Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2024 – 10:16 AM JST

PDB ID	:	8IKW
Title	:	A complex structure of PGIP-PG
Authors	:	Xiao, Y.; Chai, J.
Deposited on	:	2023-03-01
Resolution	:	1.94 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

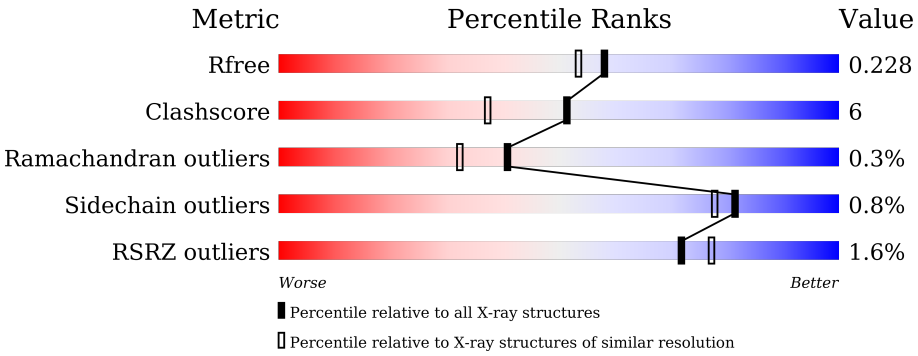
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 1.94 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	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

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	313	2% 90% 10%
1	C	313	2% 93% 7%
1	E	313	2% 89% 11%
1	G	313	2% 87% 13%
2	B	349	% 87% 12%
2	D	349	3% 88% 11%

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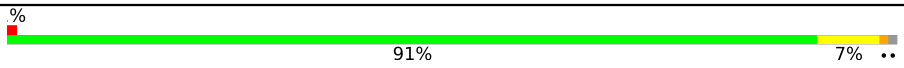
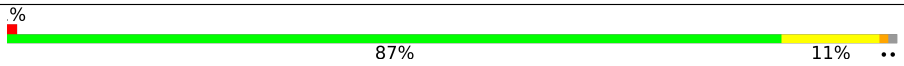
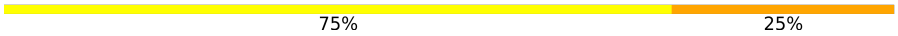
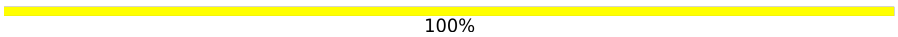
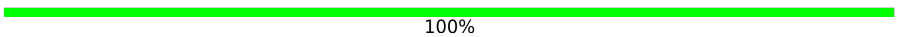
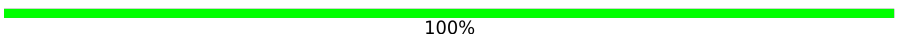
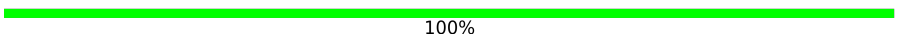
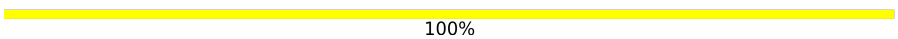
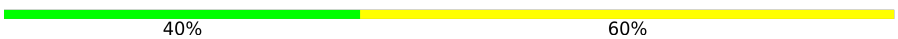
Mol	Chain	Length	Quality of chain
2	F	349	
2	H	349	
3	I	3	
4	J	4	
5	K	2	
5	L	2	
5	M	2	
5	N	2	
5	O	2	
5	P	2	
5	S	2	
5	T	2	
6	Q	3	
7	R	5	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 22453 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 Polygalacturonase inhibitor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	313	Total	C	N	O	S	0	0	0
			2392	1524	405	453	10			
1	C	313	Total	C	N	O	S	0	0	0
			2392	1524	405	453	10			
1	E	313	Total	C	N	O	S	0	0	0
			2392	1524	405	453	10			
1	G	313	Total	C	N	O	S	0	0	0
			2392	1524	405	453	10			

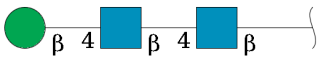
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	274	ASP	ASN	engineered mutation	UNP P58822
C	274	ASP	ASN	engineered mutation	UNP P58822
E	274	ASP	ASN	engineered mutation	UNP P58822
G	274	ASP	ASN	engineered mutation	UNP P58822

- Molecule 2 is a protein called Endo-polygalacturonase.

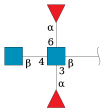
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	346	Total	C	N	O	S	0	0	0
			2520	1543	436	530	11			
2	D	346	Total	C	N	O	S	0	0	0
			2520	1543	436	530	11			
2	F	346	Total	C	N	O	S	0	0	0
			2520	1543	436	530	11			
2	H	346	Total	C	N	O	S	0	0	0
			2520	1543	436	530	11			

- Molecule 3 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
3	I	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 4 is an oligosaccharide called alpha-L-fucopyranose-(1-3)-[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
4	J	4	Total	C	N	O	0	0	0
			48	28	2	18			

- Molecule 5 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
5	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	L	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	M	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	N	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	O	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	P	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	S	2	Total	C	N	O	0	0	0
			28	16	2	10			

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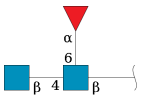
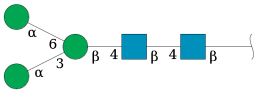
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	T	2	Total C N O 28 16 2 10	0	0	0

- Molecule 6 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
6	Q	3	Total C N O 38 22 2 14	0	0	0

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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
7	R	5	Total C N O 61 34 2 25	0	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	298	Total O 298 298	0	0
8	B	338	Total O 338 338	0	0
8	C	298	Total O 298 298	0	0
8	E	305	Total O 305 305	0	0
8	G	285	Total O 285 285	0	0
8	D	278	Total O 278 278	0	0

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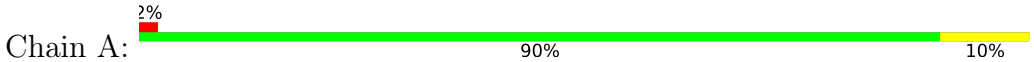
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	F	321	Total O 321 321	0	0
8	H	272	Total O 272 272	0	0

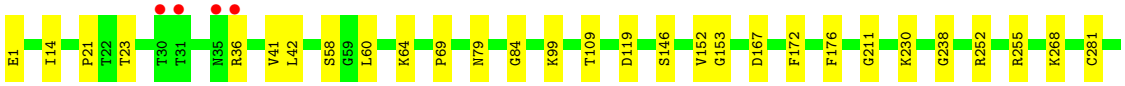
3 Residue-property plots (i)

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: Polygalacturonase inhibitor 2

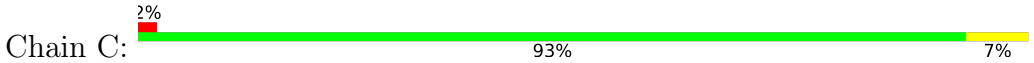
Chain A:

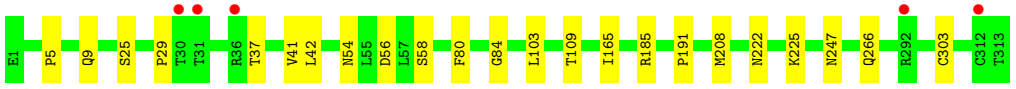




• Molecule 1: Polygalacturonase inhibitor 2

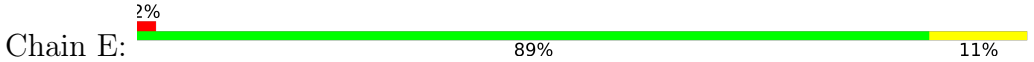
Chain C:

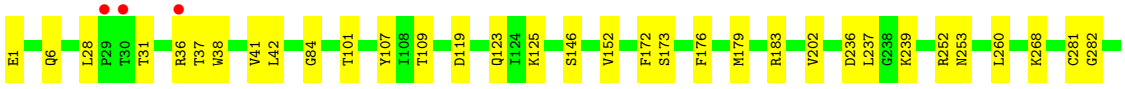


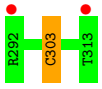


• Molecule 1: Polygalacturonase inhibitor 2

Chain E:

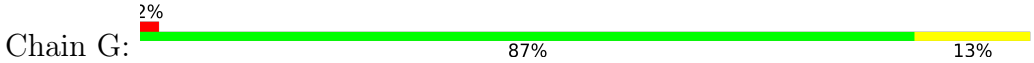


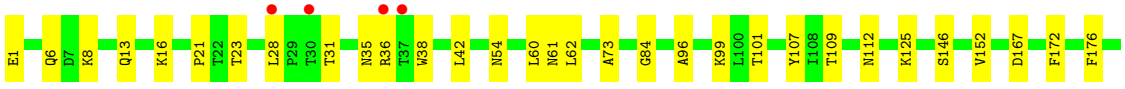


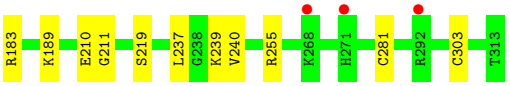


• Molecule 1: Polygalacturonase inhibitor 2

Chain G:

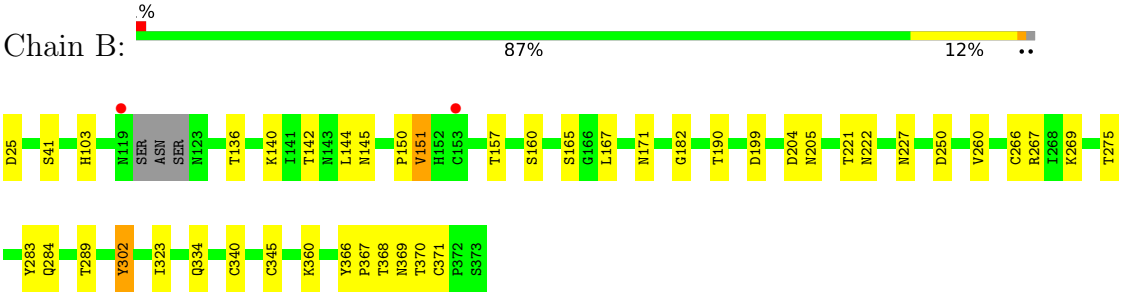






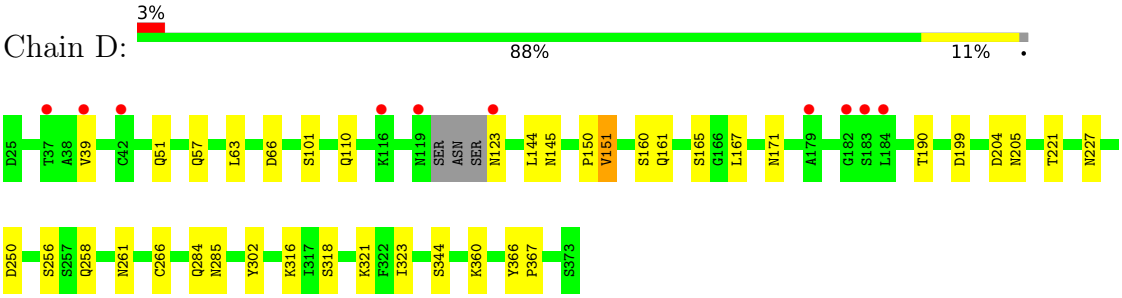
• Molecule 2: Endo-polygalacturonase

Chain B:



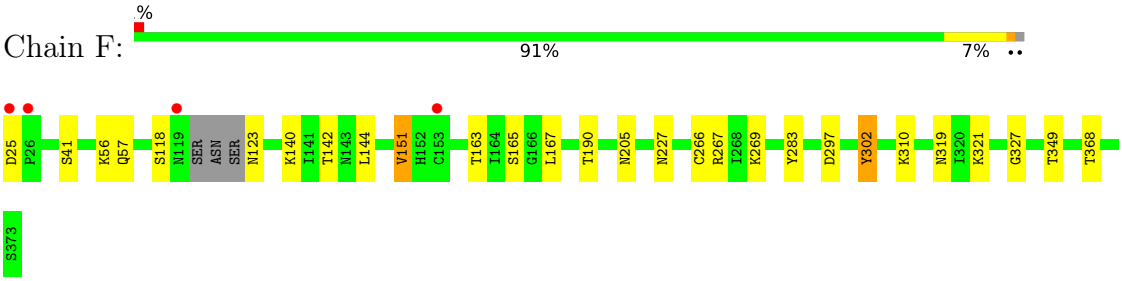
• Molecule 2: Endo-polygalacturonase

Chain D:



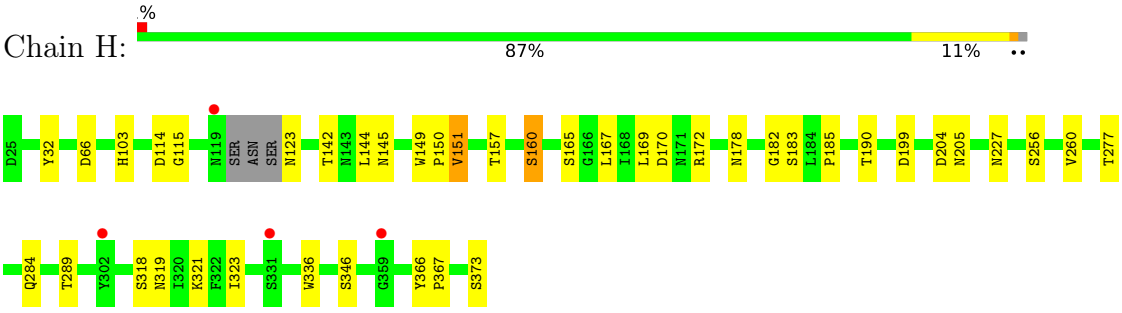
• Molecule 2: Endo-polygalacturonase

Chain F:



• Molecule 2: Endo-polygalacturonase

Chain H:

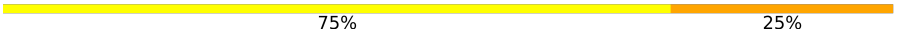


• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

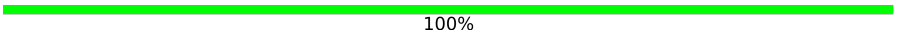
• Molecule 4: alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)][alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:



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

Chain K:

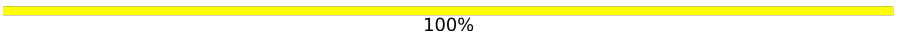


• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:

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

Chain M:



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

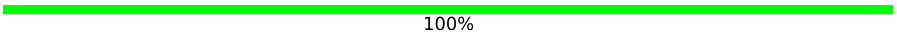
Chain N:

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

Chain O:

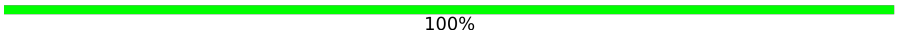
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:



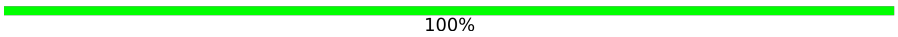
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:



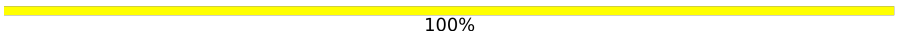
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:



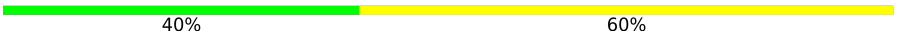
• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:



• Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	68.73Å 105.22Å 113.82Å 63.93° 89.12° 86.27°	Depositor
Resolution (Å)	34.29 – 1.94 34.29 – 1.94	Depositor EDS
% Data completeness (in resolution range)	95.4 (34.29-1.94) 95.4 (34.29-1.94)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.85 (at 1.94Å)	Xtriage
Refinement program	PHENIX v1.20.1-4487	Depositor
R, R_{free}	0.192 , 0.233 0.192 , 0.228	Depositor DCC
R_{free} test set	10099 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	19.2	Xtriage
Anisotropy	0.454	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 50.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,-k+l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	22453	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 50.02 % 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 6.8638e-05. 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: NAG, FUC, BMA, MAN

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	0.60	0/2444	0.71	1/3333 (0.0%)
1	C	0.54	0/2444	0.70	0/3333
1	E	0.55	0/2444	0.73	2/3333 (0.1%)
1	G	0.58	0/2444	0.72	1/3333 (0.0%)
2	B	0.56	0/2562	0.67	0/3487
2	D	0.55	0/2562	0.68	0/3487
2	F	0.51	0/2562	0.65	0/3487
2	H	0.48	0/2562	0.65	0/3487
All	All	0.55	0/20024	0.69	4/27280 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	303	CYS	CA-CB-SG	5.58	124.04	114.00
1	E	183	ARG	CG-CD-NE	-5.47	100.32	111.80
1	G	16	LYS	CG-CD-CE	-5.45	95.54	111.90
1	A	211	GLY	N-CA-C	5.27	126.27	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2392	0	2412	22	0
1	C	2392	0	2412	17	0
1	E	2392	0	2410	37	0
1	G	2392	0	2412	38	0
2	B	2520	0	2400	30	0
2	D	2520	0	2398	28	0
2	F	2520	0	2398	19	0
2	H	2520	0	2398	33	0
3	I	39	0	34	0	0
4	J	48	0	43	1	0
5	K	28	0	25	0	0
5	L	28	0	25	2	0
5	M	28	0	25	0	0
5	N	28	0	25	0	0
5	O	28	0	25	0	0
5	P	28	0	25	0	0
5	S	28	0	25	0	0
5	T	28	0	25	0	0
6	Q	38	0	34	1	0
7	R	61	0	52	0	0
8	A	298	0	0	9	0
8	B	338	0	0	8	0
8	C	298	0	0	10	2
8	D	278	0	0	10	1
8	E	305	0	0	19	1
8	F	321	0	0	6	0
8	G	285	0	0	20	1
8	H	272	0	0	12	1
All	All	22453	0	19603	221	3

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 6.

