



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 25, 2025 – 01:28 am BST

PDB ID : 9QAQ / pdb\_00009qaq  
Title : Human angiotensin-1 converting enzyme C-domain in complex with perindoprilat  
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Deposited on : 2025-02-28  
Resolution : 1.90 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 Phenix2.0rc1
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

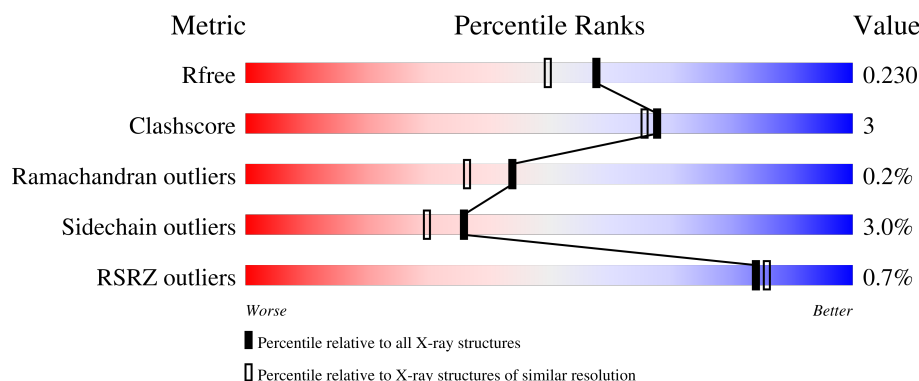
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	7293 (1.90-1.90)
Clashscore	180529	8090 (1.90-1.90)
Ramachandran outliers	177936	8022 (1.90-1.90)
Sidechain outliers	177891	8022 (1.90-1.90)
RSRZ outliers	164620	7292 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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>84%</div> <div>14%</div> <div>..</div> </div>
2	D	4	<div> <div>25%</div> <div>75%</div> </div>

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 5118 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.

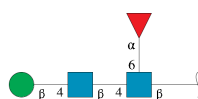
- Molecule 1 is a protein called Angiotensin-converting enzyme, soluble form.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	575	4689	3007	800	858	24	0	0	0

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	155	GLN	ASN	engineered mutation	UNP P12821
A	337	GLN	ASN	engineered mutation	UNP P12821
A	345	ASP	THR	engineered mutation	UNP P12821
A	586	GLN	ASN	engineered mutation	UNP P12821

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



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

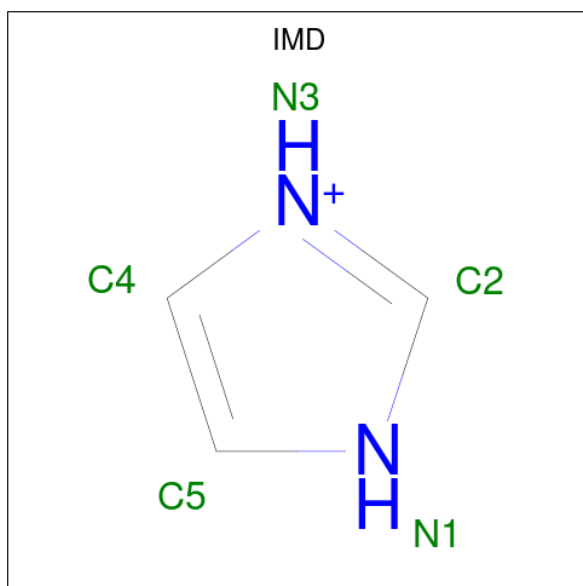
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

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



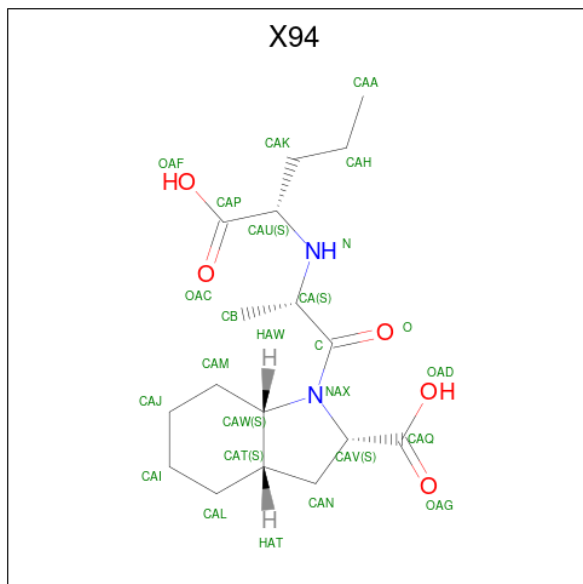
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	N	0	0
			5	3	2		

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula:  $C_2H_6O_2$ ).



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

- Molecule 7 is PERINDOPRILAT (CCD ID: X94) (formula:  $C_{17}H_{28}N_2O_5$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			24	17	2	5		

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ) (labeled as "Ligand of Interest" by depositor).



