wwPDB X-ray Structure Validation Summary Report (i)

Oct 21, 2020 – 10:22 AM BST

PDB ID	:	6ZPT
Title	:	Crystal structure of the open conformation of S2_S'-mutant human Angiotensin-1 converting enzyme N-domain.
Authors	:	Cozier, G.E.; Acharya, K.R.
Deposited on	:	2020-07-09
Resolution	:	2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

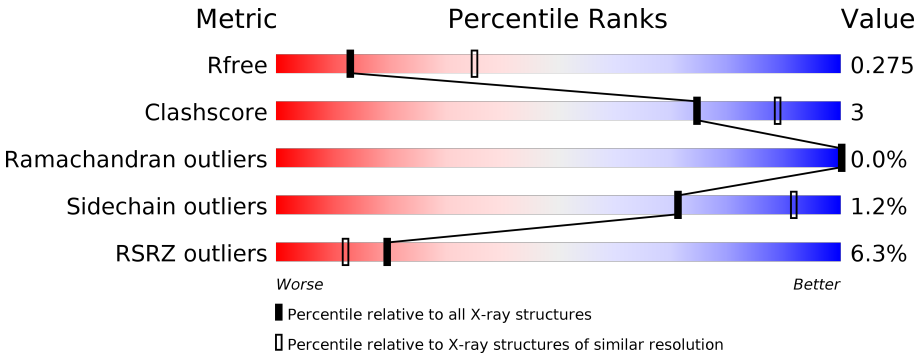
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.6

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 2.80 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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 on 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	629	6% 86% 9% ·
1	B	629	5% 89% 7% ·
1	C	629	6% 85% 9% 6%
1	D	629	8% 87% 8% ·
2	E	2	100%
3	F	2	50% 50%

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Mol	Chain	Length	Quality of chain
3	G	2	
3	H	2	

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 38972 atoms, of which 19031 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	601	Total	C	H	N	O	S	0	4	0
			9642	3171	4708	844	900	19			
1	B	601	Total	C	H	N	O	S	0	0	0
			9611	3161	4695	842	894	19			
1	C	593	Total	C	H	N	O	S	0	2	0
			9479	3111	4633	832	884	19			
1	D	601	Total	C	H	N	O	S	0	4	0
			9638	3169	4710	843	897	19			

There are 68 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	260	THR	SER	engineered mutation	UNP P12821
A	262	SER	GLU	engineered mutation	UNP P12821
A	289	GLN	ASN	engineered mutation	UNP P12821
A	354	GLU	ASP	engineered mutation	UNP P12821
A	357	VAL	SER	engineered mutation	UNP P12821
A	358	VAL	THR	engineered mutation	UNP P12821
A	369	PHE	TYR	engineered mutation	UNP P12821
A	381	GLU	ARG	engineered mutation	UNP P12821
A	431	ASP	GLU	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

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Chain	Residue	Modelled	Actual	Comment	Reference
B	131	GLN	ASN	engineered mutation	UNP P12821
B	260	THR	SER	engineered mutation	UNP P12821
B	262	SER	GLU	engineered mutation	UNP P12821
B	289	GLN	ASN	engineered mutation	UNP P12821
B	354	GLU	ASP	engineered mutation	UNP P12821
B	357	VAL	SER	engineered mutation	UNP P12821
B	358	VAL	THR	engineered mutation	UNP P12821
B	369	PHE	TYR	engineered mutation	UNP P12821
B	381	GLU	ARG	engineered mutation	UNP P12821
B	431	ASP	GLU	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
C	9	GLN	ASN	engineered mutation	UNP P12821
C	25	GLN	ASN	engineered mutation	UNP P12821
C	82	GLN	ASN	engineered mutation	UNP P12821
C	117	GLN	ASN	engineered mutation	UNP P12821
C	131	GLN	ASN	engineered mutation	UNP P12821
C	260	THR	SER	engineered mutation	UNP P12821
C	262	SER	GLU	engineered mutation	UNP P12821
C	289	GLN	ASN	engineered mutation	UNP P12821
C	354	GLU	ASP	engineered mutation	UNP P12821
C	357	VAL	SER	engineered mutation	UNP P12821
C	358	VAL	THR	engineered mutation	UNP P12821
C	369	PHE	TYR	engineered mutation	UNP P12821
C	381	GLU	ARG	engineered mutation	UNP P12821
C	431	ASP	GLU	engineered mutation	UNP P12821
C	545	ARG	GLN	engineered mutation	UNP P12821
C	576	LEU	PRO	engineered mutation	UNP P12821
C	629	LEU	-	expression tag	UNP P12821
D	9	GLN	ASN	engineered mutation	UNP P12821
D	25	GLN	ASN	engineered mutation	UNP P12821
D	82	GLN	ASN	engineered mutation	UNP P12821
D	117	GLN	ASN	engineered mutation	UNP P12821
D	131	GLN	ASN	engineered mutation	UNP P12821
D	260	THR	SER	engineered mutation	UNP P12821
D	262	SER	GLU	engineered mutation	UNP P12821
D	289	GLN	ASN	engineered mutation	UNP P12821
D	354	GLU	ASP	engineered mutation	UNP P12821
D	357	VAL	SER	engineered mutation	UNP P12821
D	358	VAL	THR	engineered mutation	UNP P12821
D	369	PHE	TYR	engineered mutation	UNP P12821

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Chain	Residue	Modelled	Actual	Comment	Reference
D	381	GLU	ARG	engineered mutation	UNP P12821
D	431	ASP	GLU	engineered mutation	UNP P12821
D	545	ARG	GLN	engineered mutation	UNP P12821
D	576	LEU	PRO	engineered mutation	UNP P12821
D	629	LEU	-	expression tag	UNP P12821

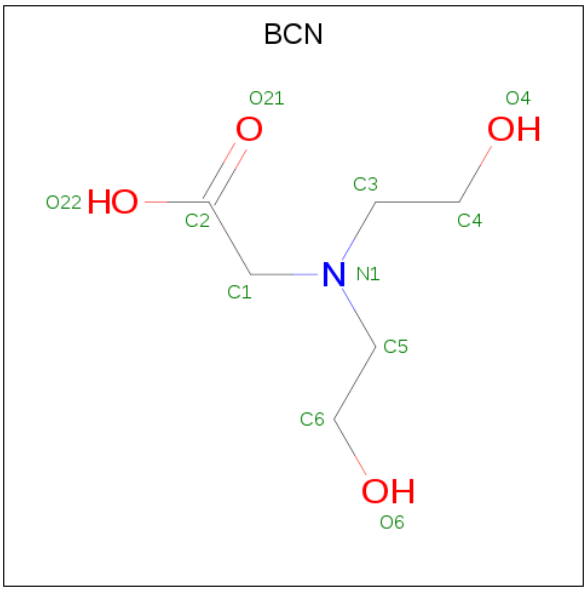
- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	2	Total	C	H	N	O	0	0	0
			55	16	27	2	10			