All (221) 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:E:31:THR:HG23	1:E:38:TRP:HE1	1.06	1.18
1:A:281:CYS:SG	8:A:666:HOH:O	2.14	1.04
1:E:36:ARG:NH1	8:E:401:HOH:O	1.93	1.02
2:B:371:CYS:SG	8:B:568:HOH:O	2.20	0.98
1:G:61:ASN:O	8:G:401:HOH:O	1.84	0.95
2:B:369:ASN:HB3	8:B:677:HOH:O	1.68	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:255:ARG:NH2	8:G:403:HOH:O	2.05	0.89
2:D:66:ASP:OD1	8:D:401:HOH:O	1.92	0.87
1:G:146:SER:OG	8:G:402:HOH:O	1.91	0.87
1:E:31:THR:HG23	1:E:38:TRP:NE1	1.88	0.87
1:E:202:VAL:HA	8:E:407:HOH:O	1.73	0.87
2:B:368:THR:HG23	2:B:370:THR:H	1.40	0.86
2:D:285:ASN:OD1	8:D:402:HOH:O	1.92	0.86
1:E:101:THR:HB	8:E:591:HOH:O	1.79	0.83
1:A:119:ASP:OD1	8:A:401:HOH:O	1.97	0.81
1:A:64:LYS:NZ	8:A:403:HOH:O	2.15	0.80
2:B:199:ASP:OD1	8:B:401:HOH:O	2.00	0.79
2:H:157:THR:OG1	8:H:401:HOH:O	1.97	0.78
1:E:6:GLN:NE2	8:E:406:HOH:O	2.18	0.77
1:A:99:LYS:NZ	8:A:402:HOH:O	2.03	0.76
1:G:99:LYS:NZ	8:G:407:HOH:O	2.20	0.75
2:B:25:ASP:N	8:B:406:HOH:O	2.21	0.74
2:H:32:TYR:HB3	8:H:584:HOH:O	1.88	0.73
1:C:266:GLN:OE1	8:C:402:HOH:O	2.06	0.72
1:G:101:THR:HB	8:G:466:HOH:O	1.89	0.72
1:E:37:THR:HG22	8:E:493:HOH:O	1.89	0.71
2:F:118:SER:HB3	2:F:151:VAL:HG11	1.73	0.71
1:E:268:LYS:NZ	8:E:408:HOH:O	2.22	0.71
1:G:189:LYS:HD3	1:G:210:GLU:HG3	1.73	0.71
1:G:42:LEU:HB2	1:G:54:ASN:HB3	1.71	0.70
1:E:31:THR:CG2	1:E:38:TRP:HE1	1.96	0.70
1:G:112:ASN:OD1	8:G:404:HOH:O	2.09	0.70
1:E:236:ASP:OD2	8:E:402:HOH:O	2.07	0.70
2:H:321:LYS:NZ	8:H:406:HOH:O	2.24	0.70
2:H:183:SER:O	8:H:402:HOH:O	2.10	0.69
1:E:119:ASP:OD1	8:E:403:HOH:O	2.09	0.69
2:H:182:GLY:O	8:H:403:HOH:O	2.11	0.69
1:G:31:THR:HG23	1:G:38:TRP:HE1	1.58	0.68
2:H:260:VAL:HG12	2:H:289:THR:HB	1.76	0.68
2:B:182:GLY:O	8:B:403:HOH:O	2.11	0.68
1:G:35:ASN:ND2	8:G:411:HOH:O	2.26	0.67
2:D:161:GLN:NE2	8:D:408:HOH:O	2.27	0.66
1:G:219:SER:OG	8:G:405:HOH:O	2.13	0.66
2:B:157:THR:OG1	8:B:402:HOH:O	2.01	0.66
1:A:1:GLU:N	8:A:406:HOH:O	2.28	0.66
1:C:191:PRO:HG3	8:C:403:HOH:O	1.95	0.64
1:G:6:GLN:NE2	8:G:410:HOH:O	2.25	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:145:ASN:ND2	8:D:409:HOH:O	2.30	0.64
2:B:144:LEU:H	2:B:167:LEU:HD22	1.63	0.64
2:B:41:SER:HB3	2:D:360:LYS:HG3	1.79	0.63
2:H:178:ASN:O	8:H:403:HOH:O	2.16	0.63
1:A:281:CYS:HB2	1:A:303:CYS:SG	2.39	0.62
2:B:221:THR:HG22	2:B:250:ASP:HB3	1.81	0.62
2:B:269:LYS:HE3	2:B:302:TYR:CE1	2.35	0.61
1:G:281:CYS:HB2	1:G:303:CYS:SG	2.39	0.61
2:B:140:LYS:NZ	8:B:404:HOH:O	2.17	0.61
1:G:189:LYS:HE2	1:G:211:GLY:HA3	1.83	0.60
1:C:222:ASN:ND2	8:C:401:HOH:O	1.99	0.60
1:E:37:THR:CG2	8:E:493:HOH:O	2.47	0.59
2:B:103:HIS:CE1	2:B:145:ASN:H	2.21	0.59
1:G:255:ARG:CZ	8:G:403:HOH:O	2.46	0.59
2:F:144:LEU:H	2:F:167:LEU:HD22	1.66	0.59
1:E:125:LYS:NZ	8:E:411:HOH:O	2.33	0.58
2:H:103:HIS:CE1	2:H:145:ASN:H	2.21	0.58
2:H:336:TRP:CD1	2:H:373:SER:HB3	2.38	0.58
2:F:57:GLN:NE2	8:F:401:HOH:O	2.22	0.58
2:H:114:ASP:OD2	2:H:123:ASN:HB2	2.03	0.57
1:C:41:VAL:O	1:C:42:LEU:HD23	2.05	0.56
1:E:281:CYS:SG	1:E:282:GLY:N	2.78	0.56
1:G:21:PRO:HB2	1:G:23:THR:HG22	1.87	0.56
1:E:28:LEU:HB2	1:E:31:THR:HG22	1.87	0.56
2:D:221:THR:HG22	2:D:250:ASP:HB3	1.88	0.56
1:A:146:SER:HA	1:A:172:PHE:CE1	2.40	0.55
2:H:172:ARG:NH2	8:H:407:HOH:O	2.28	0.55
1:E:123:GLN:NE2	8:E:405:HOH:O	2.17	0.55
1:A:230:LYS:NZ	1:A:252:ARG:HH12	2.04	0.55
1:A:238:GLY:HA3	8:A:410:HOH:O	2.07	0.55
1:G:255:ARG:NE	8:G:403:HOH:O	2.40	0.55
1:G:255:ARG:HD3	8:G:595:HOH:O	2.07	0.54
1:G:167:ASP:OD2	8:G:406:HOH:O	2.18	0.54
1:G:1:GLU:N	8:G:415:HOH:O	2.39	0.54
1:E:41:VAL:O	1:E:42:LEU:HD22	2.08	0.54
1:C:56:ASP:OD2	8:C:404:HOH:O	2.19	0.53
2:D:261:ASN:OD1	8:D:403:HOH:O	2.19	0.53
1:A:255:ARG:NH2	8:A:414:HOH:O	2.41	0.53
2:F:151:VAL:O	2:F:190:THR:HA	2.08	0.53
2:H:151:VAL:O	2:H:190:THR:HA	2.09	0.53
2:D:144:LEU:H	2:D:167:LEU:HD22	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:269:LYS:HE3	2:F:302:TYR:CZ	2.45	0.52
2:H:149:TRP:CH2	2:H:169:LEU:HB3	2.46	0.51
1:E:173:SER:HB2	8:E:660:HOH:O	2.09	0.51
2:D:266:CYS:HA	8:D:465:HOH:O	2.10	0.51
2:D:316:LYS:HZ2	2:D:318:SER:HB3	1.75	0.51
1:E:36:ARG:NH2	8:E:412:HOH:O	2.33	0.50
2:F:321:LYS:NZ	8:F:403:HOH:O	2.31	0.50
1:E:179:MET:O	8:E:407:HOH:O	2.19	0.50
1:G:8:LYS:HE2	8:G:624:HOH:O	2.11	0.50
2:D:151:VAL:O	2:D:190:THR:HA	2.11	0.50
1:C:165:ILE:O	8:C:403:HOH:O	2.18	0.50
2:D:321:LYS:HG3	8:D:425:HOH:O	2.10	0.50
2:H:160:SER:HA	2:H:199:ASP:O	2.11	0.49
2:B:222:ASN:ND2	8:B:401:HOH:O	2.36	0.49
2:H:123:ASN:ND2	8:H:417:HOH:O	2.44	0.49
2:H:123:ASN:N	8:H:417:HOH:O	2.44	0.49
1:E:239:LYS:HD3	8:E:402:HOH:O	2.12	0.49
1:A:41:VAL:O	1:A:42:LEU:HD12	2.12	0.49
1:A:21:PRO:HB2	1:A:23:THR:HG22	1.94	0.49
2:B:269:LYS:HE3	2:B:302:TYR:CZ	2.48	0.49
1:A:167:ASP:OD2	8:A:404:HOH:O	2.20	0.49
2:D:316:LYS:HD2	2:D:344:SER:O	2.11	0.48
2:D:366:TYR:CG	2:D:367:PRO:HA	2.48	0.48
1:E:252:ARG:HG2	1:E:253:ASN:OD1	2.14	0.48
8:C:697:HOH:O	5:L:2:NAG:C3	2.62	0.48
1:G:42:LEU:HD11	2:H:319:ASN:HB2	1.95	0.48
1:G:23:THR:HG21	1:G:60:LEU:HA	1.96	0.48
2:B:165:SER:HA	2:B:204:ASP:O	2.14	0.48
2:B:267:ARG:HD2	2:B:269:LYS:HD2	1.95	0.48
2:H:66:ASP:OD2	8:H:404:HOH:O	2.19	0.48
2:H:336:TRP:NE1	2:H:373:SER:HB3	2.29	0.47
1:C:5:PRO:O	1:C:9:GLN:HG3	2.14	0.47
1:G:36:ARG:N	8:G:423:HOH:O	2.48	0.47
2:D:57:GLN:N	8:D:414:HOH:O	2.42	0.47
1:G:125:LYS:HE2	8:G:485:HOH:O	2.13	0.47
2:F:123:ASN:N	8:F:418:HOH:O	2.46	0.47
2:H:172:ARG:NE	8:H:407:HOH:O	2.46	0.47
1:E:239:LYS:HD2	1:E:239:LYS:N	2.28	0.47
2:H:170:ASP:OD2	2:H:172:ARG:NH2	2.48	0.47
2:F:321:LYS:HG2	2:F:349:THR:HB	1.94	0.47
1:A:23:THR:HG21	1:A:60:LEU:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:225:LYS:NZ	1:C:247:ASN:OD1	2.38	0.47
1:E:36:ARG:NH1	8:E:412:HOH:O	2.37	0.47
1:G:62:LEU:HA	8:G:401:HOH:O	2.15	0.47
2:B:340:CYS:SG	2:B:345:CYS:SG	3.05	0.47
1:G:28:LEU:HB2	1:G:31:THR:HG22	1.97	0.47
2:B:266:CYS:HB3	2:B:283:TYR:CE2	2.50	0.47
2:B:151:VAL:O	2:B:190:THR:HA	2.15	0.47
1:A:41:VAL:C	1:A:42:LEU:HD12	2.36	0.46
1:E:202:VAL:HG23	8:E:407:HOH:O	2.16	0.46
1:C:185:ARG:NH1	8:C:412:HOH:O	2.36	0.46
1:E:42:LEU:HD13	1:E:42:LEU:HA	1.82	0.46
1:A:152:VAL:HA	1:A:176:PHE:HA	1.97	0.46
1:C:84:GLY:HA2	1:C:109:THR:O	2.16	0.46
2:D:39:VAL:HG13	2:D:63:LEU:HD23	1.98	0.45
1:C:29:PRO:HB3	8:C:671:HOH:O	2.15	0.45
1:C:80:PHE:CD2	2:D:316:LYS:HG2	2.52	0.45
2:H:144:LEU:HB2	2:H:167:LEU:HG	1.99	0.45
1:E:268:LYS:N	1:E:268:LYS:HD3	2.31	0.45
2:F:205:ASN:HA	2:F:227:ASN:O	2.16	0.45
2:D:366:TYR:CD1	2:D:367:PRO:HA	2.52	0.45
2:B:142:THR:HA	2:B:165:SER:O	2.17	0.44
2:D:199:ASP:HA	2:D:221:THR:O	2.16	0.44
4:J:3:NAG:H5	4:J:4:FUC:H61	1.99	0.44
1:A:84:GLY:HA2	1:A:109:THR:O	2.17	0.44
2:D:123:ASN:HD22	2:D:123:ASN:N	2.15	0.44
1:C:185:ARG:HA	1:C:208:MET:HE3	2.00	0.44
1:E:28:LEU:O	1:E:31:THR:HG22	2.17	0.44
1:E:36:ARG:NE	2:F:319:ASN:HD21	2.16	0.44
2:F:25:ASP:N	8:F:425:HOH:O	2.50	0.44
2:F:310:LYS:HE3	2:F:310:LYS:HB2	1.66	0.44
2:B:366:TYR:CG	2:B:367:PRO:HA	2.53	0.44
2:D:205:ASN:HA	2:D:227:ASN:O	2.18	0.43
2:F:327:GLY:HA2	8:F:667:HOH:O	2.18	0.43
1:A:14:ILE:HG23	1:A:69:PRO:HG2	1.99	0.43
1:E:268:LYS:HD3	1:E:268:LYS:H	1.83	0.43
8:C:697:HOH:O	5:L:2:NAG:O3	2.21	0.43
1:G:84:GLY:HA2	1:G:109:THR:O	2.18	0.43
2:F:142:THR:HA	2:F:165:SER:O	2.19	0.43
2:B:284:GLN:HA	2:B:323:ILE:O	2.18	0.43
2:B:205:ASN:HA	2:B:227:ASN:O	2.19	0.43
2:D:51:GLN:HG3	8:D:532:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:284:GLN:HA	2:H:323:ILE:O	2.18	0.43
1:E:1:GLU:N	8:E:424:HOH:O	2.50	0.43
1:E:84:GLY:HA2	1:E:109:THR:O	2.18	0.43
1:E:179:MET:HB3	8:E:407:HOH:O	2.19	0.43
2:F:269:LYS:HE3	2:F:302:TYR:CE1	2.53	0.43
8:F:719:HOH:O	6:Q:2:NAG:H83	2.16	0.43
2:D:165:SER:HA	2:D:204:ASP:O	2.19	0.43
2:D:160:SER:OG	2:D:161:GLN:NE2	2.51	0.43
2:F:140:LYS:HA	2:F:163:THR:O	2.19	0.43
2:D:284:GLN:HA	2:D:323:ILE:O	2.19	0.42
1:G:239:LYS:HA	1:G:239:LYS:HD3	1.96	0.42
2:B:160:SER:HA	2:B:199:ASP:O	2.19	0.42
1:C:58:SER:HA	1:C:84:GLY:O	2.20	0.42
2:H:318:SER:HA	2:H:346:SER:O	2.19	0.42
1:G:152:VAL:HA	1:G:176:PHE:HA	2.01	0.42
2:H:115:GLY:HA2	2:H:185:PRO:O	2.20	0.42
1:G:146:SER:HA	1:G:172:PHE:CE1	2.55	0.42
2:B:334:GLN:HG3	2:B:360:LYS:HB3	2.01	0.42
2:H:142:THR:HA	2:H:165:SER:O	2.19	0.42
1:A:153:GLY:HA3	2:B:275:THR:HG21	2.02	0.42
1:E:146:SER:HA	1:E:172:PHE:CE1	2.55	0.42
1:G:36:ARG:NH2	2:H:319:ASN:OD1	2.52	0.42
1:G:107:TYR:CZ	2:H:277:THR:OG1	2.73	0.42
2:D:110:GLN:OE1	2:D:110:GLN:N	2.50	0.42
1:A:79:ASN:HB2	8:A:500:HOH:O	2.19	0.42
2:H:227:ASN:HA	2:H:256:SER:O	2.20	0.42
1:G:73:ALA:HB2	1:G:96:ALA:HB1	2.01	0.42
1:A:230:LYS:HZ1	1:A:252:ARG:HH12	1.67	0.41
1:C:42:LEU:HB2	1:C:54:ASN:HB3	2.03	0.41
1:G:13:GLN:HG2	8:G:506:HOH:O	2.19	0.41
1:G:36:ARG:NE	8:G:429:HOH:O	2.53	0.41
2:F:267:ARG:HA	2:F:297:ASP:O	2.20	0.41
2:B:221:THR:HA	2:B:250:ASP:O	2.20	0.41
2:B:136:THR:HA	2:B:160:SER:O	2.20	0.41
2:D:321:LYS:NZ	8:D:425:HOH:O	2.53	0.41
1:E:268:LYS:H	1:E:268:LYS:CD	2.34	0.41
2:D:227:ASN:HA	2:D:256:SER:O	2.21	0.41
2:H:205:ASN:HA	2:H:227:ASN:O	2.21	0.41
2:H:366:TYR:CG	2:H:367:PRO:HA	2.56	0.41
2:B:260:VAL:HG12	2:B:289:THR:HB	2.02	0.41
2:H:123:ASN:CG	8:H:417:HOH:O	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:237:LEU:O	1:G:240:VAL:HG22	2.21	0.41
2:F:56:LYS:HD3	2:F:56:LYS:HA	1.87	0.41
2:F:266:CYS:HB3	2:F:283:TYR:CE2	2.56	0.41
1:A:58:SER:HA	1:A:84:GLY:O	2.21	0.40
1:C:208:MET:CE	8:C:562:HOH:O	2.69	0.40
1:E:152:VAL:HA	1:E:176:PHE:HA	2.02	0.40
1:C:185:ARG:HA	1:C:208:MET:CE	2.51	0.40
2:H:165:SER:HA	2:H:204:ASP:O	2.21	0.40
1:E:237:LEU:HD23	1:E:260:LEU:HD23	2.02	0.40
1:G:183:ARG:HH11	1:G:183:ARG:HG2	1.85	0.40

