



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 25, 2025 – 01:20 am BST

PDB ID : 9QAP / pdb\_00009qap  
Title : Human angiotensin-1 converting enzyme C-domain in complex with quinaprilat  
Authors : Gregory, K.S.; Acharya, K.R.  
Deposited on : 2025-02-28  
Resolution : 1.50 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 Phenix2.0rc1  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.45.1

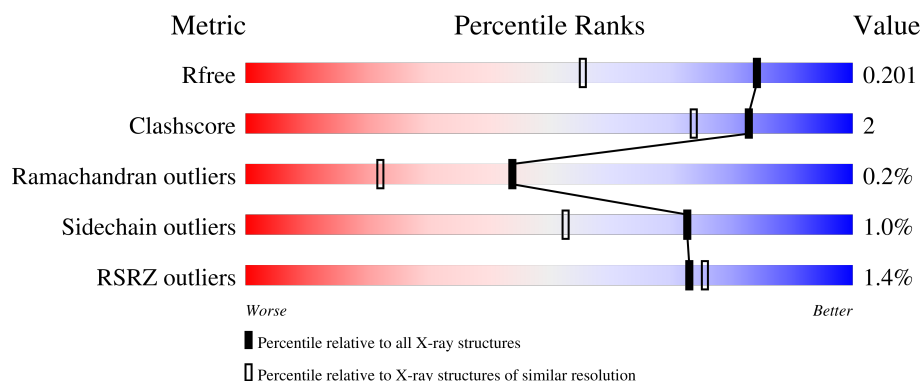
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.50 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	3717 (1.50-1.50)
Clashscore	180529	4048 (1.50-1.50)
Ramachandran outliers	177936	3970 (1.50-1.50)
Sidechain outliers	177891	3967 (1.50-1.50)
RSRZ outliers	164620	3718 (1.50-1.50)

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></div> <div>91%</div> <div>7% ..</div> </div>
2	B	6	<div> <div>17%</div> <div>83%</div> </div>

## 2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 5512 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.

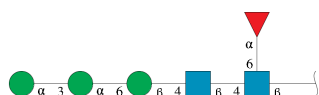
- Molecule 1 is a protein called Angiotensin-converting enzyme, soluble form.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	570	Total	C	N	O	S	0	12	0
			4753	3042	814	874	23			

There are 5 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	155	GLN	ASN	engineered mutation	UNP P12821
A	333	GLN	ASN	engineered mutation	UNP P12821
A	578	GLN	ASN	engineered mutation	UNP P12821

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



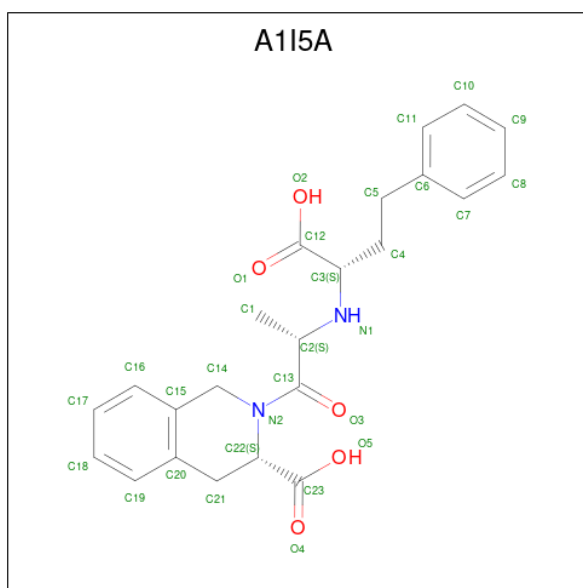
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	6	Total	C	N	O	0	0	0
			71	40	2	29			

