Full wwPDB X-ray Structure Validation Report ⓘ

Apr 10, 2025 – 04:32 pm BST

PDB ID	:	9H1A / pdb_00009h1a
Title	:	Crystal structure of Angiotensin-1 converting enzyme N-domain in complex with dual ACE/NEP inhibitor AD014
Authors	:	Cozier, G.E.; Acharya, K.R.
Deposited on	:	2024-10-09
Resolution	:	1.85 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:

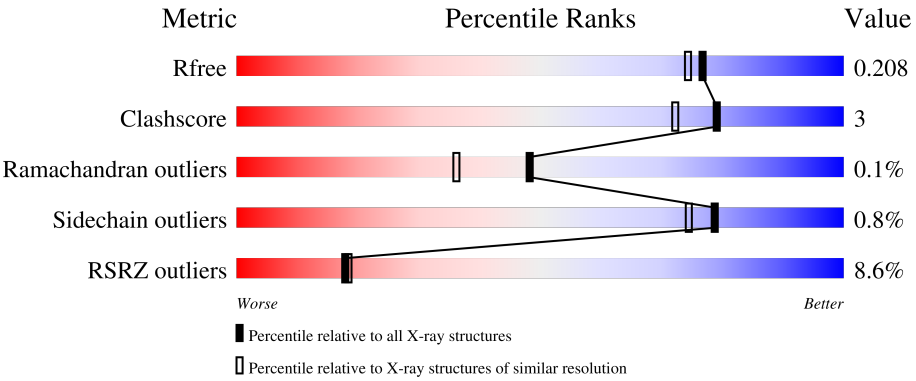
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

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 1.85 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	3097 (1.86-1.86)
Clashscore	180529	3359 (1.86-1.86)
Ramachandran outliers	177936	3335 (1.86-1.86)
Sidechain outliers	177891	3335 (1.86-1.86)
RSRZ outliers	164620	3097 (1.86-1.86)

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 <=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	5% 90% 7% .
1	B	628	11% 90% 6% .
2	C	2	50% 50%
2	E	2	50% 50%
3	D	4	25% 75%

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Mol	Chain	Length	Quality of chain
4	F	2	100%

2 Entry composition (i)

There are 18 unique types of molecules in this entry. The entry contains 20921 atoms, of which 9866 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	607	Total	C	H	N	O	S	0	15	0
			9833	3223	4807	863	921	19			
1	B	604	Total	C	H	N	O	S	0	9	0
			9733	3196	4756	855	907	19			

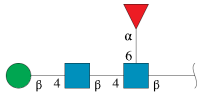
There are 16 discrepancies between the modelled and reference sequences:

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
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

- 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	H	N	O	0	0	0
			53	16	25	2	10			
2	E	2	Total	C	H	N	O	0	0	0
			53	16	25	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.

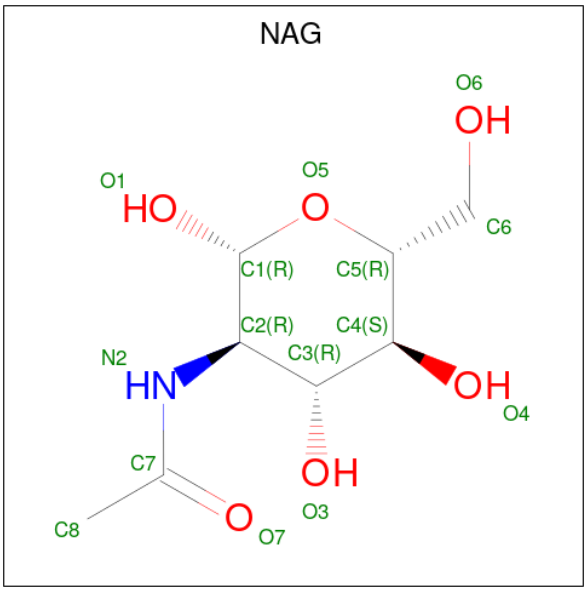


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	4	Total	C	H	N	O	0	0	0
			93	28	44	2	19			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	2	Total	C	H	N	O	0	0	0
			47	14	23	1	9			

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

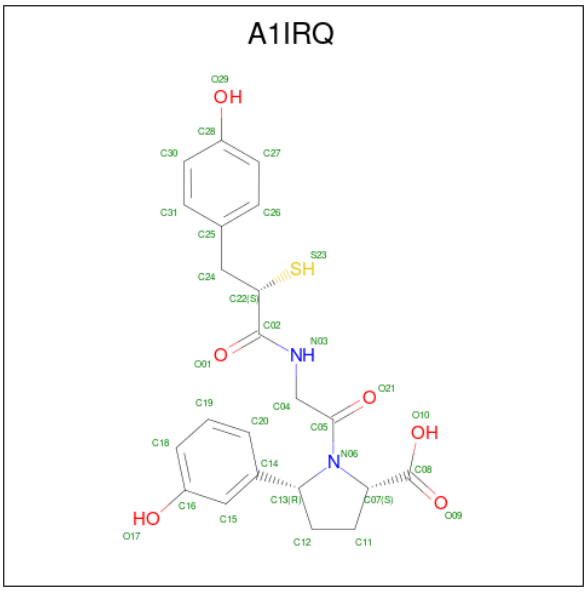


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
5	B	1	Total	C	H	N	O	0	0
			27	8	13	1	5		

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 7 is (2 {S},5 {R})-5-(3-hydroxyphenyl)-1-[2-[[(2 {S})-3-(4-hydroxyphenyl)-2-sulfanyl-propanoyl]amino]ethanoyl]pyrrolidine-2-carboxylic acid (CCD ID: A1IRQ) (formula: $C_{22}H_{24}N_2O_6S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
7	A	1	Total	C	H	N	O	S	0	0
			54	22	23	2	6	1		
7	B	1	Total	C	H	N	O	S	0	0
			54	22	23	2	6	1		

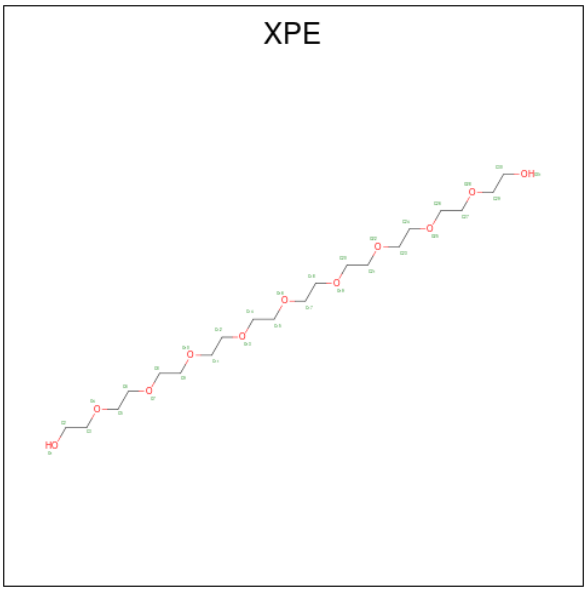
- Molecule 8 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

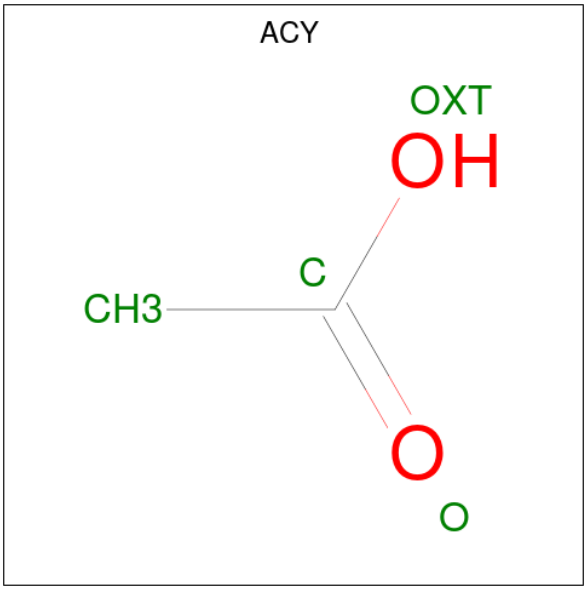
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	Mg	0	0
			1	1		
9	B	1	Total	Mg	0	0
			1	1		

- Molecule 10 is 3,6,9,12,15,18,21,24,27-NONAOXANONACOSANE-1,29-DIOL (CCD ID: XPE) (formula: $C_{20}H_{42}O_{11}$).



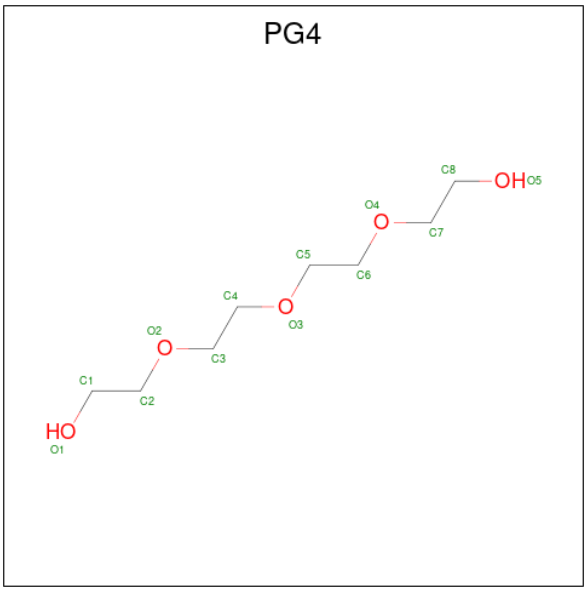
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	1	Total	C	H	O	0	0
			73	20	42	11		

- Molecule 11 is ACETIC ACID (CCD ID: ACY) (formula: $C_2H_4O_2$).



