Full wwPDB X-ray Structure Validation Report (i)

Jan 3, 2024 – 09:09 pm GMT

PDB ID	:	4V3D
Title	:	The CIDRa domain from HB3var03 PfEMP1 bound to endothelial protein C receptor
Authors	:	Lau, C.K.Y.; Turner, L.; Jespersen, J.S.; Lowe, E.D.; Petersen, B.; Wang, C.W.; Petersen, J.E.V.; Lusingu, J.; Theander, T.G.; Lavstsen, T.; Higgins, M.K.
Deposited on	:	2014-10-17
Resolution	:	2.65 Å(reported)

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

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

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

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

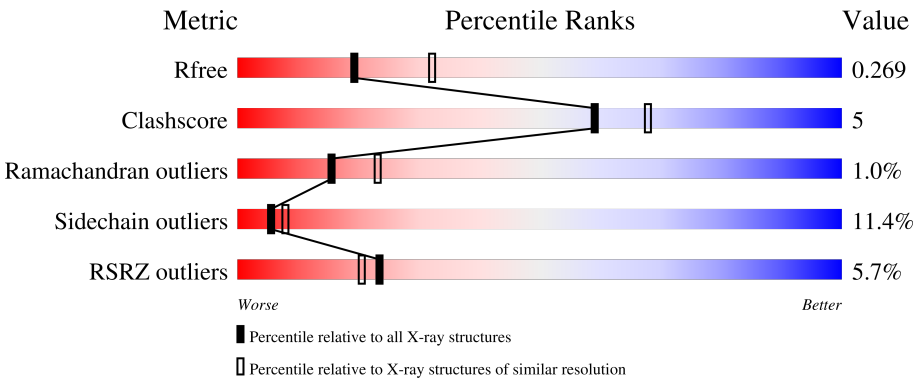
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.65 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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	251	5% 66% 16% • 16%
1	C	251	9% 55% 14% • 26%
2	B	170	% 84% 14% • •
2	D	170	3% 83% 14% • •
3	E	2	50% 50%

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Mol	Chain	Length	Quality of chain
3	G	2	50% 50%
3	I	2	100%
4	F	3	100%
4	H	3	67% 33%

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
3	NAG	E	2	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 6397 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 HB3VAR03 CIDRA DOMAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	210	1755	1116	289	339	11	0	0	0
1	C	186	1578	1016	256	295	11	0	0	0

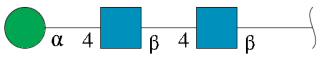
- Molecule 2 is a protein called ENDOTHELIAL PROTEIN C RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	169	1384	884	246	250	4	0	0	0
2	D	168	1376	878	245	249	4	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.

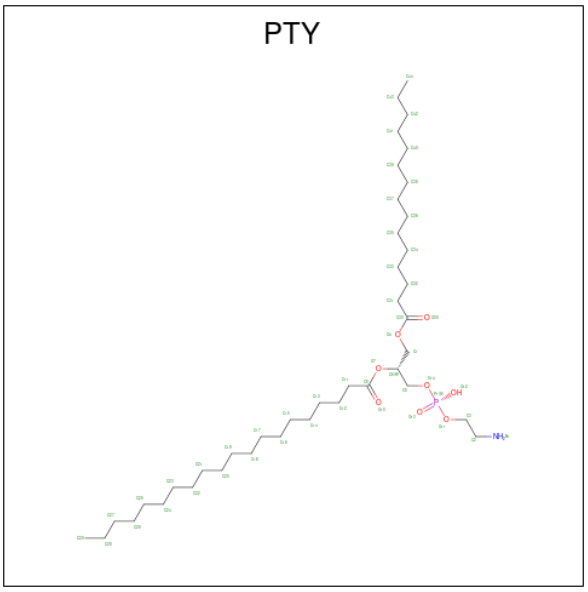
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	E	2	28	16	2	10	0	0	0
3	G	2	28	16	2	10	0	0	0
3	I	2	28	16	2	10	0	0	0

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



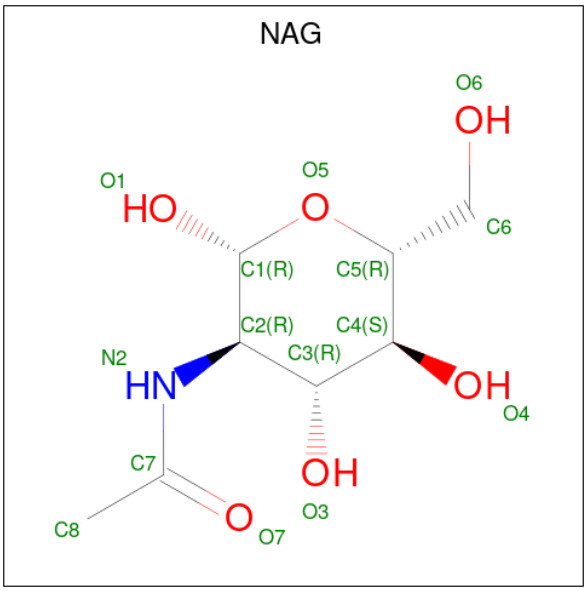
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	F	3	39	22	2	15	0	0	0
			Total	C	N	O			
4	H	3	39	22	2	15	0	0	0

- Molecule 5 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula: $C_{40}H_{80}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	B	1	50	40	1	8	1	0	0
			Total	C	N	O	P		
5	D	1	50	40	1	8	1	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



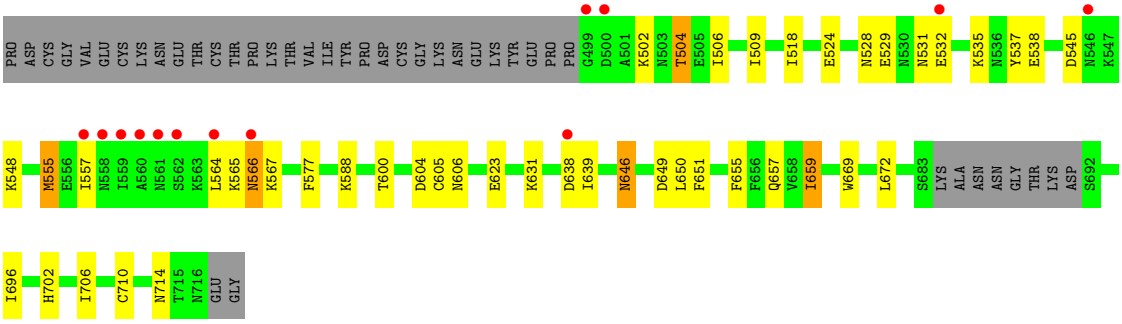
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	B	1	14	8	1	5	0	0
			Total	C	N	O		
6	B	1	14	8	1	5	0	0
			Total	C	N	O		
6	D	1	14	8	1	5	0	0

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.

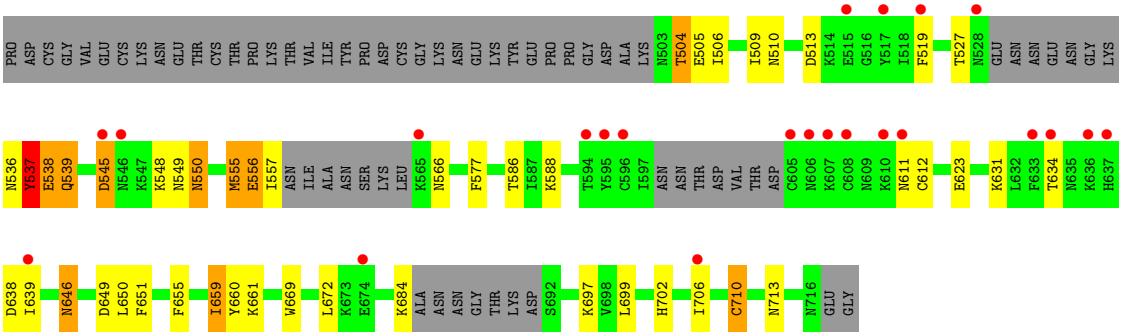
• Molecule 1: HB3VAR03 CIDRA DOMAIN

Chain A: 5% 66% 16% • 16%



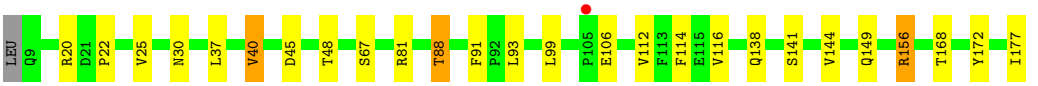
• Molecule 1: HB3VAR03 CIDRA DOMAIN

Chain C: 9% 55% 14% • 26%



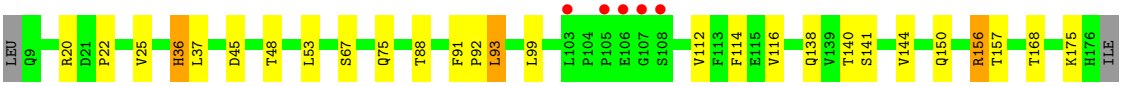
• Molecule 2: ENDOTHELIAL PROTEIN C RECEPTOR

