Full wwPDB X-ray Structure Validation Report ⓘ

Jan 11, 2021 – 05:08 PM GMT

PDB ID	:	6SNY
Title	:	Synthetic mimic of an EPCR-binding PfEMP1 bound to EPCR
Authors	:	Barber, N.M.; Higgins, M.K.
Deposited on	:	2019-08-27
Resolution	:	3.11 Å(reported)

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

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

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

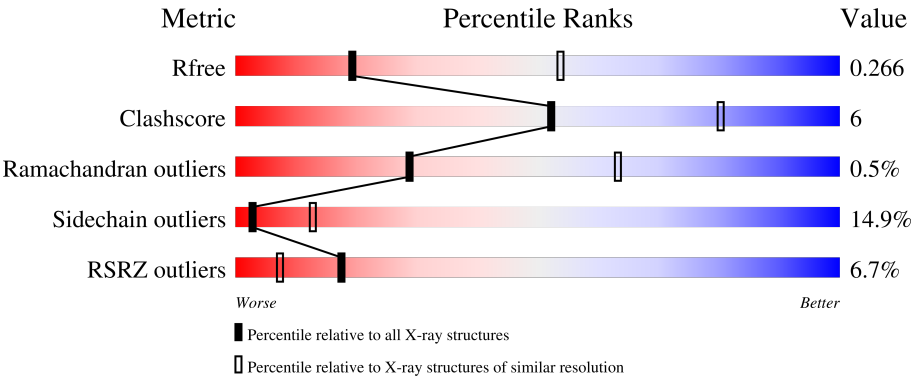
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.16
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.16

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 3.11 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	1292 (3.14-3.10)
Clashscore	141614	1389 (3.14-3.10)
Ramachandran outliers	138981	1337 (3.14-3.10)
Sidechain outliers	138945	1337 (3.14-3.10)
RSRZ outliers	127900	1260 (3.14-3.10)

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	124	15%, 53%, 30%, ·, 14%
2	B	193	2%, 70%, 16%, ·, 12%
2	C	193	4%, 70%, 16%, ·, 12%
3	D	3	33%, 67%
3	F	3	100%

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Mol	Chain	Length	Quality of chain
3	H	3	100%
4	E	2	100%
4	G	2	50% 50%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4015 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.

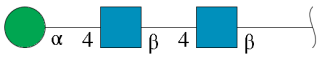
- Molecule 1 is a protein called Synthetic EPCR binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	107	Total	C	N	O	S	0	0	0
			946	584	170	190	2			

- Molecule 2 is a protein called Endothelial protein C receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	169	Total	C	N	O	S	0	0	0
			1384	884	246	250	4			
2	C	169	Total	C	N	O	S	0	0	0
			1384	884	246	250	4			

- Molecule 3 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.

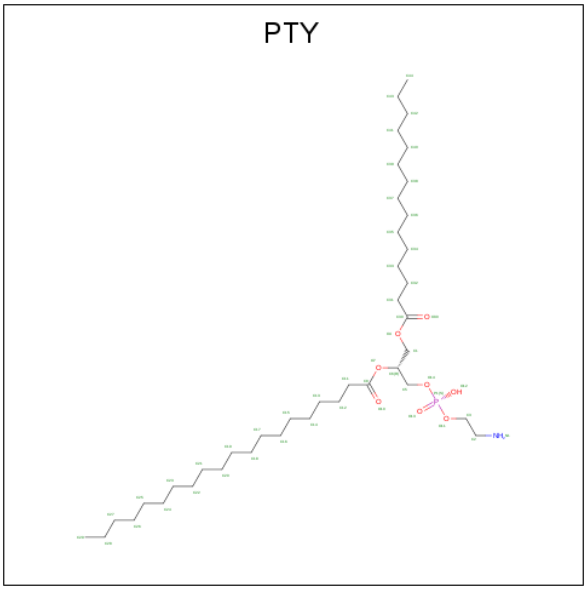


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	F	3	Total	C	N	O	13	0	0
			39	22	2	15			
3	H	3	Total	C	N	O	25	0	0
			39	22	2	15			

