



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:48 AM UTC

PDB ID : 9SS8 / pdb\_00009ss8  
Title : Human angiotensin 1-converting enzyme N-domain in complex with rentiapril  
Authors : Gregory, K.S.; Acharya, K.R.  
Deposited on : 2025-09-25  
Resolution : 2.00 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 : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

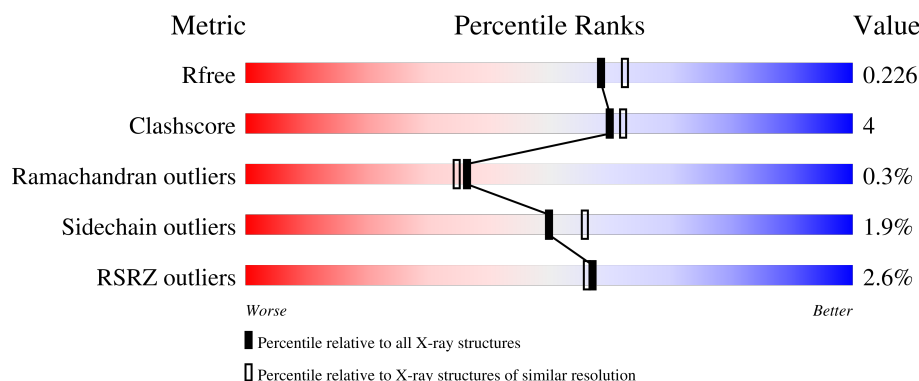
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	628	<div> <div>4%</div> <div> <div></div> <div>81%</div> <div>12%</div> <div>• •</div> </div> </div>
1	B	628	<div> <div>84%</div> <div>10%</div> <div>• •</div> </div>
2	C	2	<div> <div>100%</div> </div>
2	F	2	<div> <div>100%</div> </div>
3	D	4	<div> <div>100%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	ACT	B	711	-	-	X	-

## 2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 10989 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	604	Total	C	N	O	S	0	5	0
			4975	3192	854	910	19			
1	B	603	Total	C	N	O	S	0	8	0
			4995	3204	858	914	19			

There are 16 discrepancies between the modelled and reference sequences:

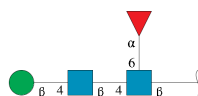
Chain	Residue	Modelled	Actual	Comment	Reference
A	9	GLN	ASN	conflict	UNP P12821
A	25	GLN	ASN	conflict	UNP P12821
A	82	GLN	ASN	conflict	UNP P12821
A	117	GLN	ASN	conflict	UNP P12821
A	131	GLN	ASN	conflict	UNP P12821
A	289	GLN	ASN	conflict	UNP P12821
A	545	ARG	GLN	conflict	UNP P12821
A	576	LEU	PRO	conflict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

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



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

- Molecule 3 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
3	D	4	Total	C	N	O	0	0	0
			49	28	2	19			

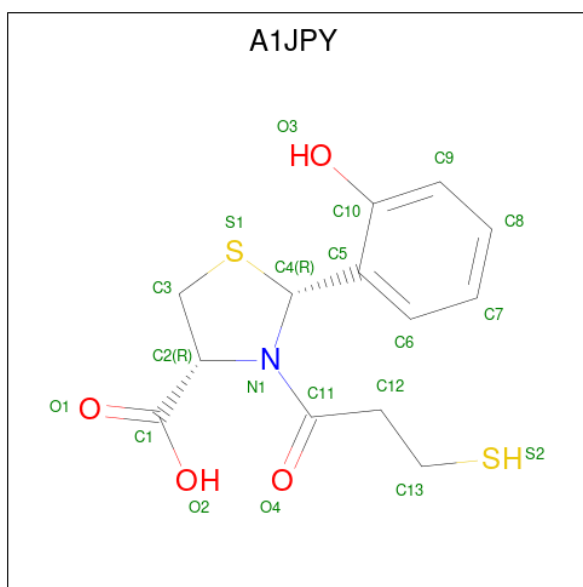
- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

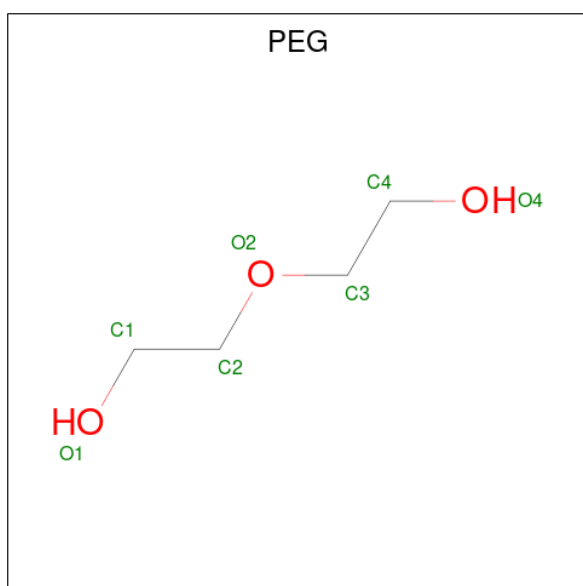
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Ca	0	0
			1	1		
5	B	1	Total	Ca	0	0
			1	1		

- Molecule 6 is Rentiapril (CCD ID: A1JPY) (formula: C<sub>13</sub>H<sub>15</sub>NO<sub>4</sub>S<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	0
			20	13	1	4	2		
6	B	1	Total	C	N	O	S	0	0
			20	13	1	4	2		

- Molecule 7 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula:  $C_4H_{10}O_3$ ).



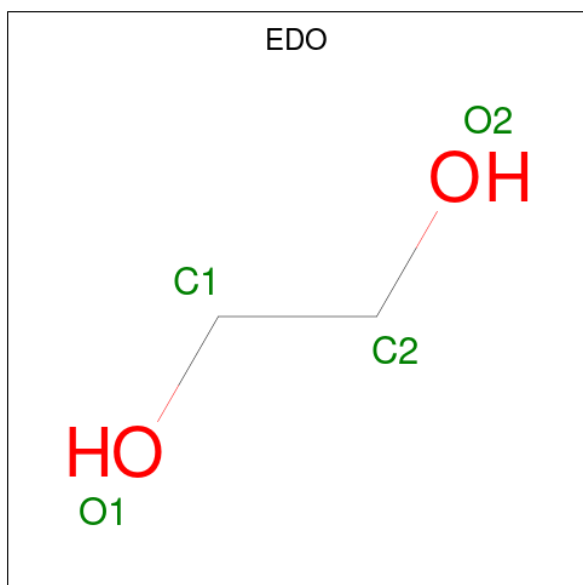
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			7	4	3		
7	A	1	Total	C	O	0	1
			14	8	6		

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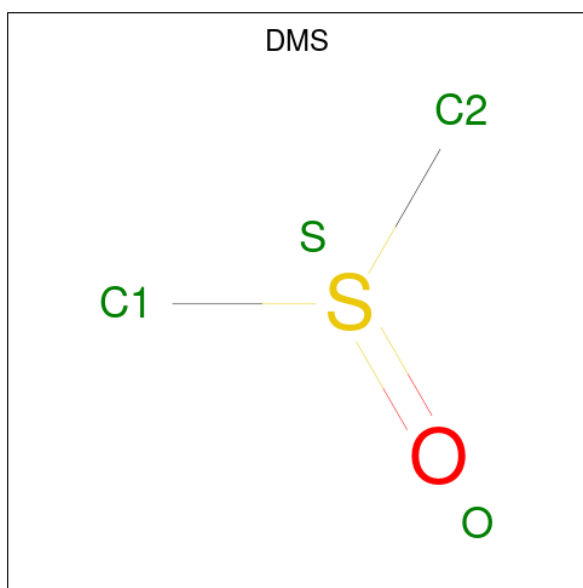
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			7	4	3		
7	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 8 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



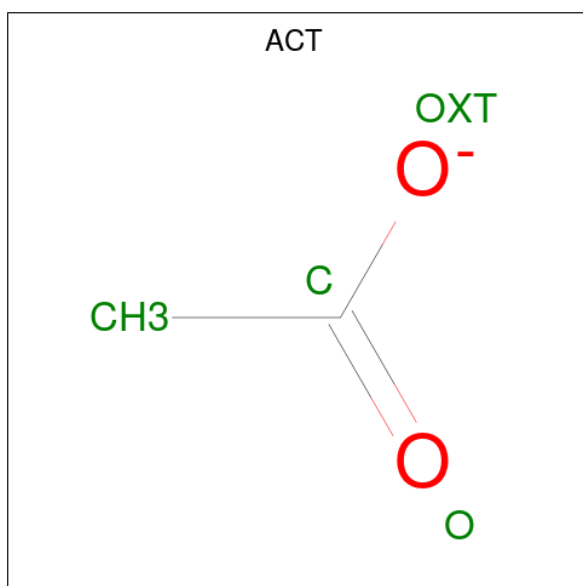
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			4	2	2		
8	A	1	Total	C	O	0	0
			4	2	2		
8	A	1	Total	C	O	0	0
			4	2	2		
8	A	1	Total	C	O	0	0
			4	2	2		
8	A	1	Total	C	O	0	0
			4	2	2		
8	A	1	Total	C	O	0	0
			4	2	2		
8	A	1	Total	C	O	0	0
			4	2	2		
8	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 9 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula:  $C_2H_6OS$ ).



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

- Molecule 10 is ACETATE ION (CCD ID: ACT) (formula:  $C_2H_3O_2$ ).



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

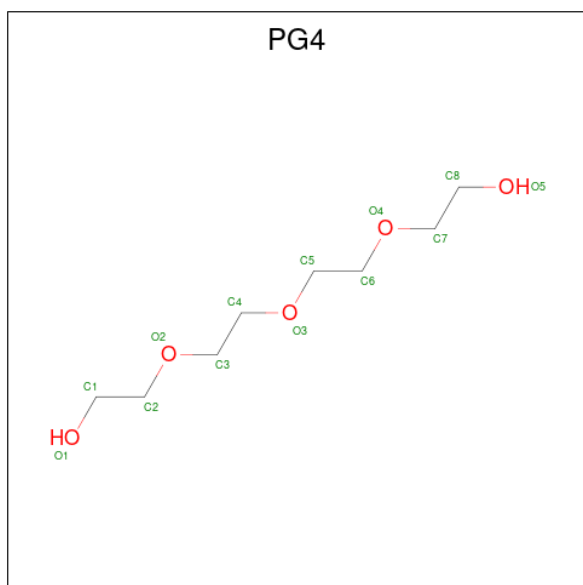
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			4	2	2		
10	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 11 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula:  $C_8H_{18}O_5$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	C	O	0	0
			13	8	5		
11	B	1	Total	C	O	0	0
			13	8	5		

- Molecule 12 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ).