Chain B: % 84% 14% • •



• Molecule 2: ENDOTHELIAL PROTEIN C RECEPTOR

Chain D: 3% 83% 14% • •



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

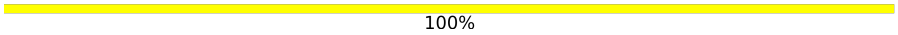
Chain E:

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

Chain G:

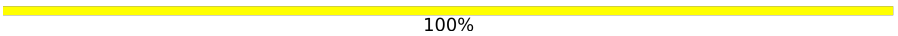
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:



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

Chain F:



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

Chain H:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	66.13Å 94.67Å 290.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	53.29 – 2.65 50.79 – 2.65	Depositor EDS
% Data completeness (in resolution range)	94.0 (53.29-2.65) 94.0 (50.79-2.65)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.94 (at 2.65Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.222 , 0.255 0.230 , 0.269	Depositor DCC
R_{free} test set	1287 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	50.9	Xtriage
Anisotropy	0.349	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 50.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6397	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% 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 (i)

5.1 Standard geometry (i)

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

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	0.53	0/1790	0.76	0/2406
1	C	0.48	0/1610	0.79	3/2157 (0.1%)
2	B	0.50	0/1422	0.74	2/1936 (0.1%)
2	D	0.45	0/1414	0.72	2/1925 (0.1%)
All	All	0.49	0/6236	0.75	7/8424 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	93	LEU	N-CA-CB	-6.30	97.80	110.40
2	B	93	LEU	N-CA-CB	-6.12	98.17	110.40
2	B	93	LEU	CA-CB-CG	5.67	128.34	115.30
2	D	93	LEU	CA-CB-CG	5.53	128.02	115.30
1	C	537	TYR	C-N-CA	5.42	135.26	121.70
1	C	556	GLU	C-N-CA	5.24	134.80	121.70
1	C	538	GLU	N-CA-C	5.12	124.83	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1755	0	1690	14	0
1	C	1578	0	1529	21	0
2	B	1384	0	1335	11	0
2	D	1376	0	1324	19	0
3	E	28	0	25	1	0
3	G	28	0	25	1	0
3	I	28	0	25	0	0
4	F	39	0	34	0	0
4	H	39	0	34	2	0
5	B	50	0	79	3	0
5	D	50	0	79	3	0
6	B	28	0	26	1	0
6	D	14	0	13	0	0
All	All	6397	0	6218	59	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (59) 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:A:696:ILE:CD1	1:A:696:ILE:CG1	1.75	1.62
1:A:538:GLU:HB2	1:A:555:MET:HE1	1.62	0.82
1:C:537:TYR:CD1	1:C:537:TYR:N	2.54	0.74
1:C:537:TYR:N	1:C:537:TYR:HD1	1.87	0.73
1:C:536:ASN:C	1:C:537:TYR:CD1	2.65	0.69
1:C:660:TYR:HD1	2:D:150:GLN:HE22	1.42	0.68
2:B:172:TYR:CD2	5:B:200:PTY:H282	2.33	0.62
1:C:505:GLU:HG2	1:C:539:GLN:HE22	1.66	0.61
2:D:93:LEU:HD23	4:H:1:NAG:H82	1.83	0.60
1:C:555:MET:O	1:C:566:ASN:HB2	2.03	0.59
6:B:205:NAG:H81	2:D:36:HIS:CE1	2.38	0.59
3:E:1:NAG:H5	3:G:2:NAG:H81	1.87	0.57
2:B:37:LEU:CD2	2:D:37:LEU:HD22	2.35	0.56
1:A:545:ASP:HB3	1:A:548:LYS:HB2	1.87	0.56
2:B:37:LEU:HD23	2:D:37:LEU:HD22	1.88	0.55
1:C:510:ASN:O	1:C:537:TYR:CD2	2.59	0.55
1:A:555:MET:HB3	1:A:567:LYS:HB3	1.88	0.55
1:C:655:PHE:O	1:C:659:ILE:HB	2.07	0.55
1:A:655:PHE:O	1:A:659:ILE:HB	2.08	0.54
2:B:168:THR:HG22	5:B:200:PTY:H281	1.89	0.54
2:D:75:GLN:HE22	2:D:156:ARG:HH11	1.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:536:ASN:C	1:C:537:TYR:HD1	2.05	0.53
1:A:504:THR:HG21	1:A:631:LYS:HB2	1.92	0.52
1:C:504:THR:HG21	1:C:631:LYS:HB2	1.92	0.52
1:C:660:TYR:CD1	2:D:150:GLN:NE2	2.78	0.50
1:A:555:MET:O	1:A:566:ASN:HA	2.11	0.50
2:D:25:VAL:CG1	2:D:45:ASP:HB3	2.43	0.49
1:A:646:ASN:ND2	1:A:649:ASP:H	2.11	0.49
1:C:538:GLU:HB3	1:C:555:MET:CE	2.44	0.48
2:D:36:HIS:CG	2:D:37:LEU:H	2.32	0.48
1:C:510:ASN:O	1:C:537:TYR:HD2	1.95	0.48
2:B:116:VAL:HG21	5:B:200:PTY:H372	1.95	0.48
1:C:646:ASN:ND2	1:C:649:ASP:H	2.11	0.47
2:D:22:PRO:HG3	2:D:91:PHE:CE2	2.49	0.47
2:B:22:PRO:HG3	2:B:91:PHE:CE2	2.49	0.47
2:D:168:THR:HG22	5:D:200:PTY:H272	1.97	0.46
1:C:519:PHE:HB2	1:C:611:ASN:OD1	2.15	0.46
2:B:40:VAL:HG11	2:D:53:LEU:HD21	1.98	0.45
2:D:156:ARG:HE	2:D:156:ARG:HB2	1.51	0.45
1:A:657:GLN:OE1	2:B:81:ARG:NH1	2.50	0.45
2:D:116:VAL:HG21	5:D:200:PTY:H371	1.99	0.44
2:D:92:PRO:O	4:H:1:NAG:H3	2.18	0.44
1:C:706:ILE:O	1:C:710:CYS:HB3	2.17	0.44
1:A:706:ILE:O	1:A:710:CYS:HB2	2.18	0.43
1:C:545:ASP:HB3	1:C:548:LYS:HB2	2.00	0.43
1:C:586:THR:HG21	1:C:699:LEU:HD11	2.01	0.43
1:A:524:GLU:O	1:A:528:ASN:HB3	2.19	0.43
1:C:651:PHE:HA	1:C:669:TRP:CZ2	2.54	0.42
2:B:25:VAL:CG1	2:B:45:ASP:HB3	2.50	0.42
2:B:141:SER:OG	2:B:144:VAL:HG23	2.19	0.42
1:A:651:PHE:HA	1:A:669:TRP:CZ2	2.54	0.42
2:D:157:THR:HG22	5:D:200:PTY:H321	2.02	0.42
1:A:518:ILE:HB	1:A:588:LYS:HG2	2.03	0.41
2:B:156:ARG:HE	2:B:156:ARG:HB2	1.55	0.41
2:D:141:SER:OG	2:D:144:VAL:HG23	2.21	0.41
1:C:660:TYR:HD1	2:D:150:GLN:NE2	2.14	0.40
2:D:25:VAL:HG12	2:D:45:ASP:HB3	2.02	0.40
1:A:702:HIS:NE2	1:A:706:ILE:HD11	2.36	0.40
1:C:702:HIS:NE2	1:C:706:ILE:HD11	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	206/251 (82%)	189 (92%)	13 (6%)	4 (2%)	8 11
1	C	176/251 (70%)	168 (96%)	7 (4%)	1 (1%)	25 37
2	B	167/170 (98%)	159 (95%)	7 (4%)	1 (1%)	25 37
2	D	166/170 (98%)	158 (95%)	7 (4%)	1 (1%)	25 37
All	All	715/842 (85%)	674 (94%)	34 (5%)	7 (1%)	15 23

