



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:01 PM UTC

PDB ID : 9SS9 / pdb_00009ss9
Title : Human angiotensin 1-converting enzyme N-domain in complex with captopril
Authors : Gregory, K.S.; Acharya, K.R.
Deposited on : 2025-09-25
Resolution : 2.50 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

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>.

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

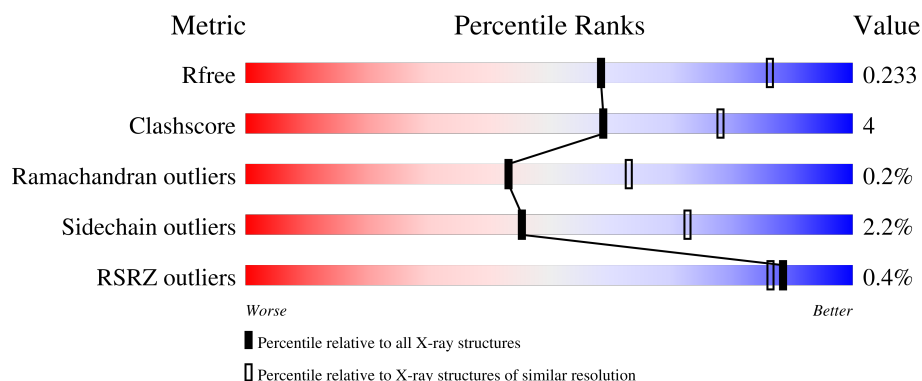
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION




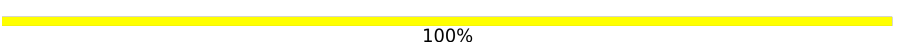
The reported resolution of this entry is 2.50 Å.

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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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 ≥ 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	 81% 14% . .
1	B	628	 82% 13% .
2	C	2	 50% 50%
2	D	2	 100%

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
4	PEG	A	708	-	-	X	-

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 10160 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	B	602	Total	C	N	O	S	0	1	0
			4928	3165	846	898	19			
1	A	602	Total	C	N	O	S	0	0	0
			4922	3162	845	896	19			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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

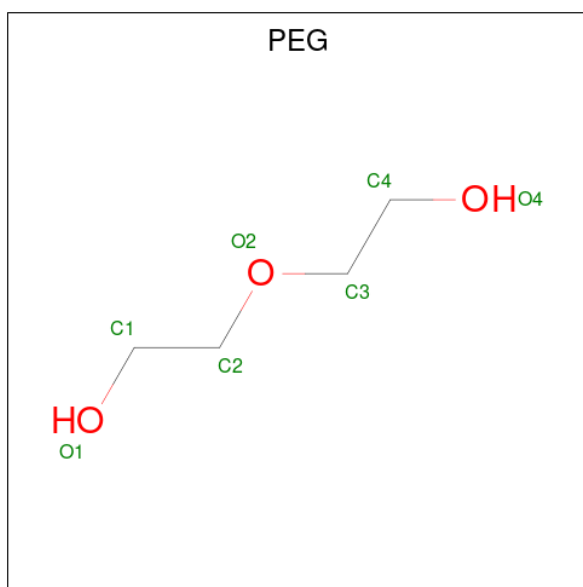


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

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

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

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



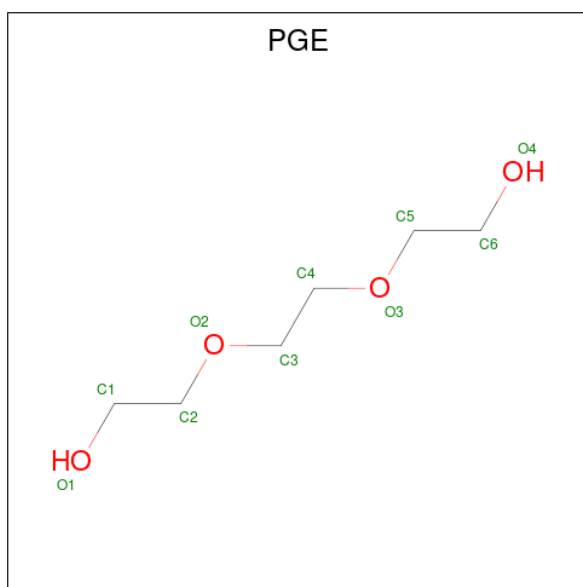
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

- Molecule 6 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



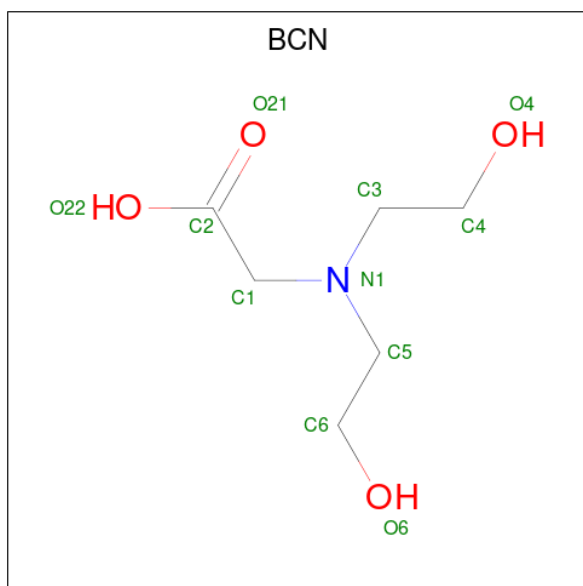
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			10	6	4		

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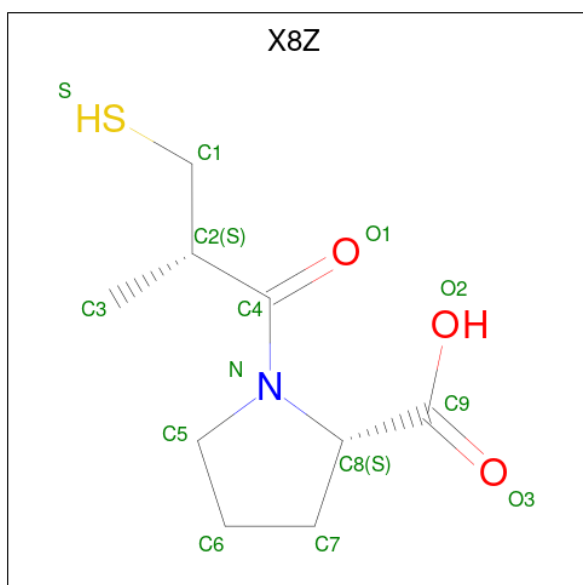
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 7 is BICINE (CCD ID: BCN) (formula: $C_6H_{13}NO_4$).



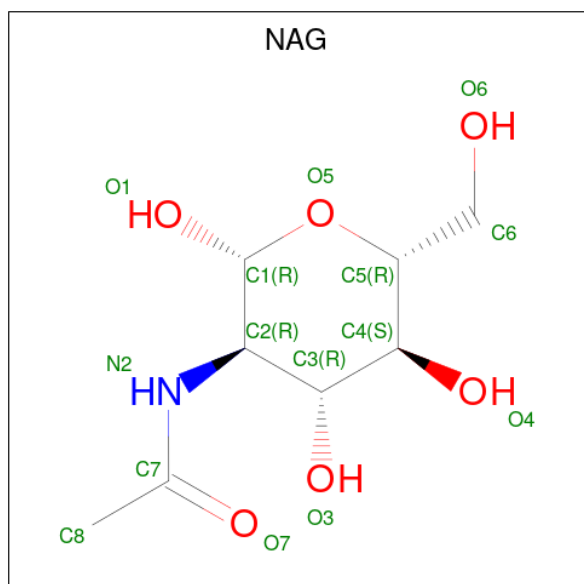
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	N	O	0	0
			11	6	1	4		

- Molecule 8 is L-CAPTOPRIL (CCD ID: X8Z) (formula: $C_9H_{15}NO_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	N	O	S	0	0
			14	9	1	3	1		