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

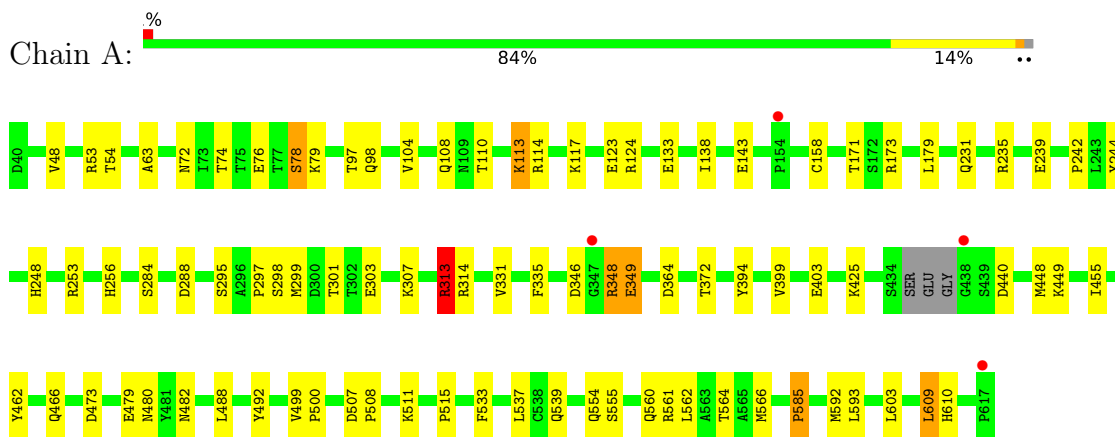
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	296	Total	O	0	0
			296	296		

### 3 Residue-property plots

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

- Molecule 1: Angiotensin-converting enzyme, soluble form



- Molecule 2: 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, $\alpha$ , $\beta$ , $\gamma$	56.48Å 85.12Å 133.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	71.93 – 1.90 71.82 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (71.93-1.90) 99.9 (71.82-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.37 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, $R_{free}$	0.169 , 0.222 0.180 , 0.230	Depositor DCC
$R_{free}$ test set	2546 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.1	Xtriage
Anisotropy	0.403	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 32.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5118	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.38% 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: CL, FUC, EDO, NAG, BMA, ZN, IMD, X94, CSO

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	0.93	2/4817 (0.0%)	1.45	42/6543 (0.6%)

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	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	555	SER	CA-CB	-5.71	1.45	1.53
1	A	248	HIS	CE1-NE2	5.35	1.38	1.32

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	585	PRO	N-CA-CB	-9.53	93.25	103.25
1	A	98	GLN	N-CA-CB	9.24	123.47	110.07
1	A	349	GLU	CB-CA-C	8.90	124.22	109.53
1	A	53	ARG	CB-CA-C	-8.77	96.22	110.79
1	A	372	THR	CA-CB-OG1	-8.34	97.10	109.60
1	A	561	ARG	CG-CD-NE	-8.19	93.98	112.00
1	A	349	GLU	N-CA-CB	-8.08	97.14	110.23
1	A	348	ARG	CB-CA-C	-7.89	98.01	109.84
1	A	561	ARG	CB-CA-C	-7.81	98.62	110.88
1	A	76	GLU	CB-CG-CD	7.60	125.53	112.60
1	A	301	THR	CA-CB-OG1	-7.40	98.50	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	346	ASP	CA-CB-CG	7.28	119.88	112.60
1	A	299	MET	CG-SD-CE	7.23	116.81	100.90
1	A	609	LEU	N-CA-CB	-6.64	99.99	110.22
1	A	473	ASP	CA-CB-CG	6.56	119.16	112.60
1	A	480	ASN	CA-CB-CG	-6.15	106.45	112.60
1	A	539	GLN	CB-CA-C	6.00	120.30	110.88
1	A	331	VAL	CA-C-N	5.99	123.97	119.66
1	A	331	VAL	C-N-CA	5.99	123.97	119.66
1	A	133	GLU	CB-CG-CD	5.97	122.75	112.60
1	A	314	ARG	CA-CB-CG	-5.93	102.24	114.10
1	A	364	ASP	CA-CB-CG	5.89	118.49	112.60
1	A	348	ARG	N-CA-CB	5.75	118.39	109.48
1	A	143	GLU	CB-CA-C	-5.56	101.56	110.79
1	A	314	ARG	CD-NE-CZ	-5.53	116.66	124.40
1	A	171	THR	CA-CB-OG1	-5.49	101.37	109.60
1	A	113	LYS	CB-CA-C	5.46	119.86	110.79
1	A	54	THR	CA-CB-OG1	5.43	117.75	109.60
1	A	63	ALA	CA-C-N	5.37	126.06	119.99
1	A	63	ALA	C-N-CA	5.37	126.06	119.99
1	A	110	THR	CA-CB-OG1	-5.37	101.55	109.60
1	A	53	ARG	N-CA-CB	5.35	117.98	110.12
1	A	97	THR	CA-CB-OG1	-5.33	101.61	109.60
1	A	313	ARG	CB-CA-C	5.26	119.52	110.79
1	A	399	VAL	N-CA-CB	5.21	119.56	110.65
1	A	482	ASN	CA-CB-CG	-5.18	107.42	112.60
1	A	314	ARG	NE-CZ-NH1	-5.13	116.37	121.50
1	A	114	ARG	NE-CZ-NH1	-5.13	116.37	121.50
1	A	244	TYR	N-CA-CB	5.12	117.43	110.01
1	A	479	GLU	CB-CA-C	-5.09	101.22	110.63
1	A	158	CYS	CB-CA-C	5.08	117.92	109.53
1	A	117	LYS	CB-CA-C	5.06	118.91	110.81

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	124	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	4689	0	4532	32	0
2	D	49	0	43	0	0
3	A	1	0	0	0	0
4	A	2	0	0	0	0
5	A	5	0	5	1	0
6	A	24	0	36	3	0
7	A	24	0	26	1	0
8	A	28	0	26	2	0
9	A	296	0	0	1	0
All	All	5118	0	4668	33	0

