Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 03:35 PM BST

PDB ID	:	5M8S
Title	:	Crystal structure of human tyrosinase related protein 1 mutant (T391V-R374S-Y362F) in complex with phenylthiourea (PTU)
Authors	:	Lai, X.; Soler-Lopez, M.; Wichers, H.J.; Dijkstra, B.W.
Deposited on	:	2016-10-29
Resolution	:	2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

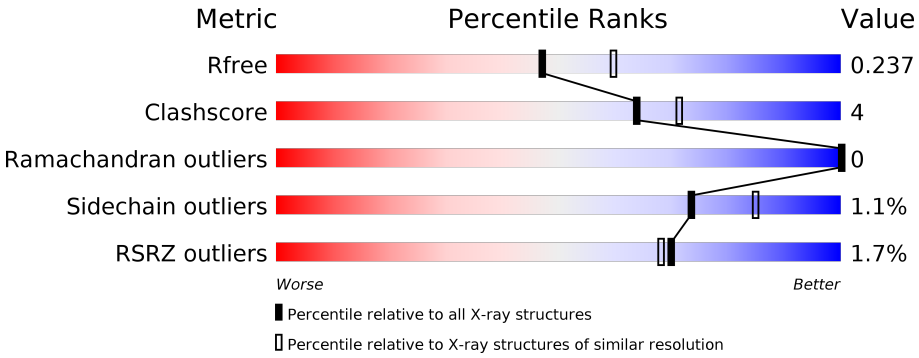
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	446	91% 9%
1	B	446	3% 89% 10%
1	C	446	2% 90% 10%
1	D	446	88% 12%
2	E	3	33% 33% 33%
2	H	3	33% 67%

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Mol	Chain	Length	Quality of chain
2	P	3	33% 67%
3	F	2	100%
3	G	2	50% 50%
3	J	2	100%
3	L	2	50% 50%
3	N	2	100%
3	O	2	100%
3	R	2	100%
3	T	2	50% 50%
4	I	2	100%
5	K	6	33% 67%
6	M	2	100%
7	Q	5	80% 20%
8	S	5	20% 80%

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
10	URS	B	516	-	X	-	-
10	URS	C	510	-	X	-	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 15622 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.

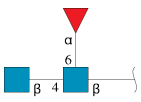
- Molecule 1 is a protein called 5,6-dihydroxyindole-2-carboxylic acid oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	446	Total	C	N	O	S	0	0	0
			3554	2231	629	671	23			
1	B	446	Total	C	N	O	S	0	0	0
			3554	2231	629	671	23			
1	C	446	Total	C	N	O	S	0	0	0
			3554	2231	629	671	23			
1	D	446	Total	C	N	O	S	0	0	0
			3554	2231	629	671	23			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	362	PHE	TYR	engineered mutation	UNP P17643
A	374	SER	ARG	engineered mutation	UNP P17643
A	391	VAL	THR	engineered mutation	UNP P17643
B	362	PHE	TYR	engineered mutation	UNP P17643
B	374	SER	ARG	engineered mutation	UNP P17643
B	391	VAL	THR	engineered mutation	UNP P17643
C	362	PHE	TYR	engineered mutation	UNP P17643
C	374	SER	ARG	engineered mutation	UNP P17643
C	391	VAL	THR	engineered mutation	UNP P17643
D	362	PHE	TYR	engineered mutation	UNP P17643
D	374	SER	ARG	engineered mutation	UNP P17643
D	391	VAL	THR	engineered mutation	UNP P17643

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

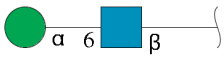


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	E	3	Total C N O 38 22 2 14	0	0	0
2	H	3	Total C N O 38 22 2 14	0	0	0
2	P	3	Total C N O 38 22 2 14	0	0	0

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

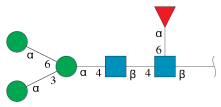
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	F	2	Total C N O 28 16 2 10	0	0	0
3	G	2	Total C N O 28 16 2 10	0	0	0
3	J	2	Total C N O 28 16 2 10	0	0	0
3	L	2	Total C N O 28 16 2 10	0	0	0
3	N	2	Total C N O 28 16 2 10	0	0	0
3	O	2	Total C N O 28 16 2 10	0	0	0
3	R	2	Total C N O 28 16 2 10	0	0	0
3	T	2	Total C N O 28 16 2 10	0	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	I	2	Total C N O 25 14 1 10	0	0	0

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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.

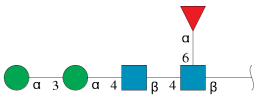


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	K	6	71	40	2	29	0	0	0

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

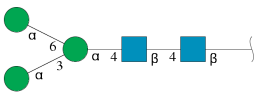
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
6	M	2	24	14	1	9	0	0	0

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-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.



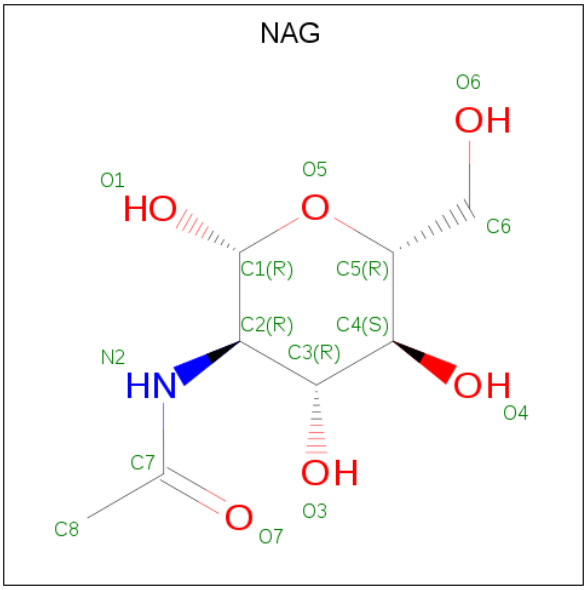
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
7	Q	5	60	34	2	24	0	0	0

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



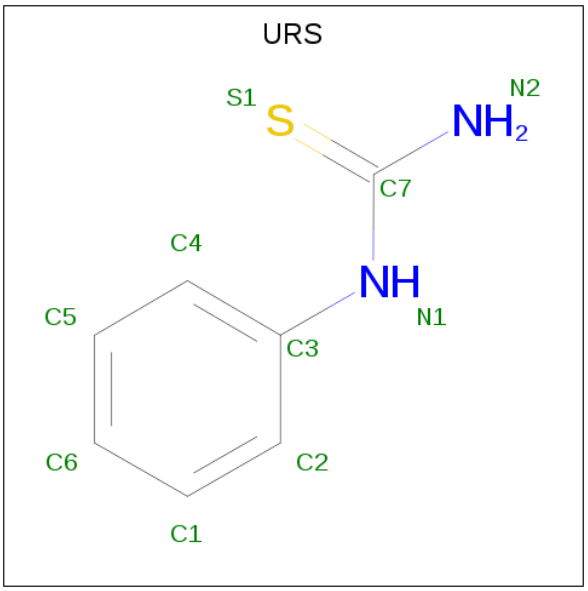
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
8	S	5	Total C N O 61 34 2 25	0	0	0

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



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

- Molecule 10 is N-PHENYLTHIOUREA (three-letter code: URS) (formula: $C_7H_8N_2S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total C N S 10 7 2 1	0	0
10	B	1	Total C N S 10 7 2 1	0	0
10	C	1	Total C N S 10 7 2 1	0	0
10	D	1	Total C N S 10 7 2 1	0	0

- Molecule 11 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	B	2	Total Zn 2 2	0	0
11	A	3	Total Zn 3 3	0	0
11	D	2	Total Zn 2 2	0	0
11	C	2	Total Zn 2 2	0	0

- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	205	Total O 205 205	0	0

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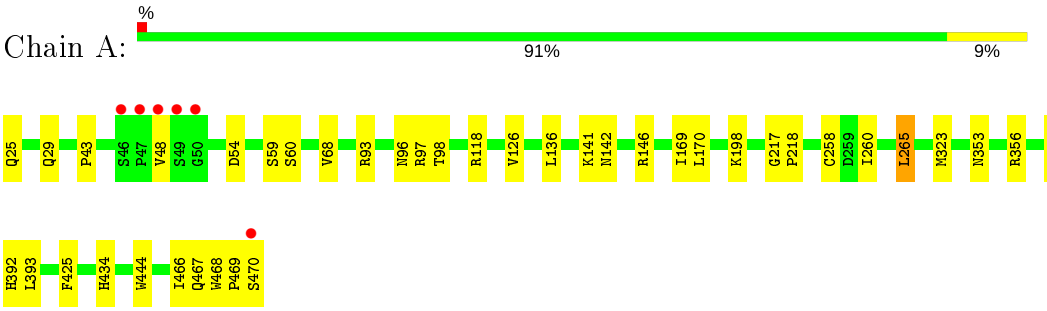
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	B	168	Total O 168 168	0	0
12	C	159	Total O 159 159	0	0
12	D	190	Total O 190 190	0	0

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.

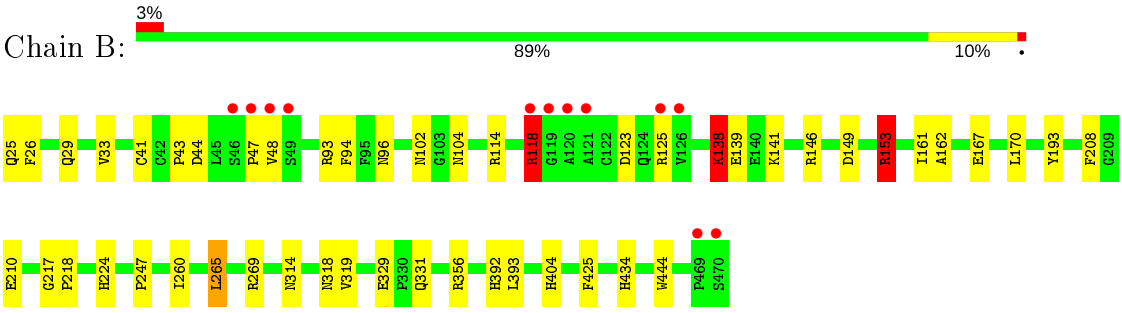
- Molecule 1: 5,6-dihydroxyindole-2-carboxylic acid oxidase

Chain A:



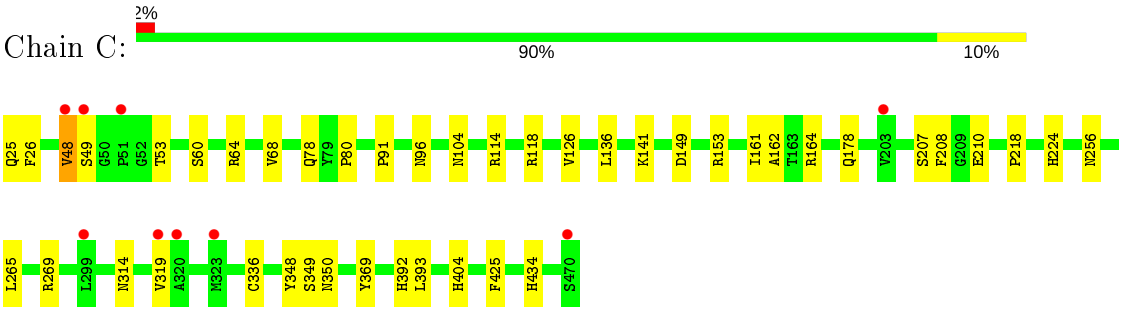
- Molecule 1: 5,6-dihydroxyindole-2-carboxylic acid oxidase

Chain B:



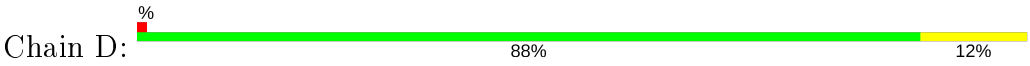
- Molecule 1: 5,6-dihydroxyindole-2-carboxylic acid oxidase

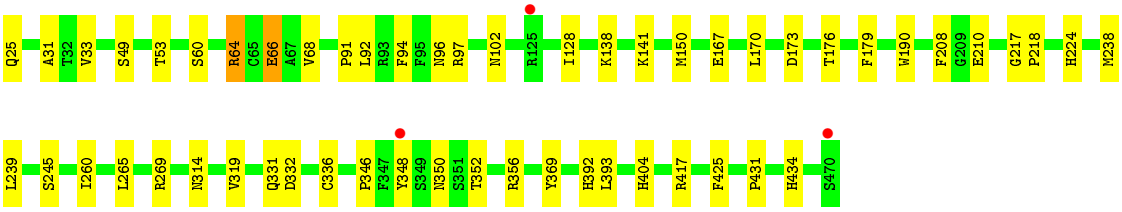
Chain C:



- Molecule 1: 5,6-dihydroxyindole-2-carboxylic acid oxidase

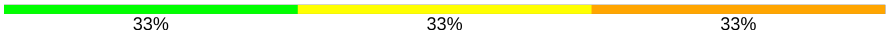
Chain D:





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

Chain E:



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

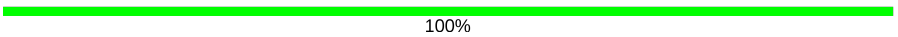
Chain H:

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

Chain P:

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

Chain F:

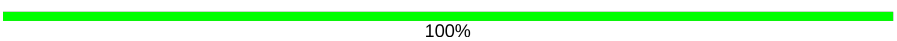


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:

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

Chain J:

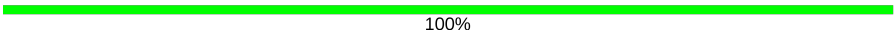


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:

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

Chain N:

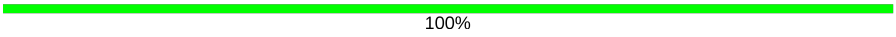


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:

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

Chain R:



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

Chain T:

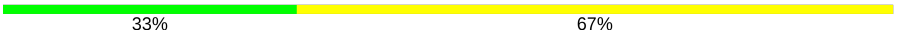
• Molecule 4: alpha-D-mannopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

• Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetami

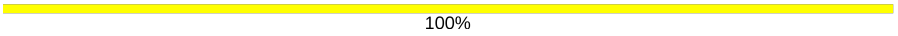
do-2-deoxy-beta-D-glucopyranose

Chain K:



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

Chain M:



• Molecule 7: alpha-D-mannopyranose-(1-3)-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 Q:

• Molecule 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	90.08Å 141.77Å 191.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.88 – 2.20 45.88 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.2 (45.88-2.20) 92.3 (45.88-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.47 (at 2.20Å)	Xtriage
Refinement program	REFMAC, PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.194 , 0.235 0.199 , 0.237	Depositor DCC
R_{free} test set	6287 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	34.5	Xtriage
Anisotropy	0.461	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 40.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	15622	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, ZN, URS, NAG, FUC

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	2/3661 (0.1%)	0.64	3/4990 (0.1%)
1	B	0.55	3/3661 (0.1%)	0.76	10/4990 (0.2%)
1	C	0.42	0/3661	0.62	2/4990 (0.0%)
1	D	0.49	3/3661 (0.1%)	0.63	0/4990
All	All	0.49	8/14644 (0.1%)	0.67	15/19960 (0.1%)

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	B	0	1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	66	GLU	CG-CD	-8.53	1.39	1.51
1	A	48	VAL	CB-CG1	6.96	1.67	1.52
1	B	118	ARG	CZ-NH1	-6.73	1.24	1.33
1	D	64	ARG	NE-CZ	-6.18	1.25	1.33
1	A	48	VAL	CB-CG2	5.51	1.64	1.52
1	B	118	ARG	CZ-NH2	-5.43	1.25	1.33
1	D	64	ARG	CZ-NH1	-5.29	1.26	1.33
1	B	153	ARG	NE-CZ	-5.07	1.26	1.33

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	146	ARG	CG-CD-NE	14.06	141.32	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	118	ARG	NE-CZ-NH1	12.62	126.61	120.30
1	B	48	VAL	CG1-CB-CG2	-8.31	97.61	110.90
1	A	48	VAL	CG1-CB-CG2	7.73	123.27	110.90
1	C	48	VAL	CG1-CB-CG2	-7.43	99.01	110.90
1	B	138	LYS	CD-CE-NZ	-7.37	94.74	111.70
1	B	138	LYS	CG-CD-CE	6.43	131.19	111.90
1	B	153	ARG	CG-CD-NE	6.17	124.76	111.80
1	B	93	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	B	153	ARG	CA-CB-CG	5.62	125.78	113.40
1	A	97	ARG	CG-CD-NE	-5.60	100.04	111.80
1	B	265	LEU	CA-CB-CG	5.49	127.93	115.30
1	B	118	ARG	NH1-CZ-NH2	-5.19	113.69	119.40
1	C	265	LEU	CA-CB-CG	5.19	127.23	115.30
1	A	265	LEU	CA-CB-CG	5.05	126.91	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	125	ARG	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	3554	0	3321	27	0
1	B	3554	0	3320	29	0
1	C	3554	0	3319	26	0
1	D	3554	0	3319	37	0
2	E	38	0	34	1	0
2	H	38	0	34	2	0
2	P	38	0	34	2	0
3	F	28	0	25	0	0
3	G	28	0	25	0	0
3	J	28	0	25	0	0
3	L	28	0	25	2	0
3	N	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	O	28	0	25	1	0
3	R	28	0	25	0	0
3	T	28	0	25	1	0
4	I	25	0	22	1	0
5	K	71	0	61	0	0
6	M	24	0	22	2	0
7	Q	60	0	52	1	0
8	S	61	0	52	0	0
9	A	14	0	13	0	0
9	C	42	0	39	1	0
10	A	10	0	8	0	0
10	B	10	0	8	0	0
10	C	10	0	8	0	0
10	D	10	0	8	0	0
11	A	3	0	0	0	0
11	B	2	0	0	0	0
11	C	2	0	0	0	0
11	D	2	0	0	0	0
12	A	205	0	0	2	0
12	B	168	0	0	0	1
12	C	159	0	0	3	1
12	D	190	0	0	4	0
All	All	15622	0	13874	121	1

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 4.