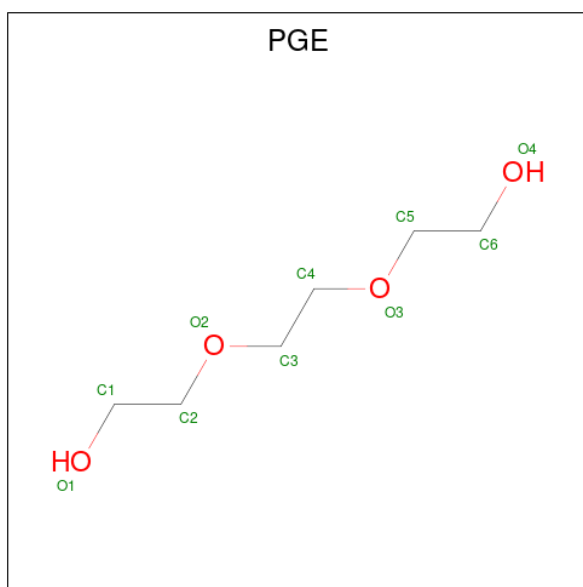


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	A	1	Total	C	N	O	0	0
			14	8	1	5		
12	B	1	Total	C	N	O	0	0
			14	8	1	5		
12	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 13 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

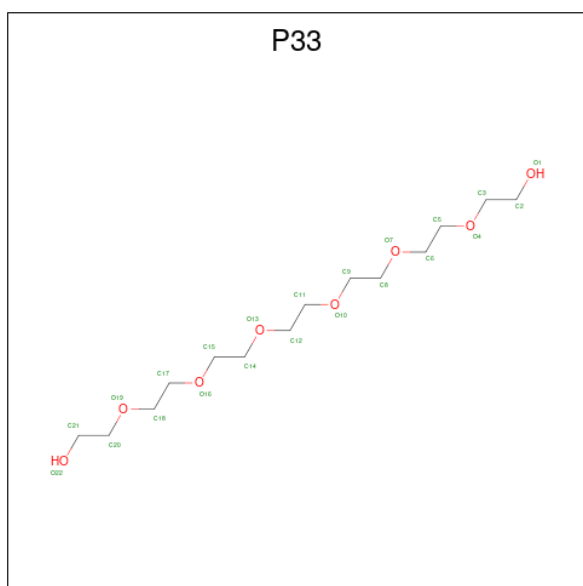
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	1	Total	Cl	0	0
			1	1		
13	B	1	Total	Cl	0	0
			1	1		

- Molecule 14 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 15 is 3,6,9,12,15,18-HEXAIOXAICOSANE-1,20-DIOL (CCD ID: P33) (formula:  $C_{14}H_{30}O_8$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	B	1	Total	C	O	0	0
			22	14	8		

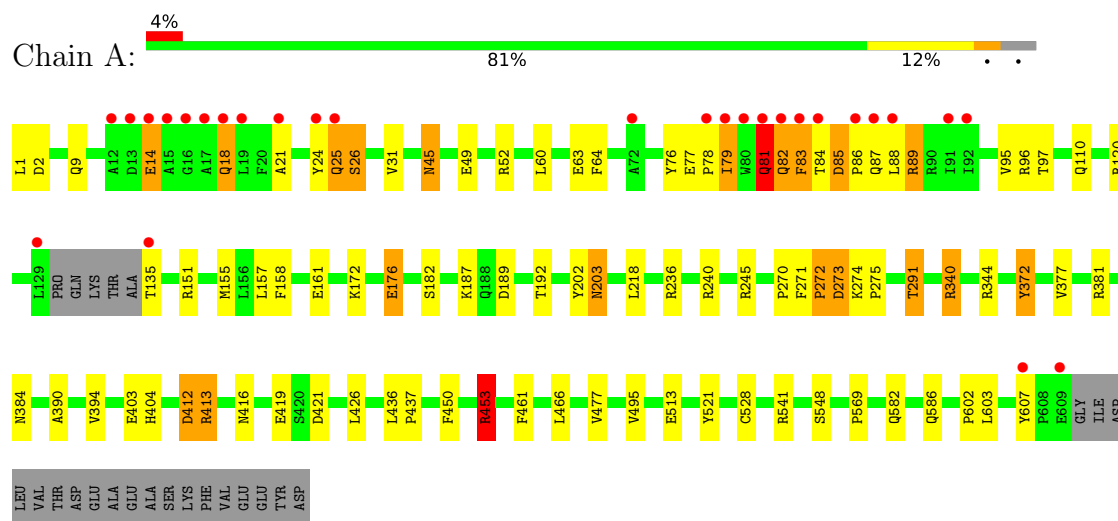
- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	360	Total 360	O 360	0	0
16	B	317	Total 317	O 317	0	0

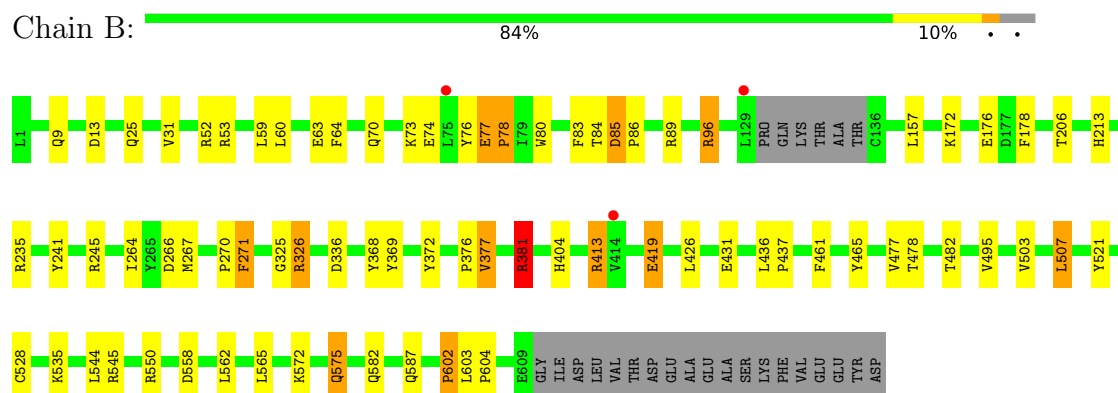
### 3 Residue-property plots

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.

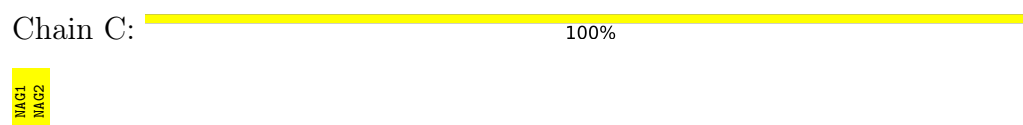
- Molecule 1: Angiotensin-converting enzyme, soluble form



- Molecule 1: Angiotensin-converting enzyme, soluble form



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




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

Chain F:  100%

MAG1  
MAG2

- Molecule 3: 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

Chain D:  100%

MAG1  
MAG2  
BMA3  
FUC4

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.95Å 77.02Å 82.89Å 88.56° 64.09° 75.23°	Depositor
Resolution (Å)	74.19 – 2.00 74.19 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.1 (74.19-2.00) 97.3 (74.19-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.34 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0431 (refmacat 0.4.105)	Depositor
R, $R_{free}$	0.173 , 0.217 0.182 , 0.226	Depositor DCC
$R_{free}$ test set	5167 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.7	Xtriage
Anisotropy	0.243	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 35.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	10989	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.74% 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: NAG, CL, EDO, ACT, FUC, DMS, BMA, A1JPY, PG4, CA, PEG, ZN, PGE, P33

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	0.97	2/5130 (0.0%)	1.46	49/6987 (0.7%)
1	B	0.91	1/5150 (0.0%)	1.34	23/7012 (0.3%)
All	All	0.94	3/10280 (0.0%)	1.40	72/13999 (0.5%)

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	7
1	B	0	7
All	All	0	14

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	21	ALA	CA-CB	-5.57	1.44	1.53
1	B	52	ARG	NE-CZ	5.57	1.39	1.33
1	A	182	SER	CA-CB	-5.47	1.44	1.53

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	291	THR	CA-CB-OG1	-16.43	84.95	109.60
1	A	18	GLN	CB-CA-C	-12.56	89.95	110.79
1	A	14	GLU	CB-CG-CD	9.60	128.91	112.60
1	A	582	GLN	CB-CA-C	-8.72	96.32	110.79
1	A	582	GLN	N-CA-CB	8.46	122.56	110.12
1	A	541	ARG	CD-NE-CZ	8.15	135.81	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	18	GLN	N-CA-CB	8.12	122.06	110.12
1	A	14	GLU	N-CA-CB	8.04	122.06	110.16
1	A	412	ASP	CB-CA-C	7.99	126.69	109.99
1	A	97	THR	CA-CB-OG1	-7.96	97.66	109.60
1	A	25	GLN	CB-CA-C	-7.44	99.20	110.88
1	B	178	PHE	CA-CB-CG	-7.12	106.68	113.80
1	B	562	LEU	N-CA-CB	-7.08	98.49	111.37
1	A	45	ASN	CA-CB-CG	7.07	119.67	112.60
1	A	84	THR	CA-CB-OG1	-7.01	99.09	109.60
1	A	419	GLU	CG-CD-OE2	-6.96	102.39	118.40
1	B	52	ARG	CB-CA-C	6.85	121.77	110.81
1	A	416	ASN	OD1-CG-ND2	-6.83	115.77	122.60
1	A	52	ARG	CD-NE-CZ	6.75	133.85	124.40
1	A	240	ARG	N-CA-CB	-6.72	99.94	110.30
1	A	541	ARG	NE-CZ-NH2	-6.72	113.15	119.20
1	A	192	THR	OG1-CB-CG2	-6.69	95.92	109.30
1	A	89	ARG	N-CA-CB	6.66	121.45	110.39
1	B	482	THR	CA-CB-OG1	-6.59	99.71	109.60
1	B	206	THR	OG1-CB-CG2	-6.58	96.14	109.30
1	A	82	GLN	CB-CA-C	6.55	121.63	110.56
1	A	49	GLU	CB-CG-CD	6.51	123.66	112.60
1	B	507	LEU	N-CA-CB	-6.43	100.67	110.12
1	B	461	PHE	CA-CB-CG	6.36	120.16	113.80
1	B	377	VAL	N-CA-CB	-6.26	102.03	110.54
1	B	587	GLN	CB-CA-C	-6.14	99.28	110.63
1	B	77	GLU	N-CA-CB	6.05	119.32	110.30
1	B	404	HIS	CA-CB-CG	-6.02	107.78	113.80
1	A	84	THR	OG1-CB-CG2	6.02	121.33	109.30
1	A	81	GLN	CB-CA-C	5.99	121.86	109.95
1	B	431	GLU	CB-CA-C	-5.92	99.73	110.56
1	B	419	GLU	CB-CA-C	-5.92	101.59	110.88
1	A	83	PHE	CA-CB-CG	5.91	119.71	113.80
1	B	13	ASP	CA-CB-CG	5.78	118.38	112.60
1	A	87	GLN	N-CA-CB	5.76	118.59	110.12
1	B	602	PRO	CB-CA-C	5.75	119.26	110.75
1	A	161	GLU	CB-CG-CD	5.74	122.36	112.60
1	A	340	ARG	CG-CD-NE	-5.69	99.48	112.00
1	B	575	GLN	CB-CA-C	-5.65	101.36	110.74
1	A	403	GLU	CB-CG-CD	5.59	122.11	112.60
1	A	461	PHE	CA-CB-CG	5.58	119.38	113.80
1	A	272	PRO	CB-CA-C	-5.50	103.07	112.26
1	A	453	ARG	CB-CG-CD	5.50	123.95	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	LEU	N-CA-CB	-5.49	101.17	110.50
1	A	586	GLN	N-CA-CB	5.48	117.96	110.01
1	B	271	PHE	N-CA-CB	-5.45	102.25	111.30
1	B	582	GLN	CB-CA-C	-5.43	101.77	110.79
1	A	189	ASP	CA-CB-CG	5.43	118.03	112.60
1	A	404	HIS	CA-CB-CG	-5.38	108.42	113.80
1	B	84	THR	CA-CB-OG1	-5.34	101.59	109.60
1	A	203	ASN	CB-CA-C	5.32	120.41	112.06
1	A	450	PHE	CA-CB-CG	5.30	119.10	113.80
1	A	384	ASN	CA-CB-CG	5.26	117.86	112.60
1	A	586	GLN	CB-CA-C	-5.26	102.62	110.88
1	A	26	SER	N-CA-C	-5.23	104.83	111.11
1	A	63	GLU	CB-CG-CD	-5.22	103.72	112.60
1	A	135	THR	OG1-CB-CG2	-5.22	98.87	109.30
1	A	421	ASP	CB-CA-C	-5.21	102.15	110.79
1	A	89	ARG	CA-C-O	5.20	125.78	119.38
1	B	266	ASP	CA-CB-CG	5.19	117.79	112.60
1	B	478	THR	CA-CB-OG1	-5.16	101.86	109.60
1	A	372	TYR	CA-CB-CG	5.15	123.16	113.90
1	A	176	GLU	CB-CA-C	-5.07	102.22	110.85
1	A	85	ASP	CA-CB-CG	5.06	117.66	112.60
1	B	582	GLN	N-CA-CB	5.05	117.55	110.12
1	B	85	ASP	CB-CA-C	5.05	120.11	110.17
1	A	602	PRO	CB-CA-C	5.05	118.84	111.22