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

All (33) 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:593:LEU:HB3	6:A:709:EDO:H12	1.52	0.90
1:A:231:GLN:HG3	1:A:235:ARG:HH21	1.57	0.70
1:A:609:LEU:C	1:A:609:LEU:HD23	2.18	0.68
1:A:179:LEU:HD11	1:A:499:VAL:HG23	1.77	0.65
1:A:284:SER:HB2	1:A:449:LYS:HE2	1.79	0.64
1:A:348:ARG:HD3	8:A:708:NAG:H82	1.84	0.59
1:A:455:ILE:HD13	1:A:592:MET:HE2	1.84	0.58
1:A:231:GLN:HG3	1:A:235:ARG:NH2	2.19	0.58
1:A:554:GLN:OE1	9:A:802:HOH:O	2.18	0.55
1:A:173:ARG:NH1	1:A:288:ASP:OD1	2.35	0.53
1:A:593:LEU:O	6:A:709:EDO:H11	2.09	0.53
1:A:295:SER:O	1:A:297:PRO:HD3	2.10	0.50
1:A:104:VAL:HG13	1:A:113:LYS:HG3	1.93	0.50
1:A:488:LEU:HD22	1:A:492:TYR:HE2	1.78	0.48
1:A:511:LYS:O	1:A:515:PRO:HD2	2.13	0.48
1:A:562:LEU:HB3	1:A:566:MET:HE2	1.94	0.48
1:A:303:GLU:OE2	1:A:307:LYS:HB2	2.15	0.46
1:A:462:TYR:O	1:A:466:GLN:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:706:X94:HAM2	7:A:706:X94:HB1C	1.96	0.46
1:A:560:GLN:O	1:A:564:THR:HG23	2.15	0.46
1:A:593:LEU:HB3	6:A:709:EDO:C1	2.34	0.45
1:A:313:ARG:HH11	1:A:313:ARG:HG2	1.80	0.45
1:A:348:ARG:CD	8:A:708:NAG:H82	2.47	0.45
1:A:609:LEU:HD22	1:A:610:HIS:CD2	2.52	0.45
1:A:335:PHE:C	1:A:335:PHE:CD1	2.95	0.44
1:A:235:ARG:O	1:A:239:GLU:HG3	2.18	0.43
1:A:507:ASP:N	1:A:508:PRO:CD	2.81	0.43
1:A:253:ARG:O	1:A:256:HIS:HB3	2.19	0.42
1:A:74:THR:O	1:A:78:SER:HB3	2.20	0.41
1:A:533:PHE:O	1:A:537:LEU:HG	2.20	0.41
1:A:448:MET:HE1	1:A:603:LEU:HD21	2.03	0.40
1:A:488:LEU:HD22	1:A:492:TYR:CE2	2.57	0.40
1:A:500:PRO:O	5:A:704:IMD:H4	2.21	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	570/578 (99%)	558 (98%)	11 (2%)	1 (0%)	44	36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	72	ASN

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	500/502 (100%)	485 (97%)	15 (3%)	36	30

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	VAL
1	A	78	SER
1	A	79	LYS
1	A	108	GLN
1	A	123	GLU
1	A	138	ILE
1	A	242	PRO
1	A	298	SER
1	A	313	ARG
1	A	349	GLU
1	A	394	TYR
1	A	403	GLU
1	A	425	LYS
1	A	440	ASP
1	A	585	PRO

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	160	GLN
1	A	610	HIS

### 5.3.3 RNA [i](#)

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	1.07	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 ⓘ

4 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	D	1	2,1	14,14,15	0.41	0	17,19,21	0.92	0
2	NAG	D	2	2	14,14,15	0.55	0	17,19,21	1.00	1 (5%)
2	BMA	D	3	2	11,11,12	1.19	1 (9%)	15,15,17	1.77	2 (13%)
2	FUC	D	4	2	10,10,11	0.69	0	14,14,16	1.33	2 (14%)

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	D	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	BMA	D	3	2	-	0/2/19/22	0/1/1/1
2	FUC	D	4	2	-	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	3	BMA	C2-C3	3.40	1.57	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3	BMA	C1-C2-C3	5.37	116.27	109.67
2	D	4	FUC	O2-C2-C3	2.91	115.96	110.14
2	D	2	NAG	C2-N2-C7	2.56	126.55	122.90
2	D	4	FUC	C2-C3-C4	-2.41	106.72	110.89
2	D	3	BMA	O3-C3-C2	2.35	114.49	109.99

There are no chirality outliers.

