



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 08:31 PM UTC

PDB ID : 7Q25 / pdb_00007q25
Title : Crystal structure of Angiotensin-1 converting enzyme N-domain in complex with dual ACE/NEP inhibitor AD012
Authors : Cozier, G.E.; Acharya, K.R.
Deposited on : 2021-10-23
Resolution : 1.60 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

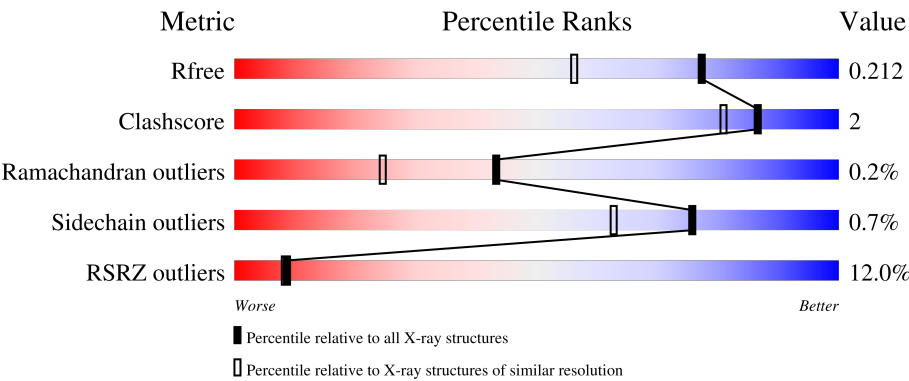
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	629	5% 93%
1	B	629	18% 91% 5%
2	C	4	75% 25%
2	E	4	50% 50%
3	D	2	50% 50%

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Mol	Chain	Length	Quality of chain
3	F	2	

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 21191 atoms, of which 9949 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.

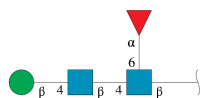
- Molecule 1 is a protein called Angiotensin-converting enzyme.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	611	Total	C	H	N	O	S	0	15	0
			9952	3269	4845	880	939	19			
1	B	606	Total	C	H	N	O	S	0	5	0
			9722	3196	4741	855	911	19			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	GLN	ASN	engineered mutation	UNP P12821
A	25	GLN	ASN	engineered mutation	UNP P12821
A	82	GLN	ASN	engineered mutation	UNP P12821
A	117	GLN	ASN	engineered mutation	UNP P12821
A	131	GLN	ASN	engineered mutation	UNP P12821
A	289	GLN	ASN	engineered mutation	UNP P12821
A	545	ARG	GLN	engineered mutation	UNP P12821
A	576	LEU	PRO	engineered mutation	UNP P12821
A	629	LEU	-	expression tag	UNP P12821
B	9	GLN	ASN	engineered mutation	UNP P12821
B	25	GLN	ASN	engineered mutation	UNP P12821
B	82	GLN	ASN	engineered mutation	UNP P12821
B	117	GLN	ASN	engineered mutation	UNP P12821
B	131	GLN	ASN	engineered mutation	UNP P12821
B	289	GLN	ASN	engineered mutation	UNP P12821
B	545	ARG	GLN	engineered mutation	UNP P12821
B	576	LEU	PRO	engineered mutation	UNP P12821
B	629	LEU	-	expression tag	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.



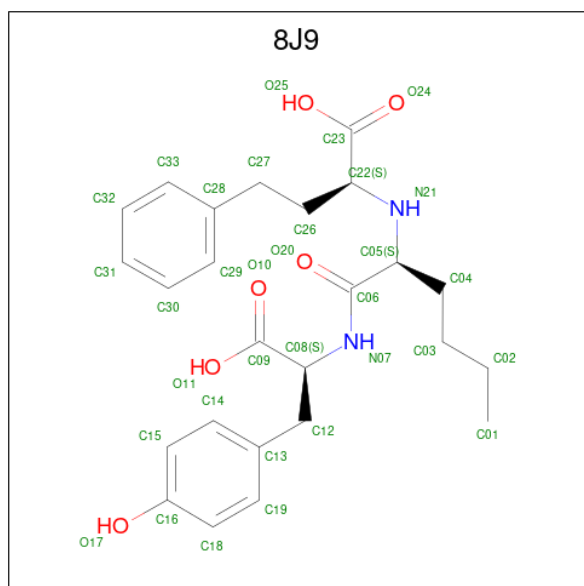
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	4	Total	C	H	N	O	0	0	0
			92	28	43	2	19			
2	E	4	Total	C	H	N	O	0	0	0
			92	28	43	2	19			

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	2	Total	C	H	N	O	0	0	0
			46	14	22	1	9			
3	F	2	Total	C	H	N	O	0	0	0
			46	14	22	1	9			

- Molecule 4 is (2 {S})-2-[[[(2 {S})-1-[[[(2 {S})-3-(4-hydroxyphenyl)-1-oxidanyl-1-oxidanylidene e-propan-2-yl]amino]-1-oxidanylidene-hexan-2-yl]amino]-4-phenyl-butanoic acid (CCD ID: 8J9) (formula: C₂₅H₃₂N₂O₆) (labeled as "Ligand of Interest" by depositor).



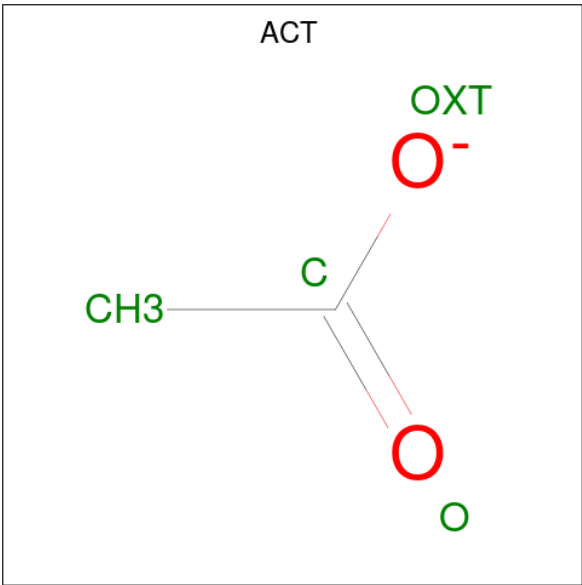
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	0	0
			63	25	30	2	6		
4	B	1	Total	C	H	N	O	0	0
			63	25	30	2	6		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



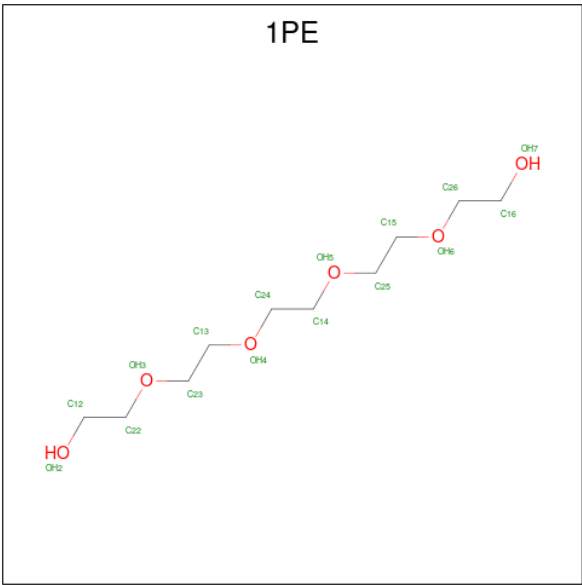
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
5	B	1	Total	C	H	N	O	0	0
			27	8	13	1	5		

- Molecule 6 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



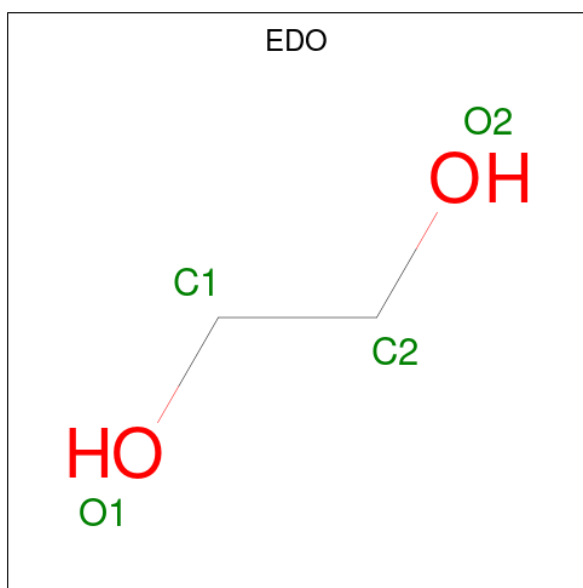
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			7	2	3	2		
6	A	1	Total	C	H	O	0	0
			7	2	3	2		
6	B	1	Total	C	H	O	0	0
			7	2	3	2		

- Molecule 7 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: C₁₀H₂₂O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	H	O	0	0
			38	10	22	6		