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	606	ASN
1	A	535	LYS
1	A	565	LYS
1	C	550	ASN
1	A	566	ASN
2	B	88	THR
2	D	88	THR

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	198/234 (85%)	175 (88%)	23 (12%)	5 7
1	C	178/234 (76%)	149 (84%)	29 (16%)	2 2
2	B	151/152 (99%)	137 (91%)	14 (9%)	9 13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	D	150/152 (99%)	139 (93%)	11 (7%)	14 21
All	All	677/772 (88%)	600 (89%)	77 (11%)	5 8

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	502	LYS
1	A	504	THR
1	A	506	ILE
1	A	509	ILE
1	A	529	GLU
1	A	531	ASN
1	A	532	GLU
1	A	537	TYR
1	A	555	MET
1	A	557	ILE
1	A	564	LEU
1	A	577	PHE
1	A	600	THR
1	A	604	ASP
1	A	605	CYS
1	A	623	GLU
1	A	638	ASP
1	A	639	ILE
1	A	646	ASN
1	A	650	LEU
1	A	659	ILE
1	A	672	LEU
1	A	714	ASN
2	B	20	ARG
2	B	30	ASN
2	B	40	VAL
2	B	48	THR
2	B	67	SER
2	B	88	THR
2	B	99	LEU
2	B	106	GLU
2	B	112	VAL
2	B	114	PHE
2	B	138	GLN
2	B	149	GLN
2	B	156	ARG

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Mol	Chain	Res	Type
2	B	177	ILE
1	C	504	THR
1	C	506	ILE
1	C	509	ILE
1	C	513	ASP
1	C	527	THR
1	C	537	TYR
1	C	539	GLN
1	C	545	ASP
1	C	549	ASN
1	C	550	ASN
1	C	555	MET
1	C	556	GLU
1	C	557	ILE
1	C	577	PHE
1	C	588	LYS
1	C	612	CYS
1	C	623	GLU
1	C	634	THR
1	C	638	ASP
1	C	639	ILE
1	C	646	ASN
1	C	650	LEU
1	C	659	ILE
1	C	661	LYS
1	C	672	LEU
1	C	684	LYS
1	C	697	LYS
1	C	710	CYS
1	C	713	ASN
2	D	20	ARG
2	D	36	HIS
2	D	48	THR
2	D	67	SER
2	D	99	LEU
2	D	112	VAL
2	D	114	PHE
2	D	138	GLN
2	D	140	THR
2	D	156	ARG
2	D	175	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	558	ASN
1	A	646	ASN
1	A	714	ASN
2	B	54	GLN
2	B	57	GLN
2	B	70	GLN
2	B	134	GLN
2	B	174	GLN
1	C	539	GLN
1	C	646	ASN
2	D	39	HIS
2	D	57	GLN
2	D	70	GLN
2	D	138	GLN
2	D	174	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

12 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	E	1	3,2	14,14,15	0.35	0	17,19,21	1.41	2 (11%)
3	NAG	E	2	3	14,14,15	0.33	0	17,19,21	0.74	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	F	1	4,2	14,14,15	0.37	0	17,19,21	1.13	1 (5%)
4	NAG	F	2	4	14,14,15	0.38	0	17,19,21	0.73	1 (5%)
4	MAN	F	3	4	11,11,12	0.35	0	15,15,17	1.52	1 (6%)
3	NAG	G	1	3,2	14,14,15	0.34	0	17,19,21	1.58	3 (17%)
3	NAG	G	2	3	14,14,15	0.27	0	17,19,21	0.84	1 (5%)
4	NAG	H	1	4,2	14,14,15	0.36	0	17,19,21	0.74	1 (5%)
4	NAG	H	2	4	14,14,15	0.30	0	17,19,21	0.69	1 (5%)
4	MAN	H	3	4	11,11,12	0.45	0	15,15,17	1.16	2 (13%)
3	NAG	I	1	3,2	14,14,15	0.42	0	17,19,21	1.95	5 (29%)
3	NAG	I	2	3	14,14,15	0.28	0	17,19,21	0.73	1 (5%)

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

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

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	1	NAG	C1-O5-C5	5.21	119.26	112.19
3	G	1	NAG	C1-O5-C5	5.05	119.04	112.19
4	F	3	MAN	C1-O5-C5	4.99	118.95	112.19
3	I	1	NAG	C1-C2-N2	4.15	117.57	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	1	NAG	C1-C2-N2	4.08	117.47	110.49
4	H	3	MAN	C1-O5-C5	3.62	117.09	112.19
4	F	1	NAG	C1-O5-C5	3.16	116.47	112.19
3	E	1	NAG	C1-O5-C5	3.03	116.30	112.19
3	G	1	NAG	O5-C1-C2	2.67	115.50	111.29
4	H	1	NAG	C1-O5-C5	2.64	115.77	112.19
3	I	1	NAG	O5-C1-C2	2.51	115.26	111.29
3	G	2	NAG	O5-C1-C2	-2.49	107.35	111.29
4	H	2	NAG	C1-O5-C5	2.40	115.44	112.19
4	F	2	NAG	C1-O5-C5	2.37	115.41	112.19
3	E	2	NAG	C1-O5-C5	2.37	115.40	112.19
3	I	1	NAG	C3-C4-C5	2.33	114.39	110.24
4	H	3	MAN	C1-C2-C3	2.28	112.46	109.67
3	I	1	NAG	C2-N2-C7	2.25	126.10	122.90
3	I	2	NAG	O5-C1-C2	-2.22	107.79	111.29
3	G	1	NAG	C1-C2-N2	2.08	114.04	110.49

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	1	NAG	O5-C5-C6-O6
4	H	1	NAG	O5-C5-C6-O6
4	F	1	NAG	C4-C5-C6-O6
4	H	1	NAG	C4-C5-C6-O6
4	F	3	MAN	C4-C5-C6-O6
4	F	3	MAN	O5-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6
4	H	3	MAN	O5-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
3	I	1	NAG	C3-C2-N2-C7
3	G	2	NAG	O5-C5-C6-O6
3	E	1	NAG	C1-C2-N2-C7
3	E	1	NAG	C3-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	1	NAG	2	0

