Full wwPDB X-ray Structure Validation Report (i)

Jan 4, 2024 – 05:00 pm GMT

PDB ID	:	5AM8
Title	:	Crystal structure of the Angiotensin-1 converting enzyme N-domain in complex with amyloid-beta 4-10
Authors	:	Masuyer, G.; Larmuth, K.M.; Douglas, R.G.; Sturrock, E.D.; Acharya, K.R.
Deposited on	:	2015-03-10
Resolution	:	1.90 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 (i) 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 (i)) were used in the production of this report:

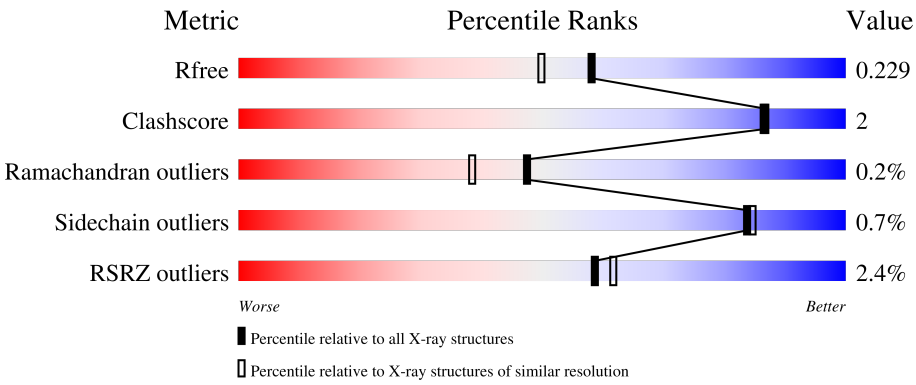
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	629	2% 91% 5% •
1	B	629	3% 91% • • •
1	C	629	% 91% 6% •
1	D	629	3% 92% 6% •
2	P	7	29% 14% 57%

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Mol	Chain	Length	Quality of chain
2	Q	7	14% 14% 29% 57%
2	R	7	29% 14% 57%
2	S	7	43% 57%
3	E	2	100%
3	F	2	50% 50%
3	H	2	50% 50%
3	K	2	100%
4	G	2	50% 50%
4	J	2	50% 50%
5	I	3	100%
6	L	4	25% 75%
7	M	4	100%

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 22316 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ANGIOTENSIN-CONVERTING ENZYME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	604	4939	3173	849	898	19	0	1	0
1	B	606	4950	3179	852	900	19	0	1	0
1	C	606	4959	3186	852	902	19	0	1	0
1	D	612	5029	3229	867	914	19	0	5	0

There are 32 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	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	ARG	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	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	ARG	engineered mutation	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	289	GLN	ASN	engineered mutation	UNP P12821

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Chain	Residue	Modelled	Actual	Comment	Reference
C	545	ARG	GLN	engineered mutation	UNP P12821
C	576	LEU	PRO	engineered mutation	UNP P12821
C	629	LEU	ARG	engineered mutation	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	289	GLN	ASN	engineered mutation	UNP P12821
D	545	ARG	GLN	engineered mutation	UNP P12821
D	576	LEU	PRO	engineered mutation	UNP P12821
D	629	LEU	ARG	engineered mutation	UNP P12821

- Molecule 2 is a protein called BETA-AMYLOID PROTEIN 42.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	P	3	15	7	3	5	0	0	1
2	Q	3	15	7	3	5	0	0	1
2	R	3	15	7	3	5	0	0	1
2	S	3	15	7	3	5	0	0	1

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

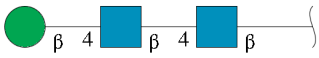
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	E	2	28	16	2	10	0	0	0
3	F	2	28	16	2	10	0	0	0
3	H	2	28	16	2	10	0	0	0
3	K	2	28	16	2	10	0	0	0

- Molecule 4 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-bet

a-D-glucopyranose.

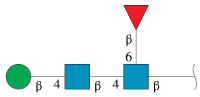
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	G	2	24	14	1	9	0	0	0
4	J	2	24	14	1	9	0	0	0

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



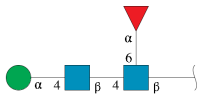
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	I	3	39	22	2	15	0	0	0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
6	L	4	49	28	2	19	0	0	0

- Molecule 7 is an oligosaccharide called alpha-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
			Total	C	N	O			
7	M	4	49	28	2	19	0	0	0

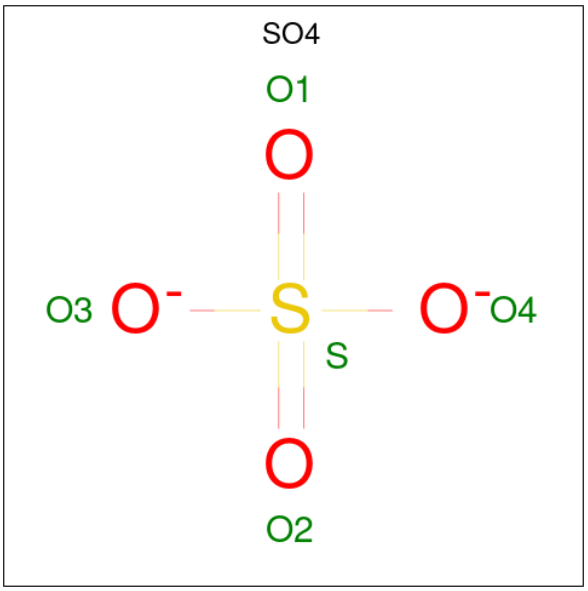
- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 9 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

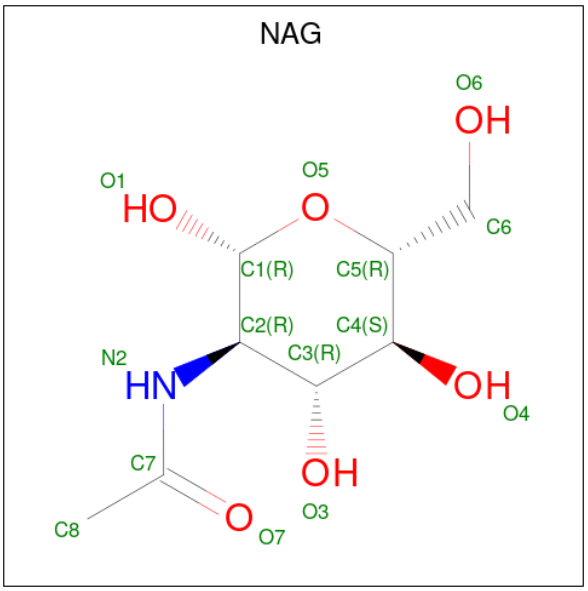
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
9	A	1	1	1	0	0
9	B	1	1	1	0	0
9	C	1	1	1	0	0
9	D	1	1	1	0	0

- Molecule 10 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



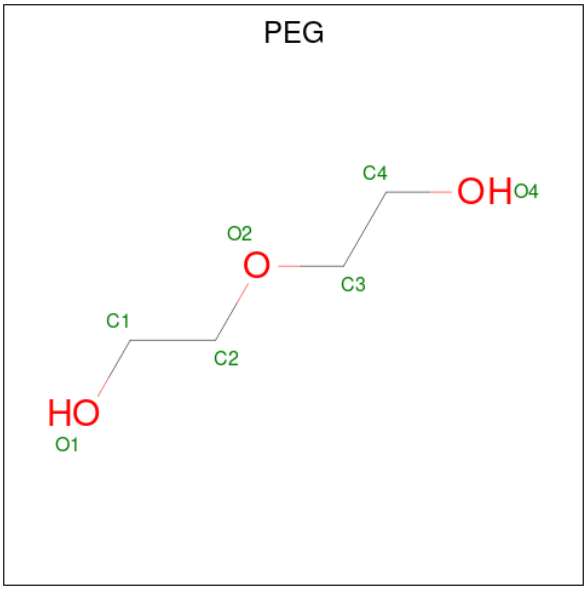
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total O S 5 4 1	0	0
10	B	1	Total O S 5 4 1	0	0
10	C	1	Total O S 5 4 1	0	0
10	D	1	Total O S 5 4 1	0	0

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 12 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

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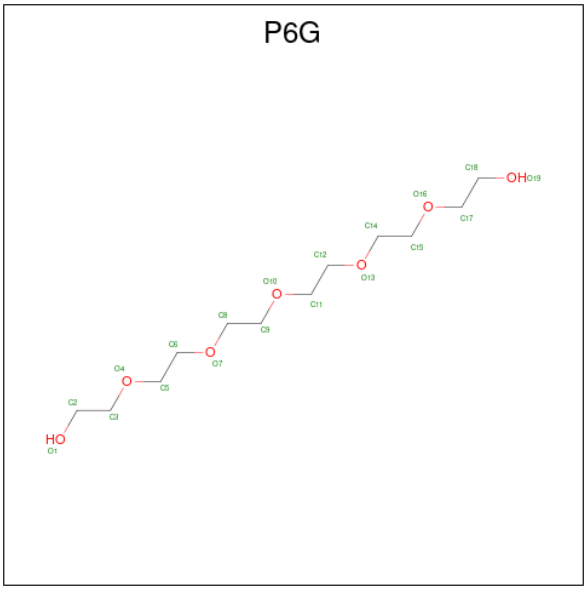
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
12	B	1	7	4	3	0	0
12	C	1	7	4	3	0	0
12	C	1	7	4	3	0	0
12	C	1	7	4	3	0	0
12	C	1	7	4	3	0	0
12	D	1	7	4	3	0	0
12	D	1	7	4	3	0	0
12	D	1	7	4	3	0	0
12	D	1	7	4	3	0	0
12	D	1	7	4	3	0	0

- Molecule 13 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: $C_{12}H_{26}O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
13	A	1	19	12	7	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
13	B	1	19	12	7	0	0
			Total	C	O		
13	D	1	19	12	7	0	0

- Molecule 14 is water.

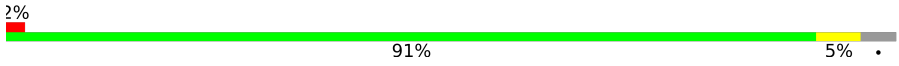
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
14	A	391	391	391	0	0
			Total	O		
14	B	458	458	458	0	0
			Total	O		
14	C	513	513	513	0	0
			Total	O		
14	D	464	464	464	0	0
			Total	O		
14	R	1	1	1	0	0
			Total	O		
14	S	2	2	2	0	0

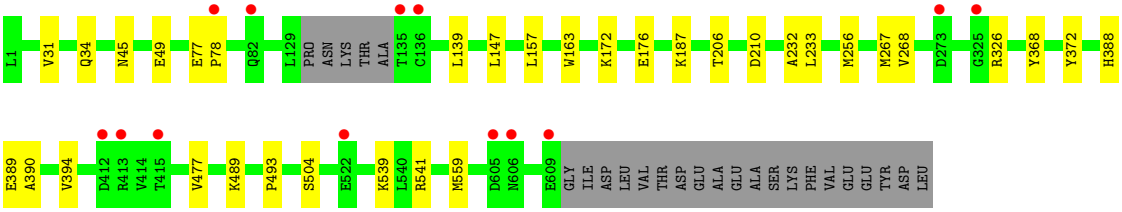
3 Residue-property plots (i)

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

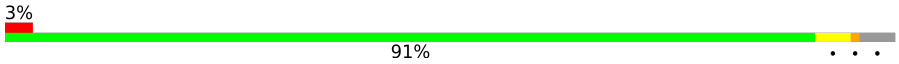
Chain A:

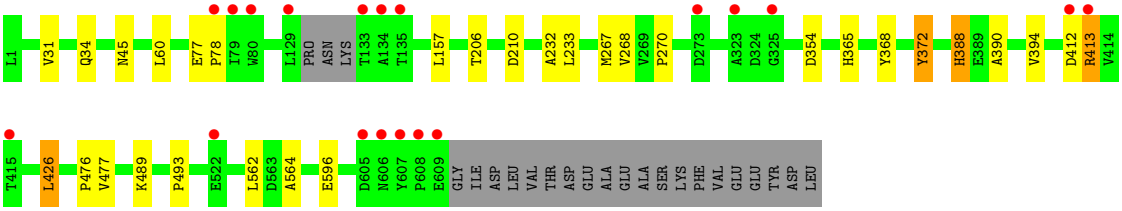




• Molecule 1: ANGIOTENSIN-CONVERTING ENZYME

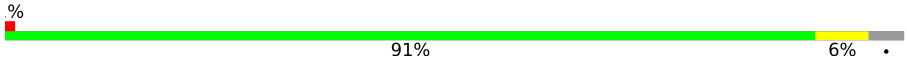
Chain B:

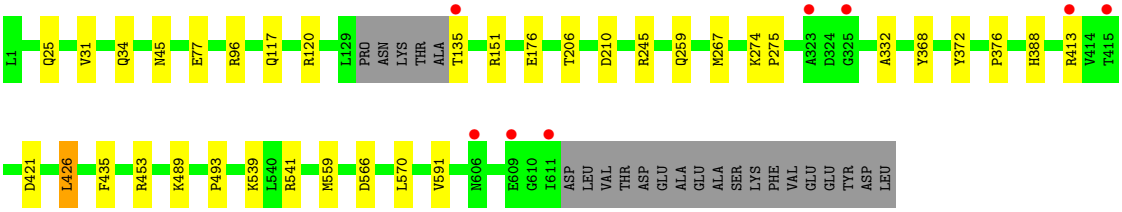




• Molecule 1: ANGIOTENSIN-CONVERTING ENZYME

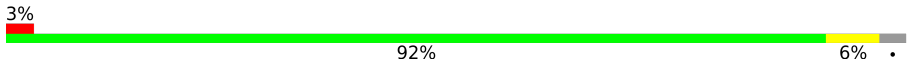
Chain C:

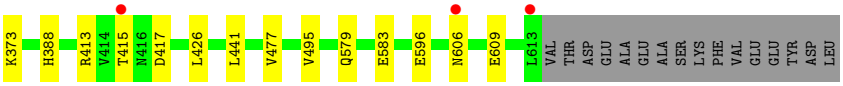




• Molecule 1: ANGIOTENSIN-CONVERTING ENZYME

Chain D:



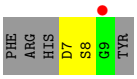


• Molecule 2: BETA-AMYLOID PROTEIN 42

Chain P: 29% 14% 57%

• Molecule 2: BETA-AMYLOID PROTEIN 42

Chain Q: 14% 14% 29% 57%



• Molecule 2: BETA-AMYLOID PROTEIN 42

Chain R: 29% 14% 57%

• Molecule 2: BETA-AMYLOID PROTEIN 42

Chain S: 43% 57%

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E: 100%

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F: 50% 50%

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H: 50% 50%

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K: 100%

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

Chain G: 50% 50%

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

Chain J: 50% 50%

• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I: 100%

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

Chain L: 25% 75%

• Molecule 7: alpha-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 M: 100%

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	73.45Å 101.76Å 114.36Å 85.23° 86.07° 81.45°	Depositor
Resolution (Å)	113.78 – 1.90 36.81 – 1.90	Depositor EDS
% Data completeness (in resolution range)	93.2 (113.78-1.90) 93.2 (36.81-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.63 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.185 , 0.224 0.194 , 0.229	Depositor DCC
R_{free} test set	12020 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	20.0	Xtriage
Anisotropy	0.428	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 46.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	22316	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.74 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.0333e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, FUL, PEG, P6G, FUC, SO4, ZN, CL, MAN, BMA

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	0.47	0/5098	0.64	1/6944 (0.0%)
1	B	0.50	0/5108	0.65	1/6957 (0.0%)
1	C	0.51	0/5117	0.67	2/6968 (0.0%)
1	D	0.51	0/5195	0.65	0/7075
2	P	1.41	0/14	1.12	0/18
2	Q	1.60	1/14 (7.1%)	0.97	0/18
2	R	1.33	0/14	1.25	0/18
2	S	1.43	0/14	0.92	0/18
All	All	0.50	1/20574 (0.0%)	0.65	4/28016 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	8	SER	C-N	-5.48	1.23	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	541	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	C	426	LEU	CA-CB-CG	-5.83	101.90	115.30
1	B	426	LEU	CA-CB-CG	-5.13	103.50	115.30
1	C	566	ASP	CB-CG-OD1	5.12	122.91	118.30

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	4939	0	4712	15	0
1	B	4950	0	4725	21	0
1	C	4959	0	4745	21	0
1	D	5029	0	4808	22	0
2	P	15	0	8	1	0
2	Q	15	0	8	1	0
2	R	15	0	8	1	0
2	S	15	0	8	0	0
3	E	28	0	25	1	0
3	F	28	0	25	0	0
3	H	28	0	25	0	0
3	K	28	0	25	0	0
4	G	24	0	22	1	0
4	J	24	0	22	1	0
5	I	39	0	34	0	0
6	L	49	0	43	0	0
7	M	49	0	43	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	A	1	0	0	0	0
9	B	1	0	0	0	0
9	C	1	0	0	0	0
9	D	1	0	0	0	0
10	A	5	0	0	0	0
10	B	5	0	0	0	0
10	C	5	0	0	0	0
10	D	5	0	0	0	0
11	A	14	0	13	0	0
11	D	28	0	26	1	0
12	A	28	0	40	3	0
12	B	35	0	50	0	0
12	C	28	0	40	0	0
12	D	35	0	50	0	0
13	A	19	0	26	1	0
13	B	19	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	D	19	0	26	3	0
14	A	391	0	0	4	0
14	B	458	0	0	3	0
14	C	513	0	0	5	0
14	D	464	0	0	2	0
14	R	1	0	0	0	0
14	S	2	0	0	0	0
All	All	22316	0	19583	85	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 (85) 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:270:PRO:HD3	1:B:426:LEU:HD22	1.67	0.75
1:A:147:LEU:HD22	1:A:256:MET:HA	1.68	0.74
1:C:206:THR:HG23	1:C:210:ASP:OD2	1.89	0.73
1:A:206:THR:HG23	1:A:210:ASP:OD2	1.91	0.71
1:B:365:HIS:HD1	1:B:388:HIS:CD2	2.09	0.70
1:D:206:THR:HG23	1:D:210:ASP:OD2	1.93	0.69
1:C:453:ARG:NH1	14:C:2414:HOH:O	2.23	0.69
1:C:413:ARG:NH2	14:C:2379:HOH:O	2.27	0.66
1:A:539:LYS:HE3	1:A:559:MET:O	1.96	0.65
1:C:176:GLU:OE1	14:C:2196:HOH:O	2.13	0.65
1:B:354:ASP:OD2	14:B:2315:HOH:O	2.15	0.63
1:B:206:THR:HG23	1:B:210:ASP:OD2	1.99	0.62
1:C:426:LEU:O	1:C:426:LEU:HG	1.99	0.61
12:A:1201:PEG:O4	13:A:1202:P6G:O19	2.19	0.60
1:B:365:HIS:HD1	1:B:388:HIS:HD2	1.49	0.60
1:C:245:ARG:HG2	1:C:591:VAL:HG11	1.83	0.59
1:B:596:GLU:OE2	11:D:1100:NAG:O7	2.19	0.59
14:C:2505:HOH:O	4:J:2:FUC:H4	2.03	0.58
1:B:157:LEU:HD11	1:B:477:VAL:HG13	1.86	0.58
1:D:235:ARG:HH11	13:D:1201:P6G:H172	1.68	0.57
1:A:233:LEU:HD23	1:A:267:MET:HE1	1.88	0.56
1:D:157:LEU:HD11	1:D:477:VAL:HG13	1.88	0.55
1:C:274:LYS:HB3	1:C:275:PRO:CD	2.37	0.54
1:B:412:ASP:O	1:B:413:ARG:CB	2.56	0.53
1:D:188:GLN:HG2	14:D:2186:HOH:O	2.08	0.53
1:D:275:PRO:HG3	1:D:413:ARG:HG2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:235:ARG:HH12	13:D:1201:P6G:H112	1.75	0.52
1:B:233:LEU:HD23	1:B:267:MET:HE1	1.93	0.51
1:A:172:LYS:O	1:A:176:GLU:HG3	2.11	0.51
1:D:596:GLU:OE2	4:G:1:NAG:O7	2.29	0.50
1:A:187:LYS:HE3	14:A:2178:HOH:O	2.10	0.50
1:D:274:LYS:HB3	1:D:275:PRO:CD	2.42	0.50
1:B:232:ALA:CB	1:B:268:VAL:HG12	2.42	0.50
1:D:579:GLN:NE2	1:D:583:GLU:OE2	2.34	0.50
1:C:539:LYS:HE3	1:C:559:MET:O	2.12	0.49
1:A:389:GLU:HB2	1:A:504:SER:HB2	1.94	0.49
1:A:77:GLU:N	1:A:78:PRO:HD2	2.28	0.49
1:C:151:ARG:HD2	1:C:267:MET:SD	2.53	0.49
12:A:1201:PEG:H22	14:A:2389:HOH:O	2.11	0.49
1:B:412:ASP:O	1:B:413:ARG:HB3	2.13	0.49
1:B:489:LYS:O	1:B:493:PRO:HD2	2.14	0.48
1:D:340[B]:ARG:HG2	1:D:373:LYS:O	2.13	0.48
1:D:270:PRO:HD3	1:D:426:LEU:HD22	1.95	0.48
1:A:489:LYS:O	1:A:493:PRO:HD2	2.14	0.48
1:D:83:PHE:HA	14:D:2006:HOH:O	2.15	0.47
1:B:31:VAL:O	1:B:34:GLN:HG3	2.15	0.46
1:D:495:VAL:O	1:D:495:VAL:HG12	2.16	0.46
1:D:31:VAL:O	1:D:34:GLN:HG3	2.15	0.45
1:C:77:GLU:OE2	1:C:96:ARG:NH2	2.49	0.45
1:D:235:ARG:NH1	13:D:1201:P6G:H172	2.31	0.45
1:C:135:THR:HG23	1:C:135:THR:O	2.17	0.45
1:B:372:TYR:OH	1:B:388:HIS:HE1	1.99	0.44
1:D:80:TRP:CE2	1:D:81:GLN:HG3	2.53	0.44
1:A:232:ALA:CB	1:A:268:VAL:HG12	2.48	0.44
1:C:245:ARG:HG2	1:C:591:VAL:CG1	2.47	0.44
1:C:25:GLN:OE1	1:C:376:PRO:HA	2.17	0.44
1:C:570:LEU:C	1:C:570:LEU:HD23	2.37	0.44
1:A:31:VAL:O	1:A:34:GLN:HG3	2.18	0.44
1:B:426:LEU:O	1:B:426:LEU:HG	2.15	0.43
1:C:541[B]:ARG:NH1	14:C:2316:HOH:O	2.51	0.43
1:D:139:LEU:HD22	1:D:163:TRP:CZ2	2.53	0.43
1:A:49:GLU:HG2	3:E:2:NAG:H82	2.00	0.43
1:C:259:GLN:O	1:C:435:PHE:HA	2.18	0.43
1:B:233:LEU:HD23	1:B:267:MET:CE	2.49	0.43
1:B:157:LEU:HD13	1:B:476:PRO:HB2	2.00	0.43
1:B:60:LEU:HD11	14:B:2001:HOH:O	2.18	0.42
1:D:606:ASN:O	1:D:609:GLU:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:332:ALA:HB3	2:R:7:ASP:HB2	2.00	0.42
1:C:117:GLN:HE22	1:C:120:ARG:HE	1.66	0.42
1:D:270:PRO:HD3	1:D:426:LEU:CD2	2.49	0.42
14:B:2323:HOH:O	2:Q:7:ASP:N	2.52	0.42
14:A:2288:HOH:O	2:P:7:ASP:N	2.53	0.42
1:A:157:LEU:HD11	1:A:477:VAL:HG13	2.02	0.41
1:B:77:GLU:HB3	1:B:78:PRO:HD3	2.02	0.41
1:D:324:ASP:OD1	1:D:326:ARG:HB2	2.21	0.41
1:C:489:LYS:O	1:C:493:PRO:HD2	2.20	0.41
1:D:415:THR:OG1	1:D:417:ASP:OD2	2.38	0.41
1:C:31:VAL:O	1:C:34:GLN:HG3	2.20	0.41
1:A:390:ALA:O	1:A:394:VAL:HG23	2.21	0.41
1:D:441:LEU:HD12	1:D:441:LEU:C	2.40	0.41
1:A:139:LEU:HD22	1:A:163:TRP:CZ2	2.56	0.41
1:C:77:GLU:HA	1:C:77:GLU:OE1	2.20	0.41
1:B:562:LEU:HD23	1:B:564:ALA:O	2.21	0.40
12:A:1203:PEG:H41	14:A:2127:HOH:O	2.20	0.40
1:B:390:ALA:O	1:B:394:VAL:HG23	2.22	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	601/629 (96%)	590 (98%)	9 (2%)	2 (0%)	41	31
1	B	603/629 (96%)	593 (98%)	8 (1%)	2 (0%)	41	31
1	C	603/629 (96%)	593 (98%)	9 (2%)	1 (0%)	47	38
1	D	613/629 (98%)	601 (98%)	11 (2%)	1 (0%)	47	38
2	P	1/7 (14%)	1 (100%)	0	0	100	100
2	Q	1/7 (14%)	1 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	R	1/7 (14%)	1 (100%)	0	0	100	100
2	S	1/7 (14%)	1 (100%)	0	0	100	100
All	All	2424/2544 (95%)	2381 (98%)	37 (2%)	6 (0%)	47	38

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	413	ARG
1	A	326	ARG
1	D	45	ASN
1	B	45	ASN
1	A	45	ASN
1	C	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	519/541 (96%)	516 (99%)	3 (1%)	86	87
1	B	519/541 (96%)	516 (99%)	3 (1%)	86	87
1	C	522/541 (96%)	518 (99%)	4 (1%)	81	82
1	D	529/541 (98%)	525 (99%)	4 (1%)	81	82
2	P	2/6 (33%)	2 (100%)	0	100	100
2	Q	2/6 (33%)	2 (100%)	0	100	100
2	R	2/6 (33%)	2 (100%)	0	100	100
2	S	2/6 (33%)	2 (100%)	0	100	100
All	All	2097/2188 (96%)	2083 (99%)	14 (1%)	84	84

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	368	TYR

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Mol	Chain	Res	Type
1	A	372	TYR
1	A	388	HIS
1	B	368	TYR
1	B	372	TYR
1	B	388	HIS
1	C	368	TYR
1	C	372	TYR
1	C	388	HIS
1	C	421	ASP
1	D	285	GLN
1	D	368	TYR
1	D	372	TYR
1	D	388	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	203	ASN
1	A	289	GLN
1	B	388	HIS
1	C	117	GLN
1	C	203	ASN
1	C	598	GLN
1	D	18	GLN
1	D	188	GLN

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)