- Molecule 8 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



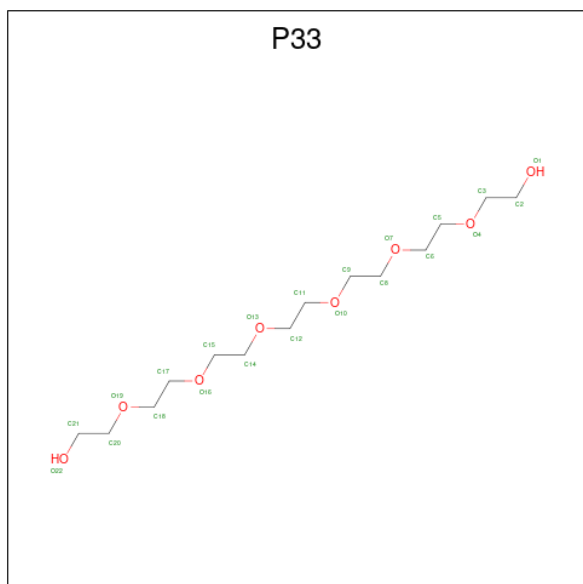
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	H	O	0	0
			10	2	6	2		
8	A	1	Total	C	H	O	0	0
			10	2	6	2		
8	A	1	Total	C	H	O	0	0
			10	2	6	2		
8	B	1	Total	C	H	O	0	0
			10	2	6	2		
8	B	1	Total	C	H	O	0	0
			10	2	6	2		

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	H	O	0	0
			17	4	10	3		
9	A	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 10 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
10	A	1	Total	C	H	O	0	0
			52	14	30	8		

- Molecule 11 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

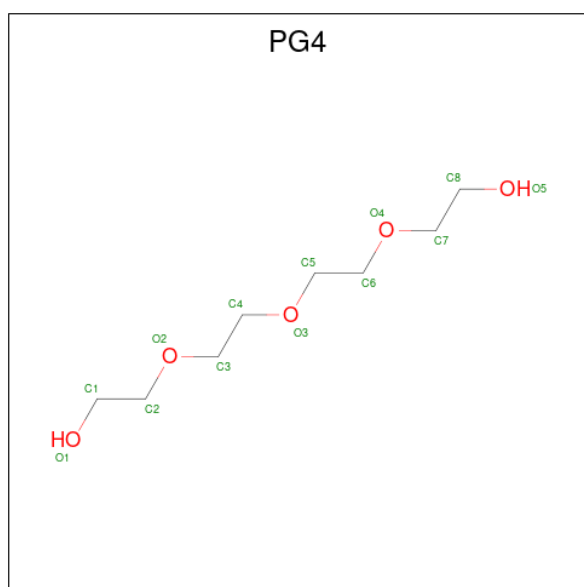
- Molecule 12 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 13 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 14 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	B	1	Total	C	H	O	0	0
			31	8	18	5		
14	B	1	Total	C	H	O	0	0
			31	8	18	5		

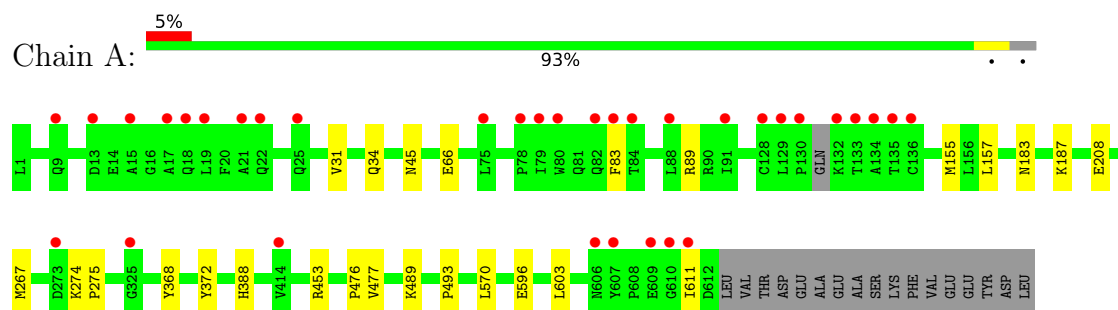
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	492	Total	O	0	3
			495	495		
15	B	301	Total	O	0	2
			303	303		

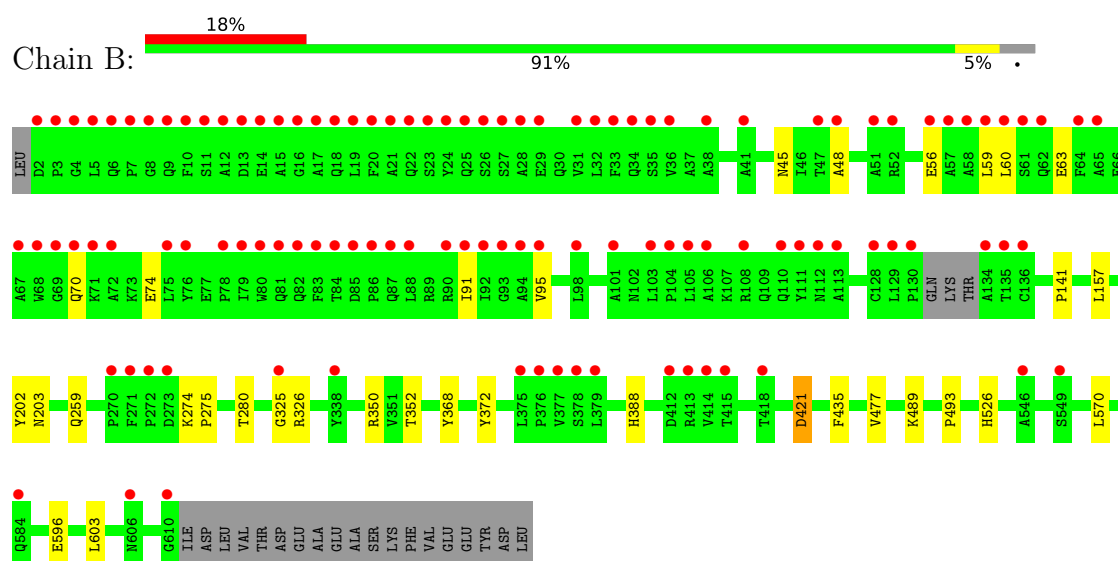
3 Residue-property plots

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.

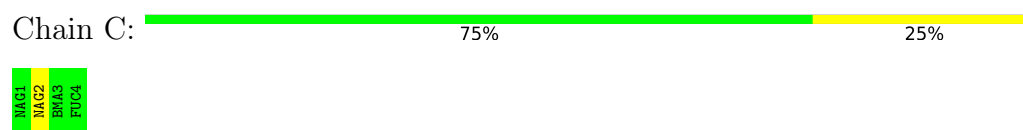
- Molecule 1: Angiotensin-converting enzyme



- Molecule 1: Angiotensin-converting enzyme



- 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



- 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

Chain E:  50% 50%



- Molecule 3: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:  50% 50%



- Molecule 3: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	72.94Å 77.48Å 82.49Å 88.39° 64.24° 74.99°	Depositor
Resolution (Å)	63.17 – 1.60 63.17 – 1.60	Depositor EDS
% Data completeness (in resolution range)	96.7 (63.17-1.60) 96.7 (63.17-1.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 1.60Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.188 , 0.212 0.188 , 0.212	Depositor DCC
R_{free} test set	2001 reflections (0.97%)	wwPDB-VP
Wilson B-factor (Å ²)	25.3	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 50.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	21191	wwPDB-VP
Average B, all atoms (Å ²)	47.0	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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 8J9, BMA, CL, EDO, ZN, NAG, FUC, PG4, P33, MG, ACT, PEG, 1PE

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	0.54	0/5263	0.54	0/7165
1	B	0.44	0/5137	0.48	0/6997
All	All	0.49	0/10400	0.51	0/14162