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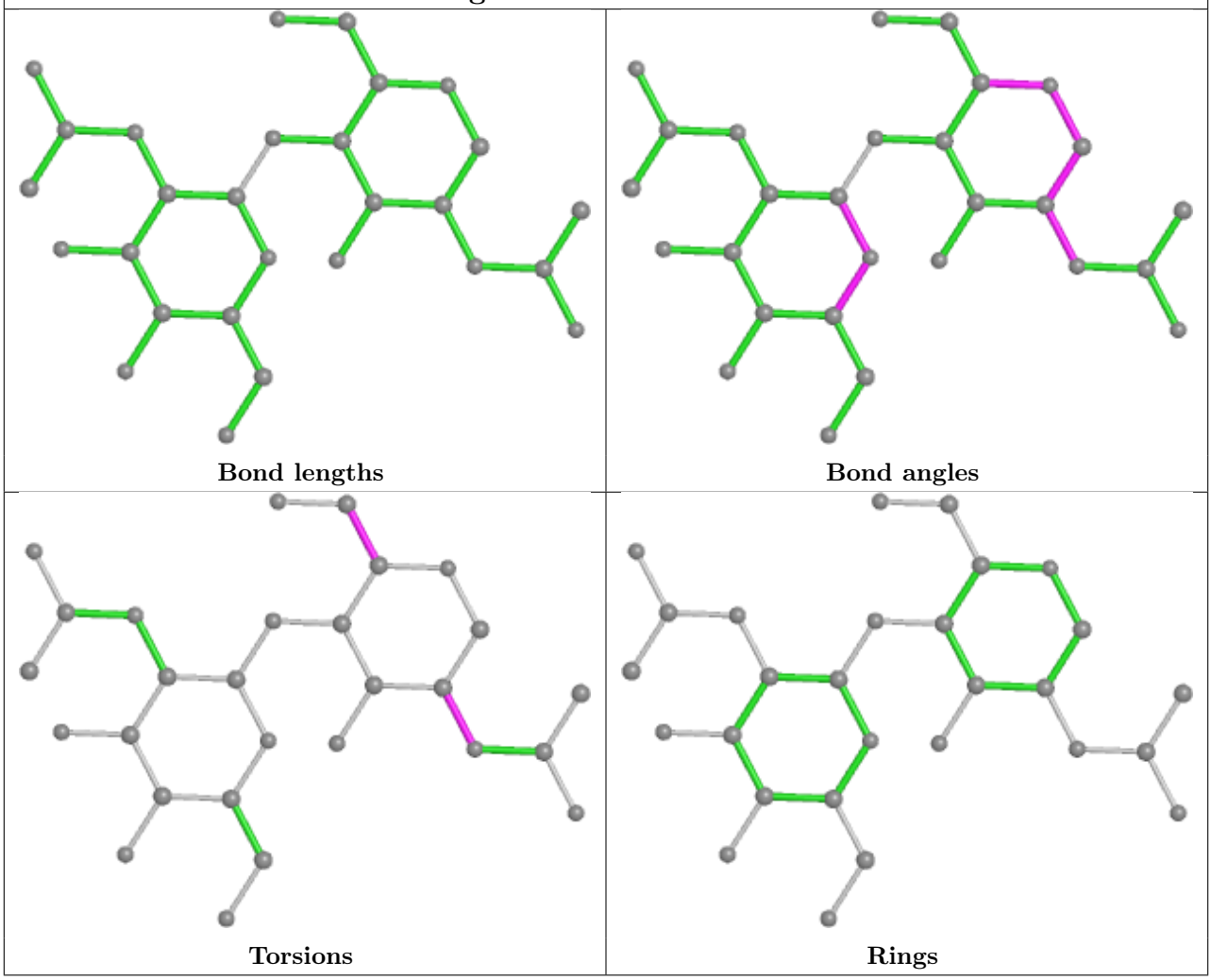
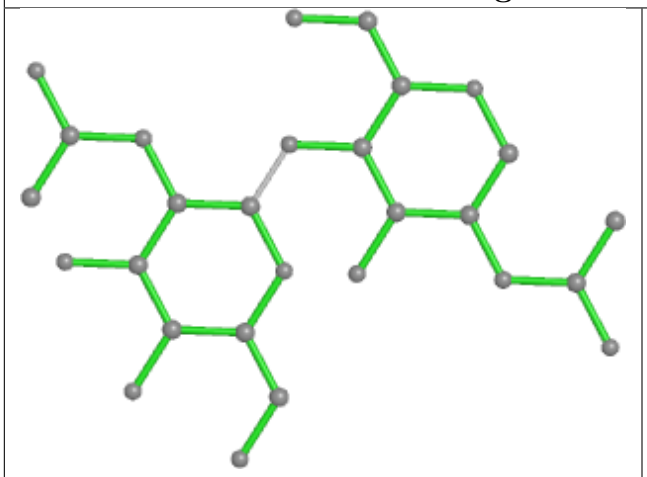
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	1	NAG	1	0
3	G	2	NAG	1	0