23 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	$\#\|Z\| > 2$
3	NAG	E	1	3,1	14,14,15	0.57	0	17,19,21	1.18	1 (5%)
3	NAG	E	2	3	14,14,15	0.57	0	17,19,21	0.79	0
3	NAG	F	1	3,1	14,14,15	0.72	0	17,19,21	0.91	0
3	NAG	F	2	3	14,14,15	0.56	0	17,19,21	1.08	1 (5%)
4	NAG	G	1	4,1	14,14,15	0.78	0	17,19,21	2.24	3 (17%)
4	FUC	G	2	4	10,10,11	0.74	0	14,14,16	1.43	2 (14%)
3	NAG	H	1	3,1	14,14,15	0.72	0	17,19,21	1.17	1 (5%)
3	NAG	H	2	3	14,14,15	0.52	0	17,19,21	0.92	0
5	NAG	I	1	5,1	14,14,15	0.62	0	17,19,21	0.82	0
5	NAG	I	2	5	14,14,15	0.68	0	17,19,21	0.76	0
5	BMA	I	3	5	11,11,12	0.38	0	15,15,17	0.80	0
4	NAG	J	1	4,1	14,14,15	0.69	0	17,19,21	2.01	5 (29%)
4	FUC	J	2	4	10,10,11	0.77	0	14,14,16	2.02	5 (35%)
3	NAG	K	1	3,1	14,14,15	0.60	0	17,19,21	1.35	2 (11%)
3	NAG	K	2	3	14,14,15	0.57	0	17,19,21	1.37	2 (11%)
6	NAG	L	1	6,1	14,14,15	0.90	1 (7%)	17,19,21	0.91	0
6	NAG	L	2	6	14,14,15	0.71	0	17,19,21	0.94	0
6	BMA	L	3	6	11,11,12	0.67	0	15,15,17	2.36	3 (20%)
6	FUL	L	4	6	10,10,11	0.88	0	14,14,16	1.50	3 (21%)
7	NAG	M	1	7,1	14,14,15	0.88	1 (7%)	17,19,21	0.94	1 (5%)
7	NAG	M	2	7	14,14,15	0.66	0	17,19,21	1.13	1 (5%)
7	MAN	M	3	7	11,11,12	0.63	0	15,15,17	2.28	4 (26%)
7	FUC	M	4	7	10,10,11	0.62	0	14,14,16	1.24	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
3	NAG	E	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
3	NAG	F	1	3,1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1
4	NAG	G	1	4,1	-	0/6/23/26	0/1/1/1
4	FUC	G	2	4	-	-	0/1/1/1
3	NAG	H	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	0/6/23/26	0/1/1/1
5	NAG	I	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	I	2	5	-	0/6/23/26	0/1/1/1
5	BMA	I	3	5	-	2/2/19/22	0/1/1/1
4	NAG	J	1	4,1	-	2/6/23/26	0/1/1/1
4	FUC	J	2	4	-	-	0/1/1/1
3	NAG	K	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	K	2	3	-	0/6/23/26	0/1/1/1
6	NAG	L	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	L	2	6	-	0/6/23/26	0/1/1/1
6	BMA	L	3	6	-	2/2/19/22	0/1/1/1
6	FUL	L	4	6	-	-	0/1/1/1
7	NAG	M	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	M	2	7	-	0/6/23/26	0/1/1/1
7	MAN	M	3	7	-	0/2/19/22	0/1/1/1
7	FUC	M	4	7	-	-	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	1	NAG	O5-C1	-2.22	1.40	1.43
7	M	1	NAG	O5-C1	-2.12	1.40	1.43

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	L	3	BMA	C1-O5-C5	7.20	121.95	112.19
4	G	1	NAG	C2-N2-C7	-5.73	114.74	122.90
7	M	3	MAN	O5-C5-C6	5.10	115.20	107.20
4	J	1	NAG	C1-C2-N2	-4.97	101.99	110.49
4	J	2	FUC	C1-C2-C3	4.51	115.21	109.67
4	G	1	NAG	C8-C7-N2	4.30	123.38	116.10
7	M	3	MAN	C3-C4-C5	4.28	117.87	110.24
6	L	3	BMA	C3-C4-C5	4.21	117.76	110.24
3	E	1	NAG	C1-O5-C5	4.04	117.67	112.19
4	G	1	NAG	O7-C7-N2	-4.01	114.58	121.95
4	J	1	NAG	C4-C3-C2	3.88	116.70	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	J	2	FUC	C3-C4-C5	3.78	115.66	109.77
4	G	2	FUC	O5-C1-C2	-3.72	105.03	110.77
7	M	3	MAN	C1-C2-C3	3.62	114.12	109.67
7	M	2	NAG	C1-C2-N2	-3.49	104.52	110.49
3	K	2	NAG	O5-C5-C6	3.15	112.14	107.20
7	M	3	MAN	C2-C3-C4	3.07	116.20	110.89
3	K	1	NAG	C1-O5-C5	3.06	116.34	112.19
4	J	1	NAG	O5-C5-C6	2.99	111.88	107.20
3	K	1	NAG	O5-C1-C2	-2.89	106.72	111.29
7	M	4	FUC	C1-C2-C3	-2.78	106.24	109.67
4	J	2	FUC	O5-C1-C2	2.75	115.02	110.77
4	J	2	FUC	C2-C3-C4	2.50	115.22	110.89
3	H	1	NAG	C1-O5-C5	2.47	115.53	112.19
6	L	4	FUL	O5-C5-C6	2.46	112.63	107.33
3	F	2	NAG	O7-C7-C8	-2.39	117.62	122.06
6	L	3	BMA	O5-C5-C4	2.38	116.61	110.83
6	L	4	FUL	C1-C2-C3	2.37	112.58	109.67
3	K	2	NAG	C3-C4-C5	-2.28	106.17	110.24
4	J	2	FUC	O5-C5-C4	-2.18	105.61	109.52
4	J	1	NAG	C2-N2-C7	2.16	125.98	122.90
6	L	4	FUL	O3-C3-C2	-2.12	105.94	109.99
4	J	1	NAG	O3-C3-C4	-2.07	105.57	110.35
4	G	2	FUC	O5-C5-C6	2.04	111.71	107.33
7	M	1	NAG	O5-C1-C2	-2.01	108.11	111.29

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	J	1	NAG	O5-C5-C6-O6
5	I	3	BMA	C4-C5-C6-O6
5	I	3	BMA	O5-C5-C6-O6
6	L	3	BMA	O5-C5-C6-O6
4	J	1	NAG	C4-C5-C6-O6
6	L	3	BMA	C4-C5-C6-O6
5	I	1	NAG	C4-C5-C6-O6
5	I	1	NAG	O5-C5-C6-O6
3	K	1	NAG	C4-C5-C6-O6

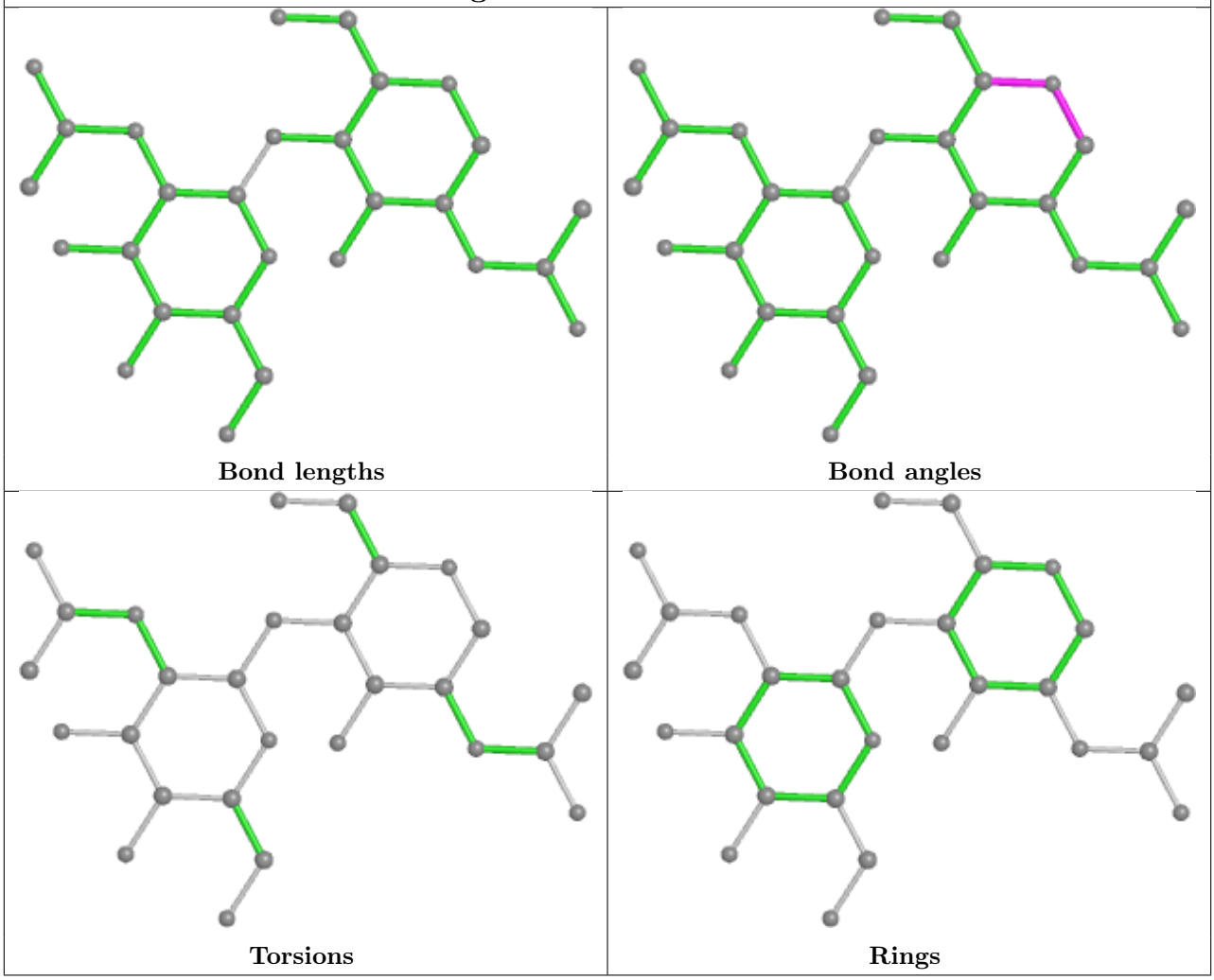
There are no ring outliers.

3 monomers are involved in 3 short contacts:

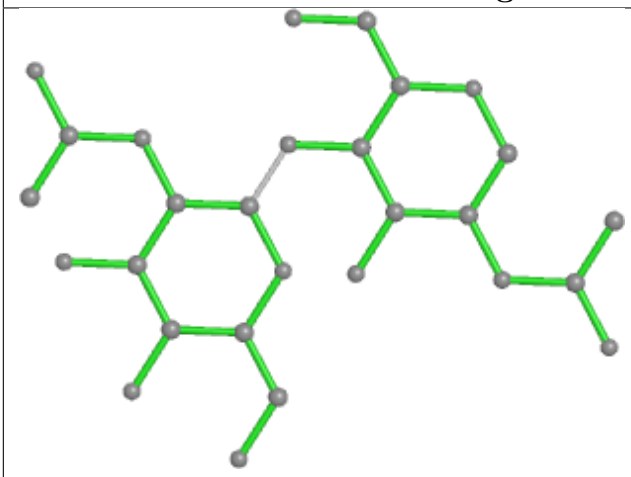
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	2	NAG	1	0
4	J	2	FUC	1	0
4	G	1	NAG	1	0