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	120	ARG	Sidechain
1	A	151	ARG	Sidechain
1	A	236	ARG	Sidechain
1	A	245	ARG	Sidechain
1	A	340	ARG	Sidechain
1	A	413	ARG	Sidechain
1	A	453	ARG	Sidechain
1	B	235	ARG	Sidechain
1	B	326	ARG	Sidechain
1	B	381	ARG	Sidechain
1	B	413	ARG	Sidechain
1	B	545	ARG	Sidechain
1	B	78	PRO	Peptide

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Mol	Chain	Res	Type	Group
1	B	96	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	4975	0	4745	46	0
1	B	4995	0	4760	35	0
2	C	28	0	25	0	0
2	F	28	0	25	0	0
3	D	49	0	43	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	20	0	0	0	0
6	B	20	0	0	0	0
7	A	21	0	30	3	0
7	B	14	0	20	2	0
8	A	32	0	48	3	0
8	B	4	0	6	0	0
9	A	4	0	6	0	0
9	B	4	0	6	0	0
10	A	8	0	6	0	0
10	B	4	0	3	2	0
11	A	13	0	18	1	0
11	B	13	0	18	4	0
12	A	14	0	13	1	0
12	B	28	0	26	0	0
13	A	1	0	0	0	0
13	B	1	0	0	0	0
14	B	10	0	14	0	0
15	B	22	0	30	0	0
16	A	360	0	0	2	0
16	B	317	0	0	4	0
All	All	10989	0	9842	87	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 4.

All (87) 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:78:PRO:O	1:A:79:ILE:HG13	1.50	1.11
1:A:77:GLU:OE1	1:A:96:ARG:NH2	1.84	1.11
1:A:78:PRO:O	1:A:79:ILE:CG1	2.29	0.80
1:A:77:GLU:CD	1:A:96:ARG:HH22	1.90	0.80
1:A:81:GLN:HG3	1:A:82:GLN:OE1	1.84	0.77
10:B:711:ACT:H3	16:B:848:HOH:O	1.88	0.74
1:A:77:GLU:CD	1:A:96:ARG:NH2	2.48	0.71
1:A:83:PHE:HA	16:A:1083:HOH:O	1.90	0.71
1:A:85:ASP:HB3	1:A:88:LEU:HB3	1.73	0.70
1:A:110:GLN:OE1	16:A:801:HOH:O	2.13	0.65
1:A:24:TYR:CZ	1:A:95:VAL:HG22	2.34	0.63
1:B:426:LEU:C	1:B:426:LEU:HD13	2.24	0.62
1:A:14:GLU:OE2	1:A:88:LEU:HD23	2.01	0.59
1:B:264[B]:ILE:HB	1:B:267:MET:HE3	1.85	0.59
1:B:477:VAL:HG12	1:B:603:LEU:HD21	1.83	0.59
1:B:550:ARG:NH2	1:B:558:ASP:OD2	2.35	0.59
1:B:381:ARG:HH22	7:B:707:PEG:H21	1.68	0.59
1:A:25:GLN:O	1:A:26:SER:C	2.45	0.58
1:A:218:LEU:HD13	1:A:436:LEU:HD13	1.85	0.58
1:B:25:GLN:OE1	1:B:376:PRO:HB2	2.05	0.57
1:A:466:LEU:HD21	7:A:716[A]:PEG:H12	1.86	0.56
1:A:77:GLU:HB3	1:A:78:PRO:HD3	1.87	0.56
1:B:157:LEU:HD11	1:B:477:VAL:HG13	1.88	0.56
1:B:507:LEU:HD13	1:B:565:LEU:CD2	2.37	0.55
1:B:59:LEU:O	1:B:63:GLU:HG3	2.08	0.53
1:A:18:GLN:NE2	1:A:88:LEU:HD22	2.24	0.53
1:A:513:GLU:OE1	8:A:712:EDO:H22	2.10	0.52
1:A:381:ARG:HG3	1:A:548:SER:HB3	1.92	0.51
10:B:711:ACT:H1	16:B:936:HOH:O	2.11	0.51
1:A:453:ARG:NH2	7:A:716[B]:PEG:H21	2.26	0.50
1:A:24:TYR:CE2	1:A:95:VAL:HG22	2.46	0.50
1:B:60:LEU:C	1:B:60:LEU:HD23	2.37	0.50
1:B:83:PHE:O	1:B:89:ARG:NH1	2.43	0.50
1:A:495:VAL:HG12	1:A:495:VAL:O	2.11	0.50
1:B:503:VAL:O	1:B:507:LEU:HB2	2.12	0.50
1:A:83:PHE:O	1:A:89:ARG:NH1	2.44	0.49
1:A:436:LEU:N	1:A:437:PRO:HD2	2.27	0.49
1:A:76:TYR:O	1:A:77:GLU:C	2.54	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:LEU:HD23	1:A:60:LEU:O	2.12	0.49
1:A:60:LEU:HD23	1:A:60:LEU:C	2.37	0.48
1:A:274:LYS:HB3	1:A:275:PRO:HD2	1.93	0.48
1:B:325:GLY:O	1:B:326:ARG:C	2.56	0.48
1:B:369:TYR:OH	11:B:709:PG4:H51	2.13	0.48
7:A:716[B]:PEG:H32	1:B:465:TYR:CE2	2.48	0.48
1:B:495:VAL:HG12	1:B:495:VAL:O	2.14	0.48
1:B:70:GLN:O	1:B:74:GLU:HG3	2.14	0.48
1:A:157:LEU:HD11	1:A:477:VAL:HG13	1.96	0.47
1:A:31:VAL:HG21	1:A:64:PHE:CD1	2.49	0.47
1:B:213:HIS:HB3	16:B:1082:HOH:O	2.15	0.47
1:B:368:TYR:CE1	1:B:544:LEU:HA	2.49	0.47
1:A:477:VAL:HG12	1:A:603:LEU:HD21	1.96	0.47
1:B:521:TYR:CD2	1:B:528:CYS:HB2	2.51	0.46
1:A:79:ILE:O	1:A:79:ILE:CG2	2.62	0.46
1:A:202:TYR:O	1:A:203:ASN:C	2.59	0.46
1:B:172:LYS:O	1:B:176:GLU:HG3	2.16	0.46
1:A:83:PHE:HB2	1:A:89:ARG:HG2	1.97	0.46
1:B:31:VAL:HG21	1:B:64:PHE:CD1	2.51	0.45
1:A:155:MET:HE3	1:A:158:PHE:HB3	1.97	0.45
1:B:76:TYR:O	1:B:80:TRP:HD1	1.99	0.45
1:A:270:PRO:HB2	1:A:271:PHE:CD2	2.51	0.45
1:B:336:ASP:H	11:B:709:PG4:H12	1.81	0.45
1:A:270:PRO:HD3	1:A:426:LEU:HD22	1.99	0.45
1:B:572:LYS:HA	1:B:575:GLN:HG3	1.99	0.45
1:A:390:ALA:O	1:A:394:VAL:HG23	2.18	0.44
1:B:503:VAL:HG12	1:B:507:LEU:HD22	1.99	0.44
1:B:80:TRP:O	1:B:89:ARG:HG2	2.17	0.44
1:A:81:GLN:CG	1:A:82:GLN:OE1	2.61	0.44
1:A:603:LEU:HD13	1:A:607:TYR:CD1	2.53	0.44
1:B:507:LEU:HD13	1:B:565:LEU:HD23	1.99	0.43
7:B:707:PEG:H12	7:B:707:PEG:H31	1.93	0.43
1:B:77:GLU:N	1:B:78:PRO:CD	2.82	0.43
11:A:713:PG4:H42	11:A:713:PG4:H21	1.54	0.42
1:A:18:GLN:CD	1:A:88:LEU:HD22	2.44	0.42
11:B:709:PG4:H82	11:B:709:PG4:H61	1.76	0.42
1:A:86:PRO:HA	1:A:89:ARG:CZ	2.49	0.42
12:A:717:NAG:H82	1:B:245:ARG:NH1	2.35	0.42
1:A:172:LYS:O	1:A:176:GLU:HG3	2.19	0.42
1:A:273:ASP:O	1:A:413:ARG:NH2	2.46	0.41
1:B:270:PRO:HB2	1:B:271:PHE:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:ARG:NH2	8:A:705:EDO:H21	2.36	0.41
1:B:436:LEU:N	1:B:437:PRO:HD2	2.35	0.41
1:B:53:ARG:HH11	1:B:53:ARG:HD3	1.74	0.41
1:B:85:ASP:HA	1:B:86:PRO:HD2	2.00	0.41
1:A:521:TYR:CD2	1:A:528:CYS:HB2	2.55	0.40
1:B:241:TYR:OH	1:B:604:PRO:HA	2.20	0.40
11:B:709:PG4:H31	16:B:815:HOH:O	2.21	0.40
1:A:569:PRO:HG3	8:A:712:EDO:H22	2.01	0.40

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	605/628 (96%)	594 (98%)	9 (2%)	2 (0%)	36	35
1	B	607/628 (97%)	594 (98%)	12 (2%)	1 (0%)	43	42
All	All	1212/1256 (96%)	1188 (98%)	21 (2%)	3 (0%)	36	42

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	79	ILE
1	B	413	ARG
1	A	45	ASN

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	525/540 (97%)	514 (98%)	11 (2%)	47	52
1	B	527/540 (98%)	518 (98%)	9 (2%)	53	60
All	All	1052/1080 (97%)	1032 (98%)	20 (2%)	50	56

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASP
1	A	9	GLN
1	A	81	GLN
1	A	187	LYS
1	A	272	PRO
1	A	273	ASP
1	A	291	THR
1	A	372	TYR
1	A	377	VAL
1	A	412	ASP
1	A	453	ARG
1	B	9	GLN
1	B	73	LYS
1	B	96	ARG
1	B	372	TYR
1	B	377	VAL
1	B	381	ARG
1	B	419	GLU
1	B	535	LYS
1	B	602	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	70	GLN
1	A	110	GLN
1	B	263	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