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

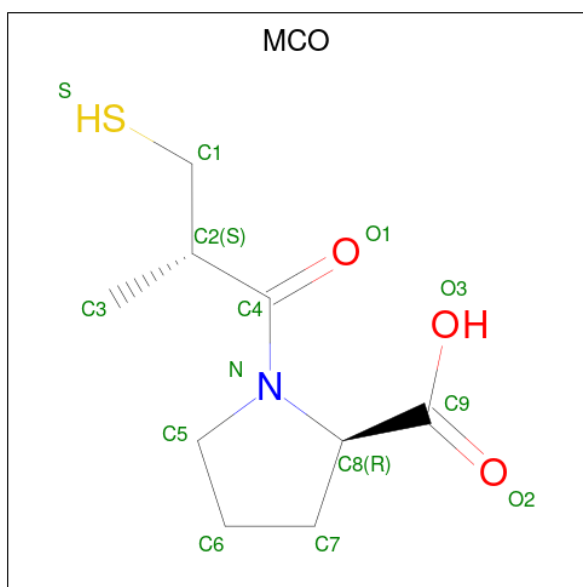


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O		0	0
			14	8	1	5			
9	A	1	Total	C	N	O		0	0
			14	8	1	5			
9	A	1	Total	C	N	O		0	0
			14	8	1	5			
9	A	1	Total	C	N	O		0	0
			14	8	1	5			

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

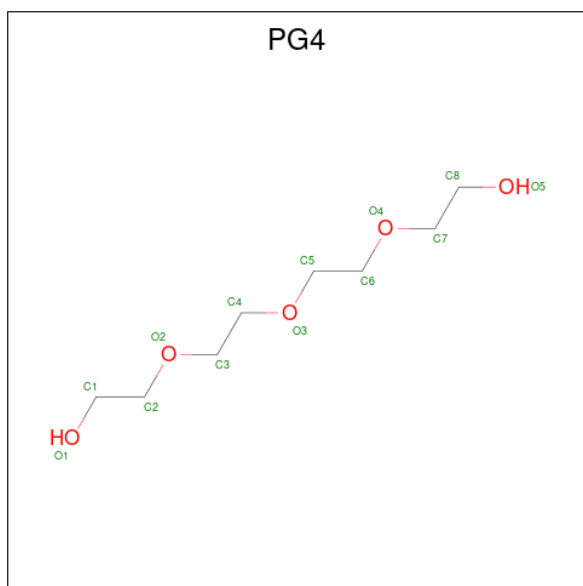
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	1	Total	Cl	0	0
			1	1		
10	A	1	Total	Cl	0	0
			1	1		

- Molecule 11 is 1-(3-MERCAPTO-2-METHYL-PROPIONYL)-PYRROLIDINE-2-CARBOXYLIC ACID (CCD ID: MCO) (formula: $C_9H_{15}NO_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	A	1	Total	C	N	O	S	0	0
			14	9	1	3	1		

- Molecule 12 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



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

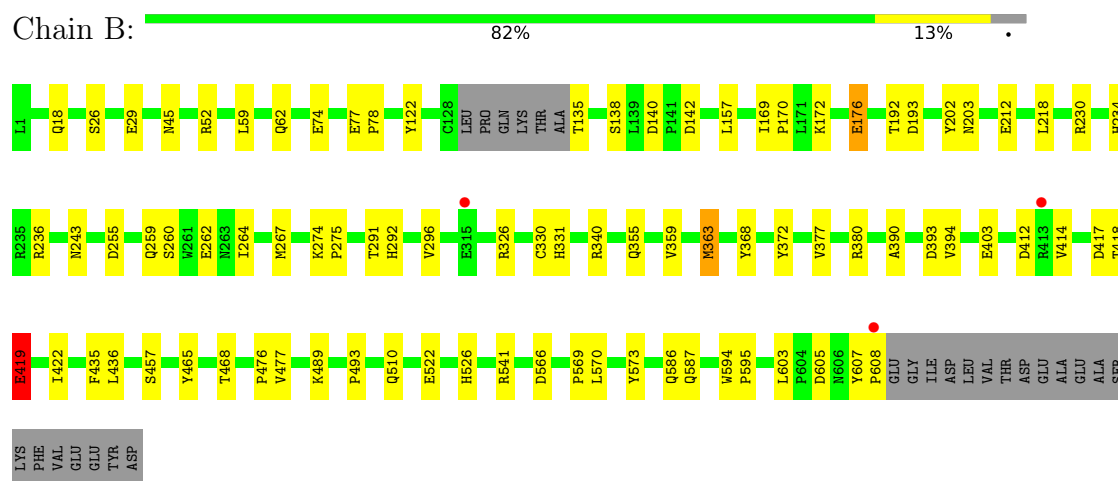
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	B	35	Total 35	O 35	0	0
13	A	34	Total 34	O 34	0	0

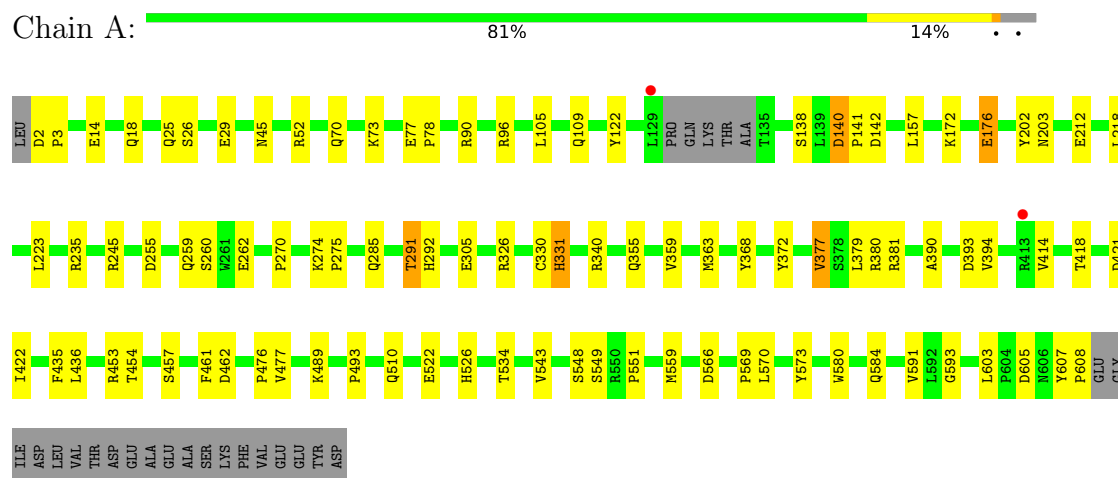
3 Residue-property plots

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



MAG1
MAG2

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

Chain D:

100%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	72.04Å 77.50Å 80.63Å 89.31° 65.33° 75.34°	Depositor
Resolution (Å)	74.55 – 2.50 74.55 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.8 (74.55-2.50) 98.6 (74.55-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0431 (refmacat 0.4.105)	Depositor
R, R_{free}	0.185 , 0.227 0.193 , 0.233	Depositor DCC
R_{free} test set	2569 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	41.8	Xtriage
Anisotropy	0.170	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 39.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10160	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.54% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: PGE, BCN, X8Z, MCO, CL, PEG, ZN, PG4, NAG, EDO

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.62	0/5077	1.11	11/6915 (0.2%)
1	B	0.65	0/5083	1.12	14/6923 (0.2%)
All	All	0.64	0/10160	1.11	25/13838 (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	5
1	B	0	2
All	All	0	7

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	291	THR	CA-CB-OG1	-8.82	96.36	109.60
1	A	291	THR	CA-CB-OG1	-8.28	97.18	109.60
1	B	393	ASP	CA-CB-CG	6.87	119.47	112.60
1	A	393	ASP	CA-CB-CG	6.81	119.41	112.60
1	B	412	ASP	CB-CA-C	-6.75	100.28	110.88
1	B	74	GLU	CB-CA-C	-6.67	100.14	110.81
1	B	363	MET	CG-SD-CE	-6.62	86.34	100.90
1	A	363	MET	CG-SD-CE	-6.45	86.72	100.90
1	B	255	ASP	CA-CB-CG	6.11	118.71	112.60
1	B	412	ASP	CA-CB-CG	5.96	118.56	112.60
1	A	584	GLN	CB-CA-C	-5.87	101.04	110.79
1	A	140	ASP	CA-CB-CG	5.86	118.46	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	255	ASP	CA-CB-CG	5.81	118.41	112.60
1	B	212	GLU	CB-CG-CD	5.79	122.45	112.60
1	B	566	ASP	CA-CB-CG	5.74	118.34	112.60
1	B	140	ASP	CA-CB-CG	5.61	118.21	112.60
1	B	419	GLU	N-CA-CB	5.57	118.92	110.28
1	A	566	ASP	CA-CB-CG	5.45	118.05	112.60
1	A	176	GLU	CB-CA-C	-5.19	102.73	110.88
1	B	586	GLN	N-CA-CB	5.18	117.58	110.07
1	B	468	THR	CA-CB-OG1	-5.12	101.92	109.60
1	A	212	GLU	CB-CG-CD	5.09	121.25	112.60
1	A	605	ASP	CA-CB-CG	5.09	117.69	112.60
1	A	331	HIS	CA-CB-CG	-5.01	108.79	113.80
1	B	176	GLU	CB-CA-C	-5.01	103.02	110.88