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

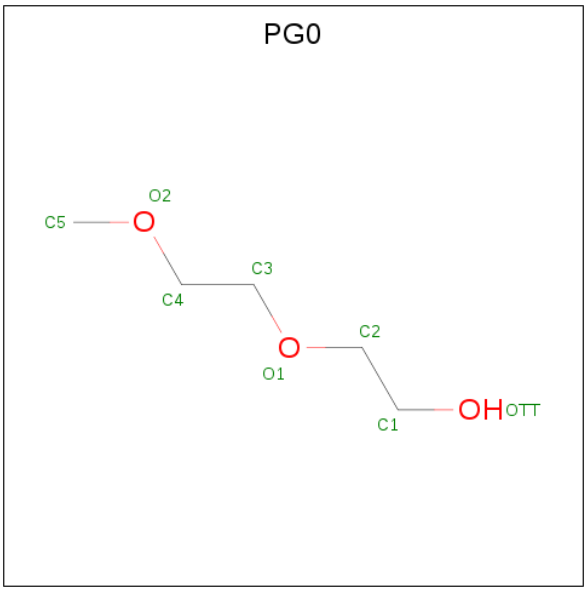
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	2	Total	C	H	N	O	0	0	0
			48	14	24	1	9			
3	G	2	Total	C	H	N	O	0	0	0
			48	14	24	1	9			
3	H	2	Total	C	H	N	O	0	0	0
			48	14	24	1	9			

- Molecule 4 is BICINE (three-letter code: BCN) (formula: $C_6H_{13}NO_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	0	0
			23	6	12	1	4		
4	B	1	Total	C	H	N	O	0	0
			23	6	12	1	4		
4	C	1	Total	C	H	N	O	0	0
			23	6	12	1	4		
4	D	1	Total	C	H	N	O	0	0
			23	6	12	1	4		

- Molecule 5 is 2-(2-METHOXYETHOXY)ETHANOL (three-letter code: PG0) (formula: $C_5H_{12}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C H O 20 5 12 3	0	0
5	A	1	Total C H O 40 10 24 6	0	1
5	B	1	Total C H O 20 5 12 3	0	0

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

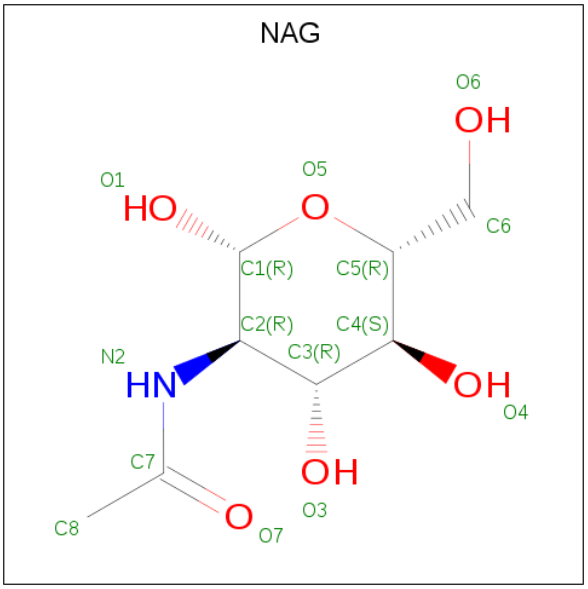
- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total Cl 1 1	0	0
7	A	1	Total Cl 1 1	0	0
7	D	1	Total Cl 1 1	0	0
7	C	1	Total Cl 1 1	0	0

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

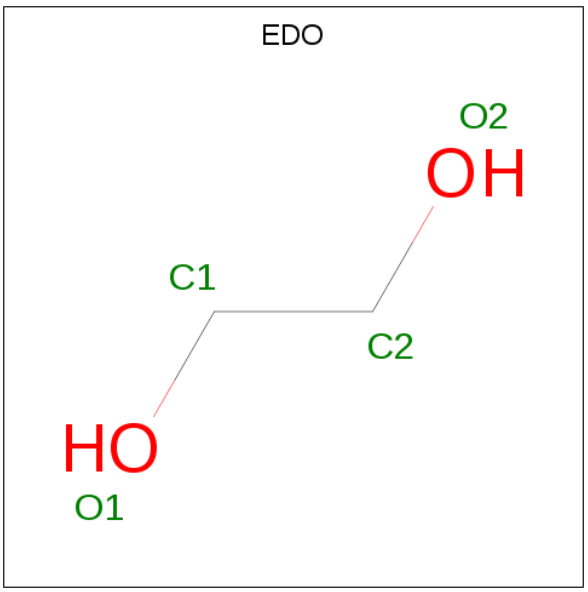
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total Ca 1 1	0	0
8	A	1	Total Ca 1 1	0	0
8	D	1	Total Ca 1 1	0	0
8	C	1	Total Ca 1 1	0	0

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
9	B	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
9	C	1	Total	C	H	N	O	0	0
			28	8	14	1	5		

- Molecule 10 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 11 is water.

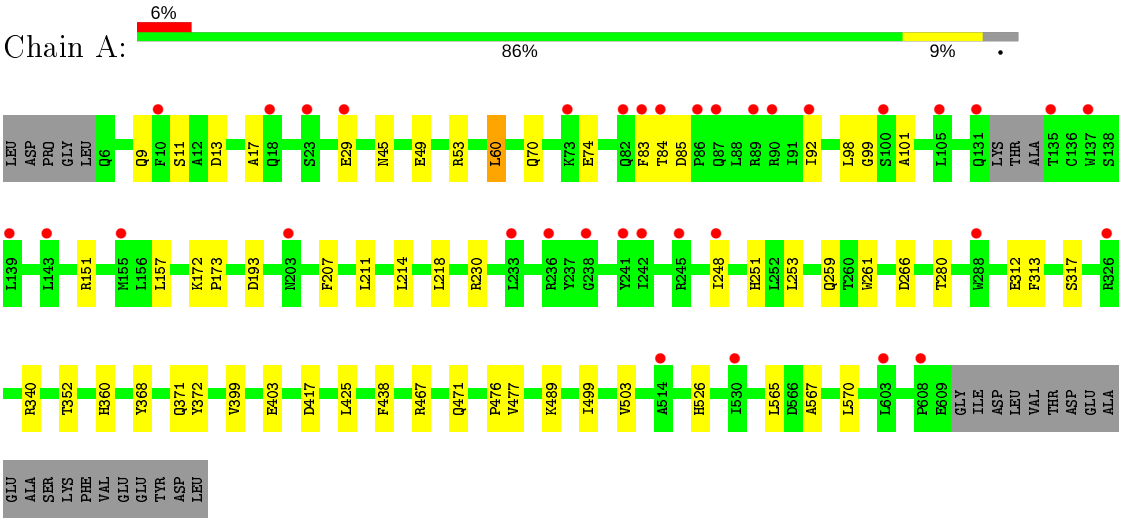
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	21	Total	O	0	0
			21	21		
11	B	10	Total	O	0	0
			10	10		
11	C	16	Total	O	0	0
			16	16		
11	D	8	Total	O	0	0
			8	8		

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.