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

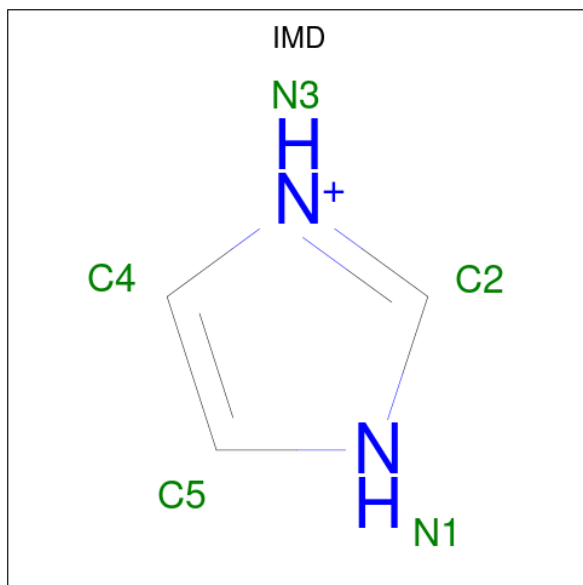
- Molecule 4 is quinaprilat (CCD ID: A1I5A) (formula: C<sub>23</sub>H<sub>26</sub>N<sub>2</sub>O<sub>5</sub>) (labeled as "Ligand of

Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			30	23	2	5		

- Molecule 5 is IMIDAZOLE (CCD ID: IMD) (formula:  $C_3H_5N_2$ ).



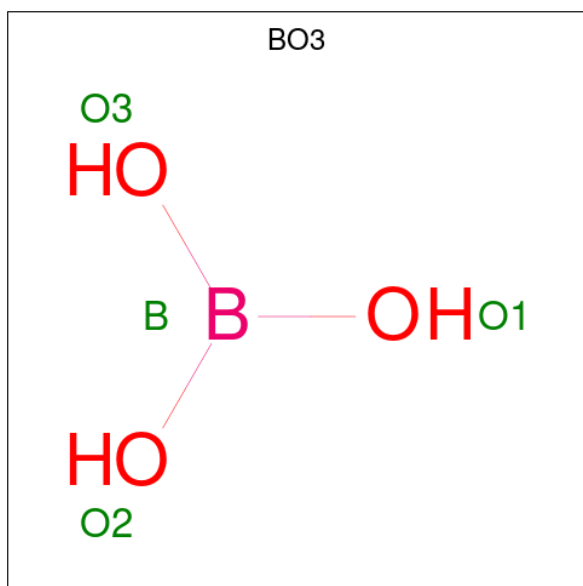
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	N	0	0
			5	3	2		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is BORIC ACID (CCD ID: BO3) (formula:  $\text{BH}_3\text{O}_3$ ).



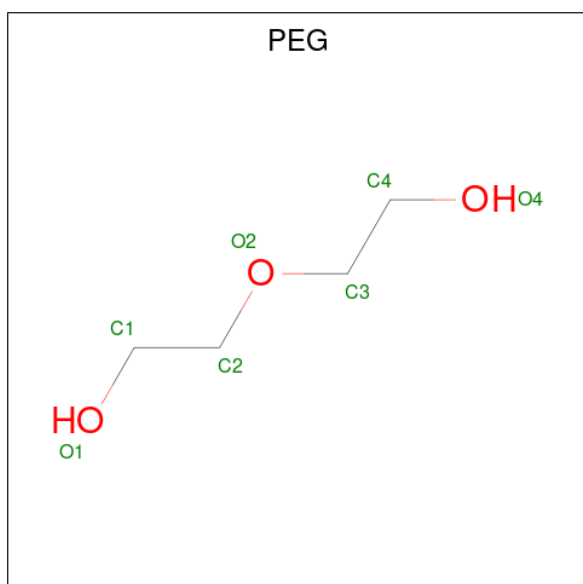
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	B	O	0	0
			4	1	3		
7	A	1	Total	B	O	0	0
			4	1	3		

- Molecule 8 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula:  $\text{C}_2\text{H}_6\text{O}_2$ ).



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

- Molecule 9 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula:  $C_4H_{10}O_3$ ).