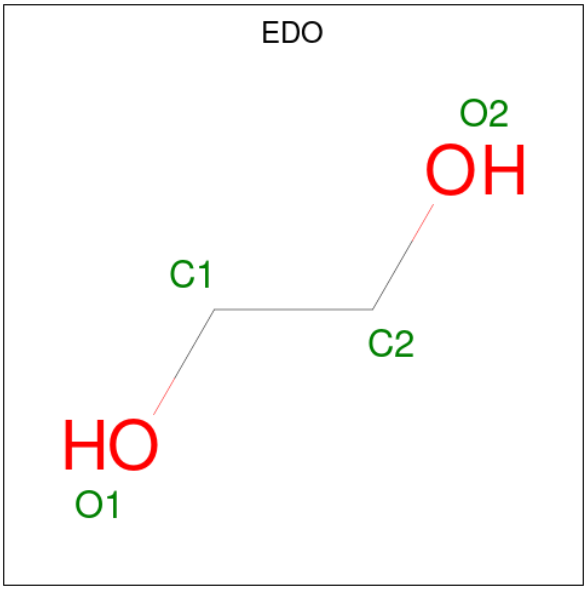
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	A	1	Total	C	H	O	0	0
			7	2	3	2		
11	B	1	Total	C	H	O	0	0
			7	2	3	2		

- 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	H	O	0	1
			31	8	18	5		

- Molecule 13 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

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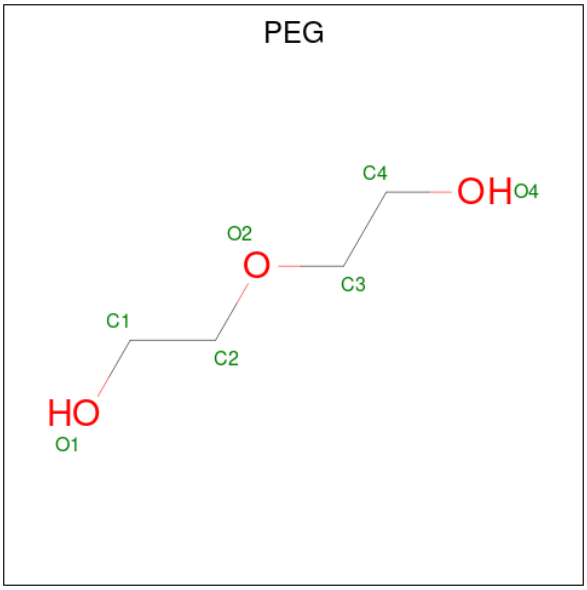
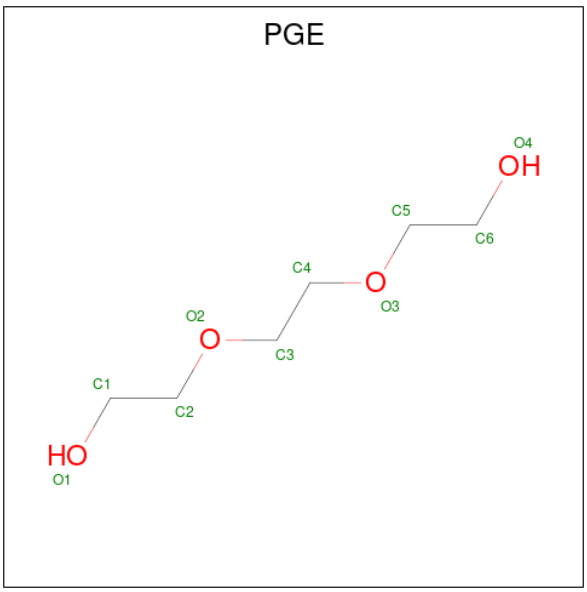
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	B	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 14 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



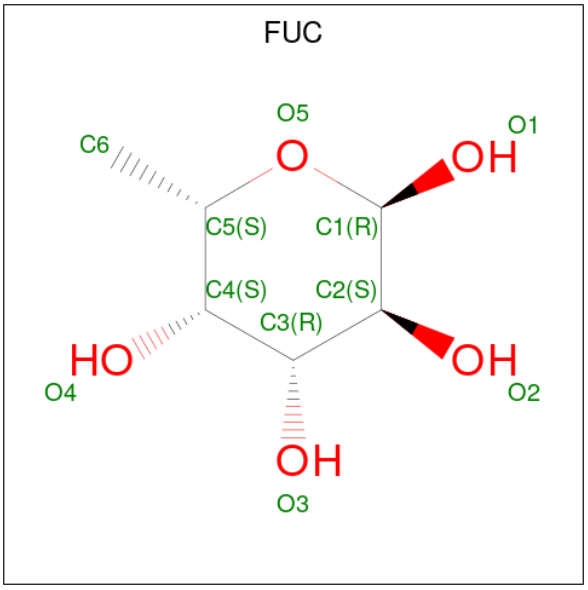
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	A	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 15 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



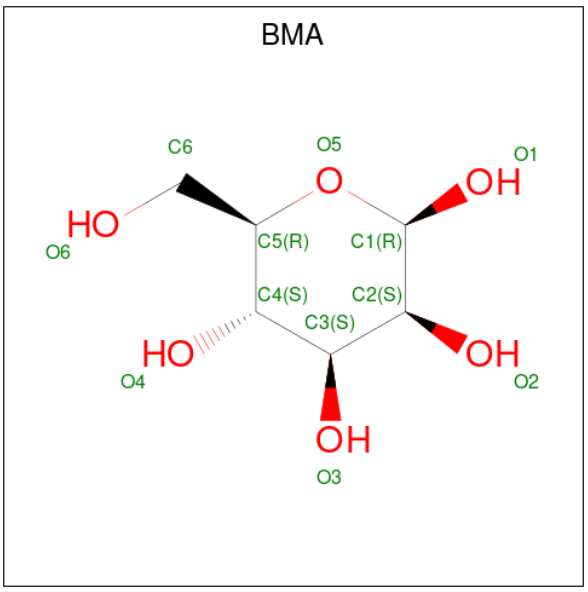
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	A	1	Total	C	H	O	0	0
			24	6	14	4		

- Molecule 16 is alpha-L-fucopyranose (CCD ID: FUC) (formula: $C_6H_{12}O_5$).



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

- Molecule 17 is beta-D-mannopyranose (CCD ID: BMA) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	B	1	Total C O 11 6 5	0	0

- Molecule 18 is water.

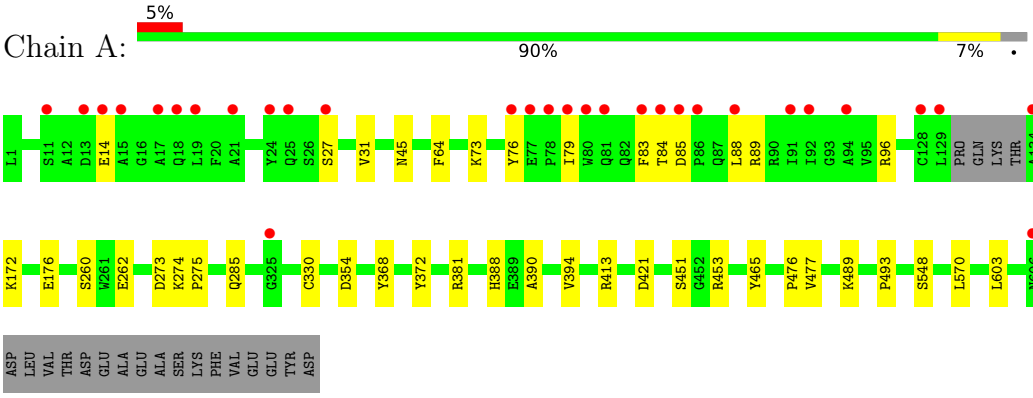
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	405	Total O 408 408	0	4
18	B	310	Total O 313 313	0	4

3 Residue-property plots (i)

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

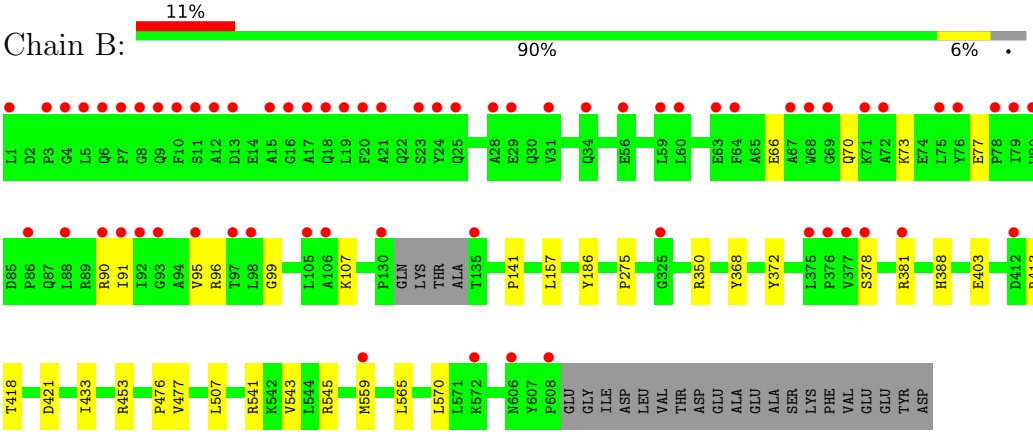
• Molecule 1: Angiotensin-converting enzyme, soluble form

Chain A:



• Molecule 1: Angiotensin-converting enzyme, soluble form

Chain B:



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

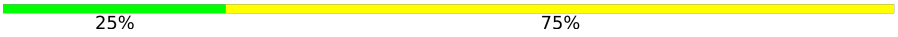
Chain C:

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

Chain E:

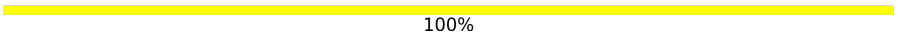
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:



• Molecule 4: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	72.93Å 77.43Å 82.63Å 88.66° 64.29° 74.92°	Depositor
Resolution (Å)	63.13 – 1.85 63.13 – 1.85	Depositor EDS
% Data completeness (in resolution range)	97.5 (63.13-1.85) 97.5 (63.13-1.85)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.16 (at 1.84Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.182 , 0.208 0.182 , 0.208	Depositor DCC
R_{free} test set	2135 reflections (1.58%)	wwPDB-VP
Wilson B-factor (Å^2)	26.7	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 44.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	20921	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.70% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: BMA, XPE, A1IRQ, PG4, PEG, NAG, CL, EDO, PGE, FUC, ZN, ACY, MG

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	0.36	0/5229	0.55	0/7121
1	B	0.34	0/5160	0.54	0/7029
All	All	0.35	0/10389	0.55	0/14150

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

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	5026	4807	4760	25	0
1	B	4977	4756	4732	23	0
2	C	28	25	25	0	0
2	E	28	25	25	1	0
3	D	49	44	43	0	0
4	F	24	23	22	0	0
5	A	14	13	13	0	0
5	B	14	13	13	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	31	23	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	31	23	0	1	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
9	A	1	0	0	0	0
9	B	1	0	0	0	0
10	A	31	42	42	0	0
11	A	4	3	3	1	0
11	B	4	3	3	0	0
12	A	13	18	18	1	0
13	A	8	12	12	0	0
13	B	8	12	12	0	0
14	A	7	10	10	0	0
15	A	10	14	14	0	0
16	B	10	0	10	2	0
17	B	11	0	10	1	0
18	A	408	0	0	7	0
18	B	313	0	0	3	0
All	All	11055	9866	9767	52	0