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	235	ARG	Sidechain
1	A	326	ARG	Sidechain
1	A	380	ARG	Sidechain
1	A	52	ARG	Sidechain
1	A	90	ARG	Sidechain
1	B	380	ARG	Sidechain
1	B	541	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	4922	0	4698	45	0
1	B	4928	0	4705	40	0
2	C	28	0	25	1	0
2	D	28	0	25	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	14	0	20	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	14	0	20	0	0
5	A	4	0	6	0	0
5	B	8	0	12	0	0
6	A	10	0	14	0	0
6	B	10	0	14	4	0
7	B	11	0	12	0	0
8	B	14	0	13	0	0
9	A	42	0	39	0	0
9	B	14	0	13	0	0
10	A	1	0	0	0	0
10	B	1	0	0	0	0
11	A	14	0	13	1	0
12	A	26	0	36	2	0
13	A	34	0	0	1	0
13	B	35	0	0	1	0
All	All	10160	0	9665	86	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 (86) 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:260:SER:OG	1:A:262:GLU:OE1	1.98	0.81
1:B:260:SER:OG	1:B:262:GLU:OE1	1.98	0.81
1:B:477:VAL:HG12	1:B:603:LEU:HD21	1.66	0.77
1:A:477:VAL:HG12	1:A:603:LEU:HD21	1.67	0.76
1:B:234:HIS:ND1	13:B:801:HOH:O	2.25	0.68
1:A:270:PRO:HB3	1:A:580:TRP:CH2	2.35	0.62
1:B:595:PRO:HA	6:B:705:PGE:H1	1.83	0.60
1:B:326:ARG:HD3	2:C:1:NAG:H82	1.85	0.57
6:B:705:PGE:H12	1:A:457:SER:O	2.05	0.56
1:A:390:ALA:O	1:A:394:VAL:HG23	2.07	0.55
1:A:29:GLU:OE1	1:A:340:ARG:NH1	2.40	0.54
1:B:403:GLU:OE2	1:B:414:VAL:HG11	2.07	0.54
1:A:593:GLY:HA3	4:A:708:PEG:H12	1.90	0.53
1:A:14:GLU:O	1:A:18:GLN:HG2	2.09	0.53
1:B:218:LEU:HD13	1:B:436:LEU:HD13	1.91	0.52
1:B:390:ALA:O	1:B:394:VAL:HG23	2.10	0.52
1:A:25:GLN:HG3	1:A:377:VAL:HB	1.90	0.52
1:A:218:LEU:HD13	1:A:436:LEU:HD13	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:LEU:HD13	1:B:476:PRO:HB2	1.91	0.51
1:B:274:LYS:O	1:B:275:PRO:C	2.55	0.50
1:B:355:GLN:O	1:B:359:VAL:HG23	2.11	0.50
1:B:29:GLU:OE1	1:B:340:ARG:NH2	2.45	0.50
1:B:172:LYS:O	1:B:176:GLU:HG3	2.11	0.50
1:A:543:VAL:HG21	1:A:559:MET:SD	2.53	0.49
1:B:340:ARG:HH21	1:B:340:ARG:HG3	1.77	0.49
1:A:275:PRO:HG2	1:A:414:VAL:HG23	1.93	0.49
1:B:417:ASP:OD2	1:B:419:GLU:HG2	2.13	0.49
1:A:292:HIS:CE1	12:A:705:PG4:H52	2.48	0.49
1:A:489:LYS:O	1:A:493:PRO:HD2	2.13	0.48
1:B:465:TYR:CE1	1:A:461:PHE:CE2	3.01	0.48
1:A:355:GLN:O	1:A:359:VAL:HG23	2.12	0.48
1:A:453:ARG:CZ	4:A:709:PEG:H41	2.44	0.48
1:A:77:GLU:N	1:A:78:PRO:HD2	2.30	0.47
1:A:245:ARG:HG2	1:A:591:VAL:CG1	2.44	0.47
1:B:52:ARG:HH11	1:B:52:ARG:HG2	1.80	0.47
1:A:223:LEU:HD11	4:A:708:PEG:H32	1.96	0.47
1:B:457:SER:HB2	4:A:708:PEG:H11	1.96	0.47
1:B:489:LYS:O	1:B:493:PRO:HD2	2.15	0.47
1:B:292:HIS:O	1:B:296:VAL:HG23	2.15	0.46
1:A:172:LYS:O	1:A:176:GLU:HG3	2.14	0.46
1:A:157:LEU:HD13	1:A:476:PRO:HB2	1.98	0.46
6:B:705:PGE:H62	6:B:705:PGE:H2	1.98	0.46
1:B:264:ILE:HB	1:B:267:MET:HE3	1.98	0.45
1:A:454:THR:OG1	1:A:462:ASP:OD2	2.26	0.45
1:B:457:SER:CB	4:A:708:PEG:H42	2.47	0.45
1:B:570:LEU:C	1:B:570:LEU:HD23	2.41	0.45
1:A:379:LEU:HD13	1:A:549:SER:HB3	1.99	0.44
1:B:510:GLN:HG2	1:B:569:PRO:HG2	2.00	0.44
1:B:77:GLU:N	1:B:78:PRO:HD2	2.32	0.44
1:B:259:GLN:O	1:B:435:PHE:HA	2.17	0.44
1:B:418:THR:O	1:B:422:ILE:HG12	2.18	0.44
1:B:157:LEU:HD11	1:B:477:VAL:HG13	1.99	0.44
1:A:105:LEU:HG	1:A:109:GLN:HE21	1.82	0.44
1:A:510:GLN:HG2	1:A:569:PRO:HG2	2.00	0.43
1:B:330:CYS:O	1:B:331:HIS:C	2.61	0.43
1:A:551:PRO:HA	13:A:814:HOH:O	2.18	0.43
1:B:192:THR:HG23	1:B:193:ASP:OD1	2.18	0.43
1:A:292:HIS:CD2	12:A:705:PG4:H32	2.54	0.43
1:A:570:LEU:C	1:A:570:LEU:HD23	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:594:TRP:CE2	6:B:705:PGE:H32	2.54	0.42
1:A:607:TYR:HA	1:A:608:PRO:HA	1.84	0.42
1:B:138:SER:O	1:B:142:ASP:HB2	2.19	0.42
1:A:138:SER:O	1:A:142:ASP:HB2	2.18	0.42
1:A:140:ASP:HA	1:A:141:PRO:HA	1.88	0.42
1:A:157:LEU:HD11	1:A:477:VAL:HG13	2.02	0.42
1:A:305:GLU:OE2	1:A:534:THR:HG21	2.20	0.42
1:B:169:ILE:N	1:B:170:PRO:HD2	2.35	0.42
1:B:202:TYR:O	1:B:203:ASN:C	2.62	0.42
1:A:526:HIS:HA	1:A:573:TYR:CE2	2.55	0.42
1:A:259:GLN:O	1:A:435:PHE:HA	2.19	0.41
1:A:381:ARG:HG3	1:A:548:SER:HB3	2.02	0.41
1:A:330:CYS:O	1:A:331:HIS:C	2.63	0.41
1:A:418:THR:O	1:A:422:ILE:HG12	2.20	0.41
1:A:379:LEU:HA	1:A:548:SER:OG	2.19	0.41
11:A:704:MCO:O1	11:A:704:MCO:C9	2.68	0.41
1:B:77:GLU:N	1:B:78:PRO:CD	2.84	0.41
1:A:122:TYR:CD1	1:A:122:TYR:C	2.99	0.41
1:A:202:TYR:O	1:A:203:ASN:C	2.62	0.41
1:B:230:ARG:HD2	1:B:243:ASN:O	2.21	0.41
1:B:59:LEU:HD23	1:B:62:GLN:OE1	2.21	0.40
1:A:274:LYS:O	1:A:275:PRO:C	2.64	0.40
1:B:526:HIS:HA	1:B:573:TYR:CE2	2.55	0.40
1:A:2:ASP:HA	1:A:3:PRO:HD3	1.98	0.40
1:B:122:TYR:CD1	1:B:122:TYR:C	2.99	0.40
1:B:607:TYR:HA	1:B:608:PRO:HD3	1.94	0.40
1:A:25:GLN:HG3	1:A:377:VAL:H	1.86	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	598/628 (95%)	586 (98%)	11 (2%)	1 (0%)	43 63
1	B	599/628 (95%)	586 (98%)	12 (2%)	1 (0%)	43 63
All	All	1197/1256 (95%)	1172 (98%)	23 (2%)	2 (0%)	43 63