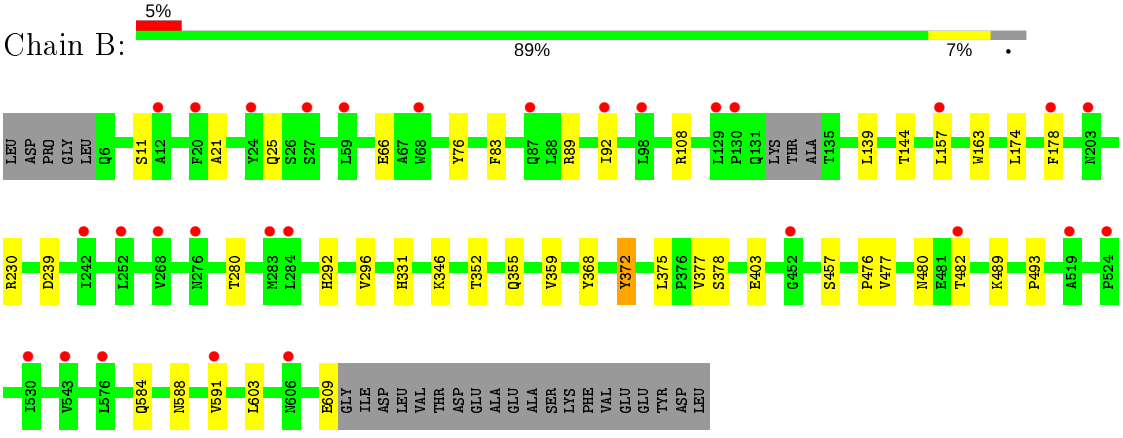
- Molecule 1: Angiotensin-converting enzyme

Chain A:



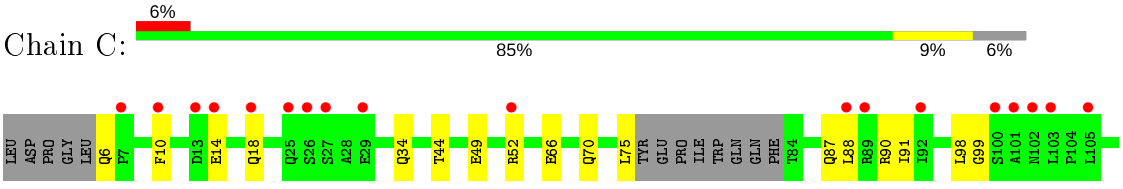
- Molecule 1: Angiotensin-converting enzyme

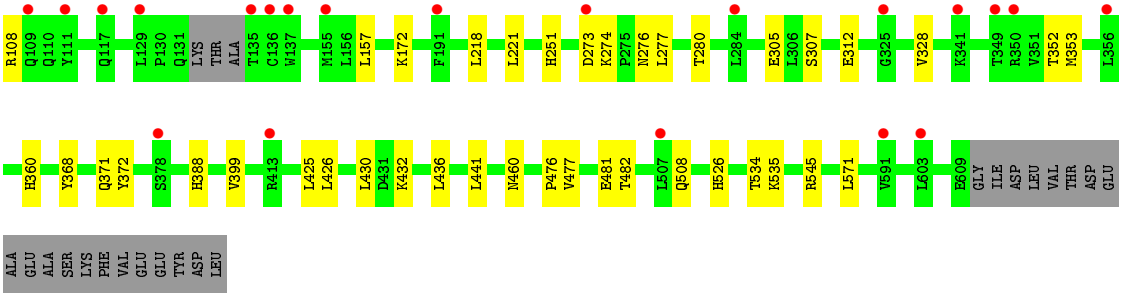
Chain B:



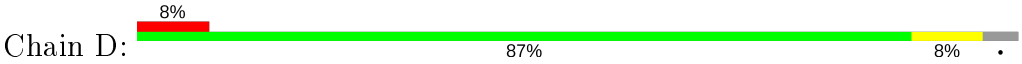
- Molecule 1: Angiotensin-converting enzyme

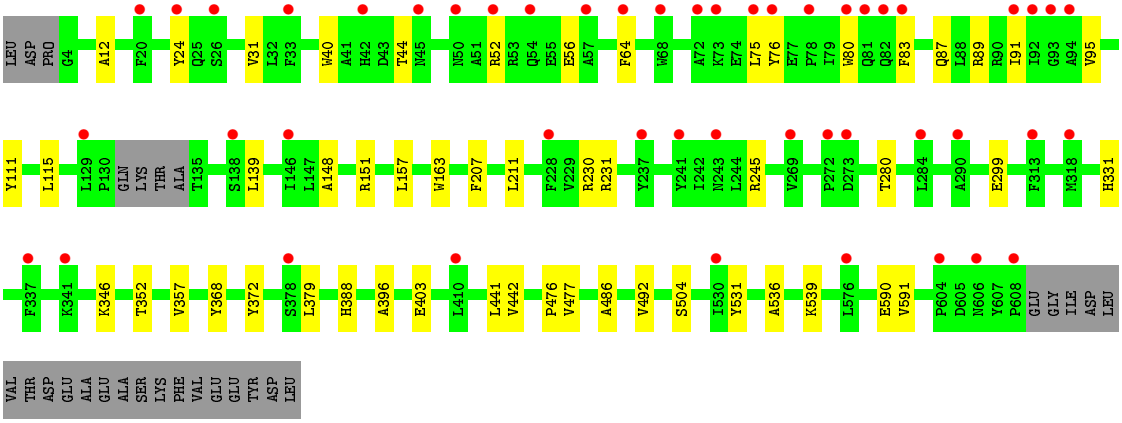
Chain C:



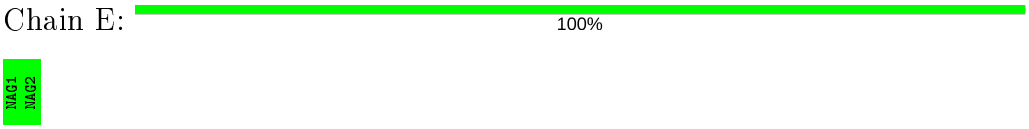


• Molecule 1: Angiotensin-converting enzyme



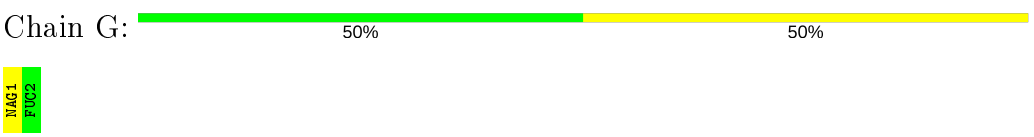


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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

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



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

Chain H:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	73.65Å 99.26Å 127.98Å 98.63° 89.63° 111.15°	Depositor
Resolution (Å)	69.05 – 2.80 91.40 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.5 (69.05-2.80) 98.9 (91.40-2.80)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.44 (at 2.82Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.224 , 0.278 0.222 , 0.275	Depositor DCC
R_{free} test set	2047 reflections (2.52%)	wwPDB-VP
Wilson B-factor (Å^2)	53.5	Xtriage
Anisotropy	0.804	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 47.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.059 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	38972	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.01% 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: ZN, NAG, CL, BCN, EDO, FUC, PG0, CA

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	0.25	0/5102	0.39	0/6950
1	B	0.25	0/5071	0.39	0/6908
1	C	0.25	0/5000	0.40	0/6808
1	D	0.25	0/5096	0.38	0/6942
All	All	0.25	0/20269	0.39	0/27608

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	4934	4708	4698	39	0
1	B	4916	4695	4695	23	0
1	C	4846	4633	4627	34	0
1	D	4928	4710	4699	28	0
2	E	28	27	25	0	0
3	F	24	24	22	2	0
3	G	24	24	22	1	0
3	H	24	24	22	0	0
4	A	11	12	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	11	12	10	0	0
4	C	11	12	11	0	0
4	D	11	12	11	0	0
5	A	24	36	36	1	0
5	B	8	12	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
9	B	28	28	26	0	0
9	C	14	14	13	0	0
10	B	4	6	6	0	0
10	C	16	24	24	0	0
10	D	12	18	18	0	0
11	A	21	0	0	1	0
11	B	10	0	0	0	0
11	C	16	0	0	1	0
11	D	8	0	0	0	0
All	All	19941	19031	18987	123	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.

The worst 5 of 123 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:B:331:HIS:O	1:B:346:LYS:NZ	2.07	0.87
1:D:157:LEU:HD11	1:D:477:VAL:HG13	1.66	0.78
1:D:40:TRP:O	1:D:44:THR:OG1	2.01	0.78
1:C:157:LEU:HD11	1:C:477:VAL:HG13	1.66	0.78
1:C:371:GLN:OE1	1:C:545:ARG:NH1	2.16	0.77

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	601/629 (96%)	578 (96%)	22 (4%)	1 (0%)	47 78
1	B	597/629 (95%)	575 (96%)	22 (4%)	0	100 100
1	C	589/629 (94%)	572 (97%)	17 (3%)	0	100 100
1	D	601/629 (96%)	575 (96%)	26 (4%)	0	100 100
All	All	2388/2516 (95%)	2300 (96%)	87 (4%)	1 (0%)	100 100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
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	521/541 (96%)	515 (99%)	6 (1%)	71 92
1	B	518/541 (96%)	512 (99%)	6 (1%)	71 92
1	C	511/541 (94%)	504 (99%)	7 (1%)	67 90
1	D	520/541 (96%)	515 (99%)	5 (1%)	76 93
All	All	2070/2164 (96%)	2046 (99%)	24 (1%)	71 92

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	372	TYR
1	C	251	HIS
1	D	388	HIS
1	B	457	SER
1	C	34	GLN

Some 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)

8 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	E	1	1,2	14,14,15	0.29	0	17,19,21	0.53	0
2	NAG	E	2	2	14,14,15	0.24	0	17,19,21	0.49	0
3	NAG	F	1	1,3	14,14,15	0.30	0	17,19,21	1.06	2 (11%)
3	FUC	F	2	3	10,10,11	0.67	0	14,14,16	0.79	0
3	NAG	G	1	1,3	14,14,15	0.19	0	17,19,21	0.55	0
3	FUC	G	2	3	10,10,11	0.72	0	14,14,16	0.94	0
3	NAG	H	1	1,3	14,14,15	0.47	0	17,19,21	0.36	0
3	FUC	H	2	3	10,10,11	0.95	0	14,14,16	0.85	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	E	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	4/6/23/26	0/1/1/1
3	FUC	F	2	3	-	-	0/1/1/1
3	NAG	G	1	1,3	-	3/6/23/26	0/1/1/1
3	FUC	G	2	3	-	-	0/1/1/1
3	NAG	H	1	1,3	-	0/6/23/26	0/1/1/1
3	FUC	H	2	3	-	-	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	1	NAG	C2-N2-C7	3.23	127.50	122.90
3	H	2	FUC	O2-C2-C1	2.31	113.87	109.15
3	F	1	NAG	C1-C2-N2	2.09	114.06	110.49

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

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

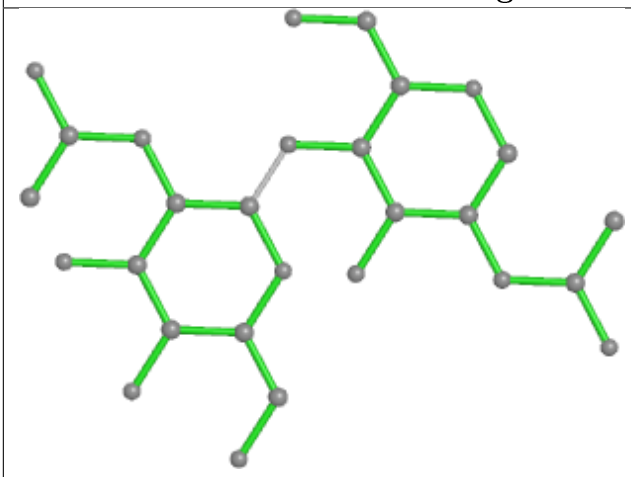
There are no ring outliers.