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

All (52) 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)
7:A:703:A1IRQ:S23	18:A:924:HOH:O	2.24	0.95
1:B:543:VAL:HG21	1:B:559:MET:HE2	1.56	0.86
1:A:157:LEU:HD11	1:A:477:VAL:HG13	1.65	0.79
1:B:416:ASN:OD1	16:B:702:FUC:H61	1.90	0.72
7:B:705:A1IRQ:S23	18:B:938:HOH:O	2.51	0.68
1:B:543:VAL:HG21	1:B:559:MET:CE	2.24	0.67
11:A:707:ACY:H3	18:A:848:HOH:O	1.94	0.66
1:A:477:VAL:HG12	1:A:603:LEU:HD21	1.77	0.65
1:A:330:CYS:O	18:A:801:HOH:O	2.14	0.64
1:A:14:GLU:OE1	1:A:84:THR:HG22	1.98	0.63
1:B:275:PRO:HG2	1:B:414:VAL:HG23	1.81	0.63
1:B:403[A]:GLU:OE2	1:B:413:ARG:NH2	2.32	0.61
1:A:285:GLN:NE2	18:A:812:HOH:O	2.37	0.58
1:B:157:LEU:HD11	1:B:477:VAL:HG13	1.86	0.57
1:A:354:ASP:OD1	18:A:802:HOH:O	2.17	0.57
1:B:66:GLU:O	1:B:70:GLN:HG3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:378:SER:O	1:B:381:ARG:NH2	2.40	0.55
1:B:91:ILE:O	1:B:95:VAL:HG23	2.08	0.54
1:B:453[B]:ARG:NH1	18:B:809:HOH:O	2.40	0.53
1:B:90:ARG:NH2	18:B:808:HOH:O	2.40	0.53
1:A:465:TYR:CE2	12:A:708[A]:PG4:H52	2.45	0.52
1:B:403[A]:GLU:OE2	1:B:413:ARG:NH1	2.43	0.52
1:A:260[A]:SER:HB2	1:A:262[A]:GLU:OE1	2.11	0.51
1:B:541:ARG:O	1:B:545:ARG:HG3	2.13	0.49
1:A:390:ALA:O	1:A:394:VAL:HG23	2.13	0.48
1:A:570:LEU:C	1:A:570:LEU:HD23	2.33	0.48
1:A:274:LYS:HB3	1:A:275:PRO:HD2	1.96	0.48
1:A:157:LEU:HD13	1:A:476:PRO:HB2	1.97	0.47
1:B:433[A]:ILE:HD11	1:B:570:LEU:HD21	1.97	0.47
1:A:27:SER:OG	18:A:803:HOH:O	2.21	0.46
1:B:157:LEU:HD13	1:B:476:PRO:HB2	1.98	0.45
1:A:489:LYS:O	1:A:493:PRO:HD2	2.16	0.45
1:A:85:ASP:HB3	1:A:88:LEU:HB3	1.98	0.45
1:A:172:LYS:O	1:A:176[B]:GLU:HG3	2.17	0.45
1:A:421:ASP:OD2	18:A:804:HOH:O	2.21	0.45
1:A:381:ARG:HG3	1:A:548:SER:HB3	1.98	0.45
1:B:418:THR:HG22	16:B:702:FUC:O4	2.17	0.45
1:A:477:VAL:HG12	1:A:603:LEU:CD2	2.47	0.44
1:A:31:VAL:HG21	1:A:64:PHE:CD2	2.53	0.44
1:B:141:PRO:HB3	1:B:350:ARG:HD3	2.00	0.44
1:B:107:LYS:HA	1:B:107:LYS:HE2	1.99	0.44
1:B:73:LYS:CG	1:B:96:ARG:HG3	2.48	0.43
1:B:73:LYS:HA	1:B:77:GLU:HB2	1.99	0.43
1:A:83:PHE:HB2	1:A:89:ARG:HG2	2.00	0.43
1:A:73:LYS:HG3	1:A:96:ARG:HG3	2.00	0.43
1:A:275:PRO:HD3	1:A:413:ARG:CZ	2.49	0.43
1:B:99:GLY:HA2	1:B:186:TYR:CE1	2.54	0.43
1:B:73:LYS:HG3	1:B:96:ARG:HG3	2.01	0.42
1:A:451:SER:OG	1:A:453:ARG:HG2	2.20	0.42
1:B:507:LEU:HD13	1:B:565:LEU:CD2	2.50	0.41
17:B:703:BMA:C1	2:E:2:NAG:H4	2.51	0.41
1:A:76:TYR:CD1	1:A:79:ILE:HD11	2.56	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	618/628 (98%)	610 (99%)	7 (1%)	1 (0%)	44 32
1	B	609/628 (97%)	598 (98%)	11 (2%)	0	100 100
All	All	1227/1256 (98%)	1208 (98%)	18 (2%)	1 (0%)	48 36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
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	535/540 (99%)	531 (99%)	4 (1%)	81 78
1	B	528/540 (98%)	524 (99%)	4 (1%)	79 74
All	All	1063/1080 (98%)	1055 (99%)	8 (1%)	79 74

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	273	ASP
1	A	368	TYR
1	A	372	TYR
1	A	388	HIS
1	B	368	TYR

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

10 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	0.69	0	17,19,21	0.90	2 (11%)
2	NAG	C	2	2	14,14,15	0.71	0	17,19,21	0.80	0
3	NAG	D	1	1,3	14,14,15	0.79	1 (7%)	17,19,21	0.74	0
3	NAG	D	2	3	14,14,15	0.76	1 (7%)	17,19,21	0.85	1 (5%)
3	BMA	D	3	3	11,11,12	0.89	0	15,15,17	1.59	1 (6%)
3	FUC	D	4	3	10,10,11	0.74	0	14,14,16	0.83	0
2	NAG	E	1	1,2	14,14,15	0.74	0	17,19,21	0.74	0
2	NAG	E	2	2	14,14,15	0.77	0	17,19,21	0.88	0
4	NAG	F	1	1,4	14,14,15	0.70	0	17,19,21	1.23	1 (5%)
4	FUC	F	2	4	10,10,11	0.68	0	14,14,16	1.09	1 (7%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	2	NAG	O5-C1	-2.06	1.40	1.43
3	D	1	NAG	O5-C1	-2.04	1.40	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	3	BMA	C1-O5-C5	4.42	118.19	112.19
4	F	1	NAG	C1-O5-C5	3.03	116.30	112.19
4	F	2	FUC	O5-C1-C2	-2.20	107.38	110.77
3	D	2	NAG	C1-O5-C5	2.18	115.14	112.19
2	C	1	NAG	O5-C1-C2	-2.15	107.89	111.29
2	C	1	NAG	C1-O5-C5	2.02	114.93	112.19

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2	NAG	C4-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
3	D	3	BMA	C4-C5-C6-O6
4	F	1	NAG	C1-C2-N2-C7
4	F	1	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
2	E	1	NAG	C4-C5-C6-O6

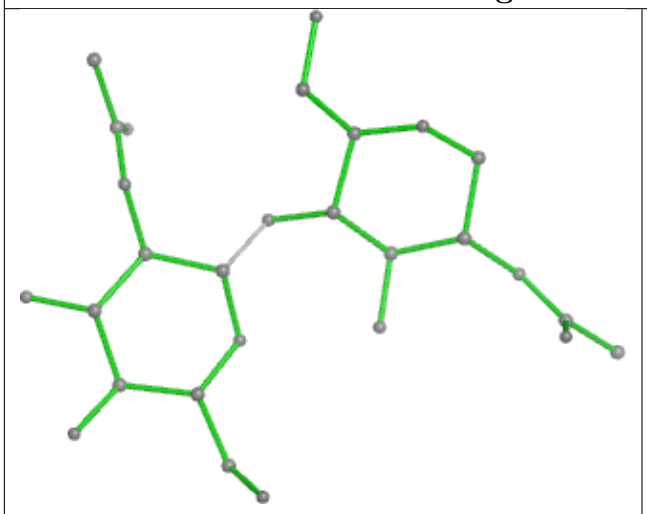
There are no ring outliers.

1 monomer is involved in 1 short contact:

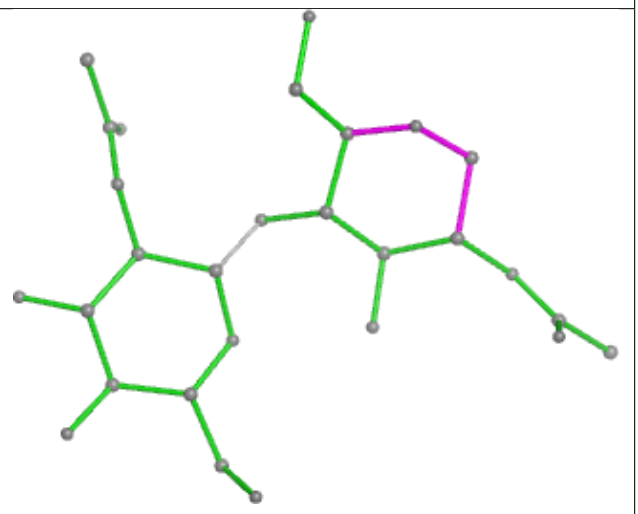
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	2	NAG	1	0