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

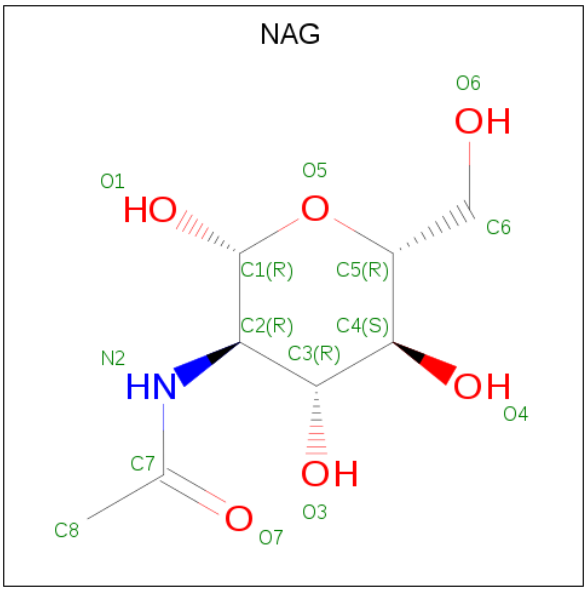
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	2	Total	C	N	O	28	0	0
			28	16	2	10			
4	G	2	Total	C	N	O	13	0	0
			28	16	2	10			

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



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

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



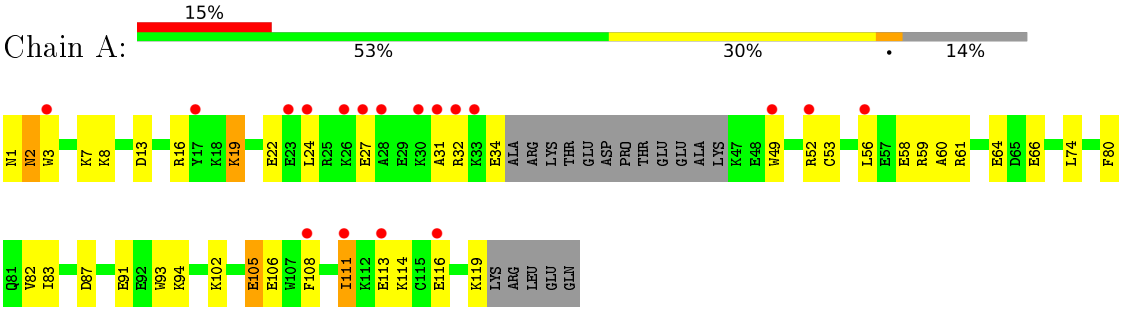
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total C N O 14 8 1 5	14	0
6	C	1	Total C N O 14 8 1 5	14	0

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.

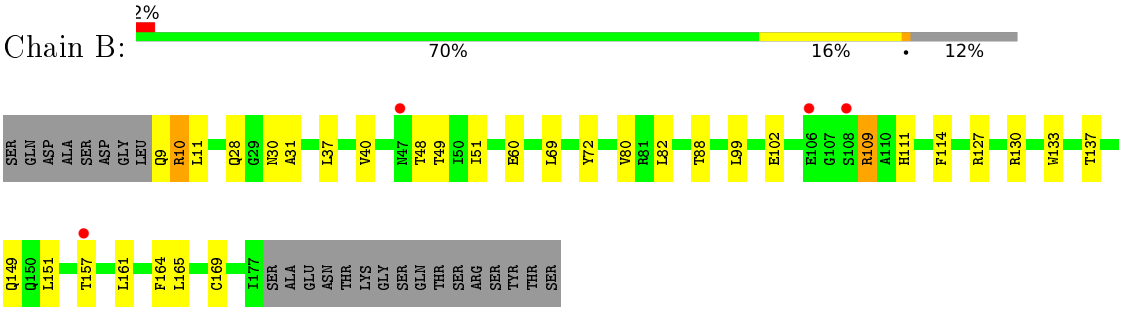
• Molecule 1: Synthetic EPCR binding protein