All (3) 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)
8:C:673:HOH:O	8:G:649:HOH:O[1_645]	1.97	0.23
8:D:525:HOH:O	8:H:452:HOH:O[1_655]	2.08	0.12
8:C:656:HOH:O	8:E:693:HOH:O[1_554]	2.15	0.05

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	311/313 (99%)	293 (94%)	18 (6%)	0	100	100
1	C	311/313 (99%)	293 (94%)	18 (6%)	0	100	100
1	E	311/313 (99%)	294 (94%)	17 (6%)	0	100	100
1	G	311/313 (99%)	293 (94%)	18 (6%)	0	100	100
2	B	342/349 (98%)	328 (96%)	12 (4%)	2 (1%)	25	13
2	D	342/349 (98%)	328 (96%)	12 (4%)	2 (1%)	25	13
2	F	342/349 (98%)	329 (96%)	12 (4%)	1 (0%)	41	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	H	342/349 (98%)	329 (96%)	11 (3%)	2 (1%)	25 13
All	All	2612/2648 (99%)	2487 (95%)	118 (4%)	7 (0%)	41 32

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	151	VAL
2	D	151	VAL
2	F	151	VAL
2	H	151	VAL
2	H	150	PRO
2	B	150	PRO
2	D	150	PRO

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	274/274 (100%)	272 (99%)	2 (1%)	84 81
1	C	274/274 (100%)	270 (98%)	4 (2%)	65 56
1	E	274/274 (100%)	272 (99%)	2 (1%)	84 81
1	G	274/274 (100%)	274 (100%)	0	100 100
2	B	289/292 (99%)	287 (99%)	2 (1%)	84 81
2	D	289/292 (99%)	285 (99%)	4 (1%)	67 58
2	F	289/292 (99%)	286 (99%)	3 (1%)	76 71
2	H	289/292 (99%)	288 (100%)	1 (0%)	92 93
All	All	2252/2264 (100%)	2234 (99%)	18 (1%)	81 78

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	ARG

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Mol	Chain	Res	Type
1	A	268	LYS
2	B	171	ASN
2	B	302	TYR
1	C	25	SER
1	C	37	THR
1	C	103	LEU
1	C	303	CYS
1	E	107	TYR
1	E	303	CYS
2	D	101	SER
2	D	171	ASN
2	D	258	GLN
2	D	302	TYR
2	F	41	SER
2	F	302	TYR
2	F	368	THR
2	H	160	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	64	GLN
2	B	103	HIS
1	C	9	GLN
1	C	102	GLN
1	C	150	ASN
1	E	48	GLN
1	E	279	ASN
1	G	150	ASN
2	D	133	GLN
2	D	145	ASN
2	D	161	GLN
2	D	258	GLN
2	F	319	ASN
2	H	103	HIS

5.3.3 RNA

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)

31 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	I	1	1,3	14,14,15	0.64	0	17,19,21	0.79	0
3	NAG	I	2	3	14,14,15	0.40	0	17,19,21	0.74	0
3	BMA	I	3	3	11,11,12	0.87	0	15,15,17	1.12	1 (6%)
4	NAG	J	1	2,4	14,14,15	1.86	1 (7%)	17,19,21	1.59	4 (23%)
4	FUC	J	2	4	10,10,11	1.12	1 (10%)	14,14,16	1.10	1 (7%)
4	NAG	J	3	4	14,14,15	0.41	0	17,19,21	0.40	0
4	FUC	J	4	4	10,10,11	1.70	1 (10%)	14,14,16	1.26	2 (14%)
5	NAG	K	1	5,2	14,14,15	0.55	0	17,19,21	0.71	0
5	NAG	K	2	5	14,14,15	0.40	0	17,19,21	0.50	0
5	NAG	L	1	1,5	14,14,15	0.38	0	17,19,21	0.70	0
5	NAG	L	2	5	14,14,15	0.60	0	17,19,21	0.60	0
5	NAG	M	1	1,5	14,14,15	0.47	0	17,19,21	0.87	2 (11%)
5	NAG	M	2	5	14,14,15	0.29	0	17,19,21	0.76	1 (5%)
5	NAG	N	1	1,5	14,14,15	0.53	0	17,19,21	0.88	2 (11%)
5	NAG	N	2	5	14,14,15	0.29	0	17,19,21	0.68	0
5	NAG	O	1	5,2	14,14,15	0.53	0	17,19,21	0.78	0
5	NAG	O	2	5	14,14,15	0.40	0	17,19,21	0.70	1 (5%)
5	NAG	P	1	5,2	14,14,15	0.59	0	17,19,21	0.77	0
5	NAG	P	2	5	14,14,15	0.39	0	17,19,21	0.57	0
6	NAG	Q	1	6,2	14,14,15	0.66	1 (7%)	17,19,21	1.17	2 (11%)
6	NAG	Q	2	6	14,14,15	0.51	0	17,19,21	0.55	0
6	FUC	Q	3	6	10,10,11	1.00	1 (10%)	14,14,16	0.73	0
7	NAG	R	1	7,2	14,14,15	0.46	0	17,19,21	0.60	0
7	NAG	R	2	7	14,14,15	0.32	0	17,19,21	0.59	0
7	BMA	R	3	7	11,11,12	0.88	0	15,15,17	1.14	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	MAN	R	4	7	11,11,12	1.04	1 (9%)	15,15,17	1.08	1 (6%)
7	MAN	R	5	7	11,11,12	1.19	1 (9%)	15,15,17	1.40	2 (13%)
5	NAG	S	1	5,2	14,14,15	0.46	0	17,19,21	0.58	0
5	NAG	S	2	5	14,14,15	0.38	0	17,19,21	0.47	0
5	NAG	T	1	5,2	14,14,15	0.27	0	17,19,21	0.77	0
5	NAG	T	2	5	14,14,15	0.39	0	17,19,21	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
3	NAG	I	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	I	2	3	-	0/6/23/26	0/1/1/1
3	BMA	I	3	3	-	0/2/19/22	0/1/1/1
4	NAG	J	1	2,4	-	2/6/23/26	0/1/1/1
4	FUC	J	2	4	-	-	0/1/1/1
4	NAG	J	3	4	-	1/6/23/26	0/1/1/1
4	FUC	J	4	4	-	-	0/1/1/1
5	NAG	K	1	5,2	-	2/6/23/26	0/1/1/1
5	NAG	K	2	5	-	0/6/23/26	0/1/1/1
5	NAG	L	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	L	2	5	-	0/6/23/26	0/1/1/1
5	NAG	M	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	M	2	5	-	0/6/23/26	0/1/1/1
5	NAG	N	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	N	2	5	-	0/6/23/26	0/1/1/1
5	NAG	O	1	5,2	-	0/6/23/26	0/1/1/1
5	NAG	O	2	5	-	0/6/23/26	0/1/1/1
5	NAG	P	1	5,2	-	0/6/23/26	0/1/1/1
5	NAG	P	2	5	-	2/6/23/26	0/1/1/1
6	NAG	Q	1	6,2	-	0/6/23/26	0/1/1/1
6	NAG	Q	2	6	-	2/6/23/26	0/1/1/1
6	FUC	Q	3	6	-	-	0/1/1/1
7	NAG	R	1	7,2	-	0/6/23/26	0/1/1/1
7	NAG	R	2	7	-	2/6/23/26	0/1/1/1
7	BMA	R	3	7	-	1/2/19/22	0/1/1/1
7	MAN	R	4	7	-	0/2/19/22	0/1/1/1
7	MAN	R	5	7	-	0/2/19/22	0/1/1/1
5	NAG	S	1	5,2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	S	2	5	-	1/6/23/26	0/1/1/1
5	NAG	T	1	5,2	-	1/6/23/26	0/1/1/1
5	NAG	T	2	5	-	2/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	1	NAG	O5-C1	-6.74	1.32	1.43
4	J	4	FUC	C1-C2	4.09	1.61	1.52
4	J	2	FUC	C2-C3	2.92	1.56	1.52
6	Q	1	NAG	O5-C1	-2.29	1.40	1.43
7	R	5	MAN	C1-C2	2.29	1.57	1.52
6	Q	3	FUC	C2-C3	2.21	1.55	1.52
7	R	4	MAN	C2-C3	2.13	1.55	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	R	5	MAN	C1-O5-C5	4.07	117.71	112.19
4	J	1	NAG	O5-C5-C6	-3.71	101.39	107.20
4	J	1	NAG	C1-O5-C5	3.52	116.96	112.19
7	R	3	BMA	C1-O5-C5	3.25	116.60	112.19
3	I	3	BMA	C1-O5-C5	3.20	116.53	112.19
7	R	4	MAN	C1-O5-C5	2.90	116.12	112.19
4	J	4	FUC	O2-C2-C1	2.74	114.75	109.15
7	R	5	MAN	O2-C2-C3	-2.57	104.98	110.14
4	J	1	NAG	O6-C6-C5	2.54	120.01	111.29
5	M	2	NAG	C1-O5-C5	2.47	115.53	112.19
5	N	1	NAG	O4-C4-C5	-2.29	103.62	109.30
6	Q	1	NAG	C1-O5-C5	2.26	115.26	112.19
5	M	1	NAG	O4-C4-C5	-2.21	103.80	109.30
5	O	2	NAG	O5-C1-C2	-2.19	107.83	111.29
7	R	3	BMA	O2-C2-C3	-2.19	105.76	110.14
4	J	1	NAG	C6-C5-C4	2.16	118.06	113.00
5	N	1	NAG	C2-N2-C7	2.11	125.91	122.90
5	M	1	NAG	C2-N2-C7	2.09	125.87	122.90
4	J	4	FUC	O5-C5-C4	2.08	113.26	109.52
6	Q	1	NAG	C1-C2-N2	-2.07	106.95	110.49
4	J	2	FUC	C1-C2-C3	-2.01	107.20	109.67

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	J	1	NAG	O5-C5-C6-O6
5	P	2	NAG	O5-C5-C6-O6
4	J	1	NAG	C4-C5-C6-O6
4	J	3	NAG	O5-C5-C6-O6
7	R	2	NAG	C4-C5-C6-O6
5	S	2	NAG	O5-C5-C6-O6
5	K	1	NAG	C4-C5-C6-O6
5	P	2	NAG	C4-C5-C6-O6
7	R	2	NAG	O5-C5-C6-O6
3	I	1	NAG	C3-C2-N2-C7
5	L	1	NAG	C3-C2-N2-C7
5	M	1	NAG	C3-C2-N2-C7
5	N	1	NAG	C3-C2-N2-C7
5	T	1	NAG	C3-C2-N2-C7
3	I	1	NAG	C4-C5-C6-O6
6	Q	2	NAG	C4-C5-C6-O6
6	Q	2	NAG	O5-C5-C6-O6
5	K	1	NAG	O5-C5-C6-O6
5	T	2	NAG	C4-C5-C6-O6
5	T	2	NAG	O5-C5-C6-O6
7	R	3	BMA	O5-C5-C6-O6

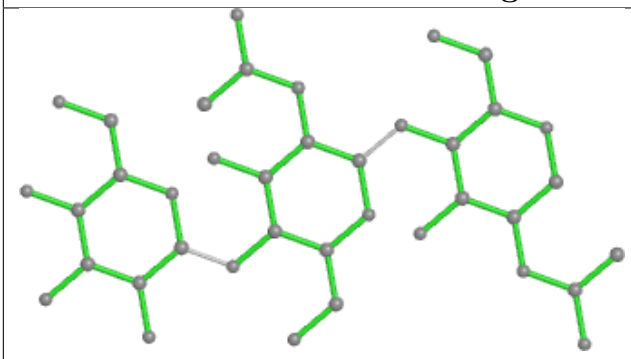
There are no ring outliers.