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

- 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 SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	1	Total	Na	0	0
			1	1		

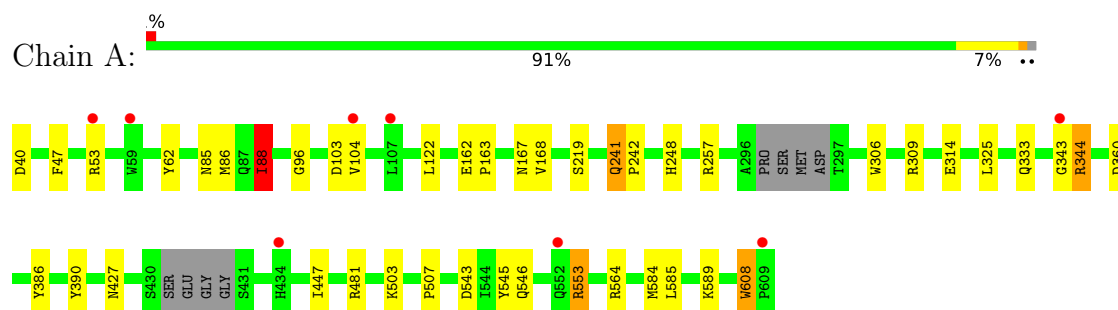
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	608	Total	O	0	0
			608	608		

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





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.72Å 85.65Å 135.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.54 – 1.50 72.44 – 1.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (72.54-1.50) 100.0 (72.44-1.50)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.43 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.8.0430 (refmacat 0.4.100)	Depositor
R, $R_{free}$	0.144 , 0.196 0.156 , 0.201	Depositor DCC
$R_{free}$ test set	5625 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.0	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 45.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	5512	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.85% 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: PEG, GOL, CSO, FUC, IMD, EDO, BO3, ZN, NAG, BMA, A1I5A, CL, NA, MAN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.84	1/4879 (0.0%)	1.15	12/6623 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	248	HIS	CE1-NE2	5.27	1.37	1.32

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	608	TRP	O-C-N	-11.49	108.10	121.32
1	A	257	ARG	CD-NE-CZ	7.21	134.50	124.40
1	A	543	ASP	CA-CB-CG	7.19	119.79	112.60
1	A	553	ARG	CB-CA-C	-6.86	99.83	110.81
1	A	47	PHE	N-CA-CB	6.48	119.41	110.01

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	481	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	553	ARG	Sidechain
1	A	564	ARG	Sidechain
1	A	608	TRP	Mainchain

## 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	4753	0	4582	21	0
2	B	71	0	61	0	0
3	A	1	0	0	0	0
4	A	30	0	0	0	0
5	A	5	0	5	0	0
6	A	6	0	8	0	0
7	A	8	0	6	1	0
8	A	20	0	30	4	0
9	A	7	0	10	2	0
10	A	2	0	0	0	0
11	A	1	0	0	0	0
12	A	608	0	0	5	0
All	All	5512	0	4702	22	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 2.

The worst 5 of 22 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:167:ASN:HB3	12:A:1255:HOH:O	1.77	0.83
1:A:589:LYS:HD3	8:A:711:EDO:H11	1.88	0.55
1:A:168:VAL:HG13	9:A:710:PEG:H21	1.89	0.54
1:A:96:GLY:HA3	1:A:122:LEU:CD2	2.41	0.50
1:A:241:GLN:HB2	1:A:242:PRO:HD3	1.93	0.50

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	575/578 (100%)	567 (99%)	7 (1%)	1 (0%)	44 22

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	344	ARG

### 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	508/502 (101%)	503 (99%)	5 (1%)	73 53

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	85	ASN
1	A	88	ILE
1	A	104	VAL
1	A	386	TYR
1	A	390	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	A	434	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	488	1	3,6,7	0.87	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	488	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

6 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	B	1	1,2	14,14,15	0.32	0	17,19,21	1.00	2 (11%)
2	NAG	B	2	2	14,14,15	0.32	0	17,19,21	0.97	1 (5%)
2	BMA	B	3	2	11,11,12	1.25	2 (18%)	15,15,17	2.03	6 (40%)
2	MAN	B	4	2	11,11,12	0.86	0	15,15,17	0.99	1 (6%)
2	MAN	B	5	2	11,11,12	0.78	0	15,15,17	1.59	3 (20%)
2	FUC	B	6	2	10,10,11	0.76	0	14,14,16	1.04	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
2	NAG	B	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	0/6/23/26	0/1/1/1
2	BMA	B	3	2	-	2/2/19/22	0/1/1/1
2	MAN	B	4	2	-	2/2/19/22	1/1/1/1
2	MAN	B	5	2	-	0/2/19/22	0/1/1/1
2	FUC	B	6	2	-	-	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3	BMA	O5-C5	2.45	1.48	1.43
2	B	3	BMA	C4-C5	2.04	1.57	1.53

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	5	MAN	C1-O5-C5	4.01	117.63	112.19
2	B	3	BMA	C1-C2-C3	4.00	114.58	109.67
2	B	3	BMA	O3-C3-C2	-3.49	103.31	109.99
2	B	5	MAN	C1-C2-C3	3.47	113.93	109.67
2	B	3	BMA	O5-C1-C2	3.11	115.57	110.77

There are no chirality outliers.