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

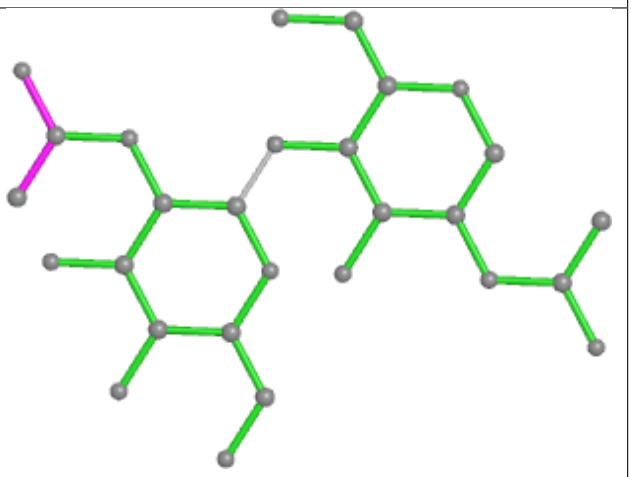
Oligosaccharide Chain E



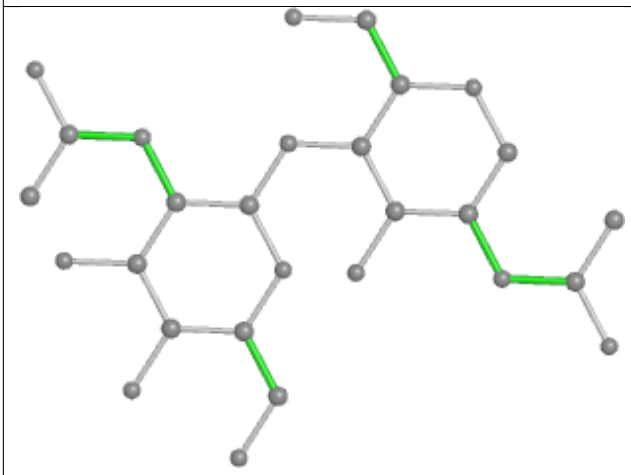
Oligosaccharide Chain F



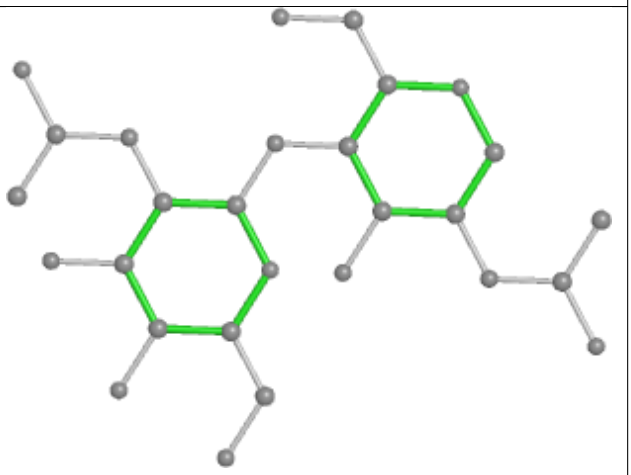
Bond lengths



Bond angles

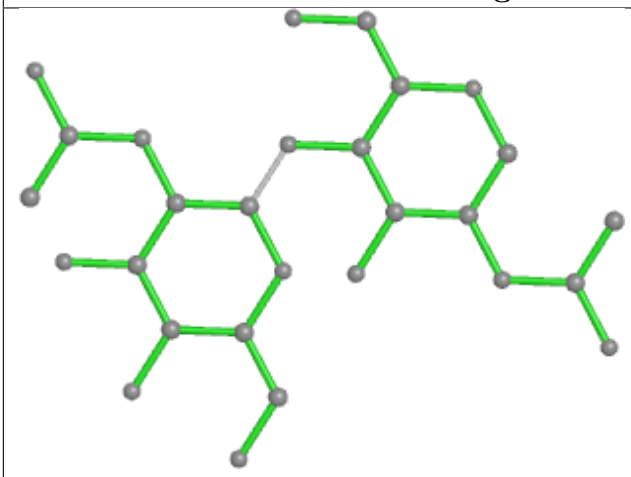


Torsions

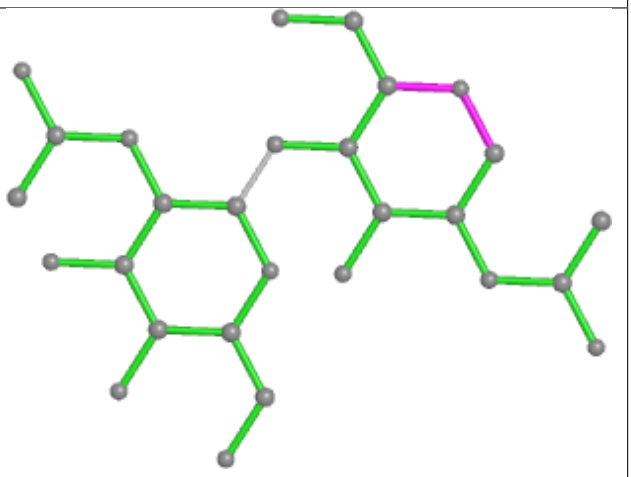


Rings

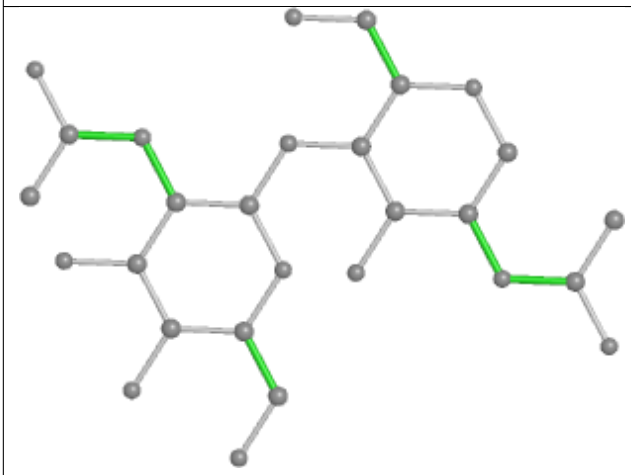
Oligosaccharide Chain H



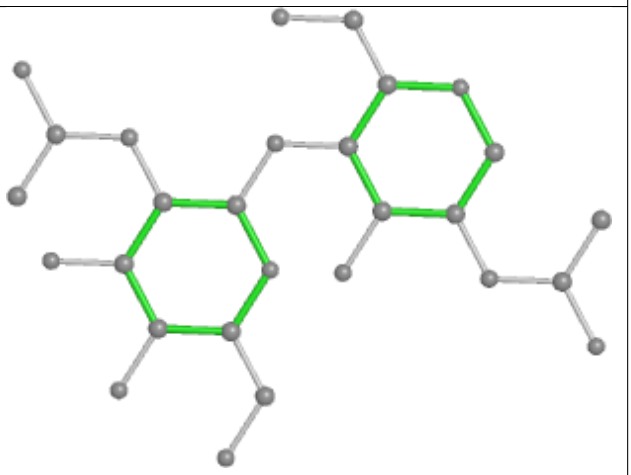
Bond lengths



Bond angles

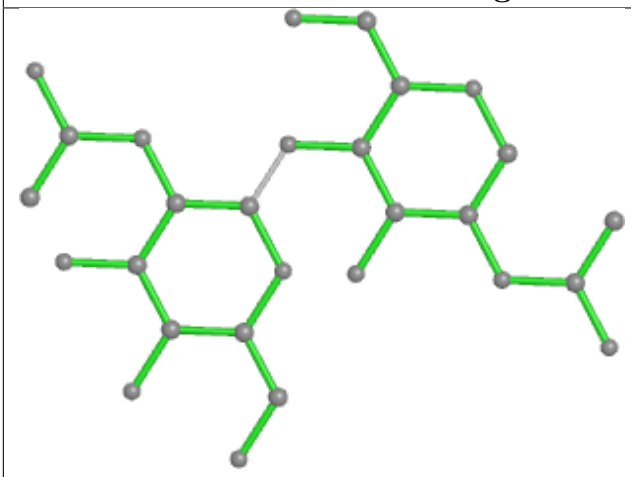


Torsions

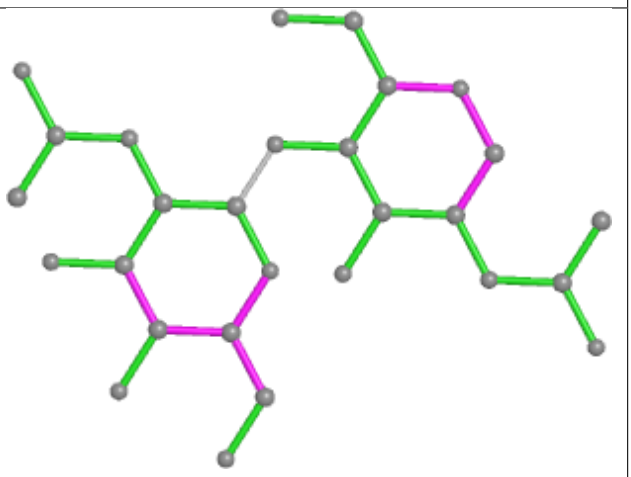


Rings

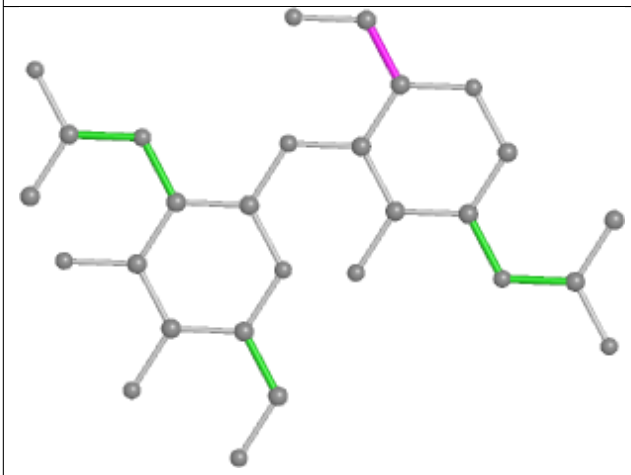
Oligosaccharide Chain K



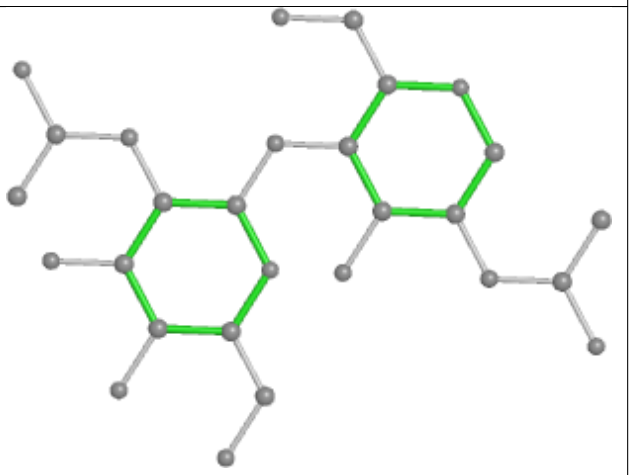
Bond lengths



Bond angles

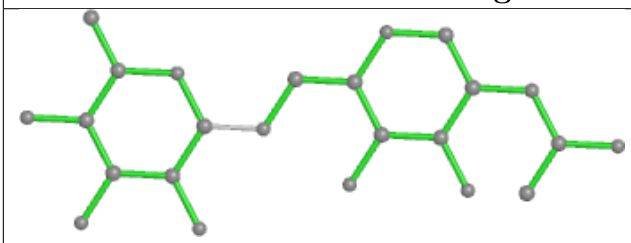


Torsions

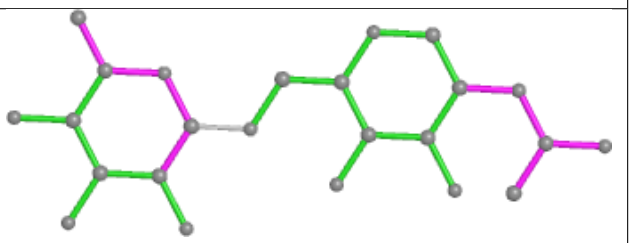


Rings

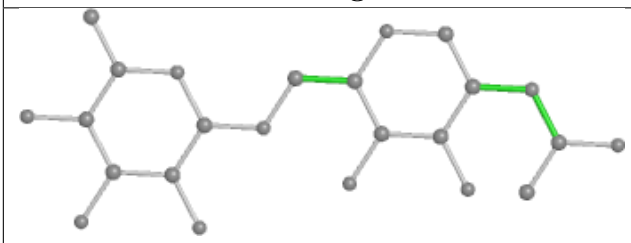
Oligosaccharide Chain G



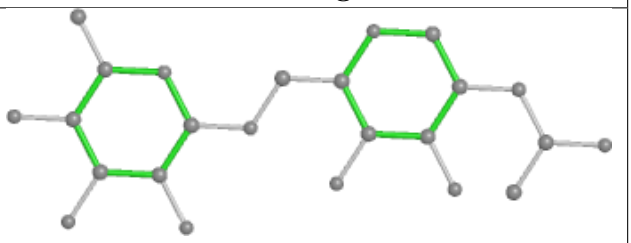
Bond lengths



Bond angles

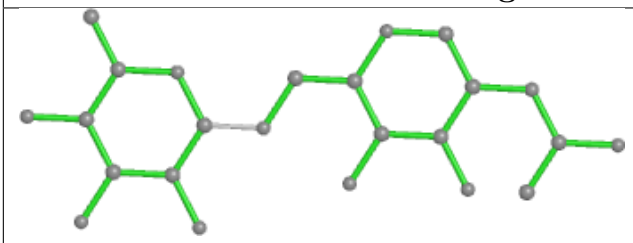


Torsions

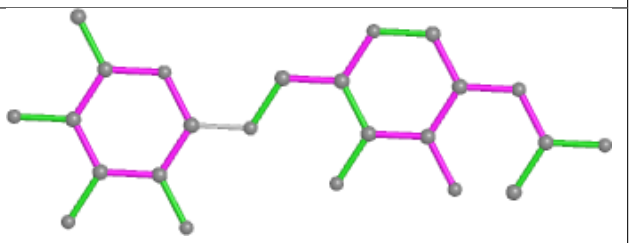


Rings

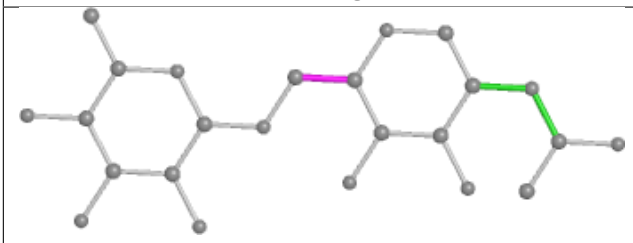
Oligosaccharide Chain J



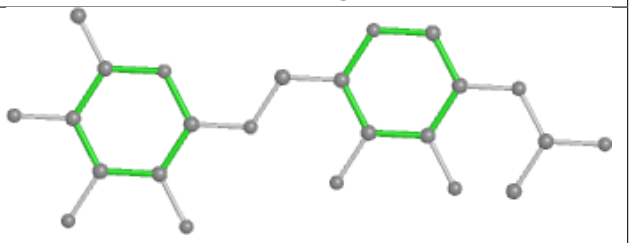
Bond lengths



Bond angles

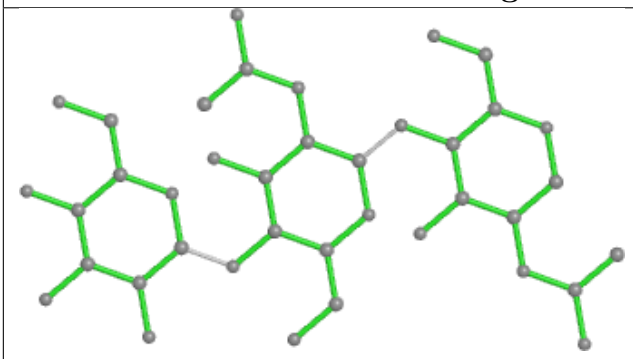


Torsions

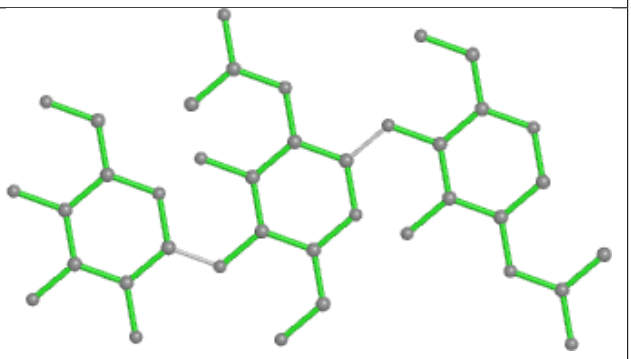


Rings

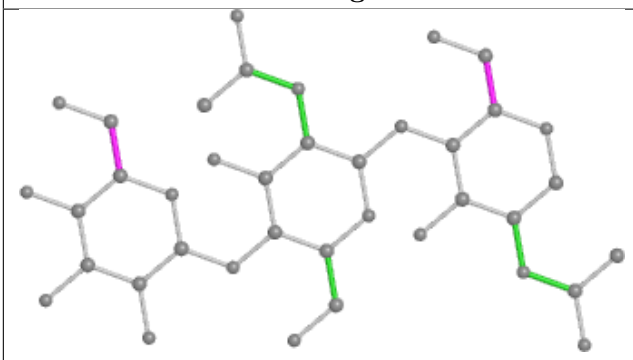
Oligosaccharide Chain I



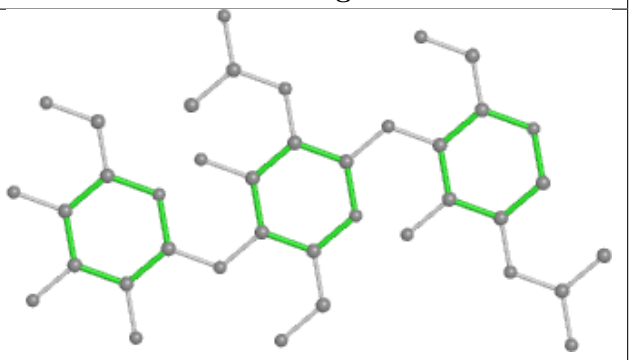
Bond lengths



Bond angles

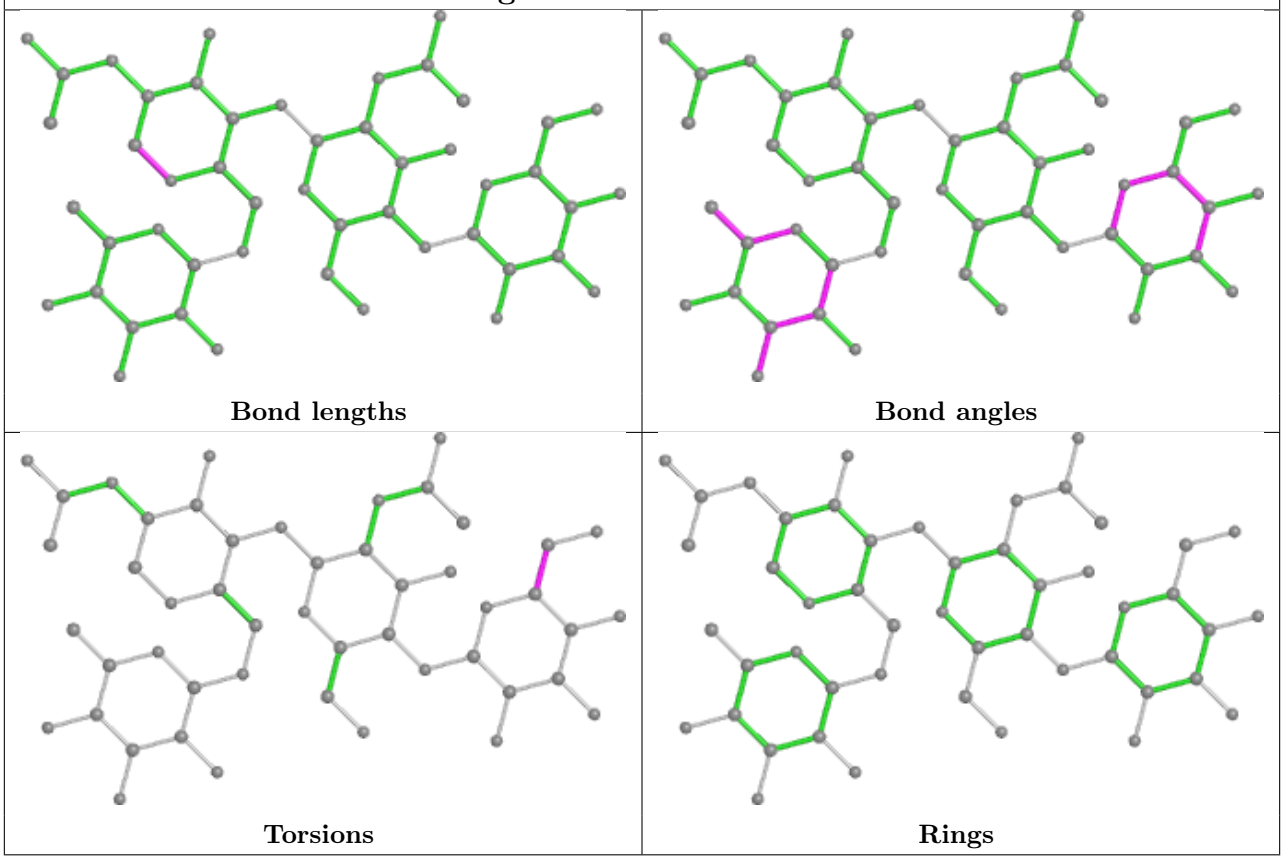


Torsions

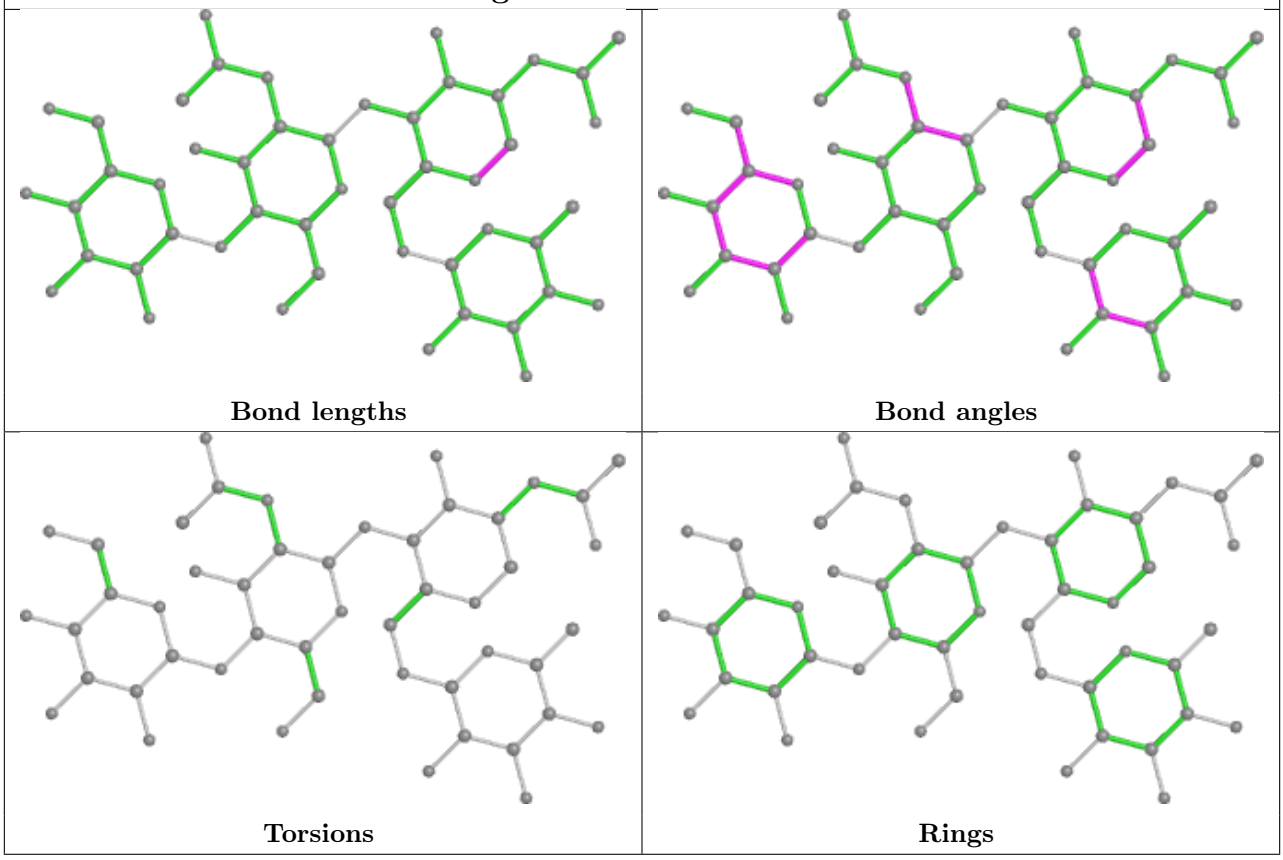


Rings

Oligosaccharide Chain L



Oligosaccharide Chain M



5.6 Ligand geometry (i)

Of 36 ligands modelled in this entry, 8 are monoatomic - leaving 28 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
12	PEG	A	1200	-	6,6,6	0.42	0	5,5,5	0.39	0
12	PEG	C	1200	-	6,6,6	0.42	0	5,5,5	0.32	0
11	NAG	A	1100	1	14,14,15	0.46	0	17,19,21	1.29	2 (11%)
13	P6G	D	1201	-	18,18,18	0.58	0	17,17,17	0.65	0
10	SO4	A	1003	-	4,4,4	0.39	0	6,6,6	0.22	0