Chain A:



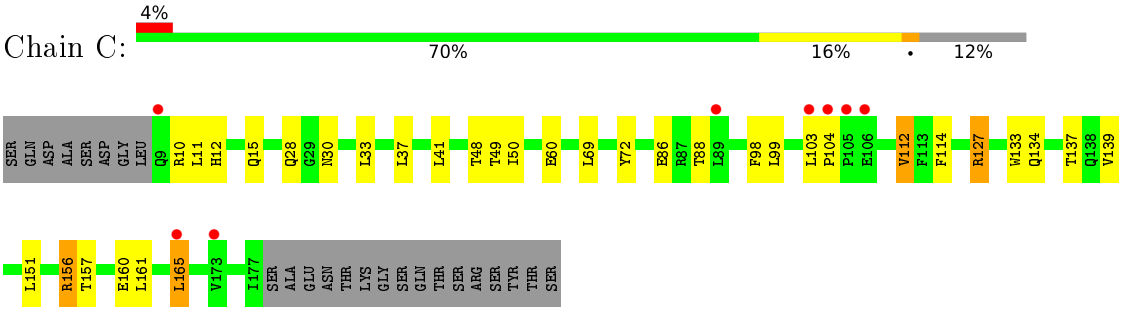
• Molecule 2: Endothelial protein C receptor

Chain B:



• Molecule 2: Endothelial protein C receptor

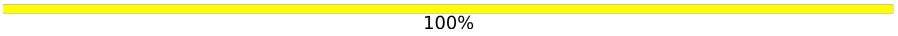
Chain C:



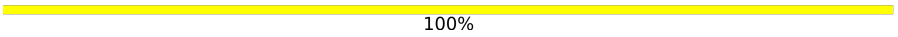
• Molecule 3: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:

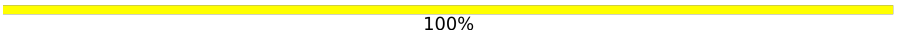
• Molecule 3: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F: 

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

Chain H: 

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

Chain E: 

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

Chain G: 

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	112.73Å 112.73Å 168.49Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.88 – 3.11 46.89 – 3.11	Depositor EDS
% Data completeness (in resolution range)	89.9 (46.88-3.11) 89.9 (46.89-3.11)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.60 (at 3.12Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.224 , 0.256 0.227 , 0.266	Depositor DCC
R_{free} test set	1025 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	105.3	Xtriage
Anisotropy	0.355	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 110.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.034 for -h,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	4015	wwPDB-VP
Average B, all atoms (Å^2)	128.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, PTY, 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	0.49	0/958	0.69	0/1267
2	B	0.55	0/1422	0.72	0/1936
2	C	0.59	0/1422	0.75	0/1936
All	All	0.55	0/3802	0.73	0/5139

There are no bond length outliers.

There are no bond angle outliers.

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	946	0	914	16	0
2	B	1384	0	1336	18	0
2	C	1384	0	1335	11	0
3	D	39	0	34	0	0
3	F	39	0	34	0	0
3	H	39	0	34	0	0
4	E	28	0	25	0	0
4	G	28	0	25	0	0
5	B	50	0	79	5	0
5	C	50	0	79	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	28	0	26	0	0
All	All	4015	0	3921	42	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 6.