4 monomers are involved in 4 short contacts:

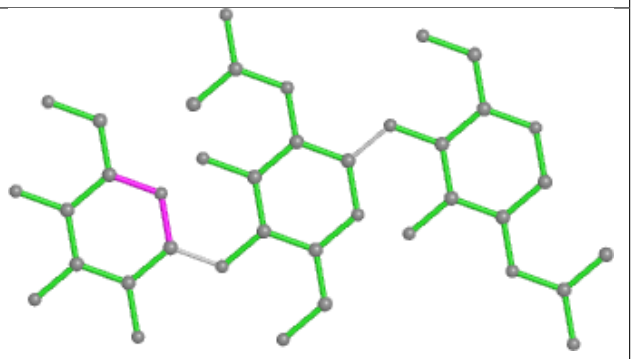
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	2	NAG	2	0
4	J	3	NAG	1	0
6	Q	2	NAG	1	0
4	J	4	FUC	1	0

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

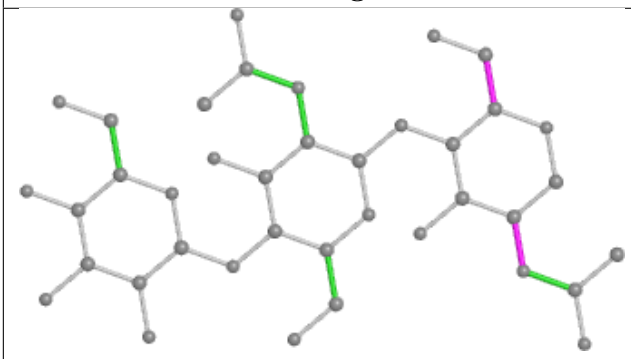
Oligosaccharide Chain I



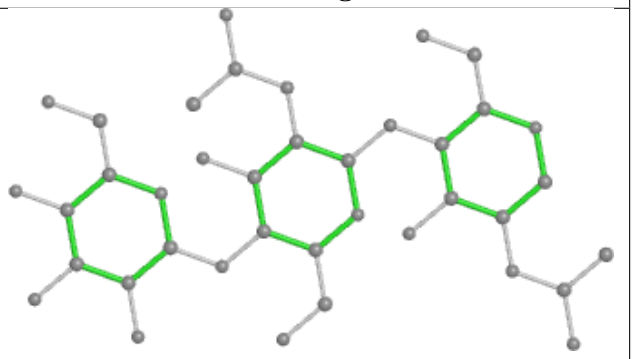
Bond lengths



Bond angles

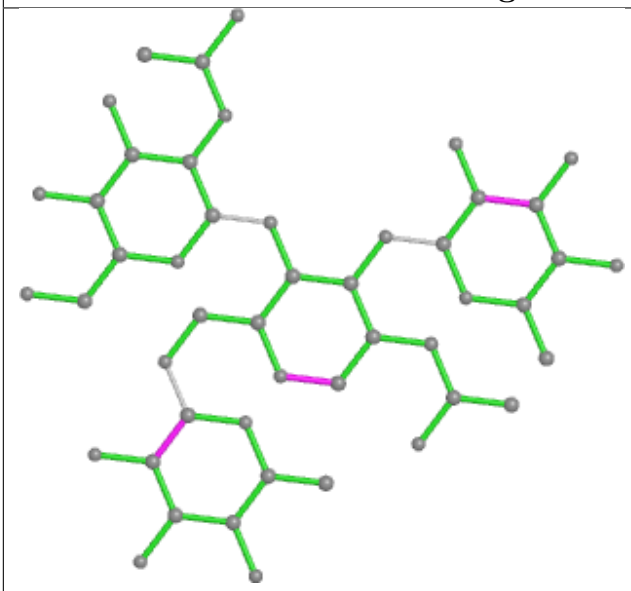


Torsions

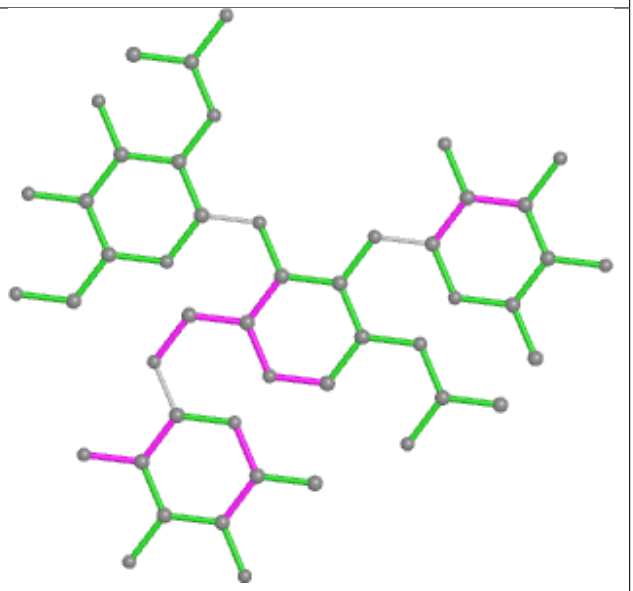


Rings

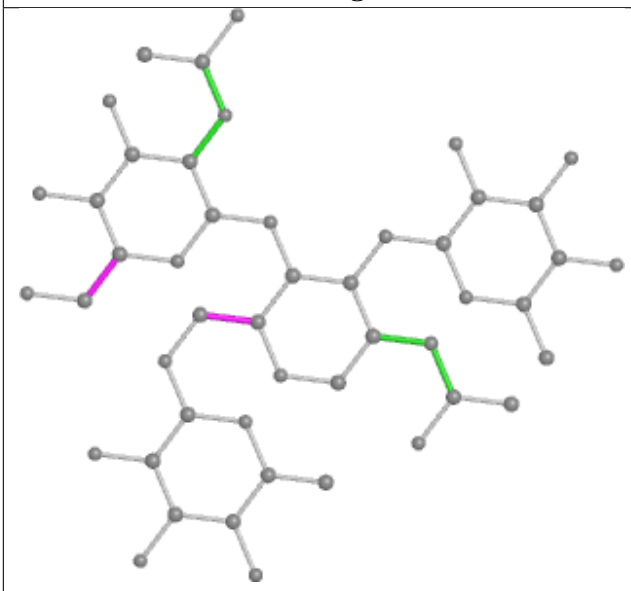
Oligosaccharide Chain J



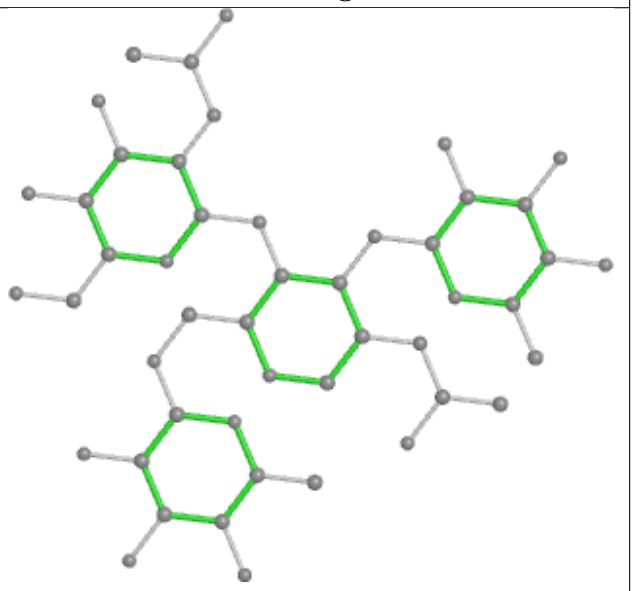
Bond lengths



Bond angles

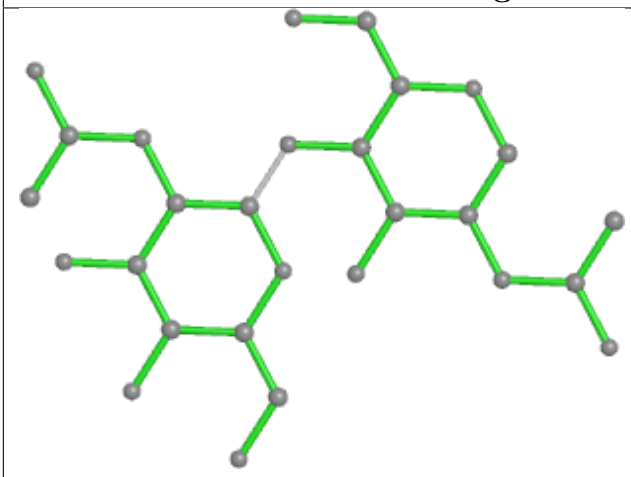


Torsions

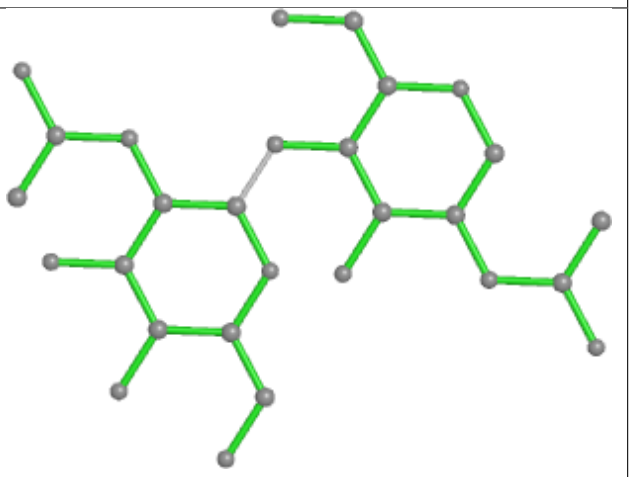


Rings

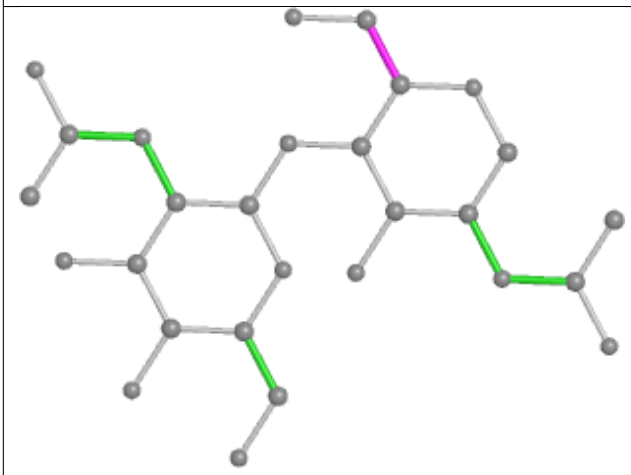
Oligosaccharide Chain K



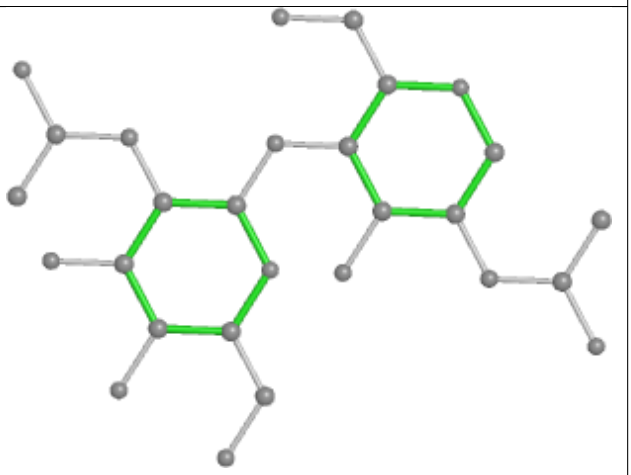
Bond lengths



Bond angles

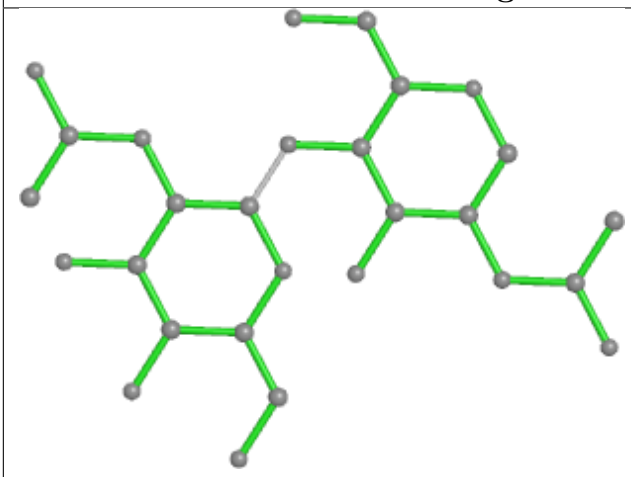


Torsions

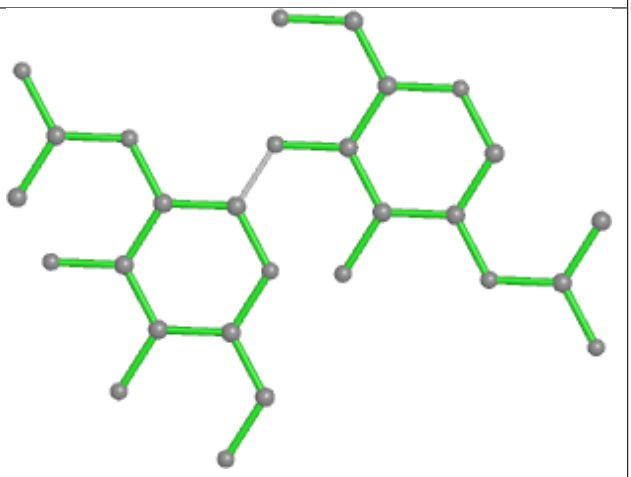


Rings

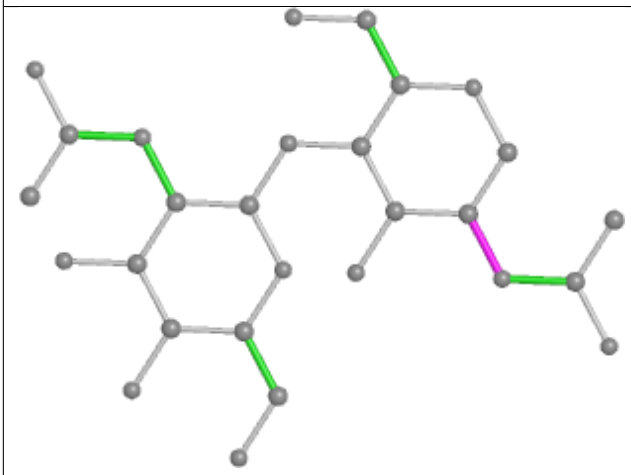
Oligosaccharide Chain L



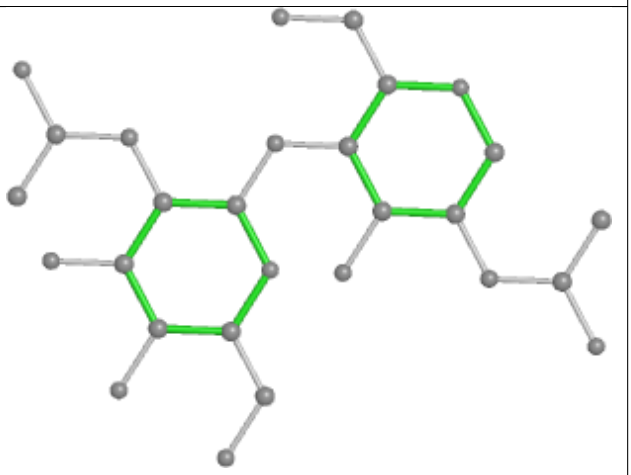
Bond lengths



Bond angles