8 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	C	1	2,1	14,14,15	0.34	0	17,19,21	1.67	4 (23%)
2	NAG	C	2	2	14,14,15	0.44	0	17,19,21	1.61	5 (29%)
3	NAG	D	1	3,1	14,14,15	0.76	0	17,19,21	1.46	2 (11%)
3	NAG	D	2	3	14,14,15	0.40	0	17,19,21	1.52	2 (11%)
3	BMA	D	3	3	11,11,12	0.93	1 (9%)	15,15,17	1.26	1 (6%)
3	FUC	D	4	3	10,10,11	1.51	2 (20%)	14,14,16	1.07	1 (7%)
2	NAG	F	1	2,1	14,14,15	0.95	1 (7%)	17,19,21	3.12	4 (23%)
2	NAG	F	2	2	14,14,15	0.76	1 (7%)	17,19,21	1.85	5 (29%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
3	NAG	D	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	4/6/23/26	0/1/1/1
3	BMA	D	3	3	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FUC	D	4	3	-	-	0/1/1/1
2	NAG	F	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	F	2	2	-	3/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	4	FUC	C2-C3	3.80	1.58	1.52
3	D	3	BMA	C2-C3	2.43	1.56	1.52
3	D	4	FUC	O4-C4	2.40	1.48	1.43
2	F	1	NAG	O4-C4	2.36	1.48	1.43
2	F	2	NAG	C1-C2	2.19	1.55	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1	NAG	C1-C2-N2	10.55	127.05	110.43
2	F	1	NAG	C2-N2-C7	4.17	128.48	122.90
2	F	2	NAG	O3-C3-C2	4.13	117.97	109.40
2	F	1	NAG	C1-O5-C5	4.11	117.69	112.19
3	D	2	NAG	C2-N2-C7	4.04	128.31	122.90
3	D	1	NAG	C1-C2-N2	-3.93	104.24	110.43
2	F	2	NAG	C1-O5-C5	3.72	117.17	112.19
2	C	1	NAG	C2-N2-C7	-3.65	118.01	122.90
2	C	2	NAG	O5-C5-C4	-3.35	102.68	110.83
2	C	1	NAG	O3-C3-C2	-3.32	102.50	109.40
2	F	2	NAG	C1-C2-N2	3.03	115.21	110.43
2	C	1	NAG	C4-C3-C2	3.02	115.45	111.02
3	D	2	NAG	C1-C2-N2	2.85	114.92	110.43
2	F	1	NAG	O4-C4-C5	2.78	116.16	109.32
2	C	2	NAG	O4-C4-C5	2.69	115.95	109.32
2	C	2	NAG	C1-O5-C5	-2.62	108.68	112.19
2	C	1	NAG	O5-C5-C4	-2.59	104.53	110.83
3	D	1	NAG	O7-C7-N2	-2.46	117.64	121.98
2	C	2	NAG	C3-C4-C5	-2.30	106.06	110.23
2	F	2	NAG	O3-C3-C4	-2.29	104.97	110.38
3	D	4	FUC	C3-C4-C5	-2.25	106.39	109.81
3	D	3	BMA	O4-C4-C3	-2.25	105.08	110.38
2	C	2	NAG	C2-N2-C7	-2.20	119.95	122.90
2	F	2	NAG	O5-C1-C2	-2.05	108.12	111.29

There are no chirality outliers.

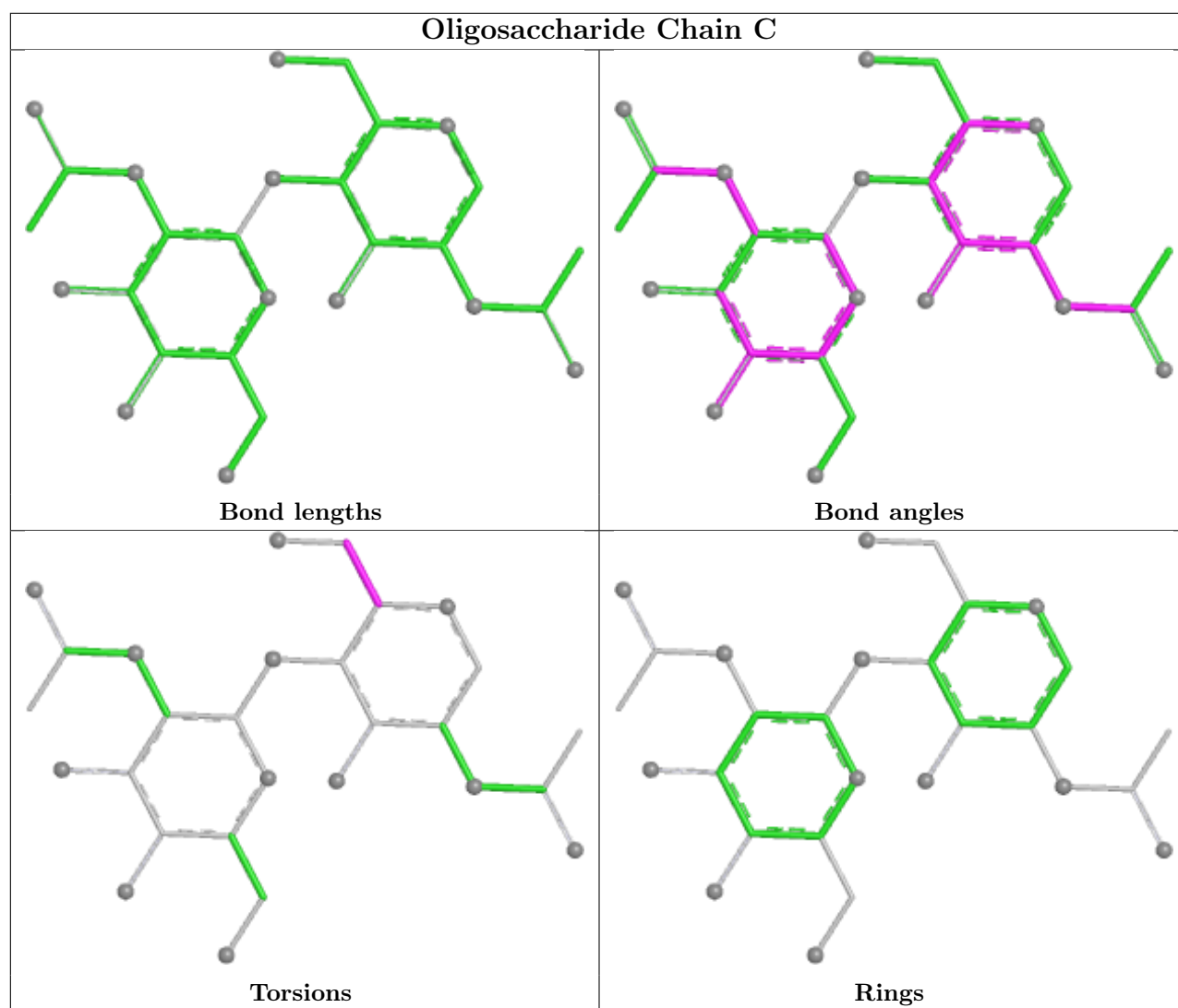
All (12) torsion outliers are listed below:

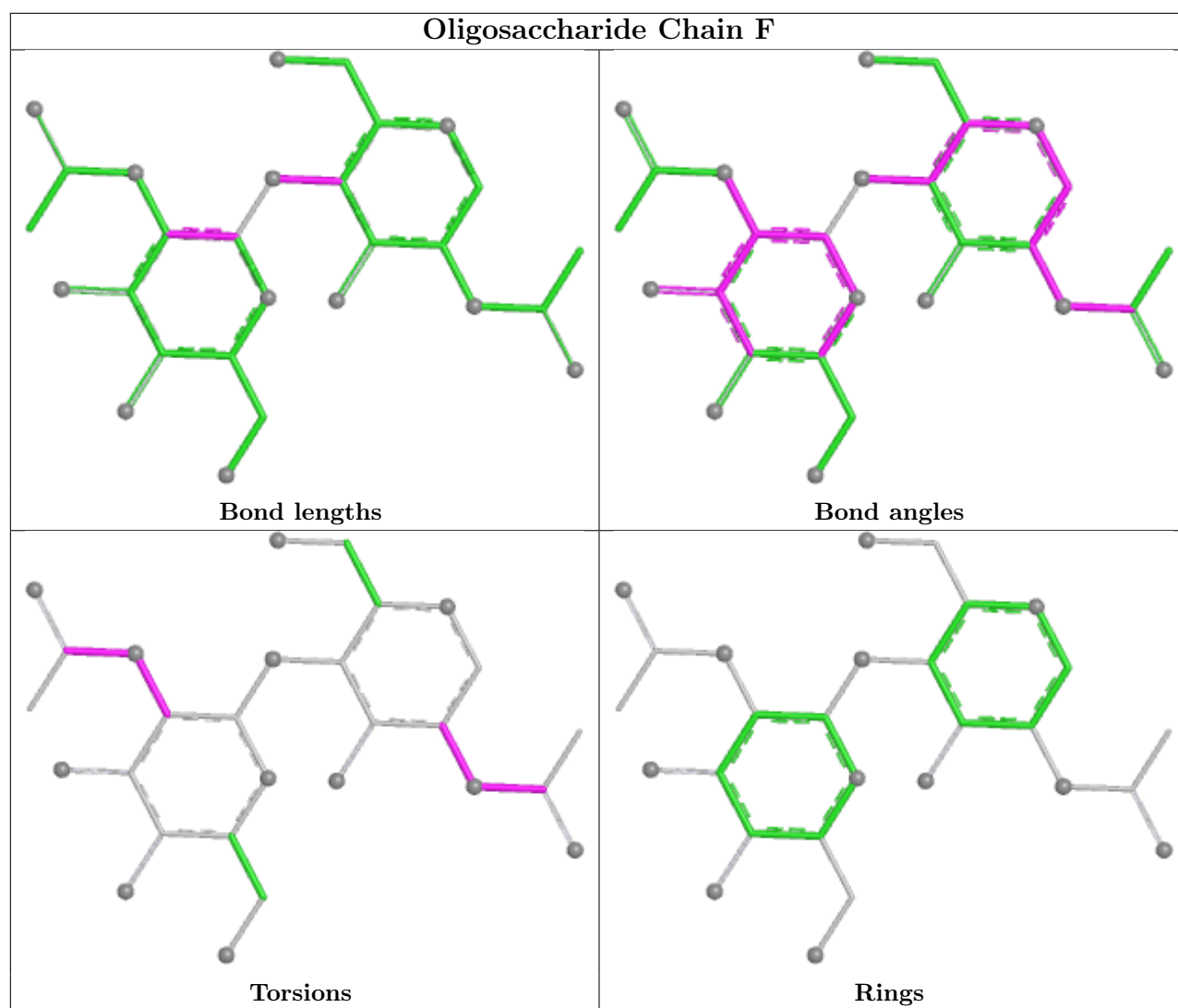
Mol	Chain	Res	Type	Atoms
2	F	1	NAG	C1-C2-N2-C7
2	F	2	NAG	C1-C2-N2-C7
2	F	2	NAG	C8-C7-N2-C2
2	F	2	NAG	O7-C7-N2-C2
3	D	2	NAG	O5-C5-C6-O6
2	F	1	NAG	C8-C7-N2-C2
3	D	2	NAG	C8-C7-N2-C2
2	F	1	NAG	O7-C7-N2-C2
3	D	2	NAG	O7-C7-N2-C2
3	D	2	NAG	C4-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6