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	45	ASN
1	B	45	ASN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	518/540 (96%)	507 (98%)	11 (2%)	47 74
1	B	519/540 (96%)	507 (98%)	12 (2%)	44 72
All	All	1037/1080 (96%)	1014 (98%)	23 (2%)	45 73

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	18	GLN
1	B	26	SER
1	B	135	THR
1	B	236	ARG
1	B	363	MET
1	B	368	TYR
1	B	372	TYR
1	B	377	VAL
1	B	419	GLU
1	B	522	GLU
1	B	587	GLN
1	B	605	ASP
1	A	26	SER
1	A	70	GLN

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Mol	Chain	Res	Type
1	A	73	LYS
1	A	96	ARG
1	A	285	GLN
1	A	291	THR
1	A	368	TYR
1	A	372	TYR
1	A	377	VAL
1	A	421	ASP
1	A	522	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	6	GLN
1	B	70	GLN
1	B	109	GLN
1	B	188	GLN
1	B	263	ASN
1	B	512	HIS
1	B	527	GLN
1	B	579	GLN
1	B	582	GLN
1	B	588	ASN
1	A	25	GLN
1	A	70	GLN
1	A	109	GLN
1	A	213	HIS
1	A	234	HIS
1	A	263	ASN
1	A	512	HIS
1	A	568	GLN
1	A	575	GLN
1	A	582	GLN
1	A	587	GLN

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 ⓘ

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	C	1	2,1	14,14,15	0.38	0	17,19,21	1.36	3 (17%)
2	NAG	C	2	2	14,14,15	0.43	0	17,19,21	1.05	2 (11%)
2	NAG	D	1	2,1	14,14,15	0.48	0	17,19,21	1.44	2 (11%)
2	NAG	D	2	2	14,14,15	0.40	0	17,19,21	0.91	2 (11%)

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	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	NAG	D	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	D	2	2	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	NAG	C2-N2-C7	4.14	128.45	122.90
2	C	1	NAG	C1-O5-C5	3.53	116.92	112.19
2	D	1	NAG	C4-C3-C2	2.71	114.99	111.02
2	D	2	NAG	C2-N2-C7	2.30	125.99	122.90
2	D	2	NAG	C1-C2-N2	2.16	113.83	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	NAG	C1-C2-N2	2.07	113.70	110.43
2	C	2	NAG	C3-C4-C5	-2.07	106.48	110.23
2	C	1	NAG	O3-C3-C2	-2.03	105.18	109.40
2	C	2	NAG	O3-C3-C2	-2.02	105.20	109.40

There are no chirality outliers.

All (6) torsion outliers are listed below:

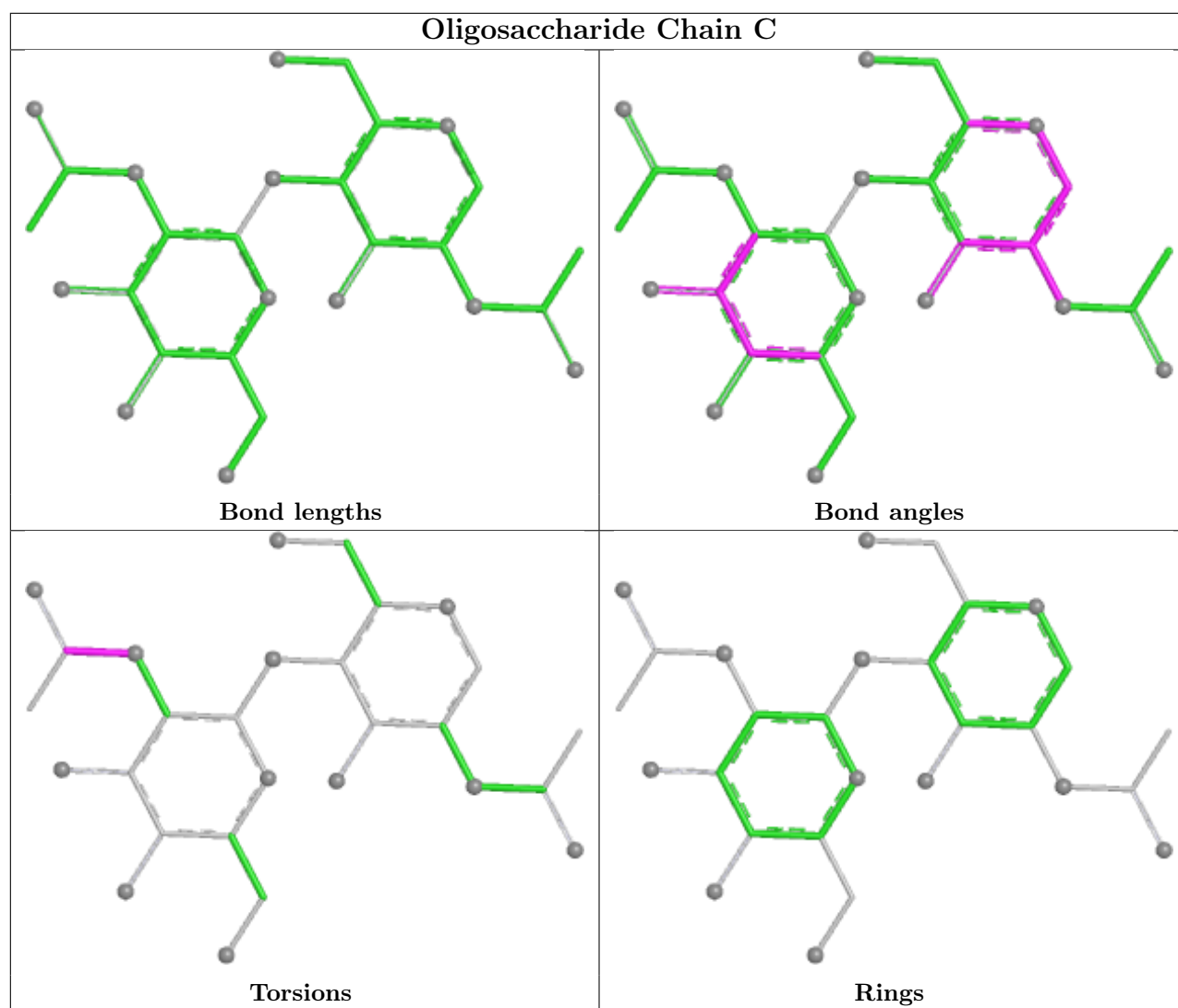
Mol	Chain	Res	Type	Atoms
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	C	2	NAG	C8-C7-N2-C2
2	C	2	NAG	O7-C7-N2-C2
2	D	2	NAG	O5-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6