All (42) 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:108:PHE:HA	1:A:111:ILE:HD12	1.54	0.89
2:B:151:LEU:HD23	2:B:157:THR:HG21	1.68	0.75
2:B:80:VAL:HG22	5:B:200:PTY:H421	1.74	0.69
2:B:169:CYS:HA	5:B:200:PTY:H291	1.77	0.66
1:A:3:TRP:CH2	1:A:7:LYS:HG2	2.37	0.59
1:A:113:GLU:O	1:A:116:GLU:HG2	2.02	0.59
1:A:82:VAL:HG11	1:A:93:TRP:HD1	1.72	0.55
1:A:3:TRP:CZ2	1:A:7:LYS:HG2	2.42	0.55
2:C:156:ARG:HA	2:C:160:GLU:HB2	1.90	0.53
1:A:24:LEU:HD21	1:A:59:ARG:HG2	1.90	0.53
2:C:15:GLN:NE2	2:C:72:TYR:HE1	2.07	0.52
2:B:151:LEU:CD2	2:B:157:THR:HG21	2.38	0.52
2:B:9:GLN:HG3	2:B:10:ARG:HG2	1.92	0.51
2:B:40:VAL:HG22	2:B:51:ILE:HG13	1.93	0.51
2:B:72:TYR:CD1	5:B:200:PTY:H112	2.46	0.50
2:C:41:LEU:HD12	2:C:50:ILE:HG12	1.95	0.49
1:A:60:ALA:HB1	1:A:111:ILE:HD13	1.94	0.49
2:B:102:GLU:OE1	2:B:111:HIS:HD2	1.96	0.48
2:B:127:ARG:HH11	2:C:127:ARG:HH12	1.64	0.46
2:B:133:TRP:CD1	2:B:151:LEU:HB3	2.51	0.46
2:C:30:ASN:HB2	2:C:37:LEU:HD11	1.96	0.46
2:B:30:ASN:HB2	2:B:37:LEU:HD11	1.98	0.46
1:A:108:PHE:HA	1:A:111:ILE:CD1	2.36	0.46
1:A:31:ALA:HB2	1:A:52:ARG:HH11	1.82	0.45
2:B:164:PHE:HB2	5:B:200:PTY:HC52	1.97	0.45
1:A:2:ASN:ND2	1:A:2:ASN:H	2.15	0.45
1:A:3:TRP:CE2	1:A:82:VAL:HG23	2.52	0.44
2:B:130:ARG:CZ	2:C:98:PHE:HE2	2.31	0.44
2:B:109:ARG:HE	2:B:109:ARG:HB3	1.61	0.43
2:C:112:VAL:CG1	2:C:165:LEU:HB3	2.49	0.43
1:A:64:GLU:OE1	1:A:105:GLU:HA	2.19	0.42
2:B:151:LEU:HA	2:B:157:THR:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:LYS:HA	1:A:22:GLU:HG2	2.01	0.42
2:C:15:GLN:NE2	2:C:72:TYR:CE1	2.88	0.41
1:A:2:ASN:HD22	1:A:2:ASN:H	1.68	0.41
1:A:80:PHE:HA	1:A:83:ILE:HG12	2.03	0.41
2:B:31:ALA:HB2	5:B:200:PTY:H201	2.02	0.41
2:C:133:TRP:CD1	2:C:151:LEU:HB3	2.55	0.41
1:A:49:TRP:HE3	1:A:52:ARG:HD2	1.86	0.41
2:C:103:LEU:HA	2:C:104:PRO:HD3	1.98	0.40
2:B:40:VAL:CG2	2:B:51:ILE:HG13	2.52	0.40
2:B:127:ARG:NH1	2:C:127:ARG:HH12	2.19	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	103/124 (83%)	100 (97%)	3 (3%)	0	100	100
2	B	167/193 (86%)	160 (96%)	6 (4%)	1 (1%)	25	59
2	C	167/193 (86%)	161 (96%)	5 (3%)	1 (1%)	25	59
All	All	437/510 (86%)	421 (96%)	14 (3%)	2 (0%)	29	63

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	88	THR
2	C	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	100/115 (87%)	76 (76%)	24 (24%)	0 2
2	B	151/171 (88%)	136 (90%)	15 (10%)	8 28
2	C	151/171 (88%)	130 (86%)	21 (14%)	3 15
All	All	402/457 (88%)	342 (85%)	60 (15%)	3 13