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

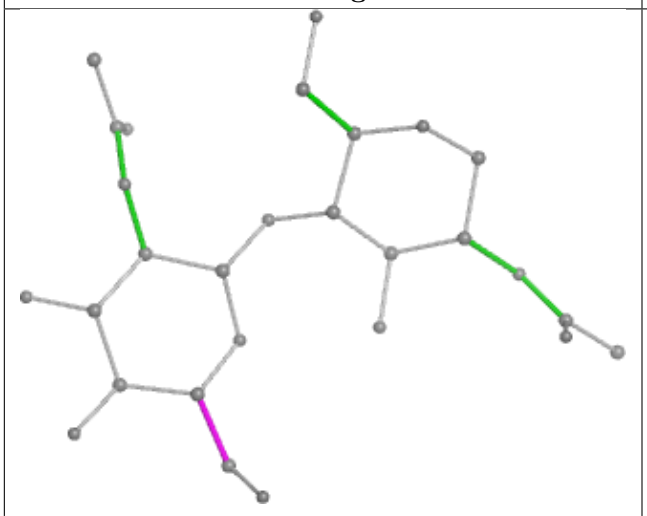
Oligosaccharide Chain C



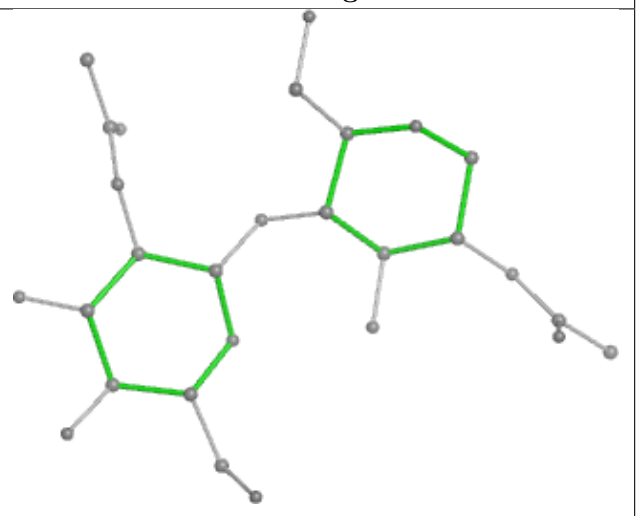
Bond lengths



Bond angles

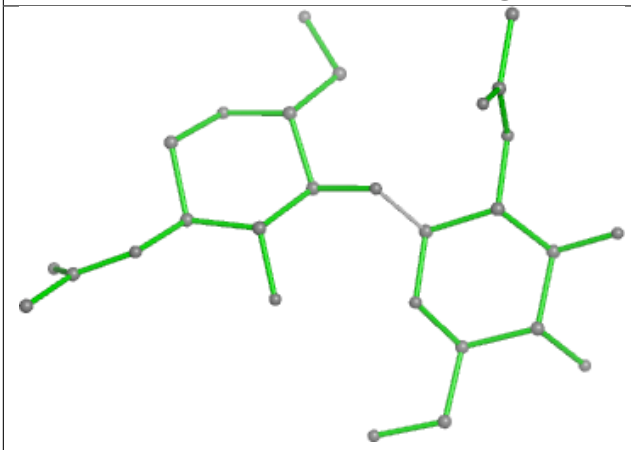


Torsions

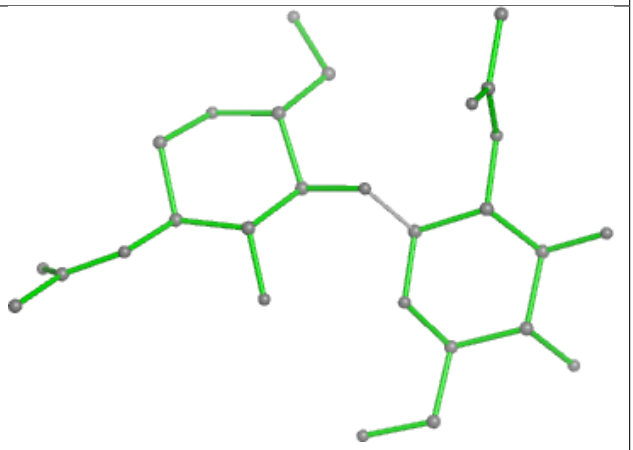


Rings

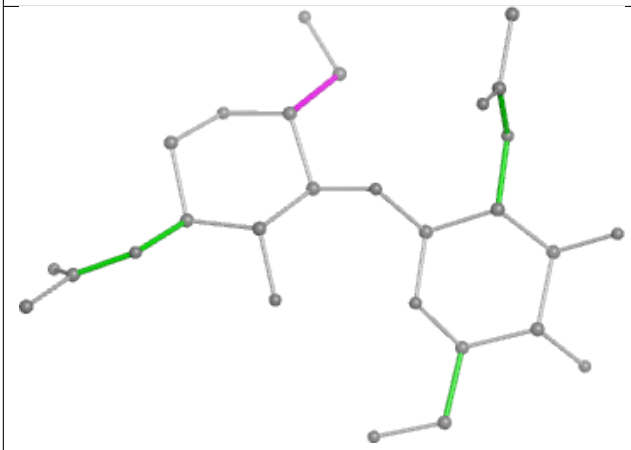
Oligosaccharide Chain E



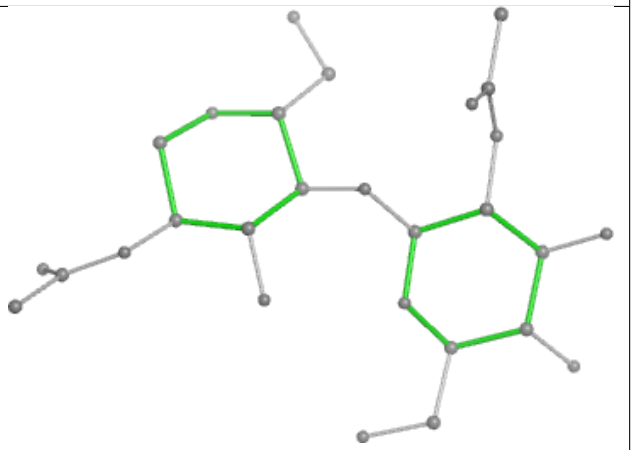
Bond lengths



Bond angles

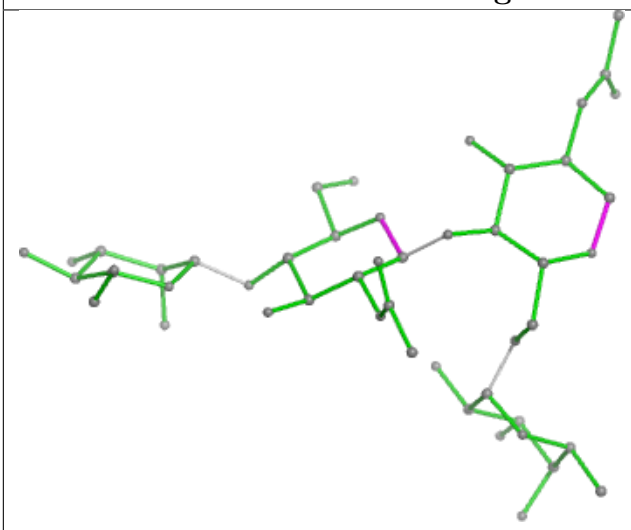


Torsions

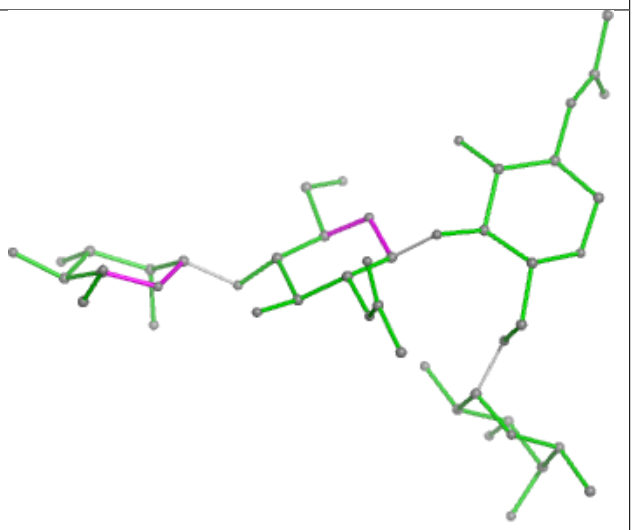


Rings

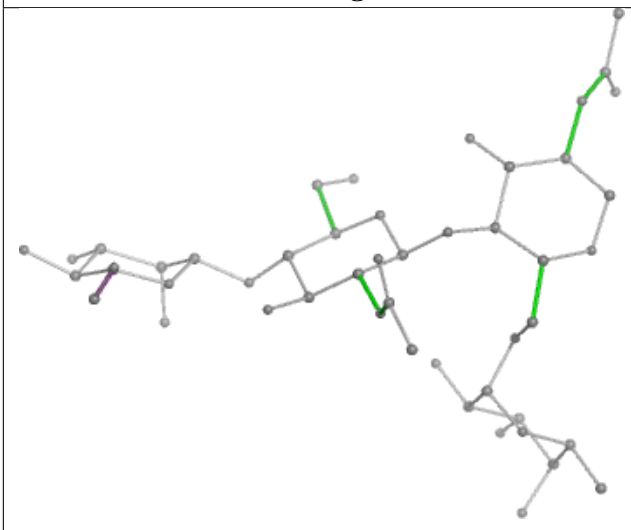
Oligosaccharide Chain D



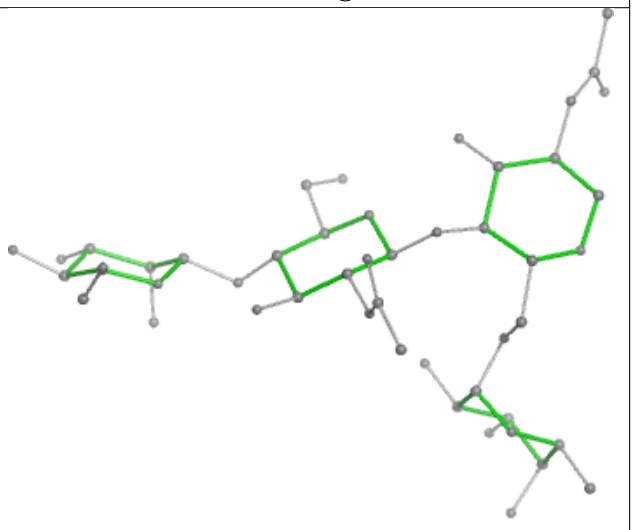
Bond lengths



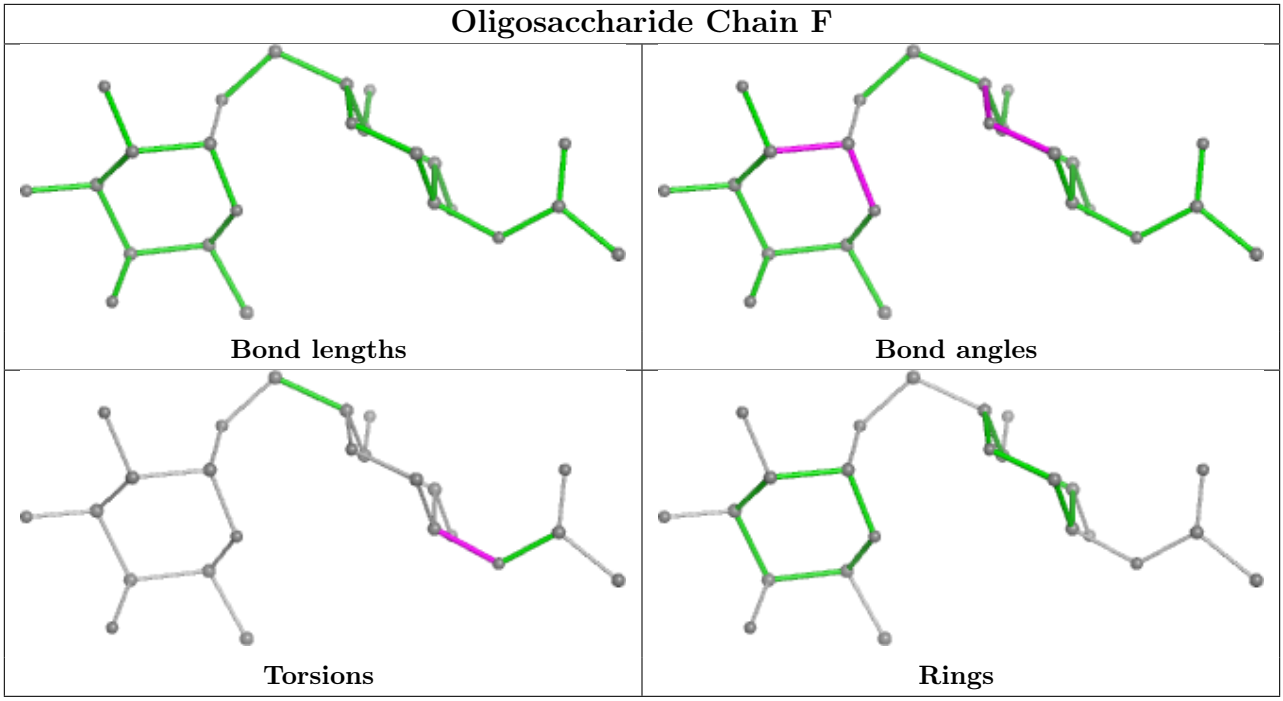
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