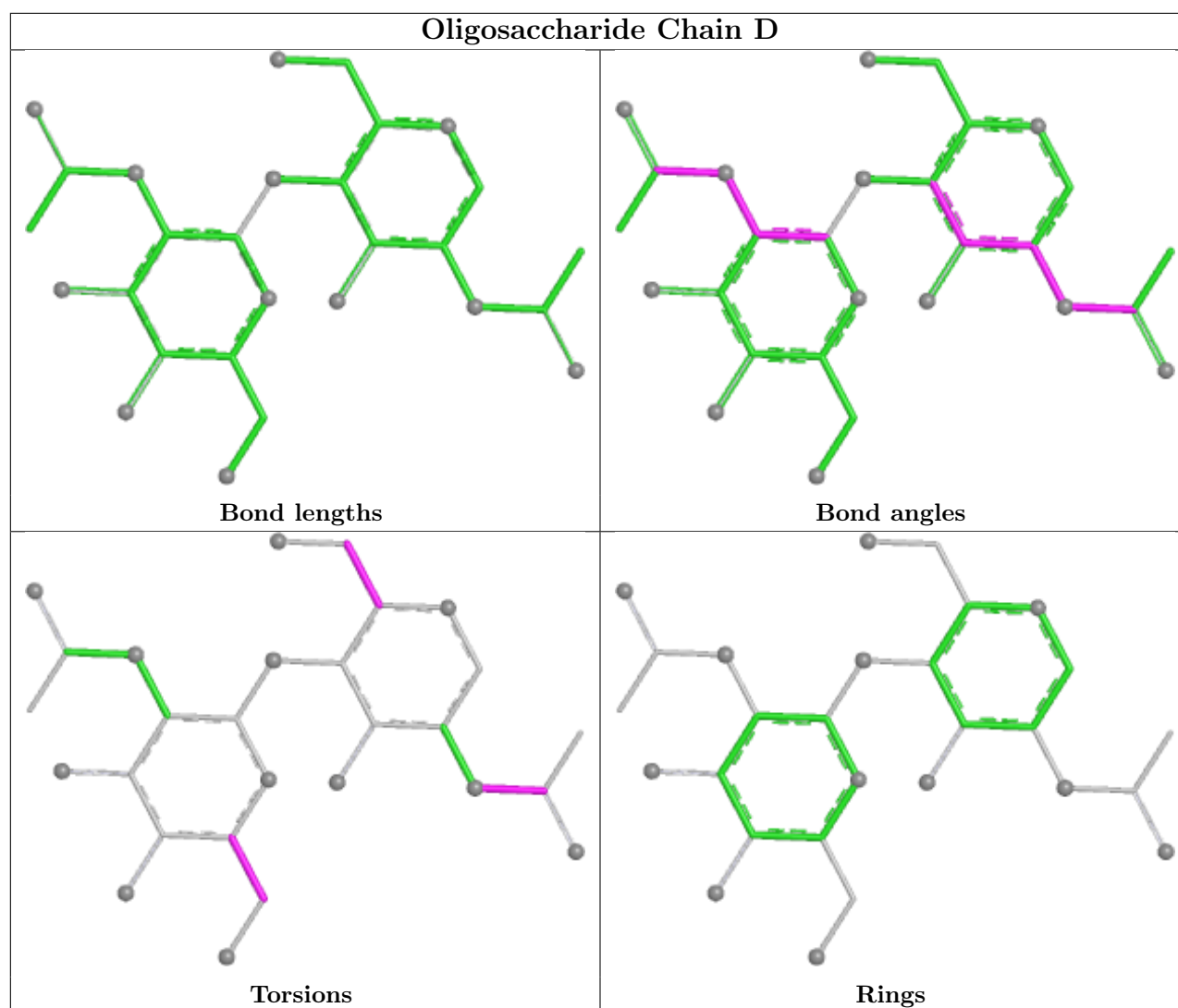
There are no ring outliers.

1 monomer is involved in 1 short contact:

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

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





5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 4 are monoatomic - leaving 18 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	$\# Z > 2$
5	EDO	A	710	-	3,3,3	0.95	0	2,2,2	1.40	0
4	PEG	A	709	-	6,6,6	0.55	0	5,5,5	0.35	0
7	BCN	B	707	-	10,10,10	0.74	0	11,11,11	0.85	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	NAG	A	702	1	14,14,15	0.45	0	17,19,21	1.33	2 (11%)
9	NAG	B	709	1	14,14,15	0.38	0	17,19,21	1.71	4 (23%)
8	X8Z	B	708	3	14,14,14	0.58	0	18,19,19	1.18	2 (11%)
9	NAG	A	711	1	14,14,15	0.49	0	17,19,21	1.21	3 (17%)
11	MCO	A	704	3	14,14,14	0.60	0	18,19,19	1.65	5 (27%)
5	EDO	B	703	-	3,3,3	0.21	0	2,2,2	0.23	0
4	PEG	A	708	-	6,6,6	0.47	0	5,5,5	0.38	0
4	PEG	B	704	-	6,6,6	0.37	0	5,5,5	0.30	0
6	PGE	B	705	-	9,9,9	0.45	0	8,8,8	0.31	0
9	NAG	A	701	1	14,14,15	0.26	0	17,19,21	0.92	0
12	PG4	A	705	-	12,12,12	0.29	0	11,11,11	0.19	0
12	PG4	A	707	-	12,12,12	0.46	0	11,11,11	0.30	0
6	PGE	A	706	-	9,9,9	0.35	0	8,8,8	0.29	0
5	EDO	B	706	-	3,3,3	0.25	0	2,2,2	0.13	0
4	PEG	B	702	-	6,6,6	0.31	0	5,5,5	0.13	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	A	710	-	-	1/1/1/1	-
4	PEG	A	709	-	-	1/4/4/4	-
7	BCN	B	707	-	-	5/10/10/10	-
9	NAG	A	702	1	-	4/6/23/26	0/1/1/1
9	NAG	B	709	1	-	4/6/23/26	0/1/1/1
8	X8Z	B	708	3	-	2/14/24/24	0/1/1/1
9	NAG	A	711	1	-	2/6/23/26	0/1/1/1
11	MCO	A	704	3	-	10/14/24/24	0/1/1/1
5	EDO	B	703	-	-	1/1/1/1	-
4	PEG	A	708	-	-	4/4/4/4	-
4	PEG	B	704	-	-	3/4/4/4	-
6	PGE	B	705	-	-	3/7/7/7	-
9	NAG	A	701	1	-	2/6/23/26	0/1/1/1
12	PG4	A	705	-	-	6/10/10/10	-
12	PG4	A	707	-	-	7/10/10/10	-
6	PGE	A	706	-	-	5/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	B	706	-	-	0/1/1/1	-
4	PEG	B	702	-	-	2/4/4/4	-

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	709	NAG	C1-C2-N2	5.25	118.71	110.43
9	A	702	NAG	C1-C2-N2	3.63	116.15	110.43
11	A	704	MCO	O2-C9-C8	-3.27	112.40	122.44
11	A	704	MCO	C5-N-C8	-3.10	107.15	112.01
9	A	711	NAG	C2-N2-C7	2.58	126.36	122.90
11	A	704	MCO	C9-C8-N	2.54	117.64	112.54
11	A	704	MCO	C7-C8-N	-2.49	99.36	103.02
9	B	709	NAG	C1-O5-C5	2.43	115.44	112.19
8	B	708	X8Z	C2-C1-S	2.38	117.12	114.04
9	A	711	NAG	C1-O5-C5	2.32	115.29	112.19
9	B	709	NAG	O5-C1-C2	-2.23	107.84	111.29
9	A	711	NAG	C1-C2-N2	2.22	113.94	110.43
11	A	704	MCO	C6-C7-C8	-2.07	99.83	104.14
9	B	709	NAG	C2-N2-C7	2.06	125.67	122.90
8	B	708	X8Z	C7-C8-N	2.06	106.04	103.02
9	A	702	NAG	C3-C4-C5	-2.06	106.50	110.23

There are no chirality outliers.

All (62) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	707	BCN	N1-C1-C2-O22
8	B	708	X8Z	S-C1-C2-C4
8	B	708	X8Z	S-C1-C2-C3
9	A	702	NAG	C8-C7-N2-C2
9	A	702	NAG	O7-C7-N2-C2
9	A	711	NAG	C8-C7-N2-C2
9	A	711	NAG	O7-C7-N2-C2
11	A	704	MCO	C7-C8-C9-O2
11	A	704	MCO	C7-C8-C9-O3
11	A	704	MCO	C2-C4-N-C8
11	A	704	MCO	S-C1-C2-C4
11	A	704	MCO	S-C1-C2-C3
11	A	704	MCO	O1-C4-N-C8

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Mol	Chain	Res	Type	Atoms
7	B	707	BCN	N1-C1-C2-O21
6	B	705	PGE	O2-C3-C4-O3
9	A	701	NAG	O5-C5-C6-O6
12	A	705	PG4	O3-C5-C6-O4
9	A	702	NAG	O5-C5-C6-O6
12	A	707	PG4	O3-C5-C6-O4
11	A	704	MCO	N-C8-C9-O2
11	A	704	MCO	N-C8-C9-O3
12	A	705	PG4	O2-C3-C4-O3
9	A	701	NAG	C4-C5-C6-O6
4	B	702	PEG	O2-C3-C4-O4
4	A	708	PEG	O2-C3-C4-O4
12	A	707	PG4	O4-C7-C8-O5
9	A	702	NAG	C4-C5-C6-O6
6	A	706	PGE	O2-C3-C4-O3
4	A	709	PEG	O1-C1-C2-O2
12	A	705	PG4	O1-C1-C2-O2
4	B	704	PEG	O2-C3-C4-O4
12	A	705	PG4	O4-C7-C8-O5
9	B	709	NAG	C4-C5-C6-O6
6	A	706	PGE	O1-C1-C2-O2
9	B	709	NAG	O5-C5-C6-O6
11	A	704	MCO	C2-C4-N-C5
4	B	702	PEG	O1-C1-C2-O2
9	B	709	NAG	C1-C2-N2-C7
6	A	706	PGE	C6-C5-O3-C4
12	A	705	PG4	C5-C6-O4-C7
4	A	708	PEG	C1-C2-O2-C3
4	A	708	PEG	O1-C1-C2-O2
4	B	704	PEG	C1-C2-O2-C3
12	A	707	PG4	C3-C4-O3-C5
6	A	706	PGE	C1-C2-O2-C3
5	B	703	EDO	O1-C1-C2-O2
9	B	709	NAG	C3-C2-N2-C7
12	A	705	PG4	C1-C2-O2-C3
11	A	704	MCO	O1-C4-N-C5
4	A	708	PEG	C4-C3-O2-C2
5	A	710	EDO	O1-C1-C2-O2
12	A	707	PG4	O1-C1-C2-O2
7	B	707	BCN	C2-C1-N1-C5
4	B	704	PEG	C4-C3-O2-C2
12	A	707	PG4	C8-C7-O4-C6