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	5107	4845	4865	16	0
1	B	4981	4741	4746	20	0
2	C	49	43	43	1	0
2	E	49	43	43	3	0
3	D	24	22	22	1	0
3	F	24	22	22	1	0
4	A	33	30	0	0	0
4	B	33	30	0	0	0
5	A	14	13	13	0	0
5	B	14	13	13	2	0
6	A	8	6	6	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	4	3	3	0	0
7	A	16	22	22	0	0
8	A	12	18	18	0	0
8	B	8	12	12	0	0
9	A	14	20	20	0	0
10	A	22	30	30	0	0
11	A	1	0	0	0	0
11	B	1	0	0	0	0
12	A	1	0	0	0	0
12	B	1	0	0	0	0
13	A	1	0	0	0	0
13	B	1	0	0	0	0
14	B	26	36	36	3	0
15	A	495	0	0	6	0
15	B	303	0	0	2	0
All	All	11242	9949	9914	43	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (43) 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:157:LEU:HD11	1:A:477:VAL:HG13	1.63	0.78
1:A:66:GLU:OE1	15:A:801:HOH:O	2.05	0.74
1:A:477:VAL:HG12	1:A:603:LEU:HD21	1.84	0.59
1:B:477:VAL:HG12	1:B:603:LEU:HD21	1.89	0.55
1:B:91:ILE:O	1:B:95:VAL:HG23	2.07	0.54
1:A:187:LYS:HE2	15:A:1211:HOH:O	2.08	0.53
2:E:1:NAG:O7	2:E:1:NAG:H3	2.08	0.53
1:B:141:PRO:HB3	1:B:350:ARG:HD3	1.93	0.51
1:A:157:LEU:HD13	1:A:476:PRO:HB2	1.94	0.50
2:E:1:NAG:O7	2:E:1:NAG:C3	2.59	0.50
15:A:1208:HOH:O	2:C:2:NAG:O7	2.19	0.49
1:B:259:GLN:O	1:B:435:PHE:HA	2.13	0.48
1:A:489:LYS:O	1:A:493:PRO:HD2	2.14	0.48
1:B:326:ARG:CG	5:B:703:NAG:H83	2.44	0.48
1:B:56:GLU:O	1:B:60:LEU:HD13	2.14	0.48
1:B:274:LYS:HB3	1:B:275:PRO:HD2	1.97	0.47
1:A:31:VAL:O	1:A:34:GLN:HG3	2.14	0.47
1:B:157:LEU:HD11	1:B:477:VAL:HG13	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:GLU:OE1	6:A:703:ACT:H1	2.15	0.46
1:A:596:GLU:OE2	3:F:1:NAG:O7	2.34	0.46
1:B:59:LEU:O	1:B:63:GLU:HG3	2.15	0.46
1:B:421:ASP:CG	1:B:526:HIS:HE2	2.24	0.45
1:A:453:ARG:HD2	15:A:869:HOH:O	2.16	0.45
1:B:570:LEU:C	1:B:570:LEU:HD23	2.42	0.45
1:A:570:LEU:C	1:A:570:LEU:HD23	2.42	0.44
1:B:489:LYS:O	1:B:493:PRO:HD2	2.18	0.44
15:A:866:HOH:O	14:B:701:PG4:C1	2.66	0.43
2:E:1:NAG:C5	2:E:4:FUC:H2	2.49	0.43
1:B:48:ALA:N	15:B:814:HOH:O	2.43	0.43
1:A:274:LYS:HB3	1:A:275:PRO:HD2	2.01	0.43
15:A:866:HOH:O	14:B:701:PG4:H11	2.19	0.43
1:B:70:GLN:O	1:B:74:GLU:HG3	2.19	0.43
1:A:267:MET:HB3	1:A:267:MET:HE2	1.83	0.42
1:B:56:GLU:O	1:B:60:LEU:CD1	2.68	0.42
14:B:701:PG4:H22	15:B:1000:HOH:O	2.20	0.42
1:B:325:GLY:O	1:B:326:ARG:C	2.62	0.42
1:A:155:MET:HE1	1:A:611:ILE:HG23	2.01	0.42
1:B:280:THR:HG23	1:B:352:THR:HA	2.02	0.42
1:B:202:TYR:O	1:B:203[A]:ASN:C	2.63	0.41
1:A:83:PHE:HB2	1:A:89:ARG:HG2	2.02	0.41
1:A:183:ASN:O	1:A:187:LYS:HG3	2.20	0.41
1:B:326:ARG:HD3	5:B:703:NAG:H83	2.02	0.40
1:B:596:GLU:OE2	3:D:1:NAG:O7	2.40	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	622/629 (99%)	612 (98%)	9 (1%)	1 (0%)	43 24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	607/629 (96%)	595 (98%)	11 (2%)	1 (0%)	43	24
All	All	1229/1258 (98%)	1207 (98%)	20 (2%)	2 (0%)	43	24

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	45	ASN
1	A	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	540/541 (100%)	537 (99%)	3 (1%)	78	66
1	B	525/541 (97%)	521 (99%)	4 (1%)	73	59
All	All	1065/1082 (98%)	1058 (99%)	7 (1%)	76	63

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	368	TYR
1	A	372	TYR
1	A	388	HIS
1	B	368	TYR
1	B	372	TYR
1	B	388	HIS
1	B	421	ASP

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

Mol	Chain	Res	Type
1	B	50	ASN
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 ⓘ

12 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	1,2	14,14,15	0.68	0	17,19,21	0.53	0
2	NAG	C	2	2	14,14,15	0.36	0	17,19,21	0.42	0
2	BMA	C	3	2	11,11,12	0.65	0	15,15,17	0.71	0
2	FUC	C	4	2	10,10,11	0.74	0	14,14,16	0.71	0
3	NAG	D	1	1,3	14,14,15	0.50	0	17,19,21	0.64	0
3	FUC	D	2	3	10,10,11	1.09	0	14,14,16	0.81	0
2	NAG	E	1	1,2	14,14,15	0.47	0	17,19,21	0.80	1 (5%)
2	NAG	E	2	2	14,14,15	0.35	0	17,19,21	0.53	0
2	BMA	E	3	2	11,11,12	0.65	0	15,15,17	0.76	0
2	FUC	E	4	2	10,10,11	1.24	1 (10%)	14,14,16	0.91	1 (7%)
3	NAG	F	1	1,3	14,14,15	0.48	0	17,19,21	0.68	1 (5%)
3	FUC	F	2	3	10,10,11	0.92	0	14,14,16	0.96	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	4	FUC	C1-C2	3.07	1.59	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1	NAG	C2-N2-C7	2.80	126.66	122.90
2	E	4	FUC	O2-C2-C1	2.32	114.55	109.22
3	F	1	NAG	C1-O5-C5	2.25	115.20	112.19

There are no chirality outliers.

All (9) torsion outliers are listed below:

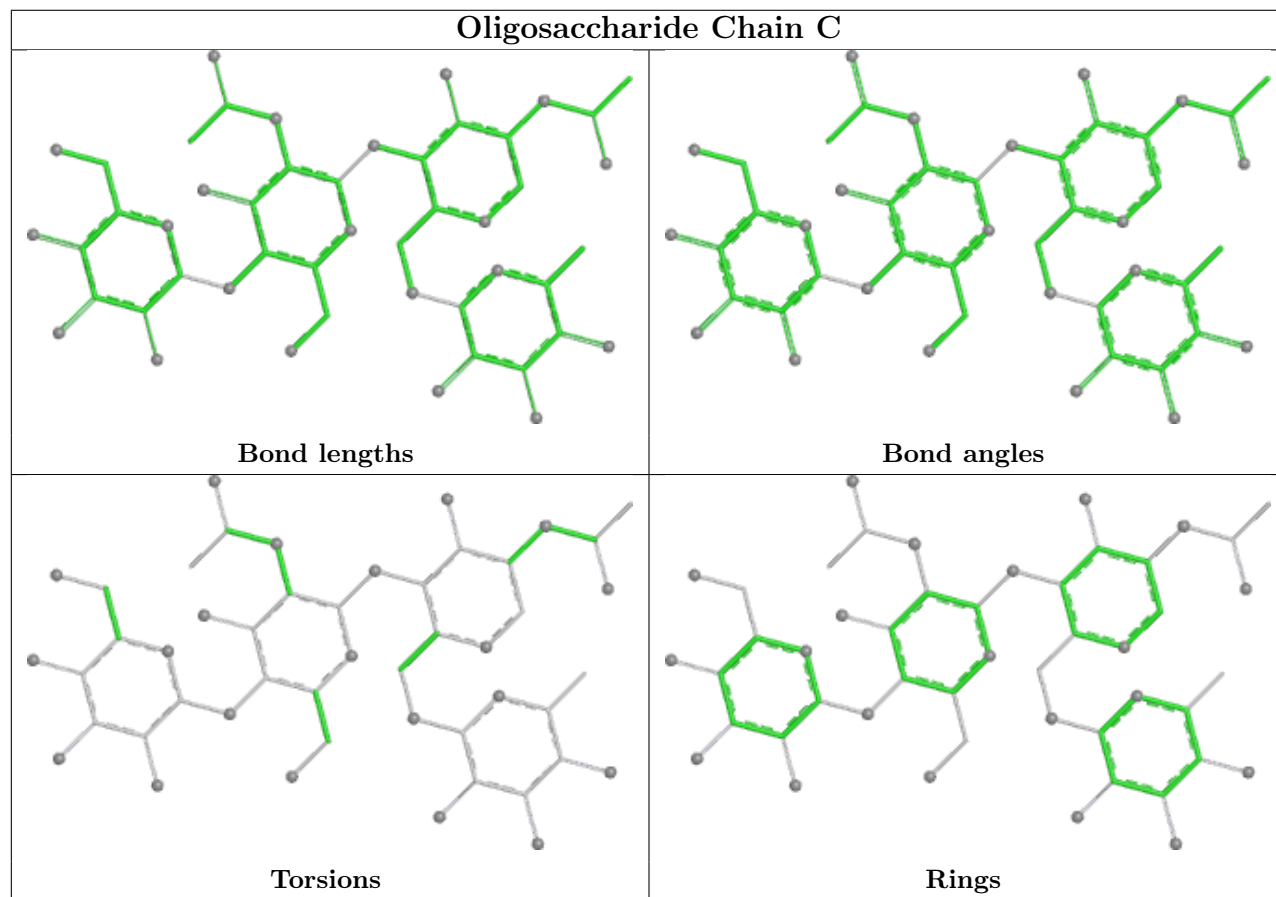
Mol	Chain	Res	Type	Atoms
2	E	1	NAG	C3-C2-N2-C7
2	E	3	BMA	O5-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
2	E	3	BMA	C4-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6