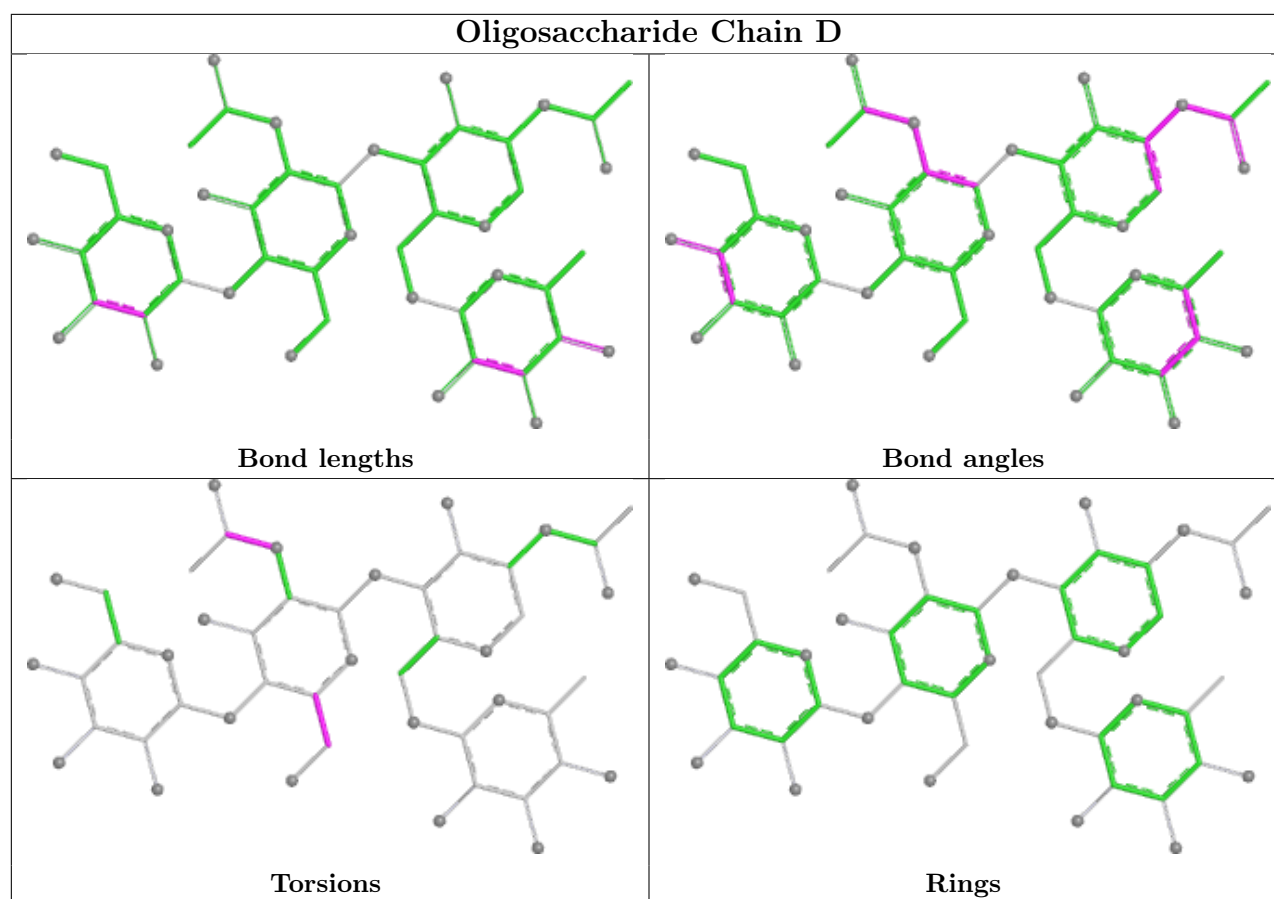
There are no ring outliers.

No monomer is involved in short contacts.

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







## 5.6 Ligand geometry [i](#)

Of 34 ligands modelled in this entry, 6 are monoatomic - leaving 28 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$
8	EDO	A	709	-	3,3,3	0.38	0	2,2,2	1.00	0
12	NAG	B	712	1	14,14,15	1.11	0	17,19,21	2.97	7 (41%)
14	PGE	B	704	-	9,9,9	0.63	0	8,8,8	0.47	0
10	ACT	A	714	-	3,3,3	2.23	2 (66%)	3,3,3	1.01	0
7	PEG	A	716[B]	-	6,6,6	0.32	0	5,5,5	0.72	0
10	ACT	B	711	-	3,3,3	1.82	2 (66%)	3,3,3	0.48	0
10	ACT	A	710	-	3,3,3	1.09	0	3,3,3	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	EDO	A	711	-	3,3,3	0.47	0	2,2,2	0.43	0
8	EDO	A	705	-	3,3,3	0.05	0	2,2,2	0.26	0
8	EDO	A	715	-	3,3,3	0.42	0	2,2,2	0.42	0
12	NAG	B	701	1	14,14,15	0.52	0	17,19,21	1.26	1 (5%)
8	EDO	A	707	-	3,3,3	0.29	0	2,2,2	0.09	0
7	PEG	A	704	-	6,6,6	0.33	0	5,5,5	0.19	0
7	PEG	B	708	-	6,6,6	0.42	0	5,5,5	0.40	0
7	PEG	A	716[A]	-	6,6,6	0.94	0	5,5,5	0.65	0
15	P33	B	705	-	21,21,21	0.69	0	20,20,20	0.58	0
8	EDO	A	712	-	3,3,3	1.34	1 (33%)	2,2,2	0.74	0
8	EDO	B	710	-	3,3,3	0.21	0	2,2,2	0.59	0
11	PG4	A	713	-	12,12,12	0.73	0	11,11,11	0.80	0
9	DMS	B	706	-	3,3,3	0.45	0	3,3,3	0.64	0
9	DMS	A	706	-	3,3,3	0.61	0	3,3,3	0.62	0
7	PEG	B	707	-	6,6,6	0.56	0	5,5,5	0.48	0
6	A1JPY	B	703	4	20,21,21	1.45	2 (10%)	24,29,29	1.21	3 (12%)
8	EDO	A	719	-	3,3,3	0.21	0	2,2,2	0.39	0
12	NAG	A	717	1	14,14,15	1.04	1 (7%)	17,19,21	1.94	5 (29%)
8	EDO	A	708	-	3,3,3	0.13	0	2,2,2	0.35	0
6	A1JPY	A	703	4	20,21,21	1.47	2 (10%)	24,29,29	1.58	3 (12%)
11	PG4	B	709	-	12,12,12	0.58	0	11,11,11	0.49	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
8	EDO	A	709	-	-	1/1/1/1	-
12	NAG	B	712	1	-	4/6/23/26	0/1/1/1
14	PGE	B	704	-	-	5/7/7/7	-
7	PEG	A	716[B]	-	-	0/4/4/4	-
8	EDO	A	711	-	-	1/1/1/1	-
8	EDO	A	705	-	-	1/1/1/1	-
8	EDO	A	715	-	-	1/1/1/1	-
12	NAG	B	701	1	-	1/6/23/26	0/1/1/1
8	EDO	A	707	-	-	0/1/1/1	-
7	PEG	A	704	-	-	2/4/4/4	-
7	PEG	B	708	-	-	3/4/4/4	-
7	PEG	A	716[A]	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	P33	B	705	-	-	10/19/19/19	-
8	EDO	A	712	-	-	1/1/1/1	-
8	EDO	B	710	-	-	1/1/1/1	-
11	PG4	A	713	-	-	3/10/10/10	-
7	PEG	B	707	-	-	4/4/4/4	-
6	A1JPY	B	703	4	-	0/15/28/28	0/2/2/2
8	EDO	A	719	-	-	1/1/1/1	-
12	NAG	A	717	1	-	4/6/23/26	0/1/1/1
8	EDO	A	708	-	-	1/1/1/1	-
6	A1JPY	A	703	4	-	0/15/28/28	0/2/2/2
11	PG4	B	709	-	-	5/10/10/10	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	703	A1JPY	C5-C4	-4.78	1.47	1.51
6	A	703	A1JPY	C11-N1	4.26	1.41	1.36
6	A	703	A1JPY	C5-C4	3.27	1.54	1.51
10	A	714	ACT	CH3-C	2.93	1.60	1.49
12	A	717	NAG	O5-C5	2.54	1.48	1.43
10	A	714	ACT	O-C	2.42	1.32	1.22
6	B	703	A1JPY	C11-N1	2.33	1.39	1.36
10	B	711	ACT	O-C	2.25	1.32	1.22
8	A	712	EDO	O2-C2	2.09	1.52	1.42
10	B	711	ACT	CH3-C	2.05	1.57	1.49

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	712	NAG	C1-C2-N2	9.44	125.31	110.43
12	A	717	NAG	C1-C2-N2	5.02	118.34	110.43
6	A	703	A1JPY	O1-C1-C2	-4.42	108.87	122.44
6	A	703	A1JPY	O2-C1-C2	3.96	126.27	113.34
12	B	712	NAG	C1-O5-C5	3.81	117.30	112.19
12	A	717	NAG	C1-O5-C5	3.46	116.82	112.19
12	B	712	NAG	O4-C4-C3	-3.44	102.27	110.38
6	A	703	A1JPY	C3-C2-C1	-3.18	105.62	111.28
6	B	703	A1JPY	C5-C4-N1	2.96	117.30	113.94
6	B	703	A1JPY	O4-C11-N1	-2.77	118.93	122.09
12	B	712	NAG	O3-C3-C2	-2.63	103.93	109.40
12	A	717	NAG	O3-C3-C2	-2.61	103.98	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	717	NAG	O3-C3-C4	2.55	116.38	110.38
12	B	701	NAG	C4-C3-C2	2.41	114.55	111.02
12	B	712	NAG	O6-C6-C5	2.30	119.17	111.33
6	B	703	A1JPY	O1-C1-C2	-2.23	115.60	122.44
12	B	712	NAG	C8-C7-N2	2.23	119.81	116.12
12	A	717	NAG	O5-C1-C2	-2.21	107.88	111.29
12	B	712	NAG	O4-C4-C5	2.15	114.62	109.32

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	B	712	NAG	C1-C2-N2-C7
12	A	717	NAG	O5-C5-C6-O6
7	B	707	PEG	C1-C2-O2-C3
15	B	705	P33	O7-C8-C9-O10
15	B	705	P33	O4-C5-C6-O7
14	B	704	PGE	O2-C3-C4-O3
11	B	709	PG4	C8-C7-O4-C6
12	A	717	NAG	C4-C5-C6-O6
12	B	712	NAG	C4-C5-C6-O6
7	A	716[A]	PEG	O2-C3-C4-O4
12	B	712	NAG	O5-C5-C6-O6
7	B	708	PEG	O2-C3-C4-O4
11	A	713	PG4	O4-C7-C8-O5
15	B	705	P33	O10-C11-C12-O13
7	A	704	PEG	O2-C3-C4-O4
11	B	709	PG4	O4-C7-C8-O5
14	B	704	PGE	O1-C1-C2-O2
7	A	716[A]	PEG	O1-C1-C2-O2
8	B	710	EDO	O1-C1-C2-O2
11	B	709	PG4	O2-C3-C4-O3
7	B	707	PEG	O2-C3-C4-O4
11	A	713	PG4	C6-C5-O3-C4
11	A	713	PG4	C4-C3-O2-C2
7	B	708	PEG	C4-C3-O2-C2
8	A	708	EDO	O1-C1-C2-O2
8	A	711	EDO	O1-C1-C2-O2
8	A	712	EDO	O1-C1-C2-O2
15	B	705	P33	O19-C20-C21-O22
15	B	705	P33	C6-C5-O4-C3
14	B	704	PGE	C6-C5-O3-C4

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Mol	Chain	Res	Type	Atoms
14	B	704	PGE	C4-C3-O2-C2
15	B	705	P33	C8-C9-O10-C11
8	A	705	EDO	O1-C1-C2-O2
11	B	709	PG4	O1-C1-C2-O2
12	A	717	NAG	C3-C2-N2-C7
7	B	708	PEG	O1-C1-C2-O2
15	B	705	P33	C11-C12-O13-C14
15	B	705	P33	C5-C6-O7-C8
15	B	705	P33	O16-C17-C18-O19
14	B	704	PGE	O3-C5-C6-O4
11	B	709	PG4	C1-C2-O2-C3
12	A	717	NAG	C1-C2-N2-C7
7	B	707	PEG	C4-C3-O2-C2
12	B	701	NAG	C4-C5-C6-O6
8	A	709	EDO	O1-C1-C2-O2
8	A	719	EDO	O1-C1-C2-O2
12	B	712	NAG	C3-C2-N2-C7
7	B	707	PEG	O1-C1-C2-O2
15	B	705	P33	C2-C3-O4-C5
8	A	715	EDO	O1-C1-C2-O2
7	A	704	PEG	O1-C1-C2-O2