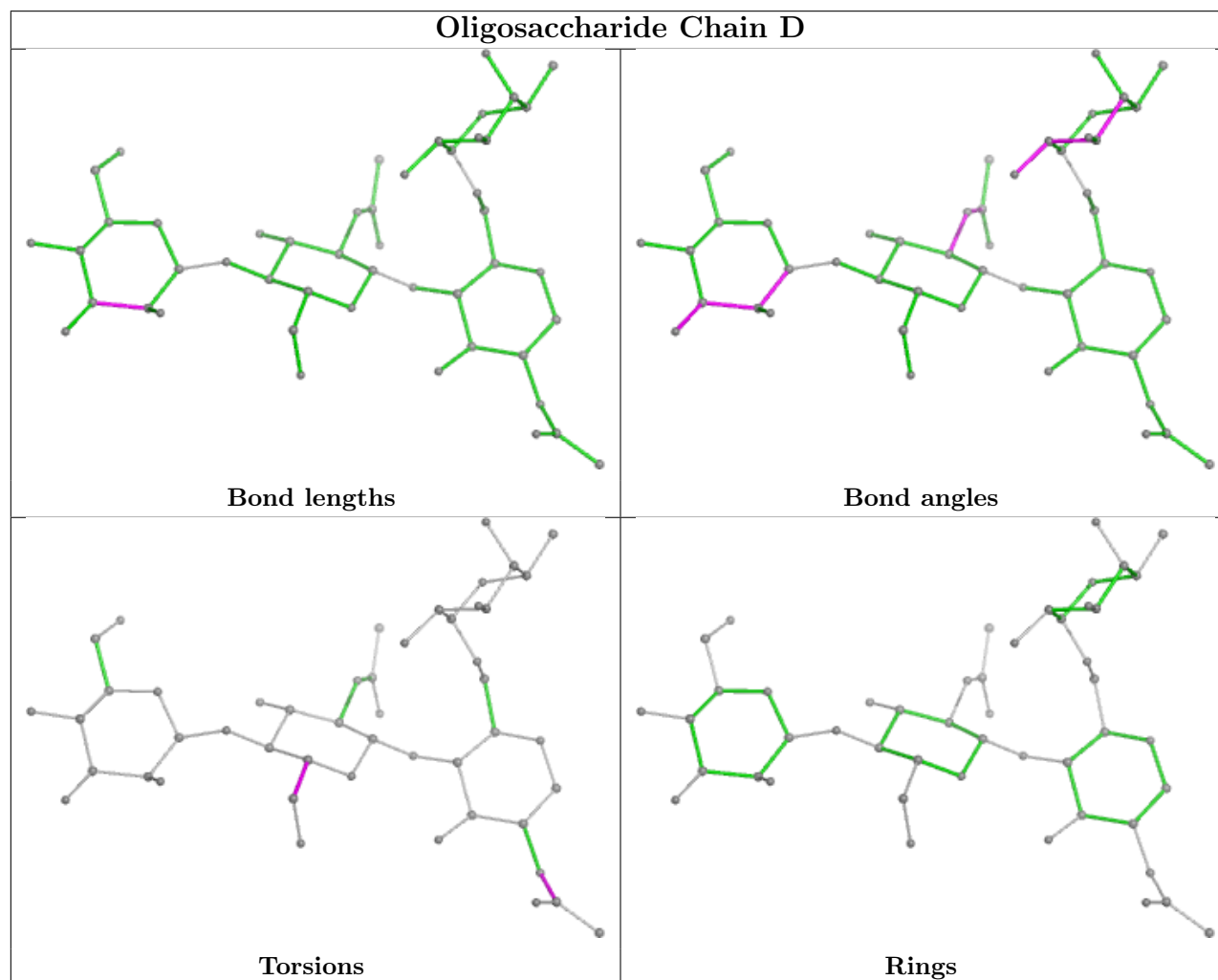
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	D	2	NAG	C4-C5-C6-O6
2	D	2	NAG	O5-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 13 ligands modelled in this entry, 3 are monoatomic - leaving 10 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	EDO	A	710	-	3,3,3	0.21	0	2,2,2	0.22	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	EDO	A	709	-	3,3,3	0.73	0	2,2,2	1.11	0
5	IMD	A	704	-	3,5,5	0.15	0	4,5,5	0.64	0
6	EDO	A	711	-	3,3,3	0.28	0	2,2,2	0.61	0
6	EDO	A	713	-	3,3,3	0.63	0	2,2,2	0.19	0
7	X94	A	706	3	25,25,25	1.00	2 (8%)	32,35,35	0.77	1 (3%)
8	NAG	A	707	-	14,14,15	0.77	0	17,19,21	1.70	3 (17%)
6	EDO	A	712	-	3,3,3	0.55	0	2,2,2	0.41	0
8	NAG	A	708	1	14,14,15	0.43	0	17,19,21	1.28	2 (11%)
6	EDO	A	705	-	3,3,3	0.29	0	2,2,2	1.35	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	EDO	A	710	-	-	1/1/1/1	-
6	EDO	A	709	-	-	1/1/1/1	-
6	EDO	A	713	-	-	1/1/1/1	-
6	EDO	A	711	-	-	1/1/1/1	-
5	IMD	A	704	-	-	-	0/1/1/1
7	X94	A	706	3	-	0/23/46/46	0/2/2/2
8	NAG	A	707	-	-	1/6/23/26	0/1/1/1
6	EDO	A	712	-	-	1/1/1/1	-
8	NAG	A	708	1	-	0/6/23/26	0/1/1/1
6	EDO	A	705	-	-	1/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	706	X94	CAV-CAQ	2.21	1.56	1.52
7	A	706	X94	OAD-CAQ	-2.09	1.23	1.30

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	707	NAG	C1-O5-C5	4.25	117.95	112.19
8	A	707	NAG	O5-C1-C2	2.51	115.25	111.29
8	A	708	NAG	O5-C5-C4	-2.34	105.14	110.83
8	A	708	NAG	C1-C2-N2	-2.21	106.70	110.49
7	A	706	X94	CAI-CAJ-CAM	2.10	115.69	111.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	707	NAG	C8-C7-N2	2.06	119.59	116.10

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	707	NAG	O5-C5-C6-O6
6	A	705	EDO	O1-C1-C2-O2
6	A	713	EDO	O1-C1-C2-O2
6	A	709	EDO	O1-C1-C2-O2
6	A	710	EDO	O1-C1-C2-O2
6	A	712	EDO	O1-C1-C2-O2
6	A	711	EDO	O1-C1-C2-O2