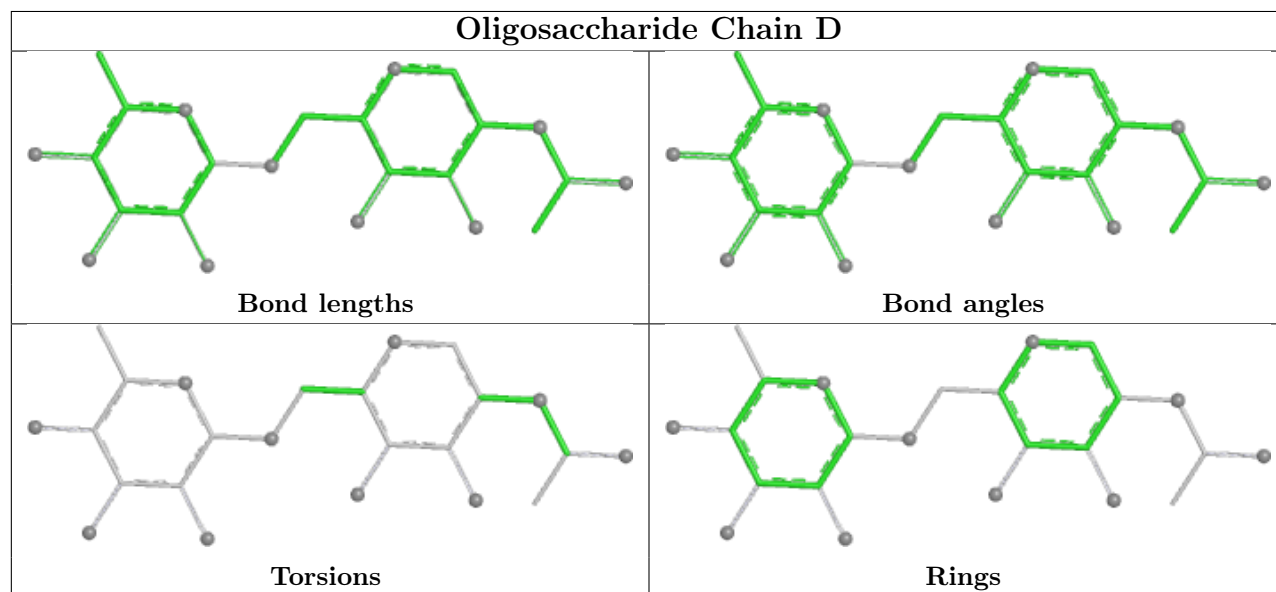
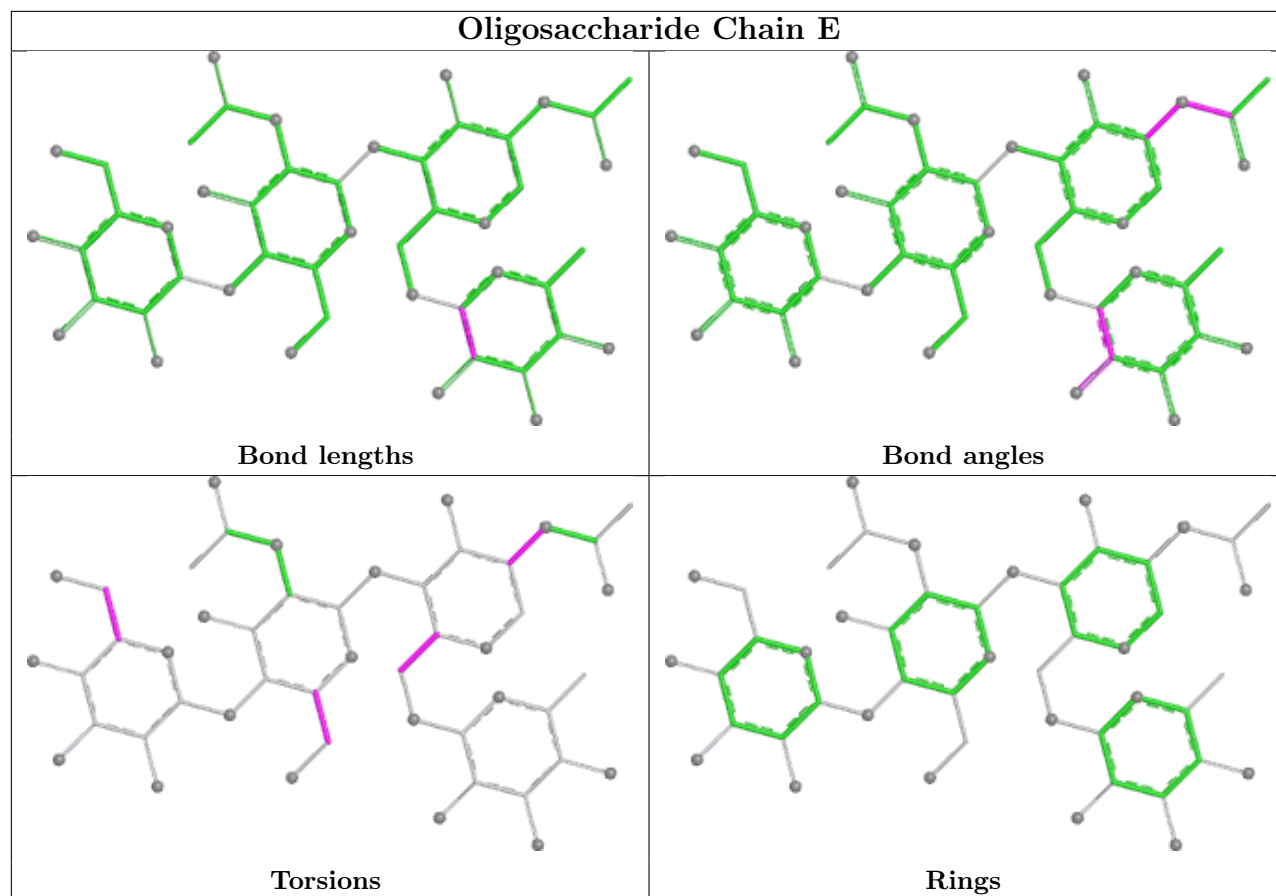
There are no ring outliers.

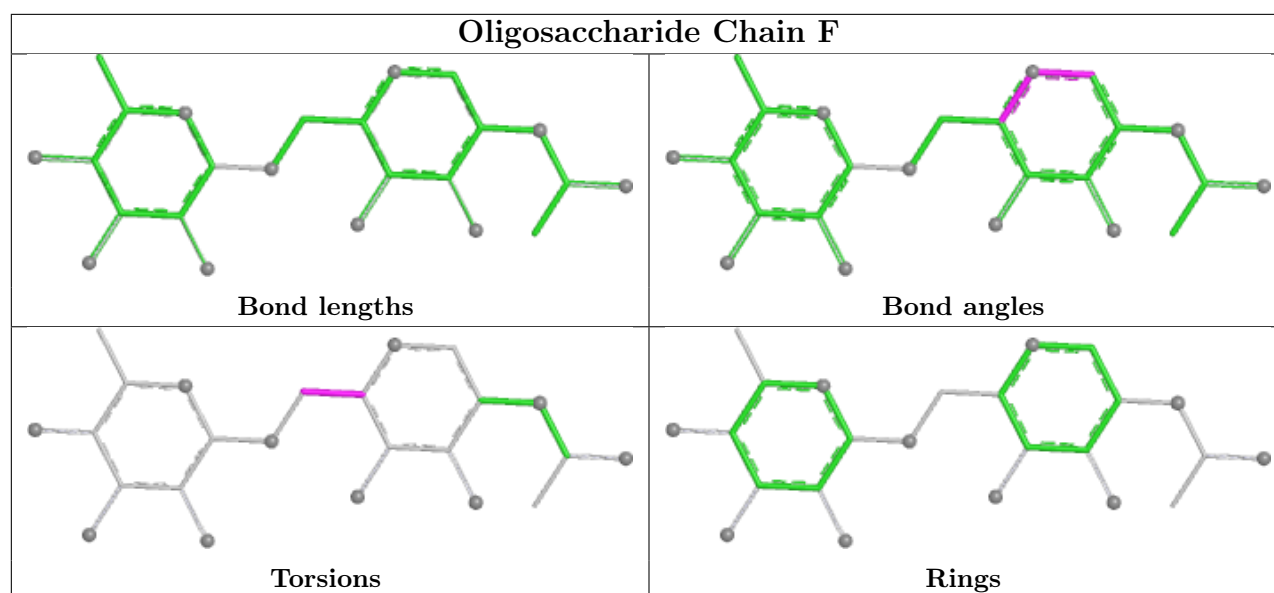
5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1	NAG	3	0
2	E	4	FUC	1	0
3	D	1	NAG	1	0
3	F	1	NAG	1	0
2	C	2	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 24 ligands modelled in this entry, 6 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	$\# Z > 2$
14	PG4	B	706	-	12,12,12	0.21	0	11,11,11	0.45	0
6	ACT	B	704	-	3,3,3	1.33	0	3,3,3	1.60	0
4	8J9	B	702	11	34,34,34	1.30	5 (14%)	44,44,44	1.61	5 (11%)
8	EDO	A	710	-	3,3,3	0.50	0	2,2,2	0.38	0
14	PG4	B	701	-	12,12,12	0.11	0	11,11,11	0.49	0
5	NAG	B	703	1	14,14,15	0.28	0	17,19,21	0.65	1 (5%)
8	EDO	A	705	-	3,3,3	0.52	0	2,2,2	0.33	0
5	NAG	A	702	1	14,14,15	0.33	0	17,19,21	0.57	0
10	P33	A	711	-	21,21,21	0.56	0	20,20,20	0.29	0
7	1PE	A	704	-	15,15,15	0.21	0	14,14,14	0.28	0
6	ACT	A	703	-	3,3,3	1.07	0	3,3,3	1.52	1 (33%)
8	EDO	B	707	-	3,3,3	0.54	0	2,2,2	0.29	0
9	PEG	A	708	-	6,6,6	0.18	0	5,5,5	0.09	0
8	EDO	B	705	-	3,3,3	0.46	0	2,2,2	0.29	0
9	PEG	A	707	-	6,6,6	0.16	0	5,5,5	0.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	ACT	A	709	-	3,3,3	1.27	0	3,3,3	1.40	0
8	EDO	A	706	-	3,3,3	0.48	0	2,2,2	0.28	0
4	8J9	A	701	11	34,34,34	1.24	3 (8%)	44,44,44	1.16	4 (9%)