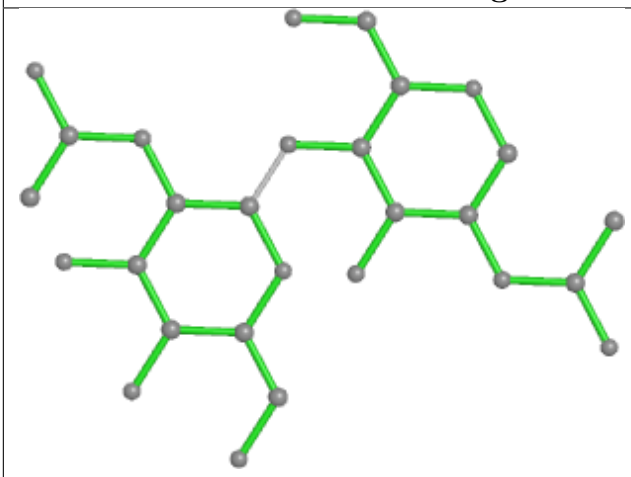


Torsions

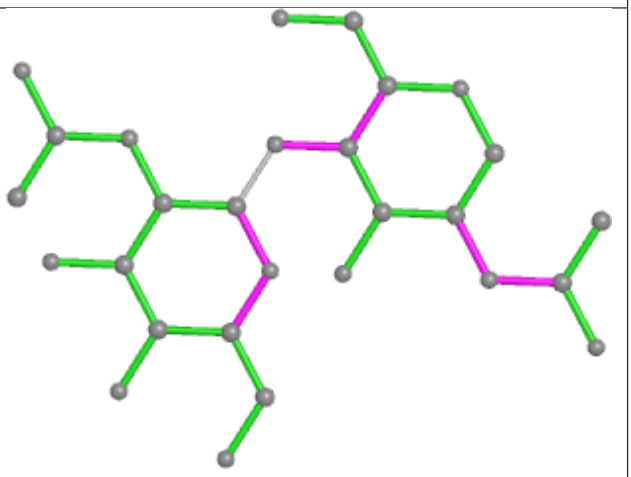


Rings

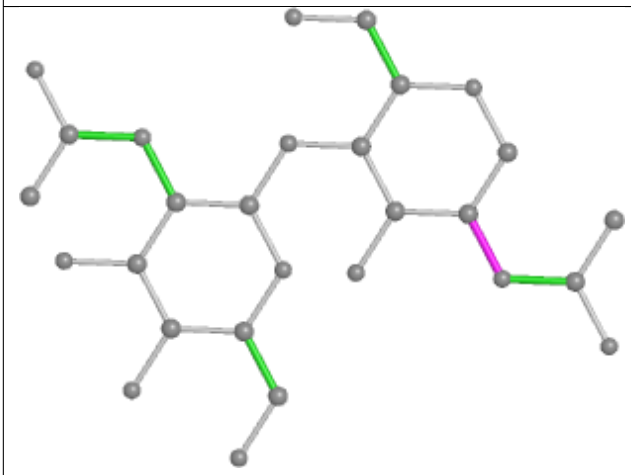
Oligosaccharide Chain M



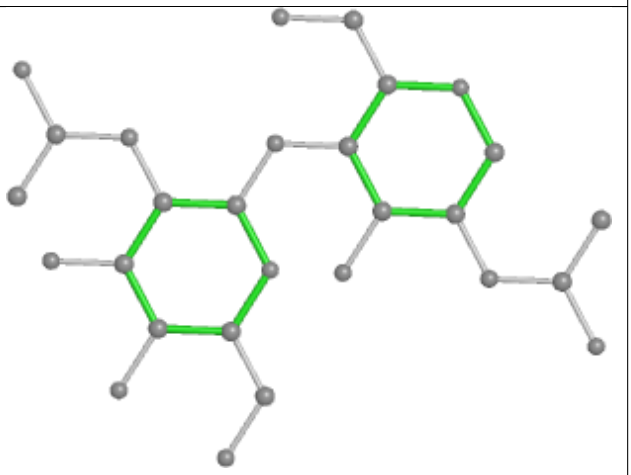
Bond lengths



Bond angles

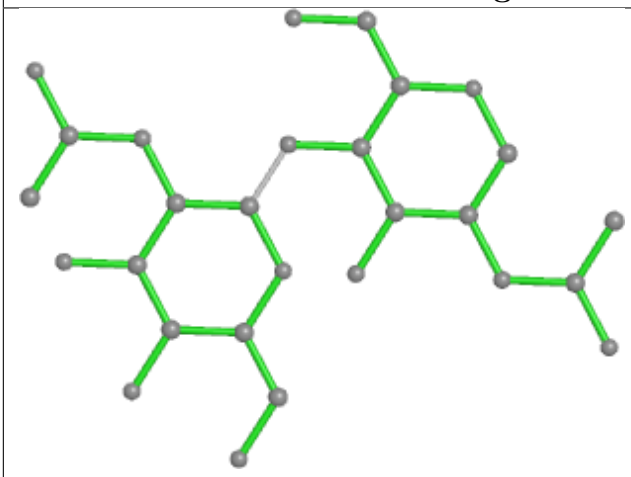


Torsions

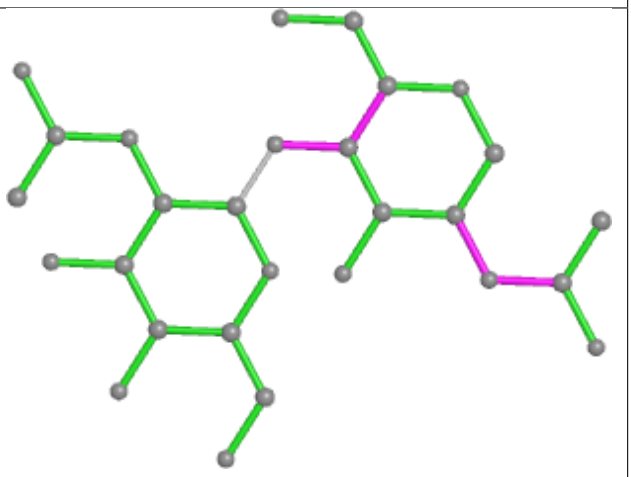


Rings

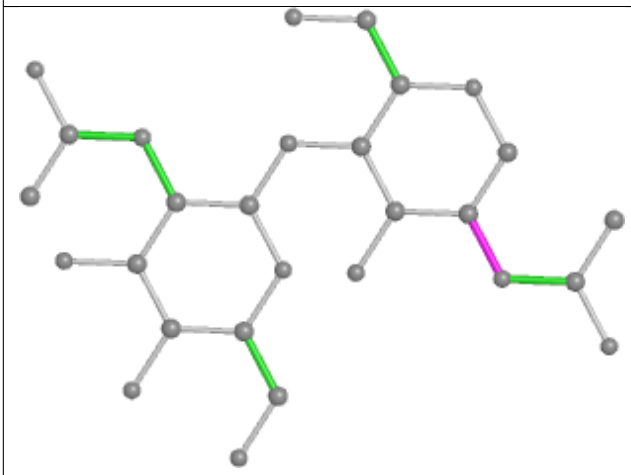
Oligosaccharide Chain N



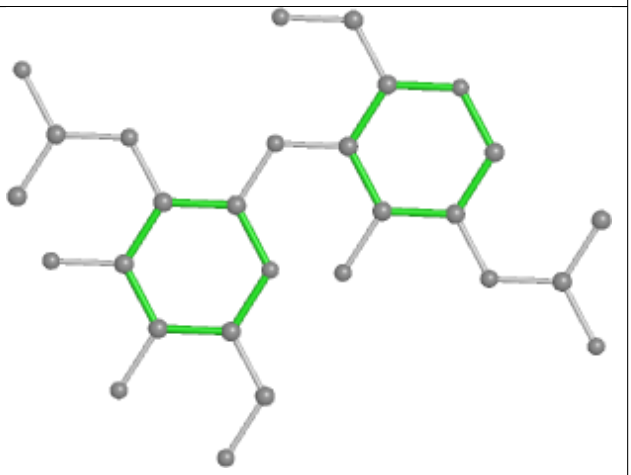
Bond lengths



Bond angles

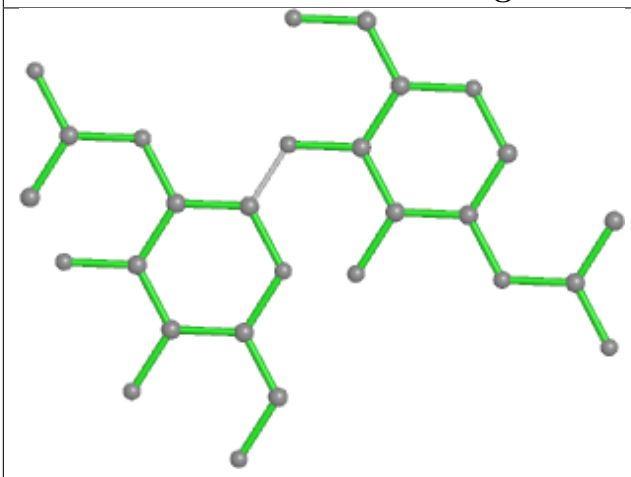


Torsions

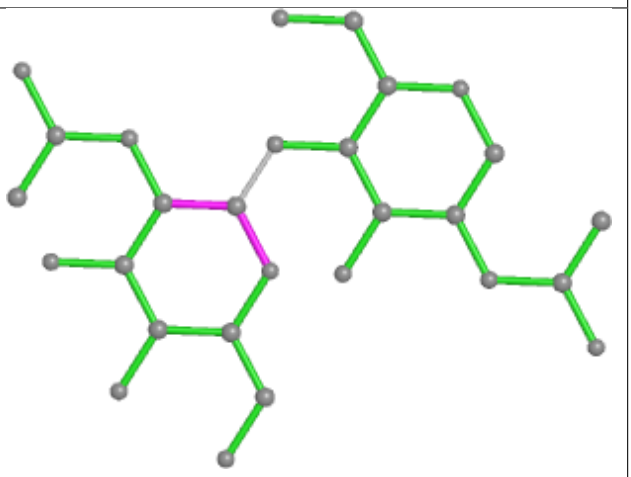


Rings

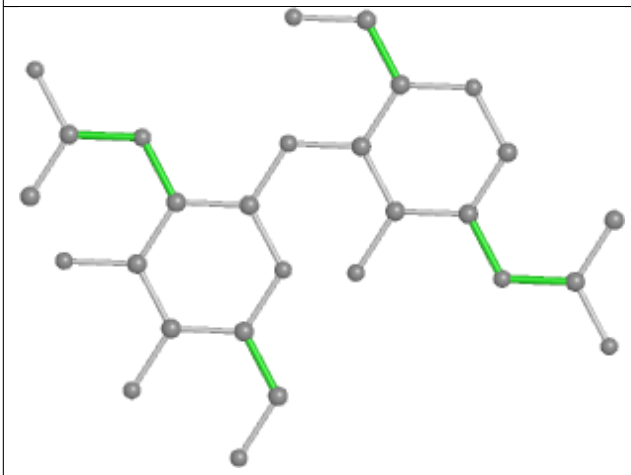
Oligosaccharide Chain O



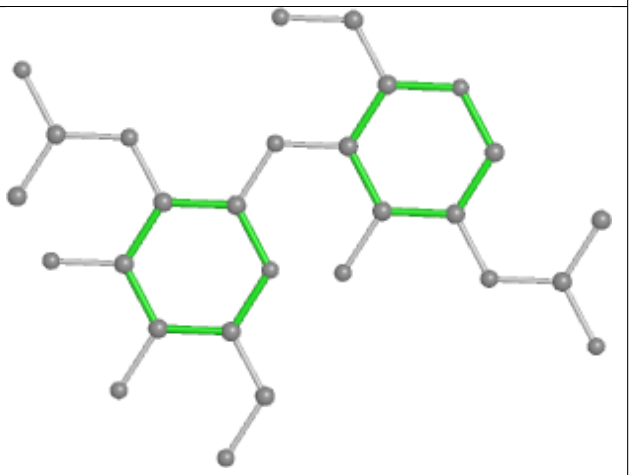
Bond lengths



Bond angles

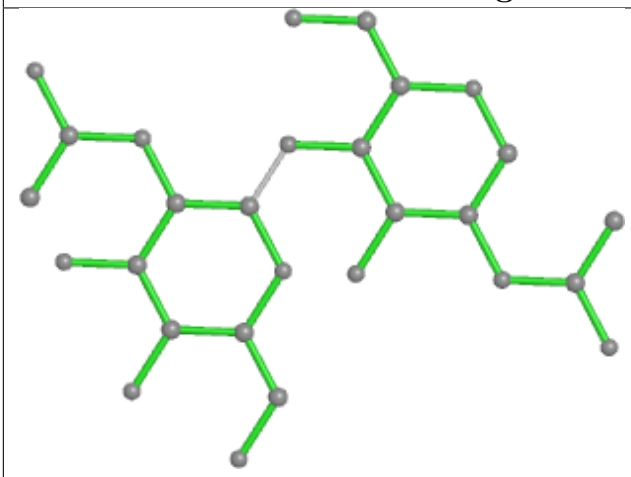


Torsions

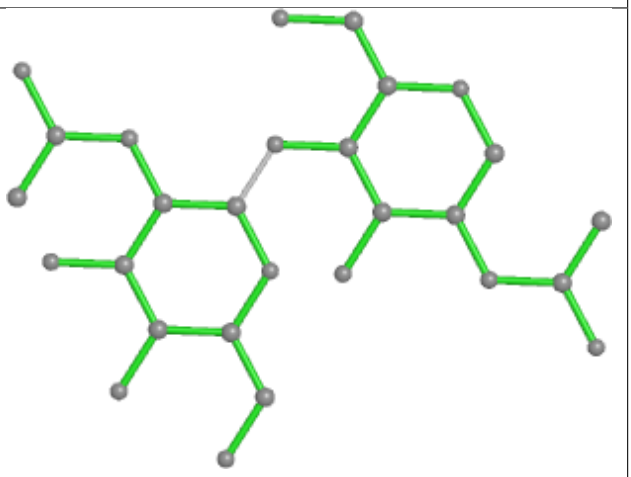


Rings

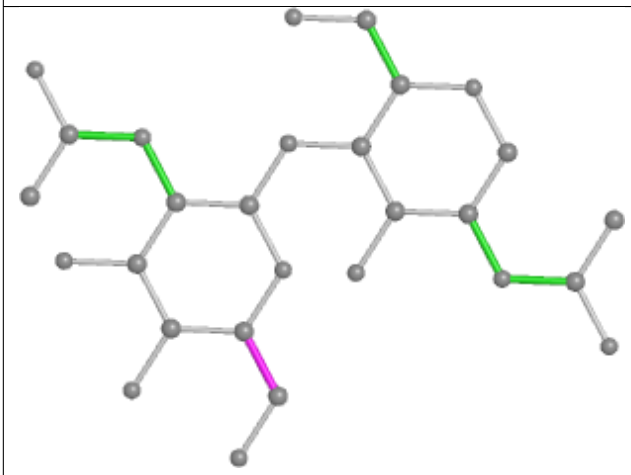
Oligosaccharide Chain P



Bond lengths



Bond angles



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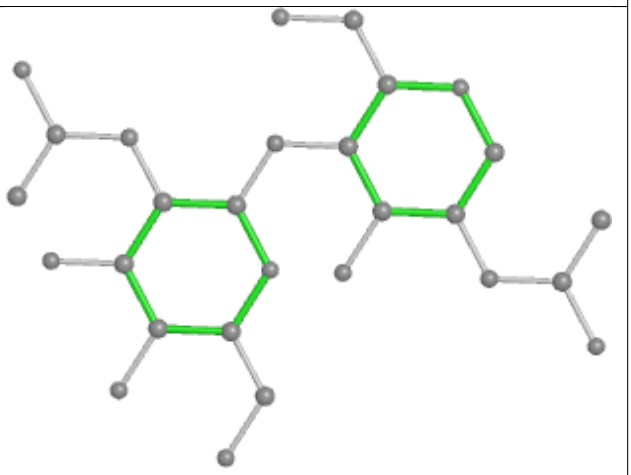
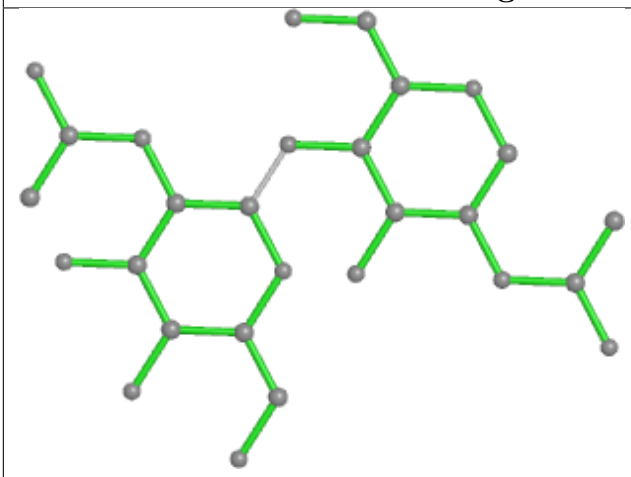
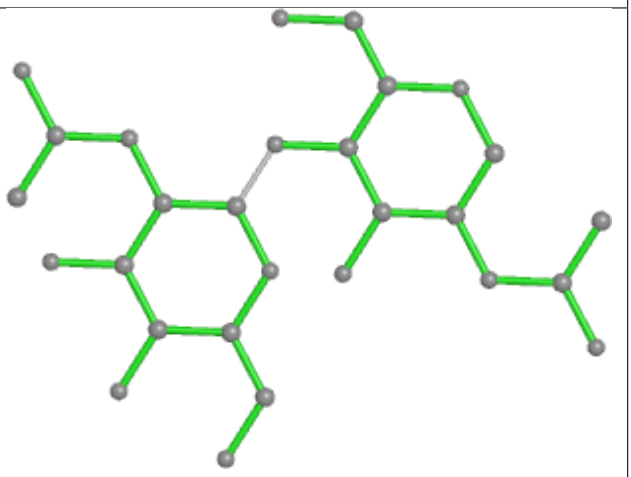


