wwPDB X-ray Structure Validation Summary Report (i)

Jan 4, 2024 – 10:07 pm GMT

PDB ID	:	5AMA
Title	:	Crystal structure of the Angiotensin-1 converting enzyme N-domain in complex with amyloid-beta 1-16
Authors	:	Masuyer, G.; Larmuth, K.M.; Douglas, R.G.; Sturrock, E.D.; Acharya, K.R.
Deposited on	:	2015-03-10
Resolution	:	1.80 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 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:

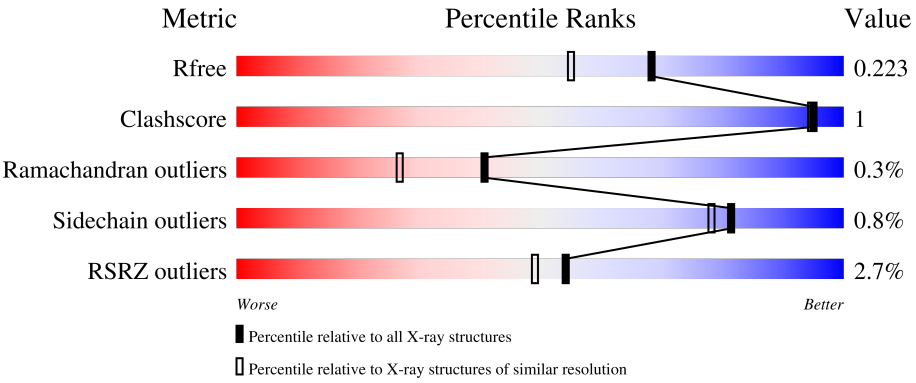
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 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% 93%
1	B	629	2% 92%
1	C	629	94%
1	D	629	5% 91% 5%
2	E	2	50% 50%

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Mol	Chain	Length	Quality of chain
2	F	2	50% 50%
2	H	2	100%
2	K	2	50% 50%
3	G	2	50% 50%
3	J	2	100%
3	M	2	50% 50%
4	I	3	33% 67%
5	L	4	25% 75%
6	N	4	50% 50%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	E	2	-	-	-	X

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 22267 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
1	A	603	Total	C	N	O	S	0	0	0
			4927	3165	846	897	19			
1	B	605	Total	C	N	O	S	0	1	0
			4939	3173	848	899	19			
1	C	609	Total	C	N	O	S	0	0	0
			4962	3189	852	902	19			
1	D	607	Total	C	N	O	S	0	1	0
			4941	3171	850	901	19			

There are 36 discrepancies between the modelled and reference sequences:

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

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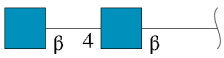
Chain	Residue	Modelled	Actual	Comment	Reference
C	82	GLN	ASN	engineered mutation	UNP P12821
C	117	GLN	ASN	engineered mutation	UNP P12821
C	131	GLN	ASN	engineered mutation	UNP P12821
C	289	GLN	ASN	engineered mutation	UNP P12821
C	545	ARG	GLN	engineered mutation	UNP P12821
C	576	LEU	PRO	engineered mutation	UNP P12821
D	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	131	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

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

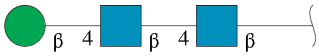


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	K	2	Total	C	N	O	0	0	0
			28	16	2	10			

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

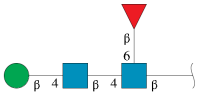
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	G	2	Total C N O 24 14 1 9	0	0	0
3	J	2	Total C N O 24 14 1 9	0	0	0
3	M	2	Total C N O 24 14 1 9	0	0	0

- Molecule 4 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.



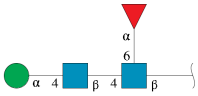
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	I	3	Total C N O 39 22 2 15	0	0	0

- Molecule 5 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.



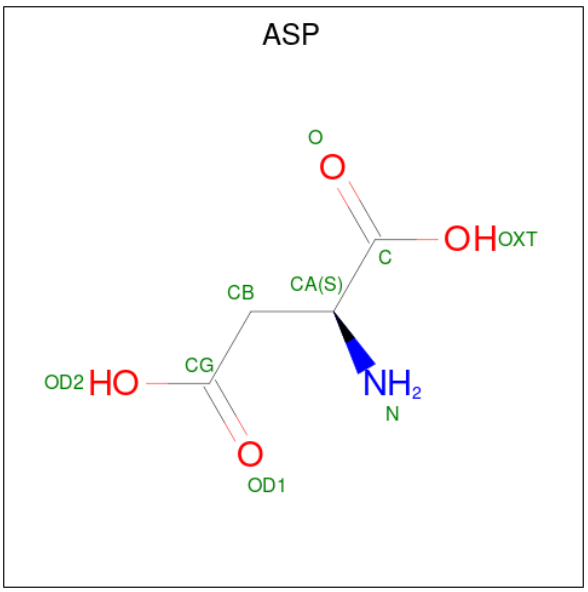
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	L	4	Total C N O 49 28 2 19	0	0	0

- Molecule 6 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.



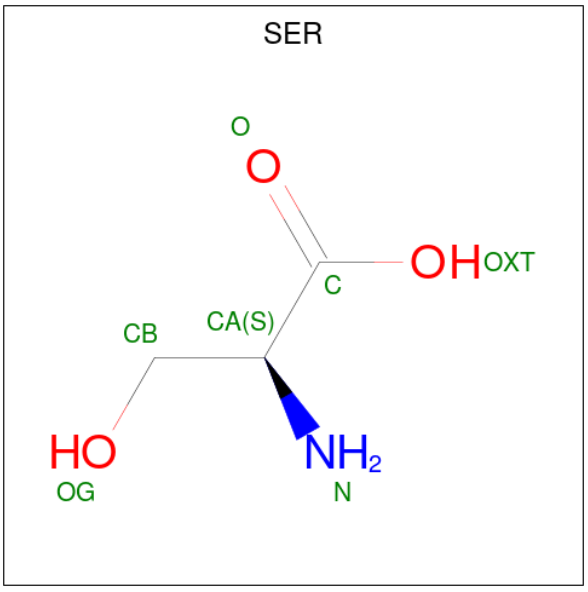
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
6	N	4	Total C N O 49 28 2 19	0	0	0

- Molecule 7 is ASPARTIC ACID (three-letter code: ASP) (formula: $C_4H_7NO_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C N O 8 4 1 3	0	0
7	B	1	Total C N O 8 4 1 3	0	0
7	C	1	Total C N O 8 4 1 3	0	0
7	D	1	Total C N O 8 4 1 3	0	0

- Molecule 8 is SERINE (three-letter code: SER) (formula: $C_3H_7NO_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C N O 7 3 1 3	0	0
8	B	1	Total C N O 7 3 1 3	0	0
8	C	1	Total C N O 7 3 1 3	0	0
8	D	1	Total C N O 7 3 1 3	0	0

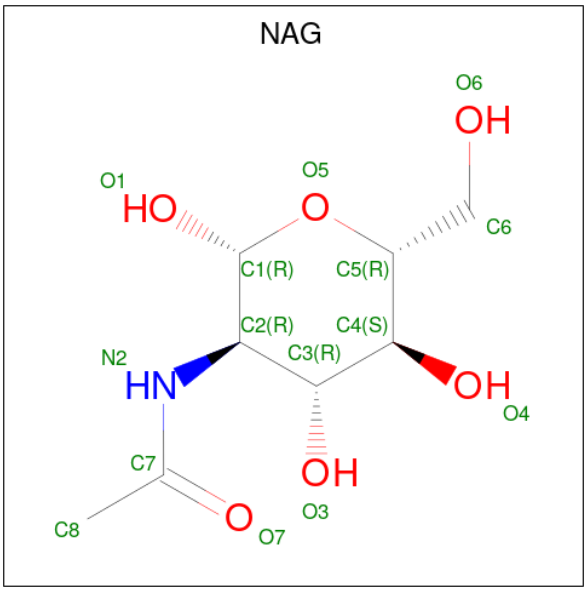
- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 10 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

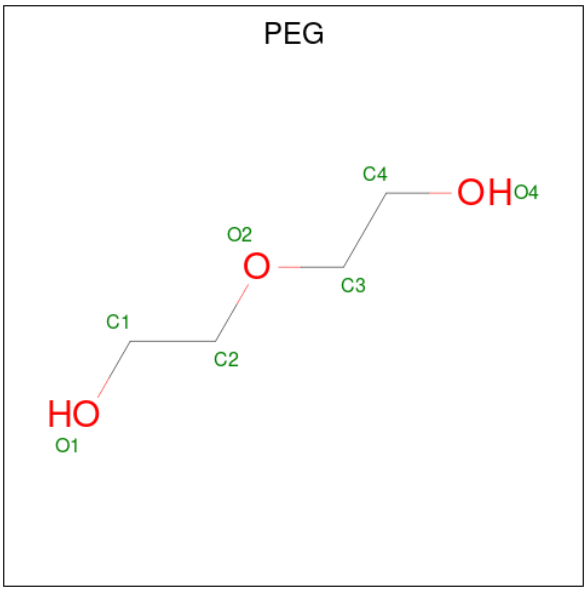
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total Cl 1 1	0	0
10	B	1	Total Cl 1 1	0	0
10	C	1	Total Cl 1 1	0	0
10	D	1	Total Cl 1 1	0	0

- 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
11	A	1	Total C N O 14 8 1 5	0	0
11	D	1	Total C N O 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
12	A	1	Total C O 7 4 3	0	0

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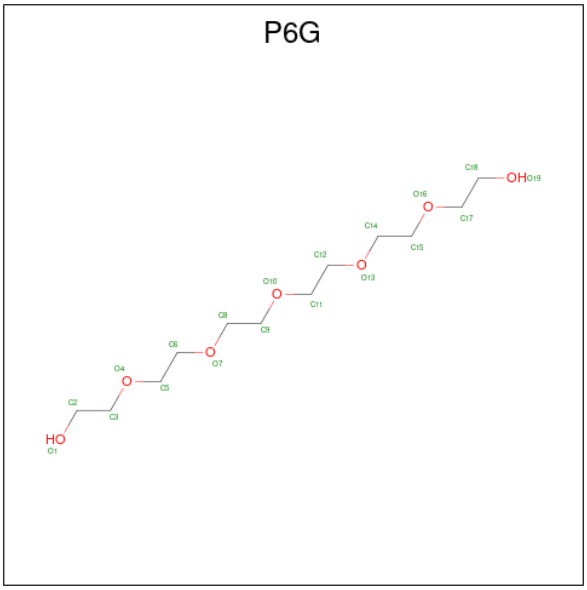
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	1	Total C O 7 4 3	0	0
12	A	1	Total C O 7 4 3	0	0
12	B	1	Total C O 7 4 3	0	0
12	B	1	Total C O 7 4 3	0	0
12	B	1	Total C O 7 4 3	0	0
12	C	1	Total C O 7 4 3	0	0
12	C	1	Total C O 7 4 3	0	0
12	D	1	Total C O 7 4 3	0	0
12	D	1	Total C O 7 4 3	0	0
12	D	1	Total C O 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
13	A	1	Total C O 19 12 7	0	0

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

- Molecule 14 is water.

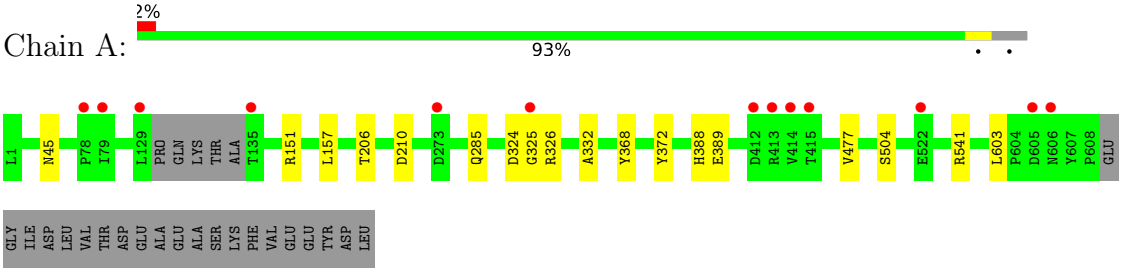
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	A	424	Total O 424 424	0	0
14	A	1	Total O 1 1	0	0
14	B	482	Total O 482 482	0	0
14	B	1	Total O 1 1	0	0
14	C	515	Total O 515 515	0	0
14	D	467	Total O 467 467	0	0

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.

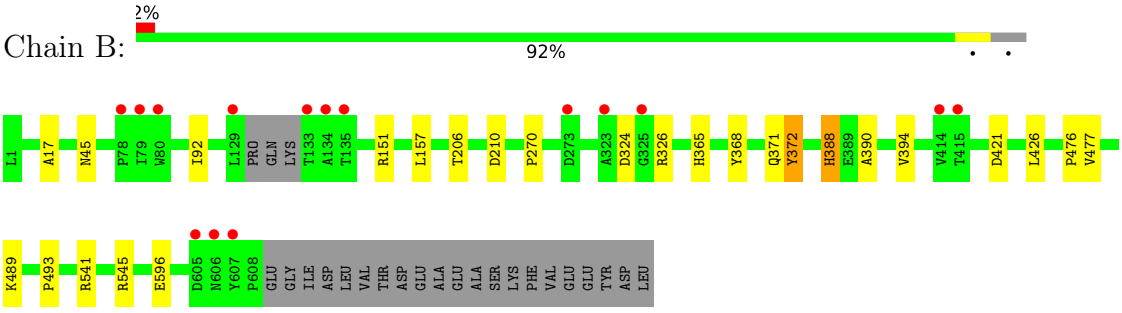
• Molecule 1: ANGIOTENSIN-CONVERTING ENZYME

Chain A:



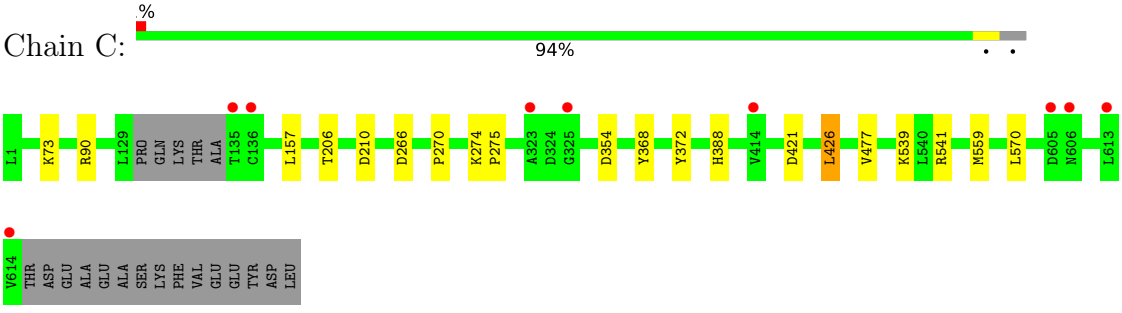
• Molecule 1: ANGIOTENSIN-CONVERTING ENZYME