All (4) torsion outliers are listed below:

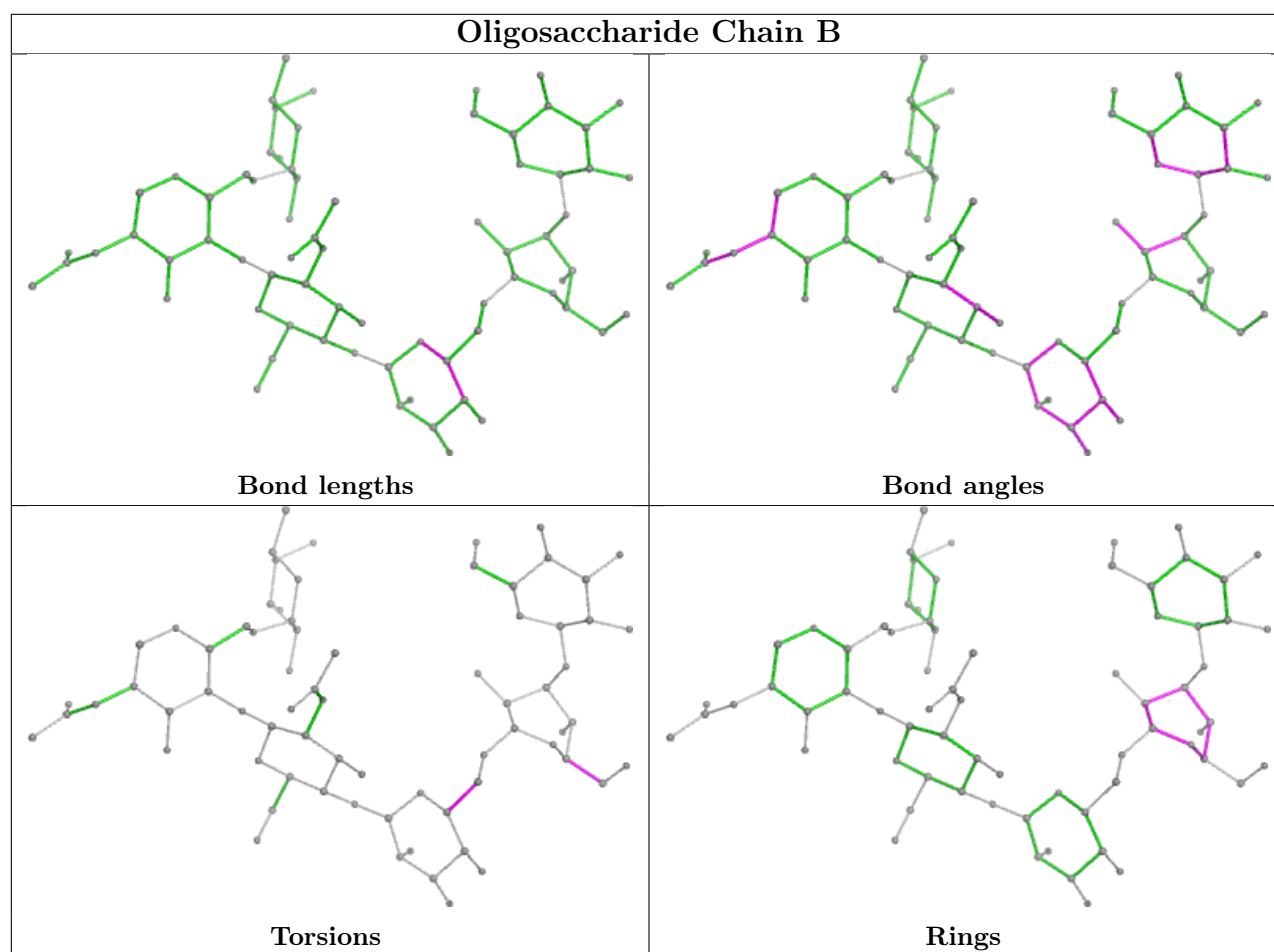
Mol	Chain	Res	Type	Atoms
2	B	3	BMA	O5-C5-C6-O6
2	B	3	BMA	C4-C5-C6-O6
2	B	4	MAN	C4-C5-C6-O6
2	B	4	MAN	O5-C5-C6-O6