Rings

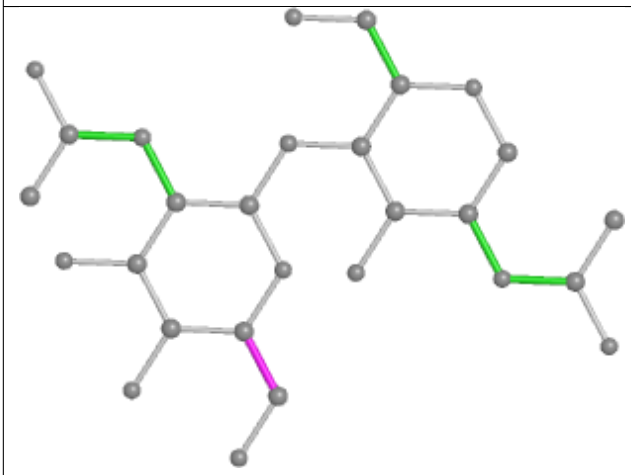
Oligosaccharide Chain S



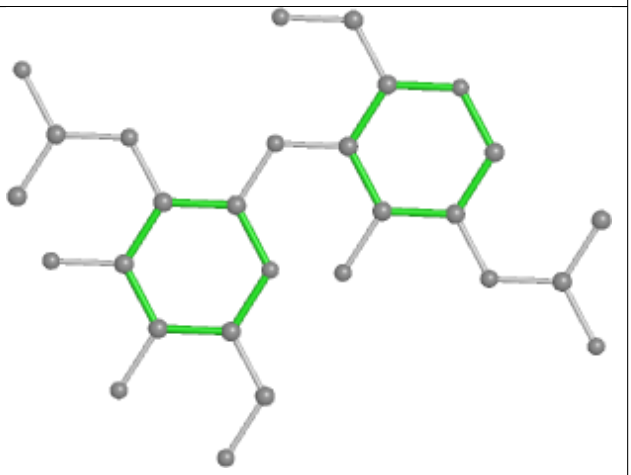
Bond lengths



Bond angles

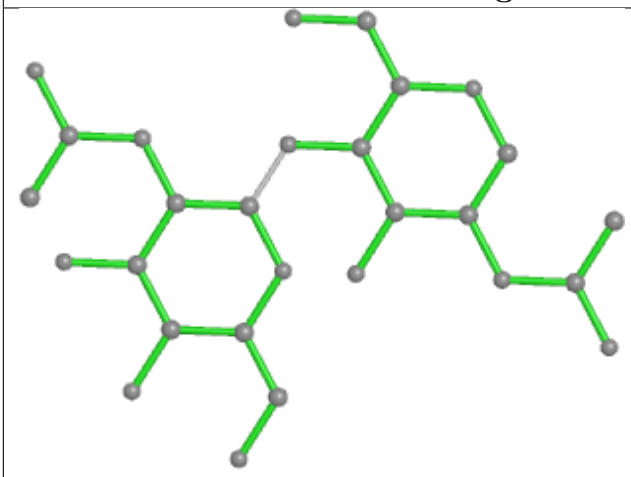


Torsions

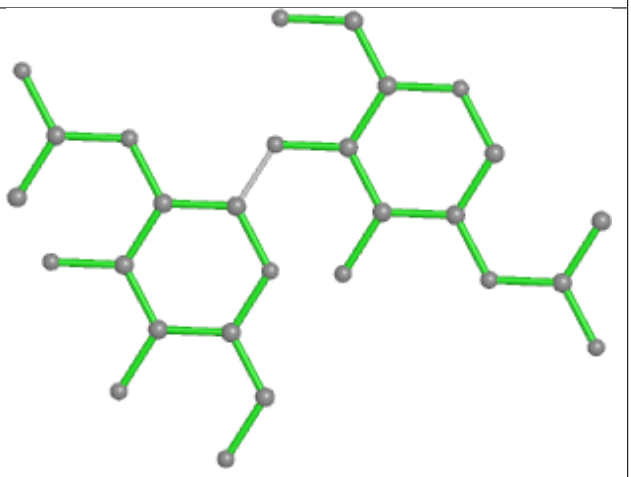


Rings

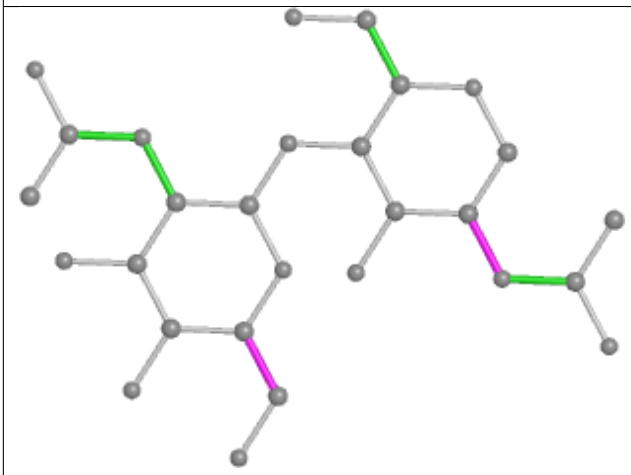
Oligosaccharide Chain T



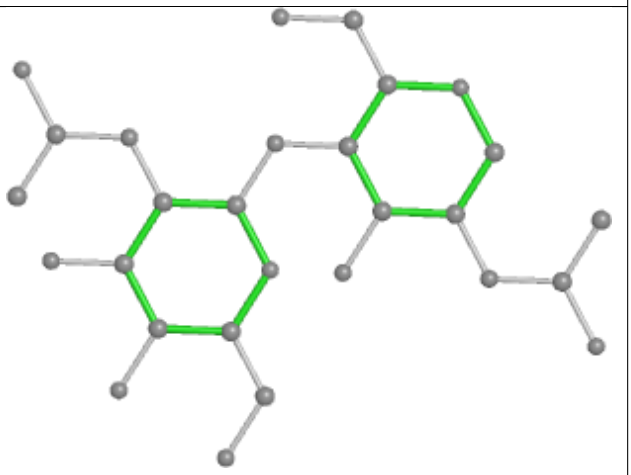
Bond lengths



Bond angles

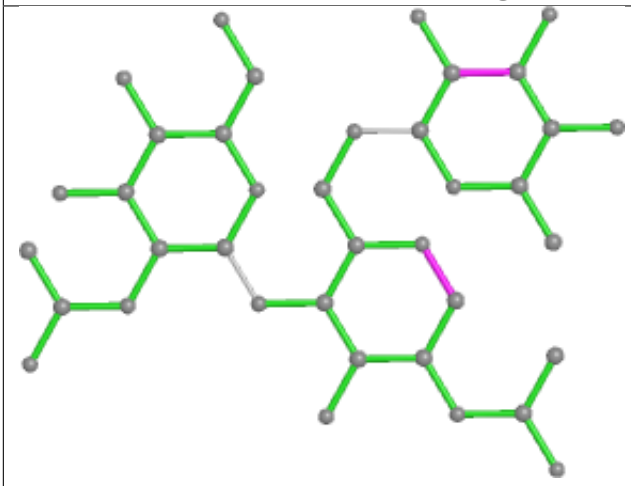


Torsions

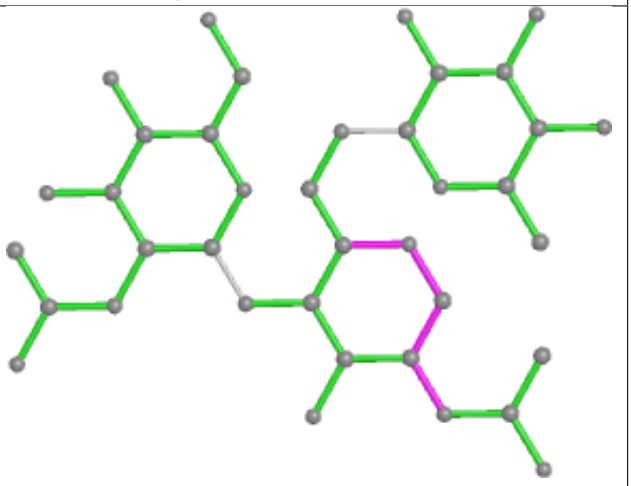


Rings

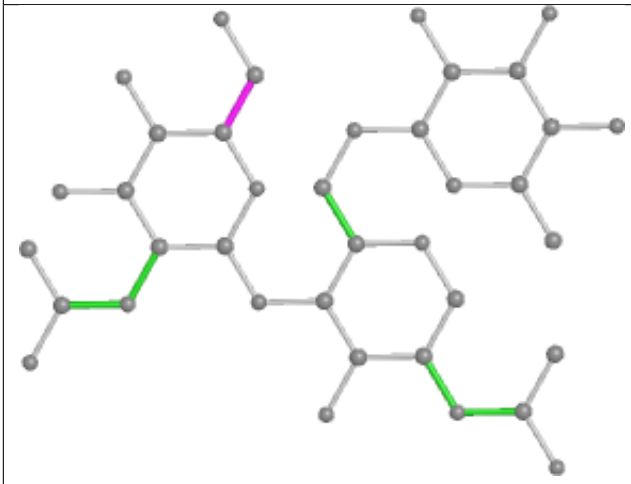
Oligosaccharide Chain Q



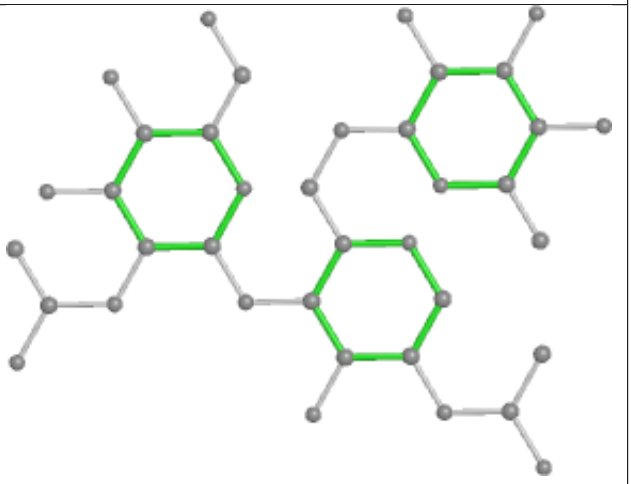
Bond lengths



Bond angles

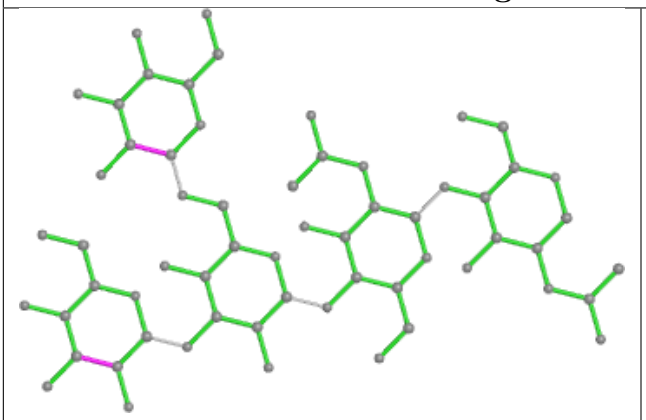


Torsions

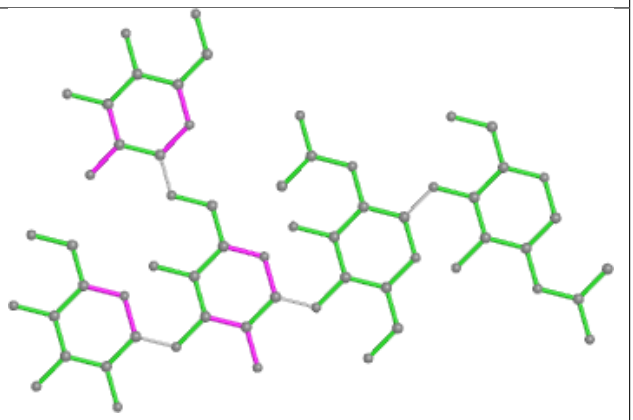


Rings

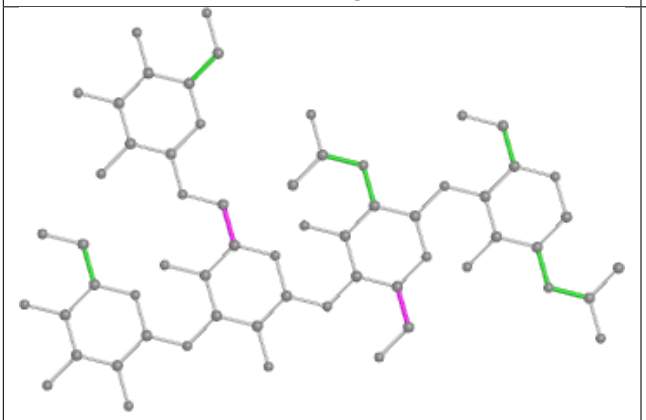
Oligosaccharide Chain R



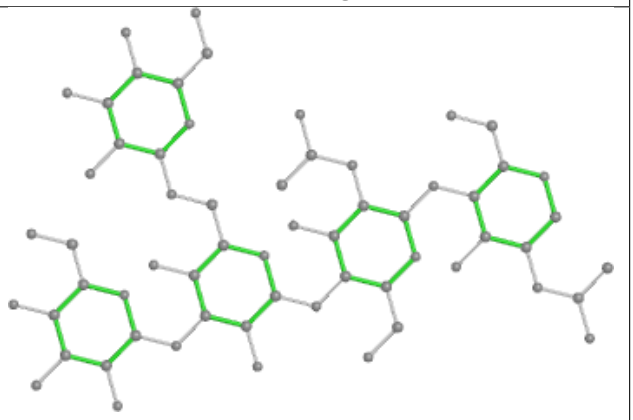
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

There are no ligands in this entry.

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	313/313 (100%)	-0.21	5 (1%)	72 77	9, 20, 35, 50	0
1	C	313/313 (100%)	-0.19	5 (1%)	72 77	11, 21, 35, 53	0
1	E	313/313 (100%)	-0.20	5 (1%)	72 77	11, 20, 35, 56	0
1	G	313/313 (100%)	-0.15	7 (2%)	62 69	10, 21, 36, 54	0
2	B	346/349 (99%)	-0.18	2 (0%)	89 92	12, 22, 33, 51	0
2	D	346/349 (99%)	0.05	10 (2%)	51 59	12, 26, 42, 57	0
2	F	346/349 (99%)	-0.10	4 (1%)	79 83	13, 22, 35, 60	0
2	H	346/349 (99%)	0.05	4 (1%)	79 83	13, 26, 39, 63	0
All	All	2636/2648 (99%)	-0.11	42 (1%)	72 77	9, 22, 37, 63	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	36	ARG	4.4
2	D	184	LEU	4.3
2	H	119	ASN	4.1
1	C	36	ARG	4.0
1	G	292	ARG	3.7
1	E	292	ARG	3.6
2	D	179	ALA	3.4
2	B	119	ASN	3.3
2	H	302	TYR	3.3
2	D	183	SER	3.2
2	D	119	ASN	3.2
1	C	31	THR	3.1
1	E	36	ARG	3.1
1	G	28	LEU	3.0
1	C	30	THR	2.8
1	A	30	THR	2.8

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Mol	Chain	Res	Type	RSRZ
2	F	153	CYS	2.8
1	C	292	ARG	2.8
2	F	119	ASN	2.8
1	E	313	THR	2.7
2	D	123	ASN	2.5
2	D	116	LYS	2.5
2	F	26	PRO	2.5
1	A	31	THR	2.4
1	C	312	CYS	2.4
1	G	30	THR	2.4
1	E	30	THR	2.3
2	D	42	CYS	2.3
1	E	29	PRO	2.3
1	A	313	THR	2.2
2	H	331	SER	2.2
1	G	271	HIS	2.2
2	F	25	ASP	2.2
1	A	35	ASN	2.1
2	D	39	VAL	2.1
2	D	182	GLY	2.1
1	G	37	THR	2.1
1	G	36	ARG	2.1
2	D	37	THR	2.1
2	B	153	CYS	2.1
2	H	359	GLY	2.1
1	G	268	LYS	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
4	FUC	J	2	10/11	0.70	0.26	53,55,58,60	0
3	BMA	I	3	11/12	0.75	0.32	49,57,63,66	0