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	ASN
1	A	2	ASN
1	A	8	LYS
1	A	13	ASP
1	A	16	ARG
1	A	19	LYS
1	A	27	GLU
1	A	32	ARG
1	A	34	GLU
1	A	53	CYS
1	A	56	LEU
1	A	58	GLU
1	A	61	ARG
1	A	66	GLU
1	A	74	LEU
1	A	87	ASP
1	A	91	GLU
1	A	94	LYS
1	A	102	LYS
1	A	105	GLU
1	A	106	GLU
1	A	111	ILE
1	A	114	LYS
1	A	119	LYS
2	B	10	ARG
2	B	11	LEU

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Mol	Chain	Res	Type
2	B	28	GLN
2	B	48	THR
2	B	49	THR
2	B	60	GLU
2	B	69	LEU
2	B	82	LEU
2	B	99	LEU
2	B	109	ARG
2	B	114	PHE
2	B	137	THR
2	B	149	GLN
2	B	161	LEU
2	B	165	LEU
2	C	10	ARG
2	C	11	LEU
2	C	12	HIS
2	C	28	GLN
2	C	33	LEU
2	C	48	THR
2	C	49	THR
2	C	60	GLU
2	C	69	LEU
2	C	86	GLU
2	C	99	LEU
2	C	112	VAL
2	C	114	PHE
2	C	127	ARG
2	C	134	GLN
2	C	137	THR
2	C	139	VAL
2	C	156	ARG
2	C	157	THR
2	C	161	LEU
2	C	165	LEU

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

Mol	Chain	Res	Type
1	A	2	ASN
2	B	15	GLN
2	B	57	GLN
2	B	111	HIS

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Mol	Chain	Res	Type
2	B	150	GLN
2	C	15	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)

13 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	D	1	3,2	14,14,15	0.42	0	17,19,21	0.82	0
3	NAG	D	2	3	14,14,15	0.36	0	17,19,21	0.80	1 (5%)
3	MAN	D	3	3	11,11,12	0.51	0	15,15,17	1.18	1 (6%)
4	NAG	E	1	2,4	14,14,15	0.47	0	17,19,21	1.30	1 (5%)
4	NAG	E	2	4	14,14,15	0.33	0	17,19,21	1.52	3 (17%)
3	NAG	F	1	3,2	14,14,15	0.27	0	17,19,21	0.84	1 (5%)
3	NAG	F	2	3	14,14,15	0.38	0	17,19,21	1.36	2 (11%)
3	MAN	F	3	3	11,11,12	0.53	0	15,15,17	1.61	2 (13%)
4	NAG	G	1	2,4	14,14,15	0.34	0	17,19,21	0.78	0
4	NAG	G	2	4	14,14,15	0.46	0	17,19,21	1.09	1 (5%)
3	NAG	H	1	3,2	14,14,15	0.36	0	17,19,21	1.06	2 (11%)
3	NAG	H	2	3	14,14,15	0.31	0	17,19,21	0.75	1 (5%)
3	MAN	H	3	3	11,11,12	0.39	0	15,15,17	0.97	1 (6%)

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	D	1	3,2	-	3/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
3	MAN	D	3	3	-	2/2/19/22	1/1/1/1
4	NAG	E	1	2,4	-	1/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1
3	NAG	F	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	MAN	F	3	3	-	1/2/19/22	0/1/1/1
4	NAG	G	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	0/6/23/26	0/1/1/1
3	NAG	H	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	H	2	3	-	0/6/23/26	0/1/1/1
3	MAN	H	3	3	-	1/2/19/22	1/1/1/1