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	4	MAN	C1-C2-C3-C4-C5-O5

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 15 ligands modelled in this entry, 4 are monoatomic - leaving 11 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	GOL	A	704	-	5,5,5	0.62	0	5,5,5	1.06	0
5	IMD	A	703	-	3,5,5	0.43	0	4,5,5	0.62	0
8	EDO	A	709	-	3,3,3	0.16	0	2,2,2	1.03	0
4	A1I5A	A	702	3	32,32,32	0.65	0	41,44,44	0.98	1 (2%)
8	EDO	A	708	-	3,3,3	0.17	0	2,2,2	0.30	0
8	EDO	A	712	-	3,3,3	0.57	0	2,2,2	0.61	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	BO3	A	706	-	3,3,3	0.10	0	3,3,3	0.33	0
8	EDO	A	707	-	3,3,3	0.27	0	2,2,2	0.53	0
7	BO3	A	705	-	3,3,3	0.25	0	3,3,3	1.63	1 (33%)
8	EDO	A	711	-	3,3,3	1.25	0	2,2,2	0.97	0
9	PEG	A	710	-	6,6,6	0.53	0	5,5,5	0.51	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	GOL	A	704	-	-	4/4/4/4	-
5	IMD	A	703	-	-	-	0/1/1/1
8	EDO	A	709	-	-	1/1/1/1	-
4	A1I5A	A	702	3	-	3/25/37/37	0/3/3/3
8	EDO	A	708	-	-	1/1/1/1	-
8	EDO	A	712	-	-	0/1/1/1	-
8	EDO	A	707	-	-	1/1/1/1	-
8	EDO	A	711	-	-	1/1/1/1	-
9	PEG	A	710	-	-	2/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	705	BO3	O3-B-O2	-2.24	112.14	119.79
4	A	702	A1I5A	C21-C22-C23	-2.22	106.32	111.18

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

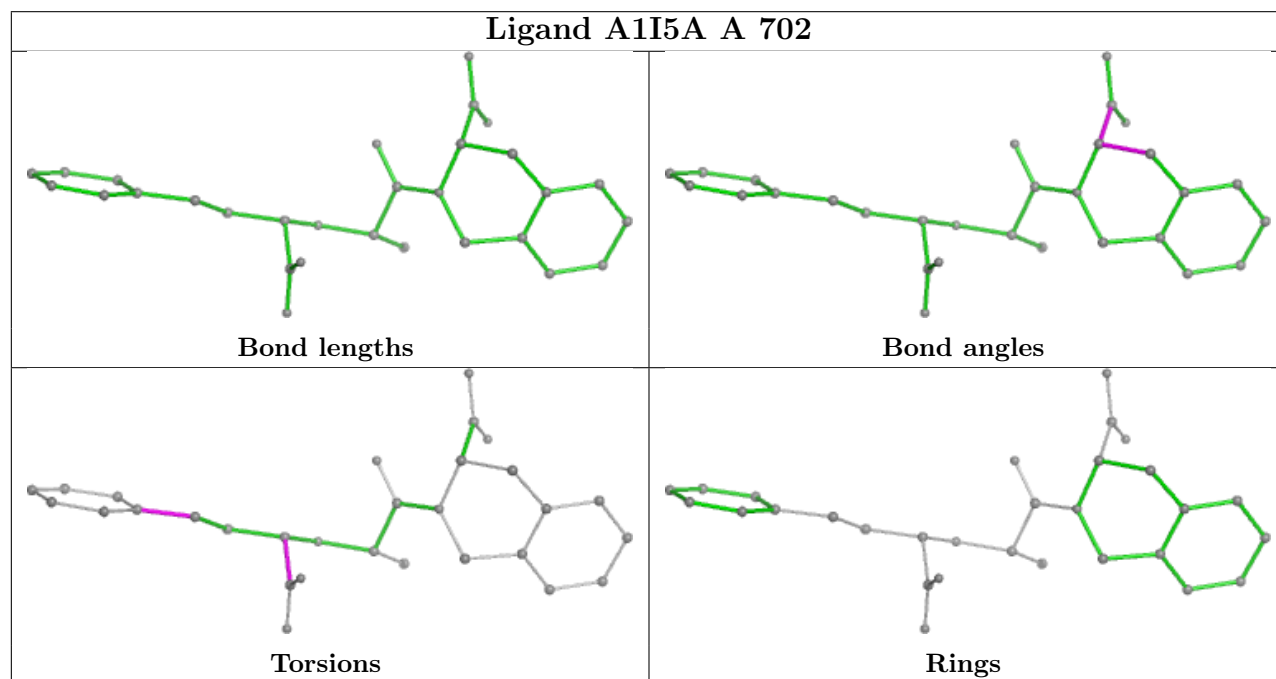
Mol	Chain	Res	Type	Atoms
6	A	704	GOL	O1-C1-C2-C3
6	A	704	GOL	C1-C2-C3-O3
6	A	704	GOL	O2-C2-C3-O3
8	A	711	EDO	O1-C1-C2-O2
9	A	710	PEG	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	708	EDO	1	0
7	A	705	BO3	1	0
8	A	711	EDO	3	0
9	A	710	PEG	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.