Of 22 ligands modelled in this entry, 6 are monoatomic - leaving 16 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	$\#\|Z\| > 2$
15	PGE	A	712	-	9,9,9	0.28	0	8,8,8	0.53	0
10	XPE	A	706	-	30,30,30	0.32	0	29,29,29	0.42	0
17	BMA	B	703	-	11,11,12	0.92	0	15,15,17	2.00	3 (20%)
13	EDO	A	709	-	3,3,3	0.30	0	2,2,2	0.13	0
13	EDO	B	710	-	3,3,3	0.28	0	2,2,2	0.22	0
14	PEG	A	711	-	6,6,6	0.26	0	5,5,5	0.26	0
7	A1IRQ	A	703	6	32,33,33	3.54	10 (31%)	40,46,46	1.71	9 (22%)
13	EDO	A	710	-	3,3,3	0.33	0	2,2,2	0.33	0
5	NAG	A	701	1	14,14,15	0.78	0	17,19,21	1.30	3 (17%)
12	PG4	A	708[A]	-	12,12,12	0.29	0	11,11,11	0.39	0
16	FUC	B	702	-	10,10,11	0.86	0	14,14,16	1.60	3 (21%)
13	EDO	B	709	-	3,3,3	0.27	0	2,2,2	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	B	701	1	14,14,15	0.66	0	17,19,21	1.01	1 (5%)
11	ACY	B	708	-	3,3,3	1.17	0	3,3,3	1.08	0
7	A1IRQ	B	705	6	32,33,33	3.52	10 (31%)	40,46,46	1.85	9 (22%)
11	ACY	A	707	-	3,3,3	1.23	0	3,3,3	0.97	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
10	XPE	A	706	-	-	11/28/28/28	-
17	BMA	B	703	-	-	0/2/19/22	0/1/1/1
13	EDO	A	709	-	-	0/1/1/1	-
13	EDO	B	710	-	-	1/1/1/1	-
14	PEG	A	711	-	-	1/4/4/4	-
7	A1IRQ	A	703	6	-	5/23/38/38	0/3/3/3
13	EDO	A	710	-	-	0/1/1/1	-
5	NAG	A	701	1	-	3/6/23/26	0/1/1/1
12	PG4	A	708[A]	-	-	5/10/10/10	-
16	FUC	B	702	-	-	-	0/1/1/1
13	EDO	B	709	-	-	0/1/1/1	-
5	NAG	B	701	1	-	2/6/23/26	0/1/1/1
15	PGE	A	712	-	-	3/7/7/7	-
7	A1IRQ	B	705	6	-	2/23/38/38	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	703	A1IRQ	C05-N06	10.96	1.50	1.36
7	B	705	A1IRQ	C05-N06	10.67	1.50	1.36
7	B	705	A1IRQ	C07-N06	8.81	1.59	1.46
7	B	705	A1IRQ	C11-C07	-8.44	1.33	1.53
7	A	703	A1IRQ	C07-N06	8.30	1.58	1.46
7	A	703	A1IRQ	C11-C07	-8.26	1.34	1.53
7	B	705	A1IRQ	C13-N06	-6.22	1.32	1.47
7	A	703	A1IRQ	C02-N03	6.14	1.47	1.33
7	A	703	A1IRQ	C13-N06	-6.08	1.32	1.47
7	B	705	A1IRQ	C02-N03	5.84	1.46	1.33
7	A	703	A1IRQ	O17-C16	4.25	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	705	A1IRQ	O17-C16	4.01	1.46	1.37
7	A	703	A1IRQ	C24-C25	3.53	1.59	1.51
7	B	705	A1IRQ	C24-C25	3.42	1.59	1.51
7	A	703	A1IRQ	O01-C02	-2.94	1.17	1.23
7	B	705	A1IRQ	O01-C02	-2.39	1.18	1.23
7	A	703	A1IRQ	C14-C13	2.13	1.55	1.51
7	A	703	A1IRQ	O21-C05	-2.12	1.18	1.23
7	B	705	A1IRQ	O21-C05	-2.09	1.18	1.23
7	B	705	A1IRQ	C14-C13	2.08	1.55	1.51

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	703	A1IRQ	C12-C13-N06	6.43	106.25	101.97
7	B	705	A1IRQ	C12-C13-N06	6.33	106.18	101.97
17	B	703	BMA	C1-O5-C5	4.67	118.52	112.19
7	B	705	A1IRQ	C24-C22-C02	-3.83	103.47	112.10
7	B	705	A1IRQ	O01-C02-C22	-3.62	116.36	121.61
7	A	703	A1IRQ	O21-C05-N06	-3.51	118.59	122.29
7	A	703	A1IRQ	C12-C13-C14	-3.26	107.30	113.61
7	B	705	A1IRQ	O21-C05-N06	-3.16	118.96	122.29
16	B	702	FUC	O5-C1-C2	3.16	115.64	110.77
7	B	705	A1IRQ	C04-N03-C02	-3.13	113.62	121.37
16	B	702	FUC	C1-C2-C3	3.01	113.37	109.67
17	B	703	BMA	C3-C4-C5	2.96	115.51	110.24
7	B	705	A1IRQ	C12-C13-C14	-2.80	108.19	113.61
5	B	701	NAG	C1-O5-C5	2.75	115.92	112.19
7	A	703	A1IRQ	C08-C07-N06	-2.72	107.74	113.01
7	A	703	A1IRQ	C11-C07-N06	2.48	105.47	103.09
7	A	703	A1IRQ	O10-C08-O09	-2.40	118.65	124.09
16	B	702	FUC	C1-O5-C5	2.38	118.17	112.78
7	A	703	A1IRQ	C04-N03-C02	-2.38	115.47	121.37
5	A	701	NAG	O5-C1-C2	-2.36	107.56	111.29
17	B	703	BMA	O4-C4-C3	-2.35	104.91	110.35
7	B	705	A1IRQ	O10-C08-C07	2.33	121.47	113.38
7	B	705	A1IRQ	O10-C08-O09	-2.31	118.85	124.09
7	A	703	A1IRQ	O10-C08-C07	2.23	121.13	113.38
5	A	701	NAG	C1-O5-C5	2.18	115.14	112.19
7	B	705	A1IRQ	C11-C07-N06	2.17	105.17	103.09
5	A	701	NAG	C2-N2-C7	2.15	125.97	122.90
7	A	703	A1IRQ	C05-C04-N03	2.00	115.91	110.94

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	703	A1IRQ	C02-C22-C24-C25
7	A	703	A1IRQ	S23-C22-C24-C25
7	B	705	A1IRQ	S23-C22-C24-C25
5	A	701	NAG	O5-C5-C6-O6
5	B	701	NAG	O5-C5-C6-O6
10	A	706	XPE	O16-C17-C18-O19
5	A	701	NAG	C4-C5-C6-O6
5	B	701	NAG	C4-C5-C6-O6
10	A	706	XPE	O4-C5-C6-O7
10	A	706	XPE	O7-C8-C9-O10
13	B	710	EDO	O1-C1-C2-O2
10	A	706	XPE	O10-C11-C12-O13
12	A	708[A]	PG4	O4-C7-C8-O5
10	A	706	XPE	O22-C23-C24-O25
10	A	706	XPE	O13-C14-C15-O16
12	A	708[A]	PG4	O3-C5-C6-O4
10	A	706	XPE	O1-C2-C3-O4
10	A	706	XPE	O19-C20-C21-O22
10	A	706	XPE	O25-C26-C27-O28
10	A	706	XPE	C9-C8-O7-C6
10	A	706	XPE	O28-C29-C30-O31
15	A	712	PGE	O1-C1-C2-O2
12	A	708[A]	PG4	C1-C2-O2-C3
7	A	703	A1IRQ	C22-C24-C25-C26
7	A	703	A1IRQ	C22-C24-C25-C31
5	A	701	NAG	C3-C2-N2-C7
12	A	708[A]	PG4	O2-C3-C4-O3
15	A	712	PGE	O3-C5-C6-O4
12	A	708[A]	PG4	O1-C1-C2-O2
7	B	705	A1IRQ	C22-C24-C25-C26
14	A	711	PEG	O1-C1-C2-O2
7	A	703	A1IRQ	O01-C02-C22-C24
15	A	712	PGE	C6-C5-O3-C4

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	B	703	BMA	1	0
7	A	703	A1IRQ	1	0

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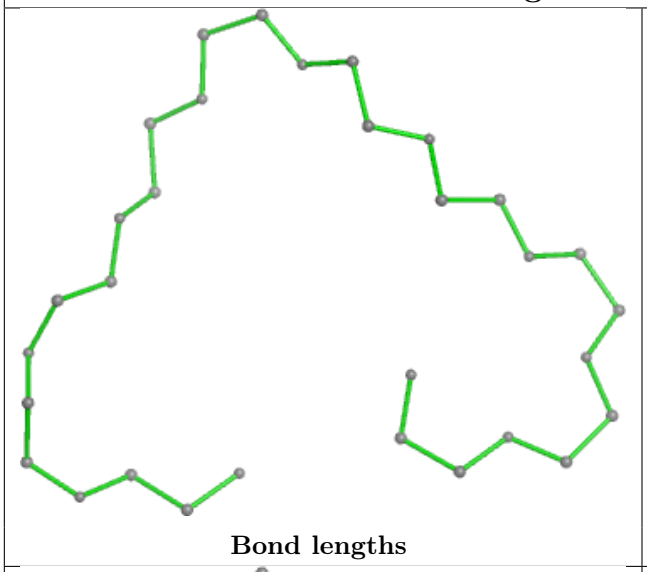
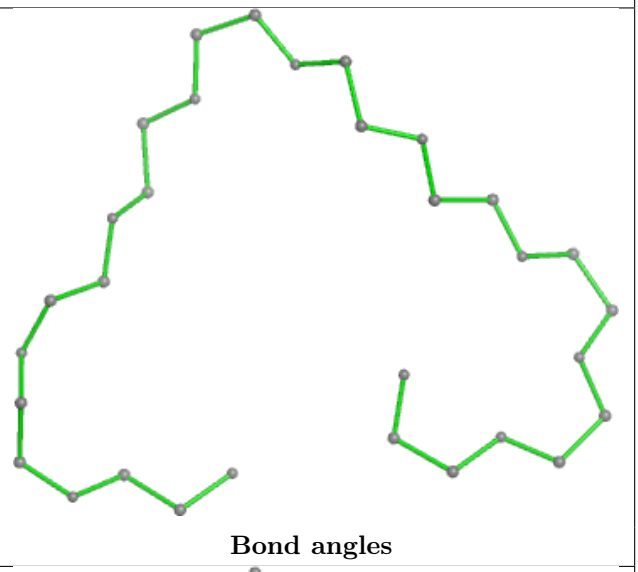
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	A	708[A]	PG4	1	0
16	B	702	FUC	2	0
7	B	705	A1IRQ	1	0
11	A	707	ACY	1	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