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

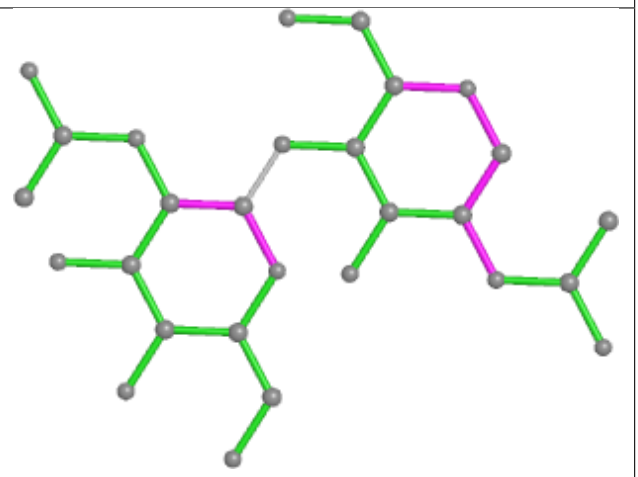
Oligosaccharide Chain E



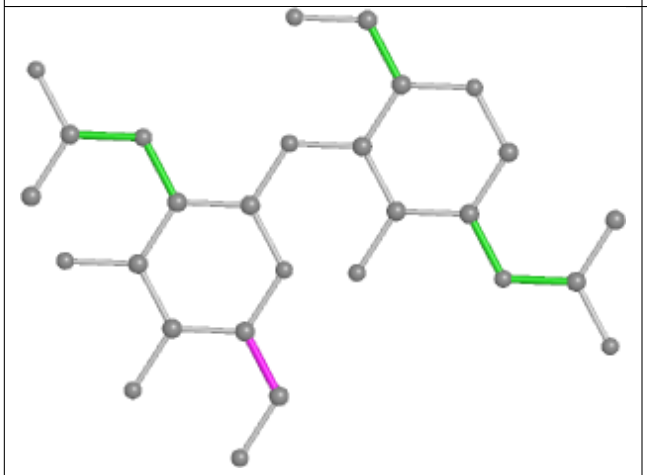
Oligosaccharide Chain G



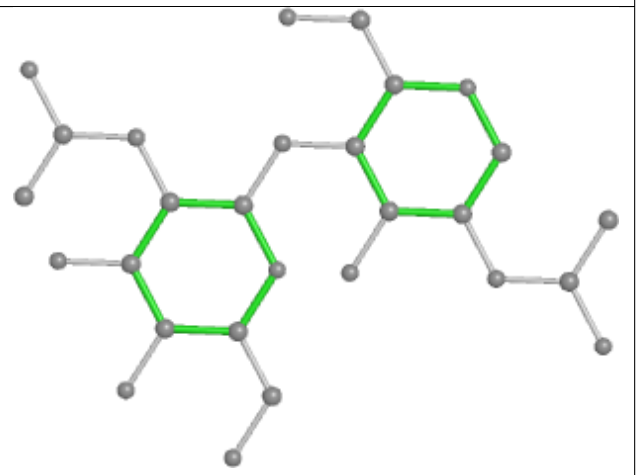
Bond lengths



Bond angles

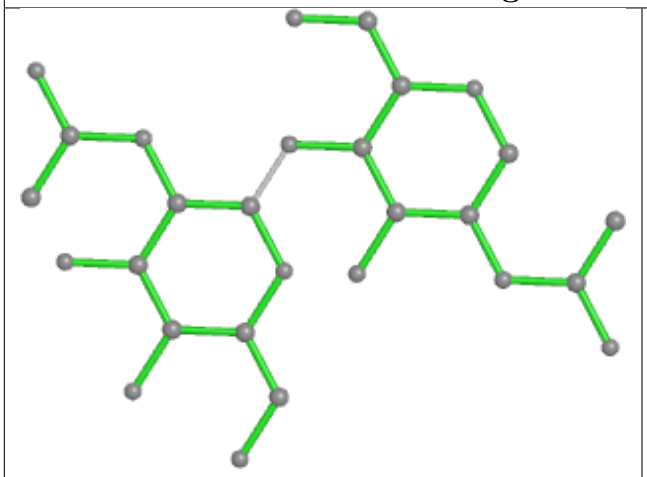


Torsions

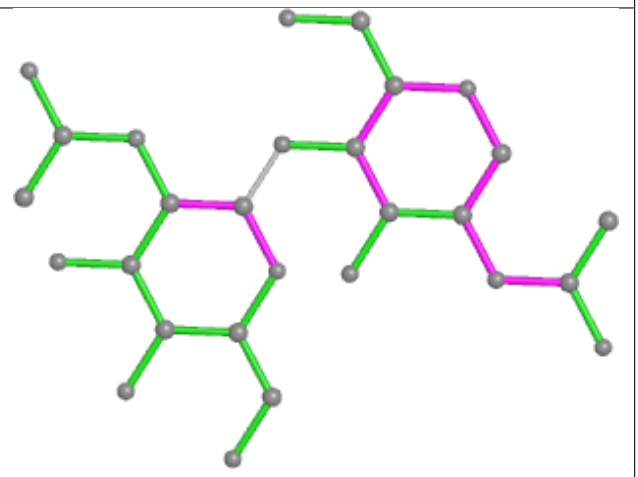


Rings

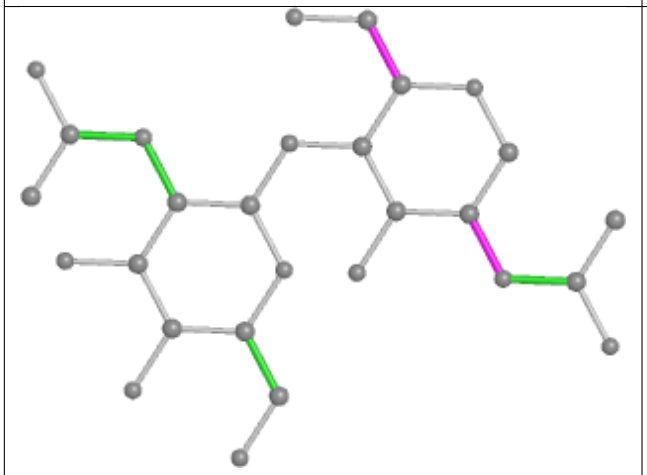
Oligosaccharide Chain I



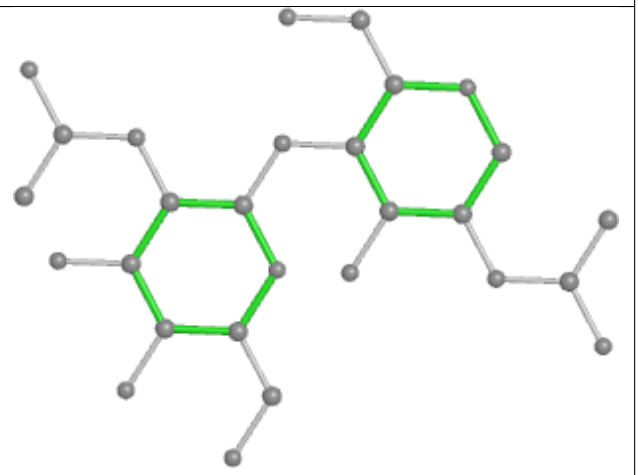
Bond lengths



Bond angles

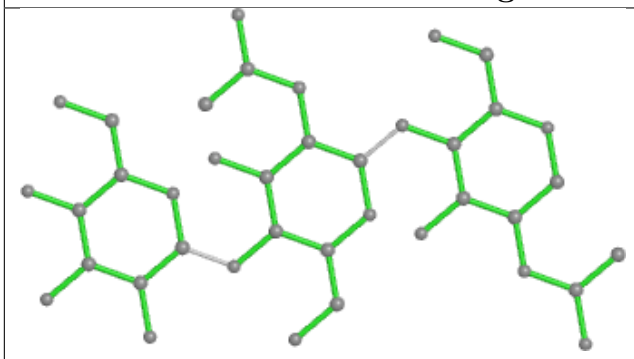


Torsions

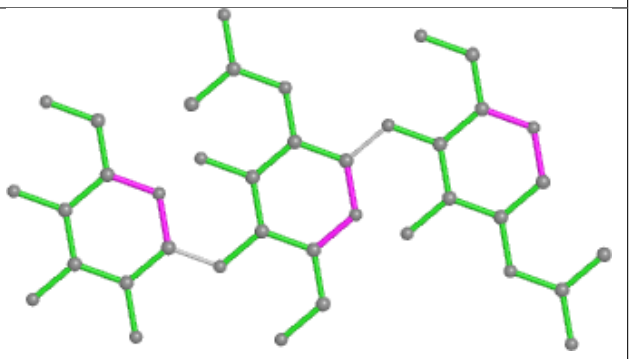


Rings

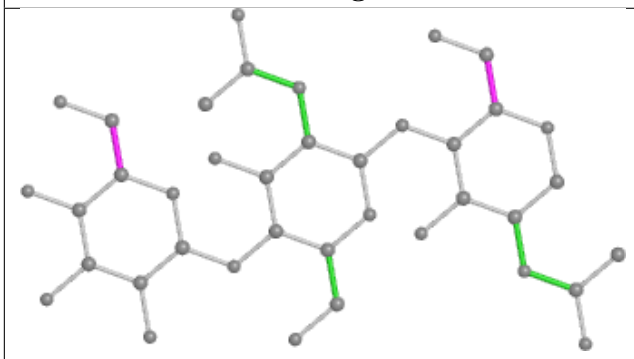
Oligosaccharide Chain F



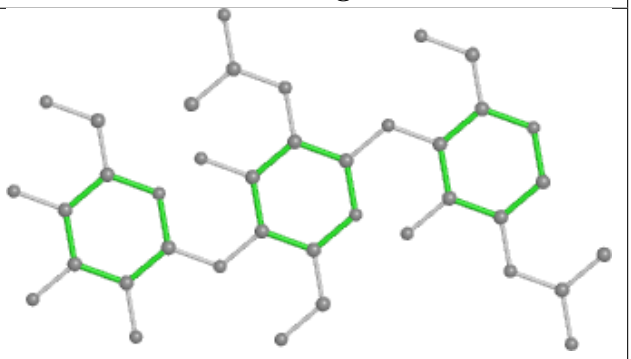
Bond lengths



Bond angles

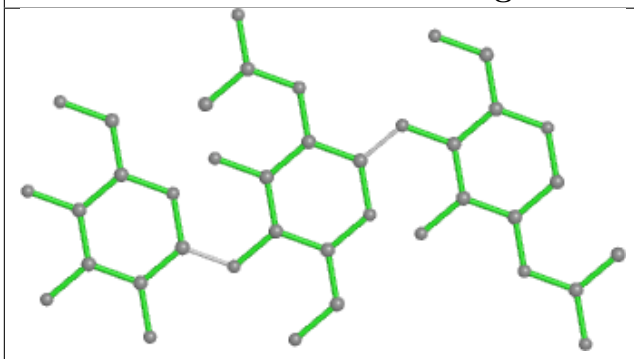


Torsions

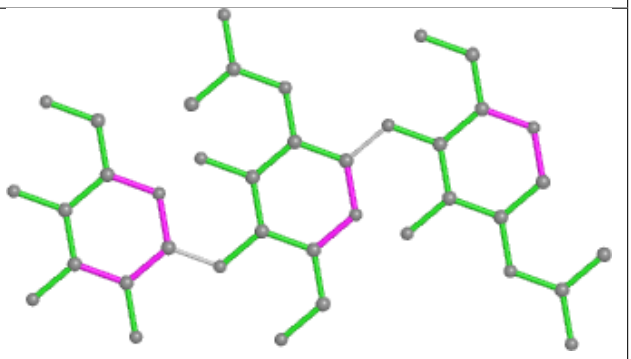


Rings

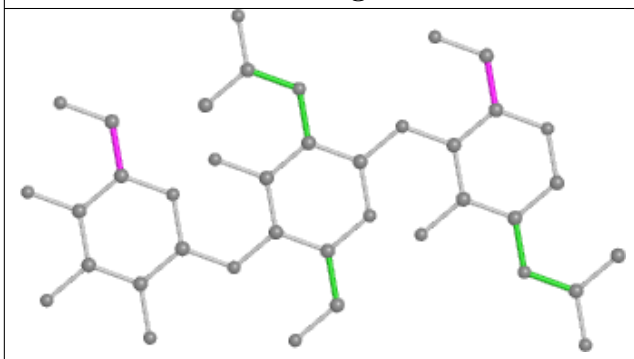
Oligosaccharide Chain H



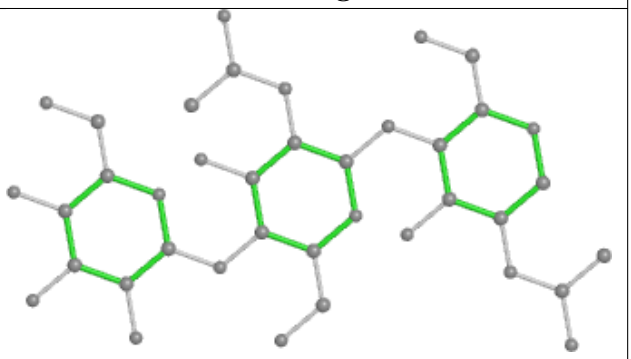
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