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	2	NAG	O5-C1-C2	4.87	118.98	111.29
3	F	2	NAG	O5-C1-C2	-4.66	103.93	111.29
3	D	3	MAN	C1-O5-C5	4.19	117.86	112.19
4	G	2	NAG	C1-O5-C5	4.12	117.78	112.19
3	F	3	MAN	C1-C2-C3	4.11	114.71	109.67
3	F	3	MAN	C1-O5-C5	3.96	117.56	112.19
4	E	1	NAG	C3-C4-C5	3.91	117.21	110.24
3	H	3	MAN	C1-O5-C5	3.49	116.92	112.19
3	H	1	NAG	C1-O5-C5	3.18	116.51	112.19
4	E	2	NAG	C1-O5-C5	3.11	116.41	112.19
3	D	2	NAG	C1-O5-C5	2.67	115.81	112.19
3	H	1	NAG	C1-C2-N2	-2.39	106.41	110.49
3	F	2	NAG	C1-O5-C5	2.31	115.33	112.19
3	F	1	NAG	C1-O5-C5	2.06	114.99	112.19
3	H	2	NAG	O5-C1-C2	-2.05	108.06	111.29
4	E	2	NAG	C2-N2-C7	2.03	125.79	122.90

There are no chirality outliers.

All (18) torsion outliers are listed below:

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

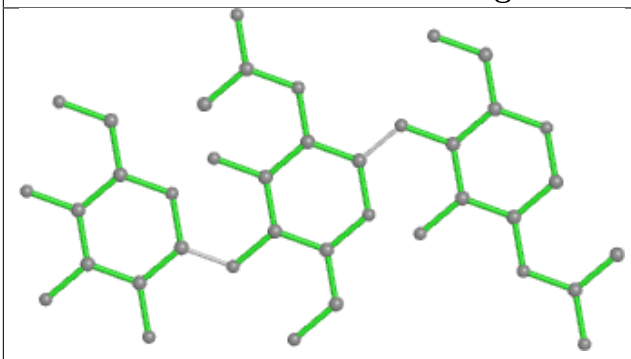
All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	3	MAN	C1-C2-C3-C4-C5-O5
3	H	3	MAN	C1-C2-C3-C4-C5-O5

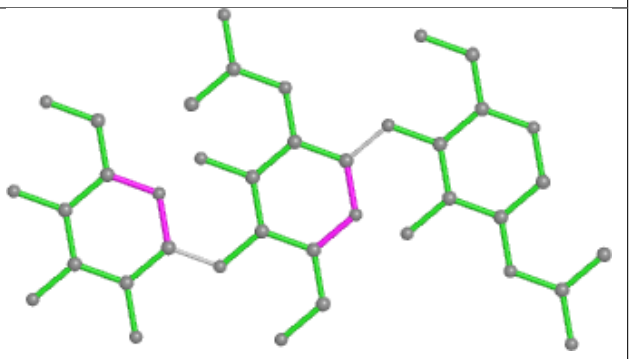
No monomer is involved in short contacts.