2 monomers are involved in 3 short contacts:

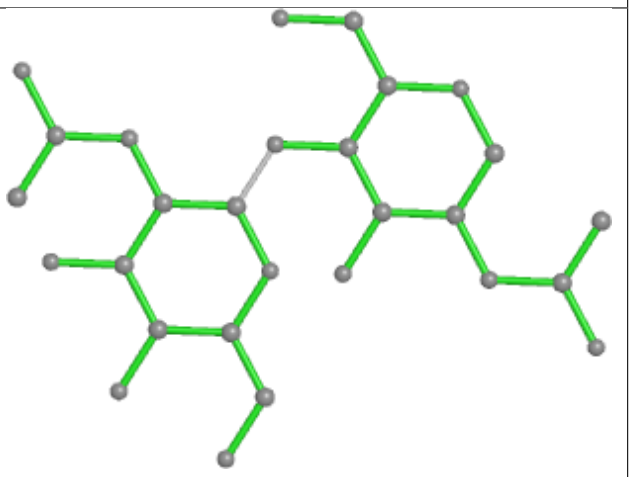
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	1	NAG	1	0
3	F	1	NAG	2	0

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

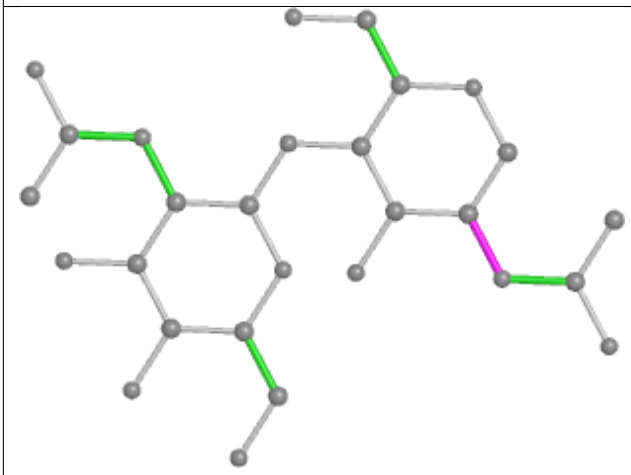
Oligosaccharide Chain E



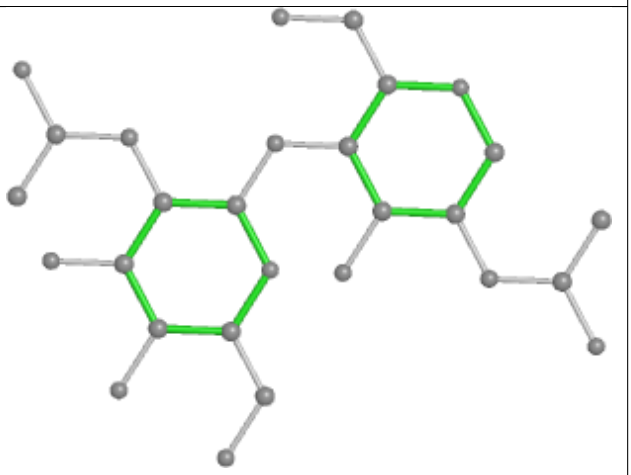
Bond lengths



Bond angles

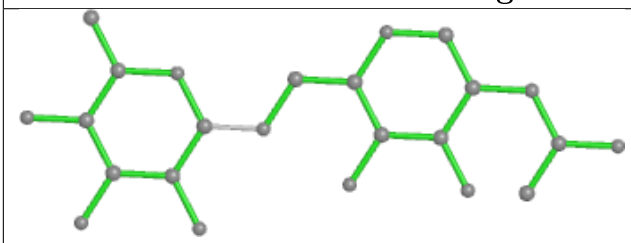


Torsions

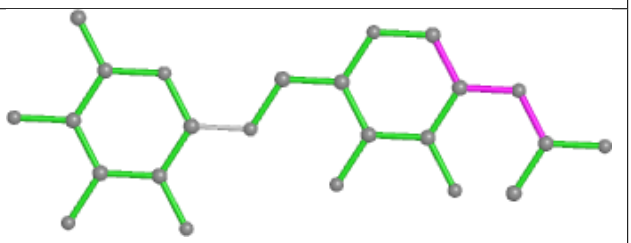


Rings

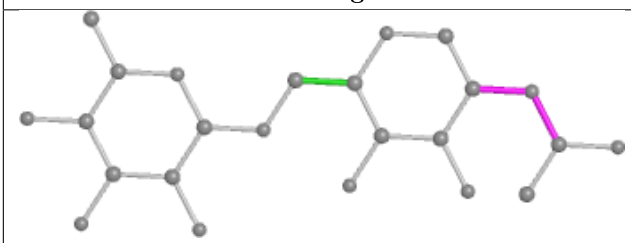
Oligosaccharide Chain F



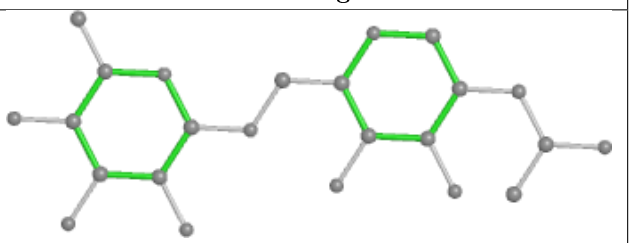
Bond lengths



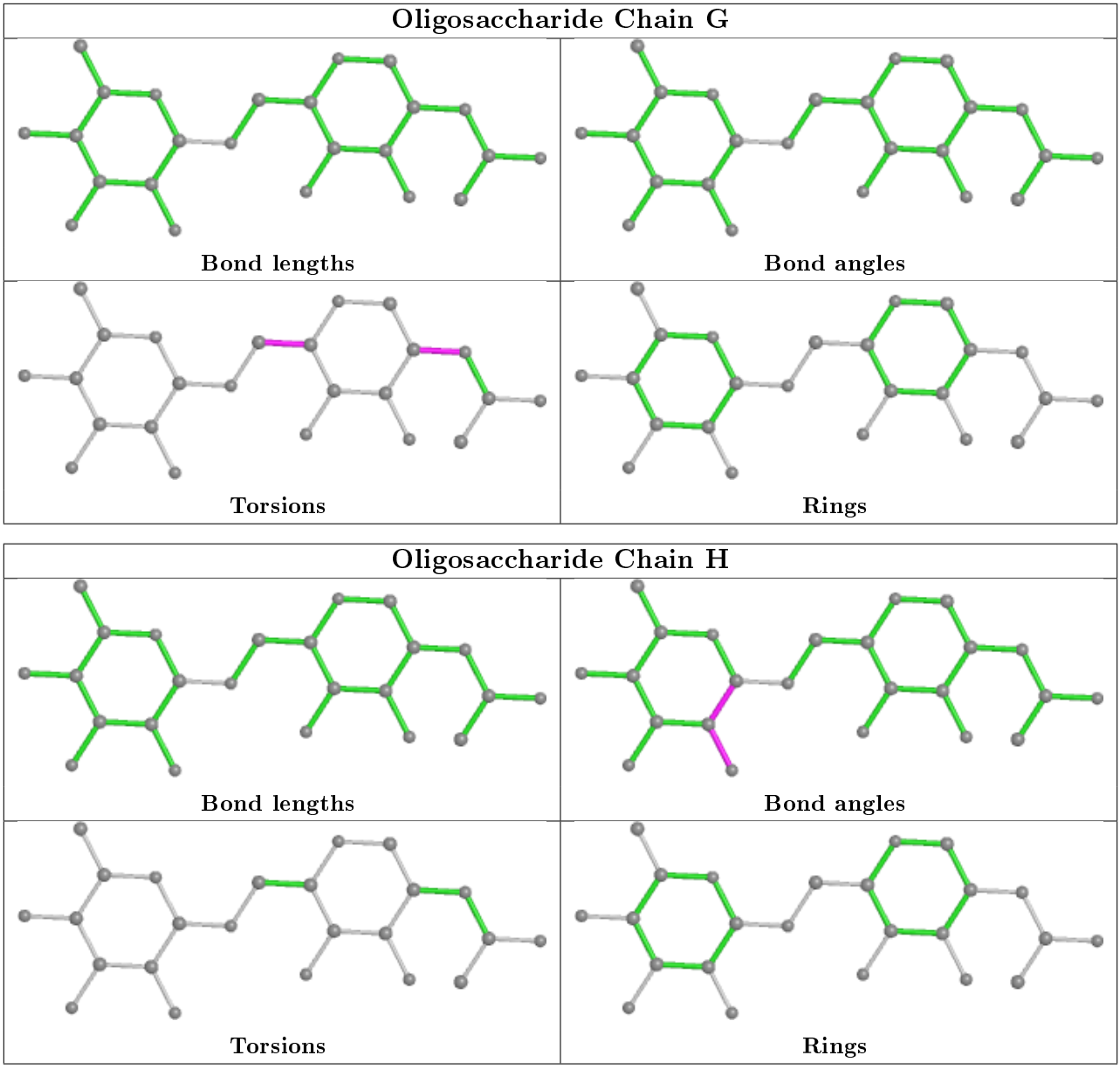
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

Of 31 ligands modelled in this entry, 12 are monoatomic - leaving 19 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	PG0	B	705	-	7,7,7	0.48	0	6,6,6	0.30	0
4	BCN	B	703	8	7,10,10	0.67	0	8,11,11	1.27	1 (12%)
4	BCN	D	703	8	7,10,10	0.68	0	8,11,11	1.08	1 (12%)
4	BCN	A	701	8	7,10,10	0.70	0	8,11,11	1.04	1 (12%)
4	BCN	C	706	8	7,10,10	0.69	0	8,11,11	1.09	1 (12%)
10	EDO	C	704	-	3,3,3	0.48	0	2,2,2	0.27	0
9	NAG	C	701	1	14,14,15	0.29	0	17,19,21	0.47	0
5	PG0	A	703[A]	-	7,7,7	0.49	0	6,6,6	0.22	0
10	EDO	B	704	-	3,3,3	0.46	0	2,2,2	0.45	0
10	EDO	C	703	-	3,3,3	0.48	0	2,2,2	0.25	0
10	EDO	D	704	-	3,3,3	0.41	0	2,2,2	0.50	0
5	PG0	A	703[B]	-	7,7,7	0.49	0	6,6,6	0.15	0
9	NAG	B	702	1	14,14,15	0.34	0	17,19,21	0.46	0
10	EDO	C	702	-	3,3,3	0.42	0	2,2,2	0.46	0
10	EDO	C	705	-	3,3,3	0.48	0	2,2,2	0.24	0
9	NAG	B	701	1	14,14,15	0.29	0	17,19,21	0.70	1 (5%)
10	EDO	D	702	-	3,3,3	0.46	0	2,2,2	0.37	0
5	PG0	A	702	-	7,7,7	0.47	0	6,6,6	0.23	0