## 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, 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%)	-0.22	8 (1%) 73 75	8, 21, 45, 66	12 (2%)

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	59	TRP	3.1
1	A	609	PRO	3.0
1	A	343	GLY	2.8
1	A	53[B]	ARG	2.4
1	A	552	GLN	2.4

### 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	488	7/8	0.98	0.04	14,14,16,19	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.

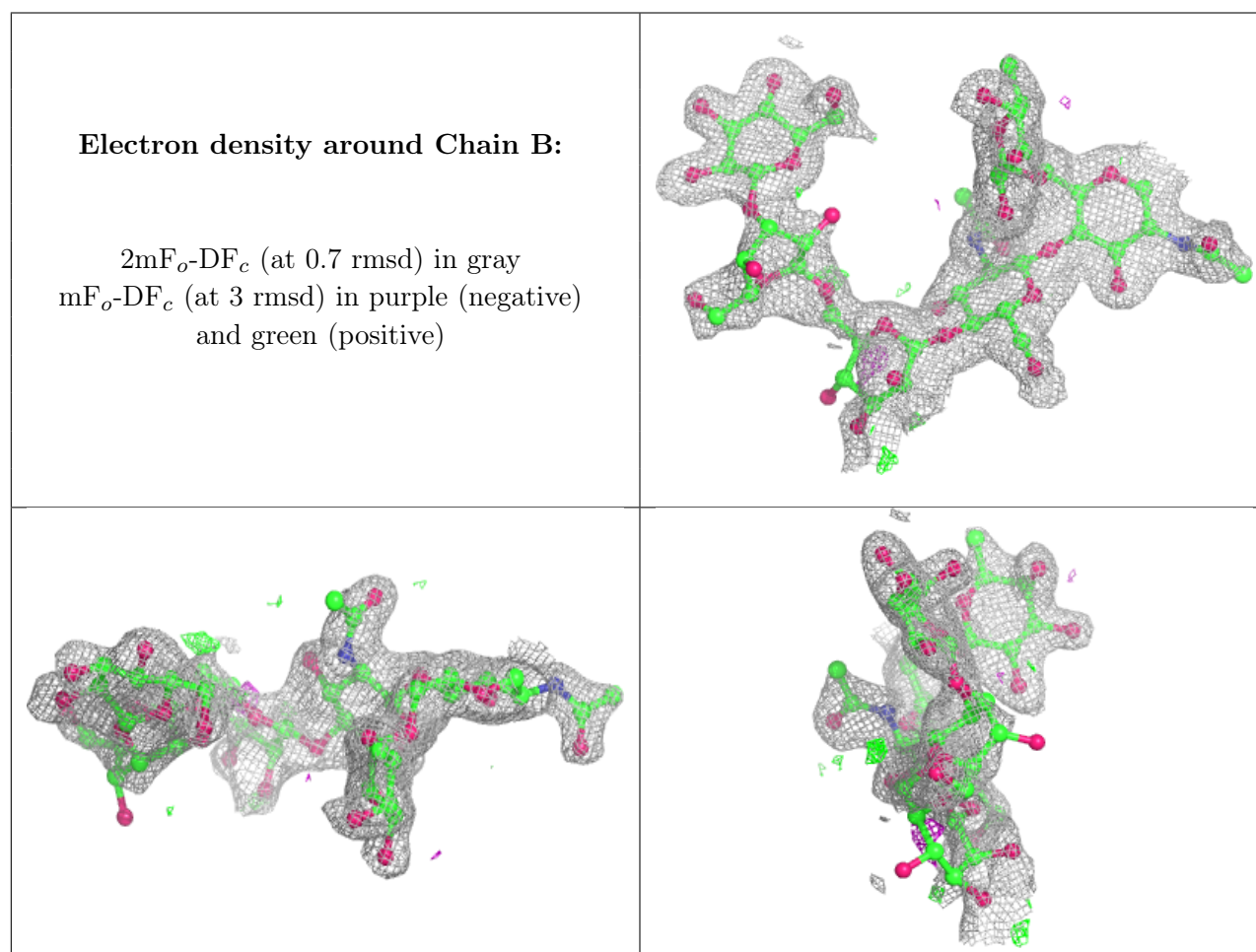
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	BMA	B	3	11/12	0.66	0.16	61,67,76,89	0