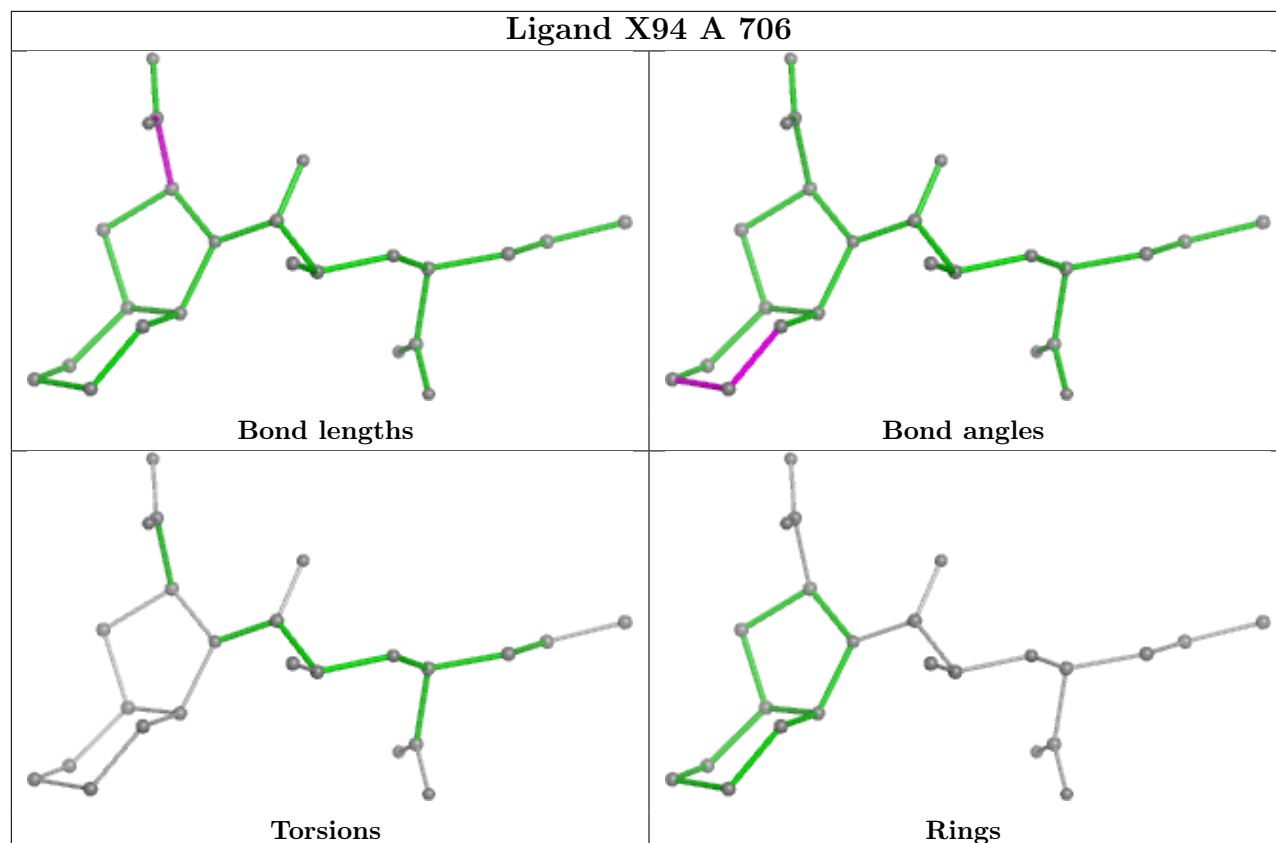
There are no ring outliers.

4 monomers are involved in 7 short contacts:

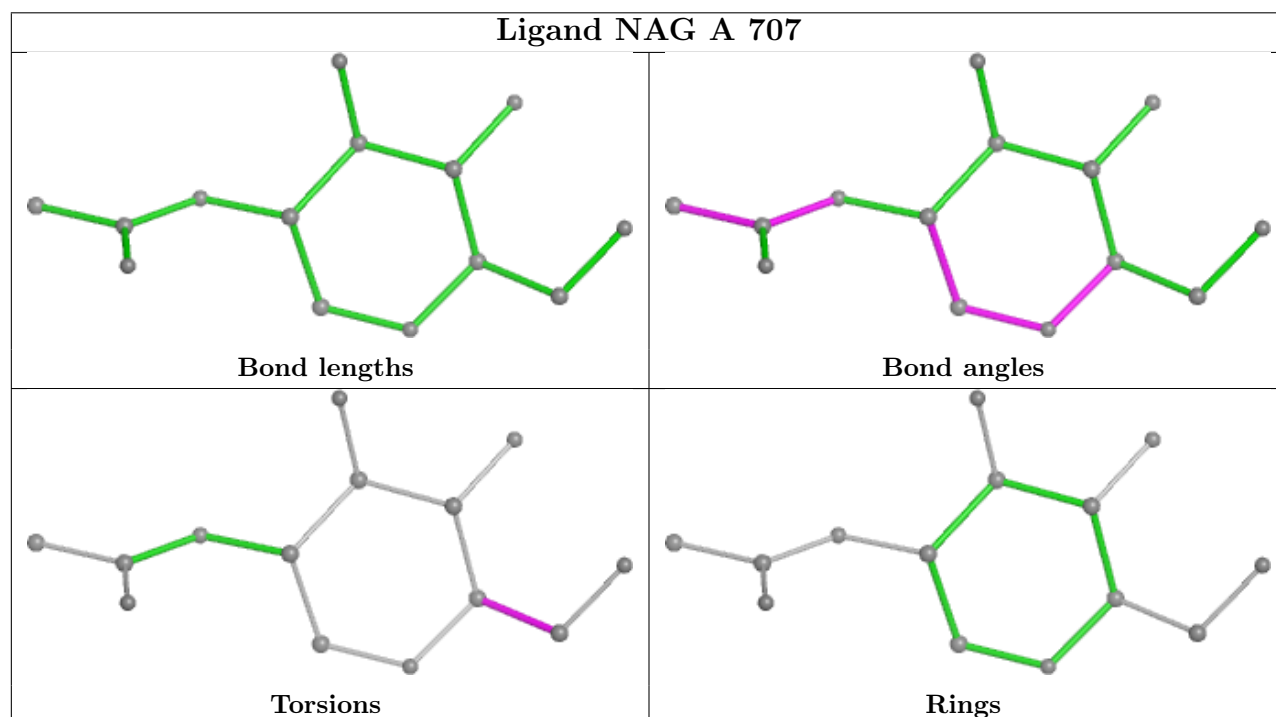
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	709	EDO	3	0
5	A	704	IMD	1	0
7	A	706	X94	1	0
8	A	708	NAG	2	0