Chain B:



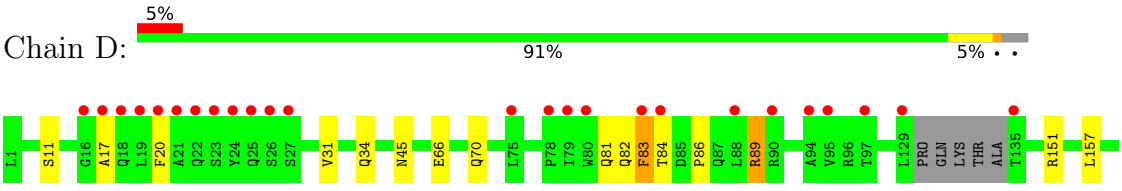
• Molecule 1: ANGIOTENSIN-CONVERTING ENZYME

Chain C:



• Molecule 1: ANGIOTENSIN-CONVERTING ENZYME

Chain D:



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

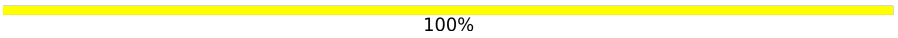
Chain E:

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

Chain F:

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

Chain H:



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

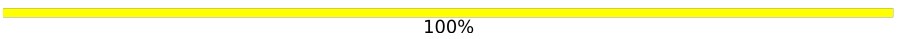
Chain K:

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

Chain G:

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

Chain J:

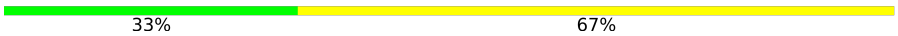


• Molecule 3: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:

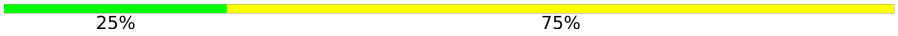
• Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:



• Molecule 5: 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:



• Molecule 6: 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 N:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	73.34Å 101.73Å 114.14Å 85.09° 85.62° 81.30°	Depositor
Resolution (Å)	113.48 – 1.80 33.27 – 1.80	Depositor EDS
% Data completeness (in resolution range)	93.5 (113.48-1.80) 93.6 (33.27-1.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.76 (at 1.81Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.187 , 0.218 0.194 , 0.223	Depositor DCC
R_{free} test set	13921 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	18.8	Xtriage
Anisotropy	0.299	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 44.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	22267	wwPDB-VP
Average B, all atoms (Å^2)	24.0	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 38.77 % 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 3.5050e-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

5.1 Standard geometry

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

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	0.48	0/5082	0.68	4/6922 (0.1%)
1	B	0.51	0/5097	0.68	2/6943 (0.0%)
1	C	0.51	0/5117	0.70	5/6970 (0.1%)
1	D	0.52	0/5096	0.69	1/6940 (0.0%)
All	All	0.51	0/20392	0.69	12/27775 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	2
All	All	0	3

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	541	ARG	NE-CZ-NH1	6.93	123.76	120.30
1	C	541	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	B	541	ARG	NE-CZ-NH1	6.11	123.36	120.30
1	D	541	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	A	326	ARG	NE-CZ-NH1	5.59	123.10	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	325	GLY	Peptide
1	D	82	GLN	Peptide
1	D	83	PHE	Peptide

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	4927	0	4703	5	0
1	B	4939	0	4712	13	0
1	C	4962	0	4736	9	0
1	D	4941	0	4718	19	0
2	E	28	0	25	0	0
2	F	28	0	25	0	0
2	H	28	0	25	0	0
2	K	28	0	25	0	0
3	G	24	0	22	1	0
3	J	24	0	22	0	0
3	M	24	0	22	1	0
4	I	39	0	34	0	0
5	L	49	0	43	0	0
6	N	49	0	43	0	0
7	A	8	0	3	1	0
7	B	8	0	3	0	0
7	C	8	0	3	0	0
7	D	8	0	3	0	0
8	A	7	0	5	0	0
8	B	7	0	5	0	0
8	C	7	0	5	0	0
8	D	7	0	5	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	1	0	0	0	0
10	B	1	0	0	0	0
10	C	1	0	0	0	0
10	D	1	0	0	0	0
11	A	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	D	14	0	13	0	0
12	A	21	0	30	1	0
12	B	21	0	30	0	0
12	C	14	0	20	0	0
12	D	21	0	30	0	0
13	A	19	0	26	1	0
13	B	38	0	52	0	0
13	C	19	0	26	0	0
13	D	38	0	52	1	0
14	A	425	0	0	0	0
14	B	483	0	0	0	0
14	C	515	0	0	2	0
14	D	467	0	0	3	0
All	All	22267	0	19479	47	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 1.

The worst 5 of 47 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:D:365:HIS:HD1	1:D:388:HIS:HD2	1.30	0.79
1:B:270:PRO:HD3	1:B:426:LEU:HD22	1.70	0.74
1:D:365:HIS:HD1	1:D:388:HIS:CD2	2.06	0.73
1:D:151:ARG:NH1	14:D:2138:HOH:O	2.16	0.72
1:D:467:ARG:HH11	1:D:471:GLN:HE22	1.37	0.72

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	599/629 (95%)	588 (98%)	9 (2%)	2 (0%)	41 27
1	B	602/629 (96%)	593 (98%)	8 (1%)	1 (0%)	47 33
1	C	605/629 (96%)	595 (98%)	10 (2%)	0	100 100
1	D	604/629 (96%)	590 (98%)	10 (2%)	4 (1%)	22 10
All	All	2410/2516 (96%)	2366 (98%)	37 (2%)	7 (0%)	41 27

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	324	ASP
1	D	83	PHE
1	D	81	GLN
1	D	84	THR
1	D	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	518/541 (96%)	514 (99%)	4 (1%)	81 78
1	B	518/541 (96%)	514 (99%)	4 (1%)	81 78
1	C	520/541 (96%)	516 (99%)	4 (1%)	81 78
1	D	518/541 (96%)	513 (99%)	5 (1%)	76 71
All	All	2074/2164 (96%)	2057 (99%)	17 (1%)	81 78

5 of 17 residues with a non-rotameric sidechain are listed below:

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	388	HIS
1	D	471	GLN
1	D	491	HIS
1	D	9	GLN
1	D	87	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)

25 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	0.42	0	17,19,21	1.16	2 (11%)
2	NAG	E	2	2	14,14,15	0.50	0	17,19,21	0.96	0
2	NAG	F	1	1,2	14,14,15	0.34	0	17,19,21	0.79	0
2	NAG	F	2	2	14,14,15	0.45	0	17,19,21	0.98	1 (5%)
3	NAG	G	1	1,3	14,14,15	0.75	0	17,19,21	1.55	5 (29%)
3	FUC	G	2	3	10,10,11	0.69	0	14,14,16	1.48	1 (7%)
2	NAG	H	1	1,2	14,14,15	0.49	0	17,19,21	0.87	1 (5%)
2	NAG	H	2	2	14,14,15	0.53	0	17,19,21	1.29	1 (5%)
4	NAG	I	1	1,4	14,14,15	0.41	0	17,19,21	0.92	1 (5%)
4	NAG	I	2	4	14,14,15	0.33	0	17,19,21	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	BMA	I	3	4	11,11,12	0.40	0	15,15,17	1.18	2 (13%)
3	NAG	J	1	1,3	14,14,15	0.69	0	17,19,21	1.61	4 (23%)
3	FUC	J	2	3	10,10,11	0.71	0	14,14,16	2.01	2 (14%)
2	NAG	K	1	1,2	14,14,15	0.49	0	17,19,21	0.96	2 (11%)
2	NAG	K	2	2	14,14,15	0.35	0	17,19,21	0.93	0
5	NAG	L	1	5,1	14,14,15	0.64	0	17,19,21	1.09	1 (5%)
5	NAG	L	2	5	14,14,15	0.43	0	17,19,21	1.06	1 (5%)
5	BMA	L	3	5	11,11,12	0.40	0	15,15,17	0.69	0
5	FUL	L	4	5	10,10,11	0.68	0	14,14,16	1.14	1 (7%)
3	NAG	M	1	1,3	14,14,15	0.72	0	17,19,21	1.69	5 (29%)
3	FUC	M	2	3	10,10,11	0.60	0	14,14,16	1.21	1 (7%)
6	NAG	N	1	1,6	14,14,15	0.46	0	17,19,21	0.89	0
6	NAG	N	2	6	14,14,15	0.48	0	17,19,21	0.75	0
6	MAN	N	3	6	11,11,12	0.57	0	15,15,17	1.62	5 (33%)
6	FUC	N	4	6	10,10,11	0.48	0	14,14,16	1.18	2 (14%)

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	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
3	NAG	G	1	1,3	-	0/6/23/26	0/1/1/1
3	FUC	G	2	3	-	-	0/1/1/1
2	NAG	H	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1
4	NAG	I	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	I	2	4	-	0/6/23/26	0/1/1/1
4	BMA	I	3	4	-	2/2/19/22	0/1/1/1
3	NAG	J	1	1,3	-	2/6/23/26	0/1/1/1
3	FUC	J	2	3	-	-	0/1/1/1
2	NAG	K	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	K	2	2	-	0/6/23/26	0/1/1/1
5	NAG	L	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	L	2	5	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BMA	L	3	5	-	2/2/19/22	0/1/1/1
5	FUL	L	4	5	-	-	0/1/1/1
3	NAG	M	1	1,3	-	2/6/23/26	0/1/1/1
3	FUC	M	2	3	-	-	0/1/1/1
6	NAG	N	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	N	2	6	-	0/6/23/26	0/1/1/1
6	MAN	N	3	6	-	0/2/19/22	0/1/1/1
6	FUC	N	4	6	-	-	0/1/1/1

There are no bond length outliers.

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	J	2	FUC	C1-C2-C3	5.90	116.92	109.67
3	G	2	FUC	O5-C1-C2	-4.32	104.11	110.77
3	J	2	FUC	O5-C1-C2	3.80	116.64	110.77
3	M	1	NAG	O5-C5-C6	3.44	112.60	107.20
3	J	1	NAG	C4-C3-C2	3.38	115.97	111.02

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

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

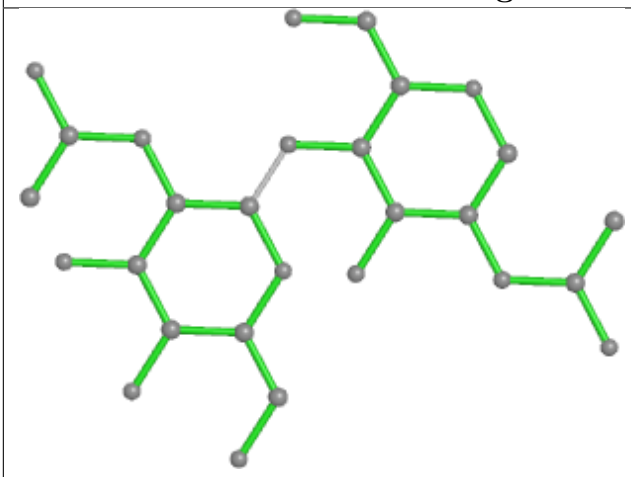
There are no ring outliers.

2 monomers are involved in 2 short contacts:

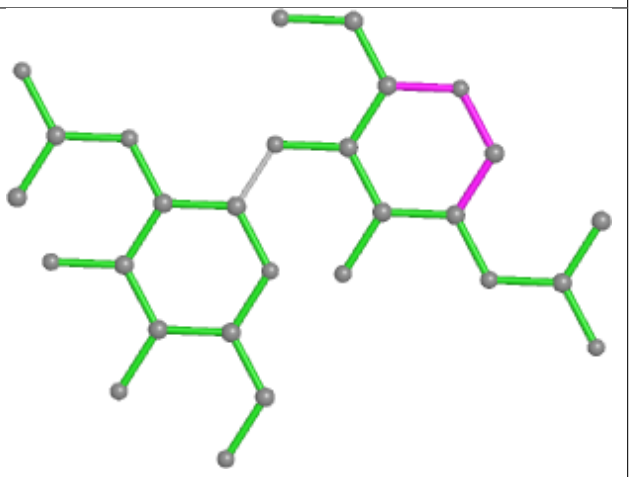
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	M	1	NAG	1	0
3	G	1	NAG	1	0