12	PEG	B	1205	-	6,6,6	0.52	0	5,5,5	0.28	0
12	PEG	D	1204	-	6,6,6	0.43	0	5,5,5	0.35	0
12	PEG	D	1203	-	6,6,6	0.50	0	5,5,5	0.16	0
12	PEG	B	1204	-	6,6,6	0.61	0	5,5,5	0.24	0
12	PEG	A	1201	-	6,6,6	0.38	0	5,5,5	0.42	0
12	PEG	B	1202	-	6,6,6	0.47	0	5,5,5	0.41	0
12	PEG	D	1202	-	6,6,6	0.50	0	5,5,5	0.38	0
13	P6G	B	1203	-	18,18,18	0.62	0	17,17,17	0.78	0
11	NAG	D	1101	1	14,14,15	0.52	0	17,19,21	1.02	1 (5%)
12	PEG	D	1205	-	6,6,6	0.62	0	5,5,5	0.49	0
13	P6G	A	1202	-	18,18,18	0.48	0	17,17,17	0.57	0
12	PEG	C	1203	-	6,6,6	0.36	0	5,5,5	0.44	0
10	SO4	B	1003	-	4,4,4	0.37	0	6,6,6	0.33	0
10	SO4	D	1003	-	4,4,4	0.48	0	6,6,6	0.27	0
12	PEG	B	1201	-	6,6,6	0.60	0	5,5,5	0.51	0
11	NAG	D	1100	1	14,14,15	0.30	0	17,19,21	0.62	0
12	PEG	A	1203	-	6,6,6	0.49	0	5,5,5	0.31	0
12	PEG	C	1202	-	6,6,6	0.34	0	5,5,5	0.56	0
12	PEG	D	1200	-	6,6,6	0.37	0	5,5,5	0.40	0
12	PEG	A	1204	-	6,6,6	0.34	0	5,5,5	0.39	0
10	SO4	C	1003	-	4,4,4	0.52	0	6,6,6	0.46	0
12	PEG	C	1201	-	6,6,6	0.43	0	5,5,5	0.31	0
12	PEG	B	1200	-	6,6,6	0.49	0	5,5,5	0.29	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
12	PEG	A	1200	-	-	3/4/4/4	-
12	PEG	C	1200	-	-	3/4/4/4	-
11	NAG	A	1100	1	-	0/6/23/26	0/1/1/1
13	P6G	D	1201	-	-	8/16/16/16	-
12	PEG	B	1205	-	-	2/4/4/4	-
12	PEG	D	1204	-	-	3/4/4/4	-
12	PEG	D	1203	-	-	0/4/4/4	-
12	PEG	B	1204	-	-	4/4/4/4	-
12	PEG	A	1201	-	-	2/4/4/4	-
12	PEG	D	1202	-	-	2/4/4/4	-
12	PEG	B	1202	-	-	1/4/4/4	-
13	P6G	B	1203	-	-	11/16/16/16	-
11	NAG	D	1101	1	-	0/6/23/26	0/1/1/1
12	PEG	D	1205	-	-	2/4/4/4	-
13	P6G	A	1202	-	-	10/16/16/16	-
12	PEG	C	1203	-	-	2/4/4/4	-
12	PEG	B	1201	-	-	3/4/4/4	-
11	NAG	D	1100	1	-	2/6/23/26	0/1/1/1
12	PEG	A	1203	-	-	1/4/4/4	-
12	PEG	C	1202	-	-	1/4/4/4	-
12	PEG	D	1200	-	-	3/4/4/4	-
12	PEG	A	1204	-	-	2/4/4/4	-
12	PEG	C	1201	-	-	1/4/4/4	-
12	PEG	B	1200	-	-	4/4/4/4	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	1100	NAG	C1-O5-C5	3.32	116.69	112.19
11	D	1101	NAG	C1-O5-C5	2.62	115.75	112.19
11	A	1100	NAG	O5-C5-C6	2.21	110.67	107.20

There are no chirality outliers.