10	EDO	D	701	-	3,3,3	0.48	0	2,2,2	0.28	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	PG0	B	705	-	-	3/5/5/5	-
4	BCN	B	703	8	-	0/8/10/10	-
4	BCN	D	703	8	-	1/8/10/10	-
4	BCN	A	701	8	-	0/8/10/10	-
4	BCN	C	706	8	-	0/8/10/10	-
10	EDO	C	704	-	-	0/1/1/1	-
9	NAG	C	701	1	-	4/6/23/26	0/1/1/1
5	PG0	A	703[A]	-	-	2/5/5/5	-
10	EDO	B	704	-	-	1/1/1/1	-
10	EDO	C	703	-	-	0/1/1/1	-
10	EDO	D	704	-	-	0/1/1/1	-
5	PG0	A	703[B]	-	-	0/5/5/5	-
9	NAG	B	702	1	-	2/6/23/26	0/1/1/1
10	EDO	C	702	-	-	0/1/1/1	-
10	EDO	C	705	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	B	701	1	-	2/6/23/26	0/1/1/1
10	EDO	D	702	-	-	0/1/1/1	-
5	PG0	A	702	-	-	2/5/5/5	-
10	EDO	D	701	-	-	0/1/1/1	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	703	BCN	C2-C1-N1	-2.82	109.47	113.48
9	B	701	NAG	C1-O5-C5	2.49	115.57	112.19
4	C	706	BCN	C2-C1-N1	-2.29	110.22	113.48
4	A	701	BCN	C2-C1-N1	-2.21	110.33	113.48
4	D	703	BCN	C2-C1-N1	-2.13	110.45	113.48

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	C	701	NAG	O5-C5-C6-O6
9	C	701	NAG	C4-C5-C6-O6
9	B	702	NAG	O5-C5-C6-O6
9	B	702	NAG	C4-C5-C6-O6
5	B	705	PG0	OTT-C1-C2-O1

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	703[A]	PG0	1	0

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	601/629 (95%)	0.71	35 (5%)	23	15	40, 59, 90, 112	0
1	B	601/629 (95%)	0.72	29 (4%)	30	21	39, 62, 96, 114	0
1	C	593/629 (94%)	0.72	39 (6%)	18	11	38, 61, 95, 113	0
1	D	601/629 (95%)	0.73	48 (7%)	12	6	41, 62, 104, 124	0
All	All	2396/2516 (95%)	0.72	151 (6%)	20	12	38, 61, 96, 124	0

The worst 5 of 151 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	89	ARG	7.8
1	C	92	ILE	7.0
1	C	25	GLN	6.5
1	A	82	GLN	5.6
1	C	101	ALA	5.3