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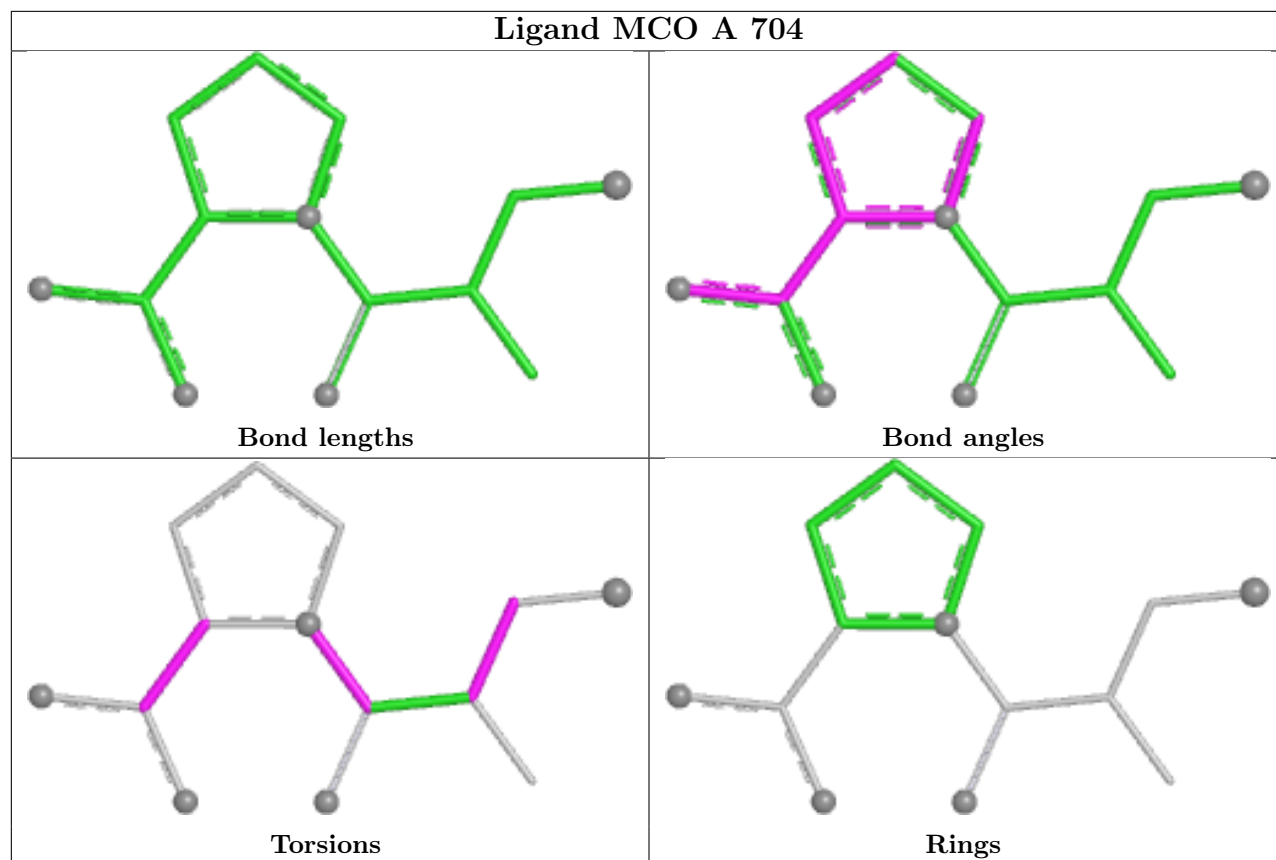
Mol	Chain	Res	Type	Atoms
7	B	707	BCN	C6-C5-N1-C3
6	A	706	PGE	O3-C5-C6-O4
12	A	707	PG4	O2-C3-C4-O3
12	A	707	PG4	C6-C5-O3-C4
6	B	705	PGE	C3-C4-O3-C5
6	B	705	PGE	C6-C5-O3-C4
7	B	707	BCN	C6-C5-N1-C1

There are no ring outliers.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	709	PEG	1	0
11	A	704	MCO	1	0
4	A	708	PEG	4	0
6	B	705	PGE	4	0
12	A	705	PG4	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 [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, 95th 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 ²)	Q<0.9
1	A	602/628 (95%)	-0.07	2 (0%) 90 87	26, 45, 71, 107	0
1	B	602/628 (95%)	-0.17	3 (0%) 87 85	19, 40, 61, 96	1 (0%)
All	All	1204/1256 (95%)	-0.12	5 (0%) 88 86	19, 43, 67, 107	1 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	608	PRO	4.9
1	A	129	LEU	3.9
1	B	413	ARG	2.1
1	A	413	ARG	2.1
1	B	315	GLU	2.1

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

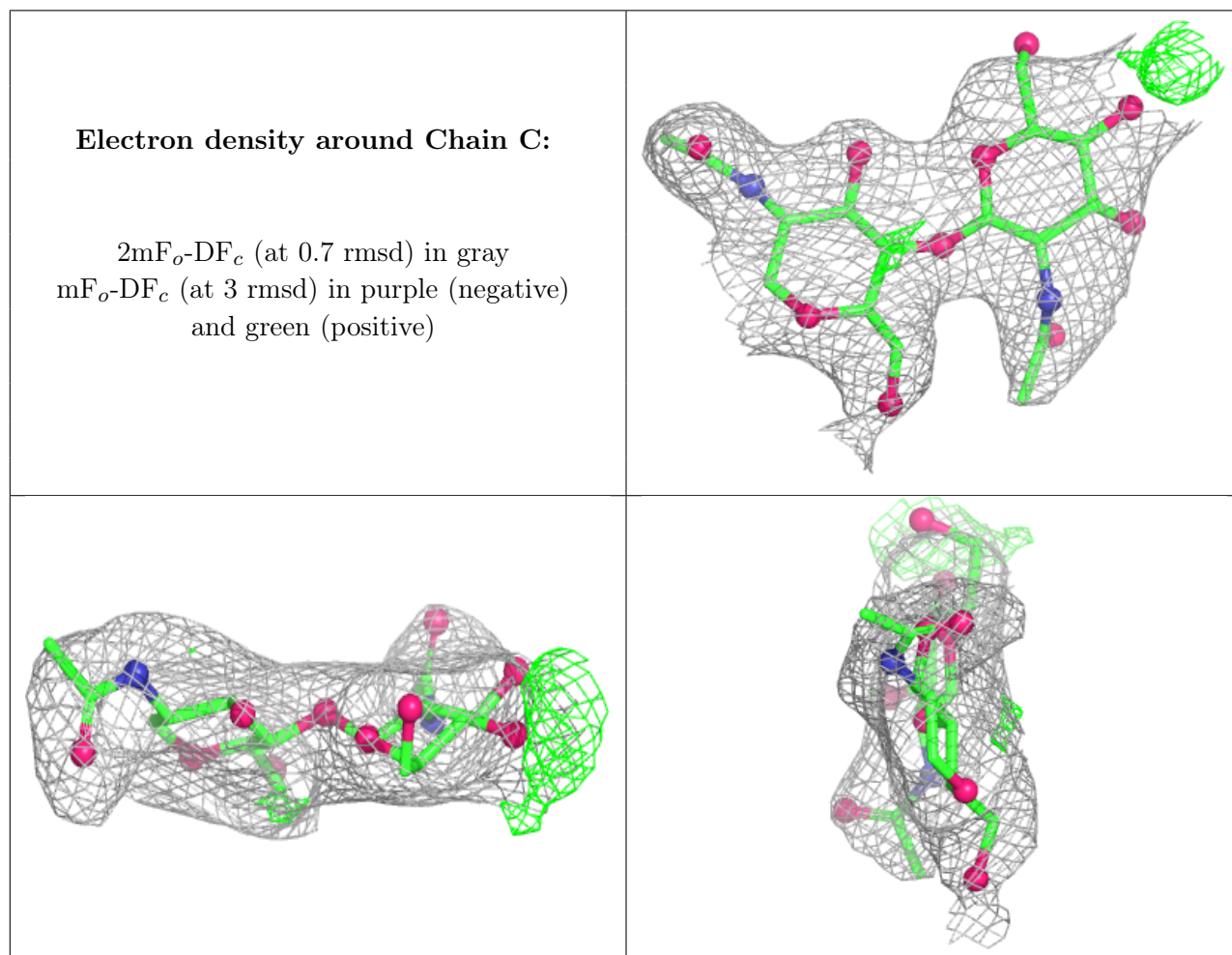
There are no non-standard protein/DNA/RNA residues in this entry.