All (121) 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:104:ASN:OD1	1:B:114:ARG:NH1	2.02	0.93
1:C:25:GLN:HG3	1:C:26:PHE:H	1.39	0.86
1:B:25:GLN:HG3	1:B:26:PHE:H	1.41	0.85
1:A:25:GLN:OE1	1:A:25:GLN:N	2.17	0.77
1:C:256:ASN:ND2	12:C:603:HOH:O	2.18	0.76
1:A:93:ARG:HE	1:D:49:SER:HB3	1.51	0.76
1:D:352:THR:HG22	1:D:369:TYR:H	1.50	0.76
1:D:49:SER:HB2	1:D:53:THR:HG21	1.65	0.75
1:C:218:PRO:HD2	1:C:434:HIS:HB3	1.74	0.69
1:D:25:GLN:N	1:D:25:GLN:CD	2.46	0.69
1:C:25:GLN:HG3	1:C:26:PHE:N	2.08	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:PRO:HD2	1:A:434:HIS:HB3	1.76	0.67
1:B:25:GLN:HG3	1:B:26:PHE:N	2.09	0.67
1:D:102:ASN:ND2	12:D:607:HOH:O	2.30	0.64
1:B:44:ASP:HB3	1:B:47:PRO:HG3	1.79	0.64
1:B:96:ASN:HD22	2:H:1:NAG:H83	1.63	0.63
1:C:149:ASP:OD2	1:C:153:ARG:NH1	2.31	0.63
12:C:601:HOH:O	6:M:1:NAG:O4	2.12	0.63
1:D:218:PRO:HD2	1:D:434:HIS:HB3	1.82	0.61
1:D:269:ARG:NH1	1:D:314:ASN:OD1	2.34	0.60
1:C:269:ARG:NH1	1:C:314:ASN:OD1	2.35	0.60
1:C:118:ARG:HD3	1:C:126:VAL:HG11	1.83	0.60
1:D:150:MET:HE3	1:D:238:MET:HG2	1.83	0.59
1:D:173:ASP:OD1	1:D:176:THR:HG22	2.03	0.59
1:A:198:LYS:NZ	12:A:602:HOH:O	2.35	0.59
1:D:96:ASN:HD22	2:P:1:NAG:H83	1.67	0.58
1:B:25:GLN:HG2	1:B:161:ILE:HA	1.85	0.58
1:C:207:SER:O	12:C:602:HOH:O	2.17	0.58
1:A:29:GLN:HG3	1:A:43:PRO:HB3	1.85	0.58
1:B:33:VAL:HG22	1:B:170:LEU:HD22	1.87	0.57
1:A:469:PRO:O	1:A:470:SER:HB3	2.03	0.57
1:B:269:ARG:NH1	1:B:314:ASN:OD1	2.35	0.56
1:B:29:GLN:HG3	1:B:43:PRO:HB3	1.88	0.56
1:D:25:GLN:OE1	1:D:190:TRP:CH2	2.59	0.56
1:B:319:VAL:N	3:L:1:NAG:O6	2.38	0.56
1:C:104:ASN:HA	1:C:114:ARG:HD2	1.88	0.55
1:C:25:GLN:HG2	1:C:161:ILE:HA	1.89	0.55
1:B:331:GLN:H	1:B:331:GLN:CD	2.10	0.55
1:C:48:VAL:HG12	1:C:48:VAL:O	2.07	0.55
1:D:331:GLN:H	1:D:331:GLN:CD	2.10	0.55
1:D:417:ARG:HD3	12:D:622:HOH:O	2.07	0.53
1:A:118:ARG:HD3	1:A:126:VAL:HG11	1.89	0.53
1:A:98:THR:HG22	1:A:444:TRP:CH2	2.44	0.52
1:A:68:VAL:HG22	1:A:98:THR:HG23	1.92	0.52
3:O:1:NAG:H61	3:O:2:NAG:O5	2.09	0.52
1:D:348:TYR:C	1:D:350:ASN:H	2.11	0.52
1:B:44:ASP:CB	1:B:47:PRO:HG3	2.40	0.52
1:A:98:THR:HG22	1:A:444:TRP:CZ2	2.45	0.51
1:A:370:ASP:HB3	1:A:373:VAL:HG23	1.92	0.51
1:D:167:GLU:H	1:D:167:GLU:CD	2.11	0.51
1:D:348:TYR:HB2	1:D:350:ASN:HB2	1.91	0.51
1:B:167:GLU:H	1:B:167:GLU:CD	2.14	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:GLN:HE21	1:B:162:ALA:H	1.57	0.50
1:B:218:PRO:HD2	1:B:434:HIS:HB3	1.94	0.50
1:C:164:ARG:HG3	1:C:178:GLN:HG3	1.92	0.50
1:C:224:HIS:CD2	1:C:404:HIS:CE1	2.99	0.50
1:A:466:ILE:O	1:A:467:GLN:NE2	2.44	0.49
1:D:224:HIS:CD2	1:D:404:HIS:CE1	3.00	0.49
1:A:323:MET:O	12:A:601:HOH:O	2.20	0.49
1:A:96:ASN:HD22	2:E:1:NAG:H83	1.77	0.48
1:B:118:ARG:O	1:B:123:ASP:N	2.45	0.48
1:A:392:HIS:CD2	1:A:393:LEU:HG	2.48	0.48
1:D:392:HIS:CD2	1:D:393:LEU:HG	2.49	0.48
1:A:54:ASP:OD1	1:A:59:SER:OG	2.25	0.48
1:B:329:GLU:HB3	1:B:331:GLN:OE1	2.15	0.47
1:D:260:ILE:O	1:D:265:LEU:O	2.32	0.47
1:B:217:GLY:O	1:B:356:ARG:HD3	2.15	0.46
1:B:149:ASP:OD2	1:B:153:ARG:NH1	2.46	0.46
1:D:94:PHE:O	2:P:3:FUC:H61	2.16	0.45
1:C:319:VAL:N	9:C:509:NAG:O6	2.49	0.45
1:B:208:PHE:CZ	1:B:210:GLU:HB2	2.52	0.45
1:D:348:TYR:CE1	1:D:431:PRO:HG3	2.52	0.45
1:A:142:ASN:O	1:A:146:ARG:HD3	2.17	0.44
1:C:68:VAL:HG11	1:C:91:PRO:HD2	2.00	0.44
1:D:128:ILE:HD12	1:D:245:SER:HB3	2.00	0.44
1:D:332:ASP:OD2	12:D:602:HOH:O	2.21	0.44
1:A:260:ILE:O	1:A:265:LEU:O	2.35	0.44
1:C:25:GLN:HA	1:C:25:GLN:OE1	2.19	0.43
1:A:169:ILE:CG2	1:A:170:LEU:HD22	2.48	0.43
1:D:31:ALA:HB1	1:D:179:PHE:CD2	2.54	0.43
1:A:169:ILE:HG23	1:A:170:LEU:HD22	1.99	0.43
1:D:64:ARG:CZ	1:D:66:GLU:OE1	2.67	0.43
1:D:150:MET:HE1	1:D:239:LEU:HD23	2.00	0.43
1:D:319:VAL:HG22	3:T:1:NAG:O6	2.18	0.43
1:B:25:GLN:OE1	1:B:25:GLN:HA	2.18	0.43
1:B:318:ASN:OD1	3:L:1:NAG:H61	2.18	0.43
1:C:25:GLN:HE21	1:C:162:ALA:H	1.66	0.43
12:D:623:HOH:O	7:Q:3:MAN:H62	2.18	0.43
1:B:260:ILE:O	1:B:265:LEU:O	2.37	0.43
1:D:141:LYS:HB3	1:D:265:LEU:HD21	2.01	0.43
1:B:138:LYS:HG2	1:B:139:GLU:OE2	2.20	0.42
1:D:92:LEU:HD23	1:D:92:LEU:HA	1.81	0.42
1:A:353:ASN:OD1	1:C:64:ARG:NH2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:136:LEU:O	1:C:141:LYS:HE3	2.19	0.42
1:D:68:VAL:HG11	1:D:91:PRO:HD2	2.02	0.42
1:C:96:ASN:HD22	6:M:1:NAG:H83	1.83	0.42
1:A:59:SER:HG	1:A:59:SER:H	1.64	0.42
1:B:392:HIS:CD2	1:B:393:LEU:HG	2.55	0.42
1:A:370:ASP:HB3	1:A:373:VAL:CG2	2.50	0.42
1:D:167:GLU:OE2	1:D:167:GLU:N	2.35	0.42
1:B:41:CYS:HB3	1:B:444:TRP:CZ2	2.54	0.42
1:C:392:HIS:CD2	1:C:393:LEU:HG	2.55	0.41
1:A:217:GLY:O	1:A:356:ARG:HD3	2.20	0.41
1:D:208:PHE:CZ	1:D:210:GLU:HB2	2.55	0.41
1:D:331:GLN:N	1:D:331:GLN:CD	2.73	0.41
1:C:78:GLN:O	1:C:80:PRO:HD3	2.20	0.41
1:B:224:HIS:CD2	1:B:404:HIS:CE1	3.08	0.41
1:C:49:SER:H	1:C:53:THR:HG21	1.85	0.41
1:D:346:PRO:HG2	1:D:348:TYR:HD2	1.86	0.41
1:B:94:PHE:O	2:H:3:FUC:H61	2.20	0.41
1:B:141:LYS:HD3	1:B:265:LEU:HD21	2.02	0.41
1:C:208:PHE:CZ	1:C:210:GLU:HB2	2.55	0.41
1:A:29:GLN:HG3	1:A:43:PRO:CB	2.51	0.41
1:D:66:GLU:O	1:D:97:ARG:HA	2.20	0.41
1:A:136:LEU:O	1:A:141:LYS:HE3	2.21	0.40
1:A:468:TRP:HA	1:A:469:PRO:HD3	1.98	0.40
1:D:33:VAL:HG22	1:D:170:LEU:HD22	2.02	0.40
1:D:217:GLY:O	1:D:356:ARG:HD3	2.22	0.40
4:I:1:NAG:H62	4:I:2:MAN:O2	2.21	0.40
1:C:348:TYR:CG	1:C:349:SER:N	2.90	0.40
1:C:350:ASN:HA	1:C:369:TYR:CD1	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:B:649:HOH:O	12:C:750:HOH:O[3_856]	2.18	0.02

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	444/446 (100%)	431 (97%)	13 (3%)	0	100	100
1	B	444/446 (100%)	430 (97%)	14 (3%)	0	100	100
1	C	444/446 (100%)	429 (97%)	15 (3%)	0	100	100
1	D	444/446 (100%)	431 (97%)	13 (3%)	0	100	100
All	All	1776/1784 (100%)	1721 (97%)	55 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	395/395 (100%)	392 (99%)	3 (1%)	81	90
1	B	395/395 (100%)	388 (98%)	7 (2%)	59	72
1	C	395/395 (100%)	392 (99%)	3 (1%)	81	90
1	D	395/395 (100%)	391 (99%)	4 (1%)	76	86
All	All	1580/1580 (100%)	1563 (99%)	17 (1%)	73	85

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	SER
1	A	258	CYS

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Mol	Chain	Res	Type
1	A	425	PHE
1	B	102	ASN
1	B	118	ARG
1	B	138	LYS
1	B	153	ARG
1	B	193	TYR
1	B	247	PRO
1	B	425	PHE
1	C	60	SER
1	C	336	CYS
1	C	425	PHE
1	D	60	SER
1	D	138	LYS
1	D	336	CYS
1	D	425	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	108	HIS
1	A	331	GLN
1	A	467	GLN
1	B	142	ASN
1	C	142	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

45 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	0.56	0	17,19,21	0.72	1 (5%)
2	NAG	E	2	2	14,14,15	0.47	0	17,19,21	0.37	0
2	FUC	E	3	2	10,10,11	1.07	0	14,14,16	1.37	2 (14%)
3	NAG	F	1	1,3	14,14,15	0.28	0	17,19,21	0.46	0
3	NAG	F	2	3	14,14,15	0.43	0	17,19,21	0.47	0
3	NAG	G	1	1,3	14,14,15	0.47	0	17,19,21	0.81	1 (5%)
3	NAG	G	2	3	14,14,15	0.40	0	17,19,21	0.45	0
2	NAG	H	1	1,2	14,14,15	0.22	0	17,19,21	0.76	1 (5%)
2	NAG	H	2	2	14,14,15	0.41	0	17,19,21	0.47	0
2	FUC	H	3	2	10,10,11	1.39	1 (10%)	14,14,16	1.55	3 (21%)
4	NAG	I	1	1,4	14,14,15	2.14	1 (7%)	17,19,21	1.10	2 (11%)
4	MAN	I	2	4	11,11,12	1.58	3 (27%)	15,15,17	1.50	2 (13%)
3	NAG	J	1	1,3	14,14,15	0.39	0	17,19,21	0.47	0
3	NAG	J	2	3	14,14,15	0.53	0	17,19,21	0.48	0
5	NAG	K	1	1,5	14,14,15	0.50	0	17,19,21	0.98	0
5	NAG	K	2	5	14,14,15	0.83	1 (7%)	17,19,21	0.81	1 (5%)
5	MAN	K	3	5	11,11,12	0.90	0	15,15,17	0.70	0
5	MAN	K	4	5	11,11,12	0.81	0	15,15,17	1.28	3 (20%)
5	MAN	K	5	5	11,11,12	1.35	2 (18%)	15,15,17	1.50	1 (6%)
5	FUC	K	6	5	10,10,11	1.32	1 (10%)	14,14,16	1.76	3 (21%)
3	NAG	L	1	1,3	14,14,15	0.44	0	17,19,21	0.87	1 (5%)
3	NAG	L	2	3	14,14,15	0.33	0	17,19,21	0.53	0
6	NAG	M	1	1,6	14,14,15	0.42	0	17,19,21	0.56	0
6	FUC	M	2	6	10,10,11	0.72	0	14,14,16	1.25	2 (14%)
3	NAG	N	1	1,3	14,14,15	0.19	0	17,19,21	0.39	0
3	NAG	N	2	3	14,14,15	0.37	0	17,19,21	0.52	0
3	NAG	O	1	1,3	14,14,15	0.41	0	17,19,21	0.90	1 (5%)
3	NAG	O	2	3	14,14,15	1.25	1 (7%)	17,19,21	1.12	3 (17%)
2	NAG	P	1	1,2	14,14,15	0.36	0	17,19,21	0.71	1 (5%)
2	NAG	P	2	2	14,14,15	0.63	1 (7%)	17,19,21	0.39	0
2	FUC	P	3	2	10,10,11	1.08	1 (10%)	14,14,16	2.03	5 (35%)
7	NAG	Q	1	1,7	14,14,15	0.74	1 (7%)	17,19,21	0.67	0
7	NAG	Q	2	7	14,14,15	0.60	0	17,19,21	0.72	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	MAN	Q	3	7	11,11,12	1.51	1 (9%)	15,15,17	1.07	1 (6%)
7	MAN	Q	4	7	11,11,12	0.87	1 (9%)	15,15,17	1.13	2 (13%)
7	FUC	Q	5	7	10,10,11	0.94	0	14,14,16	1.13	1 (7%)
3	NAG	R	1	1,3	14,14,15	0.22	0	17,19,21	0.62	0
3	NAG	R	2	3	14,14,15	0.48	0	17,19,21	0.54	0
8	NAG	S	1	1,8	14,14,15	0.42	0	17,19,21	0.64	0
8	NAG	S	2	8	14,14,15	0.60	1 (7%)	17,19,21	0.75	1 (5%)
8	MAN	S	3	8	11,11,12	0.82	0	15,15,17	1.30	1 (6%)
8	MAN	S	4	8	11,11,12	1.32	1 (9%)	15,15,17	2.10	3 (20%)
8	MAN	S	5	8	11,11,12	1.21	1 (9%)	15,15,17	1.58	2 (13%)
3	NAG	T	1	1,3	14,14,15	0.53	0	17,19,21	0.75	1 (5%)
3	NAG	T	2	3	14,14,15	0.27	0	17,19,21	0.43	0

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	L	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	L	2	3	-	0/6/23/26	0/1/1/1
6	NAG	M	1	1,6	-	2/6/23/26	0/1/1/1
6	FUC	M	2	6	-	-	0/1/1/1
3	NAG	N	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	N	2	3	-	2/6/23/26	0/1/1/1
3	NAG	O	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	O	2	3	-	2/6/23/26	0/1/1/1
2	NAG	P	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	P	2	2	-	1/6/23/26	0/1/1/1
2	FUC	P	3	2	-	-	0/1/1/1
7	NAG	Q	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	Q	2	7	-	0/6/23/26	0/1/1/1
7	MAN	Q	3	7	-	1/2/19/22	0/1/1/1
7	MAN	Q	4	7	-	2/2/19/22	0/1/1/1
7	FUC	Q	5	7	-	-	0/1/1/1
3	NAG	R	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	R	2	3	-	2/6/23/26	0/1/1/1
8	NAG	S	1	1,8	-	2/6/23/26	0/1/1/1
8	NAG	S	2	8	-	0/6/23/26	0/1/1/1
8	MAN	S	3	8	-	2/2/19/22	0/1/1/1
8	MAN	S	4	8	-	0/2/19/22	1/1/1/1
8	MAN	S	5	8	-	0/2/19/22	1/1/1/1
3	NAG	T	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	T	2	3	-	2/6/23/26	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	1	NAG	O5-C1	-7.67	1.31	1.43
7	Q	3	MAN	O5-C5	4.02	1.51	1.43
5	K	6	FUC	C1-C2	3.82	1.60	1.52
8	S	4	MAN	O5-C1	-3.78	1.37	1.43
3	O	2	NAG	C1-C2	3.76	1.58	1.52
2	H	3	FUC	O5-C5	3.72	1.51	1.43
4	I	2	MAN	C1-C2	3.00	1.59	1.52
5	K	2	NAG	O5-C1	-2.75	1.39	1.43
7	Q	1	NAG	O5-C1	-2.65	1.39	1.43
2	P	3	FUC	O5-C5	2.63	1.49	1.43
4	I	2	MAN	O5-C5	2.50	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	K	5	MAN	C4-C3	2.23	1.58	1.52
7	Q	4	MAN	O5-C5	2.22	1.47	1.43
8	S	5	MAN	C1-C2	2.19	1.57	1.52
4	I	2	MAN	C4-C5	2.14	1.57	1.53
5	K	5	MAN	O4-C4	-2.10	1.38	1.43
8	S	2	NAG	O5-C1	-2.02	1.40	1.43
2	P	2	NAG	C1-C2	2.01	1.55	1.52

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	S	4	MAN	C1-O5-C5	6.66	121.22	112.19
2	P	3	FUC	O5-C5-C4	4.74	118.03	109.52
4	I	2	MAN	C1-C2-C3	-4.18	104.53	109.67
5	K	5	MAN	C1-C2-C3	-3.83	104.95	109.67
5	K	6	FUC	C1-O5-C5	3.66	121.08	112.78
2	H	3	FUC	O5-C5-C4	3.61	116.00	109.52
7	Q	4	MAN	C1-O5-C5	3.51	116.94	112.19
2	P	3	FUC	C1-O5-C5	3.42	120.53	112.78
5	K	6	FUC	C1-C2-C3	3.36	113.79	109.67
8	S	5	MAN	C1-C2-C3	-3.28	105.63	109.67
6	M	2	FUC	C1-O5-C5	3.13	119.86	112.78
2	E	3	FUC	O5-C5-C4	2.94	114.79	109.52
4	I	2	MAN	O2-C2-C1	2.90	115.09	109.15
3	O	1	NAG	O4-C4-C3	-2.90	103.64	110.35
5	K	4	MAN	O2-C2-C3	-2.83	104.46	110.14
4	I	1	NAG	C4-C3-C2	2.77	115.08	111.02
5	K	6	FUC	O5-C1-C2	2.77	115.05	110.77
5	K	4	MAN	C1-O5-C5	2.76	115.93	112.19
8	S	3	MAN	O3-C3-C4	-2.71	104.09	110.35
3	T	1	NAG	C1-O5-C5	2.62	115.75	112.19
2	H	3	FUC	C1-O5-C5	2.60	118.68	112.78
8	S	4	MAN	O2-C2-C3	-2.54	105.04	110.14
2	H	1	NAG	C1-O5-C5	2.48	115.55	112.19
2	E	3	FUC	C1-O5-C5	2.45	118.32	112.78
2	P	3	FUC	C3-C4-C5	2.41	113.52	109.77
3	L	1	NAG	C1-O5-C5	2.40	115.44	112.19
2	P	3	FUC	O3-C3-C4	-2.37	104.86	110.35
7	Q	5	FUC	C1-O5-C5	2.35	118.11	112.78
3	O	2	NAG	C4-C3-C2	2.34	114.45	111.02
7	Q	2	NAG	O4-C4-C5	-2.34	103.49	109.30
8	S	4	MAN	O5-C1-C2	2.32	114.34	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	P	3	FUC	O5-C1-C2	2.26	114.26	110.77
4	I	1	NAG	O5-C5-C4	-2.20	105.47	110.83
2	E	1	NAG	C1-O5-C5	2.19	115.16	112.19
8	S	2	NAG	C1-O5-C5	2.19	115.15	112.19
2	P	1	NAG	C1-O5-C5	2.18	115.14	112.19
2	H	3	FUC	O3-C3-C4	-2.17	105.33	110.35
3	O	2	NAG	C1-O5-C5	-2.16	109.26	112.19
3	O	2	NAG	C2-N2-C7	2.16	125.97	122.90
7	Q	3	MAN	C1-O5-C5	2.11	115.05	112.19
5	K	2	NAG	O4-C4-C5	-2.10	104.09	109.30
6	M	2	FUC	O5-C5-C4	2.10	113.28	109.52
8	S	5	MAN	O2-C2-C1	2.09	113.43	109.15
5	K	4	MAN	C1-C2-C3	-2.07	107.12	109.67
3	G	1	NAG	C1-O5-C5	2.04	114.96	112.19
7	Q	4	MAN	O2-C2-C3	-2.02	106.10	110.14