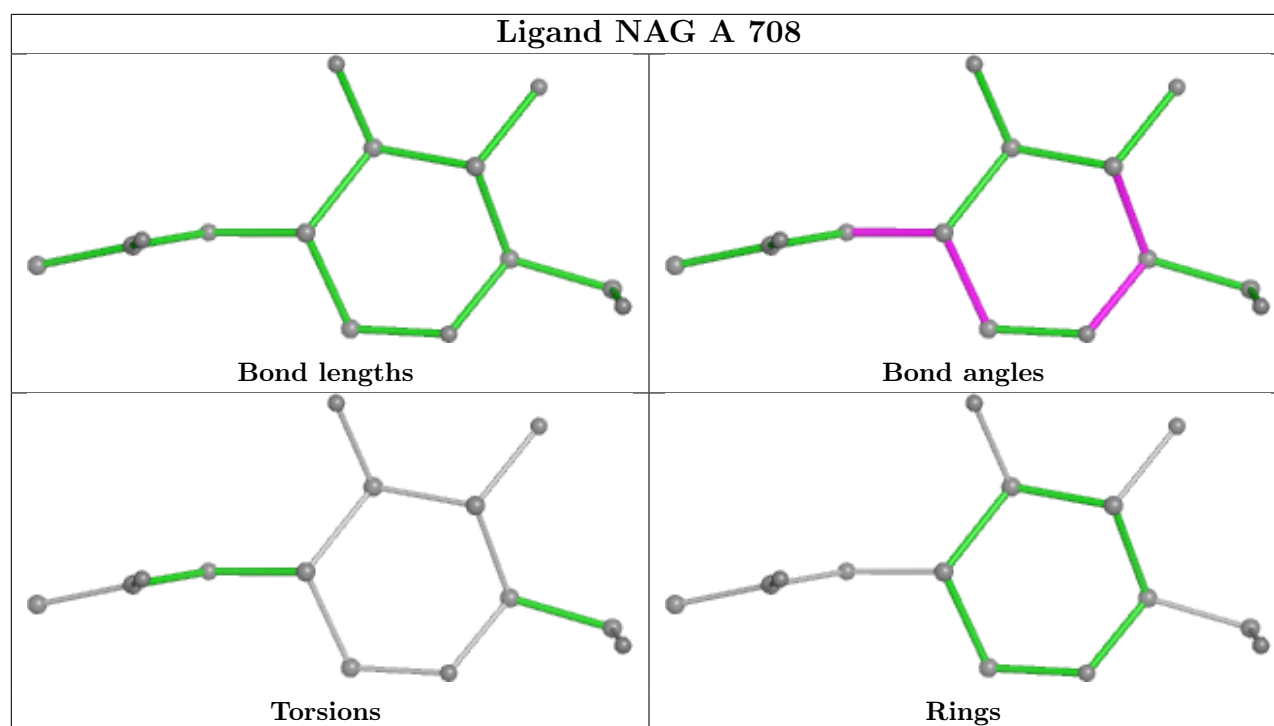
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

## Ligand X94 A 706



## Ligand NAG A 707





## 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	574/578 (99%)	-0.24	4 (0%) 84 86	18, 28, 52, 76	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	617	PRO	5.1
1	A	347	GLY	3.3
1	A	438	GLY	2.4
1	A	154	PRO	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	496	7/8	0.95	0.07	19,22,27,28	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.