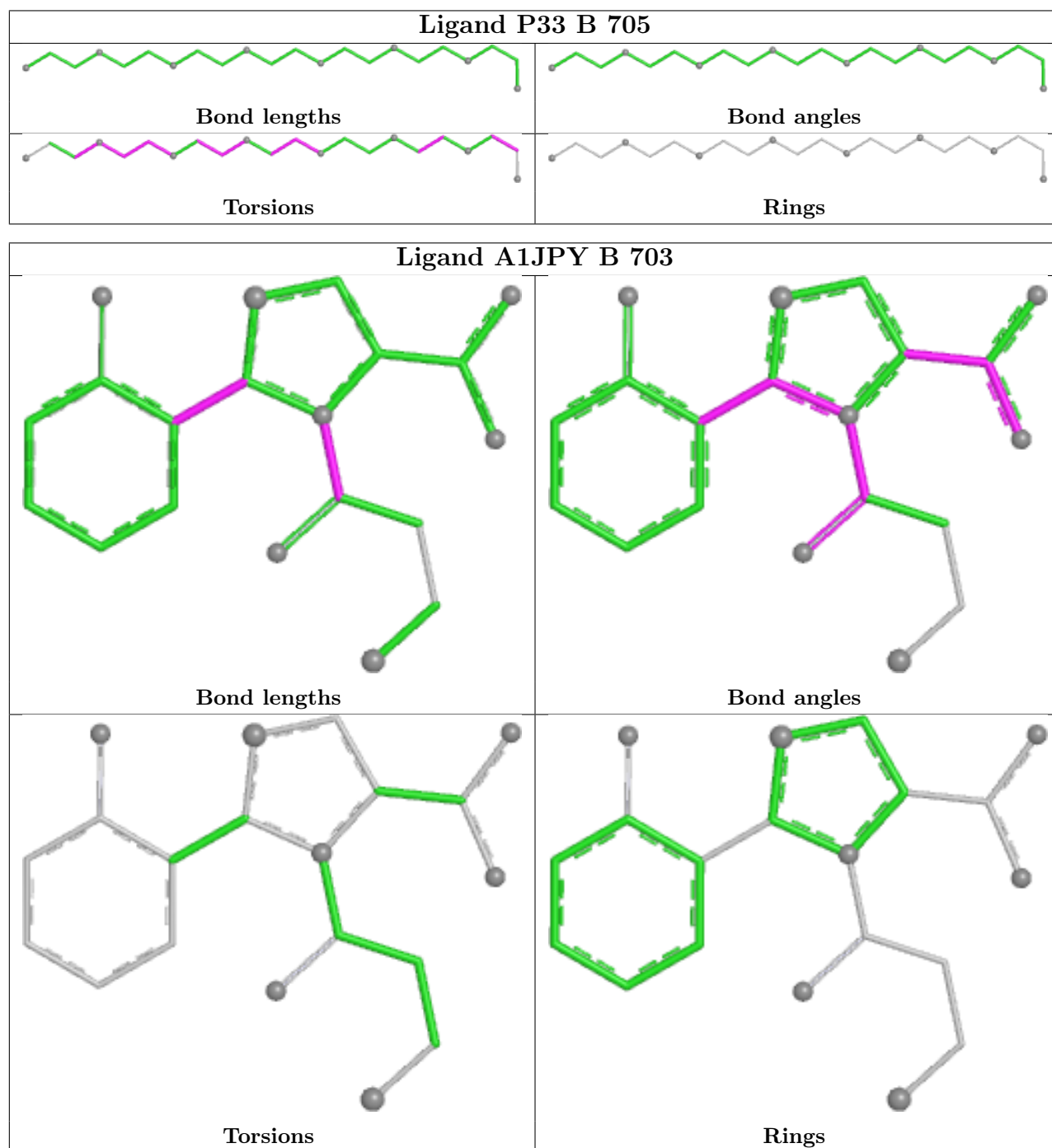
There are no ring outliers.

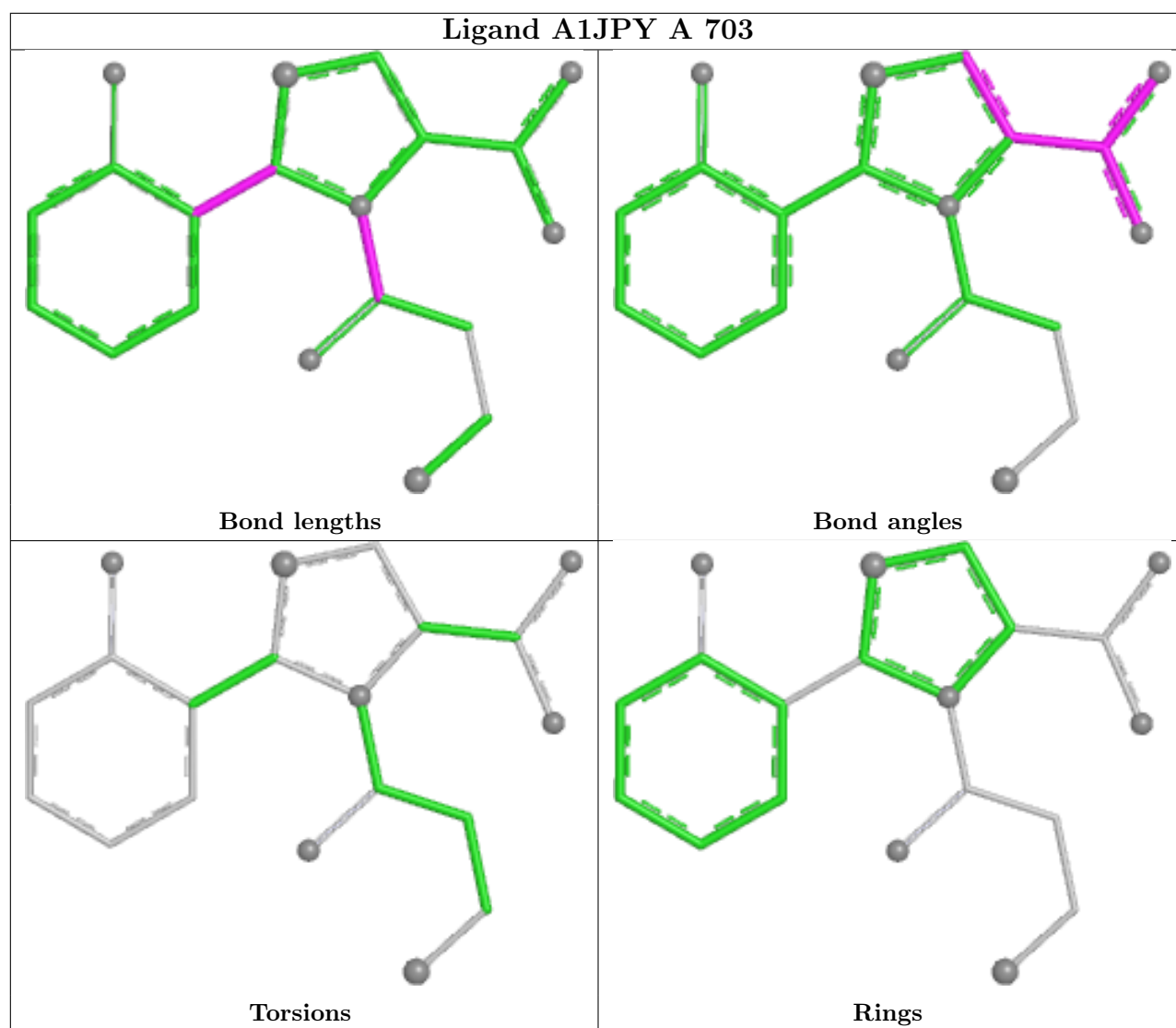
9 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	716[B]	PEG	2	0
10	B	711	ACT	2	0
8	A	705	EDO	1	0
7	A	716[A]	PEG	1	0
8	A	712	EDO	2	0
11	A	713	PG4	1	0
7	B	707	PEG	2	0
12	A	717	NAG	1	0
11	B	709	PG4	4	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	604/628 (96%)	-0.31	28 (4%) 37 36	10, 28, 57, 92	5 (0%)
1	B	603/628 (96%)	-0.18	3 (0%) 87 87	12, 33, 58, 95	8 (1%)
All	All	1207/1256 (96%)	-0.24	31 (2%) 57 56	10, 30, 58, 95	13 (1%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	414	VAL	4.9
1	A	79	ILE	4.6
1	A	83	PHE	4.6
1	A	88	LEU	4.4
1	A	80	TRP	4.1
1	A	21	ALA	4.0
1	A	129	LEU	3.9
1	B	129	LEU	3.9
1	A	135	THR	3.3
1	A	14	GLU	3.2
1	A	78	PRO	3.2
1	A	84	THR	3.1
1	A	92	ILE	3.1
1	A	72	ALA	3.1
1	A	16	GLY	3.0
1	A	91	ILE	3.0
1	A	18	GLN	2.9
1	A	24	TYR	2.7
1	A	17	ALA	2.6
1	A	15	ALA	2.5
1	A	25	GLN	2.5
1	A	12	ALA	2.5
1	A	19	LEU	2.5
1	A	609	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	607	TYR	2.4
1	A	86	PRO	2.4
1	A	82	GLN	2.3
1	A	81	GLN	2.2
1	B	75	LEU	2.2
1	A	87	GLN	2.1
1	A	13	ASP	2.0

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

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

## 6.3 Carbohydrates [i](#)

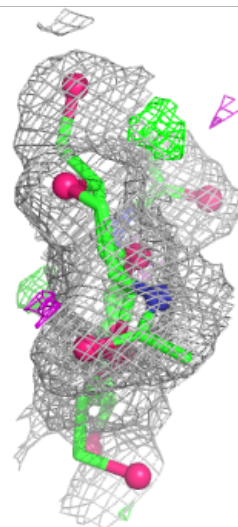
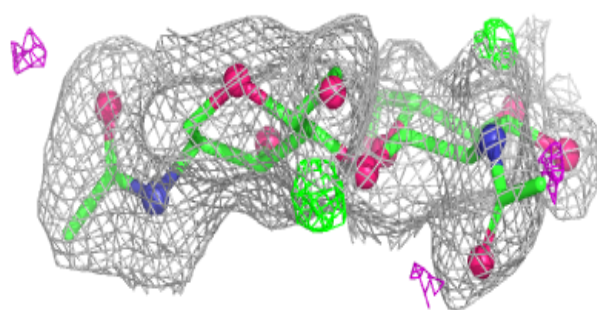
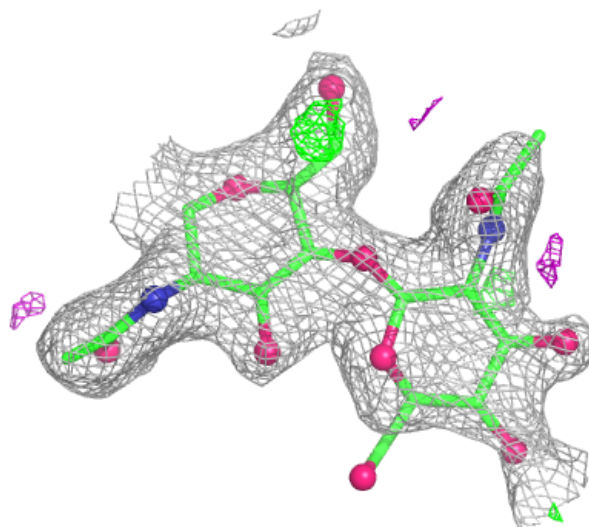
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	NAG	C	2	14/15	0.72	0.15	46,63,81,86	0
2	NAG	C	1	14/15	0.85	0.10	40,50,65,72	0
2	NAG	F	1	14/15	-	-	46,64,74,77	0
2	NAG	F	2	14/15	-	-	56,73,83,86	0
3	FUC	D	4	10/11	0.85	0.13	43,52,60,63	0
3	BMA	D	3	11/12	0.86	0.11	44,60,68,71	0
3	NAG	D	2	14/15	0.92	0.08	39,49,62,75	0
3	NAG	D	1	14/15	0.94	0.08	32,40,48,50	0