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	R	2	NAG	O5-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6
5	K	3	MAN	O5-C5-C6-O6
3	R	2	NAG	C4-C5-C6-O6
7	Q	1	NAG	O5-C5-C6-O6
2	H	2	NAG	C4-C5-C6-O6
4	I	1	NAG	O5-C5-C6-O6
4	I	1	NAG	C4-C5-C6-O6
8	S	3	MAN	O5-C5-C6-O6
5	K	3	MAN	C4-C5-C6-O6
5	K	1	NAG	O5-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
3	O	1	NAG	C4-C5-C6-O6
3	O	1	NAG	O5-C5-C6-O6
5	K	1	NAG	C4-C5-C6-O6
3	O	2	NAG	C8-C7-N2-C2
3	O	2	NAG	O7-C7-N2-C2
2	H	1	NAG	C8-C7-N2-C2
2	H	1	NAG	O7-C7-N2-C2
2	P	1	NAG	C8-C7-N2-C2
2	P	1	NAG	O7-C7-N2-C2
5	K	1	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
5	K	1	NAG	O7-C7-N2-C2
3	O	1	NAG	C8-C7-N2-C2
3	O	1	NAG	O7-C7-N2-C2
2	E	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2
6	M	1	NAG	C8-C7-N2-C2
6	M	1	NAG	O7-C7-N2-C2
7	Q	4	MAN	C4-C5-C6-O6
8	S	3	MAN	C4-C5-C6-O6
5	K	4	MAN	C4-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
3	N	2	NAG	O5-C5-C6-O6
7	Q	1	NAG	C4-C5-C6-O6
3	N	2	NAG	C4-C5-C6-O6
7	Q	4	MAN	O5-C5-C6-O6
5	K	4	MAN	O5-C5-C6-O6
8	S	1	NAG	C4-C5-C6-O6
7	Q	3	MAN	O5-C5-C6-O6
8	S	1	NAG	O5-C5-C6-O6
3	T	2	NAG	C4-C5-C6-O6
3	T	2	NAG	O5-C5-C6-O6
3	J	2	NAG	C4-C5-C6-O6
2	P	2	NAG	O5-C5-C6-O6

All (3) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	S	4	MAN	C1-C2-C3-C4-C5-O5
5	K	5	MAN	C1-C2-C3-C4-C5-O5
8	S	5	MAN	C1-C2-C3-C4-C5-O5

13 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	2	MAN	1	0
2	P	3	FUC	1	0
3	O	2	NAG	1	0
4	I	1	NAG	1	0
2	H	1	NAG	1	0
7	Q	3	MAN	1	0

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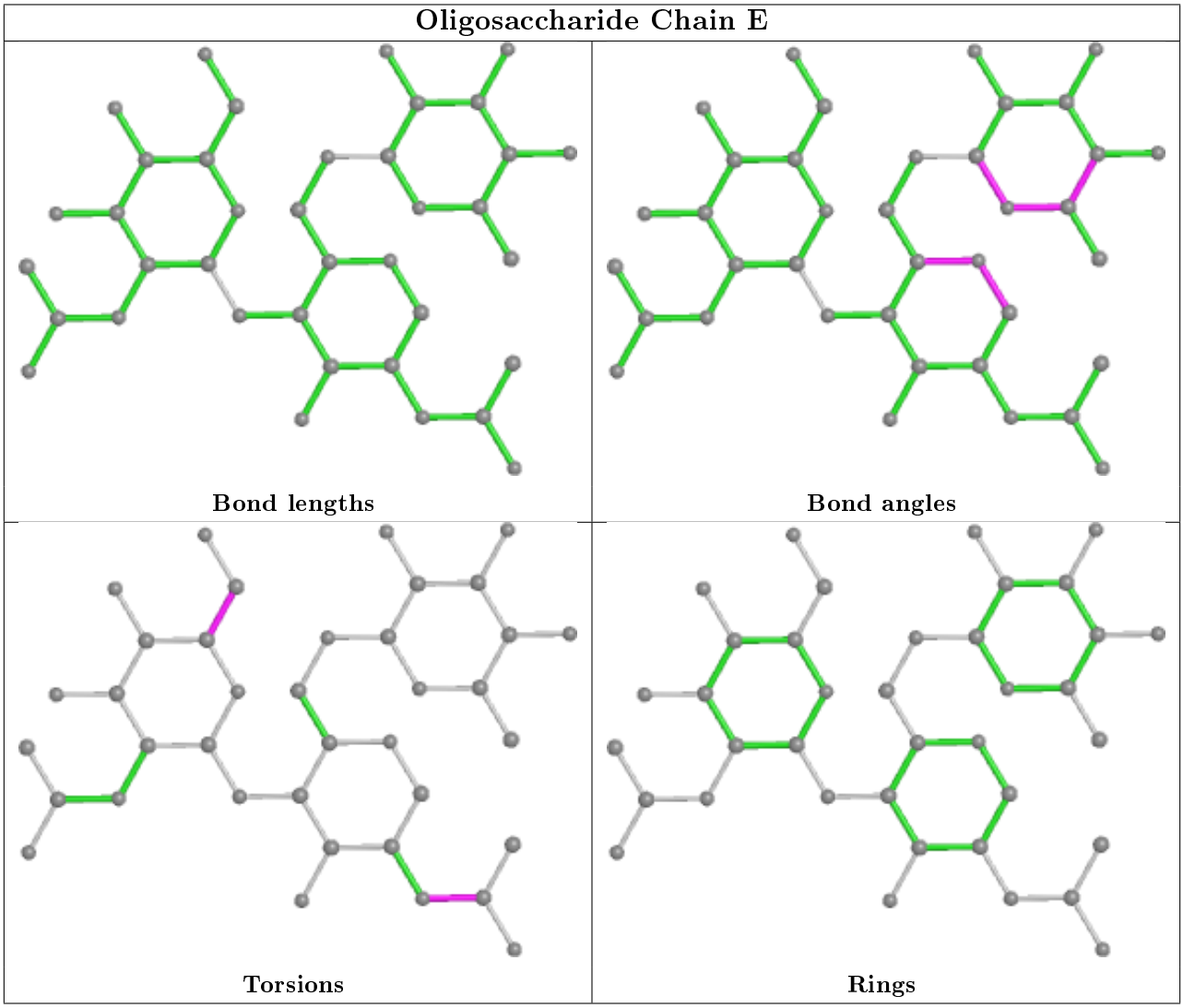
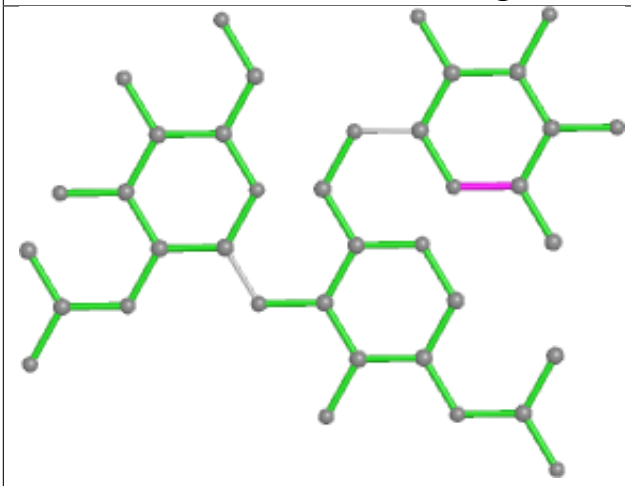
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	P	1	NAG	1	0
2	H	3	FUC	1	0
3	O	1	NAG	1	0
2	E	1	NAG	1	0
3	T	1	NAG	1	0
6	M	1	NAG	2	0
3	L	1	NAG	2	0

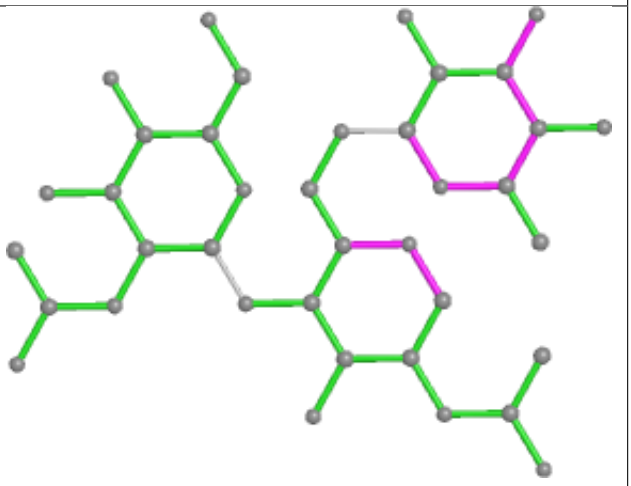
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