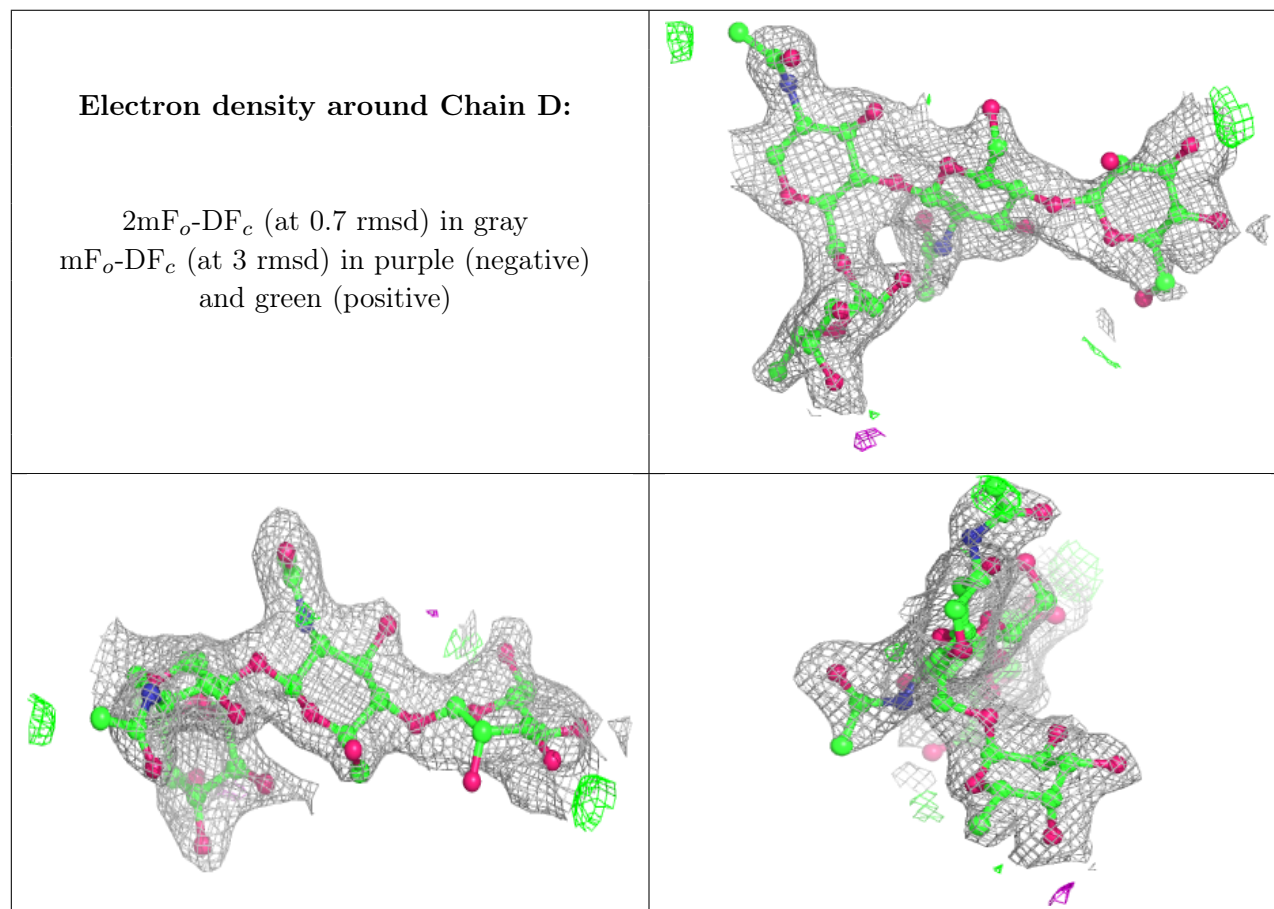
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	NAG	D	1	14/15	-	-	36,44,58,62	0
2	NAG	D	2	14/15	-	-	38,56,65,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	BMA	D	3	11/12	-	-	60,71,86,108	0
2	FUC	D	4	10/11	-	-	43,49,52,57	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.

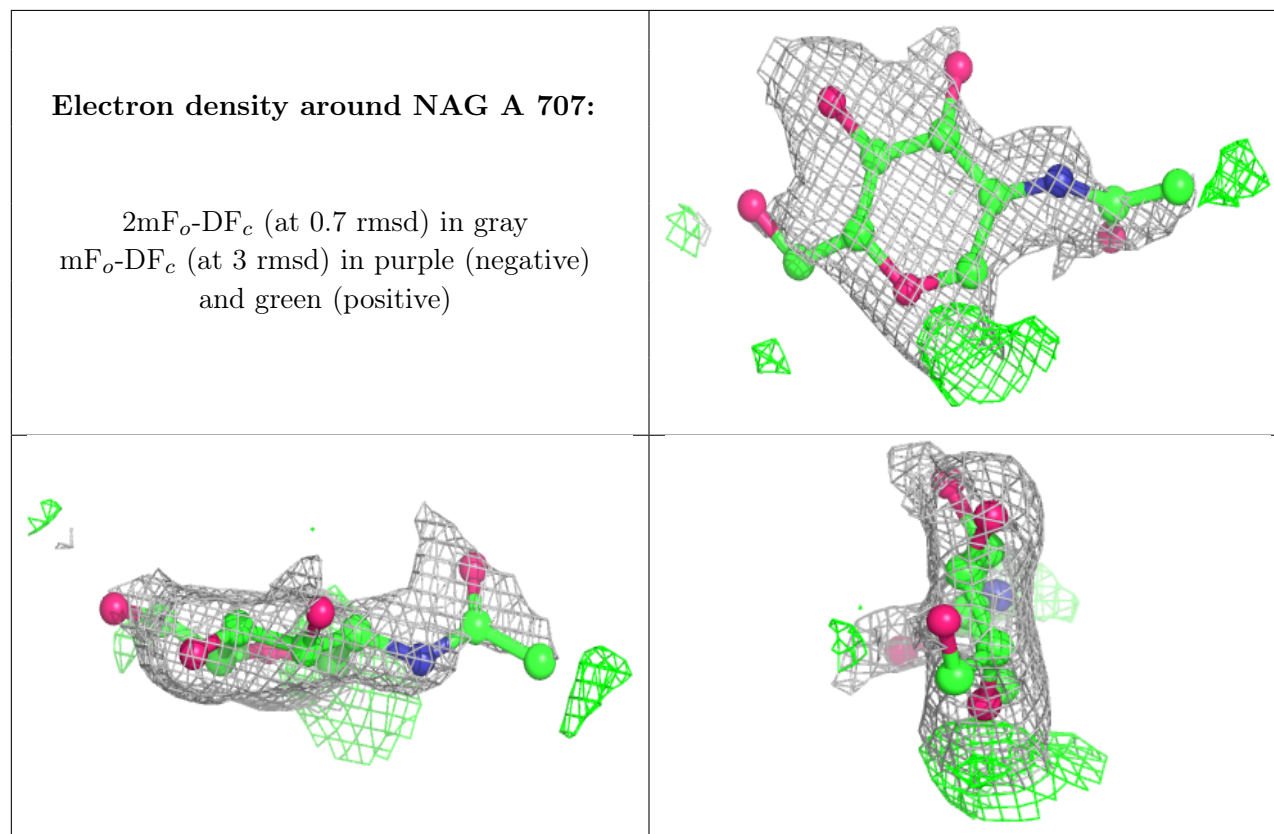
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	EDO	A	711	4/4	0.73	0.18	47,54,56,62	0
8	NAG	A	707	14/15	0.76	0.18	35,58,64,67	14
6	EDO	A	713	4/4	0.77	0.18	44,52,52,54	0
6	EDO	A	712	4/4	0.80	0.17	46,52,58,64	0