All (70) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	D	1100	NAG	O5-C5-C6-O6
13	B	1203	P6G	O7-C8-C9-O10
11	D	1100	NAG	C4-C5-C6-O6
12	A	1201	PEG	O2-C3-C4-O4
12	C	1200	PEG	O2-C3-C4-O4
12	C	1202	PEG	O1-C1-C2-O2
12	A	1204	PEG	O1-C1-C2-O2
12	B	1204	PEG	O2-C3-C4-O4
13	A	1202	P6G	O1-C2-C3-O4
13	D	1201	P6G	O10-C11-C12-O13
13	D	1201	P6G	O7-C8-C9-O10
12	B	1200	PEG	O1-C1-C2-O2
13	A	1202	P6G	O7-C8-C9-O10
13	A	1202	P6G	O13-C14-C15-O16
12	C	1200	PEG	O1-C1-C2-O2
13	A	1202	P6G	O16-C17-C18-O19
13	D	1201	P6G	C8-C9-O10-C11
13	B	1203	P6G	C8-C9-O10-C11
13	B	1203	P6G	O10-C11-C12-O13
12	A	1200	PEG	O2-C3-C4-O4
12	B	1200	PEG	O2-C3-C4-O4
12	B	1201	PEG	O1-C1-C2-O2
12	D	1205	PEG	O1-C1-C2-O2
13	B	1203	P6G	O1-C2-C3-O4
12	B	1201	PEG	O2-C3-C4-O4
12	B	1200	PEG	C1-C2-O2-C3
12	B	1205	PEG	O2-C3-C4-O4
12	B	1202	PEG	C1-C2-O2-C3
12	C	1201	PEG	C4-C3-O2-C2
13	A	1202	P6G	C9-C8-O7-C6
13	B	1203	P6G	C6-C5-O4-C3
12	D	1204	PEG	C1-C2-O2-C3
12	D	1202	PEG	C4-C3-O2-C2
13	B	1203	P6G	C2-C3-O4-C5
12	A	1204	PEG	O2-C3-C4-O4
12	C	1203	PEG	C4-C3-O2-C2
12	A	1201	PEG	C1-C2-O2-C3
12	D	1200	PEG	O2-C3-C4-O4
13	B	1203	P6G	O16-C17-C18-O19
12	C	1200	PEG	C1-C2-O2-C3
12	B	1201	PEG	C4-C3-O2-C2
13	D	1201	P6G	O13-C14-C15-O16
13	A	1202	P6G	C2-C3-O4-C5

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Mol	Chain	Res	Type	Atoms
13	B	1203	P6G	C11-C12-O13-C14
13	A	1202	P6G	O4-C5-C6-O7
12	D	1205	PEG	C4-C3-O2-C2
13	A	1202	P6G	C5-C6-O7-C8
12	B	1204	PEG	O1-C1-C2-O2
12	D	1200	PEG	O1-C1-C2-O2
13	A	1202	P6G	C12-C11-O10-C9
13	B	1203	P6G	C5-C6-O7-C8
12	A	1203	PEG	C1-C2-O2-C3
12	D	1200	PEG	C4-C3-O2-C2
12	B	1204	PEG	C1-C2-O2-C3
12	A	1200	PEG	C1-C2-O2-C3
13	A	1202	P6G	O10-C11-C12-O13
12	B	1204	PEG	C4-C3-O2-C2
12	D	1204	PEG	C4-C3-O2-C2
12	D	1204	PEG	O2-C3-C4-O4
13	D	1201	P6G	C11-C12-O13-C14
13	D	1201	P6G	C12-C11-O10-C9
12	C	1203	PEG	O1-C1-C2-O2
12	B	1205	PEG	C4-C3-O2-C2
13	B	1203	P6G	O4-C5-C6-O7
12	A	1200	PEG	O1-C1-C2-O2
12	D	1202	PEG	C1-C2-O2-C3
13	B	1203	P6G	O13-C14-C15-O16
13	D	1201	P6G	C9-C8-O7-C6
12	B	1200	PEG	C4-C3-O2-C2
13	D	1201	P6G	O4-C5-C6-O7

There are no ring outliers.

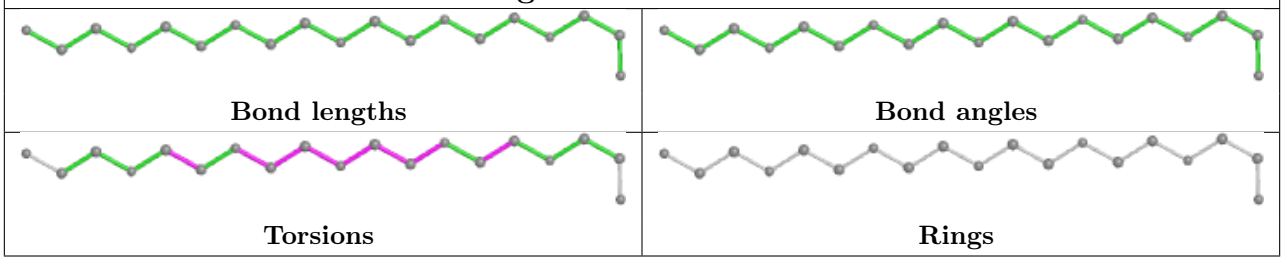
5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	D	1201	P6G	3	0
12	A	1201	PEG	2	0
13	A	1202	P6G	1	0
11	D	1100	NAG	1	0
12	A	1203	PEG	1	0

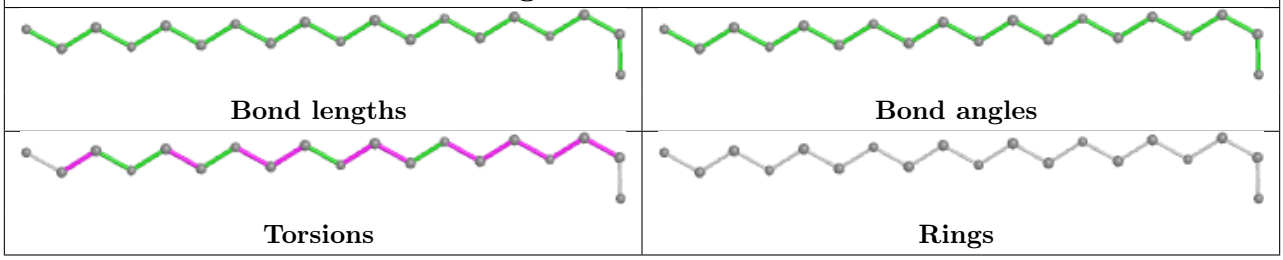
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

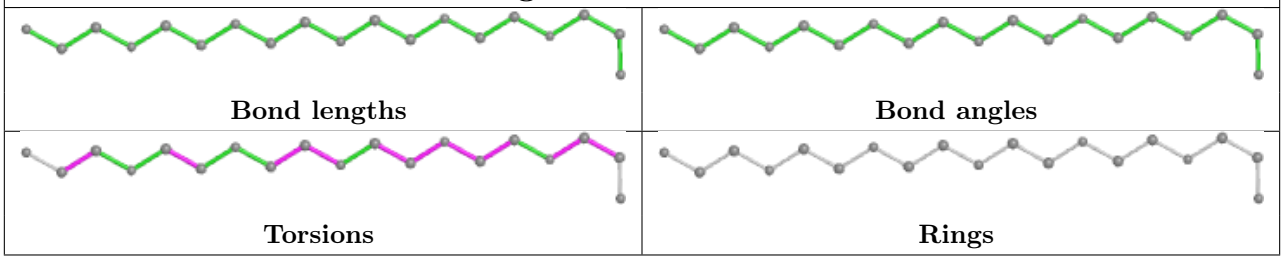
Ligand P6G D 1201



Ligand P6G B 1203



Ligand P6G A 1202



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	604/629 (96%)	-0.13	13 (2%) 62 64	15, 25, 46, 73	0
1	B	606/629 (96%)	-0.14	19 (3%) 49 51	13, 23, 43, 68	0
1	C	606/629 (96%)	-0.29	8 (1%) 77 79	12, 20, 36, 69	0
1	D	612/629 (97%)	-0.17	17 (2%) 53 56	11, 20, 42, 81	0
2	P	3/7 (42%)	1.12	0 100 100	23, 23, 23, 29	0
2	Q	3/7 (42%)	1.49	1 (33%) 0 0	19, 19, 19, 28	0
2	R	3/7 (42%)	0.34	0 100 100	20, 20, 22, 29	0
2	S	3/7 (42%)	0.39	0 100 100	18, 18, 19, 27	0
All	All	2440/2544 (95%)	-0.18	58 (2%) 59 62	11, 22, 42, 81	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	325	GLY	8.7
1	B	325	GLY	7.2
1	B	134	ALA	6.5
1	D	130	PRO	5.8
1	B	135	THR	5.2
1	A	415	THR	5.0
1	D	79	ILE	4.9
1	D	613	LEU	4.9
1	D	134	ALA	4.5
1	A	606	ASN	4.5
1	C	135	THR	4.4
1	D	131	ASN	4.3
1	A	413	ARG	4.2
1	A	135	THR	4.1
1	C	611	ILE	4.1
1	A	325	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	80	TRP	3.6
1	A	78	PRO	3.6
1	C	413	ARG	3.5
1	B	129	LEU	3.5
1	C	606	ASN	3.5
1	B	606	ASN	3.4
1	D	132	LYS	3.3
1	B	609	GLU	3.3
1	C	325	GLY	3.2
1	A	412	ASP	3.1
1	B	605	ASP	3.0
1	B	415	THR	3.0
1	D	135	THR	3.0
1	B	607	TYR	2.9
1	B	79	ILE	2.8
1	C	609	GLU	2.7
1	D	19	LEU	2.7
1	D	323	ALA	2.5
1	A	605	ASP	2.5
2	Q	9	GLY	2.5
1	B	412	ASP	2.5
1	A	82	GLN	2.4
1	D	80	TRP	2.4
1	B	78	PRO	2.4
1	D	129	LEU	2.3
1	A	273	ASP	2.3
1	D	78	PRO	2.3
1	B	323	ALA	2.3
1	C	415	THR	2.3
1	A	609	GLU	2.3
1	B	273	ASP	2.3
1	B	522	GLU	2.2
1	A	522	GLU	2.2
1	D	72	ALA	2.1
1	B	413	ARG	2.1
1	A	136	CYS	2.1
1	B	133	THR	2.1
1	D	606	ASN	2.1
1	D	415	THR	2.0
1	C	323	ALA	2.0
1	B	608	PRO	2.0
1	D	88	LEU	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)

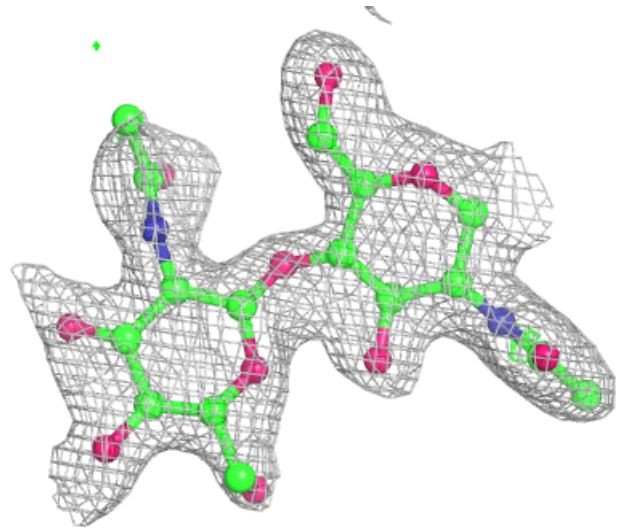
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

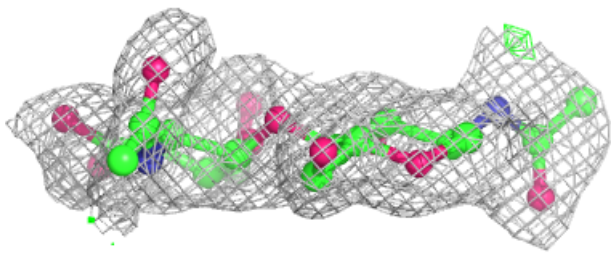
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	FUC	J	2	10/11	0.61	0.32	54,61,65,69	0
3	NAG	H	2	14/15	0.67	0.39	62,69,75,79	0
7	MAN	M	3	11/12	0.69	0.23	55,59,60,61	0
5	BMA	I	3	11/12	0.71	0.25	64,67,69,70	0
6	BMA	L	3	11/12	0.78	0.21	45,48,53,54	0
4	FUC	G	2	10/11	0.78	0.20	46,50,52,53	0
3	NAG	E	2	14/15	0.79	0.38	57,62,64,65	0
4	NAG	G	1	14/15	0.80	0.13	33,36,43,44	0
6	FUL	L	4	10/11	0.82	0.19	43,47,49,51	0
3	NAG	H	1	14/15	0.83	0.22	38,42,49,58	0
4	NAG	J	1	14/15	0.85	0.15	34,40,48,50	0
3	NAG	F	2	14/15	0.86	0.31	66,67,70,75	0
3	NAG	K	2	14/15	0.86	0.30	43,47,54,57	0
3	NAG	F	1	14/15	0.88	0.23	62,64,68,70	0
7	NAG	M	2	14/15	0.90	0.13	39,45,49,54	0
5	NAG	I	2	14/15	0.91	0.24	51,54,57,62	0
3	NAG	E	1	14/15	0.91	0.26	36,38,44,51	0
7	FUC	M	4	10/11	0.91	0.15	37,40,44,44	0
6	NAG	L	2	14/15	0.92	0.15	36,40,46,46	0
3	NAG	K	1	14/15	0.93	0.15	27,31,35,38	0
5	NAG	I	1	14/15	0.93	0.14	46,48,51,52	0
7	NAG	M	1	14/15	0.95	0.11	30,33,35,36	0
6	NAG	L	1	14/15	0.96	0.10	29,30,34,38	0