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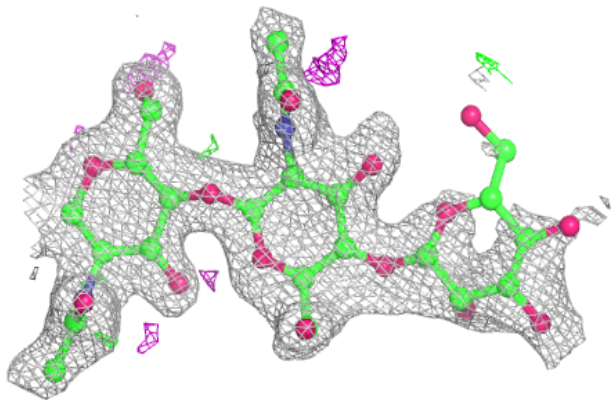
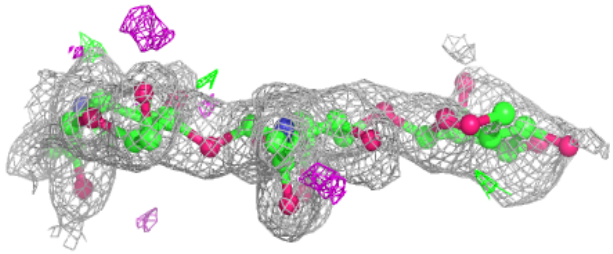
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NAG	O	1	14/15	0.77	0.31	40,47,57,58	0
4	FUC	J	4	10/11	0.79	0.29	48,56,64,65	0
6	NAG	Q	1	14/15	0.79	0.26	47,51,55,58	0
6	FUC	Q	3	10/11	0.79	0.39	48,52,58,60	0
4	NAG	J	1	14/15	0.80	0.15	35,42,51,56	0
6	NAG	Q	2	14/15	0.80	0.32	47,55,61,68	0
5	NAG	T	2	14/15	0.80	0.18	42,48,57,64	0
5	NAG	K	2	14/15	0.81	0.23	43,49,57,66	0
5	NAG	O	2	14/15	0.81	0.30	45,55,61,63	0
5	NAG	M	2	14/15	0.81	0.21	32,46,54,56	0
5	NAG	P	2	14/15	0.83	0.24	46,50,54,55	0
7	MAN	R	5	11/12	0.83	0.20	38,43,50,51	0
5	NAG	T	1	14/15	0.84	0.14	31,38,48,58	0
7	BMA	R	3	11/12	0.84	0.18	38,43,49,50	0
5	NAG	S	1	14/15	0.84	0.21	34,42,47,47	0
4	NAG	J	3	14/15	0.85	0.23	46,52,56,61	0
5	NAG	S	2	14/15	0.86	0.25	45,50,55,56	0
7	MAN	R	4	11/12	0.87	0.21	38,44,51,57	0
5	NAG	P	1	14/15	0.88	0.19	39,43,48,53	0
5	NAG	L	2	14/15	0.88	0.25	31,42,52,53	0
3	NAG	I	2	14/15	0.89	0.17	24,35,43,47	0
5	NAG	L	1	14/15	0.90	0.12	20,23,30,30	0
7	NAG	R	2	14/15	0.91	0.17	33,40,46,55	0
5	NAG	N	2	14/15	0.91	0.14	27,35,43,48	0
5	NAG	M	1	14/15	0.92	0.11	17,23,33,34	0
3	NAG	I	1	14/15	0.92	0.12	17,22,28,29	0
5	NAG	N	1	14/15	0.92	0.10	19,25,27,32	0
7	NAG	R	1	14/15	0.92	0.10	31,34,40,41	0
5	NAG	K	1	14/15	0.93	0.14	28,35,41,42	0

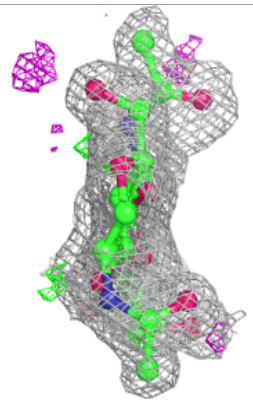
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain I:

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

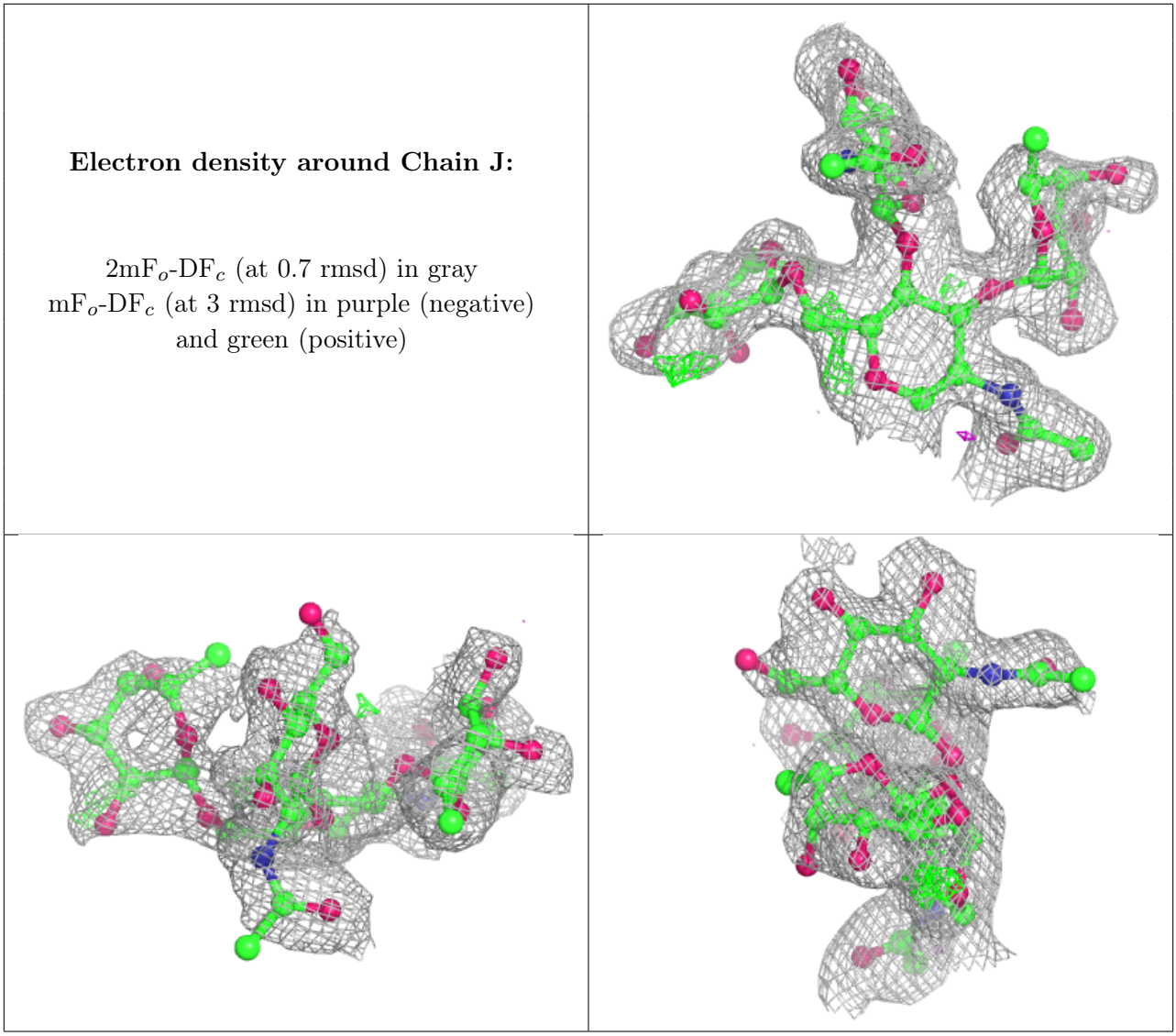






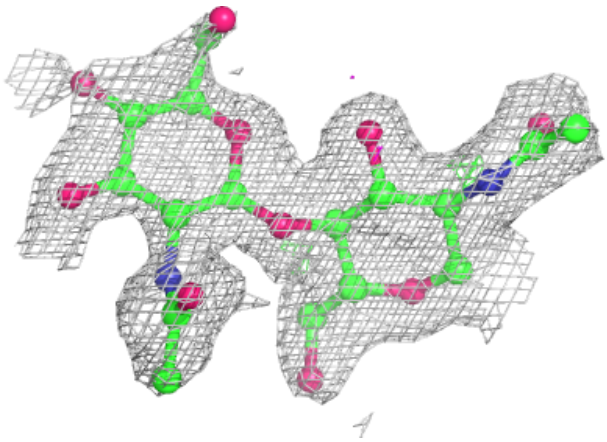
Electron density around Chain J:

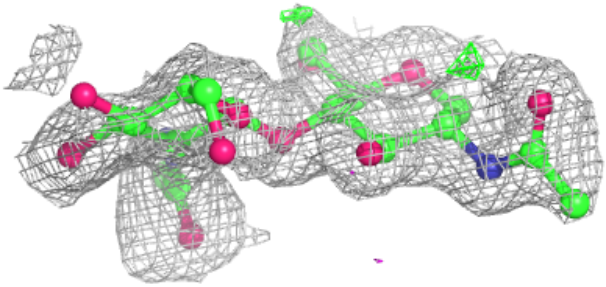
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

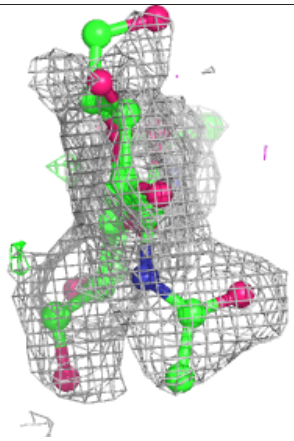


Electron density around Chain K:

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

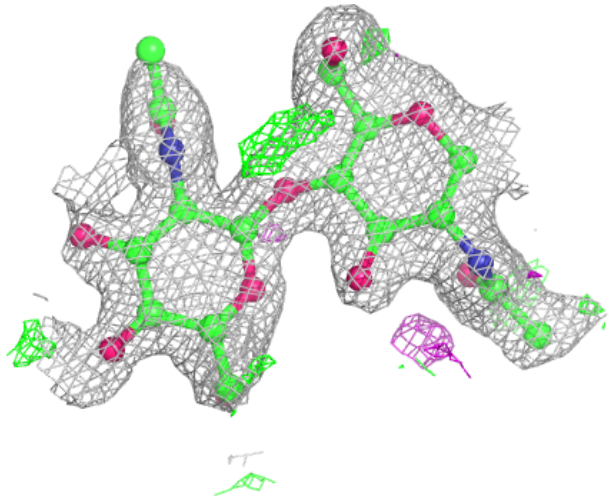


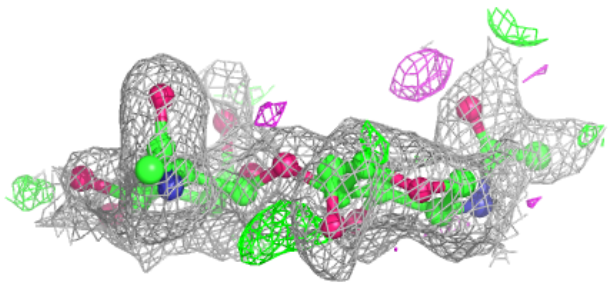


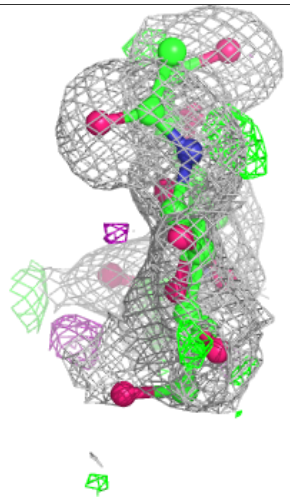


Electron density around Chain L:

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

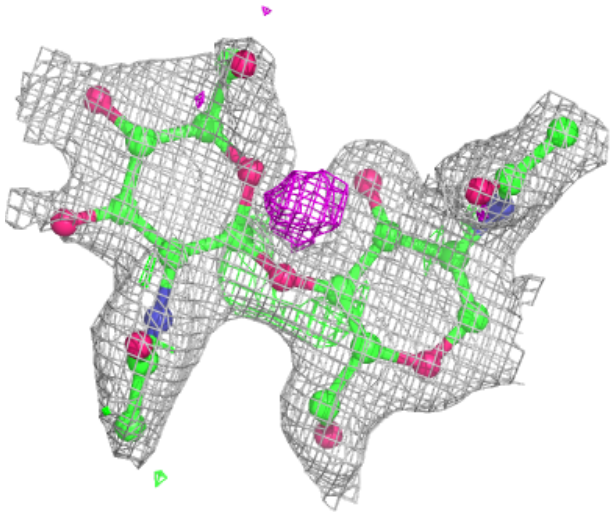


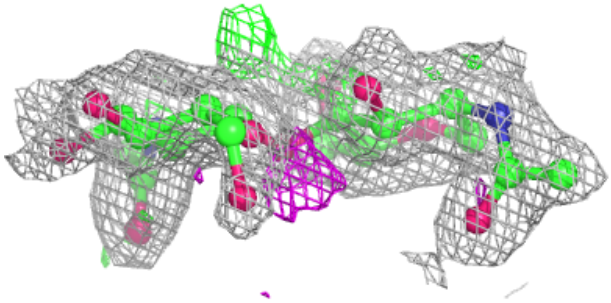


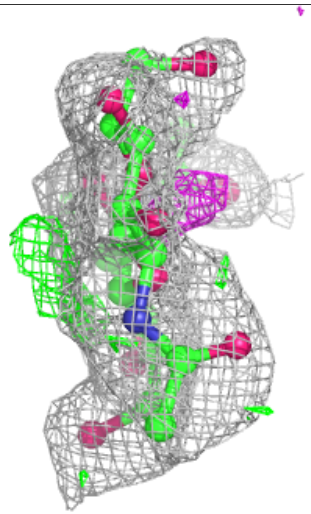


Electron density around Chain M:

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

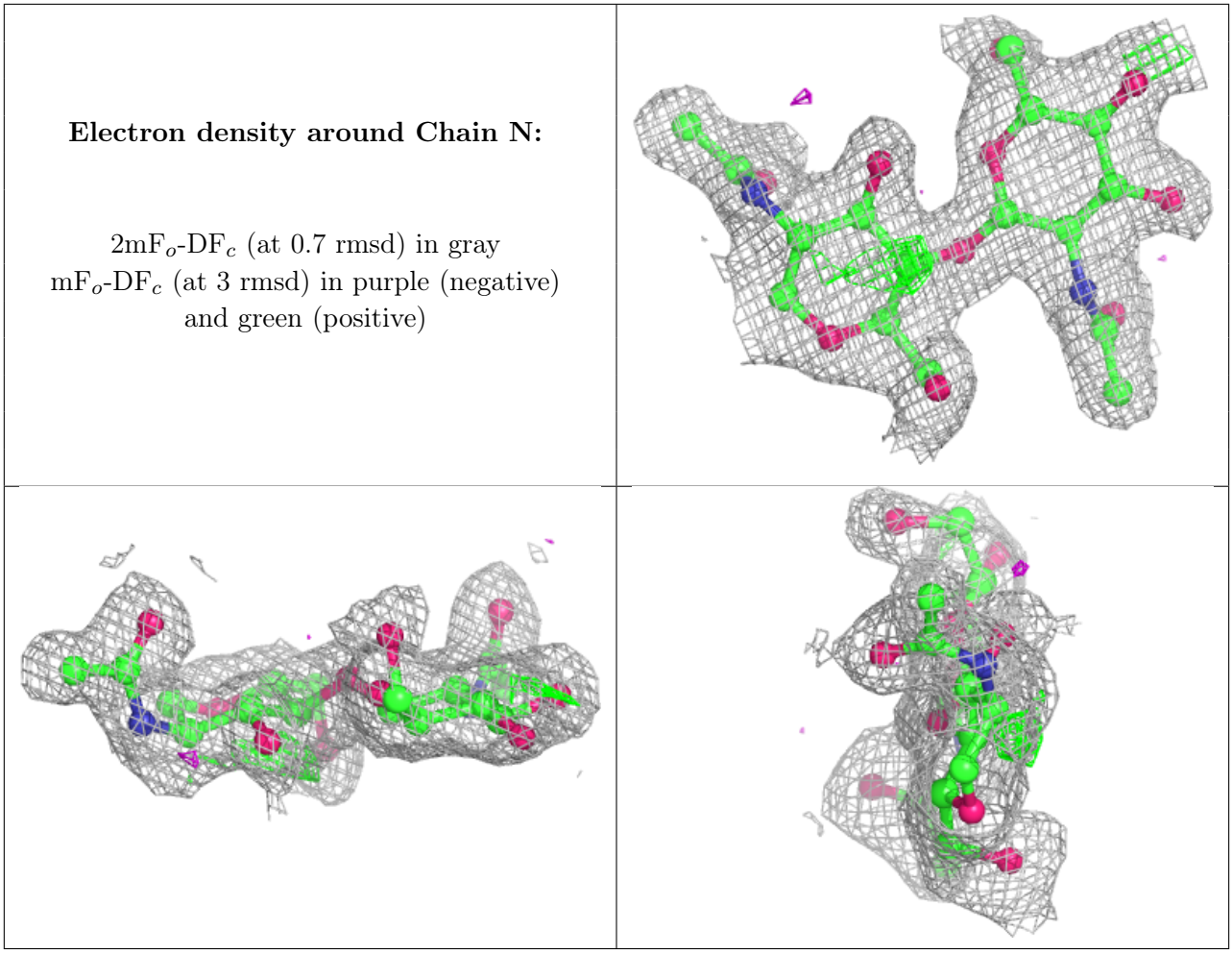






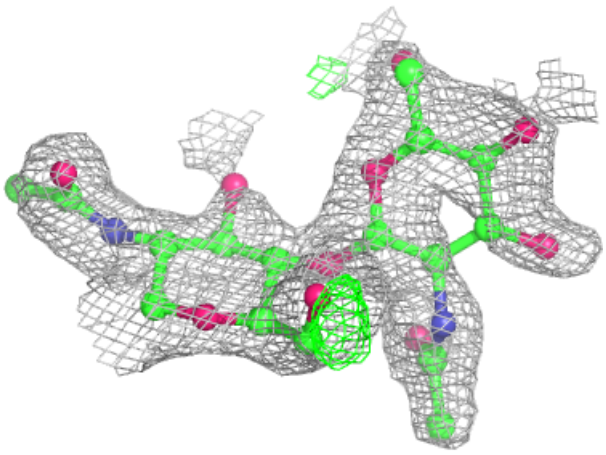
Electron density around Chain N:

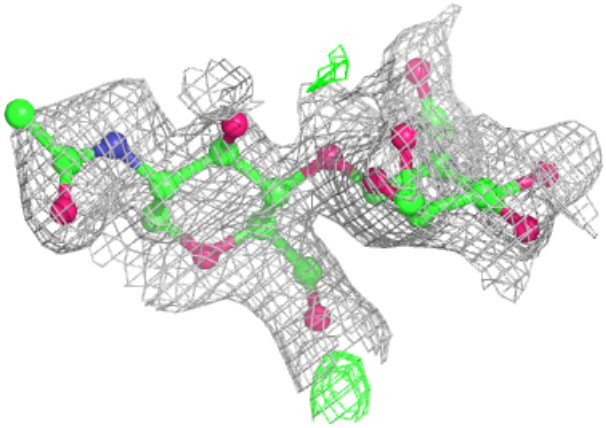
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

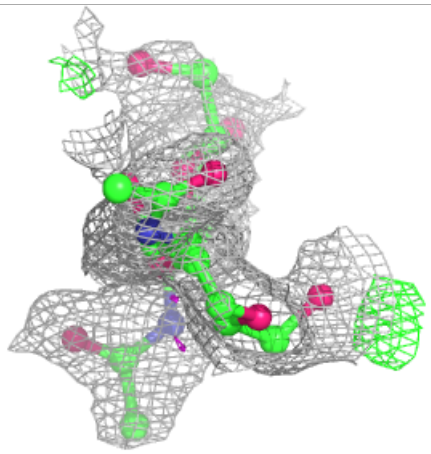


Electron density around Chain O:

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

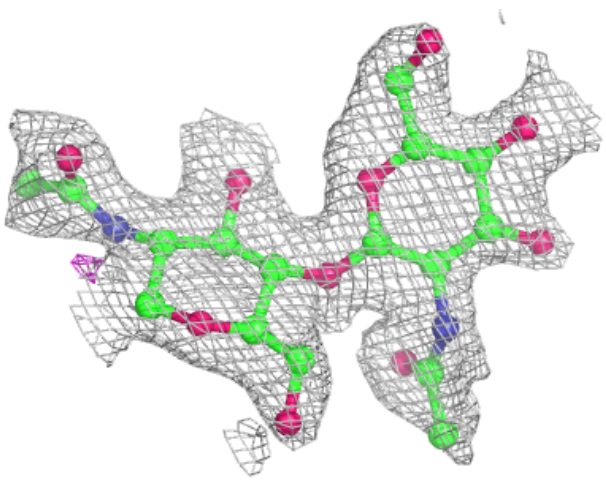


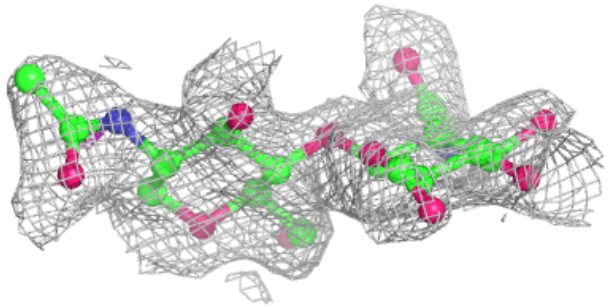




Electron density around Chain P:

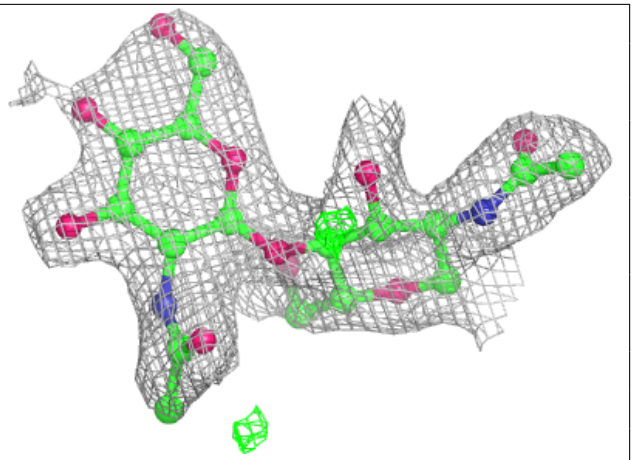
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

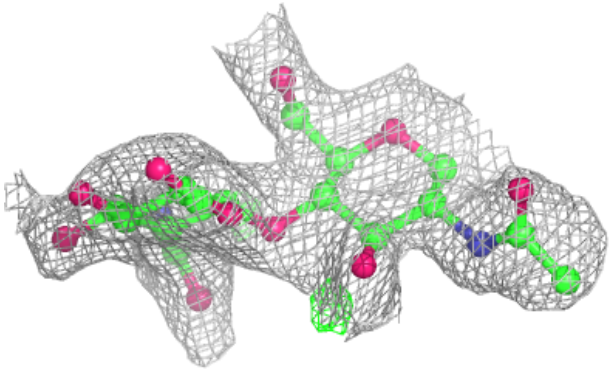


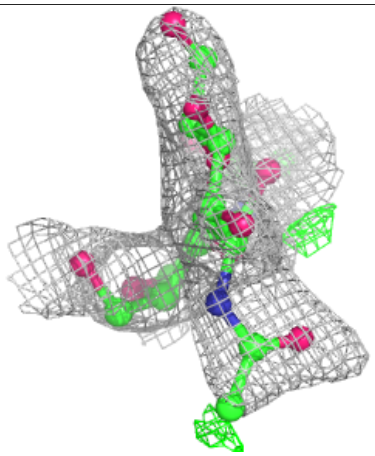


Electron density around Chain S:

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

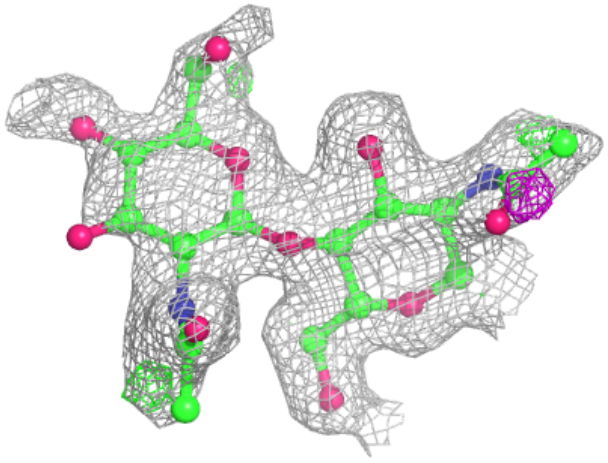


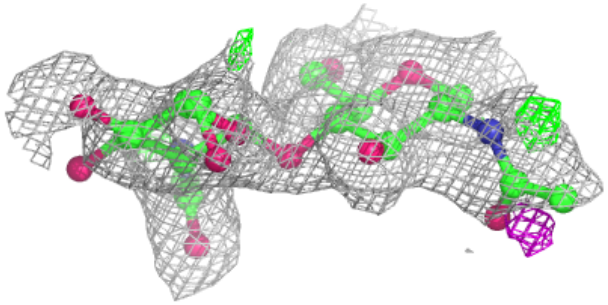


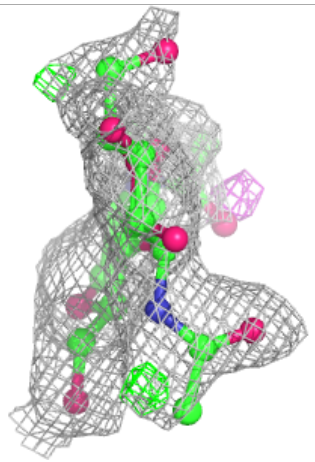


Electron density around Chain T:

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

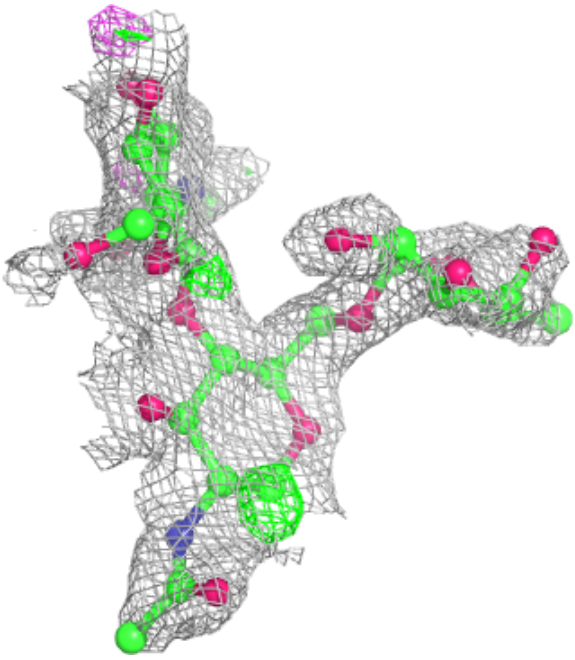


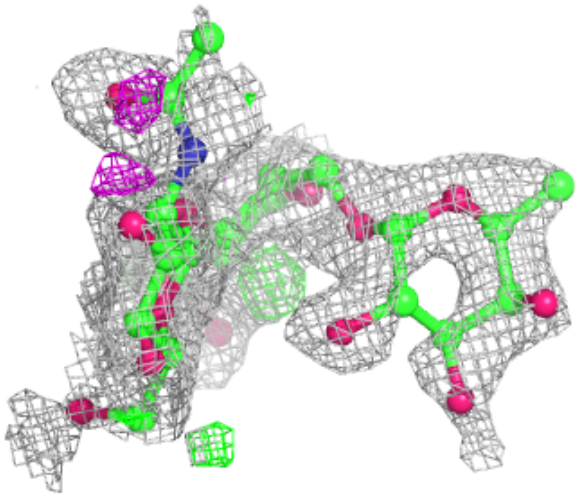


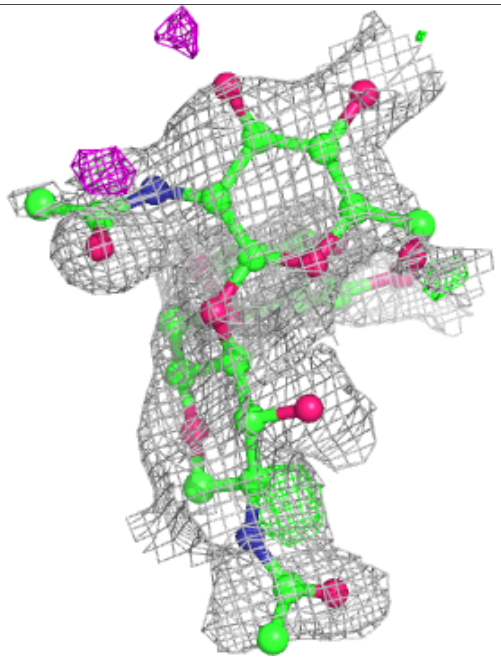


Electron density around Chain Q:

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

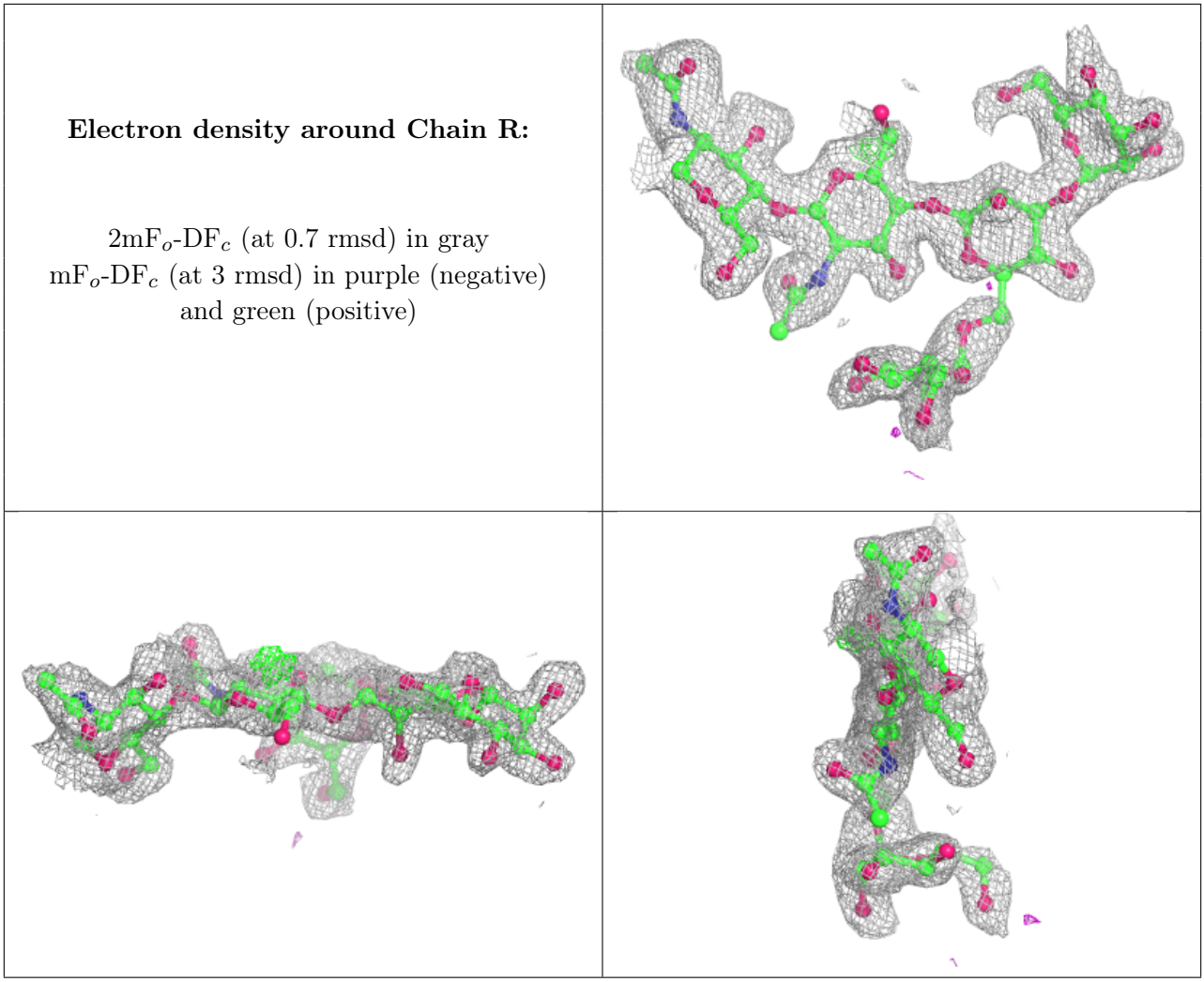






Electron density around Chain R:

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



6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.