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

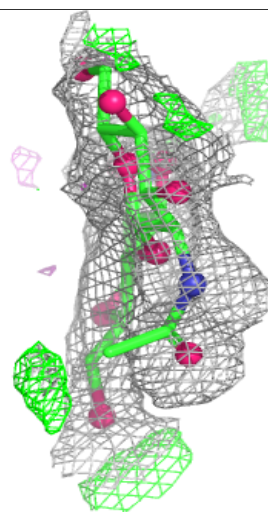
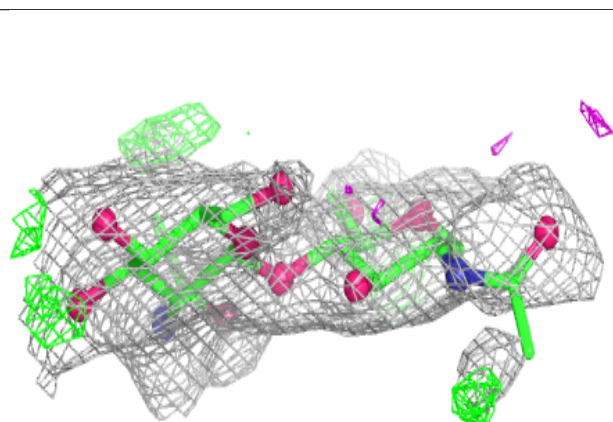
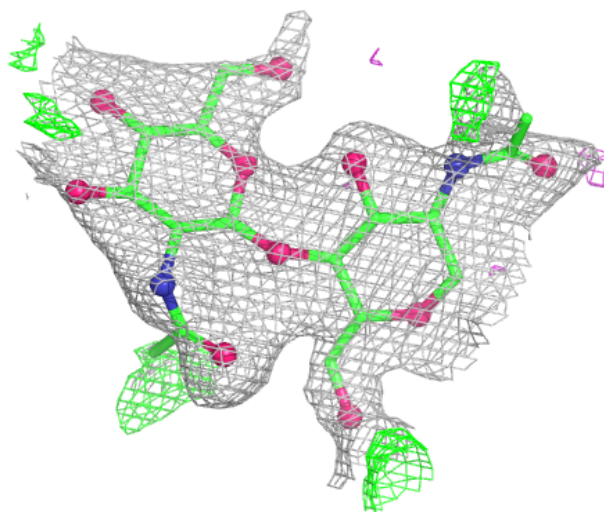
**Electron density around Chain C:**

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

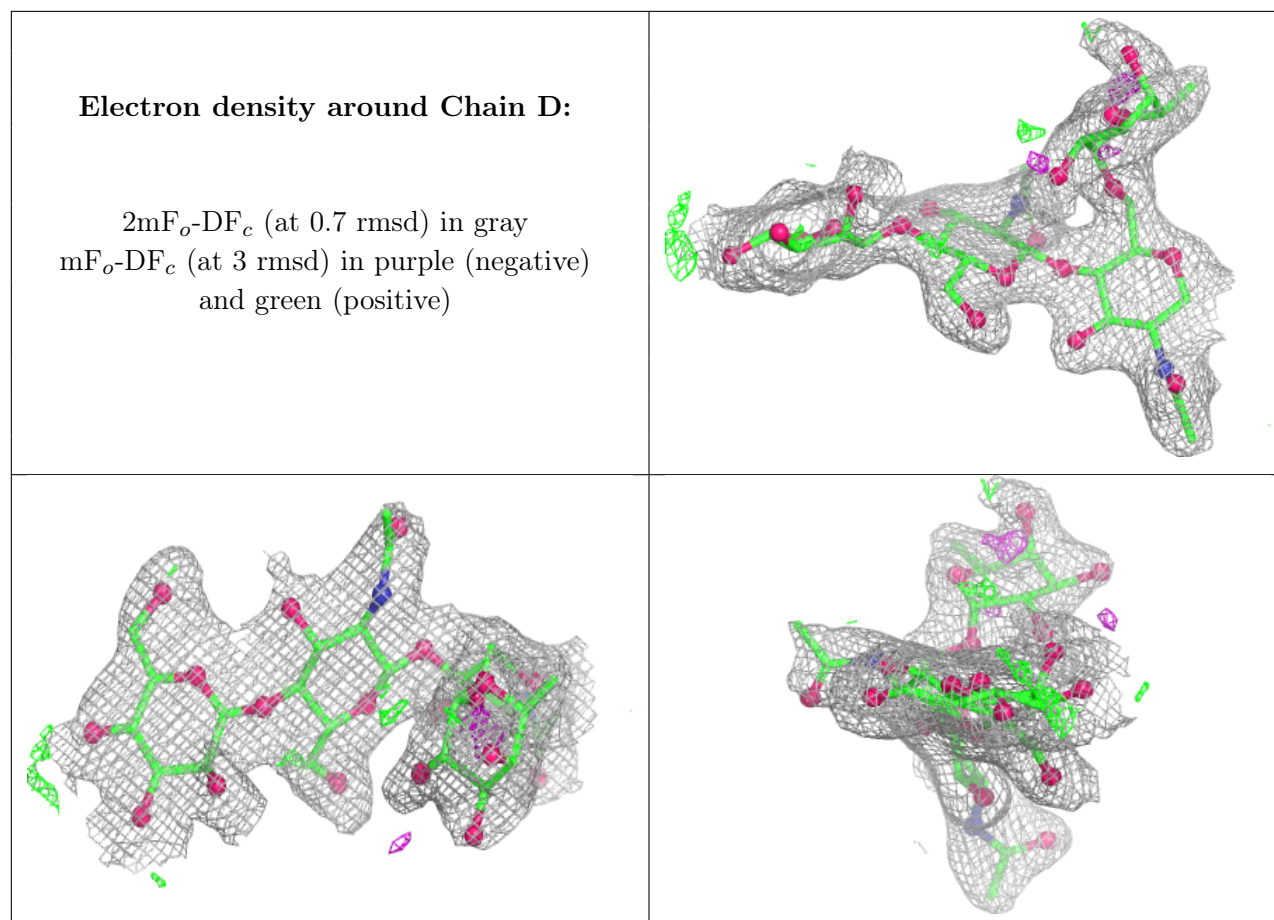


**Electron density around Chain F:**

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







## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
7	PEG	A	716[A]	7/7	0.68	0.37	42,45,51,56	7
7	PEG	A	716[B]	7/7	0.68	0.37	24,26,28,29	7
12	NAG	A	717	14/15	0.80	0.14	34,42,57,61	0
12	NAG	B	712	14/15	0.80	0.13	37,46,56,63	0
8	EDO	A	711	4/4	0.82	0.20	54,62,63,67	0
8	EDO	A	719	4/4	0.82	0.14	50,58,59,62	0
8	EDO	A	712	4/4	0.83	0.15	43,44,50,56	0
11	PG4	A	713	13/13	0.84	0.14	45,53,66,67	0
7	PEG	B	707	7/7	0.85	0.18	47,58,69,70	0
8	EDO	A	715	4/4	0.87	0.12	53,55,58,58	0
11	PG4	B	709	13/13	0.87	0.13	37,54,69,70	0
10	ACT	A	714	4/4	0.87	0.12	37,37,42,44	0

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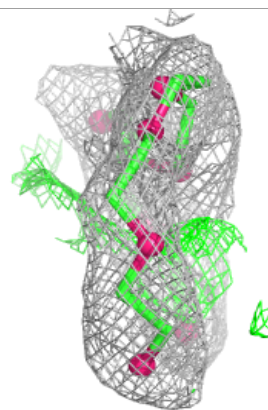
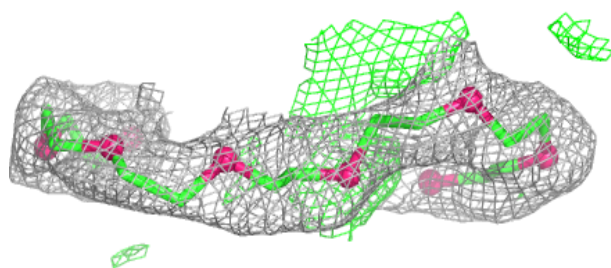
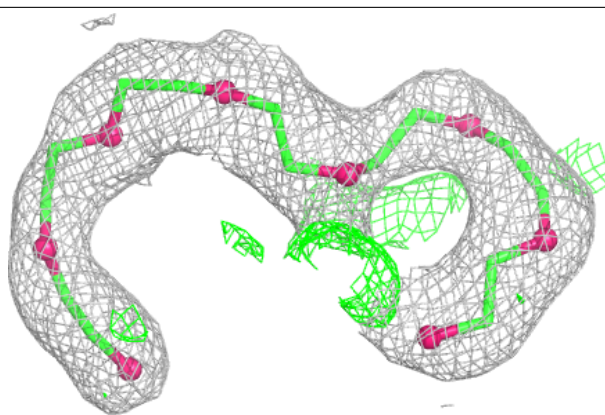
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
10	ACT	B	711	4/4	0.87	0.13	34,42,49,55	0
14	PGE	B	704	10/10	0.87	0.15	44,55,78,98	0
8	EDO	A	705	4/4	0.88	0.14	52,56,57,62	0
8	EDO	A	709	4/4	0.89	0.11	41,48,48,52	0
7	PEG	B	708	7/7	0.89	0.11	48,50,57,58	0
8	EDO	A	707	4/4	0.89	0.10	50,51,53,54	0
8	EDO	B	710	4/4	0.90	0.14	54,56,57,58	0
12	NAG	B	701	14/15	0.90	0.09	42,48,55,64	0
7	PEG	A	704	7/7	0.91	0.09	46,49,64,71	0
15	P33	B	705	22/22	0.91	0.12	45,52,62,72	0
5	CA	B	714	1/1	0.92	0.08	58,58,58,58	0
8	EDO	A	708	4/4	0.93	0.10	50,52,52,57	0
10	ACT	A	710	4/4	0.95	0.10	46,49,50,51	0
6	A1JPY	B	703	20/20	0.98	0.04	18,21,22,23	0
9	DMS	A	706	4/4	0.98	0.06	22,23,25,26	0
6	A1JPY	A	703	20/20	0.98	0.04	16,17,20,22	0
5	CA	A	702	1/1	0.99	0.08	39,39,39,39	0
9	DMS	B	706	4/4	0.99	0.07	19,22,23,24	0
13	CL	A	718	1/1	0.99	0.04	20,20,20,20	0
4	ZN	A	701	1/1	0.99	0.02	18,18,18,18	0
4	ZN	B	702	1/1	0.99	0.02	20,20,20,20	0
13	CL	B	713	1/1	1.00	0.03	24,24,24,24	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.