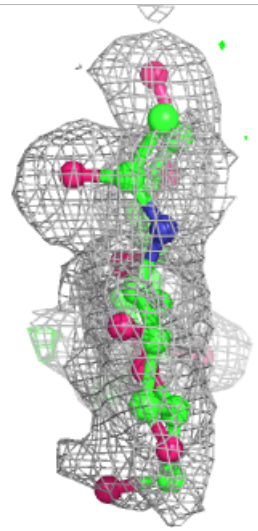
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

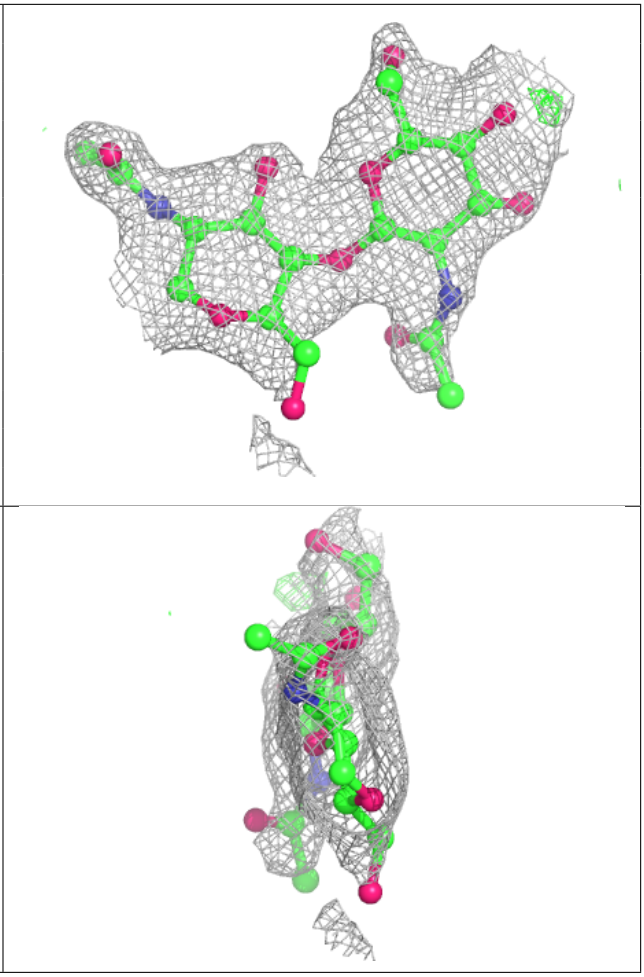






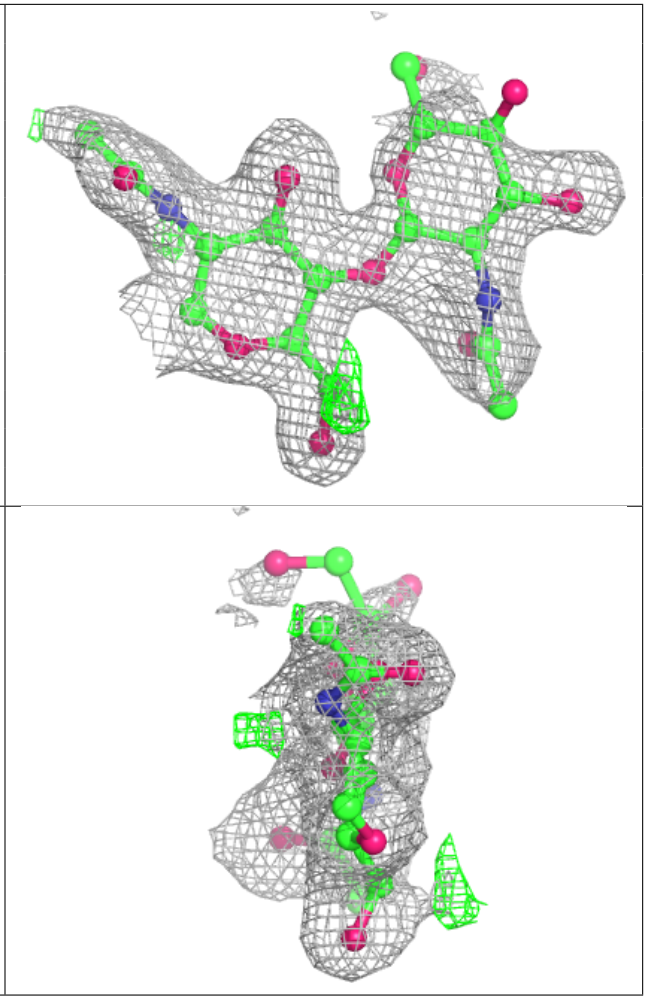
Electron density around Chain F:

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



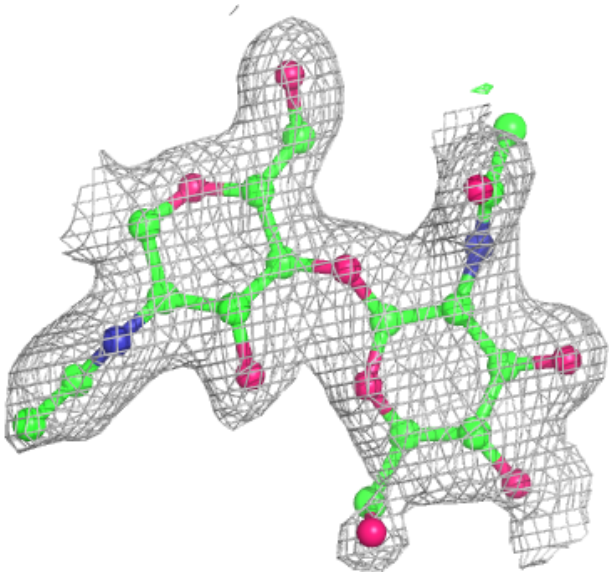
Electron density around Chain H:

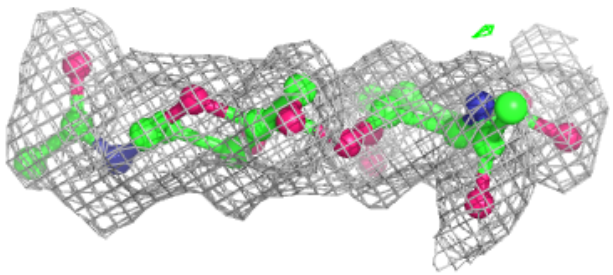
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

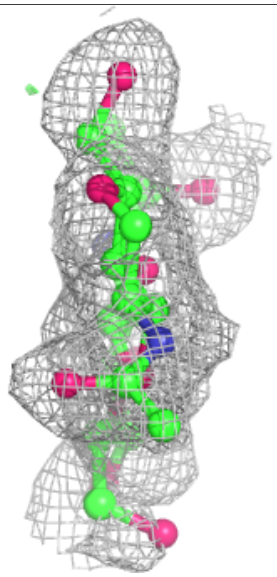


Electron density around Chain K:

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

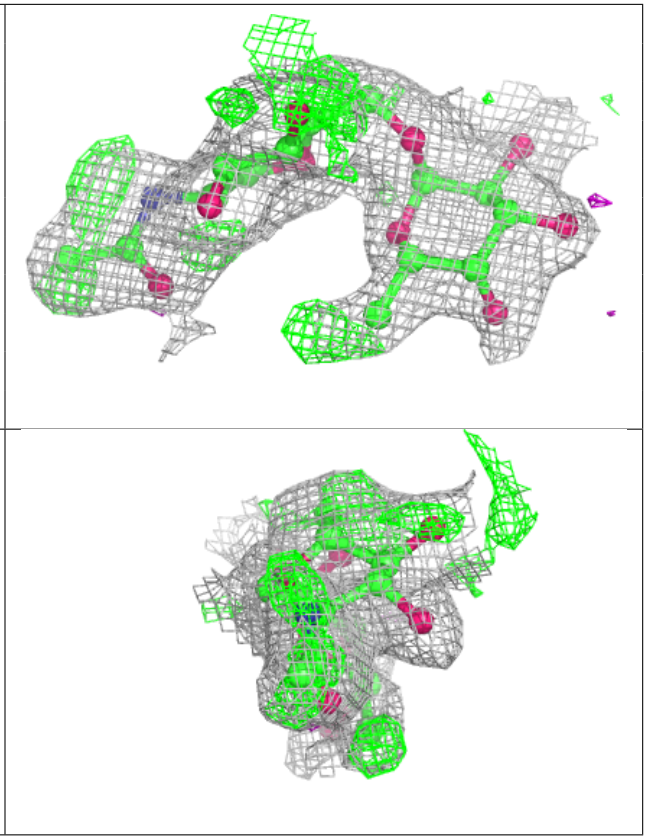






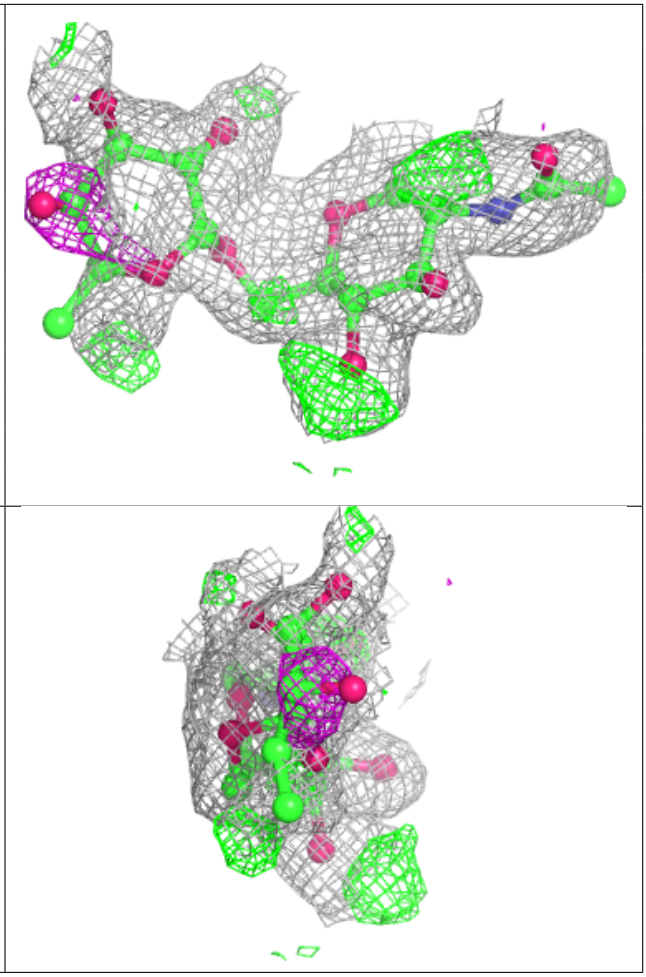
Electron density around Chain G:

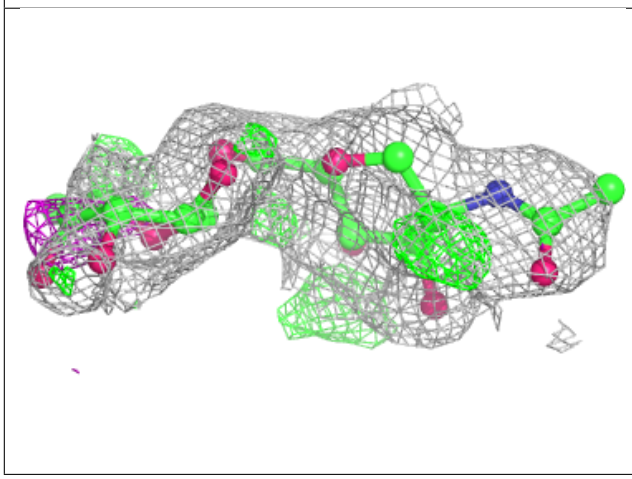
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain J:

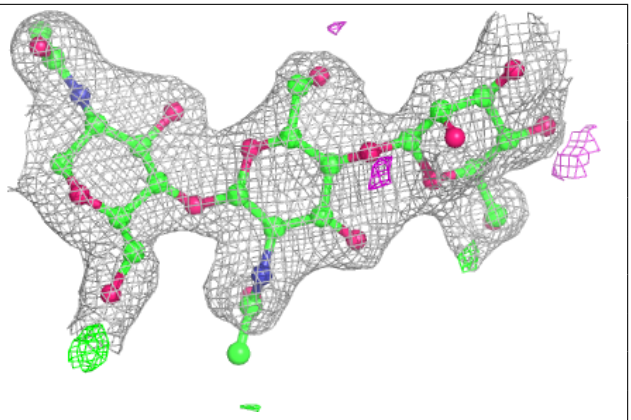
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

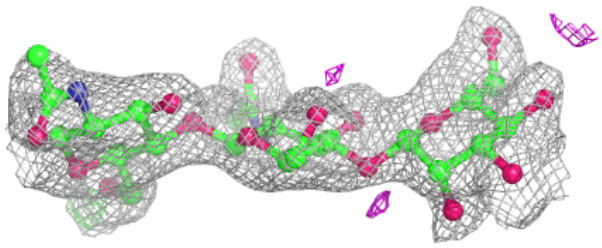


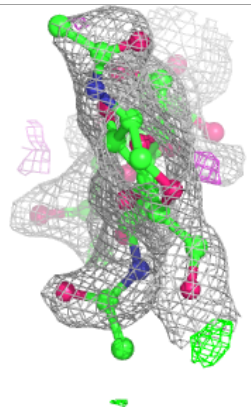


Electron density around Chain I:

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

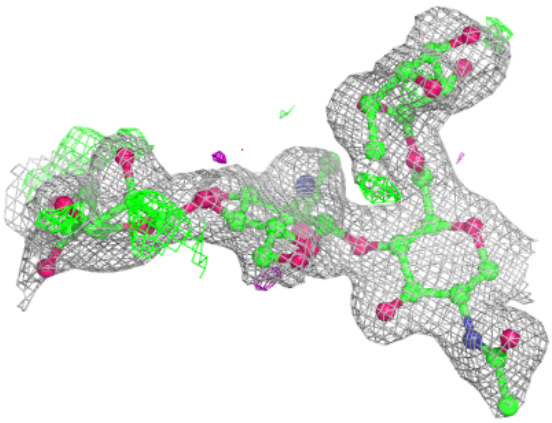


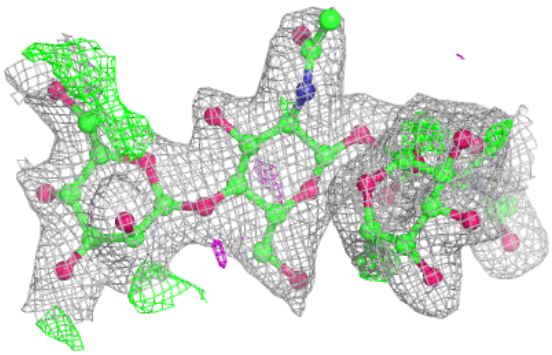


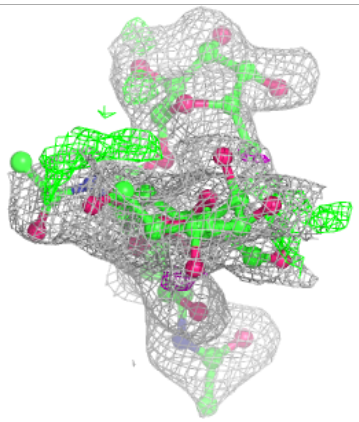


Electron density around Chain L:

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

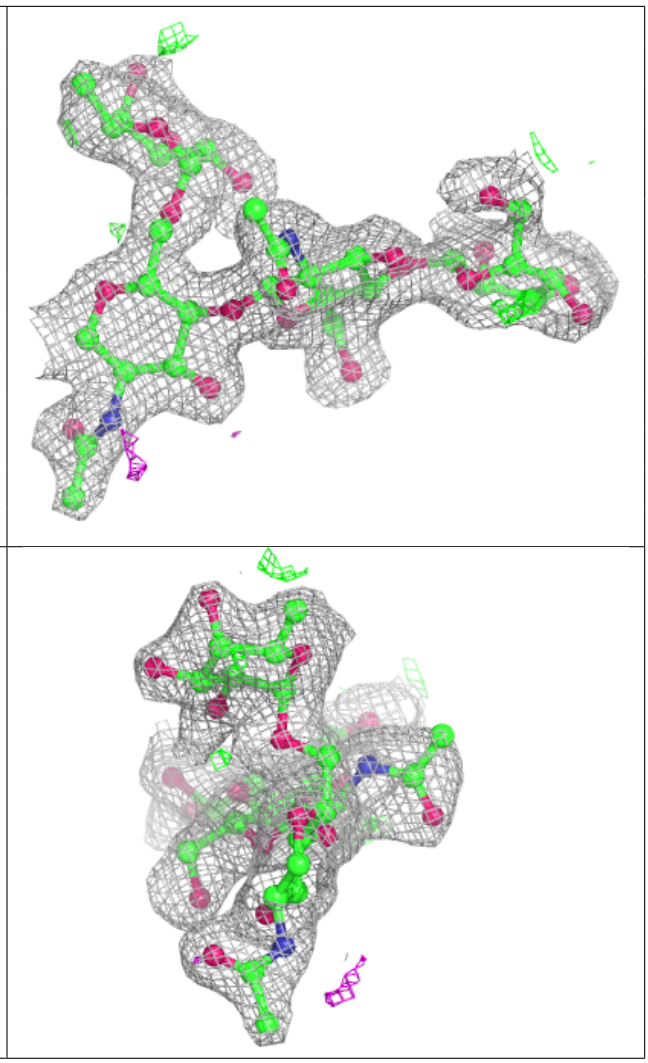






Electron density around Chain M:

$2mF_o$-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(Å^2)	Q<0.9
10	SO4	D	1003	5/5	0.63	0.29	69,69,79,84	0
12	PEG	B	1201	7/7	0.71	0.25	41,43,46,47	0
11	NAG	A	1100	14/15	0.72	0.19	42,47,52,60	0
12	PEG	B	1200	7/7	0.74	0.26	59,61,62,63	0
13	P6G	B	1203	19/19	0.77	0.16	37,39,51,51	0
12	PEG	B	1205	7/7	0.78	0.32	50,51,54,58	0
12	PEG	C	1202	7/7	0.78	0.26	46,47,50,52	0
11	NAG	D	1100	14/15	0.78	0.14	30,36,40,42	0
12	PEG	B	1204	7/7	0.80	0.24	49,51,53,53	0

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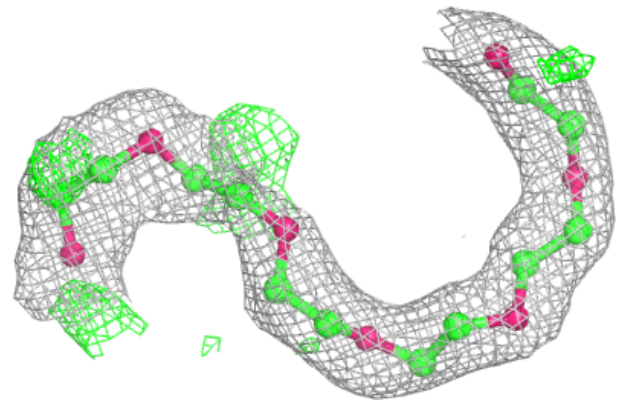
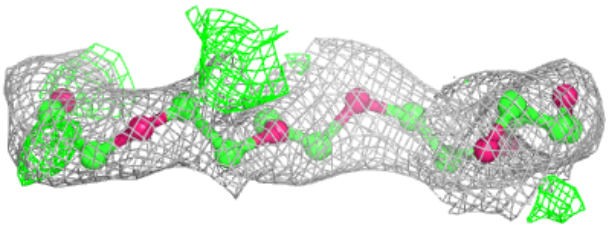
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
10	SO4	A	1003	5/5	0.80	0.25	74,80,84,88	0
12	PEG	D	1200	7/7	0.81	0.19	52,53,55,60	0
12	PEG	D	1202	7/7	0.82	0.16	52,55,58,58	0
11	NAG	D	1101	14/15	0.82	0.23	37,41,46,46	0
12	PEG	D	1205	7/7	0.83	0.18	37,40,42,43	0
12	PEG	D	1203	7/7	0.83	0.20	46,49,53,53	0
12	PEG	A	1200	7/7	0.84	0.22	47,48,52,54	0
12	PEG	A	1204	7/7	0.84	0.24	50,52,54,55	0
12	PEG	A	1201	7/7	0.85	0.13	40,43,45,45	0
12	PEG	C	1200	7/7	0.86	0.13	43,44,45,47	0
13	P6G	D	1201	19/19	0.87	0.14	31,36,50,51	0
10	SO4	B	1003	5/5	0.88	0.18	71,73,75,77	0
12	PEG	B	1202	7/7	0.88	0.12	33,33,34,34	0
10	SO4	C	1003	5/5	0.88	0.18	60,62,65,74	0
12	PEG	D	1204	7/7	0.89	0.24	43,45,53,55	0
12	PEG	A	1203	7/7	0.89	0.27	49,50,52,52	0
13	P6G	A	1202	19/19	0.90	0.11	36,39,40,41	0
12	PEG	C	1201	7/7	0.92	0.22	36,38,43,47	0
12	PEG	C	1203	7/7	0.93	0.20	41,43,44,46	0
9	CL	B	1002	1/1	0.99	0.09	16,16,16,16	0
8	ZN	B	1001	1/1	1.00	0.08	16,16,16,16	0
8	ZN	C	1001	1/1	1.00	0.06	15,15,15,15	0
8	ZN	D	1001	1/1	1.00	0.07	15,15,15,15	0
9	CL	A	1002	1/1	1.00	0.09	18,18,18,18	0
8	ZN	A	1001	1/1	1.00	0.06	19,19,19,19	0
9	CL	C	1002	1/1	1.00	0.08	15,15,15,15	0
9	CL	D	1002	1/1	1.00	0.07	14,14,14,14	0

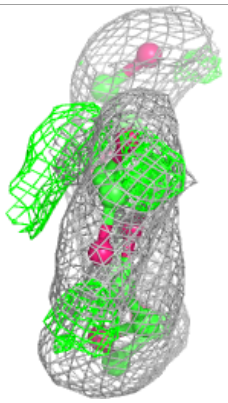
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around P6G B 1203:

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

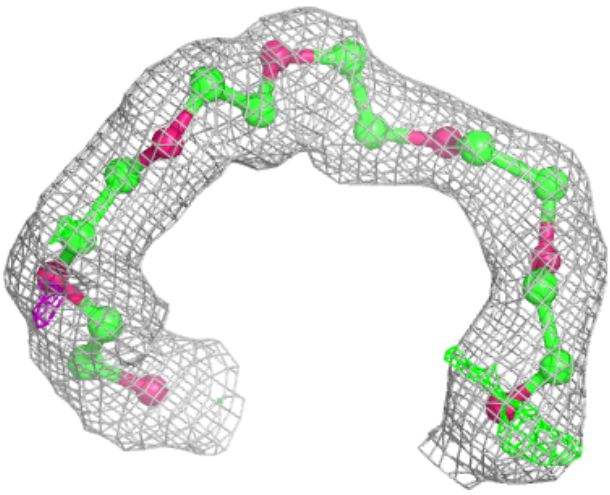


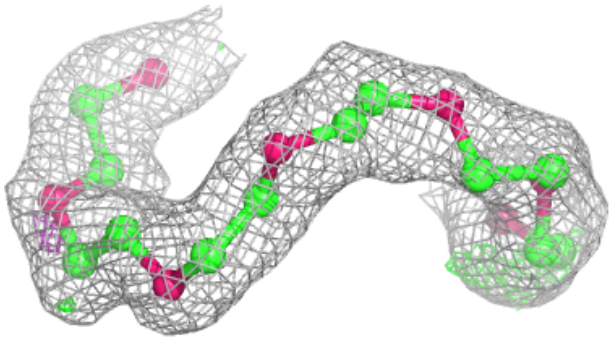


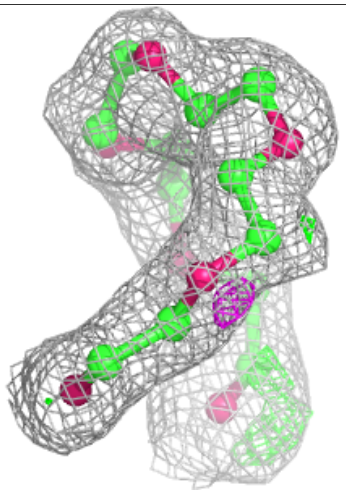


Electron density around P6G D 1201:

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

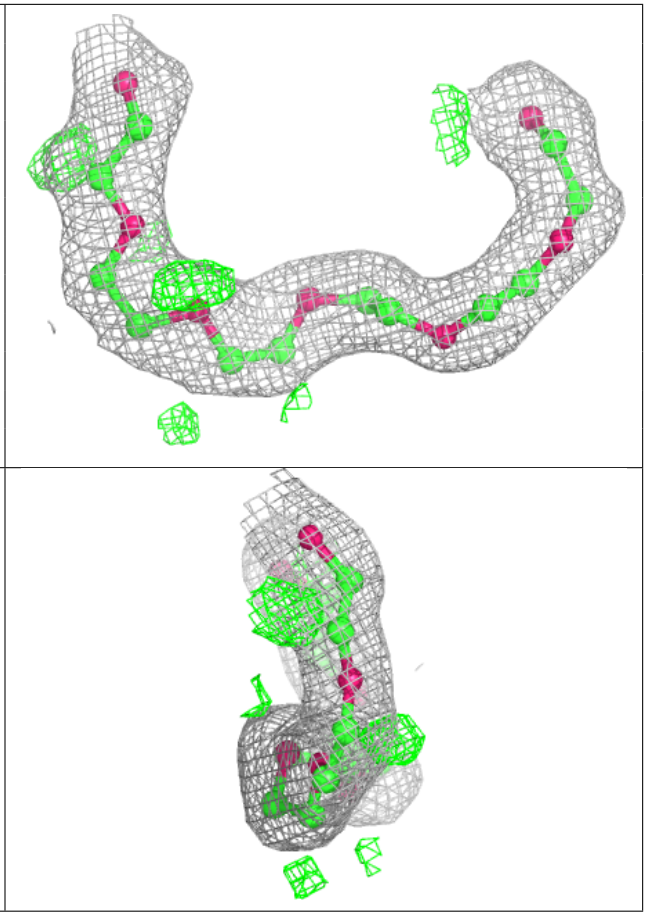






Electron density around P6G A 1202:

$2mF_o$-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.