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, 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	2	14/15	0.81	0.15	94,114,136,137	0
3	NAG	H	1	14/15	0.82	0.23	51,69,92,111	0

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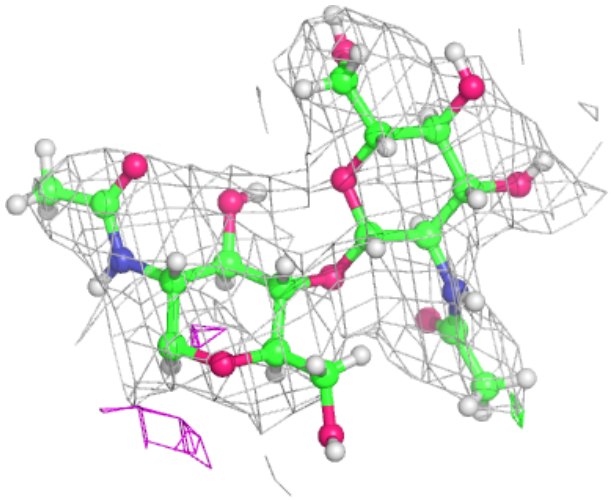
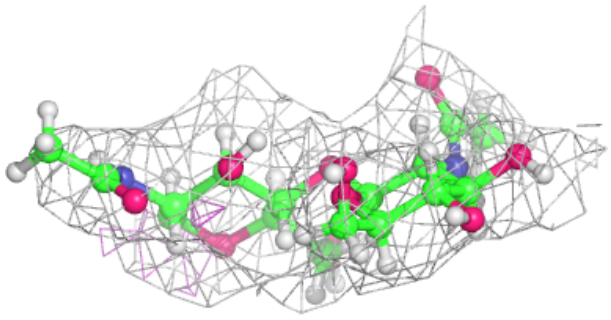
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	FUC	H	2	10/11	0.82	0.34	67,85,102,106	0
3	FUC	G	2	10/11	0.83	0.32	79,95,108,115	0
3	FUC	F	2	10/11	0.84	0.28	68,85,101,116	0
3	NAG	G	1	14/15	0.84	0.28	68,82,98,101	0
2	NAG	E	1	14/15	0.85	0.23	72,92,113,117	0
3	NAG	F	1	14/15	0.86	0.21	58,71,82,86	0

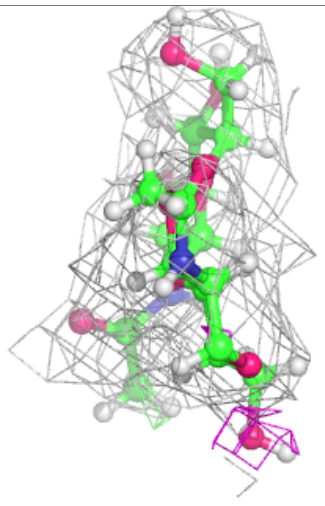
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain E:

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

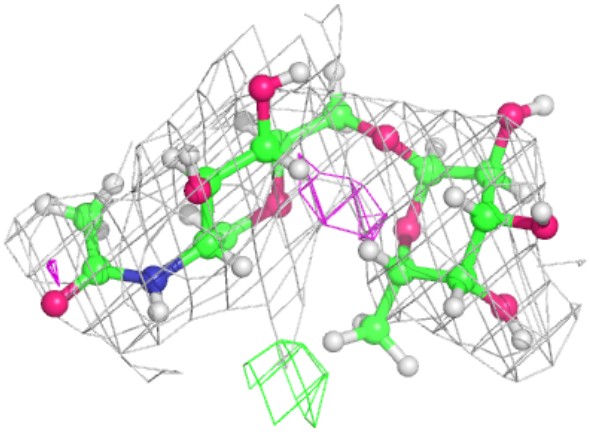


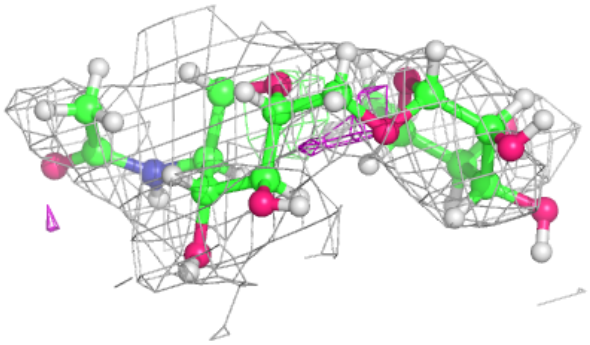


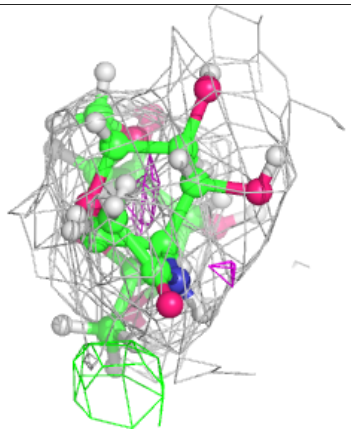


Electron density around Chain F:

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

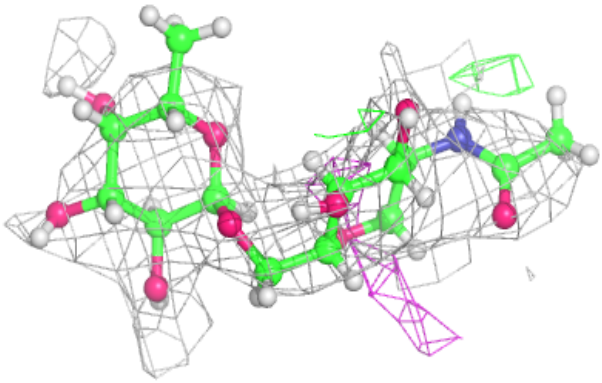


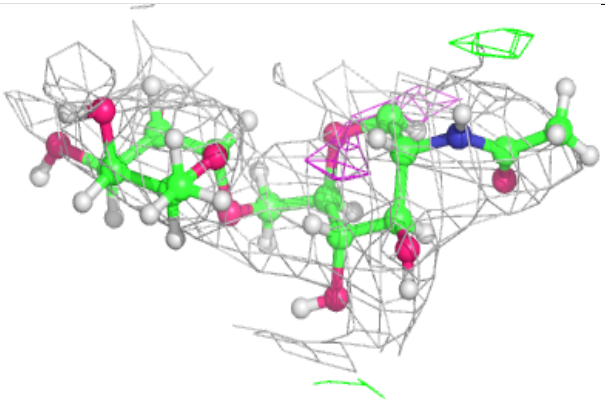


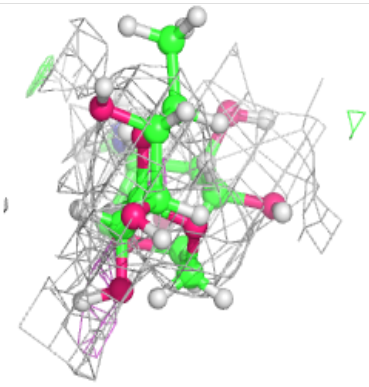


Electron density around Chain G:

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

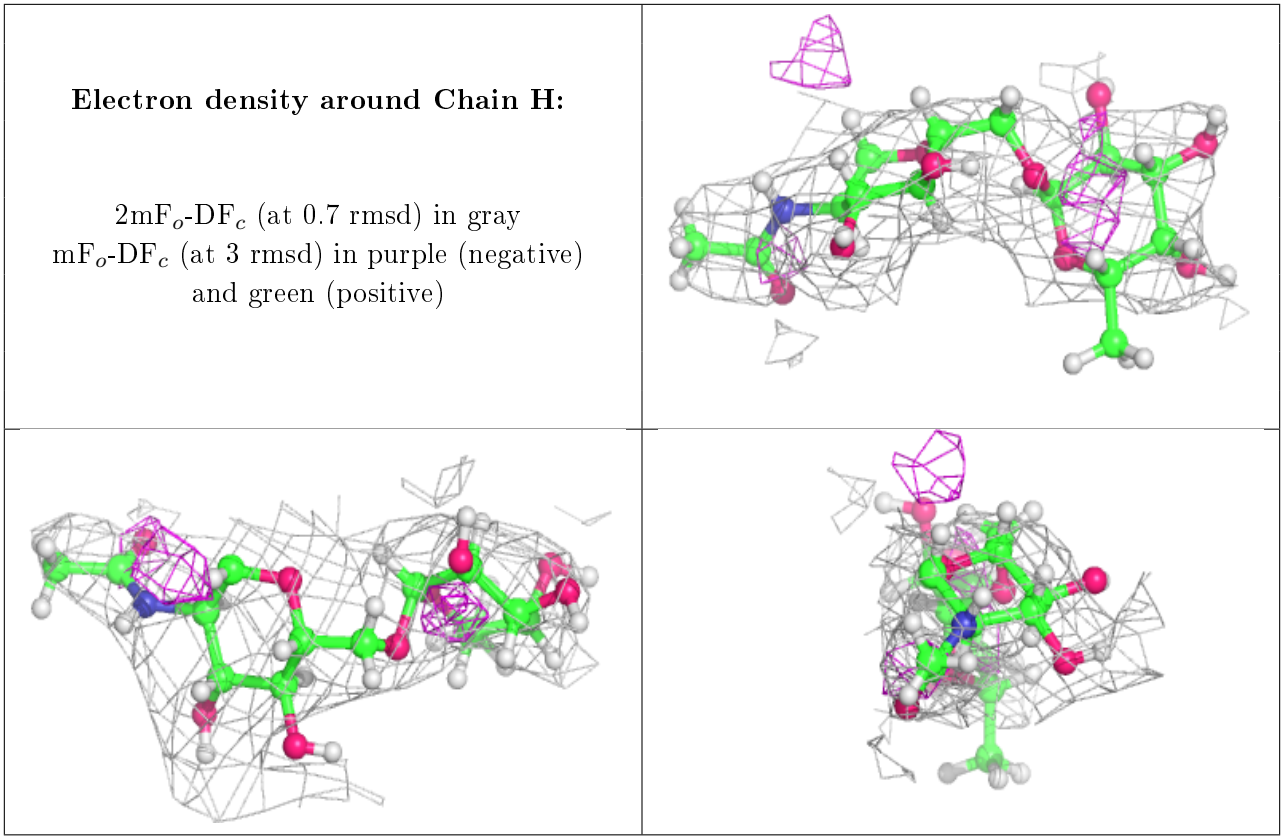






Electron density around Chain H:

$2mF_o$-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
9	NAG	C	701	14/15	0.49	0.37	96,112,132,134	0
10	EDO	D	702	4/4	0.60	0.24	57,70,84,84	0
5	PG0	A	703[B]	8/8	0.61	0.34	52,62,74,76	20
5	PG0	A	703[A]	8/8	0.61	0.34	52,63,74,75	20
10	EDO	C	705	4/4	0.65	0.24	59,71,82,82	0
10	EDO	C	704	4/4	0.67	0.24	60,72,87,87	0
9	NAG	B	701	14/15	0.67	0.24	85,99,116,119	0
10	EDO	D	701	4/4	0.71	0.28	58,70,80,83	0
9	NAG	B	702	14/15	0.78	0.19	56,76,98,104	0
10	EDO	C	703	4/4	0.80	0.29	61,73,88,88	0
8	CA	C	709	1/1	0.80	0.25	69,69,69,69	0
4	BCN	A	701	11/11	0.83	0.23	48,64,70,83	0
5	PG0	A	702	8/8	0.84	0.28	58,75,77,77	0
4	BCN	C	706	11/11	0.85	0.22	57,69,80,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
10	EDO	C	702	4/4	0.85	0.18	60,72,75,84	0
10	EDO	B	704	4/4	0.87	0.21	67,80,83,93	0
7	CL	D	706	1/1	0.89	0.16	50,50,50,50	0
5	PG0	B	705	8/8	0.89	0.17	58,76,87,87	0
8	CA	B	708	1/1	0.90	0.11	60,60,60,60	0
4	BCN	D	703	11/11	0.90	0.22	49,59,73,76	0
10	EDO	D	704	4/4	0.91	0.16	57,68,77,84	0
7	CL	B	707	1/1	0.92	0.29	60,60,60,60	0
4	BCN	B	703	11/11	0.92	0.23	50,61,69,73	0
8	CA	A	706	1/1	0.93	0.09	55,55,55,55	0
8	CA	D	707	1/1	0.94	0.23	58,58,58,58	0
7	CL	A	705	1/1	0.96	0.11	54,54,54,54	0
7	CL	C	708	1/1	0.98	0.34	44,44,44,44	0
6	ZN	C	707	1/1	0.98	0.22	44,44,44,44	0
6	ZN	D	705	1/1	0.98	0.25	57,57,57,57	0
6	ZN	A	704	1/1	0.98	0.23	37,37,37,37	0
6	ZN	B	706	1/1	1.00	0.25	49,49,49,49	0

6.5 Other polymers

There are no such residues in this entry.