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
14	PG4	B	706	-	-	6/10/10/10	-
4	8J9	B	702	11	-	5/33/33/33	0/2/2/2
8	EDO	A	710	-	-	0/1/1/1	-
14	PG4	B	701	-	-	7/10/10/10	-
5	NAG	B	703	1	-	4/6/23/26	0/1/1/1
8	EDO	A	705	-	-	0/1/1/1	-
5	NAG	A	702	1	-	0/6/23/26	0/1/1/1
10	P33	A	711	-	-	11/19/19/19	-
7	1PE	A	704	-	-	0/13/13/13	-
8	EDO	B	707	-	-	0/1/1/1	-
8	EDO	B	705	-	-	0/1/1/1	-
9	PEG	A	707	-	-	1/4/4/4	-
9	PEG	A	708	-	-	2/4/4/4	-
8	EDO	A	706	-	-	1/1/1/1	-
4	8J9	A	701	11	-	5/33/33/33	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	701	8J9	C06-N07	4.46	1.43	1.34
4	B	702	8J9	O24-C23	4.31	1.34	1.22
4	B	702	8J9	C06-N07	3.85	1.42	1.34
4	A	701	8J9	O10-C09	2.73	1.30	1.22
4	A	701	8J9	O24-C23	2.67	1.30	1.22
4	B	702	8J9	O10-C09	2.15	1.28	1.22
4	B	702	8J9	O17-C16	2.08	1.41	1.37
4	B	702	8J9	C22-C23	-2.03	1.47	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	702	8J9	O25-C23-O24	-7.70	106.60	124.08
4	A	701	8J9	O20-C06-N07	-3.58	116.55	122.96
4	B	702	8J9	O25-C23-C22	3.12	124.05	113.51
4	A	701	8J9	O20-C06-C05	2.40	125.50	120.48
4	B	702	8J9	O20-C06-N07	-2.23	118.97	122.96
4	A	701	8J9	C19-C13-C14	2.22	121.53	118.23
5	B	703	NAG	C1-O5-C5	2.21	115.14	112.19
4	A	701	8J9	C05-N21-C22	-2.11	110.97	115.67
4	B	702	8J9	O24-C23-C22	2.07	128.92	122.26
6	A	703	ACT	OXT-C-O	2.03	129.56	122.03
4	B	702	8J9	C05-N21-C22	-2.02	111.17	115.67

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	711	P33	O4-C5-C6-O7
10	A	711	P33	O10-C11-C12-O13
14	B	701	PG4	O3-C5-C6-O4
10	A	711	P33	O13-C14-C15-O16
10	A	711	P33	O19-C20-C21-O22
14	B	701	PG4	O4-C7-C8-O5
4	A	701	8J9	N07-C08-C12-C13
14	B	701	PG4	O2-C3-C4-O3
14	B	701	PG4	O1-C1-C2-O2
14	B	706	PG4	O1-C1-C2-O2
9	A	708	PEG	O1-C1-C2-O2
9	A	708	PEG	O2-C3-C4-O4
14	B	706	PG4	O2-C3-C4-O3
4	A	701	8J9	C09-C08-C12-C13
4	B	702	8J9	N07-C08-C12-C13
4	B	702	8J9	C09-C08-C12-C13
10	A	711	P33	C6-C5-O4-C3
10	A	711	P33	C18-C17-O16-C15
14	B	701	PG4	C1-C2-O2-C3
14	B	706	PG4	C3-C4-O3-C5
14	B	701	PG4	C3-C4-O3-C5
10	A	711	P33	O7-C8-C9-O10
10	A	711	P33	C5-C6-O7-C8
5	B	703	NAG	C3-C2-N2-C7
9	A	707	PEG	O1-C1-C2-O2
10	A	711	P33	O16-C17-C18-O19
5	B	703	NAG	C4-C5-C6-O6

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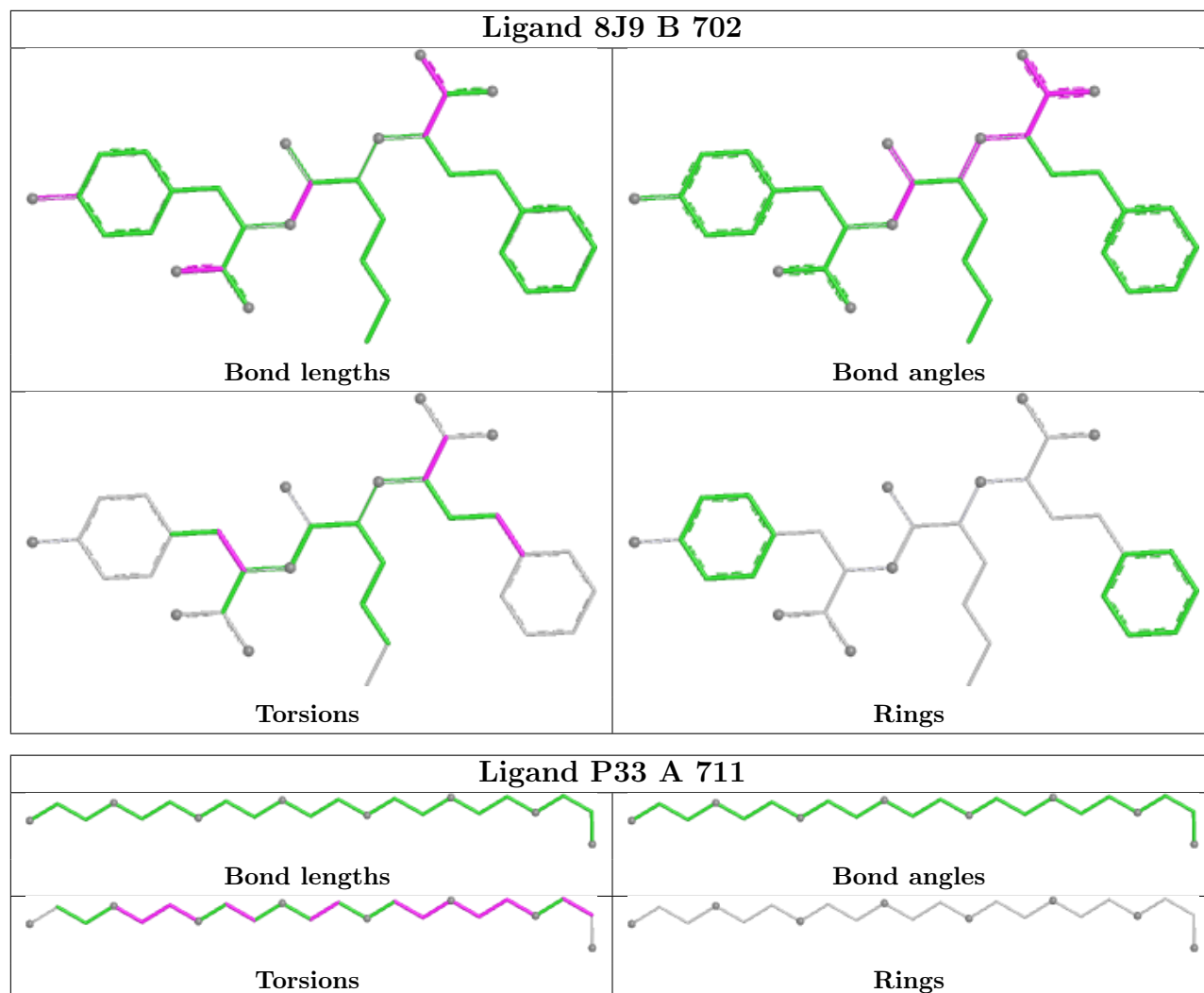
Mol	Chain	Res	Type	Atoms
10	A	711	P33	C17-C18-O19-C20
14	B	706	PG4	C4-C3-O2-C2
5	B	703	NAG	O5-C5-C6-O6
4	B	702	8J9	C26-C27-C28-C33
4	B	702	8J9	C26-C27-C28-C29
5	B	703	NAG	C1-C2-N2-C7
8	A	706	EDO	O1-C1-C2-O2
4	A	701	8J9	C26-C27-C28-C33
14	B	706	PG4	O3-C5-C6-O4
4	A	701	8J9	C26-C27-C28-C29
14	B	706	PG4	C8-C7-O4-C6
14	B	701	PG4	C8-C7-O4-C6
4	B	702	8J9	N21-C22-C23-O24
10	A	711	P33	C14-C15-O16-C17
4	A	701	8J9	N21-C22-C23-O25