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

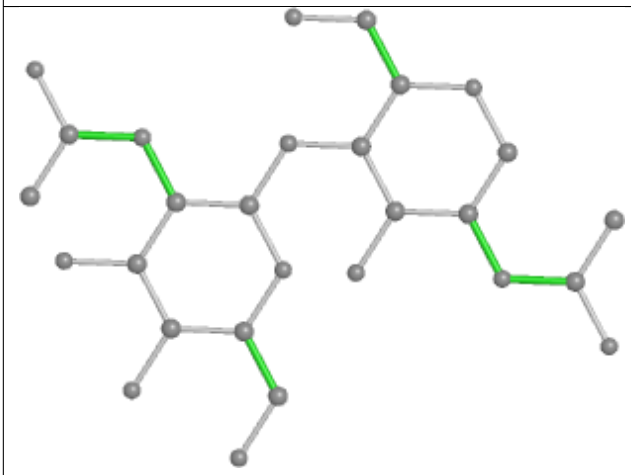
Oligosaccharide Chain E



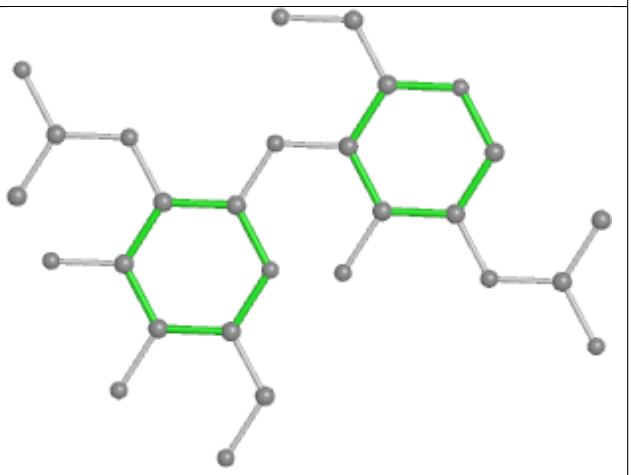
Bond lengths



Bond angles

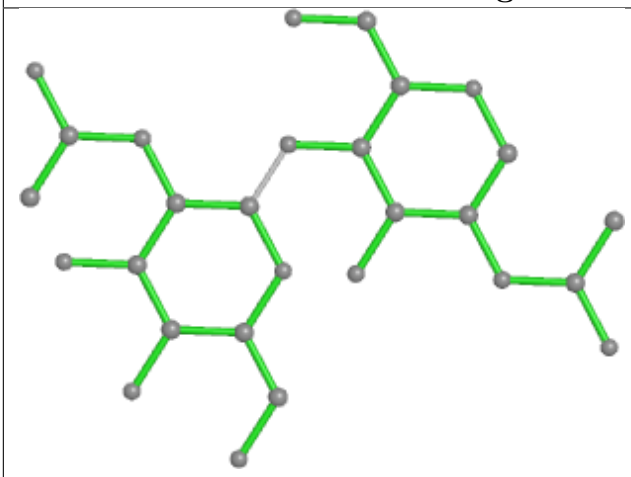


Torsions

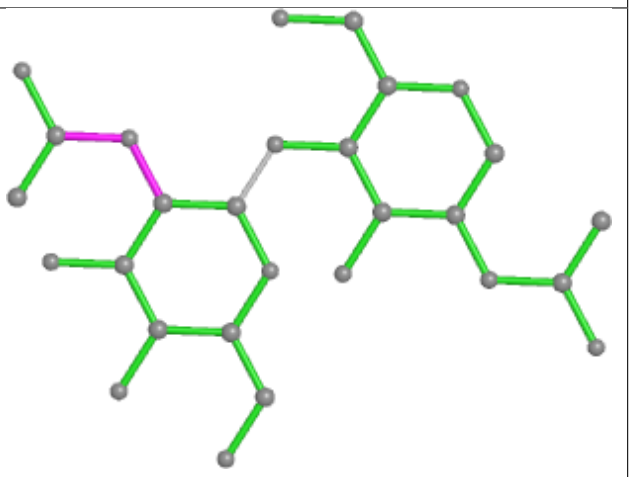


Rings

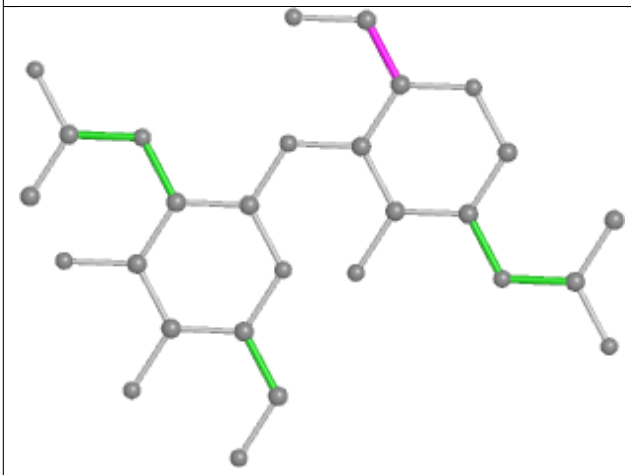
Oligosaccharide Chain F



Bond lengths



Bond angles



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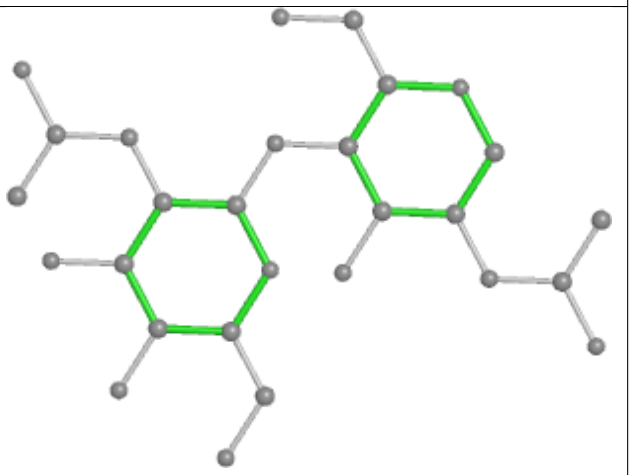
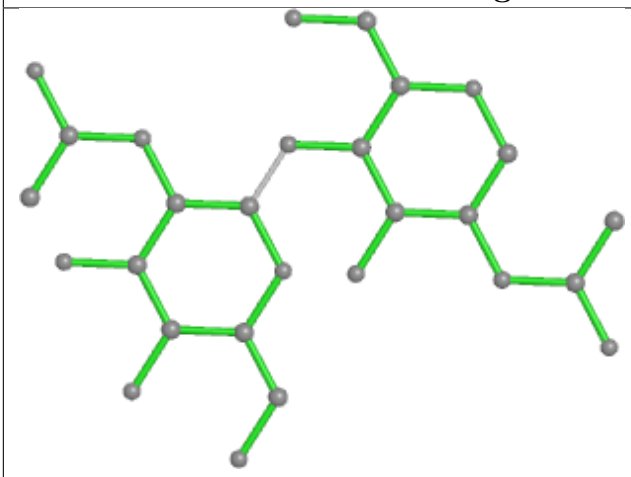
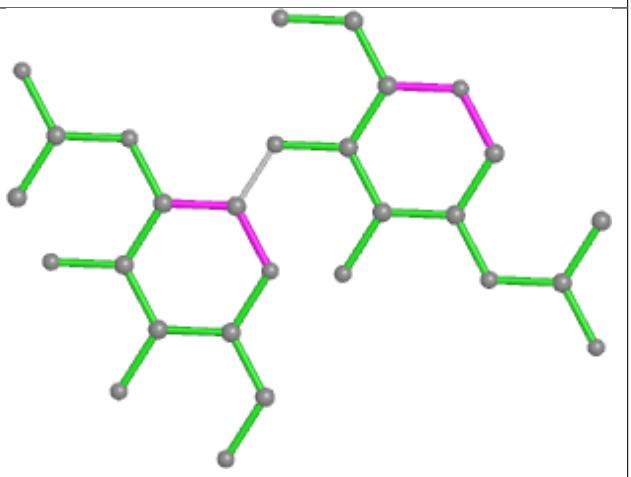