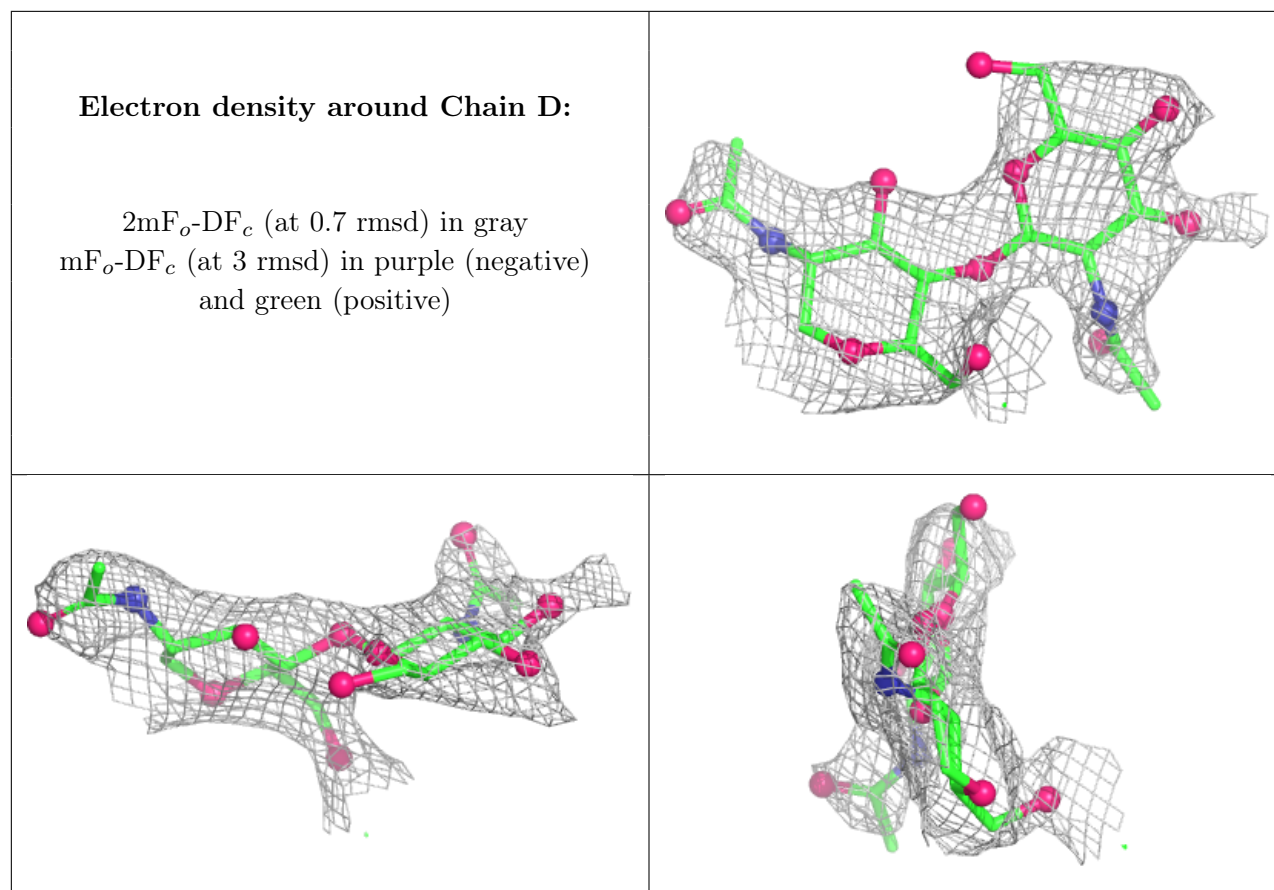
6.3 Carbohydrates [i](#)

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, 95th 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 ²)	Q<0.9
2	NAG	D	1	14/15	0.73	0.13	66,74,81,82	0
2	NAG	C	2	14/15	0.76	0.13	47,63,75,81	0
2	NAG	D	2	14/15	0.78	0.12	64,73,79,82	0
2	NAG	C	1	14/15	0.91	0.09	37,49,57,57	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 ⓘ

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, 95th 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.

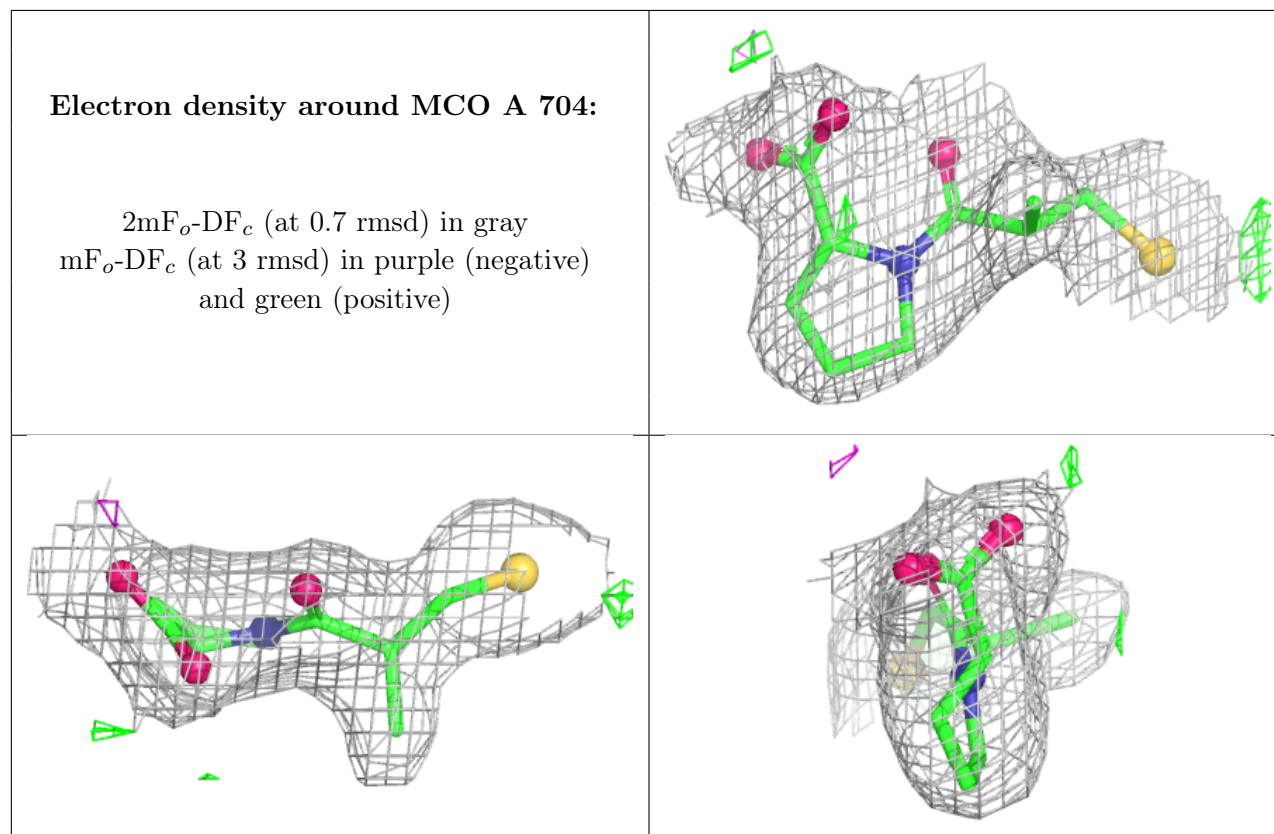
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	NAG	A	711	14/15	0.74	0.12	64,79,83,84	0
5	EDO	A	710	4/4	0.79	0.19	44,51,51,55	0
7	BCN	B	707	11/11	0.82	0.18	59,69,71,72	0
4	PEG	A	709	7/7	0.85	0.16	55,64,66,68	0
5	EDO	B	706	4/4	0.86	0.12	44,46,48,50	0
9	NAG	B	709	14/15	0.87	0.12	40,54,57,62	0
9	NAG	A	702	14/15	0.89	0.10	55,62,64,66	0
4	PEG	B	704	7/7	0.89	0.17	50,61,65,66	0
12	PG4	A	707	13/13	0.89	0.14	52,59,75,76	0
6	PGE	B	705	10/10	0.90	0.14	50,55,60,61	0
6	PGE	A	706	10/10	0.90	0.11	54,59,61,62	0
9	NAG	A	701	14/15	0.90	0.09	52,55,64,67	0
4	PEG	B	702	7/7	0.91	0.10	43,48,52,53	0