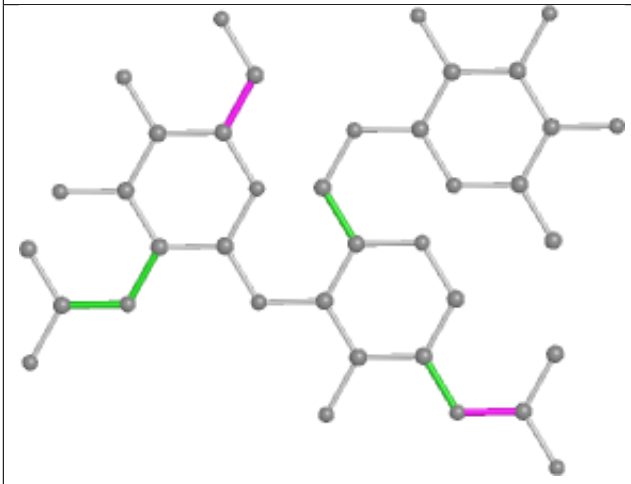
Oligosaccharide Chain H



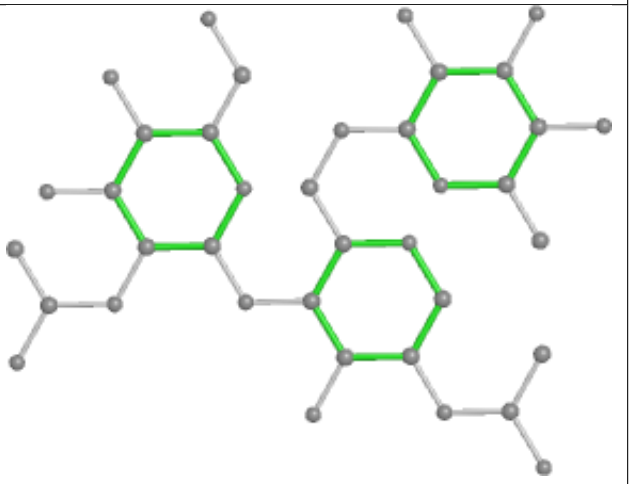
Bond lengths



Bond angles

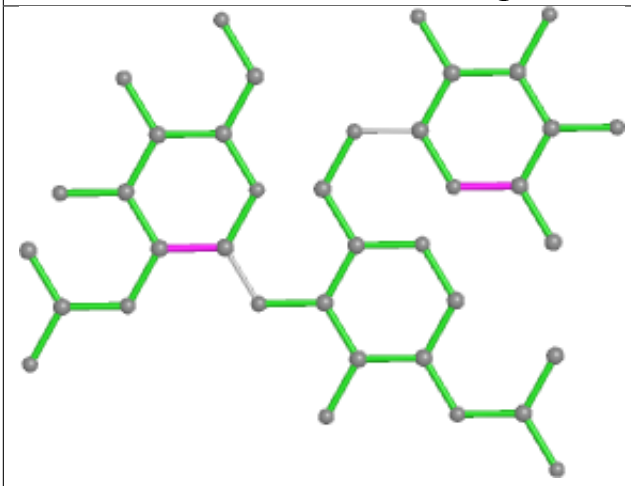


Torsions

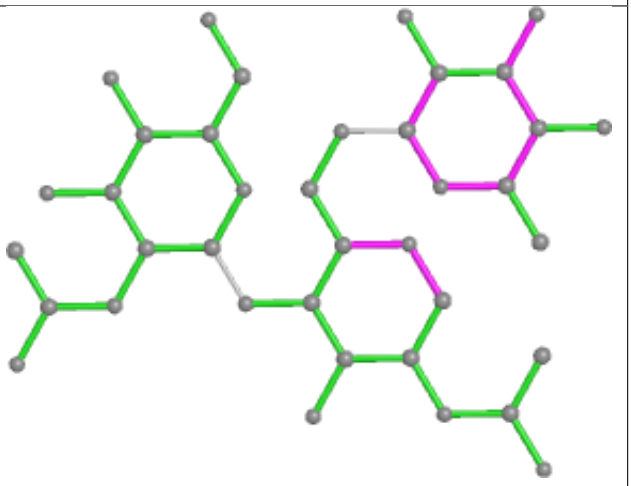


Rings

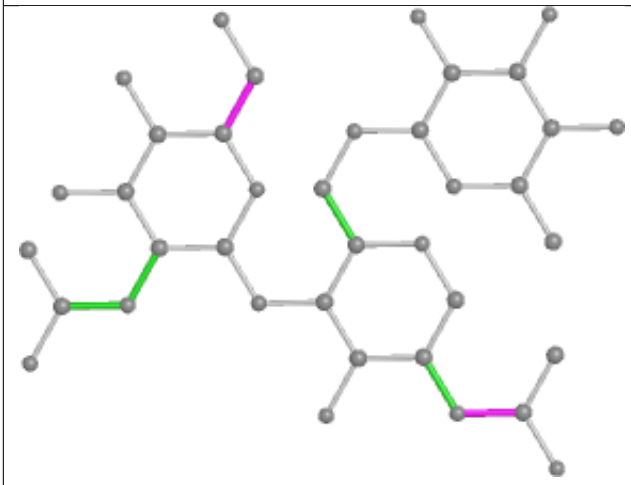
Oligosaccharide Chain P



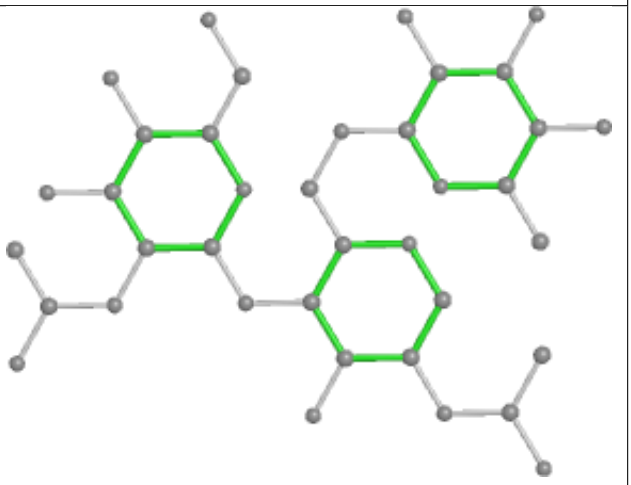
Bond lengths



Bond angles

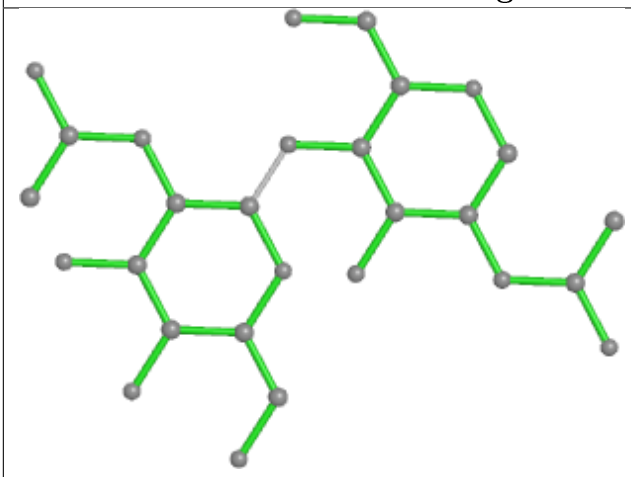


Torsions

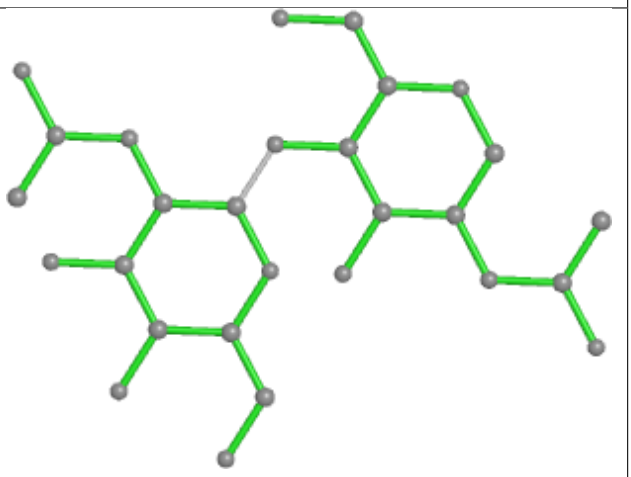


Rings

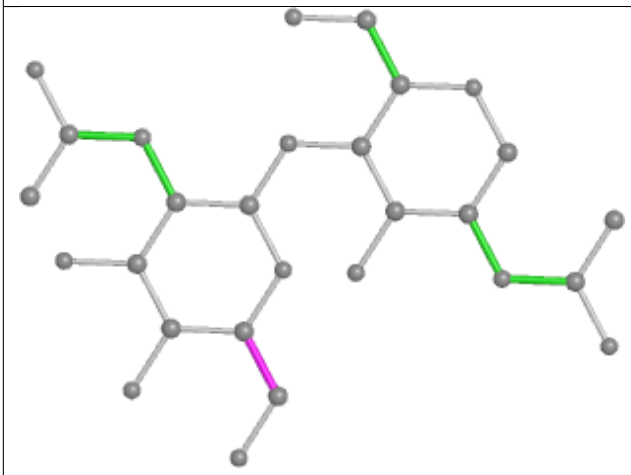
Oligosaccharide Chain F



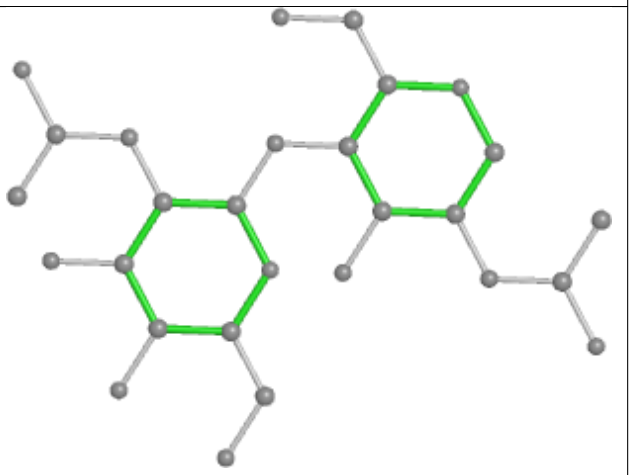
Bond lengths



Bond angles

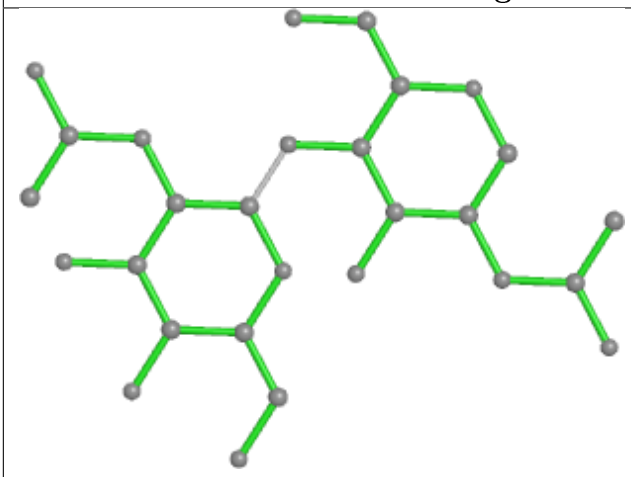


Torsions

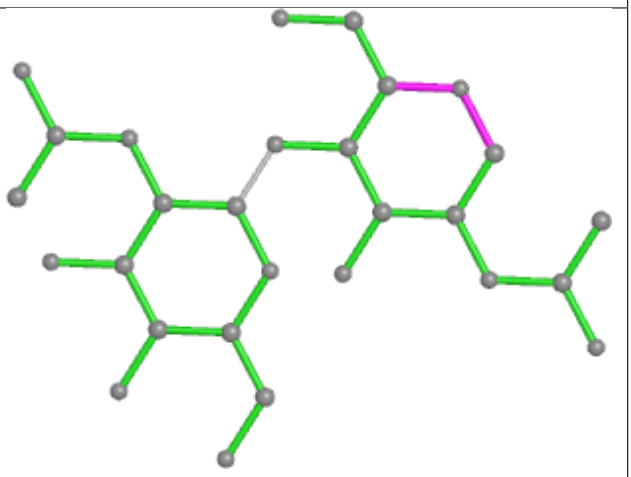


Rings

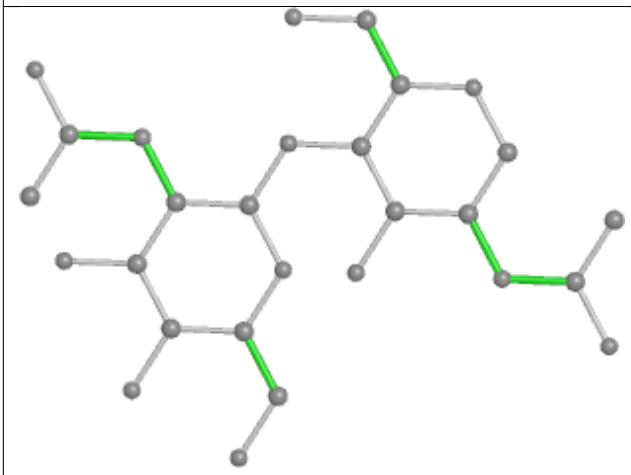
Oligosaccharide Chain G



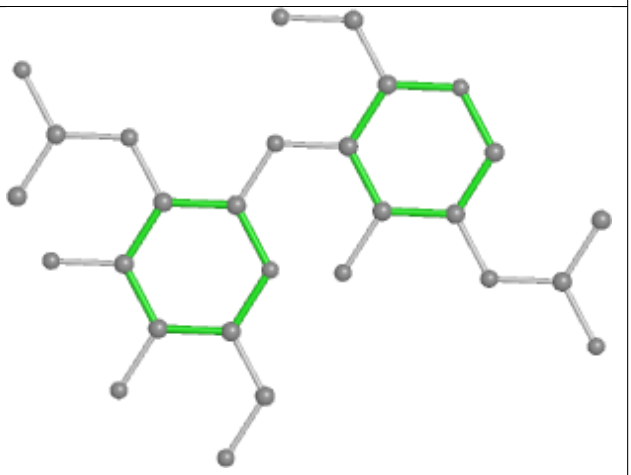
Bond lengths



Bond angles

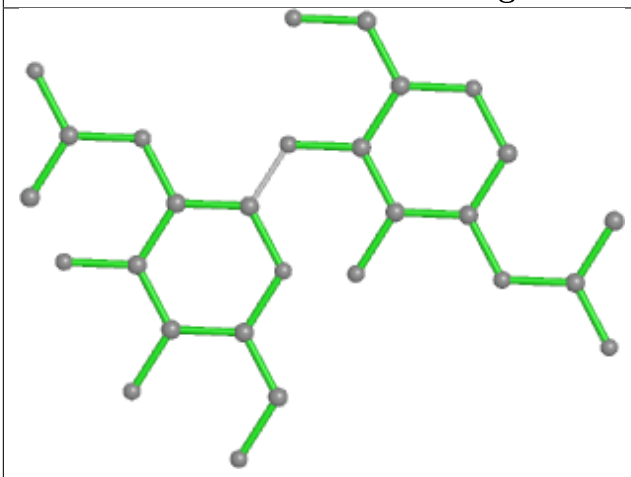


Torsions

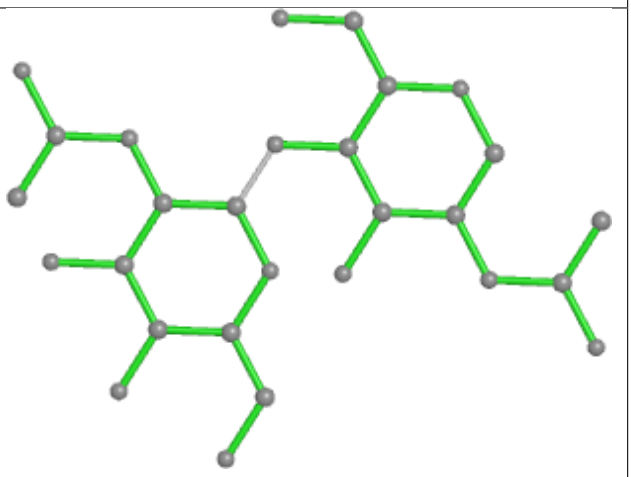


Rings

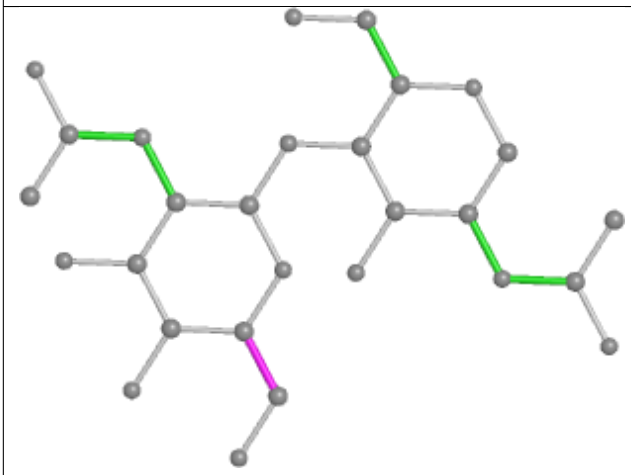
Oligosaccharide Chain J



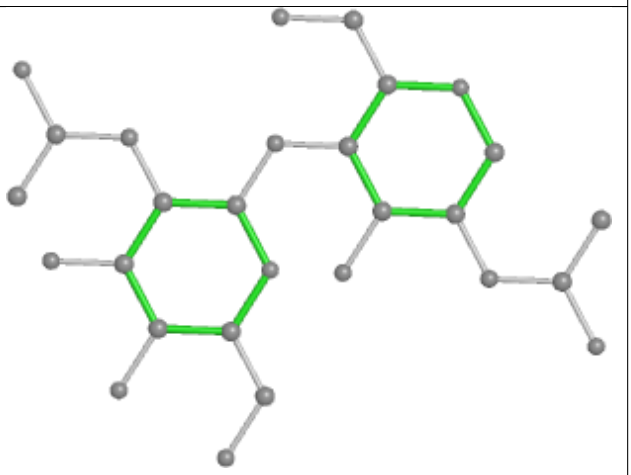
Bond lengths



Bond angles

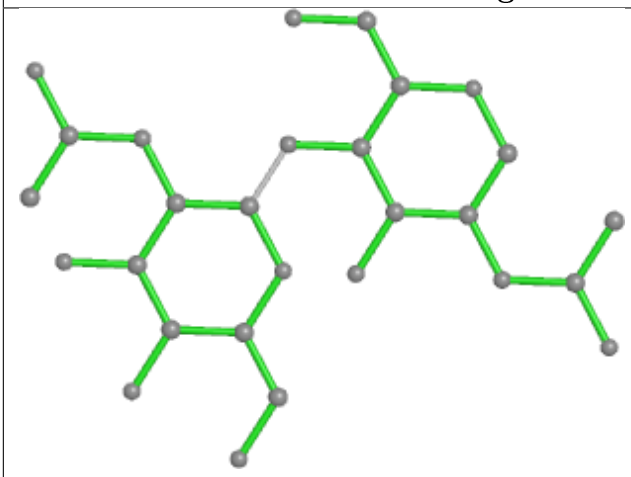


Torsions

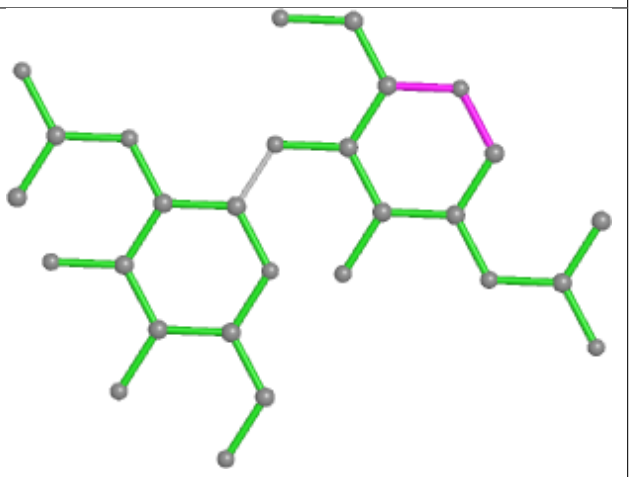


Rings

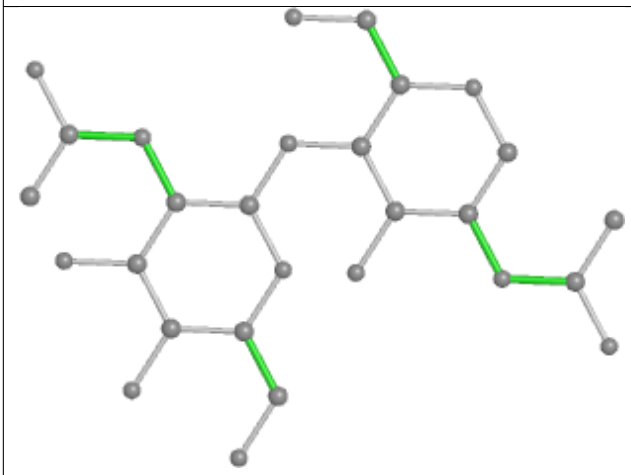
Oligosaccharide Chain L



Bond lengths



Bond angles



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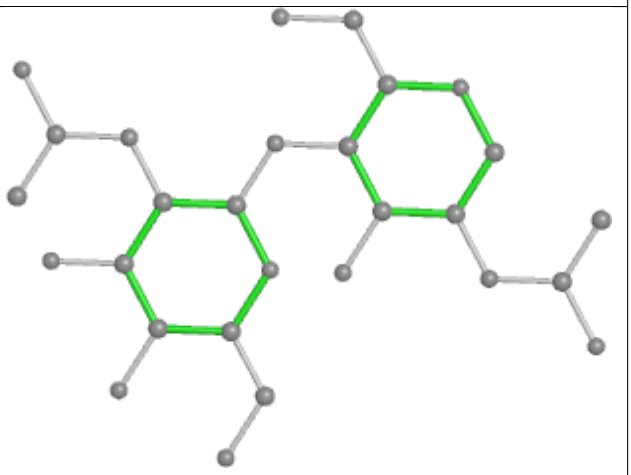
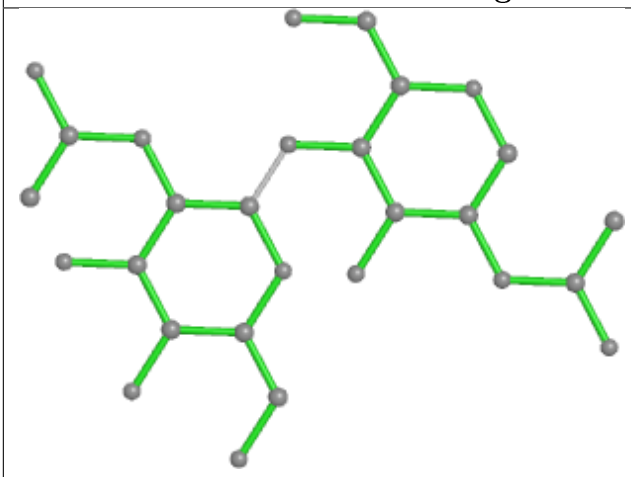
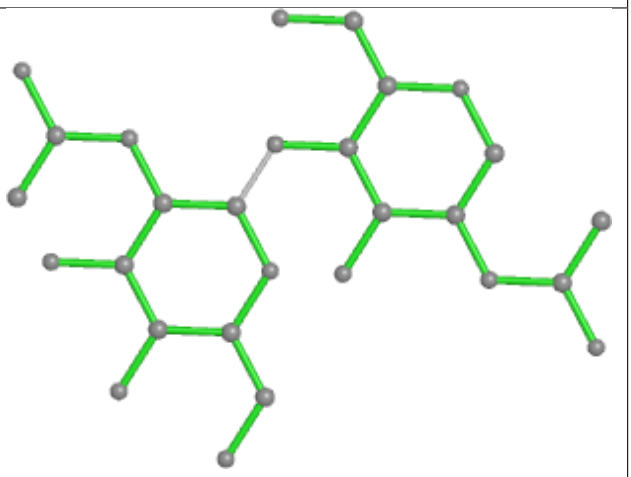


Rings

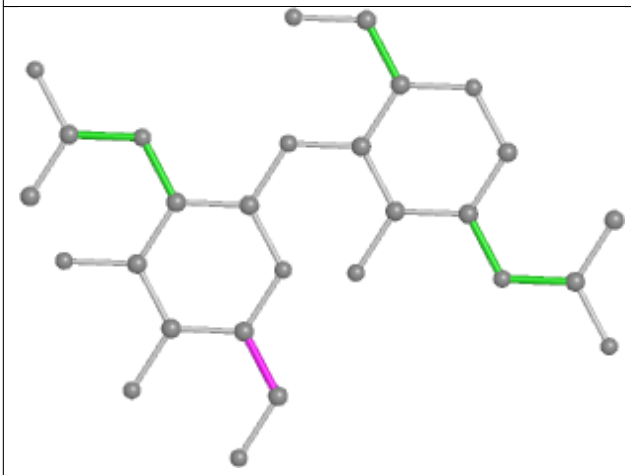
Oligosaccharide Chain N



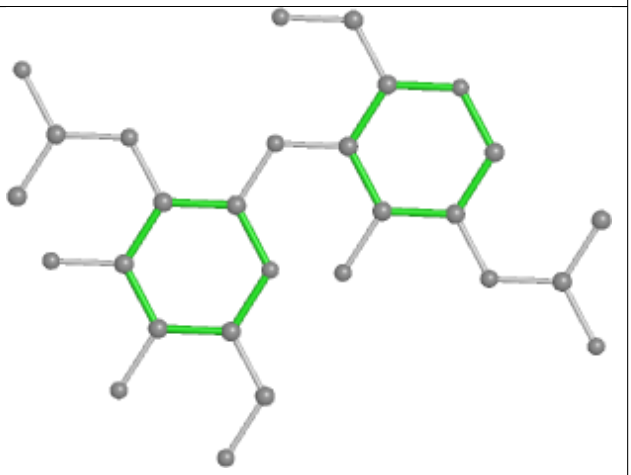
Bond lengths



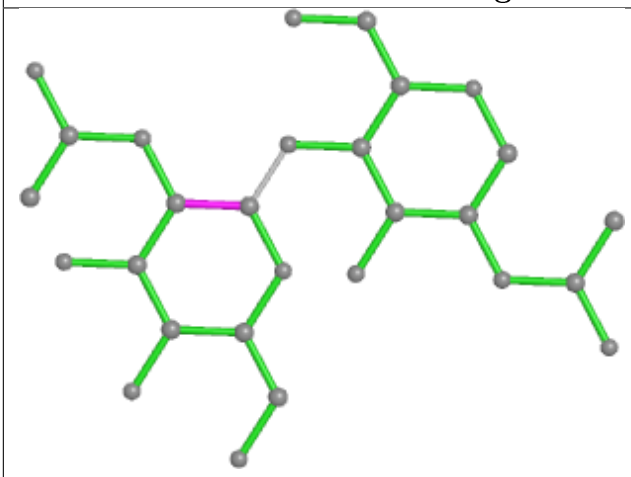
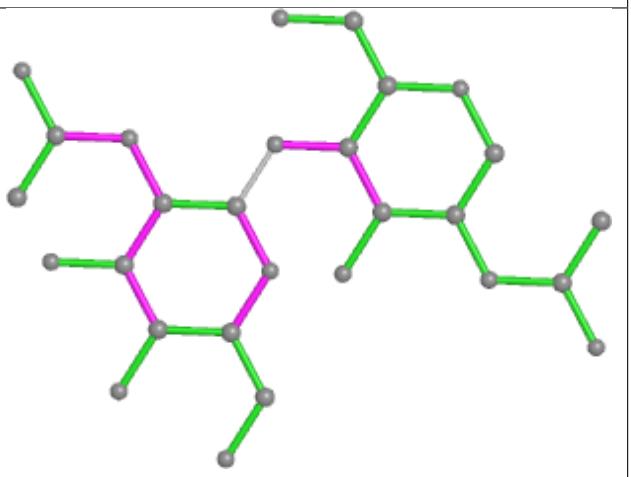
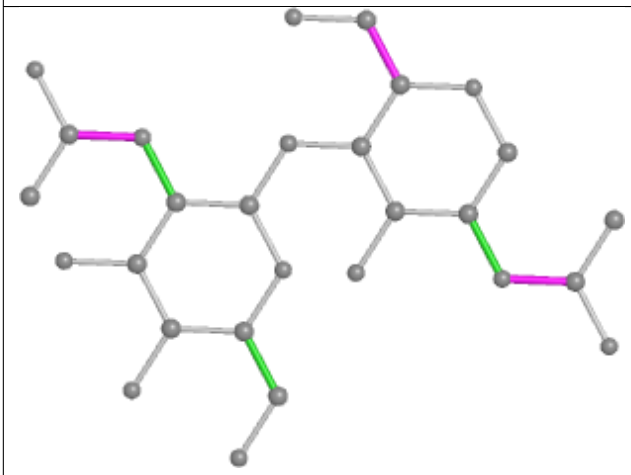
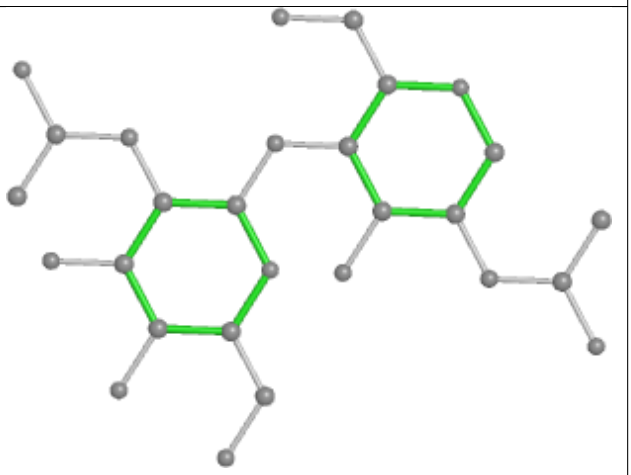
Bond angles