Rings

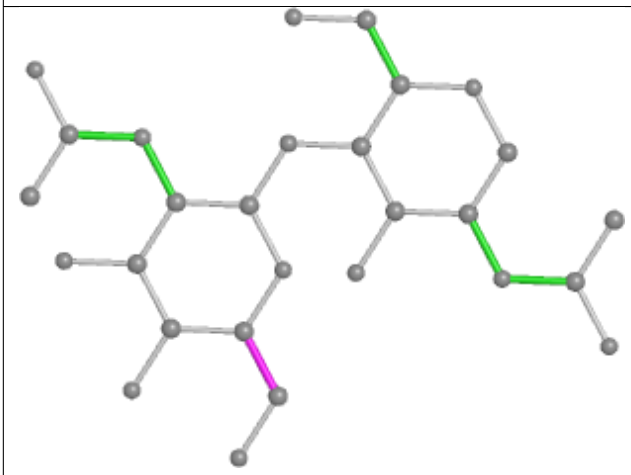
Oligosaccharide Chain H



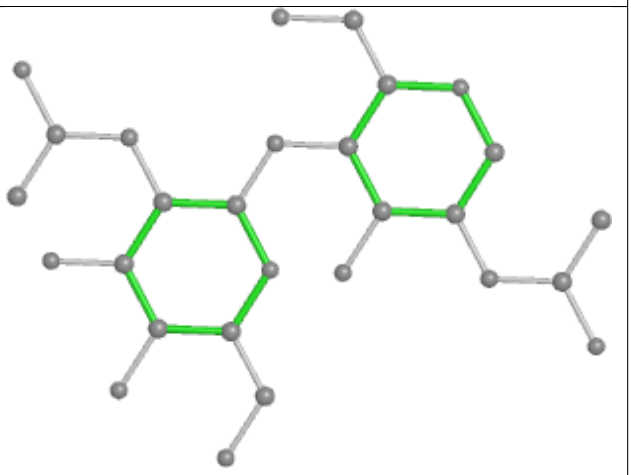
Bond lengths



Bond angles

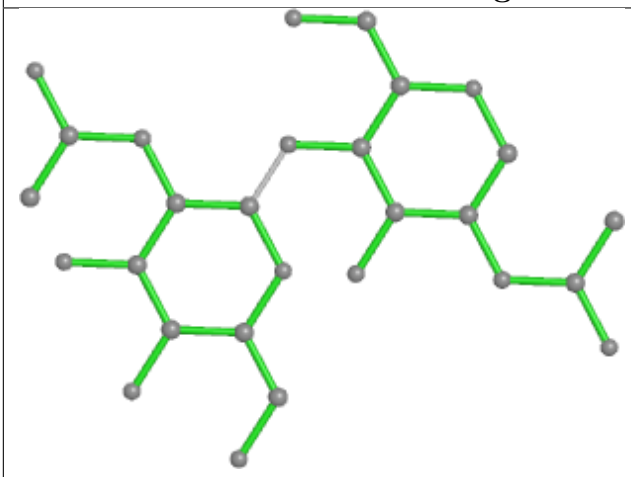


Torsions

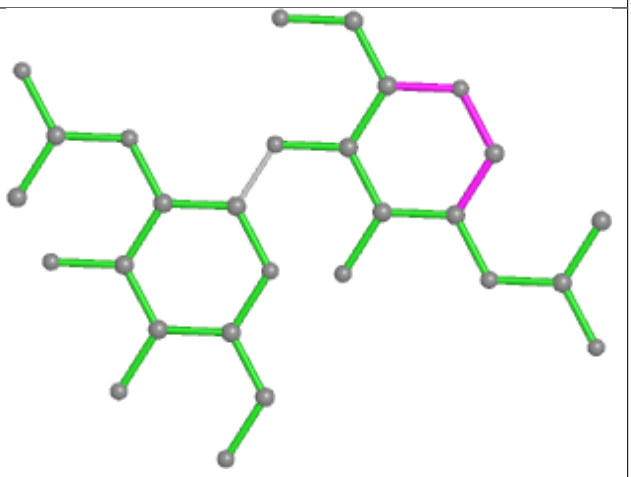


Rings

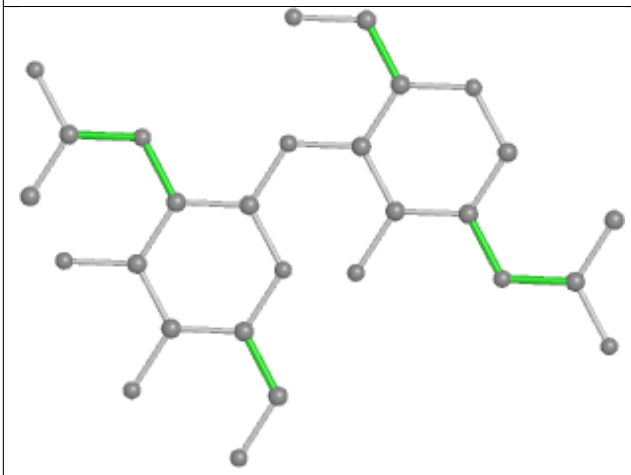
Oligosaccharide Chain K



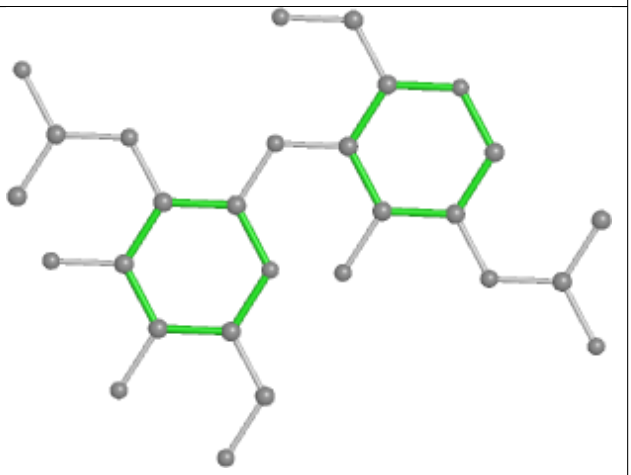
Bond lengths



Bond angles

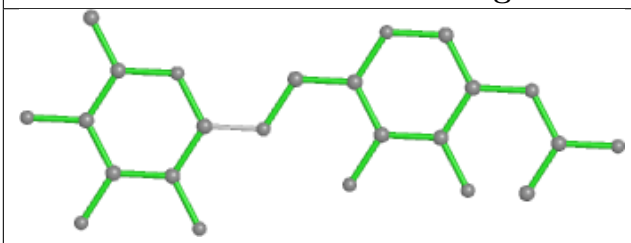


Torsions

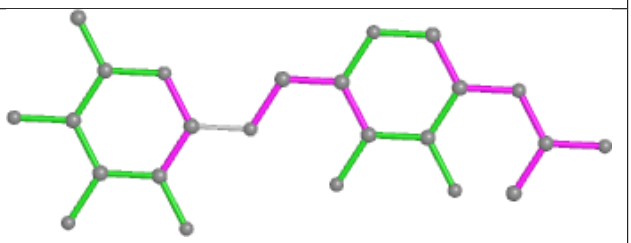


Rings

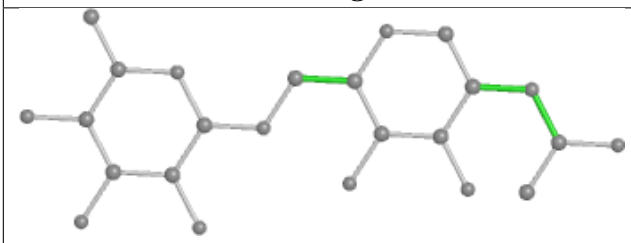
Oligosaccharide Chain G



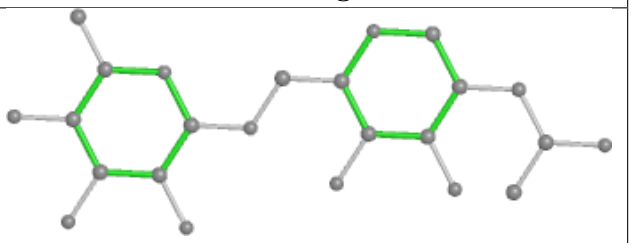
Bond lengths



Bond angles

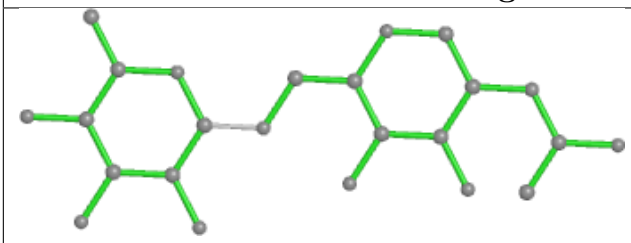


Torsions

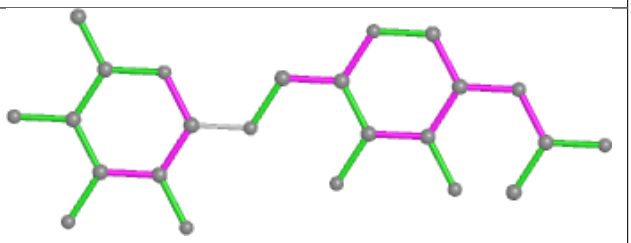


Rings

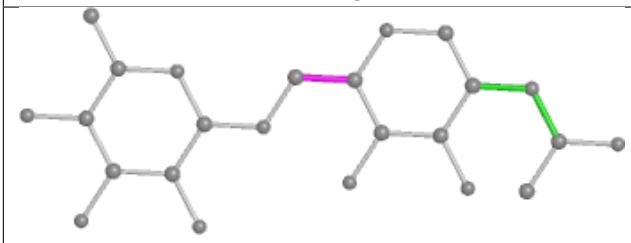
Oligosaccharide Chain J



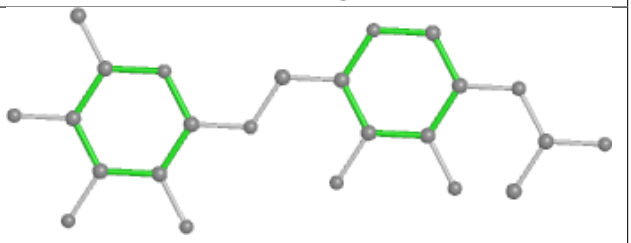
Bond lengths



Bond angles

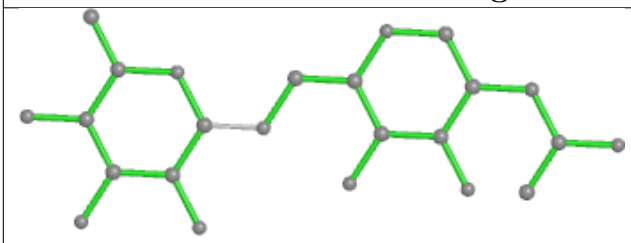


Torsions

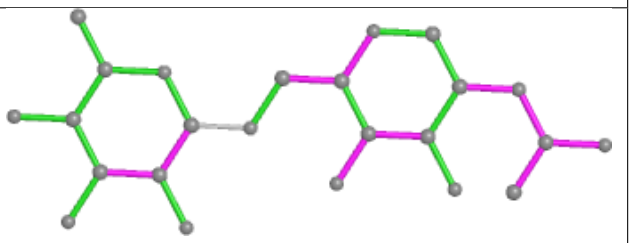


Rings

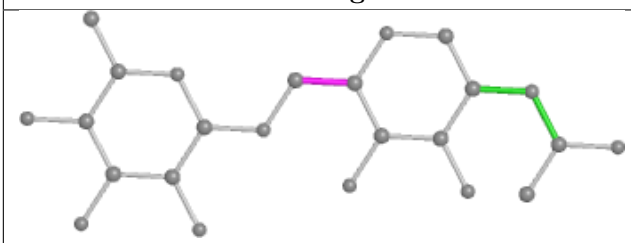
Oligosaccharide Chain M



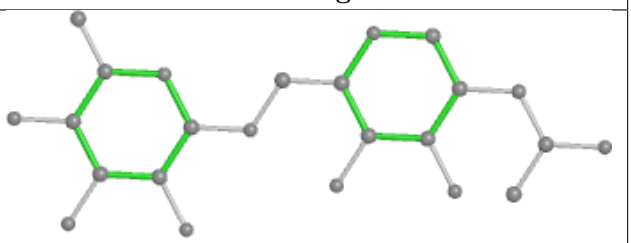
Bond lengths



Bond angles

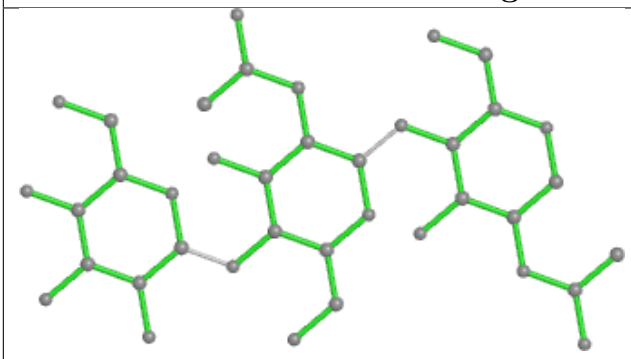


Torsions

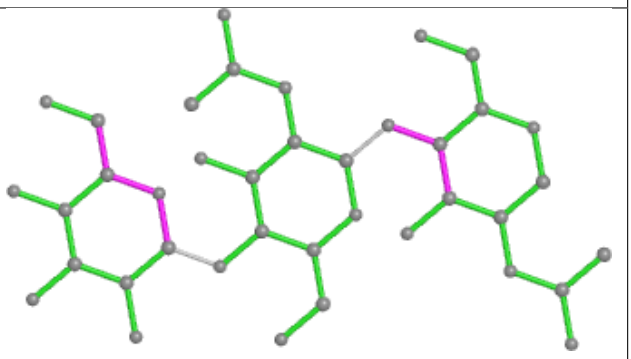


Rings

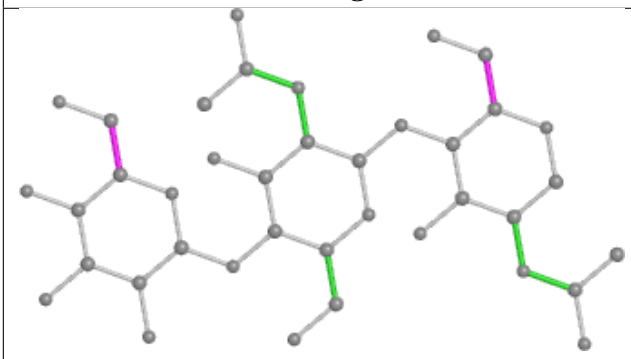
Oligosaccharide Chain I



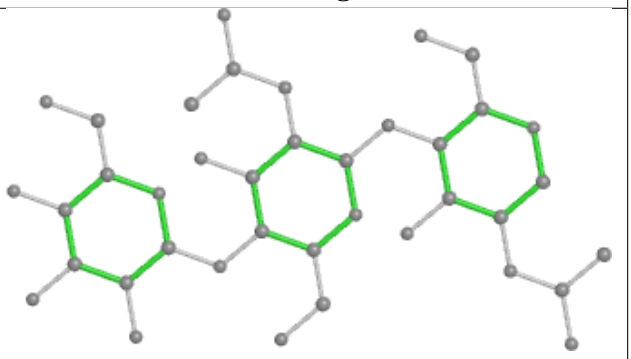
Bond lengths



Bond angles

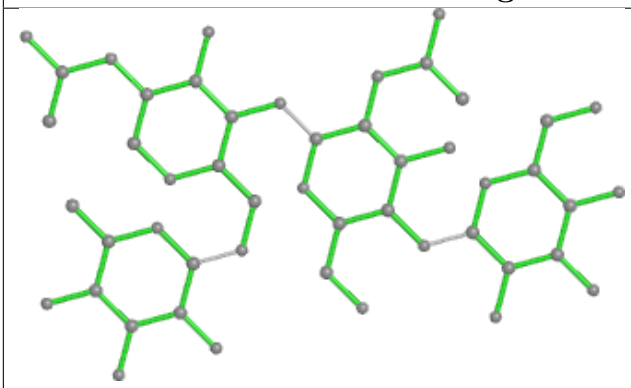


Torsions

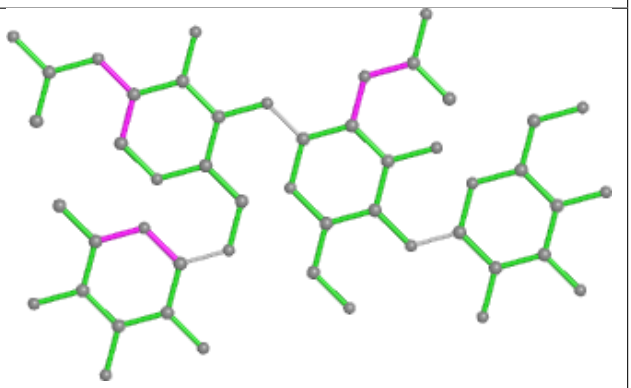


Rings

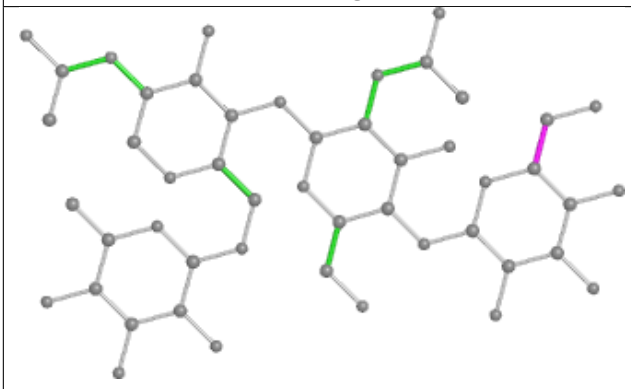
Oligosaccharide Chain L



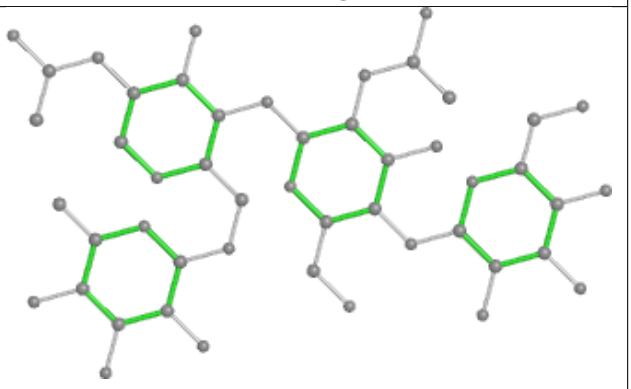
Bond lengths



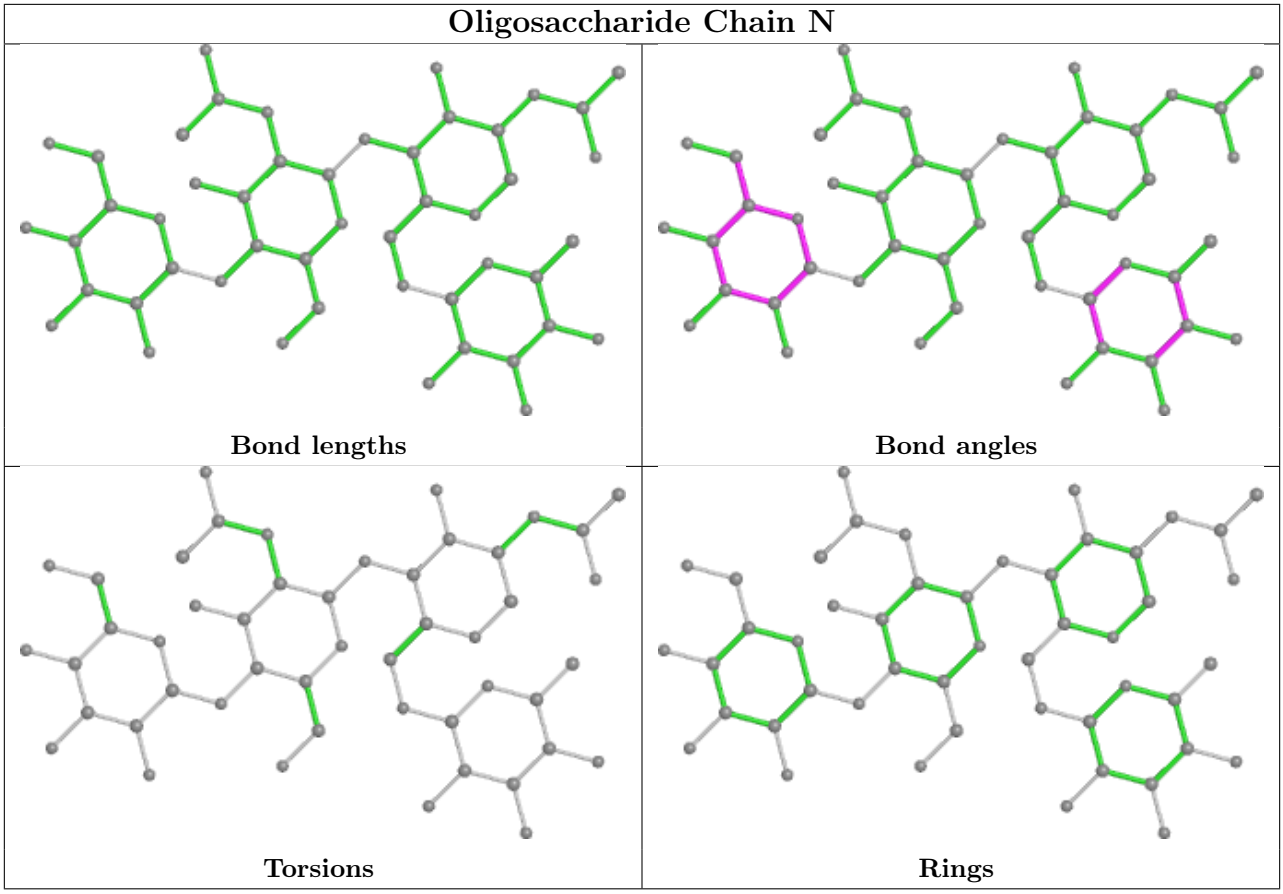
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