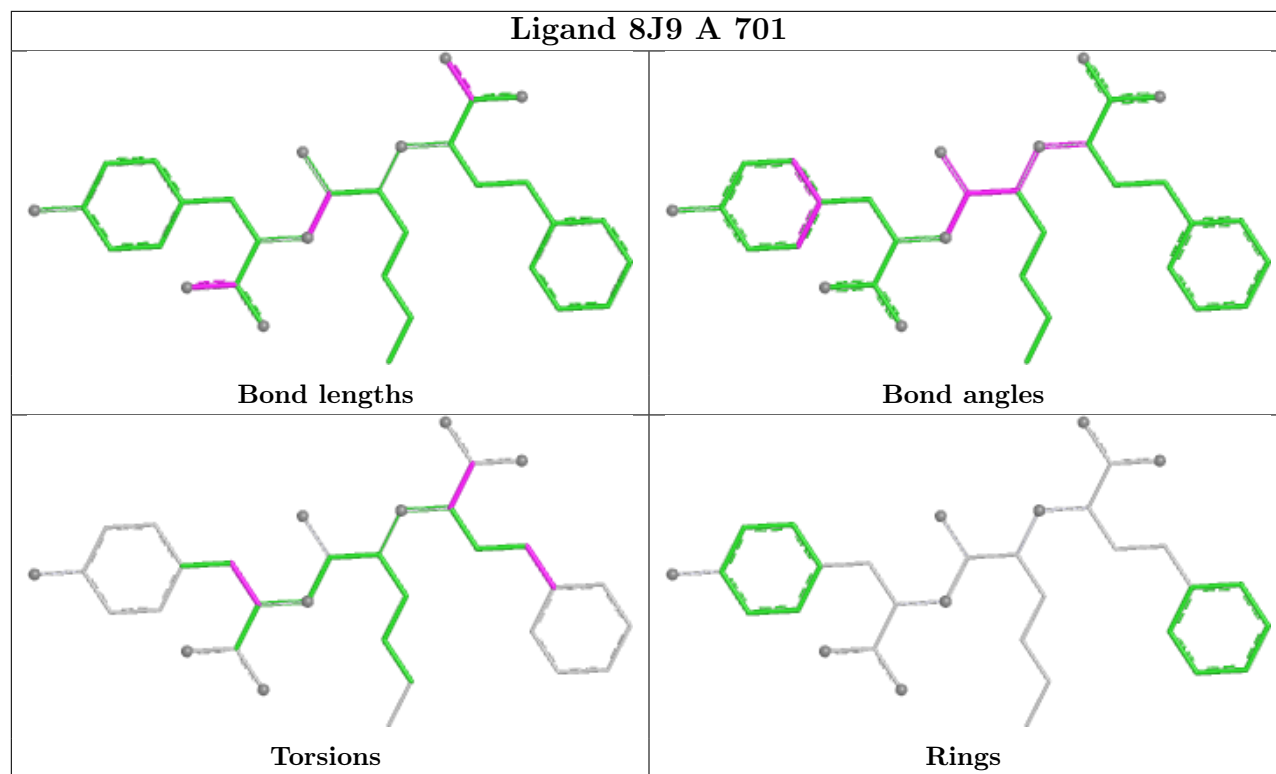
There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	B	701	PG4	3	0
5	B	703	NAG	2	0
6	A	703	ACT	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 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, 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	611/629 (97%)	0.04	34 (5%) 30 31	11, 35, 67, 127	15 (2%)
1	B	606/629 (96%)	0.78	112 (18%) 3 3	15, 49, 97, 136	5 (0%)
All	All	1217/1258 (96%)	0.41	146 (11%) 9 8	11, 41, 92, 136	20 (1%)

All (146) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	19	LEU	7.5
1	B	92	ILE	6.5
1	B	20	PHE	6.4
1	B	10	PHE	6.1
1	B	5	LEU	6.0
1	A	79	ILE	6.0
1	B	15	ALA	5.9
1	B	67	ALA	5.9
1	A	132	LYS	5.6
1	A	130	PRO	5.4
1	B	11	SER	5.2
1	B	75	LEU	5.2
1	B	83	PHE	5.1
1	B	68	TRP	5.0
1	B	80	TRP	5.0
1	B	378	SER	5.0
1	B	28	ALA	4.9
1	B	31	VAL	4.8
1	B	377	VAL	4.7
1	B	24	TYR	4.7
1	B	18	GLN	4.6
1	B	8	GLY	4.6
1	B	17	ALA	4.6
1	B	78	PRO	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	95	VAL	4.5
1	B	4	GLY	4.5
1	B	12	ALA	4.4
1	B	105	LEU	4.4
1	A	129	LEU	4.3
1	B	84	THR	4.3
1	B	91	ILE	4.3
1	B	130	PRO	4.3
1	B	72	ALA	4.3
1	B	88	LEU	4.3
1	B	64	PHE	4.2
1	A	325	GLY	4.2
1	B	13	ASP	4.1
1	B	16	GLY	4.0
1	B	79	ILE	4.0
1	B	76	TYR	3.9
1	B	94	ALA	3.9
1	B	414	VAL	3.8
1	B	610	GLY	3.8
1	A	78	PRO	3.8
1	B	59	LEU	3.7
1	B	21	ALA	3.7
1	A	17	ALA	3.7
1	B	9	GLN	3.7
1	A	83	PHE	3.7
1	B	7	PRO	3.6
1	B	65	ALA	3.6
1	B	81	GLN	3.6
1	B	3	PRO	3.5
1	B	135	THR	3.5
1	B	48	ALA	3.5
1	B	71	LYS	3.5
1	B	25	GLN	3.5
1	B	134	ALA	3.4
1	B	85	ASP	3.4
1	B	14	GLU	3.4
1	B	60	LEU	3.4
1	B	106	ALA	3.4
1	B	34	GLN	3.4
1	B	69	GLY	3.4
1	A	607	TYR	3.3
1	A	606	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	414	VAL	3.3
1	B	23	SER	3.3
1	A	134	ALA	3.3
1	B	111	TYR	3.2
1	A	25	GLN	3.2
1	B	375	LEU	3.2
1	A	611	ILE	3.2
1	B	379	LEU	3.2
1	B	33	PHE	3.2
1	A	84	THR	3.2
1	A	135	THR	3.2
1	B	272	PRO	3.1
1	B	58	ALA	3.1
1	B	29	GLU	3.1
1	A	80	TRP	3.1
1	B	22	GLN	3.0
1	B	86	PRO	3.0
1	B	103	LEU	3.0
1	B	27	SER	3.0
1	B	412	ASP	3.0
1	B	56	GLU	3.0
1	B	2	ASP	2.9
1	A	21	ALA	2.9
1	A	75	LEU	2.9
1	B	90	ARG	2.9
1	A	15	ALA	2.8
1	B	93	GLY	2.8
1	B	26	SER	2.8
1	B	47	THR	2.8
1	B	52	ARG	2.8
1	A	133	THR	2.7
1	B	101	ALA	2.7
1	B	98	LEU	2.7
1	B	82	GLN	2.7
1	B	606	ASN	2.7
1	A	136	CYS	2.7
1	B	270	PRO	2.6
1	B	376	PRO	2.6
1	B	271	PHE	2.6
1	B	129	LEU	2.6
1	A	609	GLU	2.6
1	B	51	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	70	GLN	2.6
1	B	32	LEU	2.6
1	A	19	LEU	2.5
1	B	6	GLN	2.5
1	A	91	ILE	2.5
1	B	113	ALA	2.5
1	B	415	THR	2.5
1	B	57	ALA	2.5
1	B	35	SER	2.4
1	A	128	CYS	2.4
1	A	18	GLN	2.4
1	B	108	ARG	2.4
1	B	87	GLN	2.3
1	B	41	ALA	2.3
1	B	418	THR	2.3
1	B	61	SER	2.3
1	A	9[A]	GLN	2.3
1	B	38	ALA	2.2
1	B	136	CYS	2.2
1	B	110	GLN	2.2
1	B	62	GLN	2.2
1	B	112	ASN	2.2
1	B	273	ASP	2.2
1	B	338	TYR	2.2
1	B	549	SER	2.2
1	B	104	PRO	2.1
1	A	82	GLN	2.1
1	B	546	ALA	2.1
1	A	13	ASP	2.1
1	B	413	ARG	2.1
1	B	36	VAL	2.1
1	B	584	GLN	2.1
1	A	88	LEU	2.1
1	B	325	GLY	2.0
1	B	128	CYS	2.0
1	A	22	GLN	2.0
1	A	610	GLY	2.0
1	A	273	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates