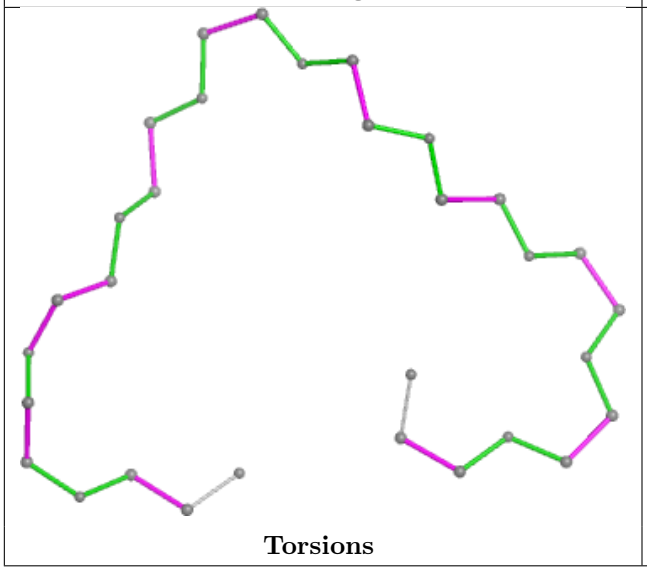
Ligand XPE A 706



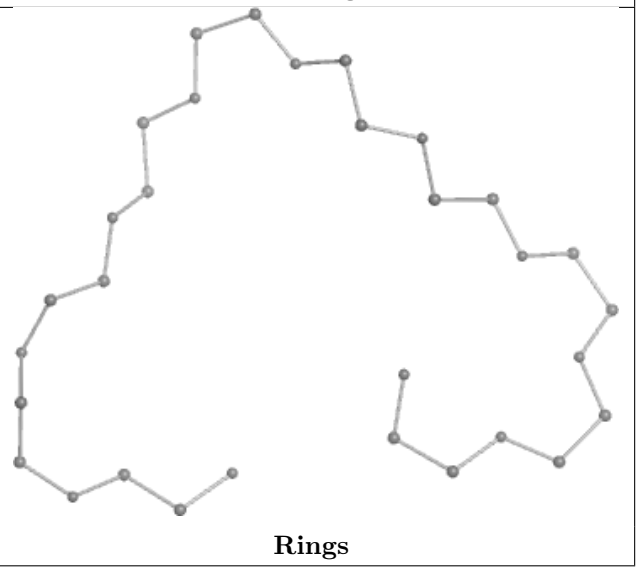
Bond lengths



Bond angles

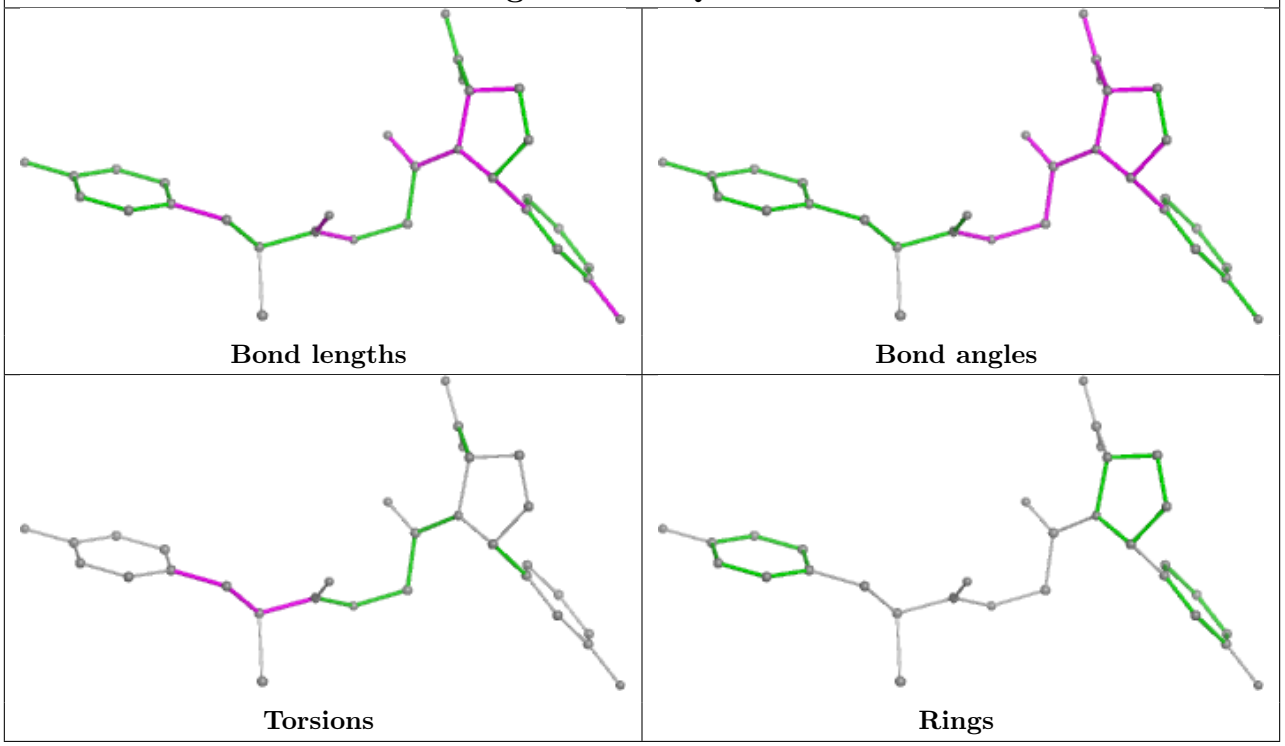


Torsions

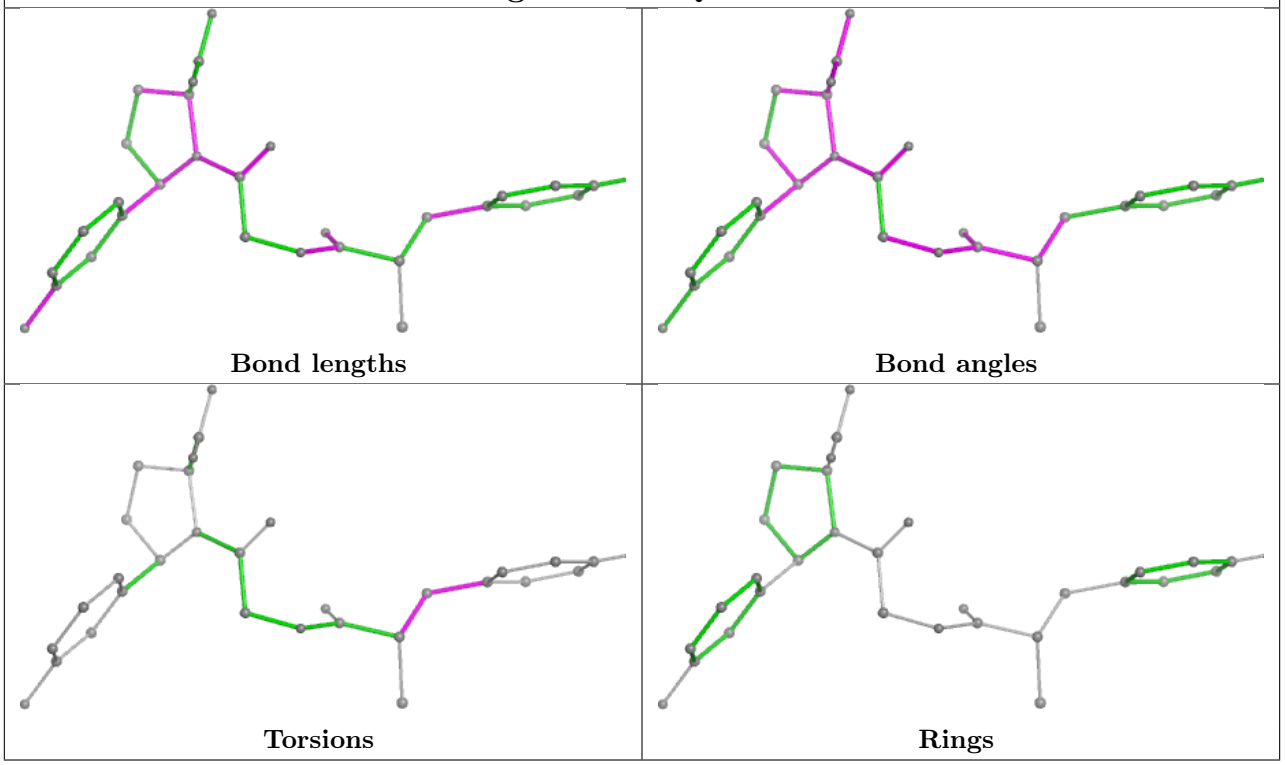


Rings

Ligand A1IRQ A 703



Ligand A1IRQ B 705



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^{th} 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	607/628 (96%)	-0.13	34 (5%)	31	33	12, 34, 72, 108	9 (1%)
1	B	604/628 (96%)	0.33	70 (11%)	11	10	13, 45, 85, 110	5 (0%)
All	All	1211/1256 (96%)	0.10	104 (8%)	18	18	12, 38, 82, 110	14 (1%)