Of 35 ligands modelled in this entry, 8 are monoatomic - leaving 27 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	C	1200	-	6,6,6	0.42	0	5,5,5	0.29	0
12	PEG	D	1205	-	6,6,6	0.51	0	5,5,5	0.22	0
13	P6G	A	1202	-	18,18,18	0.46	0	17,17,17	0.42	0
13	P6G	B	1204	-	18,18,18	0.54	0	17,17,17	0.52	0
13	P6G	C	1202	-	18,18,18	0.52	0	17,17,17	0.40	0
12	PEG	B	1201	-	6,6,6	0.52	0	5,5,5	0.37	0
8	SER	A	908	-	5,6,6	0.88	0	5,7,7	1.35	1 (20%)
12	PEG	A	1201	-	6,6,6	0.44	0	5,5,5	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	P6G	B	1203	-	18,18,18	0.67	0	17,17,17	0.90	0
7	ASP	D	907	-	6,7,8	0.92	0	5,8,10	0.79	0
8	SER	C	908	-	5,6,6	0.75	0	5,7,7	1.60	2 (40%)
12	PEG	C	1201	-	6,6,6	0.48	0	5,5,5	0.42	0
12	PEG	A	1204	-	6,6,6	0.40	0	5,5,5	0.40	0
13	P6G	D	1203	-	18,18,18	0.52	0	17,17,17	0.35	0
11	NAG	D	1102	1	14,14,15	0.54	0	17,19,21	1.14	0
12	PEG	D	1200	-	6,6,6	0.40	0	5,5,5	0.34	0
7	ASP	C	907	-	6,7,8	0.89	0	5,8,10	0.53	0
8	SER	D	908	-	5,6,6	0.87	0	5,7,7	1.41	2 (40%)
7	ASP	B	907	-	6,7,8	0.88	0	5,8,10	1.13	0
8	SER	B	908	-	5,6,6	1.00	1 (20%)	5,7,7	1.53	1 (20%)
11	NAG	A	1100	1	14,14,15	0.45	0	17,19,21	1.02	2 (11%)
12	PEG	D	1202	-	6,6,6	0.47	0	5,5,5	0.36	0
7	ASP	A	907	-	6,7,8	0.95	0	5,8,10	0.95	0
12	PEG	B	1202	-	6,6,6	0.46	0	5,5,5	0.31	0
13	P6G	D	1201	-	18,18,18	0.61	0	17,17,17	0.94	1 (5%)
12	PEG	A	1200	-	6,6,6	0.43	0	5,5,5	0.42	0
12	PEG	B	1200	-	6,6,6	0.42	0	5,5,5	0.38	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	C	1200	-	-	2/4/4/4	-
12	PEG	D	1205	-	-	2/4/4/4	-
13	P6G	A	1202	-	-	5/16/16/16	-
13	P6G	B	1204	-	-	10/16/16/16	-
13	P6G	C	1202	-	-	7/16/16/16	-
12	PEG	B	1201	-	-	1/4/4/4	-
8	SER	A	908	-	-	0/6/6/6	-
12	PEG	A	1201	-	-	1/4/4/4	-
13	P6G	B	1203	-	-	12/16/16/16	-
7	ASP	D	907	-	-	2/5/6/8	-
8	SER	C	908	-	-	0/6/6/6	-
12	PEG	C	1201	-	-	1/4/4/4	-
12	PEG	A	1204	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	P6G	D	1203	-	-	5/16/16/16	-
11	NAG	D	1102	1	-	0/6/23/26	0/1/1/1
12	PEG	D	1200	-	-	2/4/4/4	-
7	ASP	C	907	-	-	0/5/6/8	-
8	SER	D	908	-	-	0/6/6/6	-
7	ASP	B	907	-	-	3/5/6/8	-
8	SER	B	908	-	-	0/6/6/6	-
11	NAG	A	1100	1	-	0/6/23/26	0/1/1/1
12	PEG	D	1202	-	-	1/4/4/4	-
7	ASP	A	907	-	-	2/5/6/8	-
12	PEG	B	1202	-	-	3/4/4/4	-
13	P6G	D	1201	-	-	8/16/16/16	-
12	PEG	A	1200	-	-	3/4/4/4	-
12	PEG	B	1200	-	-	3/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	908	SER	OXT-C	-2.18	1.23	1.30

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	908	SER	OXT-C-O	-2.71	117.94	124.09
11	A	1100	NAG	O5-C5-C6	2.54	111.18	107.20
8	C	908	SER	OXT-C-O	-2.48	118.47	124.09
8	C	908	SER	OXT-C-CA	2.47	121.79	113.38
13	D	1201	P6G	O16-C17-C18	2.44	120.79	110.07

There are no chirality outliers.

5 of 75 torsion outliers are listed below:

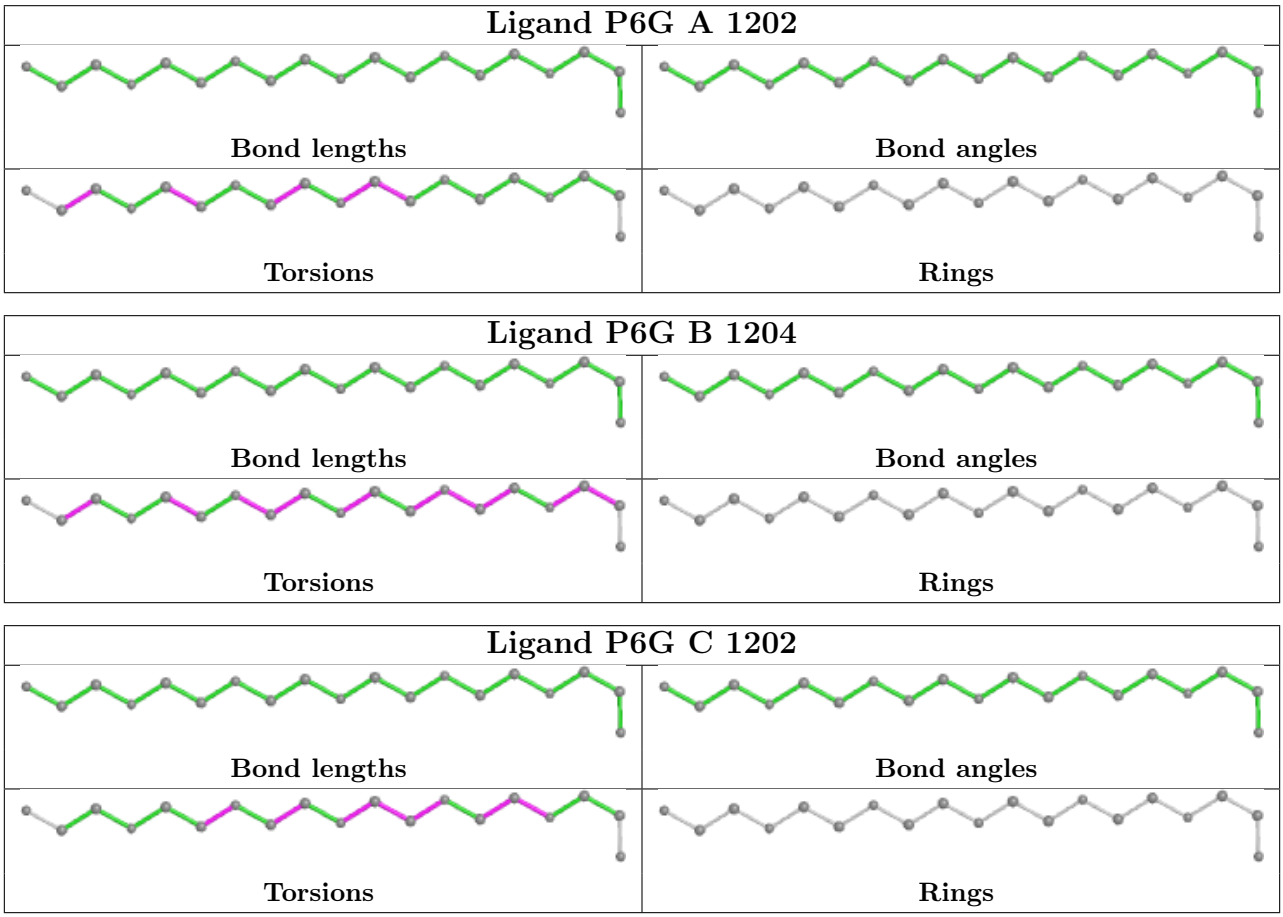
Mol	Chain	Res	Type	Atoms
7	B	907	ASP	O-C-CA-CB
7	B	907	ASP	C-CA-CB-CG
13	B	1204	P6G	O16-C17-C18-O19
13	B	1203	P6G	O7-C8-C9-O10
13	B	1204	P6G	O10-C11-C12-O13

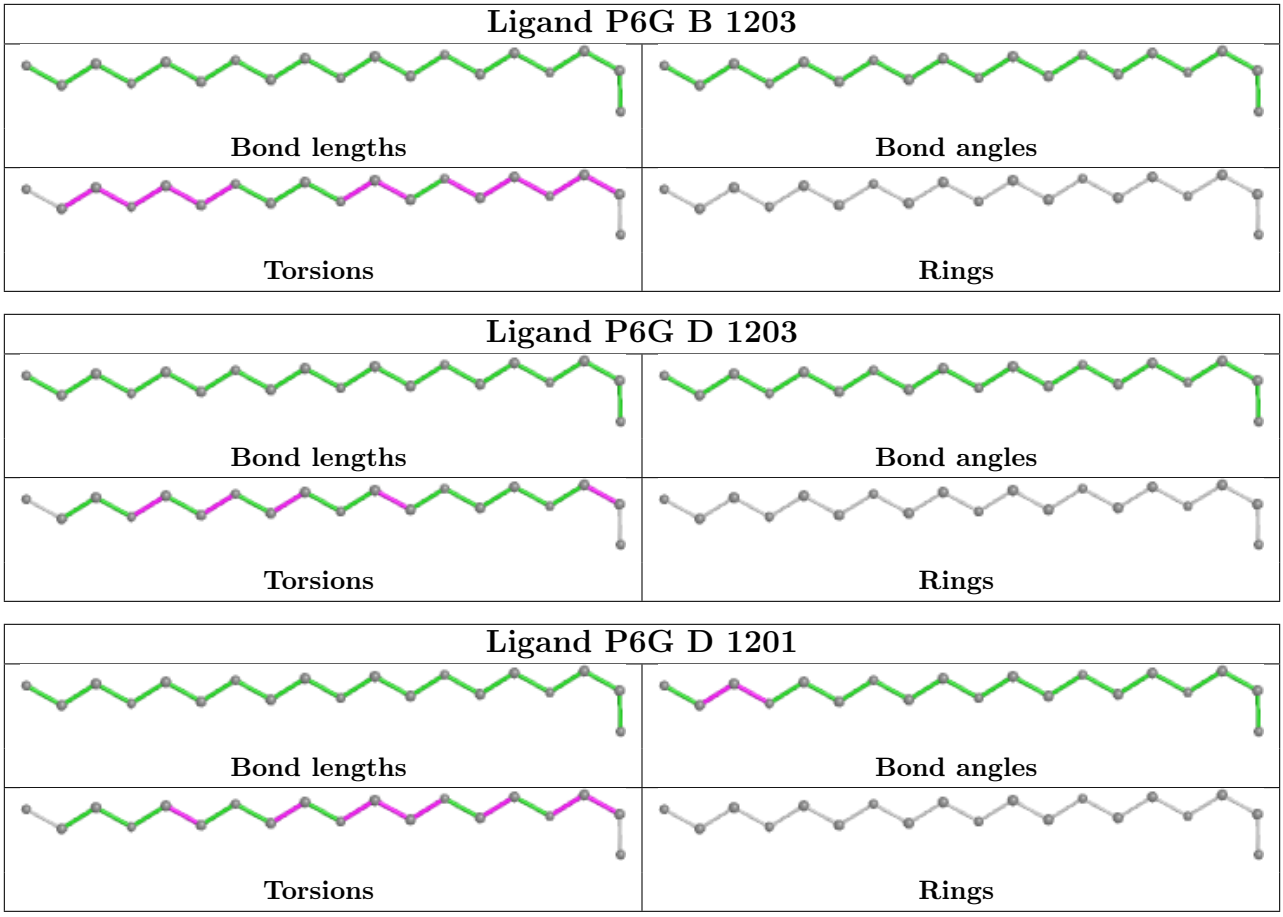
There are no ring outliers.

4 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	A	1202	P6G	1	0
12	A	1201	PEG	1	0
7	A	907	ASP	1	0
13	D	1201	P6G	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.





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	603/629 (95%)	-0.22	13 (2%)	62	57	14, 24, 42, 69	0
1	B	605/629 (96%)	-0.21	15 (2%)	57	52	12, 21, 37, 69	0
1	C	609/629 (96%)	-0.35	9 (1%)	73	70	12, 19, 35, 59	0
1	D	607/629 (96%)	-0.14	29 (4%)	30	25	12, 20, 43, 60	0
All	All	2424/2516 (96%)	-0.23	66 (2%)	54	49	12, 21, 41, 69	0

The worst 5 of 66 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	135	THR	7.0
1	A	415	THR	6.6
1	B	134	ALA	6.4
1	D	88	LEU	6.1
1	B	325	GLY	5.7

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
3	FUC	J	2	10/11	0.57	0.38	54,58,61,62	0
6	MAN	N	3	11/12	0.64	0.26	61,63,65,65	0

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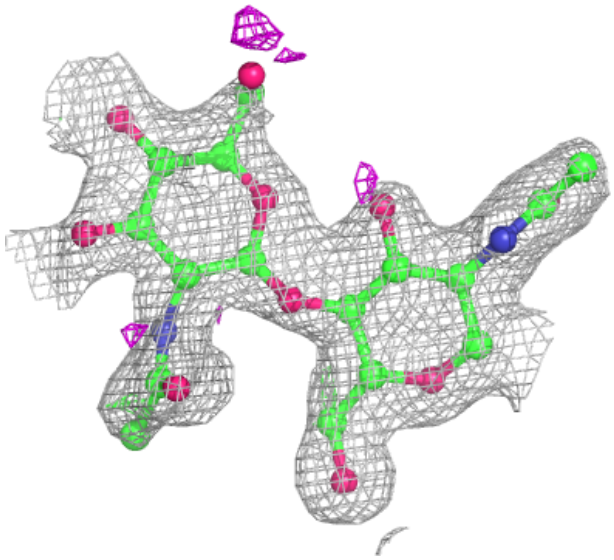
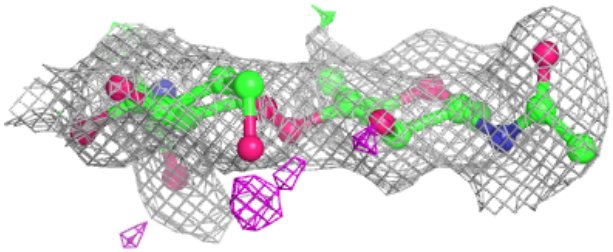
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	FUC	G	2	10/11	0.69	0.25	43,47,48,49	0
3	FUC	M	2	10/11	0.70	0.29	50,54,56,56	0
2	NAG	H	2	14/15	0.70	0.39	56,59,61,61	0
2	NAG	E	2	14/15	0.71	0.42	54,59,60,61	0
5	FUL	L	4	10/11	0.72	0.19	44,48,50,50	0
3	NAG	G	1	14/15	0.79	0.13	29,34,39,40	0
3	NAG	M	1	14/15	0.80	0.14	30,35,40,44	0
2	NAG	K	2	14/15	0.80	0.30	40,44,48,49	0
2	NAG	F	2	14/15	0.81	0.33	65,66,68,68	0
2	NAG	H	1	14/15	0.82	0.26	37,39,44,50	0
2	NAG	F	1	14/15	0.83	0.26	61,63,66,69	0
4	BMA	I	3	11/12	0.83	0.30	60,63,64,65	0
6	NAG	N	2	14/15	0.85	0.16	42,49,53,57	0
6	FUC	N	4	10/11	0.85	0.17	40,42,45,45	0
5	BMA	L	3	11/12	0.86	0.18	40,42,45,47	0
3	NAG	J	1	14/15	0.87	0.15	32,38,43,46	0
4	NAG	I	2	14/15	0.87	0.23	47,49,52,56	0
2	NAG	E	1	14/15	0.88	0.21	34,37,41,47	0
5	NAG	L	2	14/15	0.91	0.14	32,34,39,41	0
6	NAG	N	1	14/15	0.92	0.10	31,34,36,38	0
2	NAG	K	1	14/15	0.92	0.15	28,31,33,36	0
5	NAG	L	1	14/15	0.94	0.09	27,29,32,37	0
4	NAG	I	1	14/15	0.95	0.13	38,40,43,43	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:

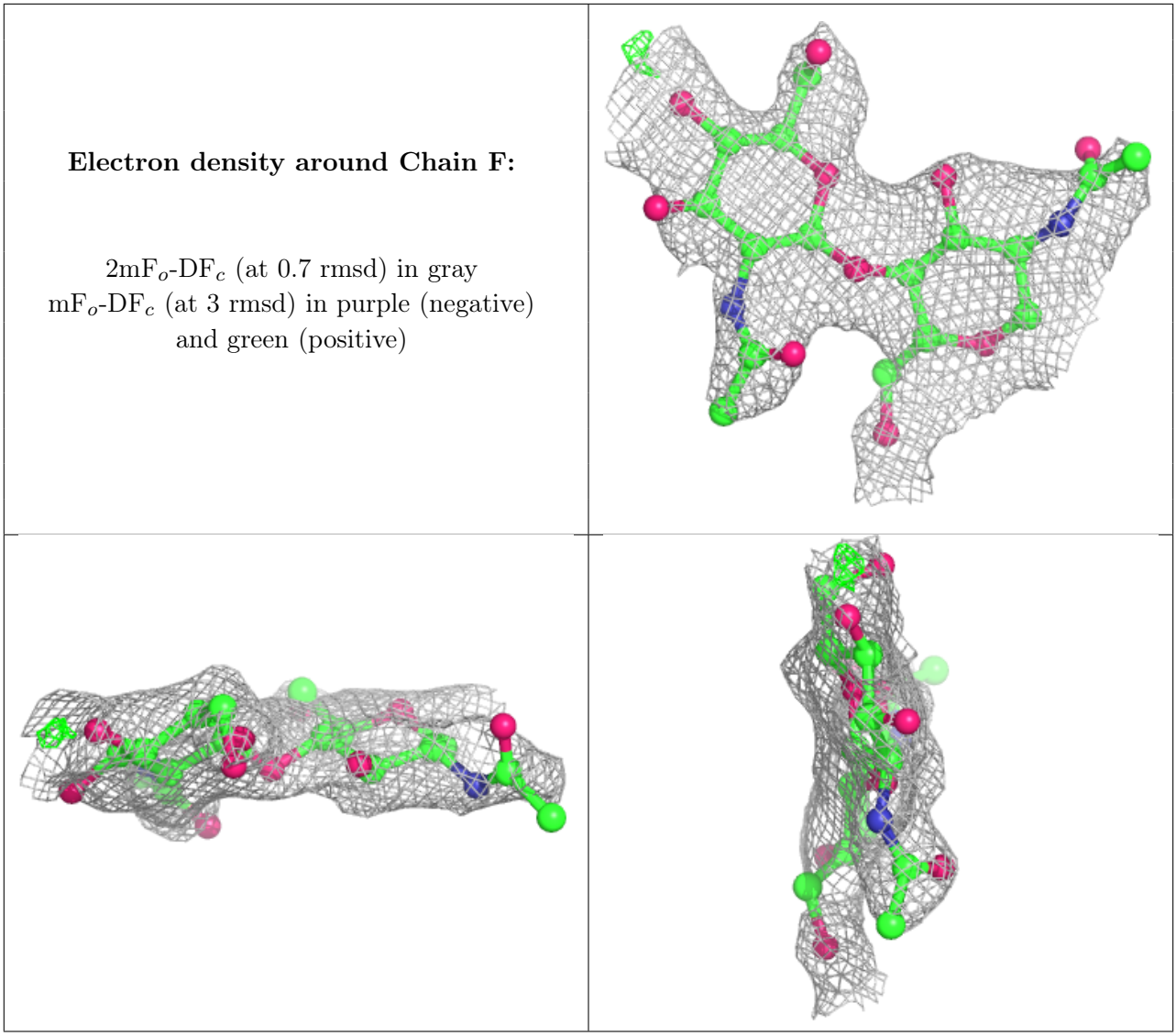
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





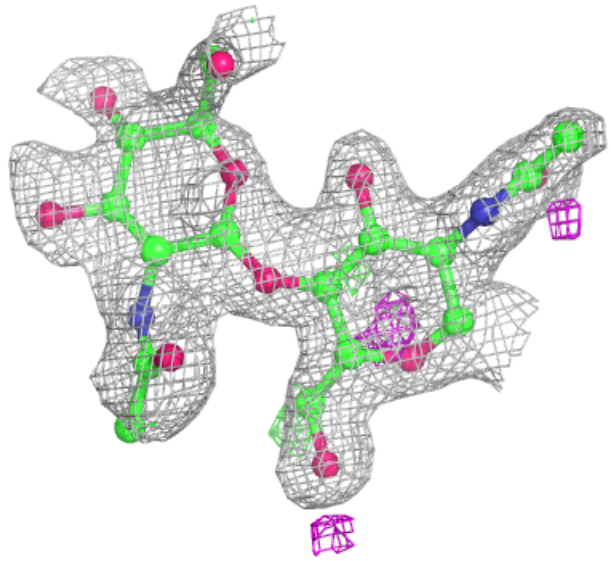
Electron density around Chain F:

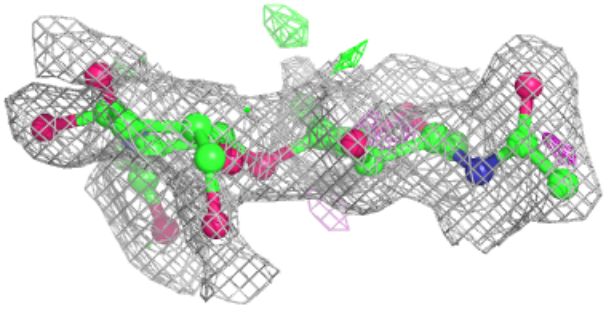
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

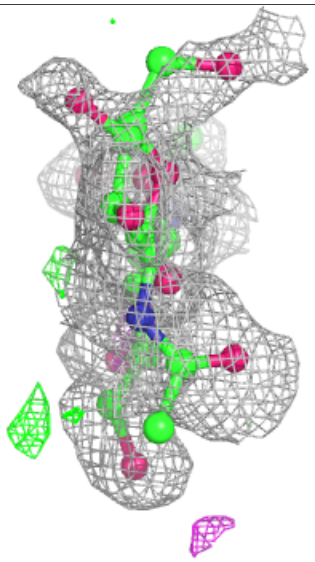


Electron density around Chain H:

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

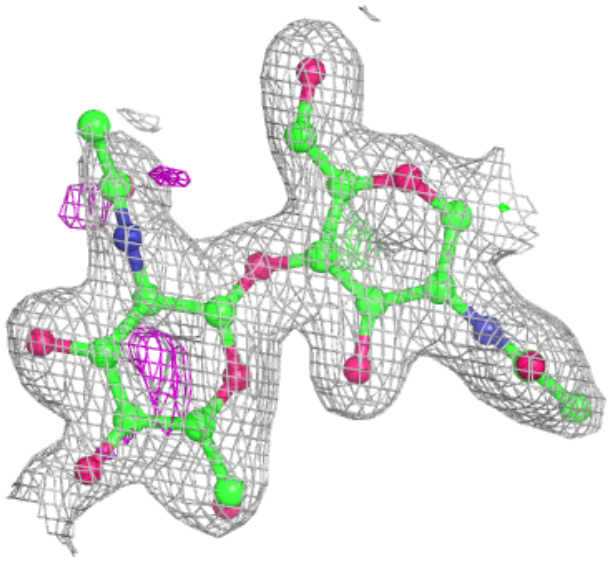


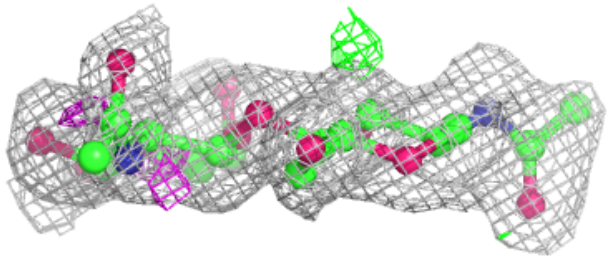


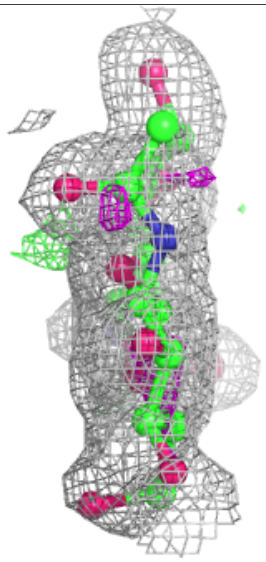


Electron density around Chain K:

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

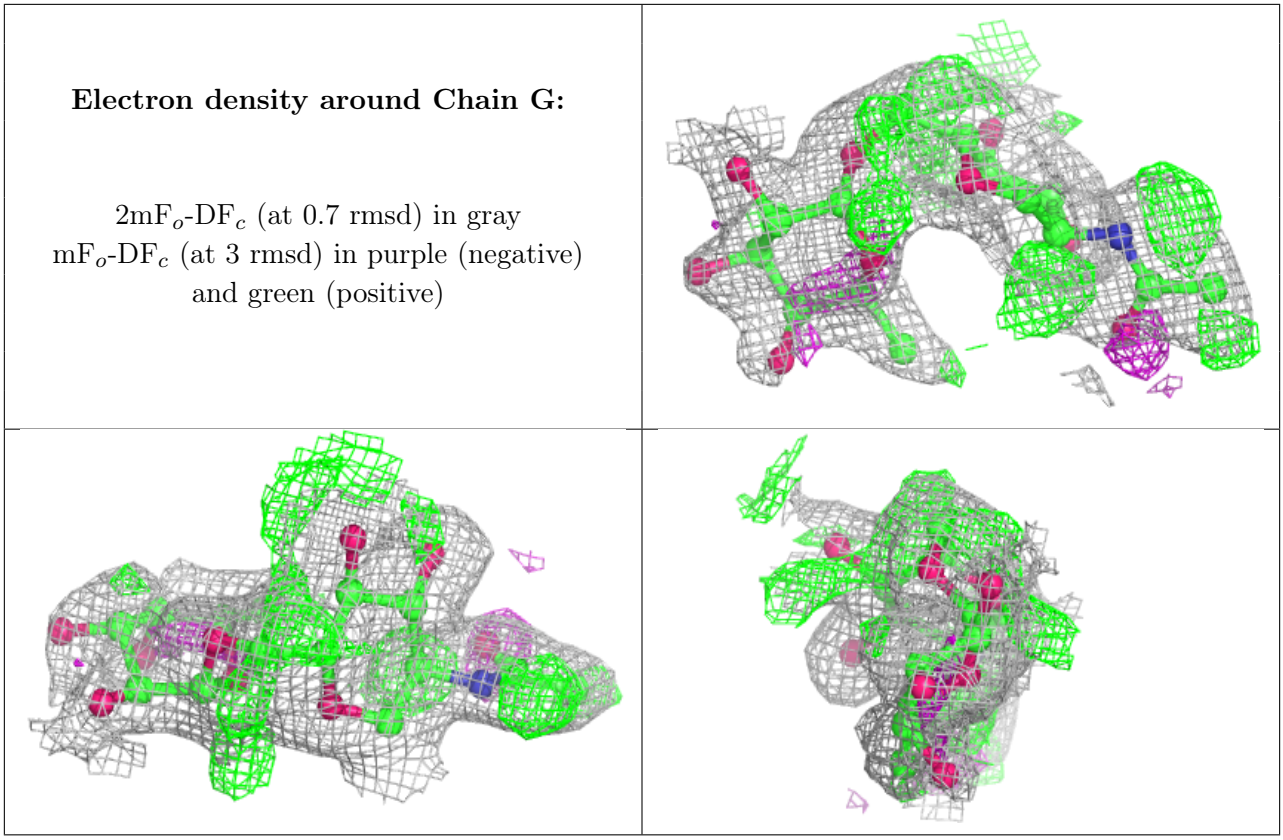






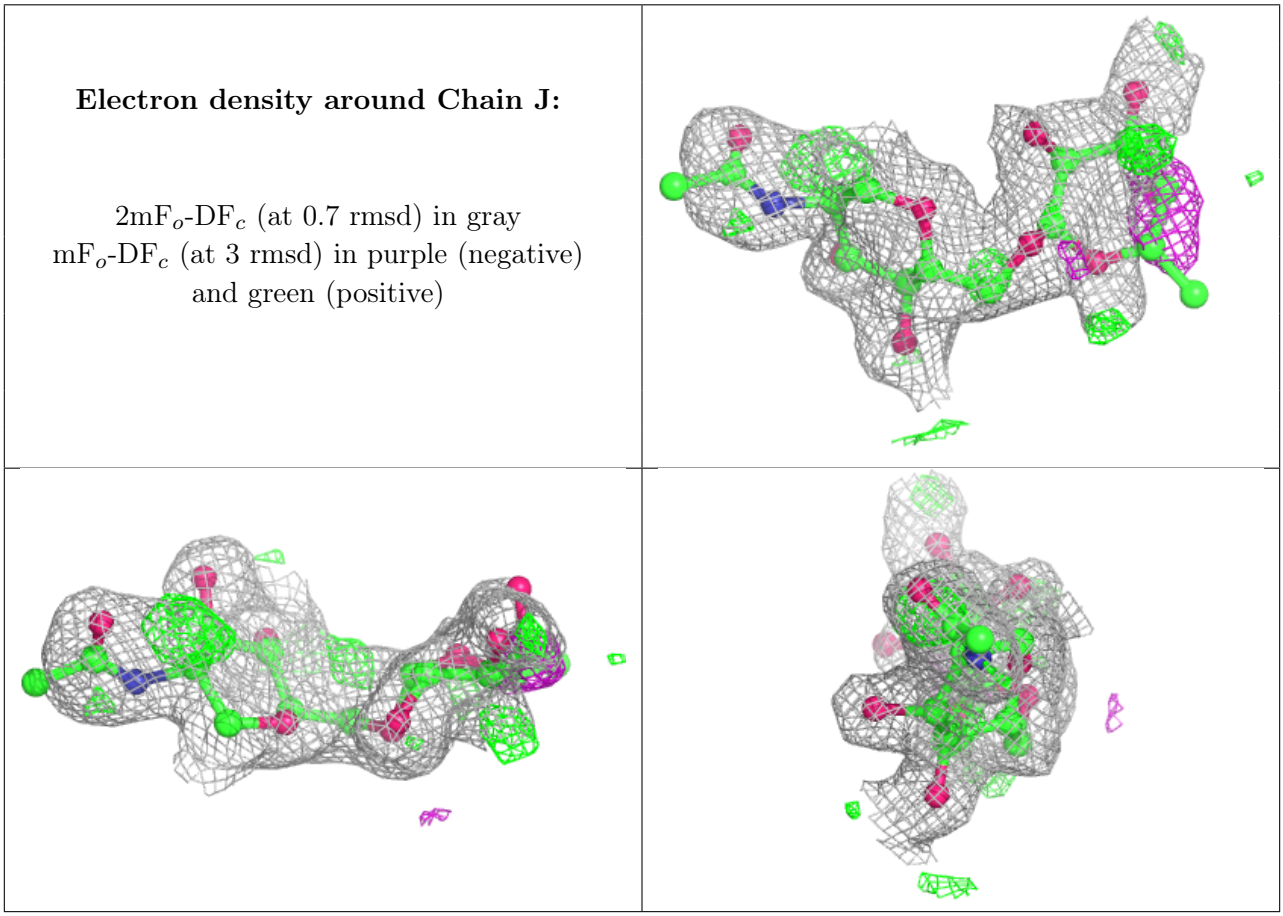
Electron density around Chain G:

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



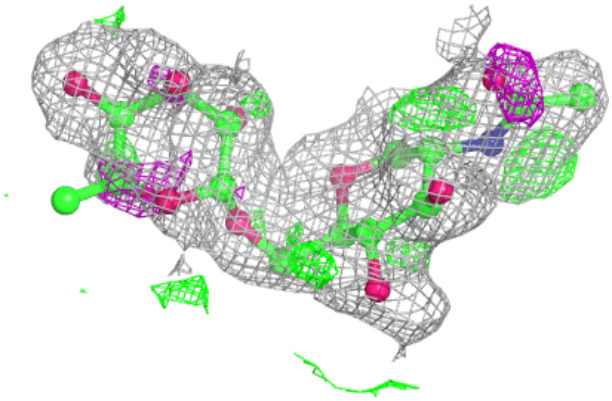
Electron density around Chain J:

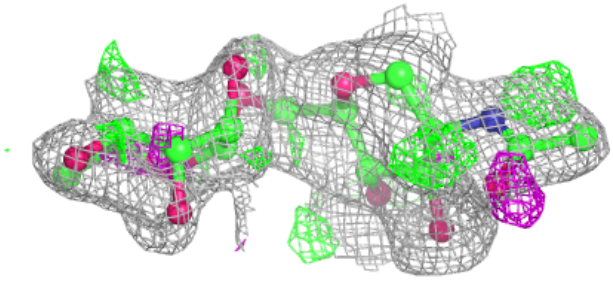
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

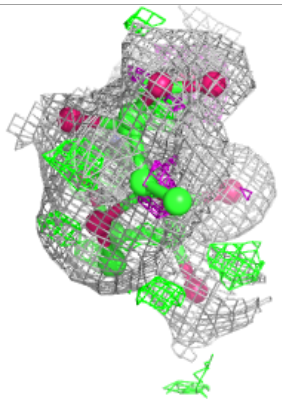


Electron density around Chain M:

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

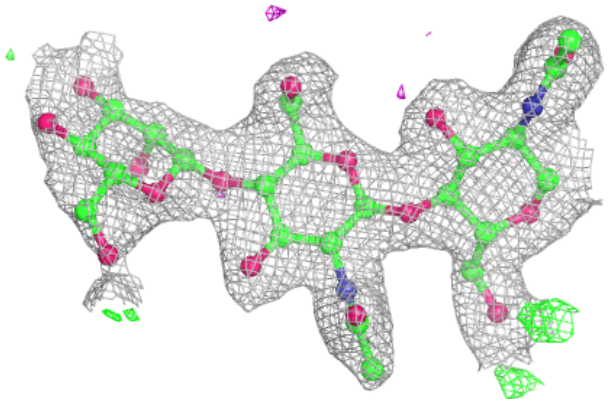


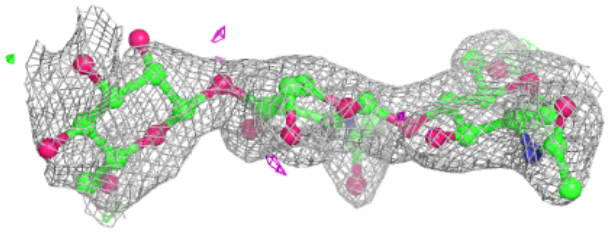


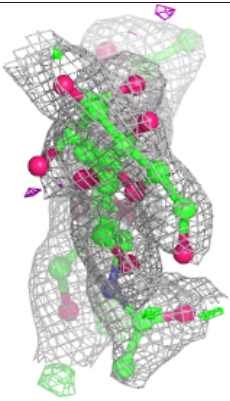


Electron density around Chain I:

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

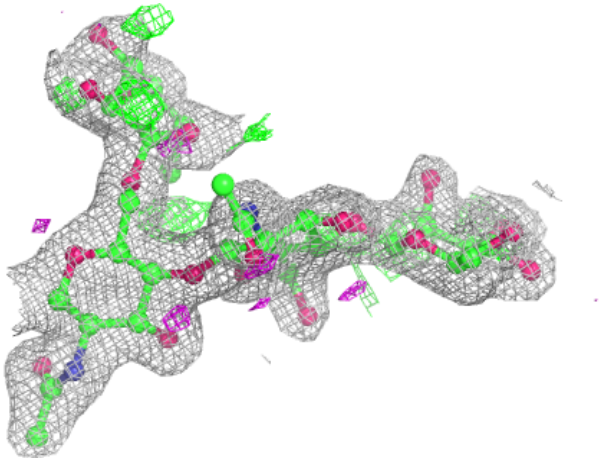


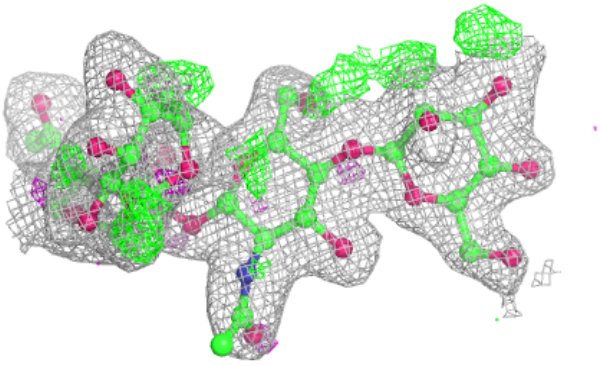


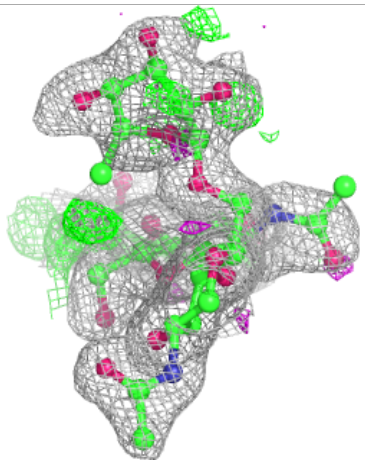


Electron density around Chain L:

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

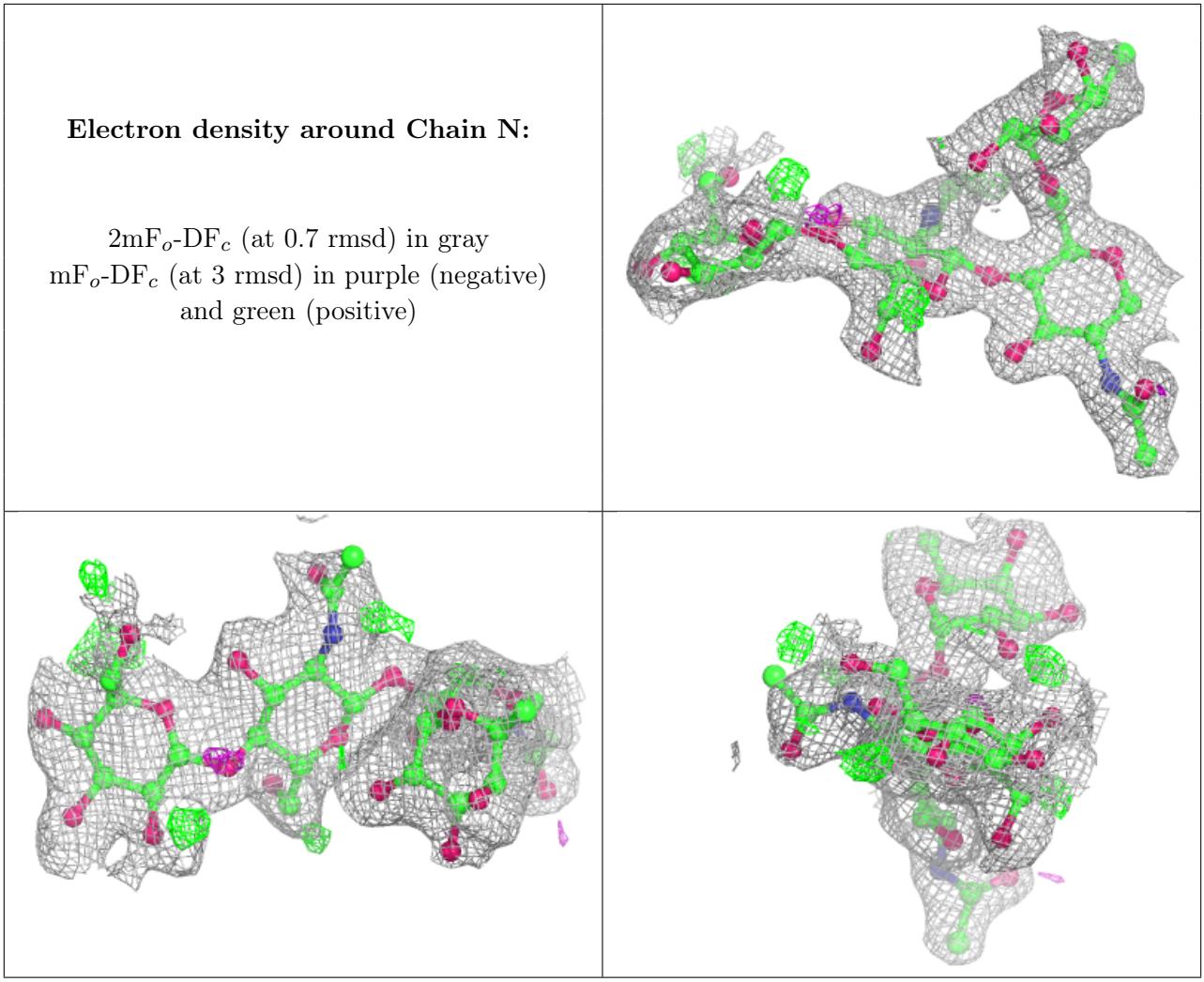






Electron density around Chain N:

$2mF_o$-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
13	P6G	C	1202	19/19	0.66	0.25	44,57,61,63	0
12	PEG	B	1201	7/7	0.72	0.18	45,46,47,48	0
13	P6G	B	1204	19/19	0.74	0.27	48,55,65,66	0
11	NAG	D	1102	14/15	0.74	0.26	36,37,40,40	0
13	P6G	D	1203	19/19	0.77	0.21	44,56,64,64	0
13	P6G	B	1203	19/19	0.79	0.16	36,39,47,47	0
12	PEG	D	1205	7/7	0.79	0.20	43,44,48,49	0
11	NAG	A	1100	14/15	0.80	0.17	37,42,47,50	0
12	PEG	B	1202	7/7	0.81	0.18	41,41,42,43	0

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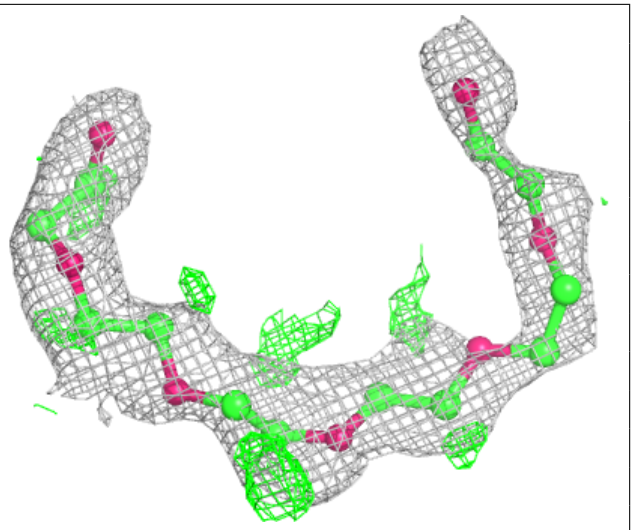
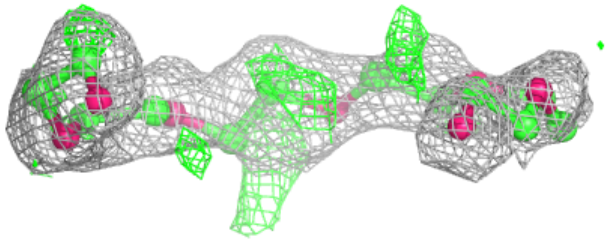
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
12	PEG	D	1200	7/7	0.82	0.15	51,51,53,55	0
12	PEG	A	1204	7/7	0.84	0.22	40,40,43,44	0
12	PEG	A	1200	7/7	0.85	0.18	53,53,54,54	0
12	PEG	C	1200	7/7	0.86	0.13	44,45,48,49	0
13	P6G	A	1202	19/19	0.86	0.12	33,39,43,44	0
13	P6G	D	1201	19/19	0.86	0.14	27,30,42,43	0
7	ASP	B	907	8/9	0.86	0.17	22,27,36,37	0
12	PEG	B	1200	7/7	0.87	0.19	61,61,62,63	0
12	PEG	D	1202	7/7	0.87	0.14	48,48,49,50	0
12	PEG	A	1201	7/7	0.87	0.15	40,42,45,46	0
12	PEG	C	1201	7/7	0.88	0.17	38,39,43,44	0
7	ASP	C	907	8/9	0.90	0.13	18,23,29,31	0
7	ASP	D	907	8/9	0.91	0.14	20,25,36,37	0
7	ASP	A	907	8/9	0.91	0.16	21,26,36,37	0
8	SER	B	908	7/7	0.94	0.15	18,20,23,25	0
8	SER	C	908	7/7	0.95	0.08	17,19,21,23	0
8	SER	A	908	7/7	0.95	0.10	20,22,24,26	0
8	SER	D	908	7/7	0.97	0.09	20,21,22,25	0
9	ZN	D	1001	1/1	1.00	0.04	17,17,17,17	0
10	CL	A	1002	1/1	1.00	0.07	18,18,18,18	0
10	CL	B	1002	1/1	1.00	0.06	16,16,16,16	0
10	CL	C	1002	1/1	1.00	0.06	14,14,14,14	0
10	CL	D	1002	1/1	1.00	0.05	15,15,15,15	0
9	ZN	A	1001	1/1	1.00	0.04	18,18,18,18	0
9	ZN	B	1001	1/1	1.00	0.05	17,17,17,17	0
9	ZN	C	1001	1/1	1.00	0.04	15,15,15,15	0