*Continued on next page...*

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MAN	B	4	11/12	0.85	0.11	62,68,76,78	0
2	NAG	B	2	14/15	0.90	0.10	50,54,66,69	0
2	MAN	B	5	11/12	0.91	0.10	41,52,61,61	0
2	FUC	B	6	10/11	0.92	0.09	43,47,50,52	0
2	NAG	B	1	14/15	0.94	0.08	42,49,51,58	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.



## 6.4 Ligands [i](#)

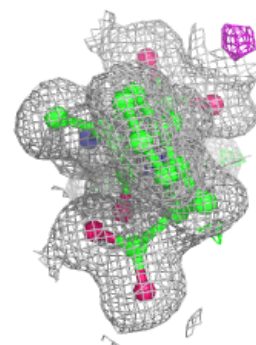
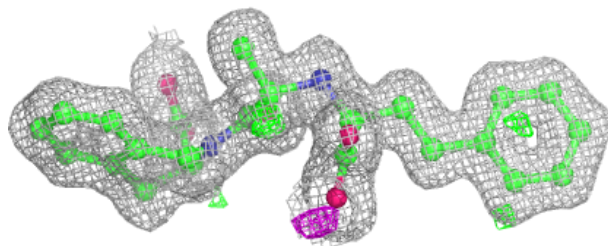
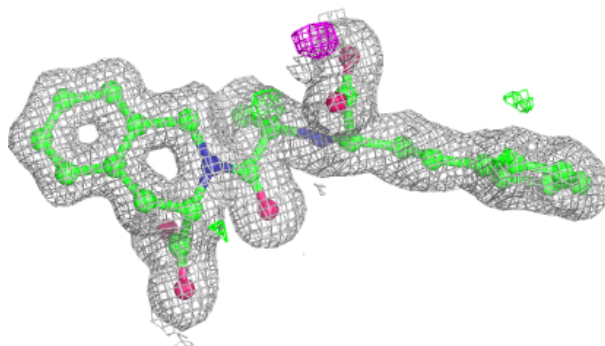
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
8	EDO	A	708	4/4	0.86	0.14	52,61,65,67	0
9	PEG	A	710	7/7	0.87	0.14	43,51,54,60	0
8	EDO	A	709	4/4	0.89	0.11	41,42,44,54	0
8	EDO	A	707	4/4	0.89	0.12	53,53,53,62	0
8	EDO	A	712	4/4	0.90	0.12	38,42,44,48	0
8	EDO	A	711	4/4	0.90	0.13	31,38,39,39	0
7	BO3	A	706	4/4	0.91	0.14	69,74,76,81	0
7	BO3	A	705	4/4	0.94	0.09	33,35,37,40	0
6	GOL	A	704	6/6	0.94	0.11	19,37,44,52	0
5	IMD	A	703	5/5	0.97	0.05	25,25,26,26	0
4	A1I5A	A	702	30/30	0.98	0.05	11,14,18,21	0
3	ZN	A	701	1/1	1.00	0.02	13,13,13,13	0
10	CL	A	713	1/1	1.00	0.02	14,14,14,14	0
10	CL	A	714	1/1	1.00	0.02	15,15,15,15	0
11	NA	A	715	1/1	1.00	0.04	19,19,19,19	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.