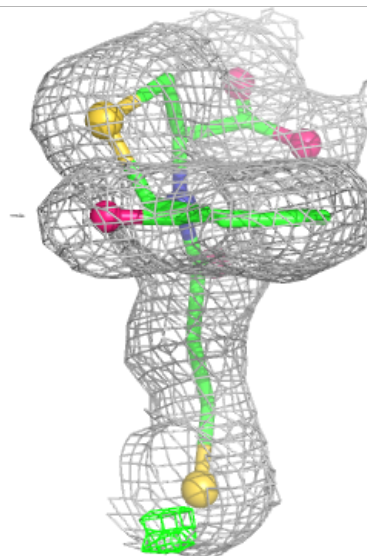
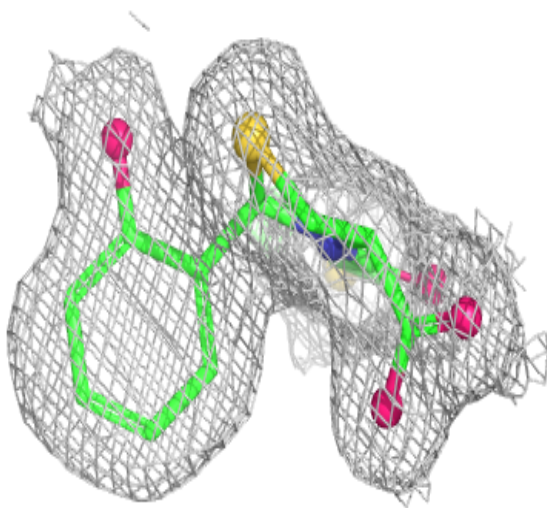
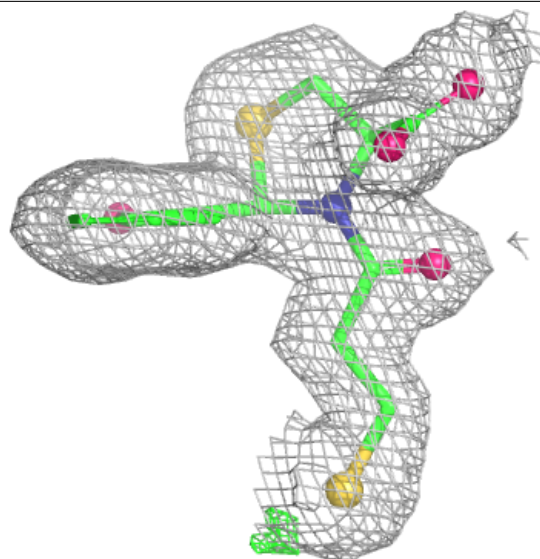
**Electron density around P33 B 705:**

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



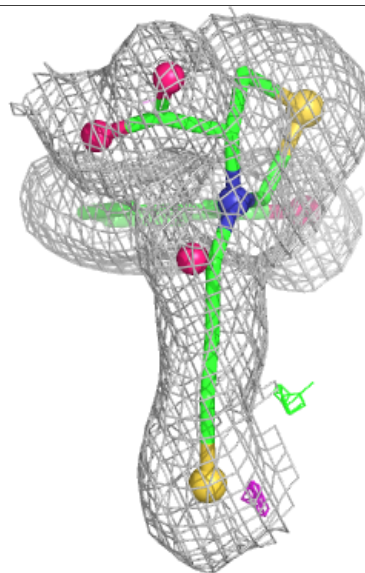
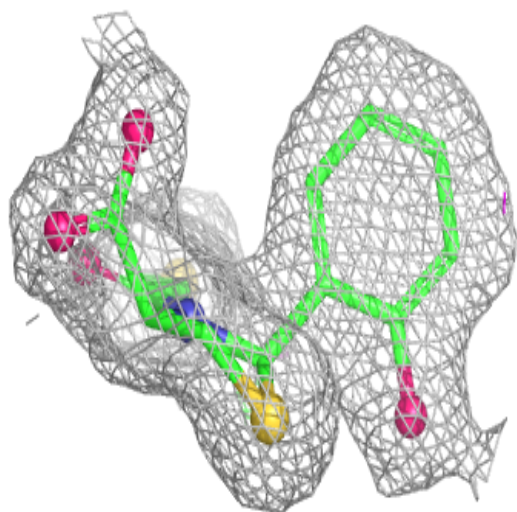
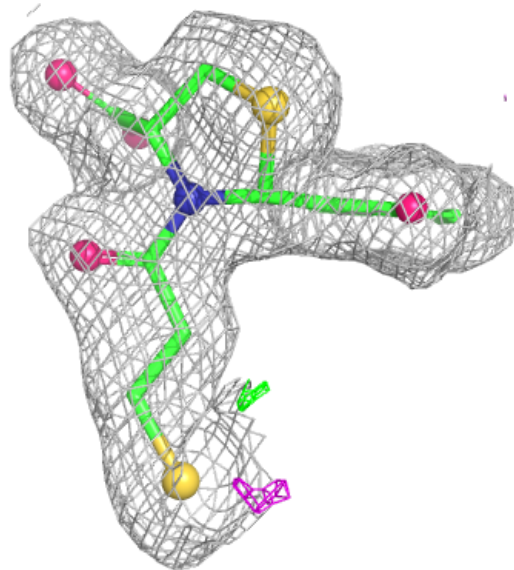
**Electron density around A1JPY B 703:**

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



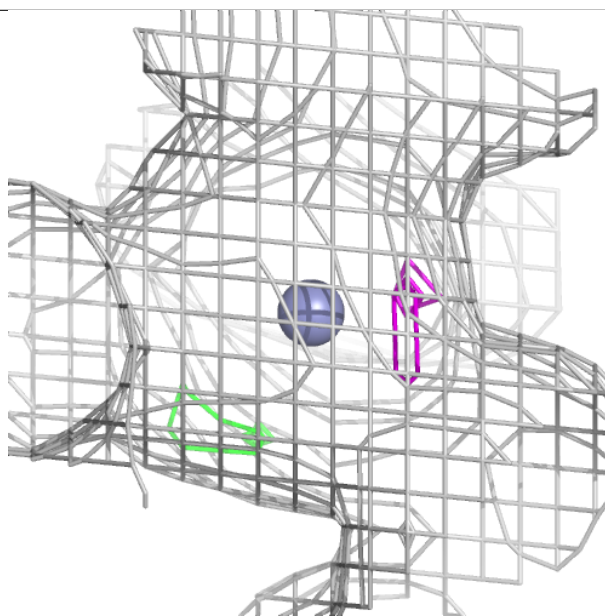
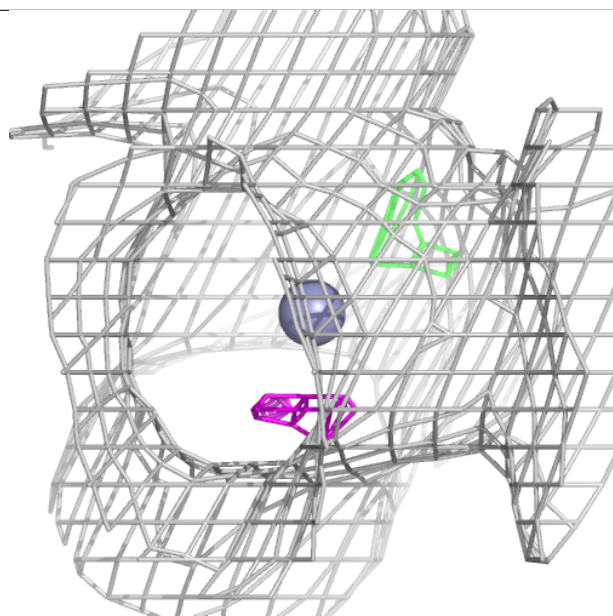
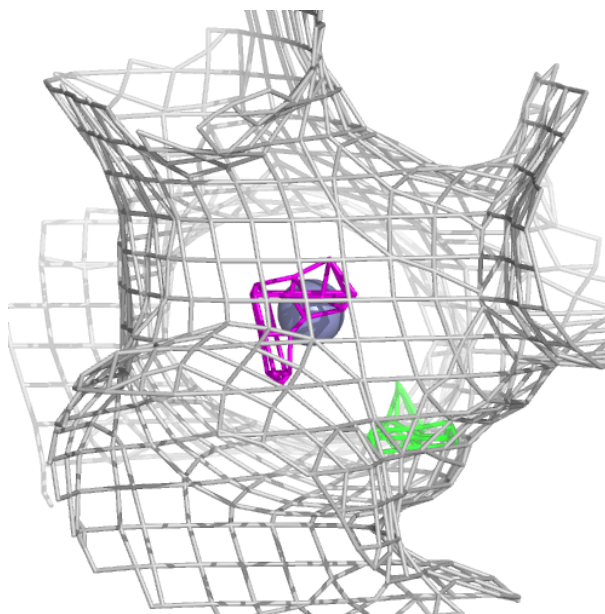
**Electron density around A1JPY A 703:**

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



**Electron density around ZN A 701:**

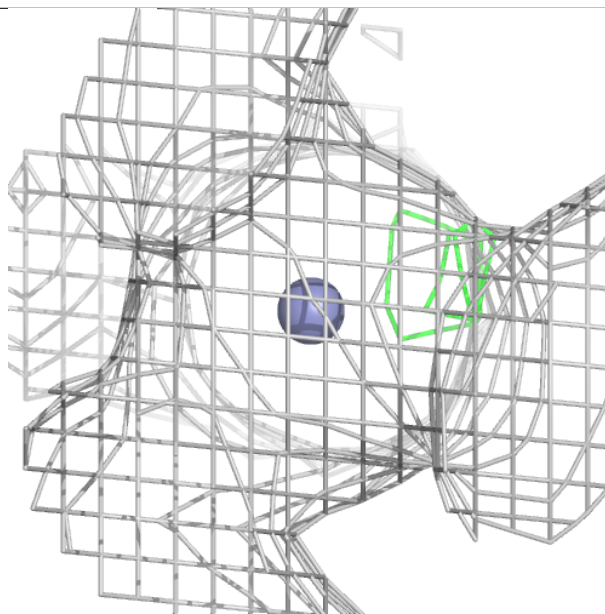
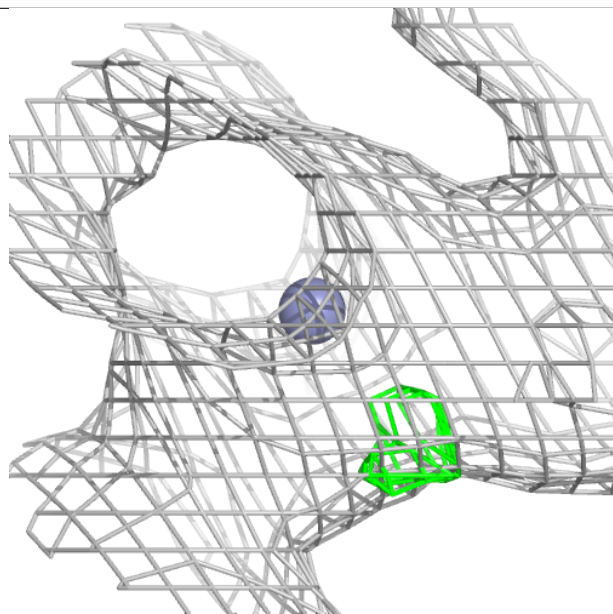
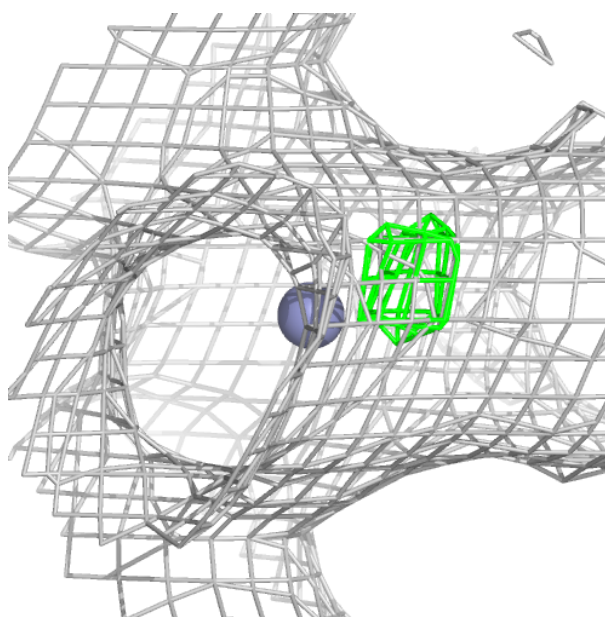
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around ZN B 702:**

$2mF_o-DF_c$  (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.