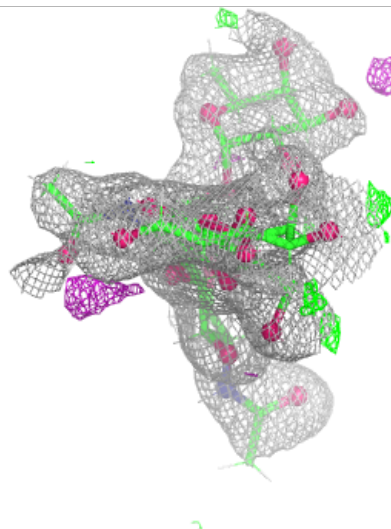
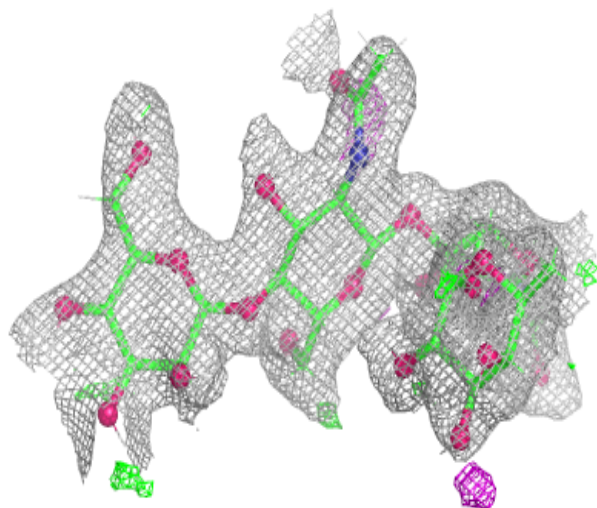
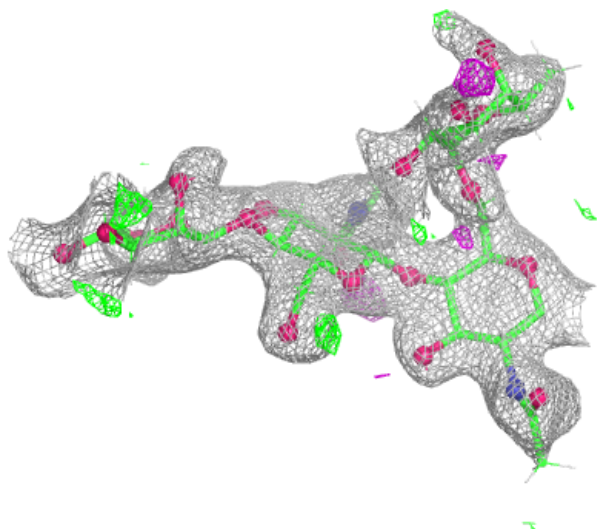
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BMA	E	3	11/12	0.57	0.15	88,108,129,136	0
3	FUC	D	2	10/11	0.66	0.24	66,94,114,130	0
2	FUC	E	4	10/11	0.71	0.19	66,98,126,146	0
2	NAG	E	1	14/15	0.71	0.16	62,87,101,108	0
3	FUC	F	2	10/11	0.77	0.17	53,95,117,119	0
3	NAG	F	1	14/15	0.80	0.15	35,61,77,92	0
2	NAG	E	2	14/15	0.80	0.13	77,92,108,113	0
2	BMA	C	3	11/12	0.81	0.12	66,80,96,99	0
3	NAG	D	1	14/15	0.86	0.14	36,61,74,75	0
2	FUC	C	4	10/11	0.88	0.12	55,66,79,81	0
2	NAG	C	2	14/15	0.89	0.11	37,64,76,84	0
2	NAG	C	1	14/15	0.93	0.10	32,47,69,69	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.

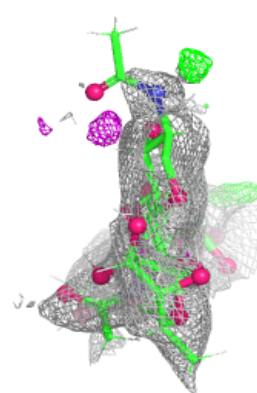
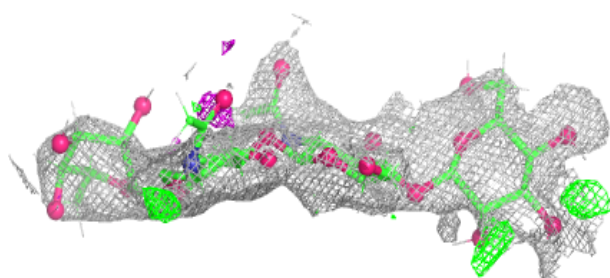
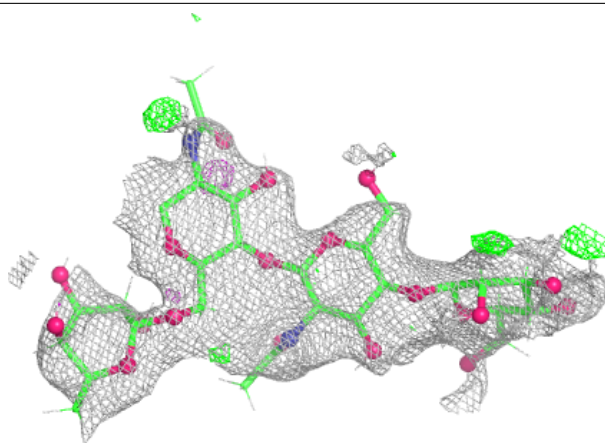
Electron density around Chain C:

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

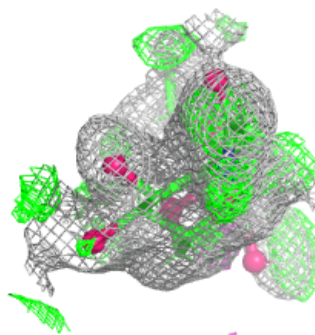
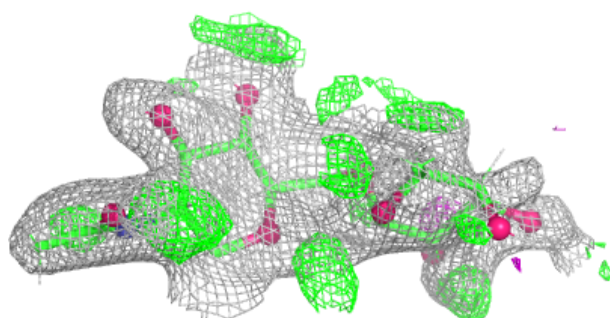
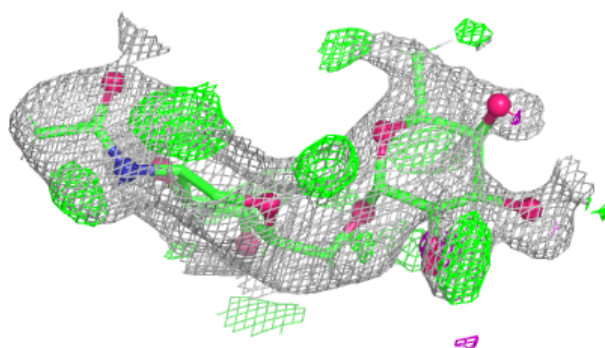


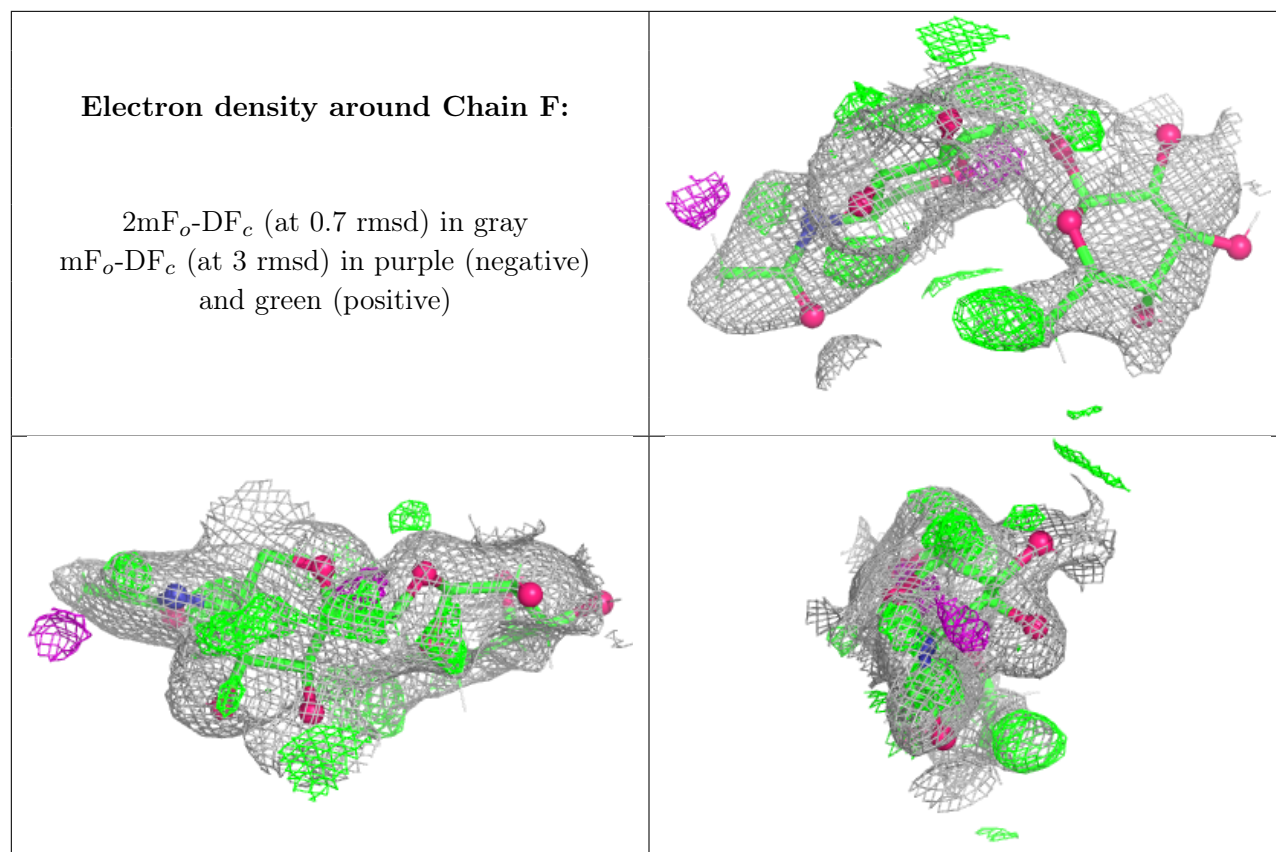
Electron density around Chain E:

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

**Electron density around Chain D:**

$2mF_o-DF_c$ (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, 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($\text{\AA}^2$)	Q<0.9
5	NAG	B	703	14/15	0.72	0.16	86,107,134,140	0
8	EDO	B	707	4/4	0.76	0.17	47,64,77,81	0
8	EDO	A	710	4/4	0.81	0.15	49,59,68,82	0
9	PEG	A	708	7/7	0.81	0.15	51,73,89,89	0
6	ACT	B	704	4/4	0.84	0.19	42,52,63,65	0
10	P33	A	711	22/22	0.84	0.16	41,72,89,106	0
5	NAG	A	702	14/15	0.86	0.12	48,68,88,97	0
8	EDO	A	705	4/4	0.87	0.14	56,67,75,79	0
14	PG4	B	701	13/13	0.88	0.12	44,62,80,90	0
6	ACT	A	709	4/4	0.90	0.12	52,55,64,64	0
8	EDO	B	705	4/4	0.90	0.10	54,65,79,79	0
8	EDO	A	706	4/4	0.91	0.10	45,55,65,78	0
13	MG	A	714	1/1	0.92	0.13	40,40,40,40	0
14	PG4	B	706	13/13	0.92	0.10	25,49,68,84	0

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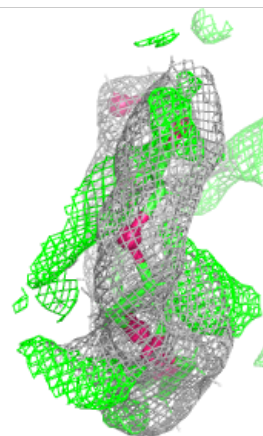
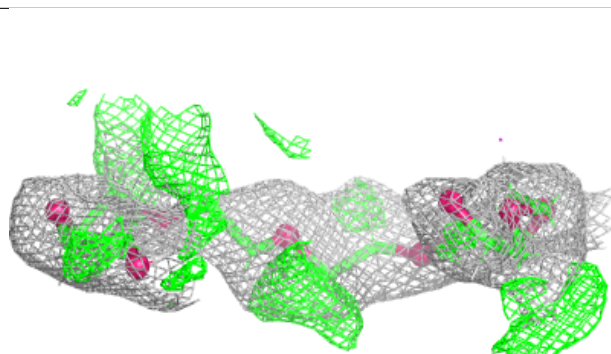
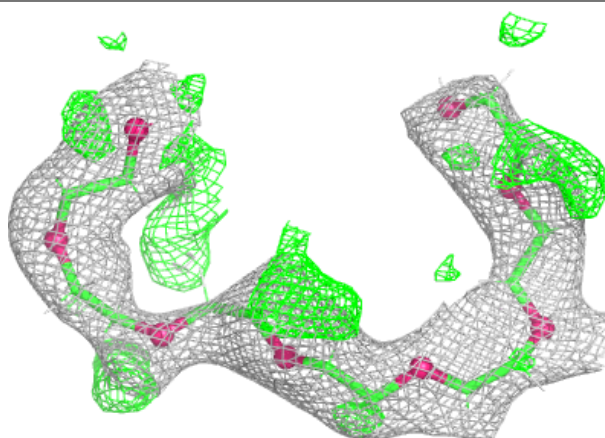
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	PEG	A	707	7/7	0.94	0.10	37,55,69,71	0
6	ACT	A	703	4/4	0.95	0.12	34,37,41,51	0
7	1PE	A	704	16/16	0.96	0.07	26,43,65,66	0
13	MG	B	710	1/1	0.96	0.07	30,30,30,30	0
4	8J9	B	702	33/33	0.97	0.06	21,31,41,48	0
12	CL	B	709	1/1	0.97	0.07	29,29,29,29	0
4	8J9	A	701	33/33	0.97	0.06	23,30,37,39	0
11	ZN	B	708	1/1	0.99	0.03	24,24,24,24	0
12	CL	A	713	1/1	1.00	0.04	22,22,22,22	0
11	ZN	A	712	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.

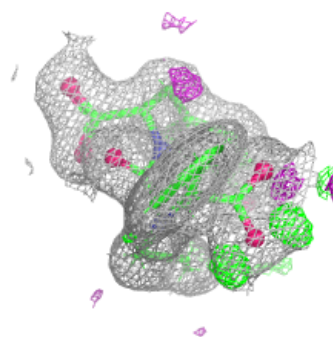
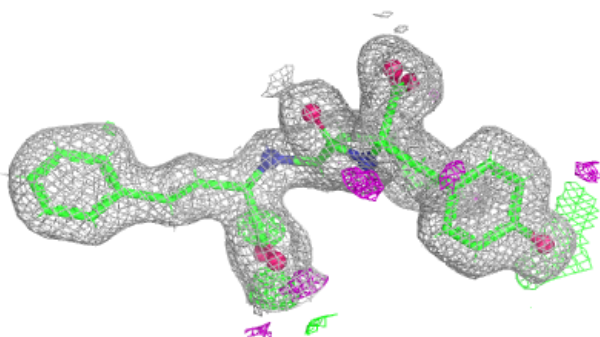
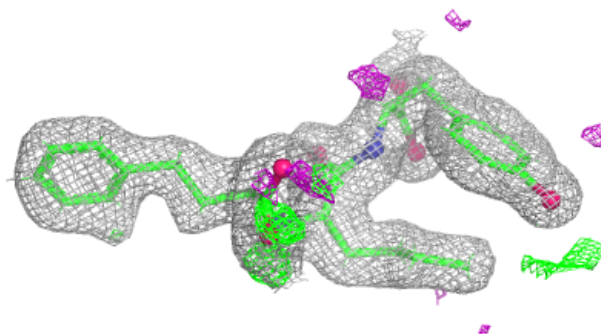
Electron density around P33 A 711:

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

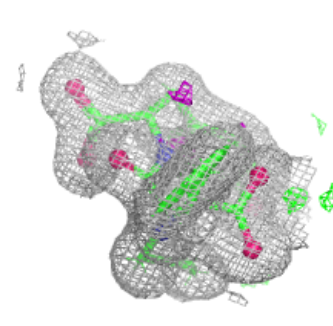
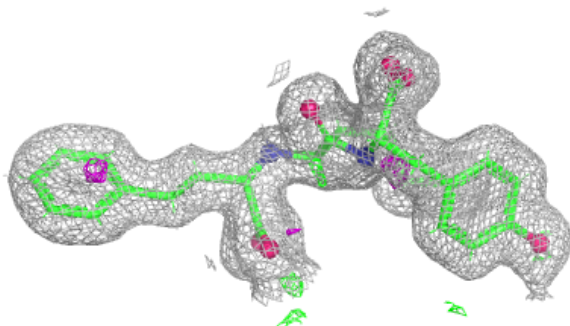
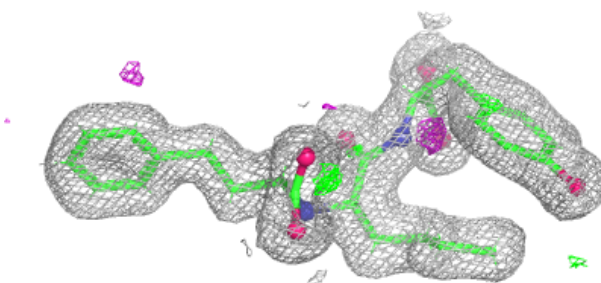


Electron density around 8J9 B 702:

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

**Electron density around 8J9 A 701:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.