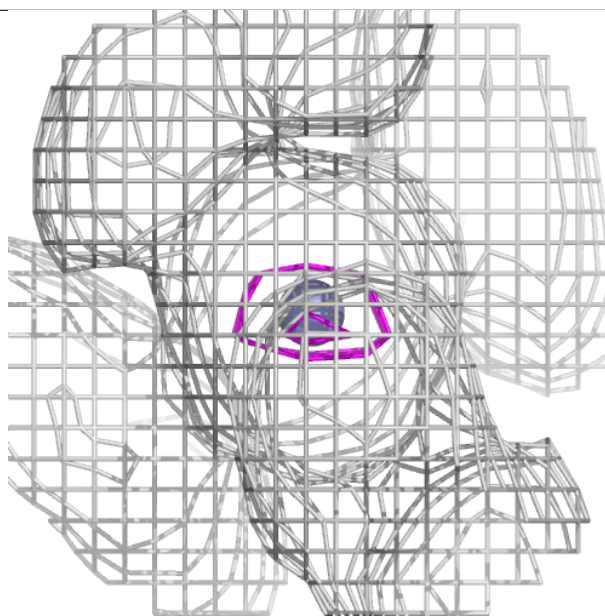
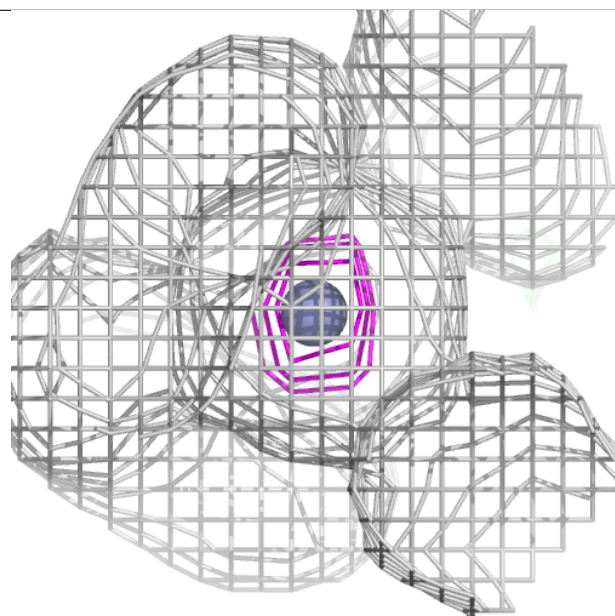
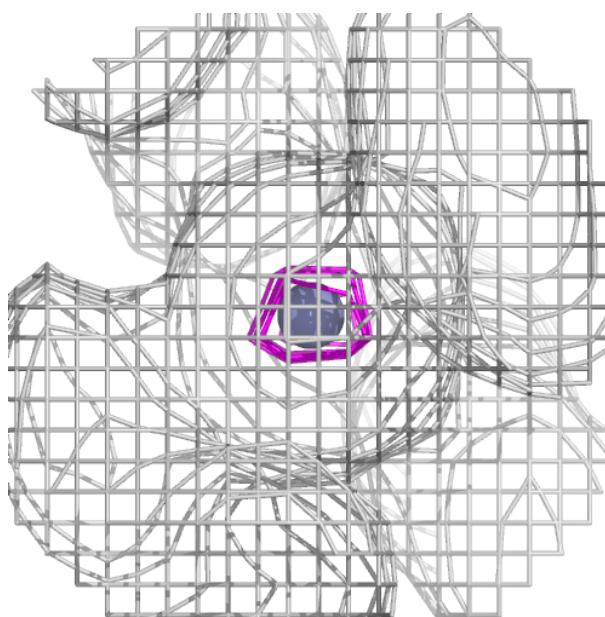
**Electron density around A1I5A A 702:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (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.