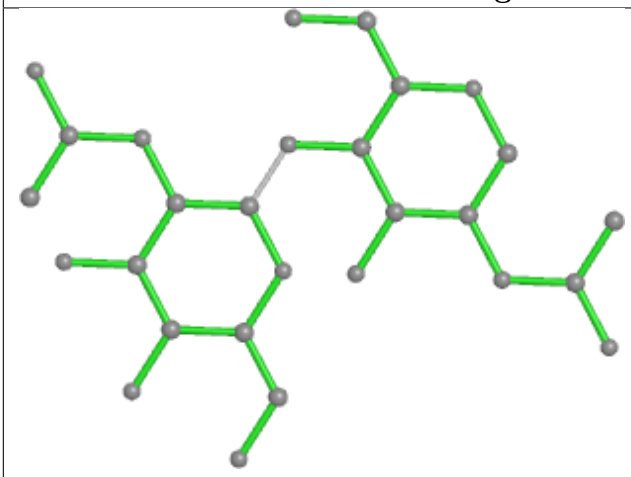
Torsions



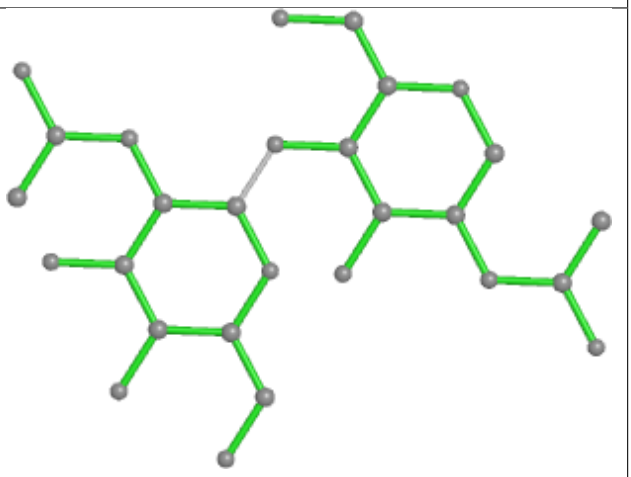
Rings

Oligosaccharide Chain O	
 Bond lengths	 Bond angles
 Torsions	 Rings

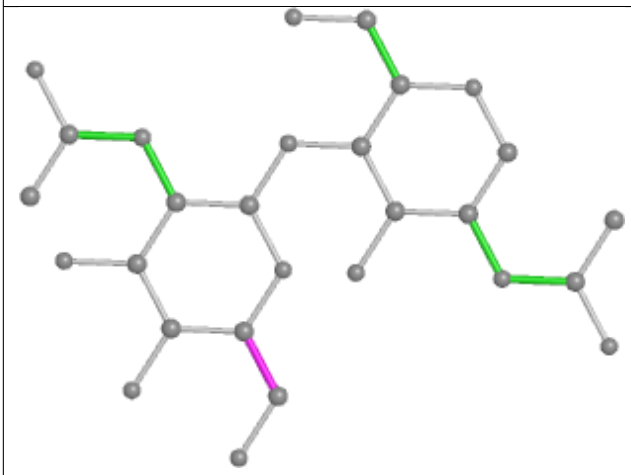
Oligosaccharide Chain R



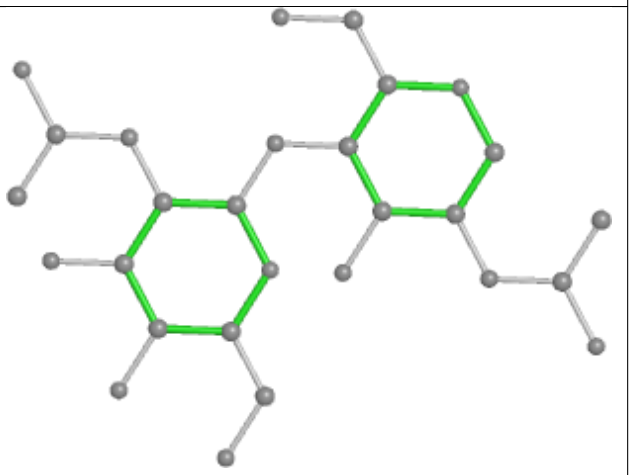
Bond lengths



Bond angles

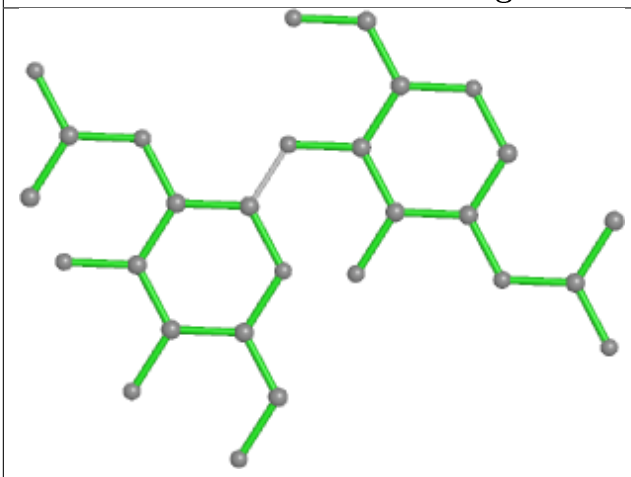


Torsions

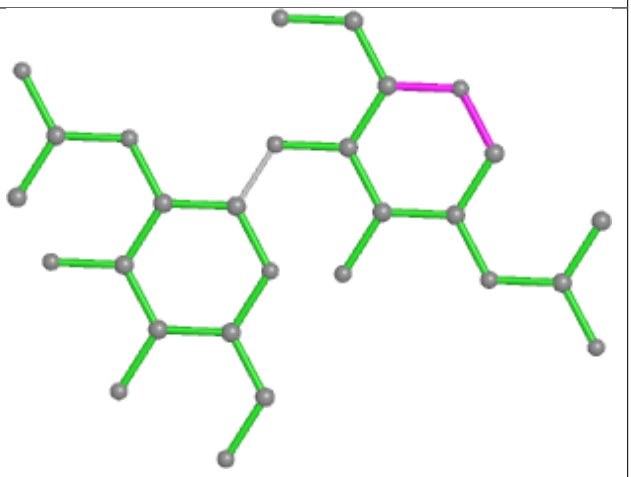


Rings

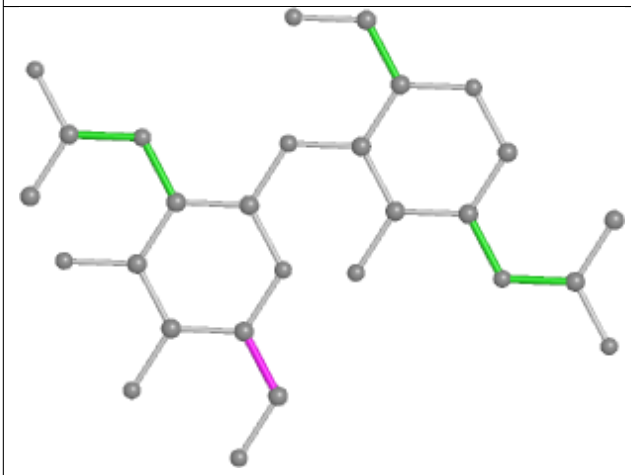
Oligosaccharide Chain T



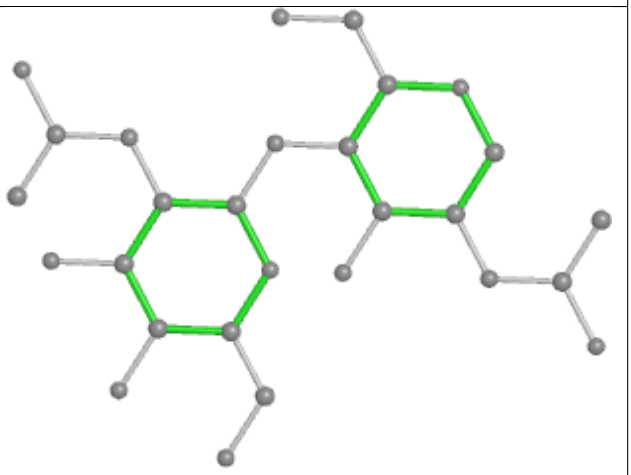
Bond lengths



Bond angles

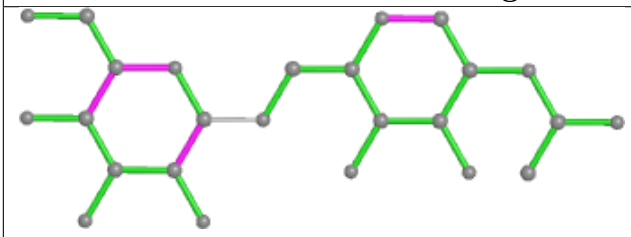


Torsions

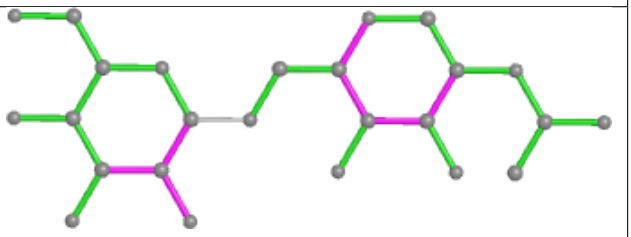


Rings

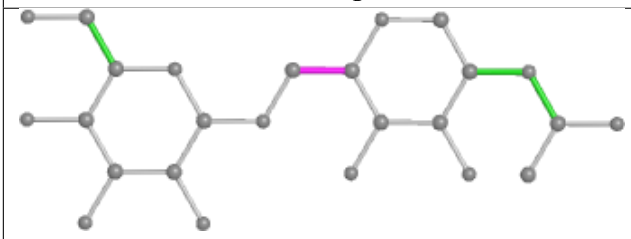
Oligosaccharide Chain I



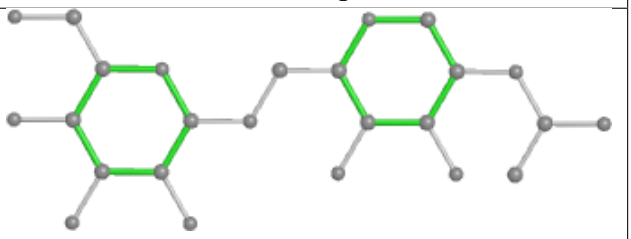
Bond lengths



Bond angles

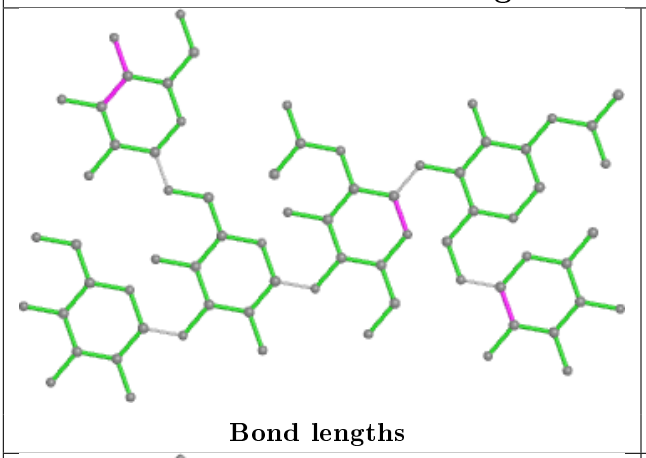


Torsions

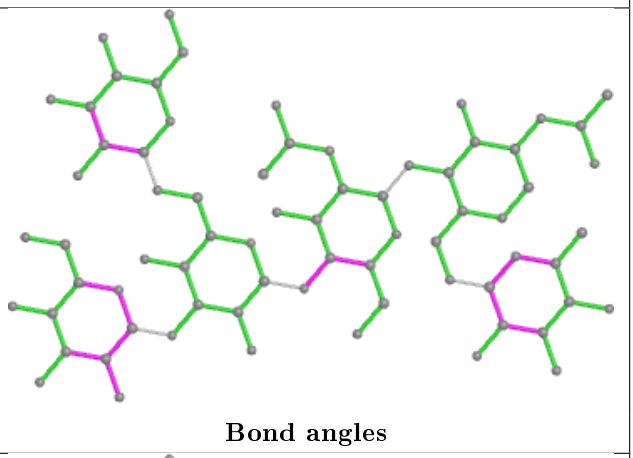


Rings

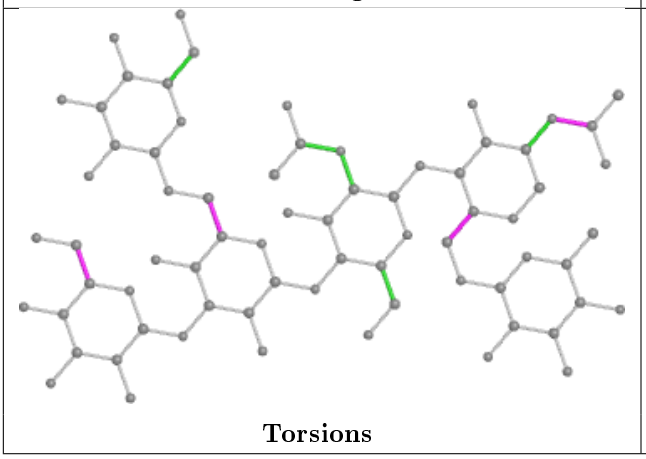
Oligosaccharide Chain K



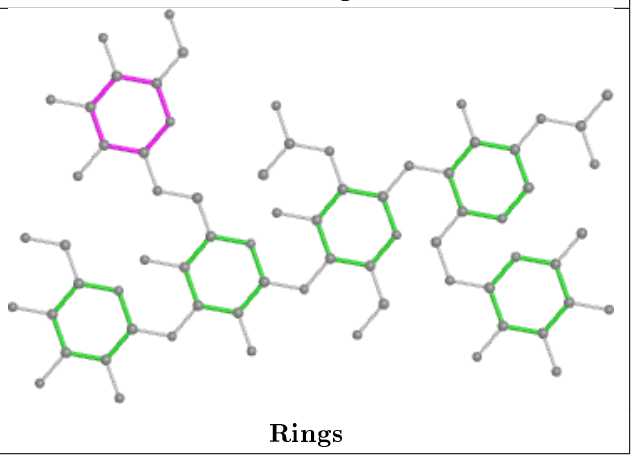
Bond lengths



Bond angles

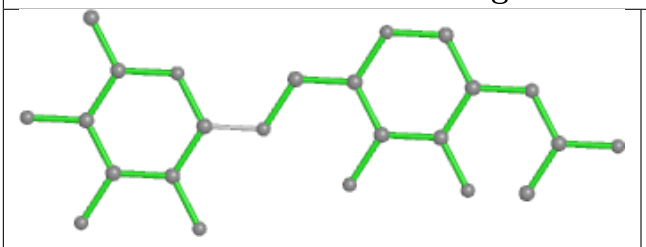


Torsions

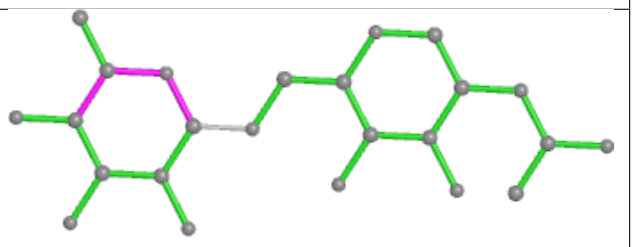


Rings

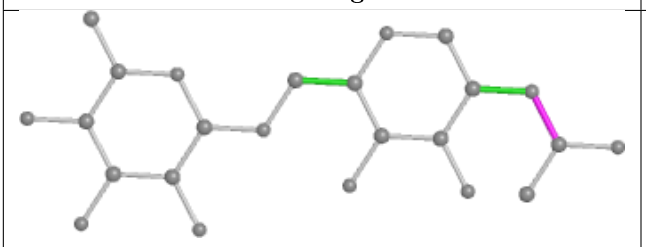
Oligosaccharide Chain M



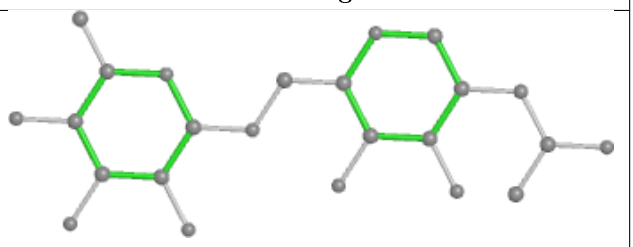
Bond lengths



Bond angles

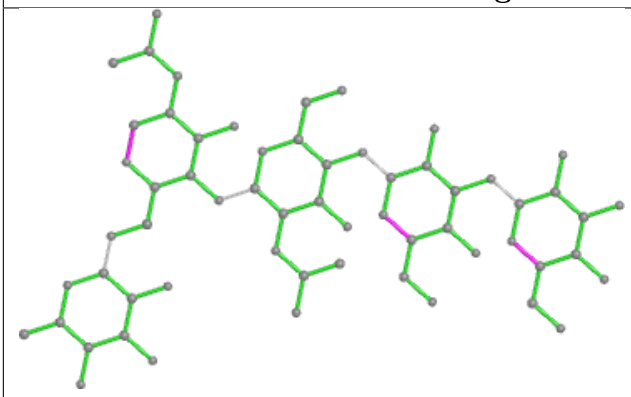


Torsions

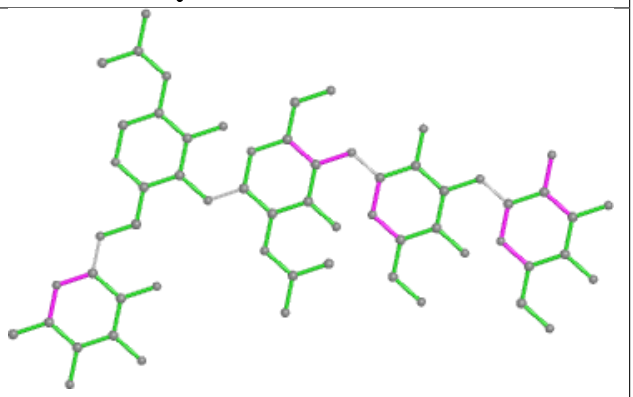


Rings

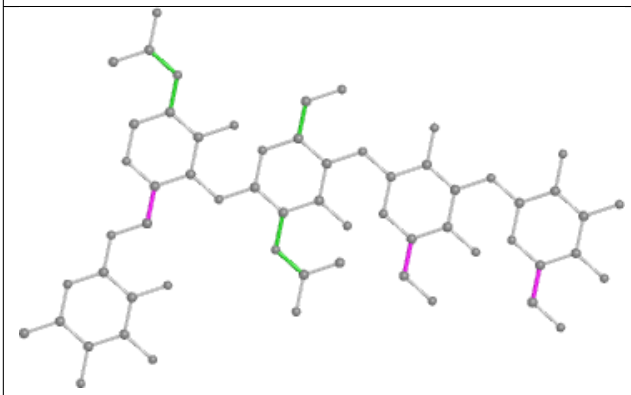
Oligosaccharide Chain Q



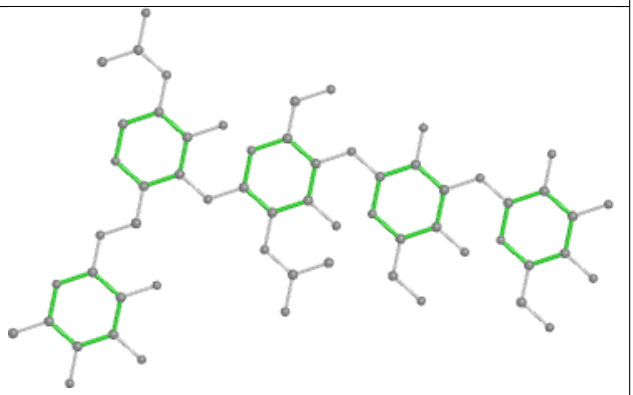
Bond lengths



Bond angles

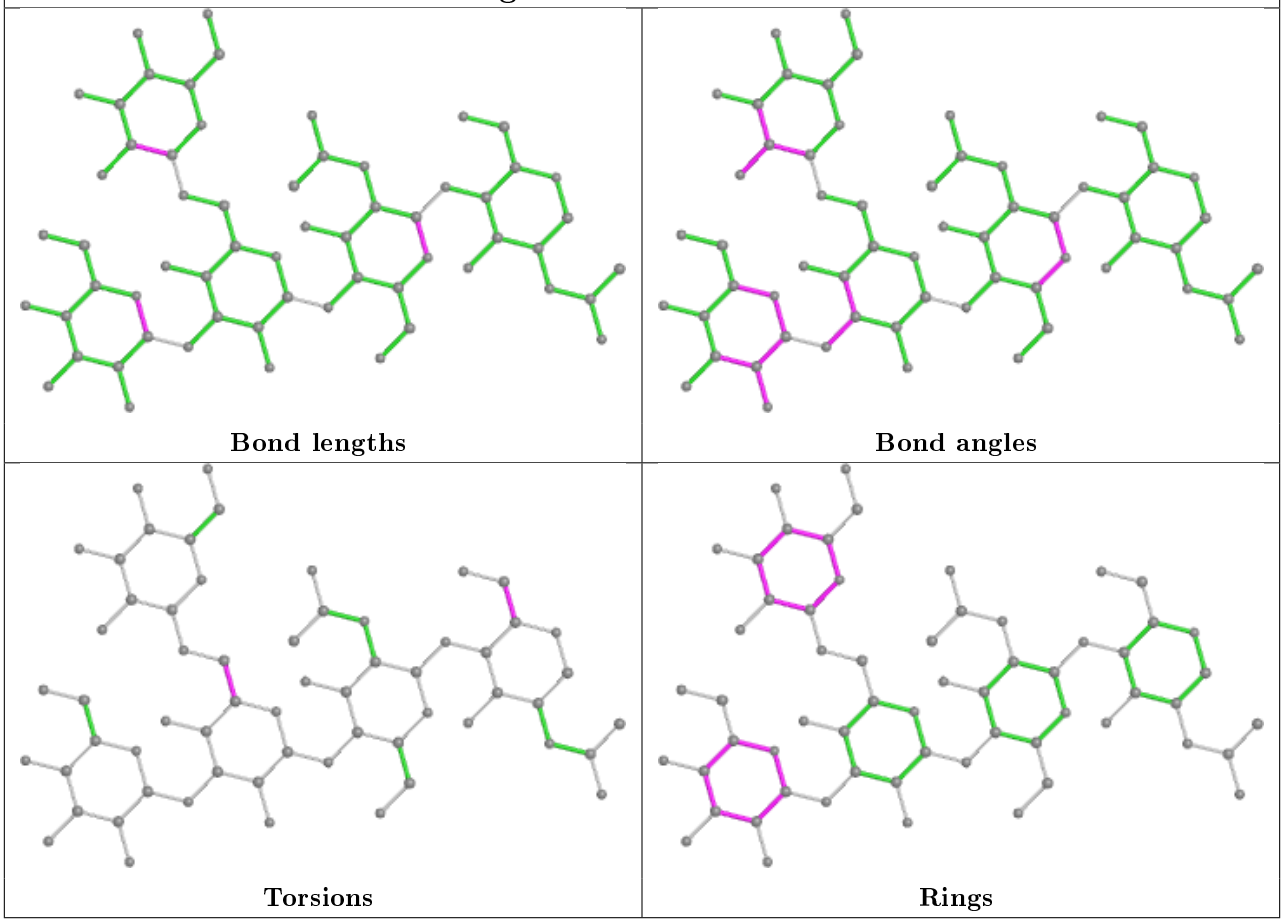


Torsions



Rings

Oligosaccharide Chain S



5.6 Ligand geometry (i)

Of 17 ligands modelled in this entry, 9 are monoatomic - leaving 8 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	$\#\|Z\| > 2$
10	URS	B	516	-	10,10,10	5.25	9 (90%)	11,12,12	1.23	2 (18%)
10	URS	A	509	-	10,10,10	5.04	9 (90%)	11,12,12	0.99	0
10	URS	C	510	-	10,10,10	5.27	9 (90%)	11,12,12	1.15	1 (9%)
10	URS	D	518	-	10,10,10	4.99	10 (100%)	11,12,12	0.87	0
9	NAG	C	509	1	14,14,15	0.93	1 (7%)	17,19,21	1.06	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	NAG	C	504	1	14,14,15	1.36	3 (21%)	17,19,21	1.26	2 (11%)
9	NAG	C	503	1	14,14,15	0.31	0	17,19,21	0.50	0
9	NAG	A	504	1	14,14,15	1.66	2 (14%)	17,19,21	1.22	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	URS	B	516	-	-	0/4/4/4	0/1/1/1
10	URS	A	509	-	-	0/4/4/4	0/1/1/1
10	URS	C	510	-	-	2/4/4/4	0/1/1/1
10	URS	D	518	-	-	0/4/4/4	0/1/1/1
9	NAG	C	509	1	-	0/6/23/26	0/1/1/1
9	NAG	C	504	1	-	2/6/23/26	0/1/1/1
9	NAG	C	503	1	-	2/6/23/26	0/1/1/1
9	NAG	A	504	1	-	0/6/23/26	0/1/1/1

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	510	URS	C4-C3	8.41	1.53	1.39
10	B	516	URS	C4-C3	8.21	1.53	1.39
10	D	518	URS	C4-C3	8.12	1.52	1.39
10	A	509	URS	C4-C3	7.70	1.52	1.39
10	C	510	URS	C7-N1	7.12	1.47	1.34
10	B	516	URS	C7-S1	-6.98	1.59	1.69
10	B	516	URS	C1-C2	6.76	1.53	1.38
10	C	510	URS	C1-C2	6.64	1.52	1.38
10	D	518	URS	C1-C2	6.45	1.52	1.38
10	A	509	URS	C1-C2	6.41	1.52	1.38
10	A	509	URS	C7-N1	6.35	1.45	1.34
10	D	518	URS	C7-N1	6.28	1.45	1.34
10	A	509	URS	C7-S1	-6.11	1.60	1.69
10	B	516	URS	C7-N1	6.04	1.45	1.34
10	C	510	URS	C6-C5	5.99	1.53	1.38
10	B	516	URS	C6-C5	5.91	1.53	1.38
10	C	510	URS	C7-S1	-5.73	1.61	1.69
10	D	518	URS	C6-C5	5.56	1.52	1.38
10	A	509	URS	C6-C5	5.28	1.52	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	D	518	URS	C7-S1	-5.13	1.62	1.69
9	A	504	NAG	O5-C1	-4.95	1.35	1.43
10	A	509	URS	C2-C3	-4.52	1.31	1.39
10	C	510	URS	C2-C3	-4.06	1.32	1.39
10	B	516	URS	C2-C3	-4.06	1.32	1.39
10	D	518	URS	C2-C3	-3.82	1.32	1.39
9	C	504	NAG	O5-C1	-3.74	1.37	1.43
10	A	509	URS	C5-C4	-3.42	1.31	1.38
10	D	518	URS	C5-C4	-3.40	1.31	1.38
9	C	509	NAG	O5-C1	3.24	1.48	1.43
10	B	516	URS	C5-C4	-3.09	1.32	1.38
10	D	518	URS	C7-N2	-3.05	1.26	1.32
9	A	504	NAG	C1-C2	2.98	1.56	1.52
10	C	510	URS	C7-N2	-2.97	1.26	1.32
10	B	516	URS	C7-N2	-2.96	1.27	1.32
10	C	510	URS	C5-C4	-2.91	1.32	1.38
10	A	509	URS	C7-N2	-2.83	1.27	1.32
10	C	510	URS	C3-N1	2.54	1.46	1.41