5 ligands 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	$\#\|Z\| > 2$
5	PTY	D	200	-	49,49,49	0.49	0	52,54,54	0.61	2 (3%)
6	NAG	B	205	2	14,14,15	0.40	0	17,19,21	0.71	1 (5%)
6	NAG	D	208	2	14,14,15	0.30	0	17,19,21	2.13	3 (17%)
5	PTY	B	200	-	49,49,49	0.46	0	52,54,54	0.63	1 (1%)
6	NAG	B	206	2	14,14,15	0.32	0	17,19,21	1.78	3 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PTY	D	200	-	-	22/53/53/53	-
6	NAG	B	205	2	-	0/6/23/26	0/1/1/1
6	NAG	D	208	2	-	1/6/23/26	0/1/1/1
5	PTY	B	200	-	-	25/53/53/53	-
6	NAG	B	206	2	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	208	NAG	C1-C2-N2	7.48	123.27	110.49
6	B	206	NAG	C1-C2-N2	5.42	119.75	110.49
6	B	206	NAG	C1-O5-C5	3.73	117.24	112.19
6	D	208	NAG	O5-C1-C2	-3.35	106.00	111.29
5	B	200	PTY	O14-P1-O13	-2.65	98.70	109.07
6	B	205	NAG	C1-C2-N2	2.20	114.25	110.49
5	D	200	PTY	O14-P1-O13	-2.15	100.65	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	200	PTY	O11-P1-O13	-2.09	100.91	109.07
6	B	206	NAG	O5-C1-C2	-2.06	108.03	111.29
6	D	208	NAG	C2-N2-C7	2.04	125.81	122.90

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	200	PTY	N1-C2-C3-O11
5	D	200	PTY	C5-O14-P1-O13
6	B	206	NAG	O5-C5-C6-O6
6	B	206	NAG	C4-C5-C6-O6
6	B	206	NAG	C1-C2-N2-C7
6	D	208	NAG	C1-C2-N2-C7
5	D	200	PTY	C30-C31-C32-C33
5	D	200	PTY	C31-C32-C33-C34
5	D	200	PTY	C34-C35-C36-C37
5	B	200	PTY	C15-C16-C17-C18
5	B	200	PTY	C18-C19-C20-C21
5	D	200	PTY	C19-C20-C21-C22
5	B	200	PTY	C19-C20-C21-C22
5	D	200	PTY	C22-C23-C24-C25
5	B	200	PTY	C34-C35-C36-C37
5	B	200	PTY	C16-C17-C18-C19
5	D	200	PTY	C25-C26-C27-C28
5	B	200	PTY	C38-C39-C40-C41
5	B	200	PTY	C13-C14-C15-C16
5	B	200	PTY	C24-C25-C26-C27
5	B	200	PTY	C31-C32-C33-C34
5	D	200	PTY	C11-C12-C13-C14
5	B	200	PTY	C14-C15-C16-C17
5	D	200	PTY	C15-C16-C17-C18
5	B	200	PTY	C35-C36-C37-C38
5	B	200	PTY	C23-C24-C25-C26
5	B	200	PTY	C25-C26-C27-C28
5	B	200	PTY	C30-C31-C32-C33
5	D	200	PTY	C40-C41-C42-C43
5	D	200	PTY	C26-C27-C28-C29
5	B	200	PTY	C26-C27-C28-C29
5	B	200	PTY	C41-C42-C43-C44
5	B	200	PTY	C37-C38-C39-C40
5	B	200	PTY	C21-C22-C23-C24

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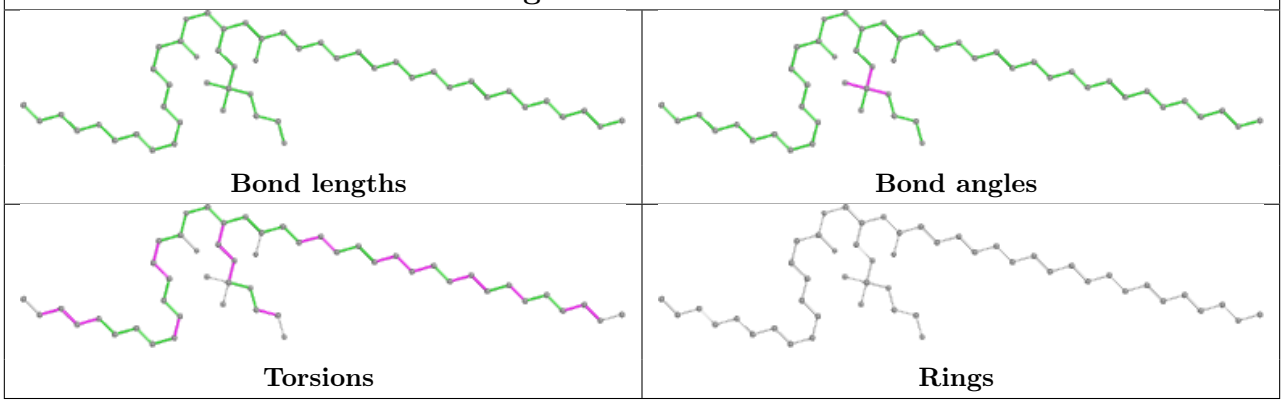
Mol	Chain	Res	Type	Atoms
5	D	200	PTY	C20-C21-C22-C23
5	D	200	PTY	O14-C5-C6-C1
5	D	200	PTY	O14-C5-C6-O7
5	D	200	PTY	C41-C42-C43-C44
5	D	200	PTY	C12-C13-C14-C15
5	D	200	PTY	C5-O14-P1-O11
5	B	200	PTY	C39-C40-C41-C42
5	B	200	PTY	C6-C5-O14-P1
5	D	200	PTY	C6-C5-O14-P1
5	B	200	PTY	C17-C18-C19-C20
5	D	200	PTY	C39-C40-C41-C42
5	B	200	PTY	O4-C1-C6-C5
5	B	200	PTY	C32-C33-C34-C35
5	B	200	PTY	O4-C1-C6-O7
5	D	200	PTY	C17-C18-C19-C20
5	B	200	PTY	C11-C12-C13-C14
5	D	200	PTY	C16-C17-C18-C19

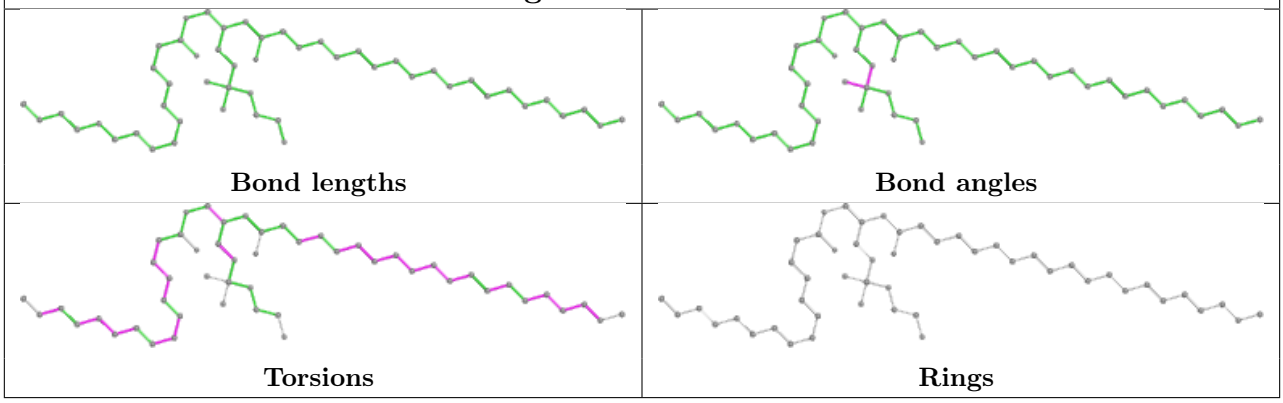
There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	200	PTY	3	0
6	B	205	NAG	1	0
5	B	200	PTY	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand PTY D 200	
 Bond lengths	Bond angles
Torsions	Rings