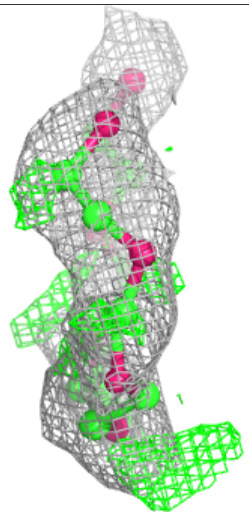
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around P6G C 1202:

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

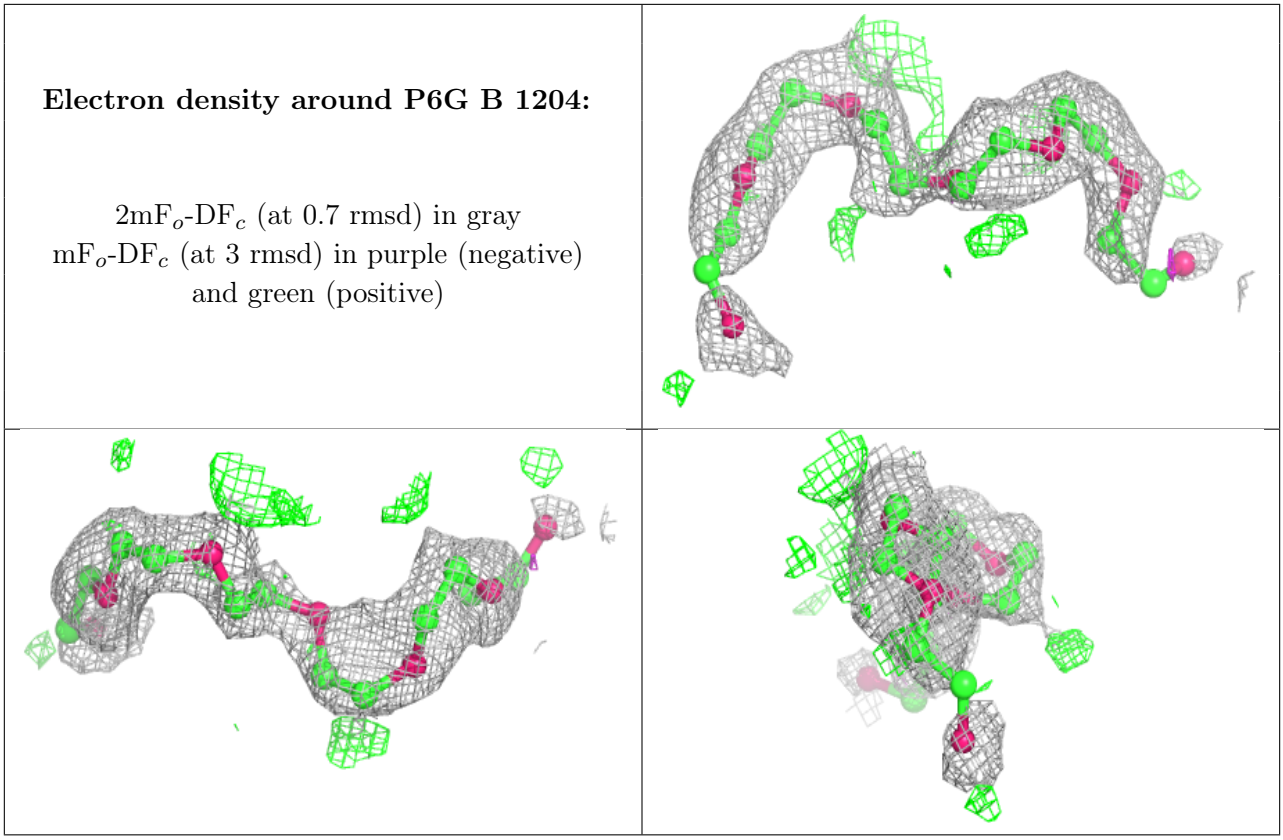






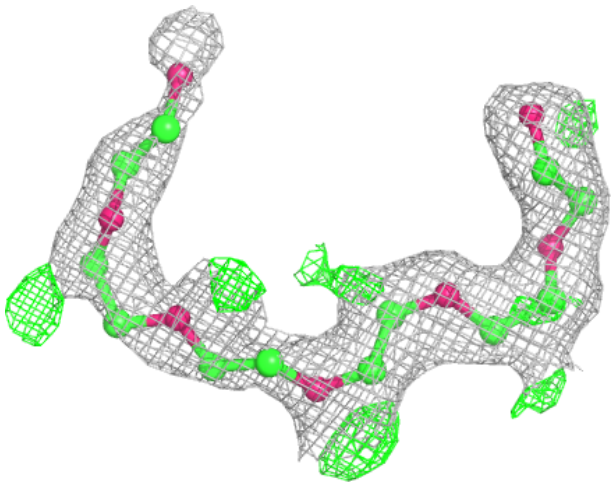
Electron density around P6G B 1204:

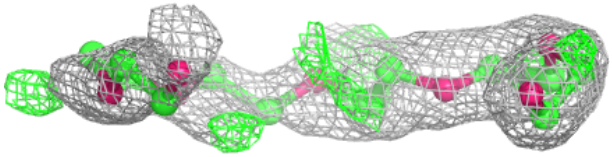
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

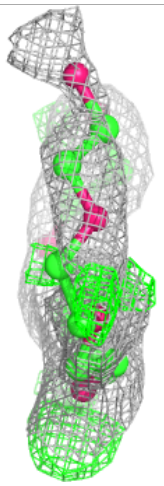


Electron density around P6G D 1203:

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

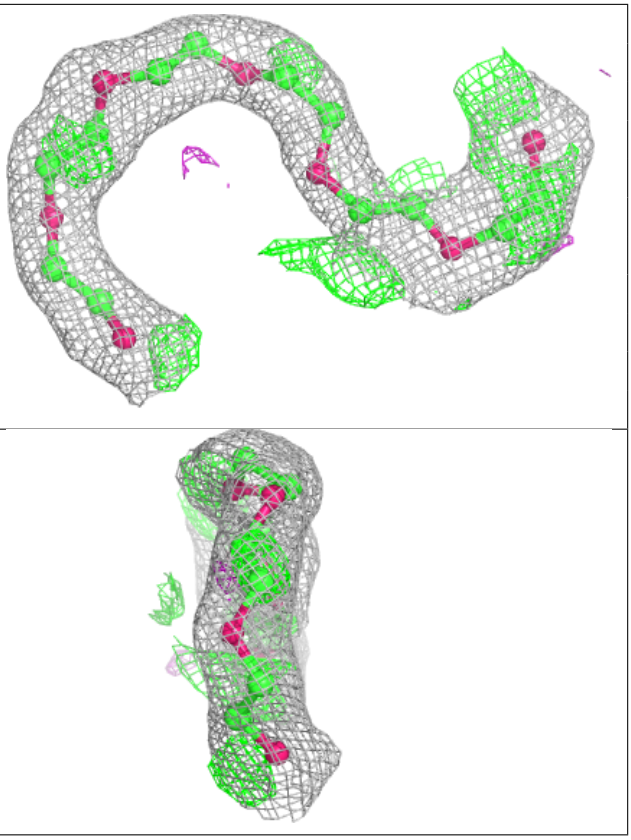






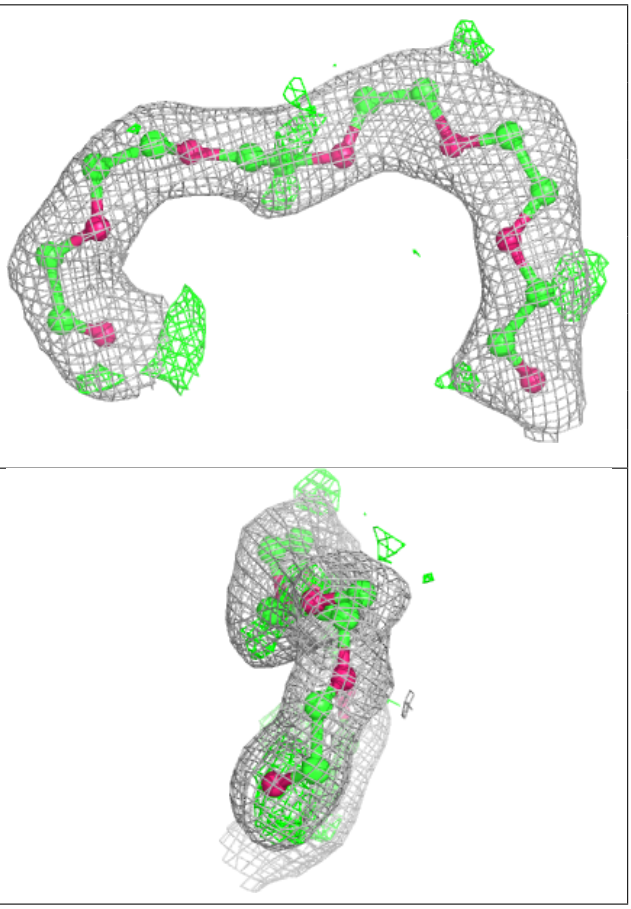
Electron density around P6G B 1203:

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



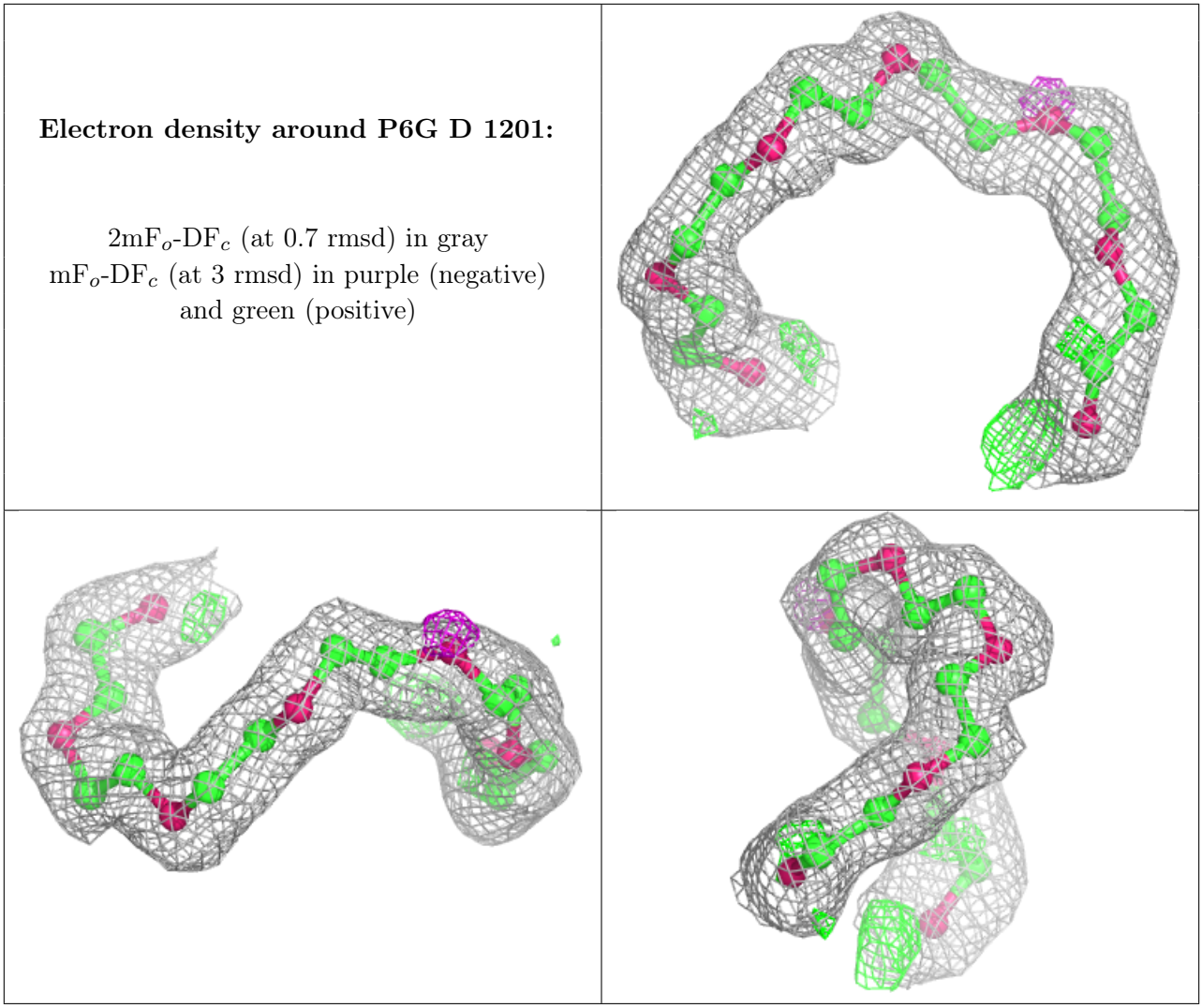
Electron density around P6G A 1202:

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



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)



6.5 Other polymers

There are no such residues in this entry.