9	C	504	NAG	C1-C2	2.52	1.56	1.52
10	A	509	URS	C6-C1	-2.18	1.32	1.38
10	D	518	URS	C6-C1	-2.13	1.32	1.38
10	D	518	URS	C3-N1	2.10	1.45	1.41
9	C	504	NAG	C3-C2	2.07	1.56	1.52
10	B	516	URS	C6-C1	-2.06	1.32	1.38

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	C	504	NAG	C4-C3-C2	4.01	116.90	111.02
9	C	509	NAG	C1-O5-C5	3.81	117.36	112.19
9	A	504	NAG	C4-C3-C2	3.75	116.51	111.02
10	C	510	URS	S1-C7-N2	-3.08	118.95	123.15
10	B	516	URS	N2-C7-N1	2.72	122.42	117.43
9	A	504	NAG	O5-C5-C4	-2.46	104.85	110.83
9	C	504	NAG	O5-C5-C4	-2.42	104.95	110.83
10	B	516	URS	S1-C7-N1	-2.12	116.50	121.07

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	C	503	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
9	C	503	NAG	O5-C5-C6-O6
9	C	504	NAG	O5-C5-C6-O6
9	C	504	NAG	C4-C5-C6-O6
10	C	510	URS	C4-C3-N1-C7
10	C	510	URS	C2-C3-N1-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	C	509	NAG	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	446/446 (100%)	-0.18	6 (1%) 77 75	26, 41, 58, 82	0
1	B	446/446 (100%)	-0.10	12 (2%) 54 52	27, 43, 63, 87	0
1	C	446/446 (100%)	-0.19	9 (2%) 65 63	29, 43, 62, 84	0
1	D	446/446 (100%)	-0.20	3 (0%) 87 86	28, 43, 60, 93	0
All	All	1784/1784 (100%)	-0.17	30 (1%) 70 68	26, 42, 61, 93	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	126	VAL	7.4
1	A	48	VAL	5.5
1	B	118	ARG	5.5
1	B	119	GLY	4.9
1	A	470	SER	4.9
1	C	49	SER	4.4
1	B	47	PRO	4.3
1	D	470	SER	4.3
1	A	49	SER	4.1
1	C	320	ALA	4.0
1	B	48	VAL	4.0
1	B	125	ARG	2.8
1	B	49	SER	2.8
1	C	203	VAL	2.7
1	A	50	GLY	2.7
1	B	46	SER	2.6
1	B	120	ALA	2.6
1	C	470	SER	2.4
1	D	125	ARG	2.4
1	B	121	ALA	2.4
1	C	51	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	319	VAL	2.3
1	B	469	PRO	2.2
1	C	48	VAL	2.2
1	C	323	MET	2.2
1	C	299	LEU	2.2
1	A	47	PRO	2.1
1	D	348	TYR	2.1
1	B	470	SER	2.1
1	A	46	SER	2.0

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

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

6.3 Carbohydrates (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	O	2	14/15	0.67	0.29	79,89,97,99	0
2	NAG	E	2	14/15	0.71	0.27	72,82,89,91	0
2	NAG	E	1	14/15	0.77	0.15	55,64,76,81	0
2	NAG	P	2	14/15	0.80	0.29	57,74,80,82	0
8	MAN	S	4	11/12	0.80	0.21	54,63,72,82	0
3	NAG	O	1	14/15	0.81	0.16	60,66,77,86	0
4	NAG	I	1	14/15	0.82	0.18	63,68,70,72	0
5	MAN	K	5	11/12	0.82	0.16	63,69,75,76	0
8	MAN	S	5	11/12	0.82	0.19	58,62,66,69	0
5	FUC	K	6	10/11	0.83	0.26	66,73,75,78	0
4	MAN	I	2	11/12	0.83	0.24	78,79,81,83	0
2	NAG	H	2	14/15	0.84	0.18	50,59,68,78	0
2	NAG	P	1	14/15	0.84	0.17	51,55,62,70	0
2	FUC	E	3	10/11	0.84	0.20	58,68,76,79	0
3	NAG	N	2	14/15	0.85	0.28	59,71,76,77	0
3	NAG	G	2	14/15	0.86	0.22	55,62,70,72	0
6	NAG	M	1	14/15	0.86	0.19	51,58,64,64	0
7	FUC	Q	5	10/11	0.86	0.18	51,56,62,66	0
7	MAN	Q	3	11/12	0.87	0.12	47,52,55,57	0

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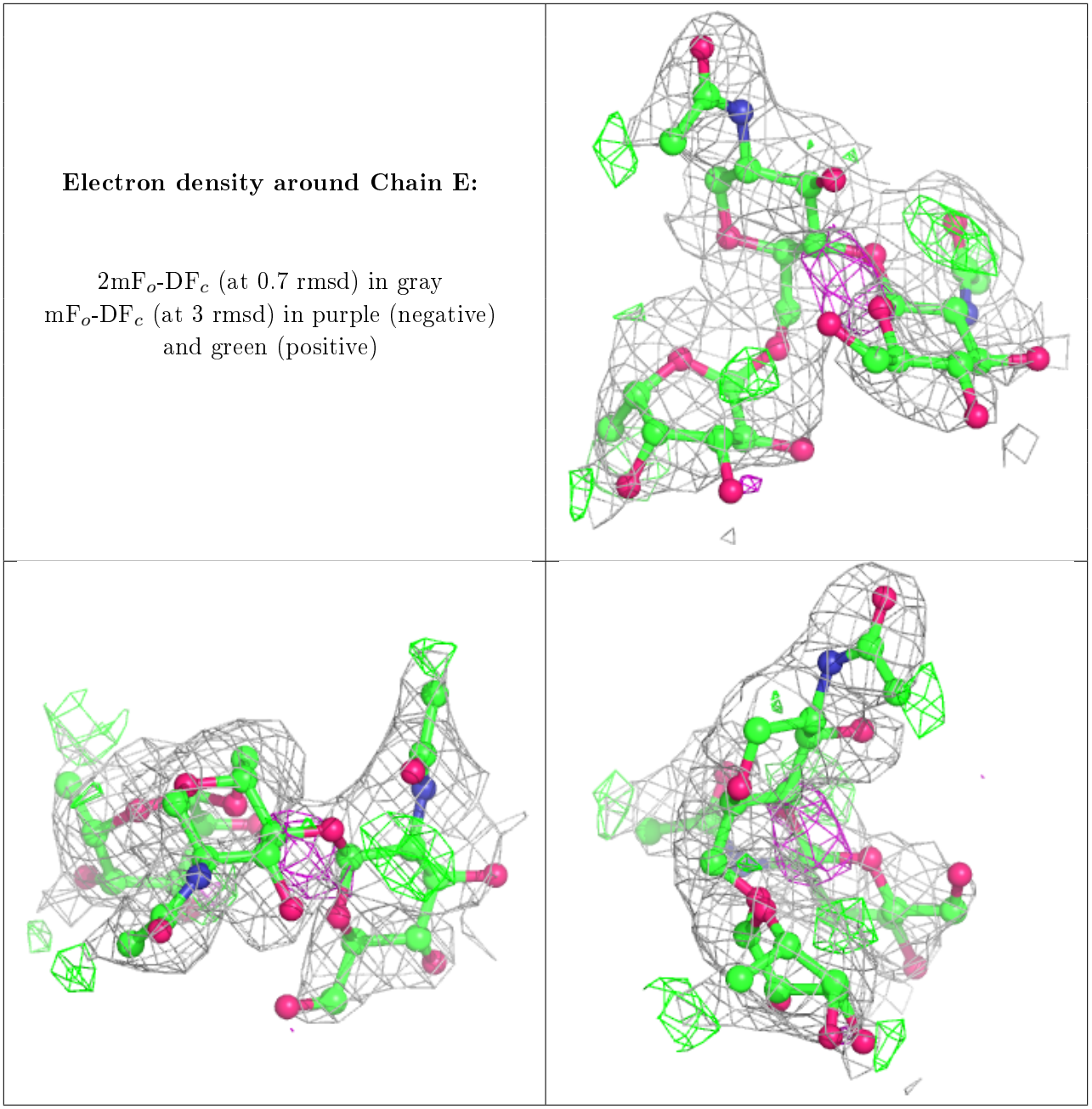
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	FUC	M	2	10/11	0.87	0.20	54,64,68,68	0
8	NAG	S	1	14/15	0.87	0.21	52,62,69,70	0
3	NAG	T	1	14/15	0.89	0.12	42,49,60,63	0
5	MAN	K	4	11/12	0.89	0.19	61,67,72,76	0
3	NAG	T	2	14/15	0.89	0.28	60,66,76,80	0
2	FUC	P	3	10/11	0.89	0.21	51,60,63,68	0
5	MAN	K	3	11/12	0.90	0.12	50,56,61,68	0
7	MAN	Q	4	11/12	0.90	0.15	50,53,58,59	0
2	NAG	H	1	14/15	0.90	0.12	50,55,63,71	0
3	NAG	R	2	14/15	0.90	0.15	51,58,65,68	0
3	NAG	L	2	14/15	0.91	0.16	43,57,65,75	0
3	NAG	J	2	14/15	0.91	0.17	56,60,65,67	0
7	NAG	Q	2	14/15	0.91	0.11	48,51,55,55	0
3	NAG	G	1	14/15	0.91	0.10	41,48,57,60	0
8	MAN	S	3	11/12	0.92	0.14	46,50,56,62	0
3	NAG	L	1	14/15	0.92	0.11	34,46,56,59	0
3	NAG	F	2	14/15	0.92	0.18	56,64,67,73	0
2	FUC	H	3	10/11	0.93	0.11	49,56,65,67	0
5	NAG	K	1	14/15	0.94	0.12	38,43,50,60	0
3	NAG	N	1	14/15	0.94	0.14	53,58,64,70	0
5	NAG	K	2	14/15	0.95	0.09	40,46,48,56	0
7	NAG	Q	1	14/15	0.95	0.08	39,46,52,61	0
8	NAG	S	2	14/15	0.95	0.13	37,48,58,59	0
3	NAG	R	1	14/15	0.96	0.10	41,47,51,52	0
3	NAG	J	1	14/15	0.96	0.10	42,49,51,56	0
3	NAG	F	1	14/15	0.97	0.10	44,47,53,57	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.