Ligand PTY B 200	
 Bond lengths	Bond angles
Torsions	Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	210/251 (83%)	0.25	13 (6%)	20	17	27, 56, 110, 123	0
1	C	186/251 (74%)	0.75	23 (12%)	4	2	41, 81, 131, 155	0
2	B	169/170 (99%)	-0.05	1 (0%)	89	89	25, 44, 80, 126	0
2	D	168/170 (98%)	0.15	5 (2%)	50	47	38, 61, 98, 147	0
All	All	733/842 (87%)	0.28	42 (5%)	23	20	25, 61, 116, 155	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	559	ILE	8.2
1	C	595	TYR	6.6
1	A	560	ALA	6.5
1	C	633	PHE	6.4
1	C	634	THR	5.7
1	C	607	LYS	5.4
1	A	561	ASN	5.3
1	C	565	LYS	4.7
1	A	562	SER	4.5
1	A	558	ASN	4.3
1	C	545	ASP	4.2
1	A	557	ILE	4.1
1	A	564	LEU	3.9
1	C	519	PHE	3.8
1	C	517	TYR	3.7
1	C	610	LYS	3.3
1	C	594	THR	3.2
1	C	611	ASN	3.2
1	C	637	HIS	3.1
1	C	606	ASN	3.1
1	A	532	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	105	PRO	3.0
1	C	639	ILE	3.0
2	D	106	GLU	3.0
2	D	108	SER	2.8
2	D	105	PRO	2.8
1	A	499	GLY	2.8
1	C	528	ASN	2.6
1	C	674	GLU	2.5
1	C	515	GLU	2.5
1	C	546	ASN	2.5
1	C	596	CYS	2.4
1	C	636	LYS	2.4
1	C	605	CYS	2.4
1	A	546	ASN	2.4
1	A	638	ASP	2.2
2	D	107	GLY	2.2
2	D	103	LEU	2.1
1	A	566	ASN	2.1
1	C	706	ILE	2.1
1	A	500	ASP	2.0
1	C	608	CYS	2.0

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

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

6.3 Carbohydrates (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	E	2	14/15	0.50	0.42	148,160,169,172	0
4	MAN	F	3	11/12	0.63	0.35	77,82,93,101	0
4	MAN	H	3	11/12	0.66	0.25	119,122,132,135	0
3	NAG	E	1	14/15	0.73	0.33	141,148,153,156	0
3	NAG	G	1	14/15	0.81	0.30	101,103,113,114	0
3	NAG	G	2	14/15	0.81	0.29	91,97,104,107	0
3	NAG	I	1	14/15	0.85	0.23	94,101,104,106	0

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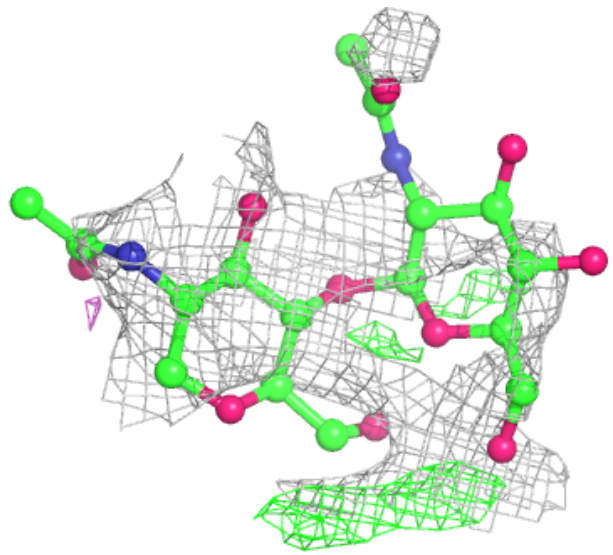
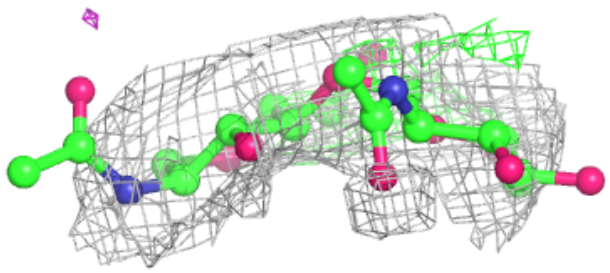
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	I	2	14/15	0.88	0.16	106,112,118,118	0
4	NAG	H	2	14/15	0.92	0.14	87,95,105,113	0
4	NAG	H	1	14/15	0.92	0.17	53,64,72,82	0
4	NAG	F	2	14/15	0.96	0.12	42,45,52,63	0
4	NAG	F	1	14/15	0.97	0.14	35,42,46,49	0

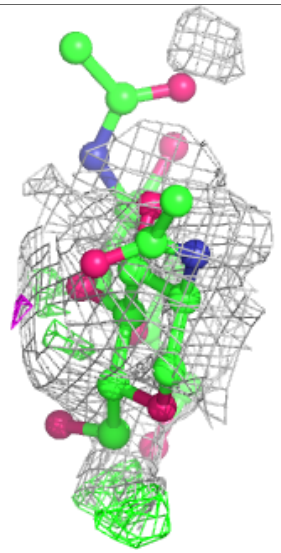
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

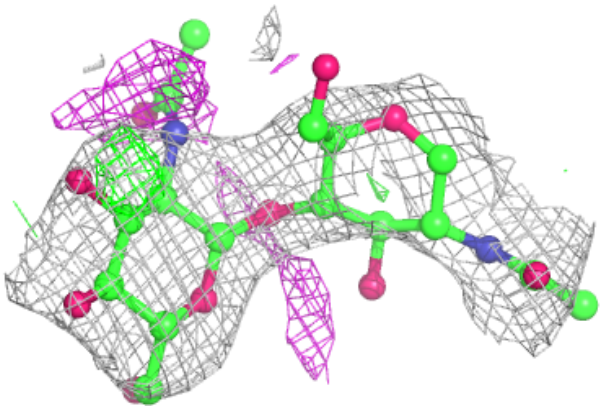


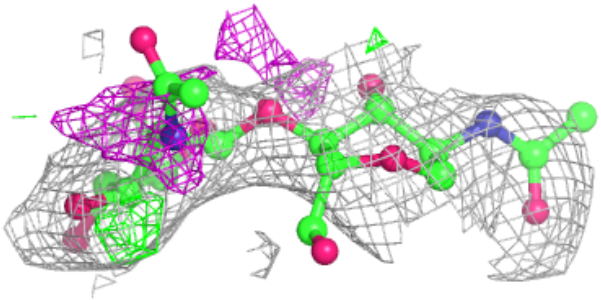


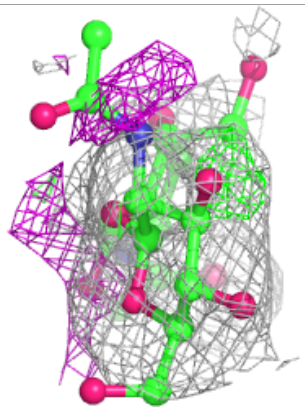


Electron density around Chain G:

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

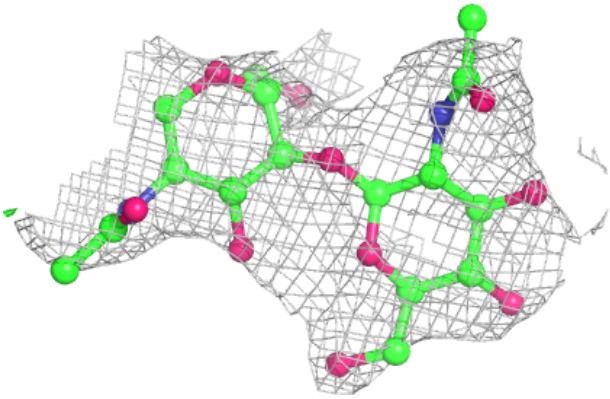


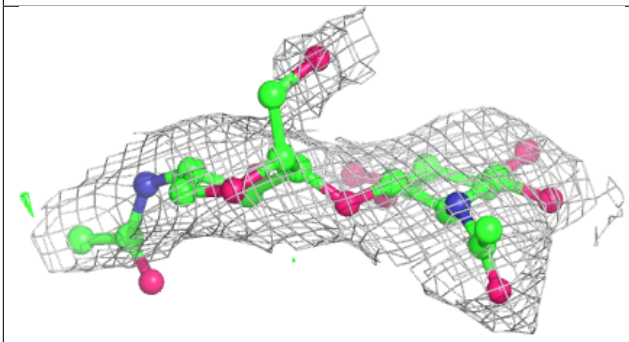


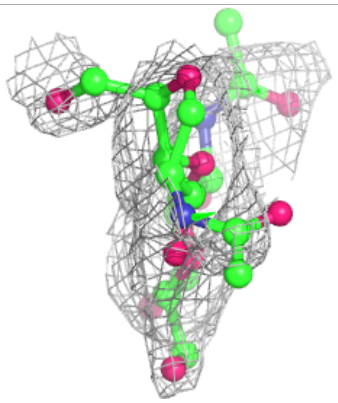


Electron density around Chain I:

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

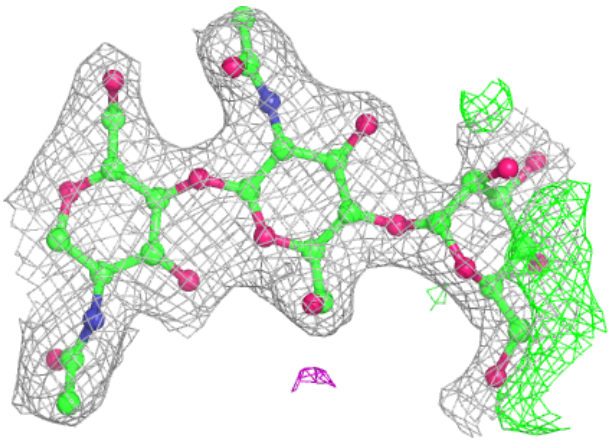


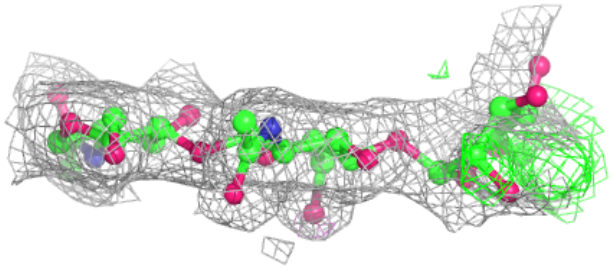


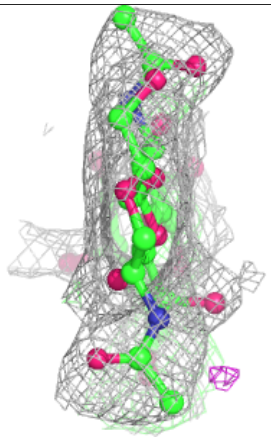


Electron density around Chain F:

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

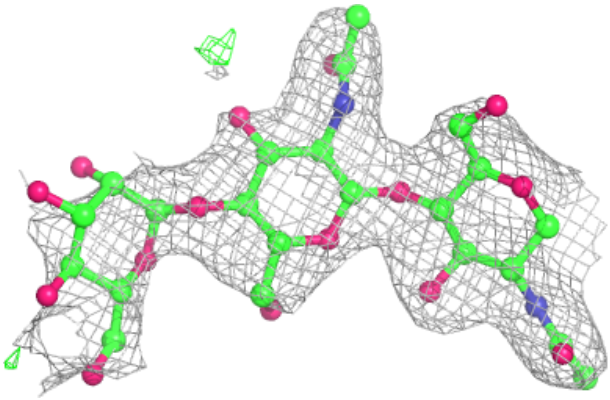


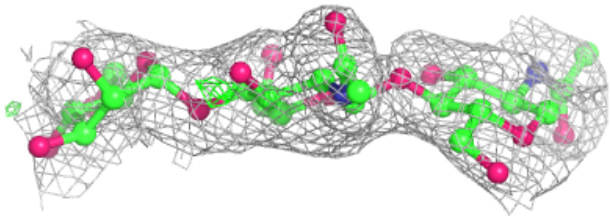


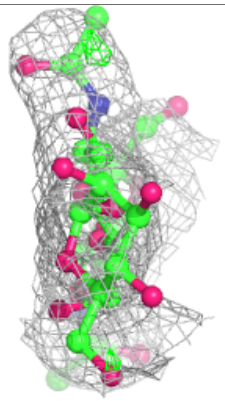


Electron density around Chain H:

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







6.4 Ligands (i)

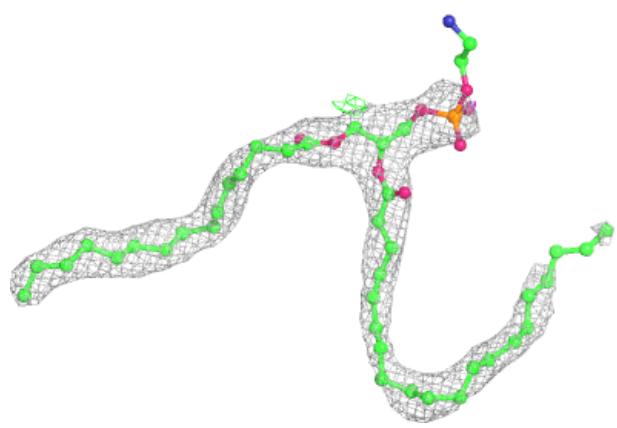
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

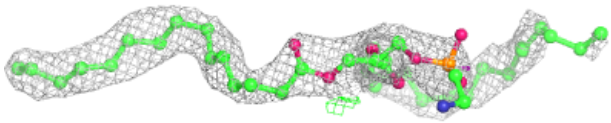
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	NAG	B	206	14/15	0.71	0.23	88,97,102,102	0
6	NAG	D	208	14/15	0.71	0.23	103,109,115,120	0
5	PTY	D	200	50/50	0.86	0.29	36,61,118,118	0
6	NAG	B	205	14/15	0.91	0.14	39,46,52,57	0
5	PTY	B	200	50/50	0.92	0.22	29,41,76,82	0

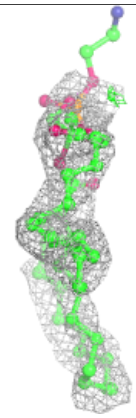
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PTY D 200:

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

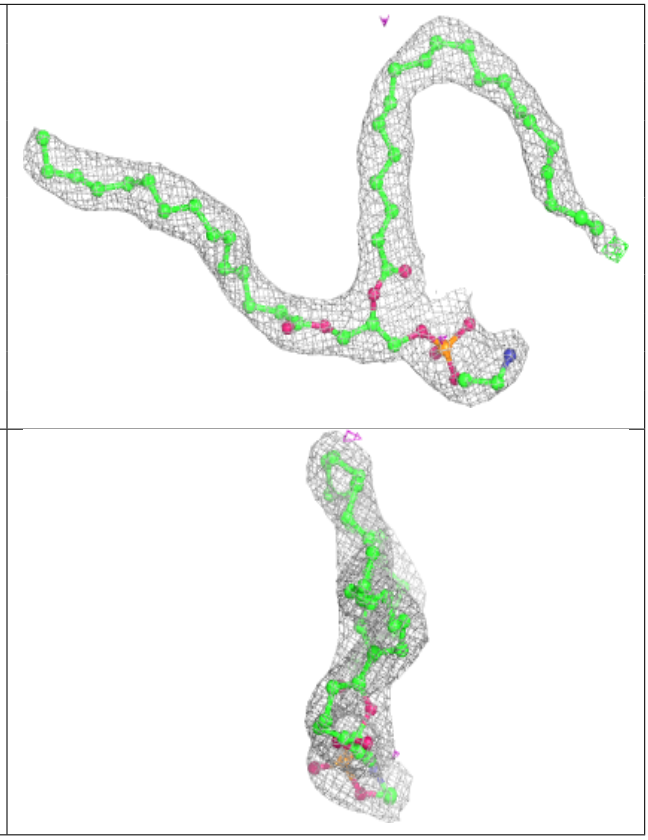






Electron density around PTY B 200:

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



6.5 Other polymers (i)

There are no such residues in this entry.