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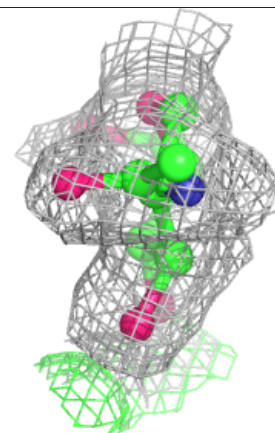
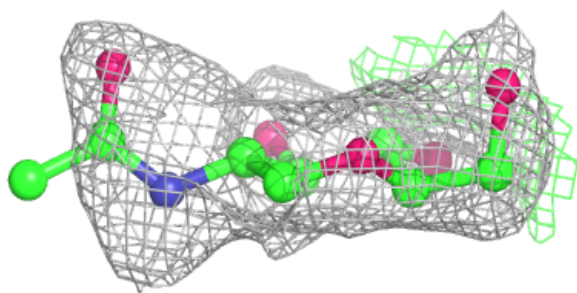
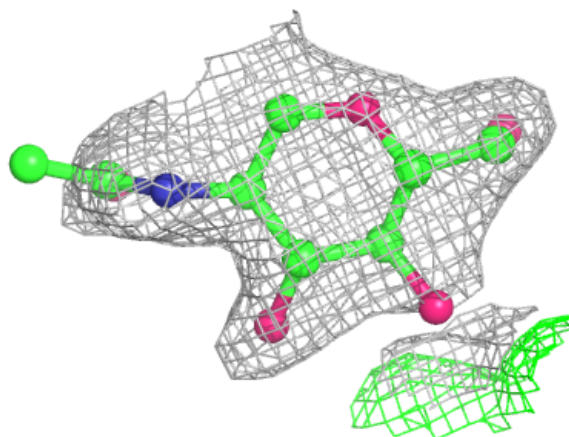
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
8	NAG	A	708	14/15	0.80	0.12	56,61,68,74	0
6	EDO	A	709	4/4	0.81	0.18	42,53,54,55	0
6	EDO	A	710	4/4	0.88	0.15	57,59,60,64	0
6	EDO	A	705	4/4	0.90	0.13	51,55,55,58	0
5	IMD	A	704	5/5	0.96	0.07	35,35,36,36	0
7	X94	A	706	24/24	0.96	0.06	22,24,27,28	0
4	CL	A	702	1/1	0.99	0.02	24,24,24,24	0
3	ZN	A	701	1/1	1.00	0.02	21,21,21,21	0
4	CL	A	703	1/1	1.00	0.04	22,22,22,22	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 NAG A 708:**

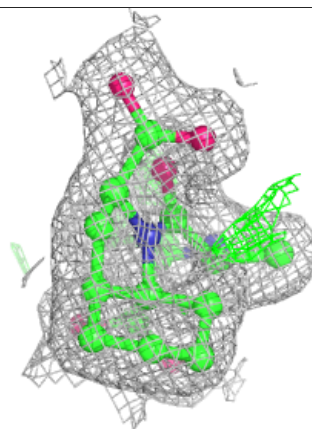
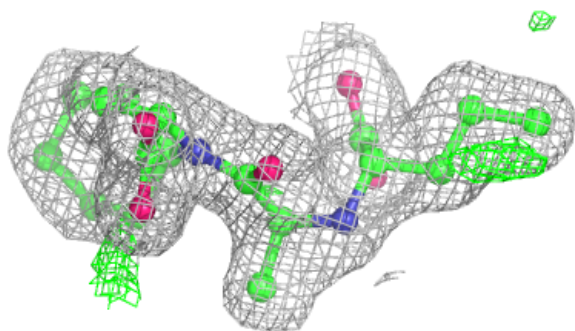
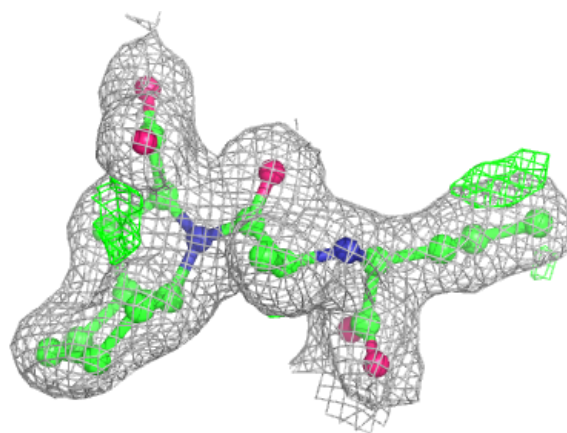
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around X94 A 706:**

$2mF_o-DF_c$  (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.