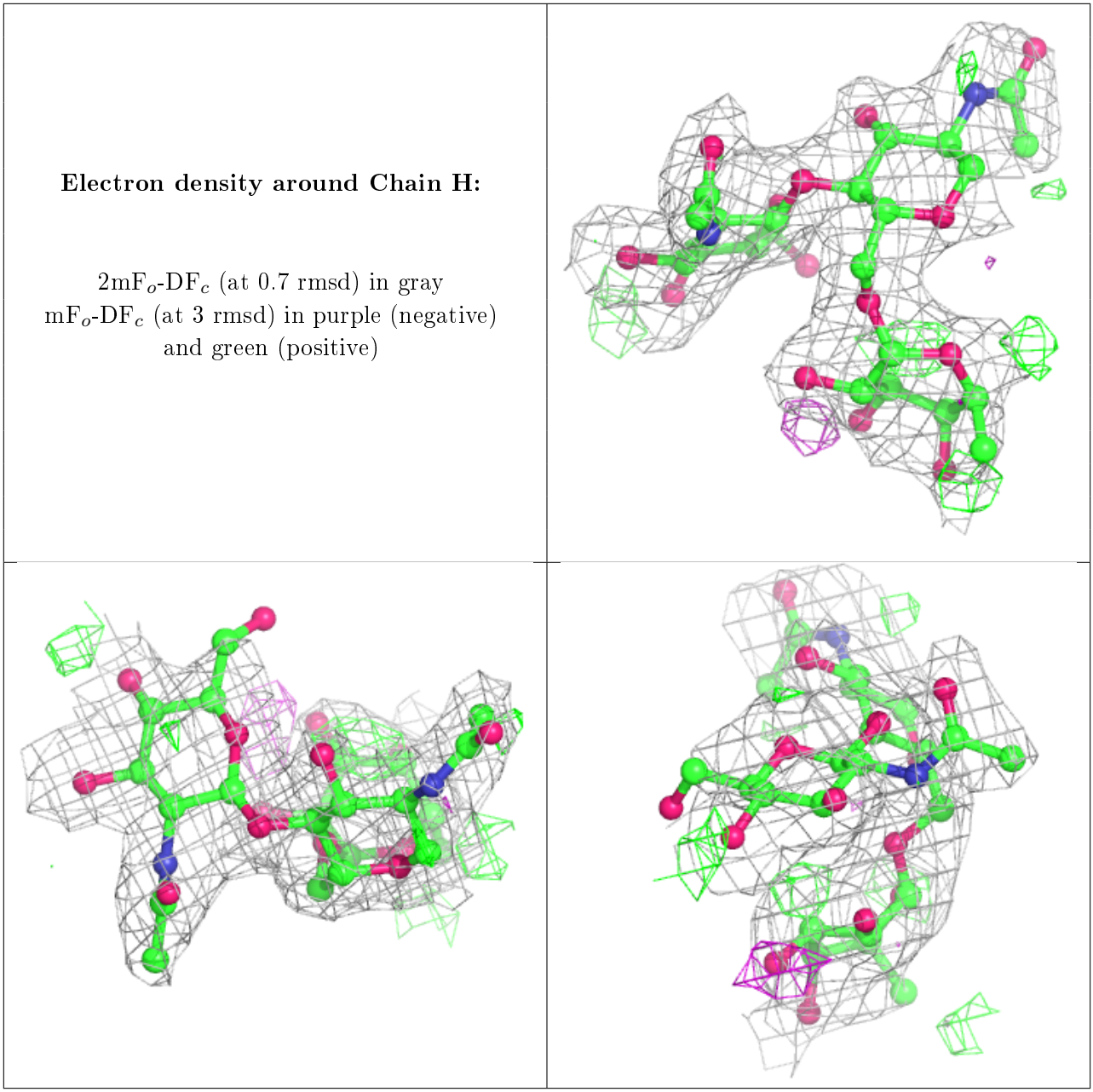
Electron density around Chain E:

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



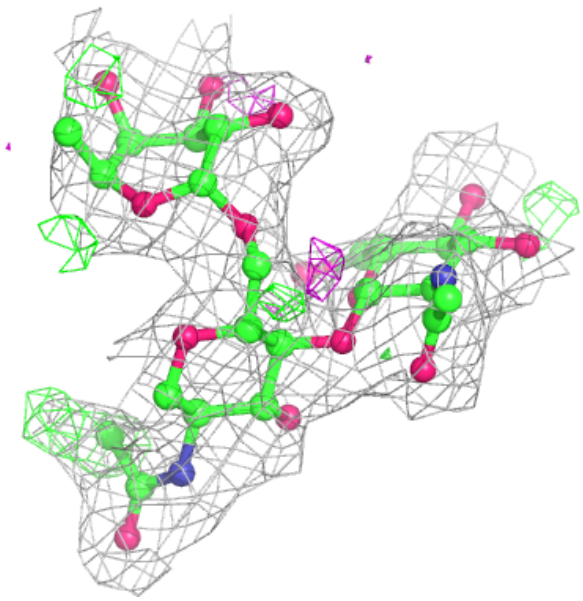
Electron density around Chain H:

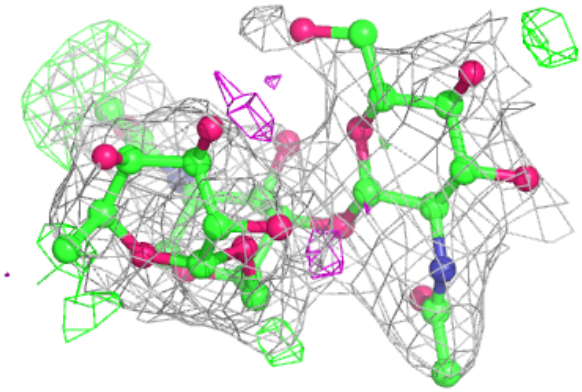
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

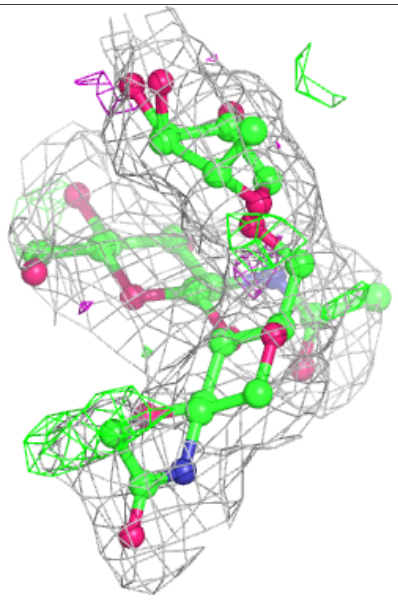


Electron density around Chain P:

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

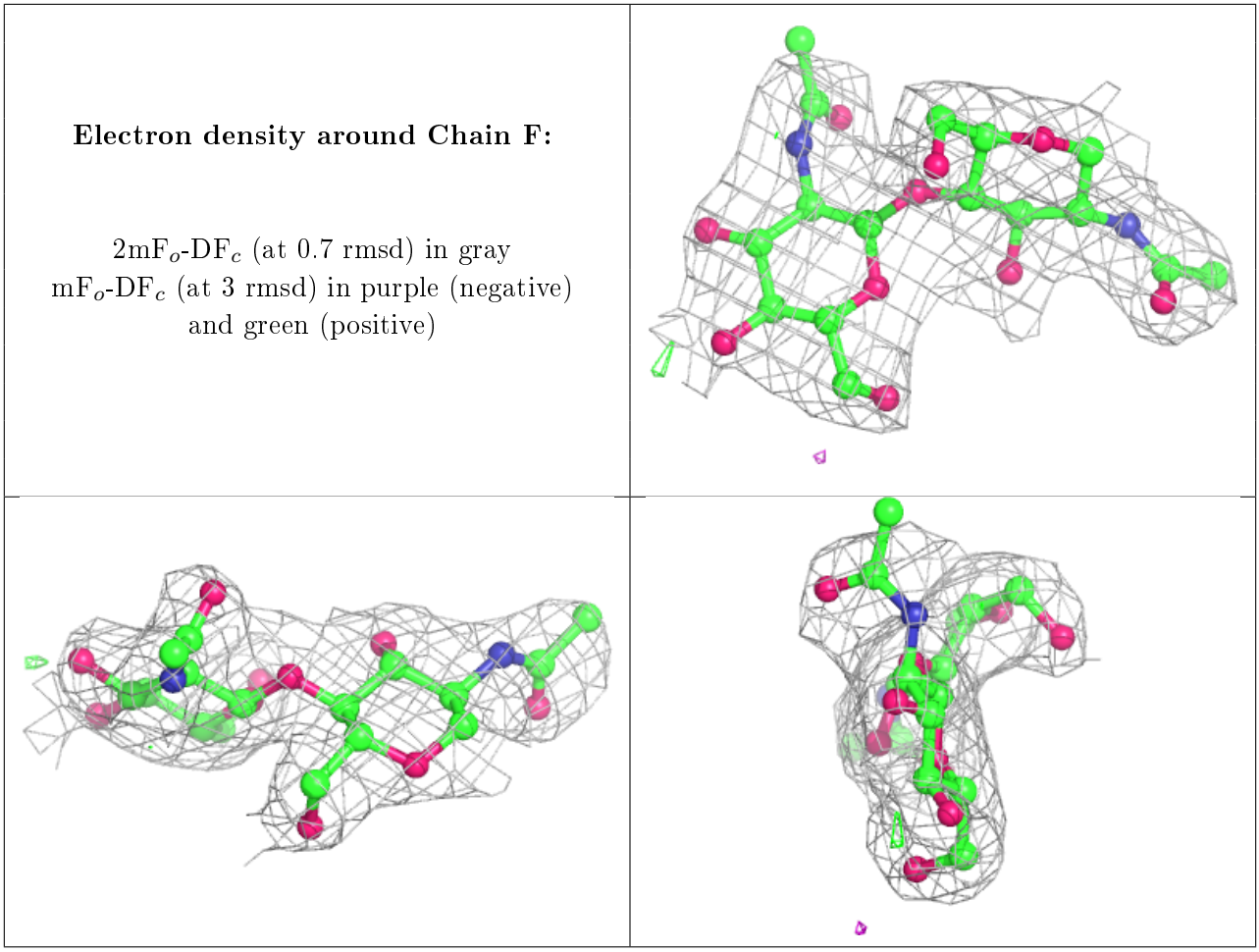






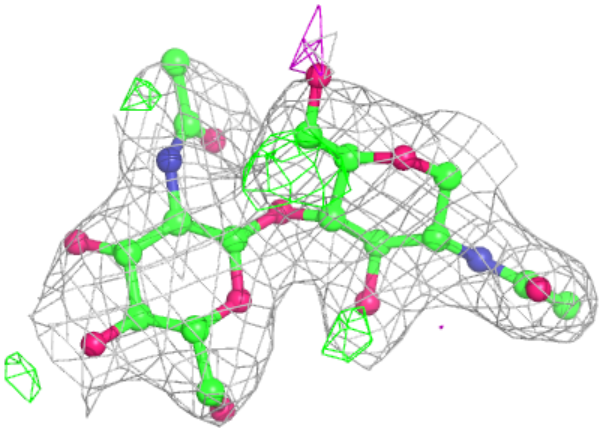
Electron density around Chain F:

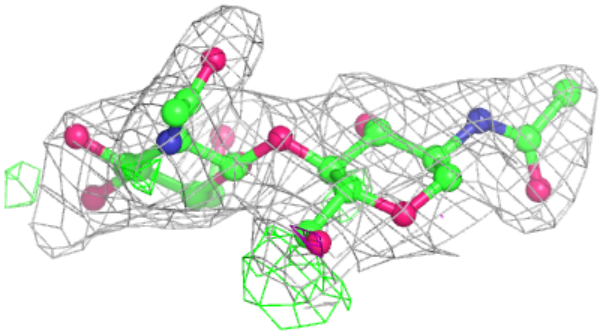
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

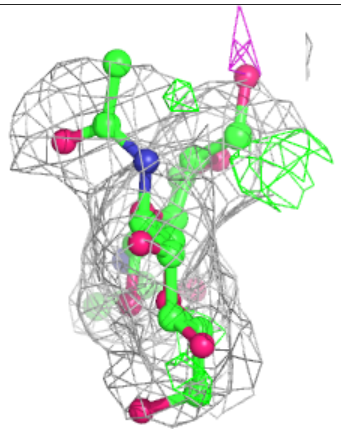


Electron density around Chain G:

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

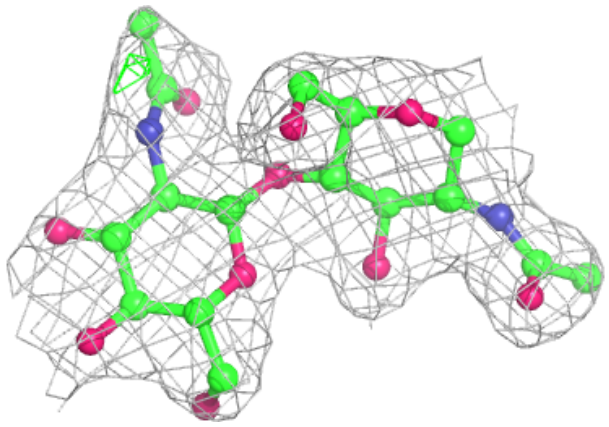


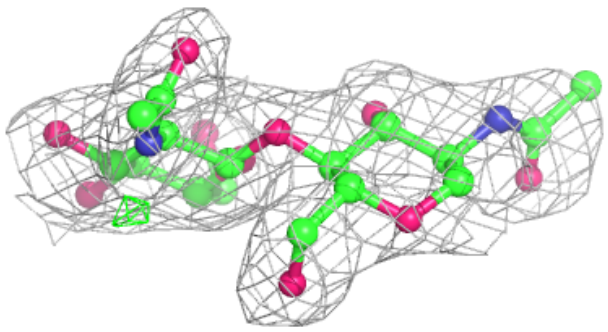


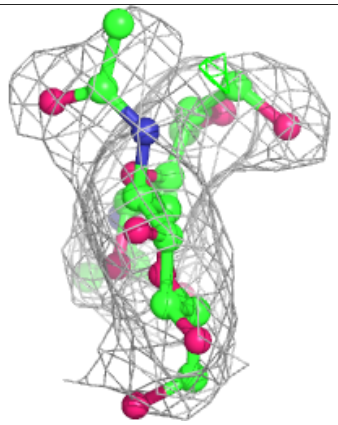


Electron density around Chain J:

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

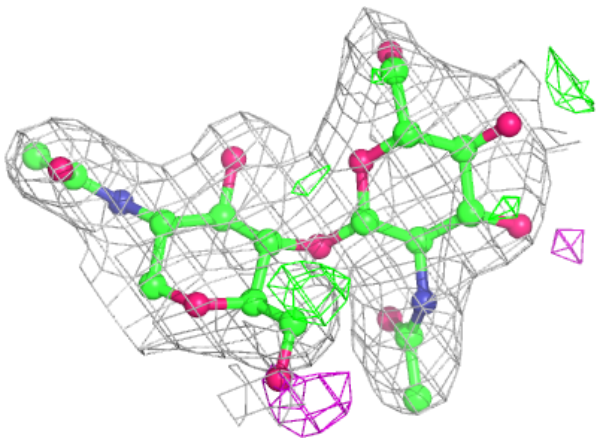


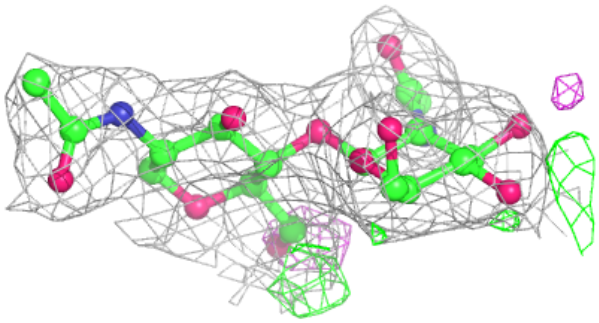


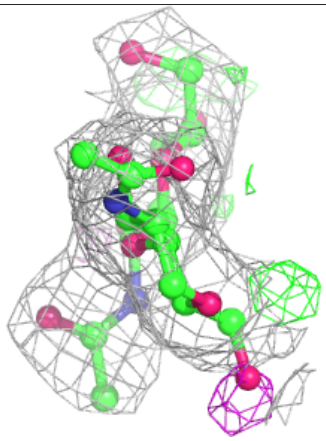


Electron density around Chain L:

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

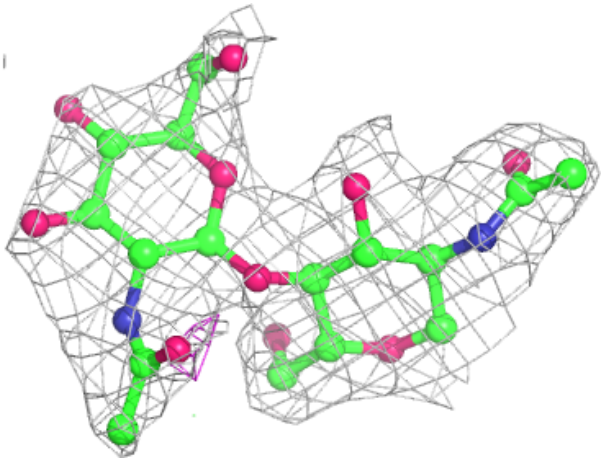


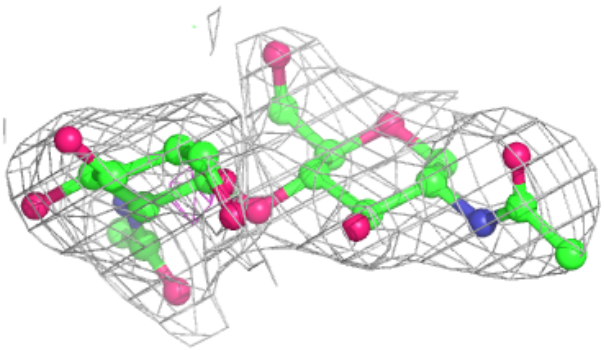


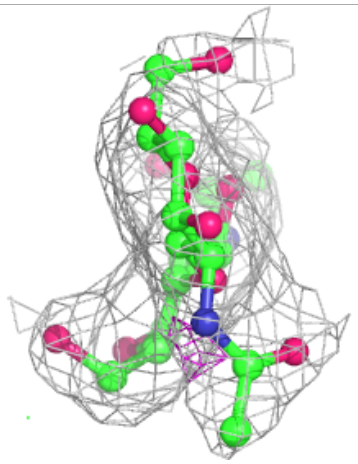


Electron density around Chain N:

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

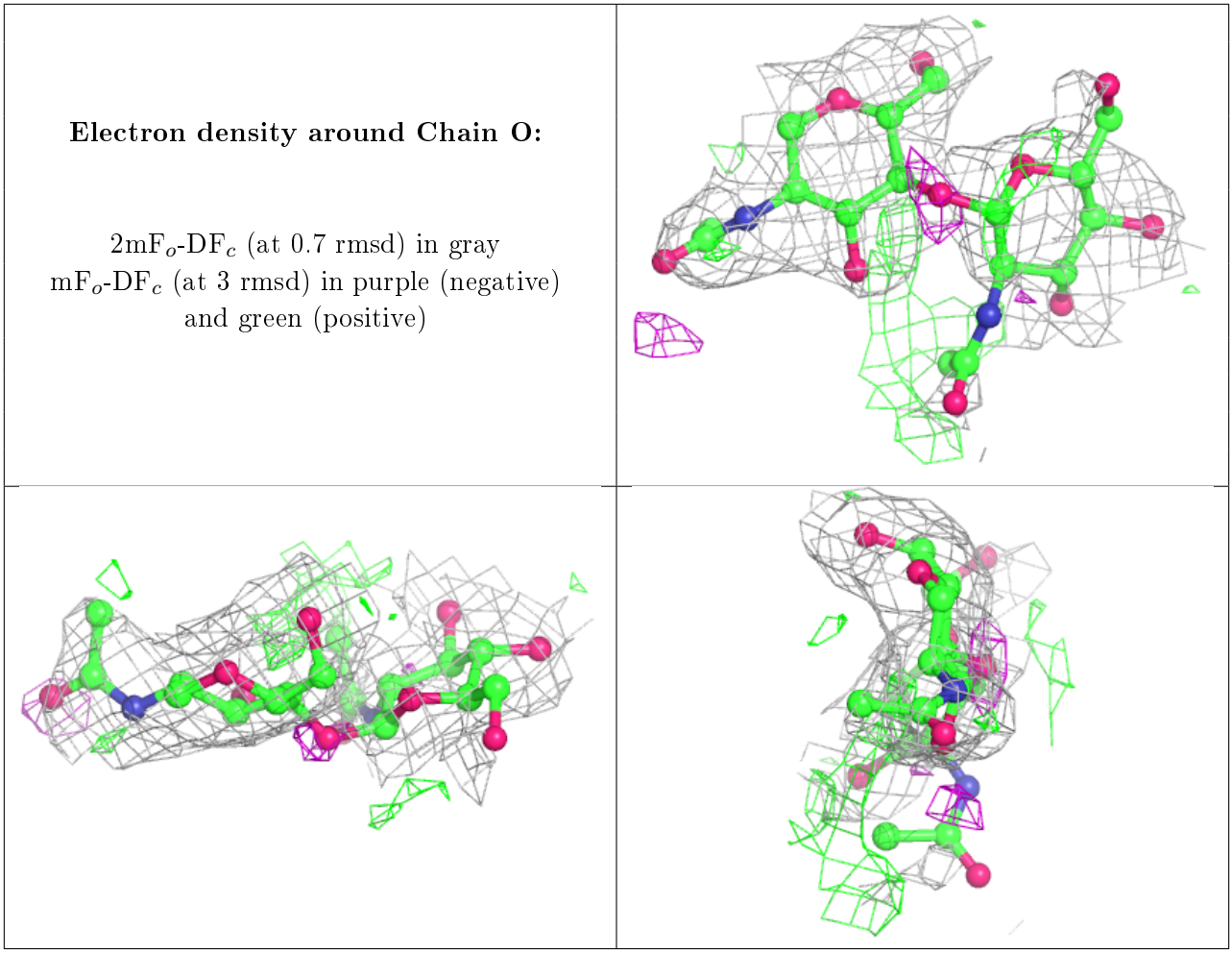






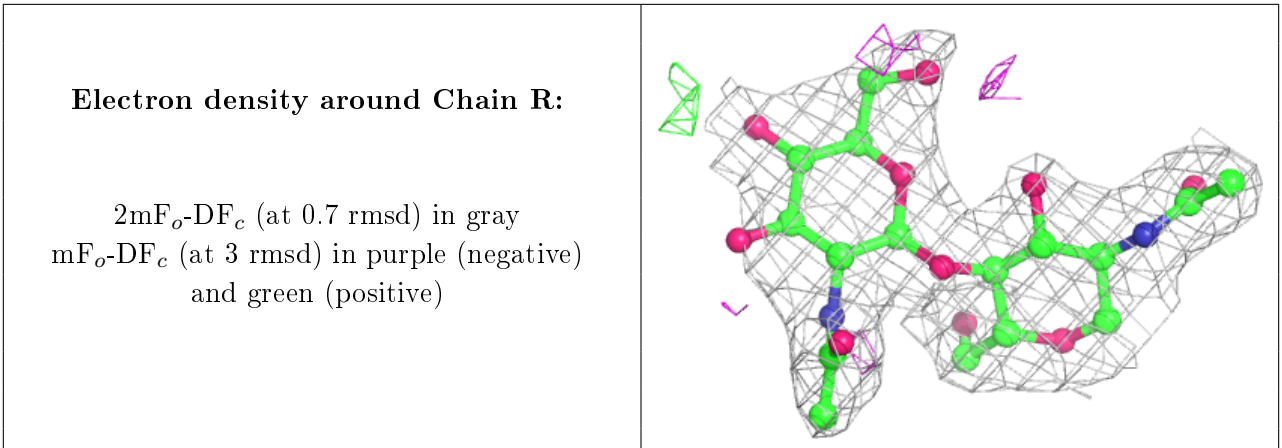
Electron density around Chain O:

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



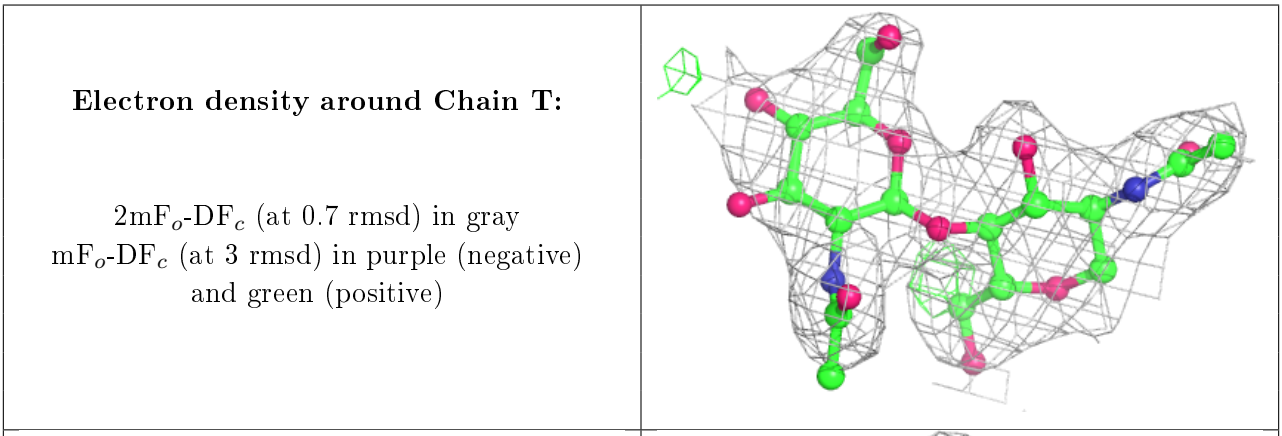
Electron density around Chain R:

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



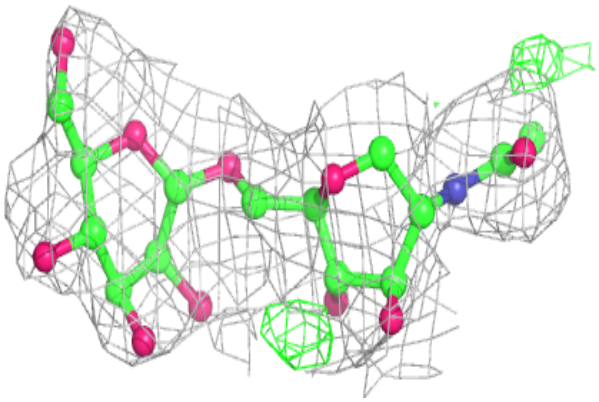
Electron density around Chain T:

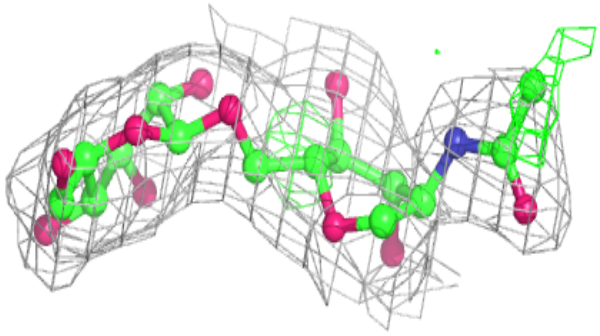
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

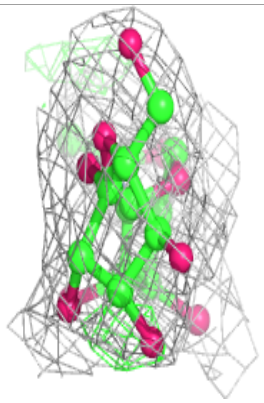


Electron density around Chain I:

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

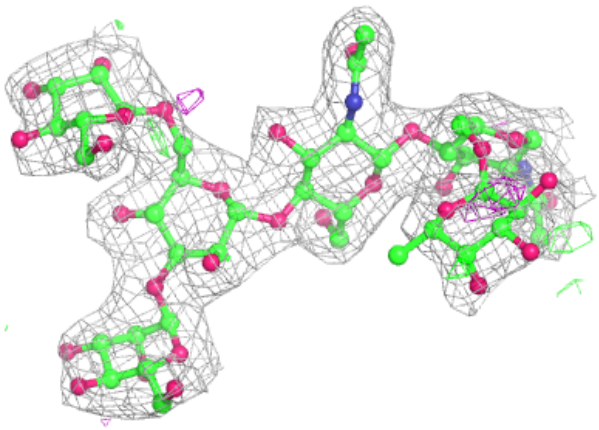


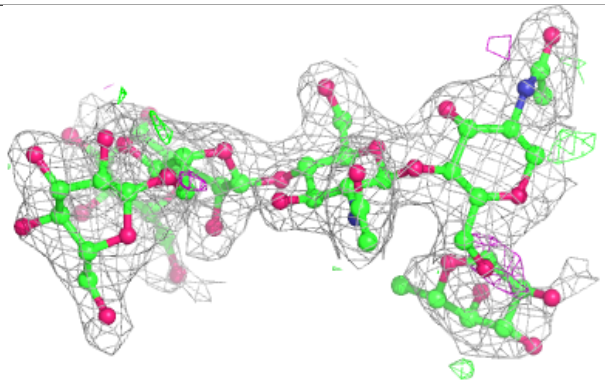


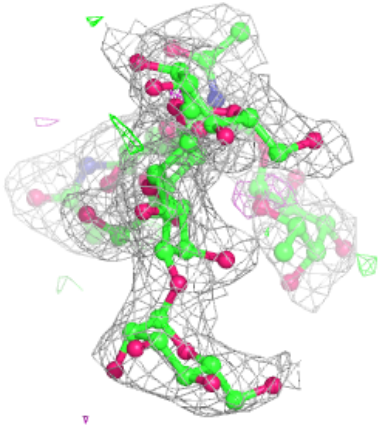


Electron density around Chain K:

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

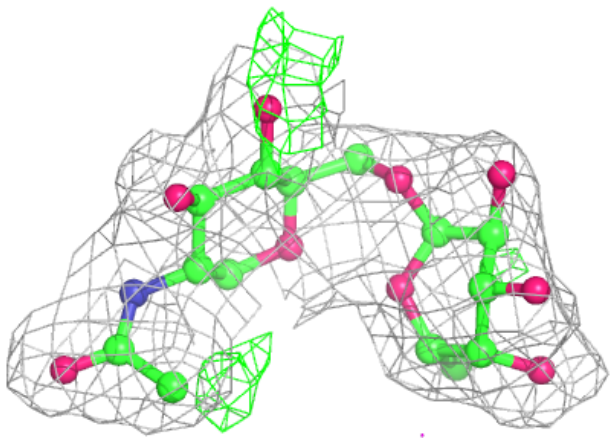


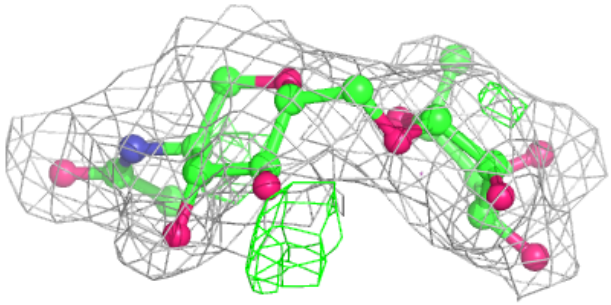


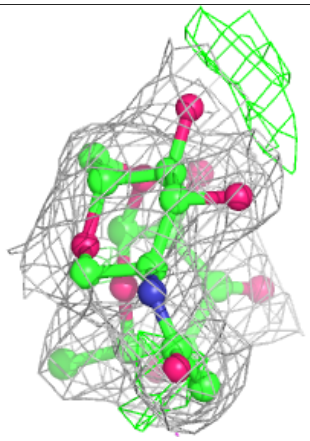


Electron density around Chain M:

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

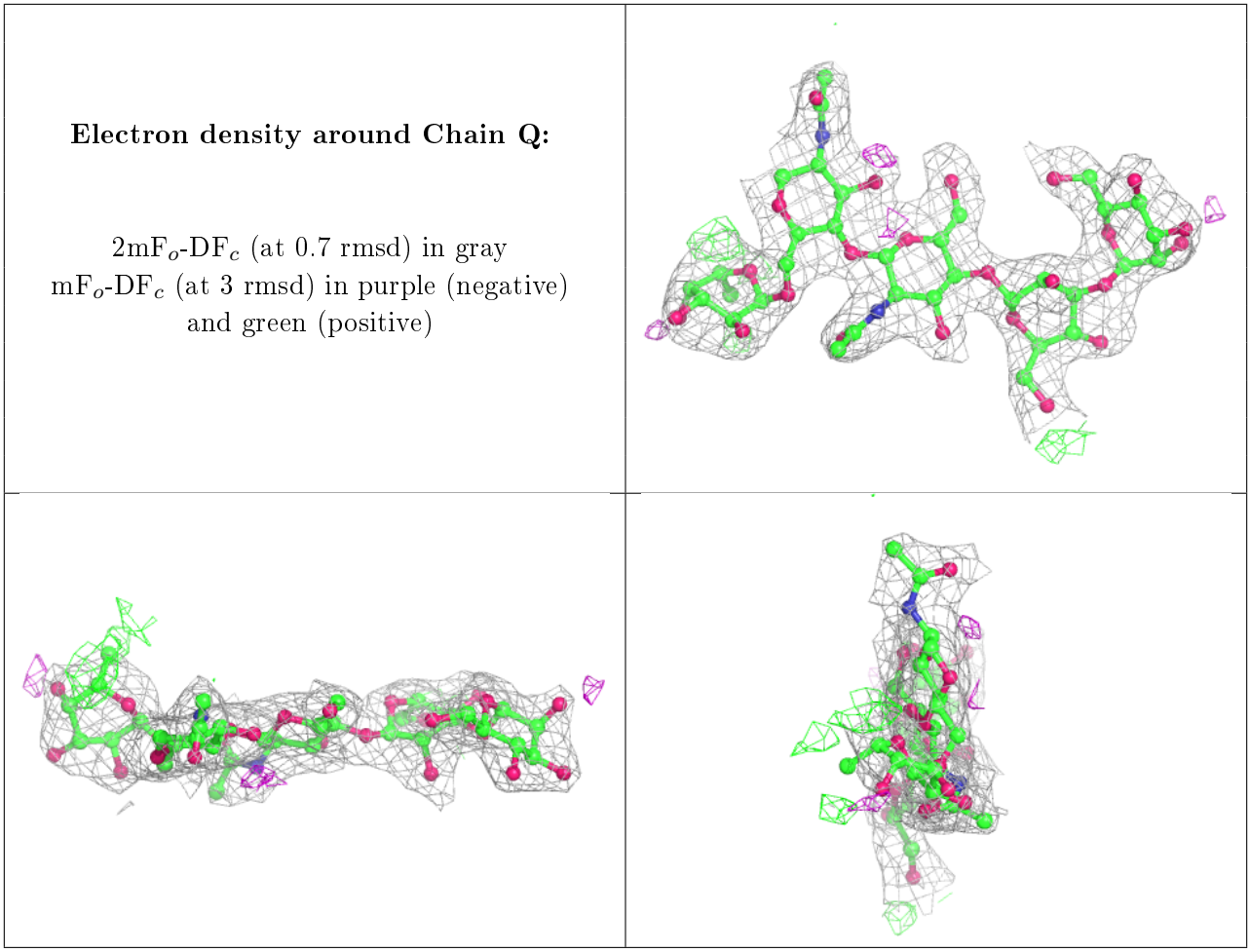






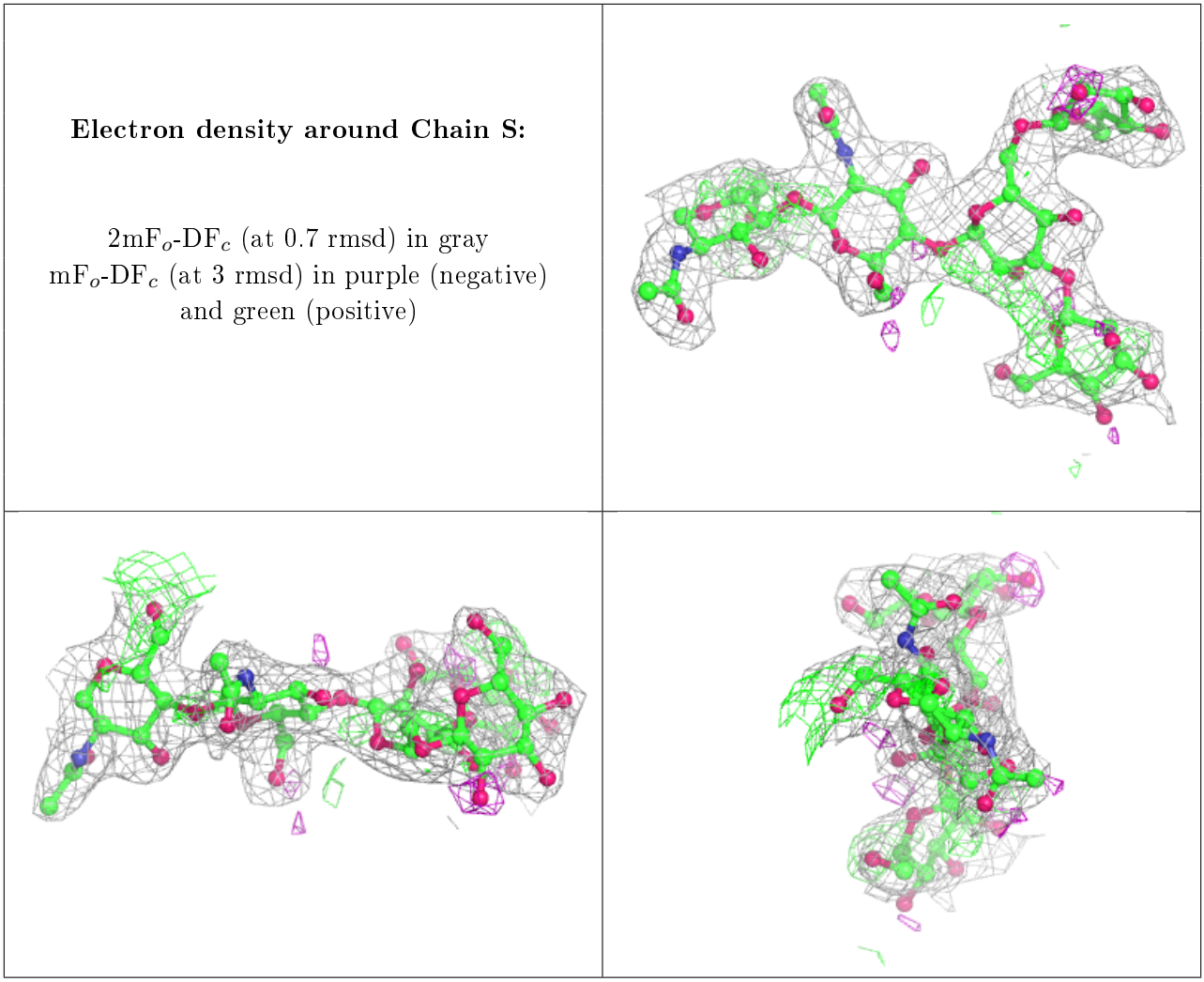
Electron density around Chain Q:

$2mF_o$-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 S:

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



6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	NAG	A	504	14/15	0.72	0.26	58,69,73,73	0
9	NAG	C	504	14/15	0.81	0.21	61,68,76,82	0
9	NAG	C	503	14/15	0.87	0.13	47,52,55,57	0
9	NAG	C	509	14/15	0.88	0.15	49,58,64,66	0
10	URS	C	510	10/10	0.94	0.13	43,46,49,52	0
10	URS	B	516	10/10	0.97	0.12	32,35,38,38	0
10	URS	D	518	10/10	0.97	0.12	34,39,41,43	0
10	URS	A	509	10/10	0.97	0.14	35,37,40,40	0
11	ZN	C	512	1/1	0.98	0.16	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
11	ZN	B	517	1/1	0.99	0.14	29,29,29,29	0
11	ZN	A	512	1/1	0.99	0.08	51,51,51,51	0
11	ZN	C	511	1/1	0.99	0.16	35,35,35,35	0
11	ZN	D	519	1/1	1.00	0.15	30,30,30,30	0
11	ZN	A	511	1/1	1.00	0.15	29,29,29,29	0
11	ZN	D	520	1/1	1.00	0.16	30,30,30,30	0
11	ZN	A	510	1/1	1.00	0.16	29,29,29,29	0
11	ZN	B	518	1/1	1.00	0.14	30,30,30,30	0

6.5 Other polymers (i)

There are no such residues in this entry.