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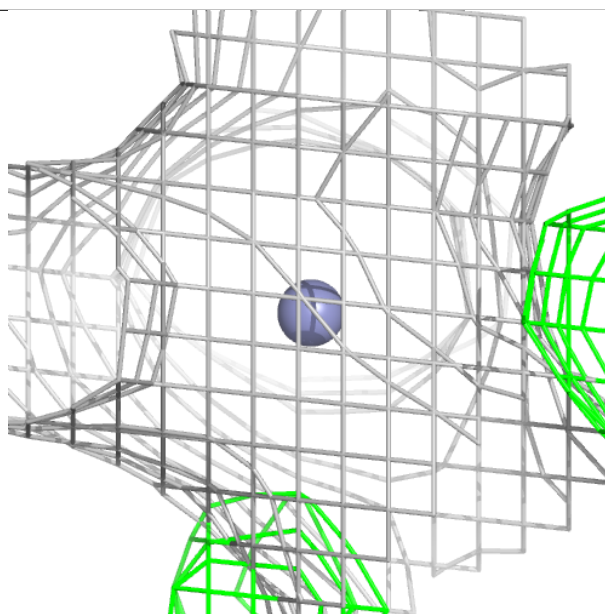
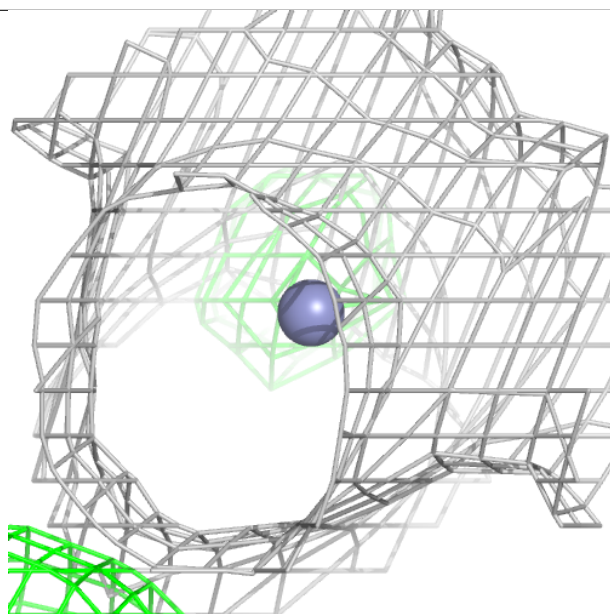
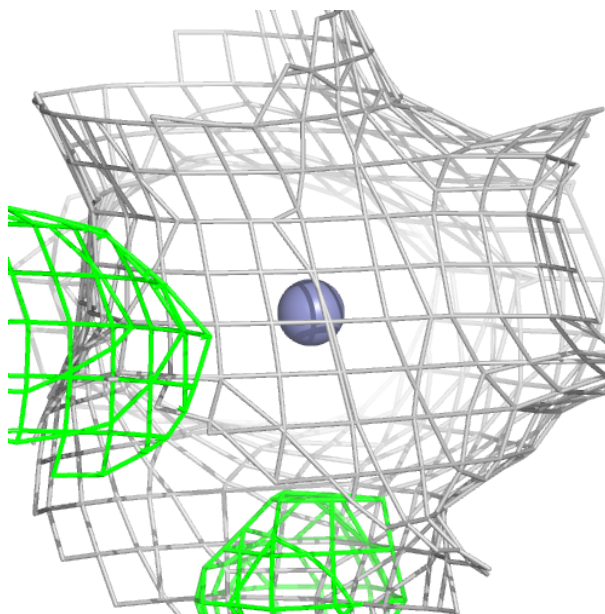
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
12	PG4	A	705	13/13	0.92	0.11	51,54,59,63	0
4	PEG	A	708	7/7	0.92	0.13	42,45,56,57	0
5	EDO	B	703	4/4	0.95	0.14	46,52,57,57	0
8	X8Z	B	708	14/14	0.95	0.07	30,37,44,44	0
11	MCO	A	704	14/14	0.97	0.08	35,44,47,49	0
10	CL	B	710	1/1	0.98	0.05	37,37,37,37	0
3	ZN	B	701	1/1	0.99	0.02	35,35,35,35	0
3	ZN	A	703	1/1	0.99	0.02	36,36,36,36	0
10	CL	A	712	1/1	0.99	0.05	35,35,35,35	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.



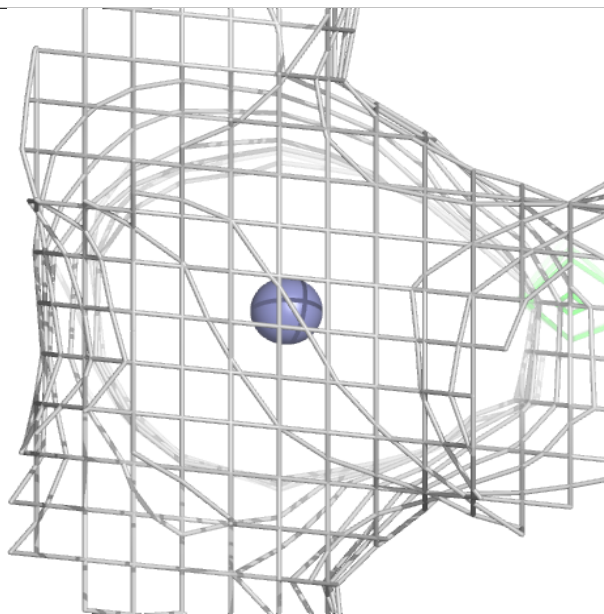
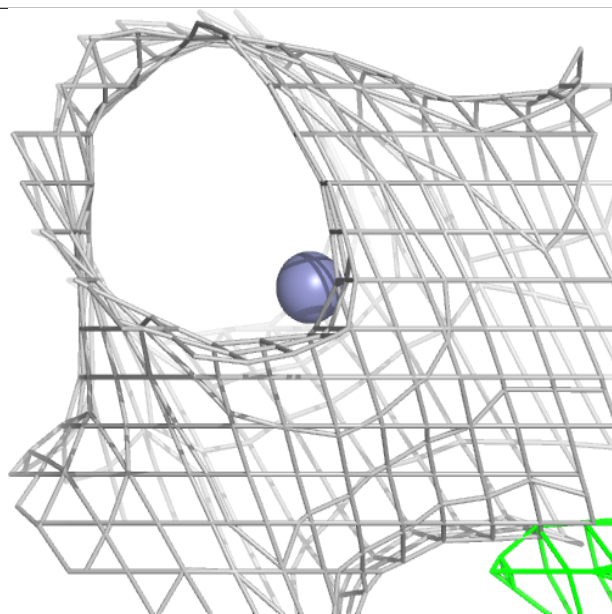
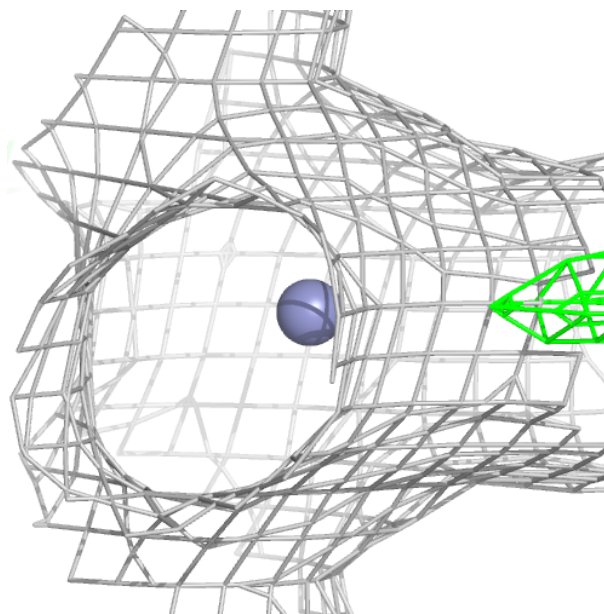
Electron density around ZN B 701:

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



Electron density around ZN 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)



6.5 Other polymers ⓘ

There are no such residues in this entry.