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	79	ILE	5.9
1	A	88	LEU	5.5
1	A	134	ALA	5.5
1	B	20	PHE	5.1
1	B	19	LEU	5.1
1	B	15	ALA	5.1
1	B	92	ILE	4.9
1	B	11	SER	4.7
1	A	80	TRP	4.5
1	A	21	ALA	4.4
1	A	611	ILE	4.2
1	A	15	ALA	4.1
1	A	129	LEU	4.1
1	B	1	LEU	4.1
1	A	78	PRO	4.1
1	B	25	GLN	4.0
1	A	607	TYR	3.9
1	B	21	ALA	3.9
1	B	414	VAL	3.8
1	A	325	GLY	3.8
1	B	75	LEU	3.7
1	A	17	ALA	3.7
1	B	24	TYR	3.6
1	B	76	TYR	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	84	THR	3.6
1	B	325	GLY	3.6
1	A	83	PHE	3.5
1	A	606	ASN	3.5
1	A	14	GLU	3.5
1	B	86	PRO	3.5
1	B	17	ALA	3.5
1	B	78	PRO	3.4
1	B	18	GLN	3.4
1	A	86	PRO	3.4
1	B	105	LEU	3.3
1	B	10	PHE	3.3
1	B	8	GLY	3.3
1	B	5	LEU	3.3
1	A	84	THR	3.3
1	B	68	TRP	3.2
1	B	28	ALA	3.2
1	B	83	PHE	3.2
1	B	130	PRO	3.2
1	B	4	GLY	3.1
1	B	7	PRO	3.0
1	B	13	ASP	3.0
1	B	412	ASP	3.0
1	B	82	GLN	3.0
1	B	106	ALA	3.0
1	B	59	LEU	3.0
1	B	29	GLU	2.9
1	B	23	SER	2.9
1	B	91	ILE	2.9
1	A	81	GLN	2.9
1	B	606	ASN	2.9
1	B	375	LEU	2.9
1	B	90	ARG	2.9
1	B	95	VAL	2.9
1	B	80	TRP	2.9
1	A	135	THR	2.8
1	B	31	VAL	2.8
1	B	12	ALA	2.8
1	B	377	VAL	2.8
1	B	6	GLN	2.8
1	B	9	GLN	2.8
1	A	13	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	64	PHE	2.7
1	A	94	ALA	2.6
1	B	79	ILE	2.6
1	A	24	TYR	2.6
1	A	85	ASP	2.6
1	A	92	ILE	2.6
1	B	81	GLN	2.6
1	B	135	THR	2.5
1	A	11	SER	2.5
1	B	67	ALA	2.5
1	B	16	GLY	2.4
1	B	93	GLY	2.4
1	A	19	LEU	2.4
1	B	56	GLU	2.4
1	B	3	PRO	2.4
1	A	91	ILE	2.4
1	B	72	ALA	2.4
1	A	610	GLY	2.4
1	B	34	GLN	2.4
1	B	97	THR	2.4
1	A	25	GLN	2.3
1	B	71	LYS	2.3
1	B	63	GLU	2.3
1	B	378	SER	2.3
1	B	376	PRO	2.3
1	B	60	LEU	2.3
1	B	88	LEU	2.3
1	B	69	GLY	2.2
1	A	76	TYR	2.2
1	B	572	LYS	2.2
1	B	559	MET	2.2
1	B	98	LEU	2.2
1	A	77	GLU	2.2
1	B	608	PRO	2.1
1	A	27	SER	2.1
1	A	18	GLN	2.1
1	A	128	CYS	2.0
1	B	381	ARG	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)

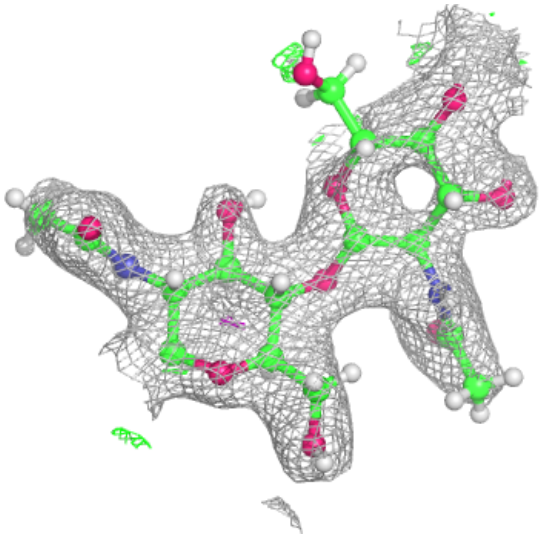
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

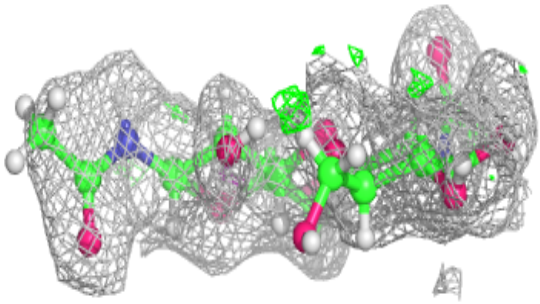
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	E	1	14/15	0.72	0.15	64,79,91,95	0
2	NAG	C	2	14/15	0.73	0.16	65,92,127,134	0
3	BMA	D	3	11/12	0.75	0.13	59,76,86,93	0
2	NAG	E	2	14/15	0.76	0.15	73,88,107,107	0
4	FUC	F	2	10/11	0.76	0.15	60,73,85,91	0
3	FUC	D	4	10/11	0.85	0.15	44,59,69,74	0
4	NAG	F	1	14/15	0.86	0.12	39,57,72,82	0
2	NAG	C	1	14/15	0.86	0.12	47,61,86,93	0
3	NAG	D	2	14/15	0.88	0.11	40,60,70,75	0
3	NAG	D	1	14/15	0.94	0.08	35,47,61,61	0

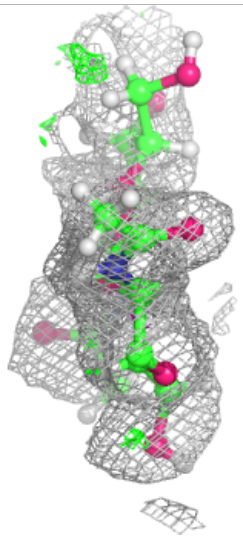
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

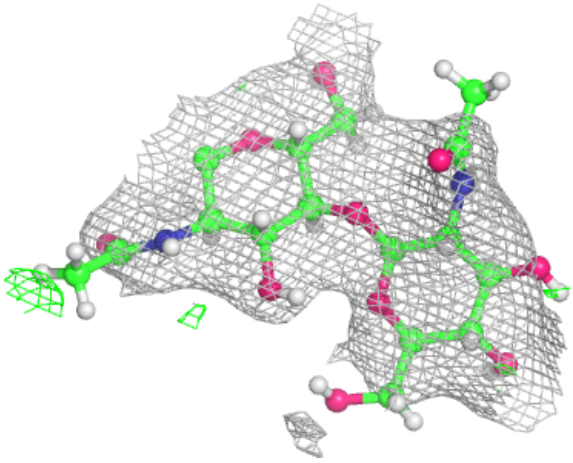


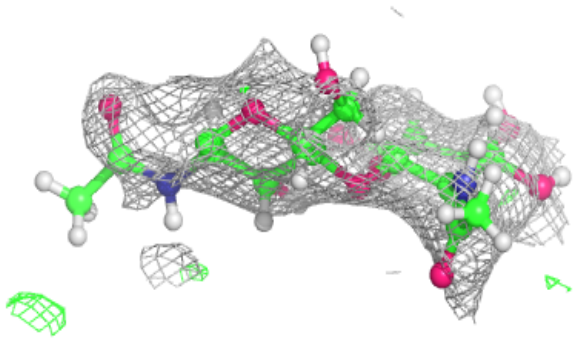


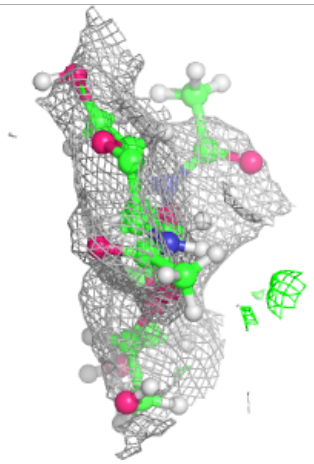


Electron density around Chain E:

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

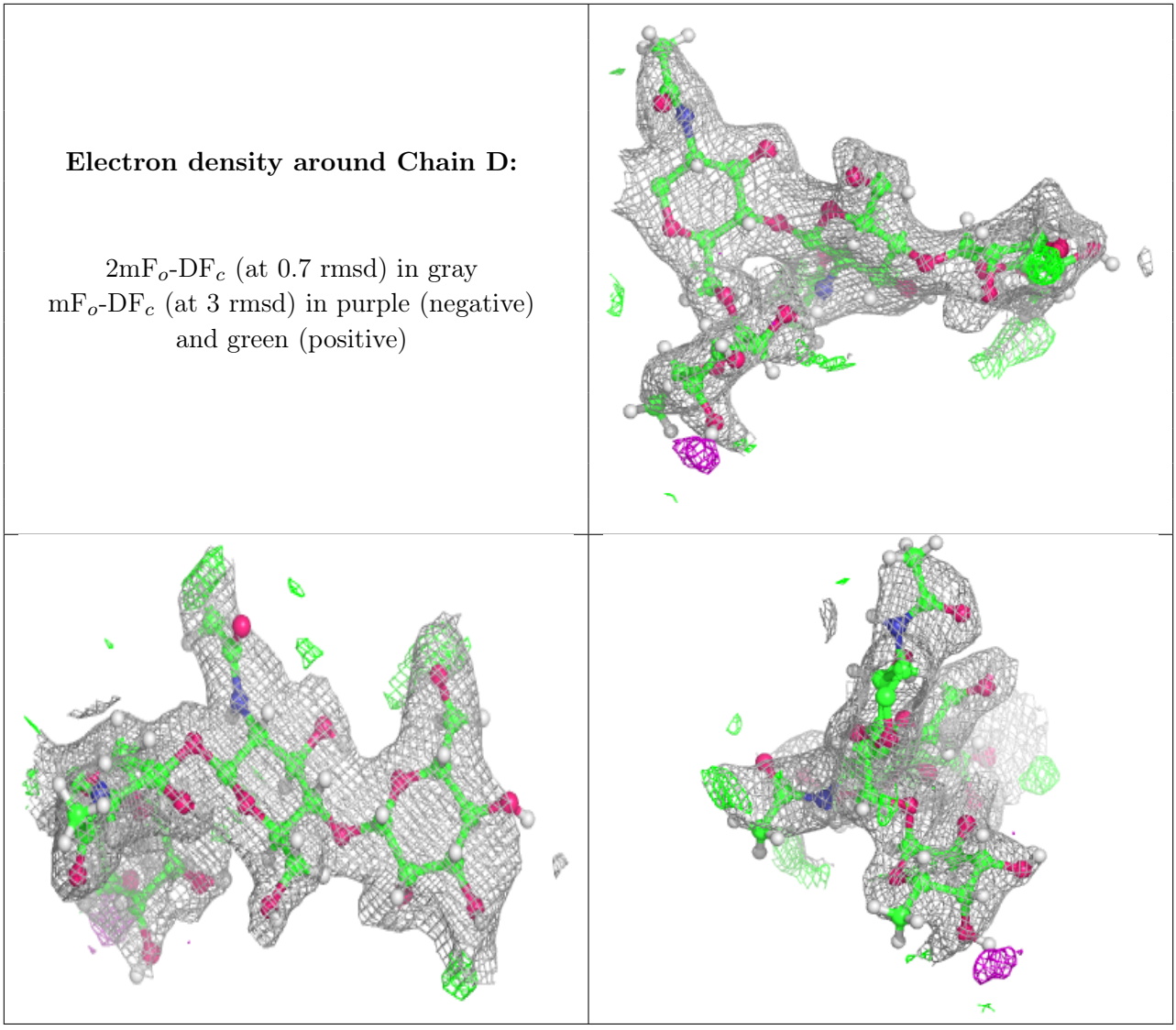






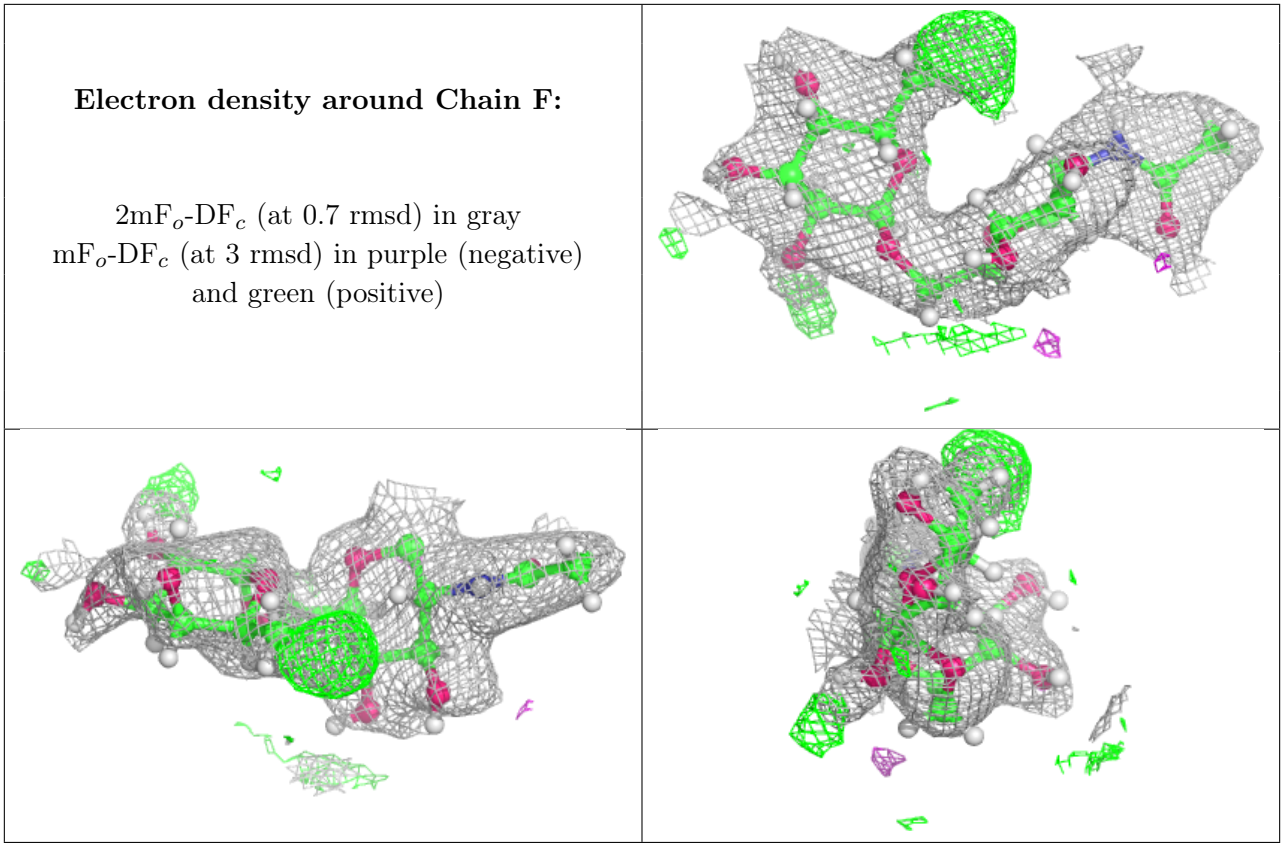
Electron density around Chain D:

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



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

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^{th} 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
17	BMA	B	703	11/12	0.57	0.16	89,97,102,104	0
16	FUC	B	702	10/11	0.66	0.17	75,81,90,93	0
5	NAG	B	701	14/15	0.69	0.17	59,87,103,106	0
13	EDO	A	709	4/4	0.85	0.13	55,67,71,76	0
12	PG4	A	708[A]	13/13	0.86	0.14	33,44,53,60	31
13	EDO	A	710	4/4	0.86	0.17	34,55,59,71	0
5	NAG	A	701	14/15	0.87	0.13	36,50,62,71	0
15	PGE	A	712	10/10	0.88	0.13	44,59,76,79	0
11	ACY	B	708	4/4	0.88	0.14	35,42,54,55	0
10	XPE	A	706	31/31	0.88	0.12	41,57,69,77	0
7	A1IRQ	B	705	31/31	0.90	0.12	23,45,77,93	0
14	PEG	A	711	7/7	0.91	0.09	45,60,74,74	0
7	A1IRQ	A	703	31/31	0.92	0.11	20,40,77,89	0
13	EDO	B	709	4/4	0.93	0.10	53,64,73,73	0

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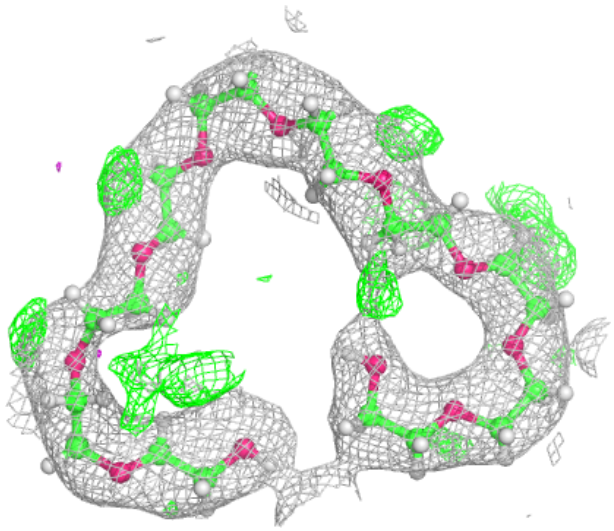
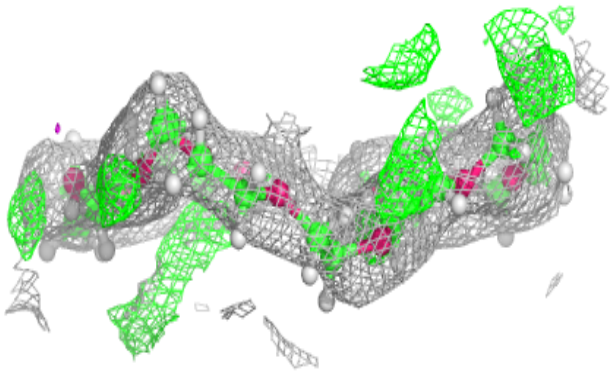
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
13	EDO	B	710	4/4	0.93	0.10	48,58,64,70	0
9	MG	A	705	1/1	0.95	0.06	35,35,35,35	1
11	ACY	A	707	4/4	0.95	0.11	24,28,46,50	0
9	MG	B	707	1/1	0.97	0.05	38,38,38,38	0
8	CL	B	706	1/1	0.98	0.04	27,27,27,27	0
8	CL	A	704	1/1	0.99	0.03	20,20,20,20	0
6	ZN	A	702	1/1	1.00	0.03	25,25,25,25	0
6	ZN	B	704	1/1	1.00	0.02	25,25,25,25	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 XPE A 706:

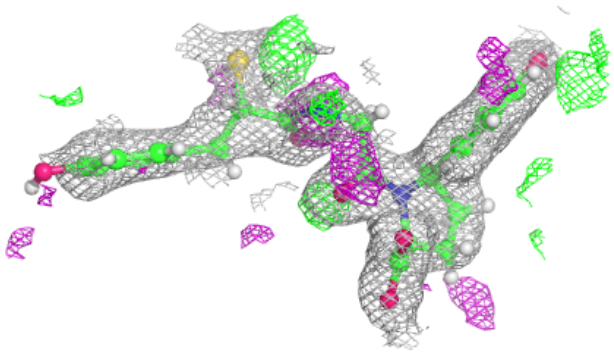
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

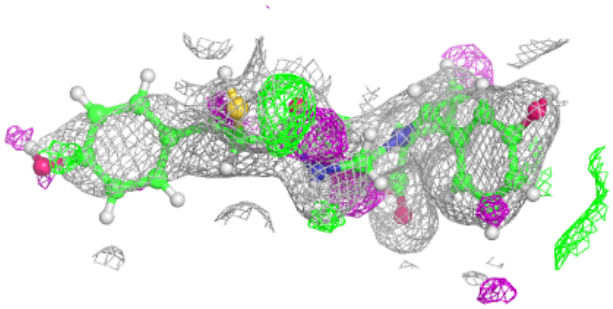


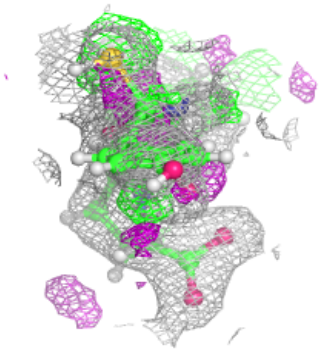


Electron density around A1IRQ B 705:

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

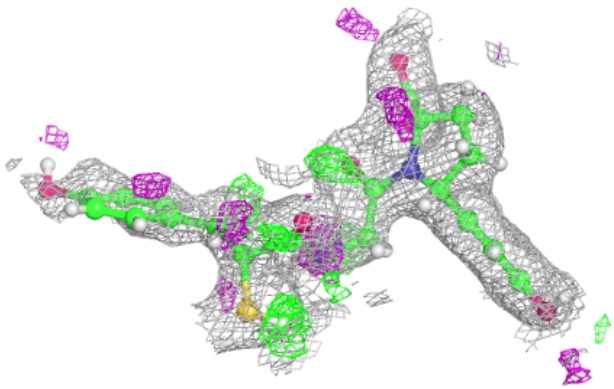


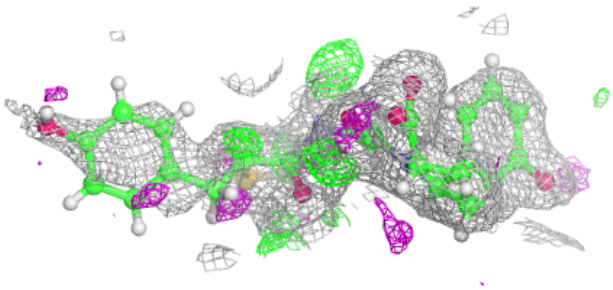


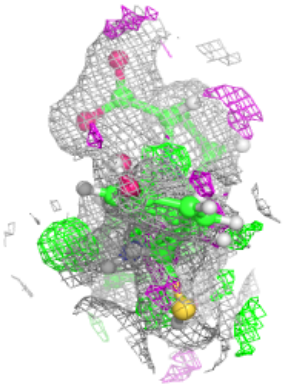


Electron density around A1IRQ A 703:

$2mF_o$-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 (i)

There are no such residues in this entry.