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

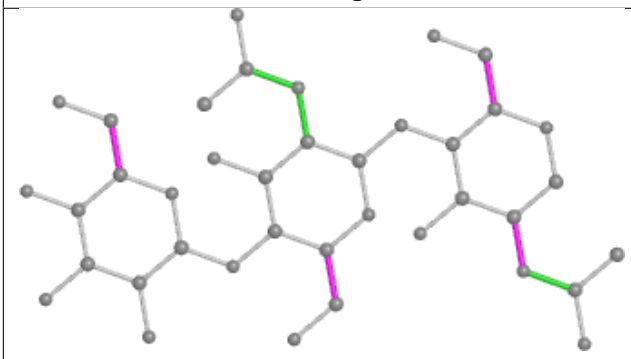
Oligosaccharide Chain D



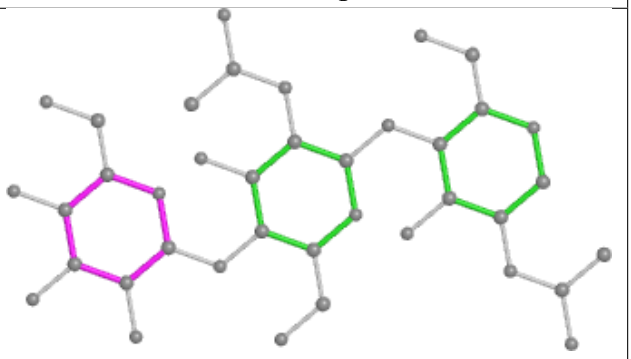
Bond lengths



Bond angles

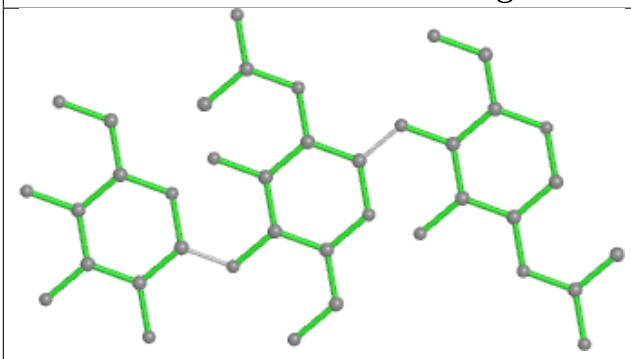


Torsions

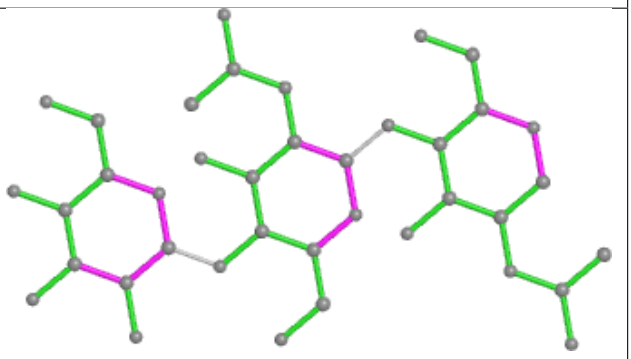


Rings

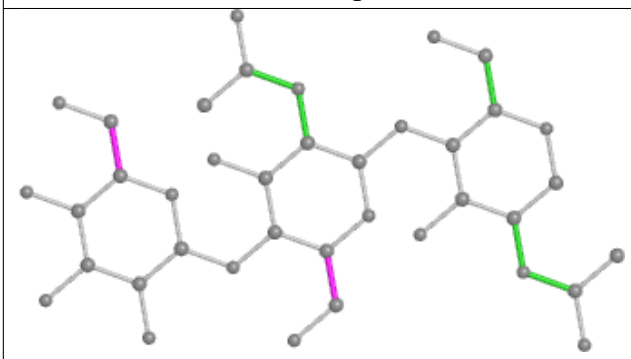
Oligosaccharide Chain F



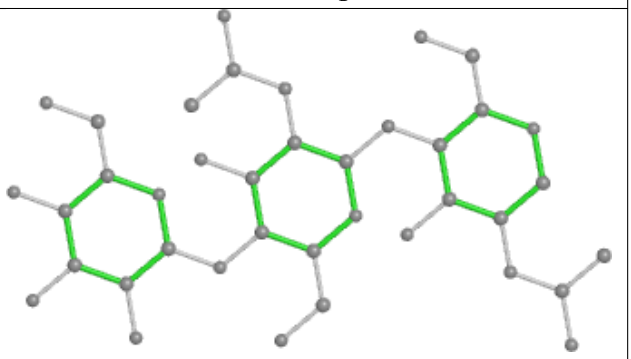
Bond lengths



Bond angles

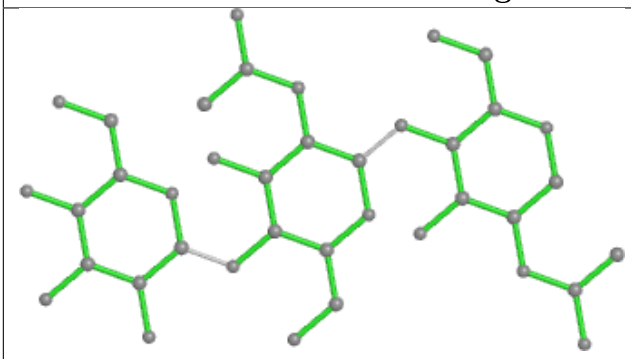


Torsions

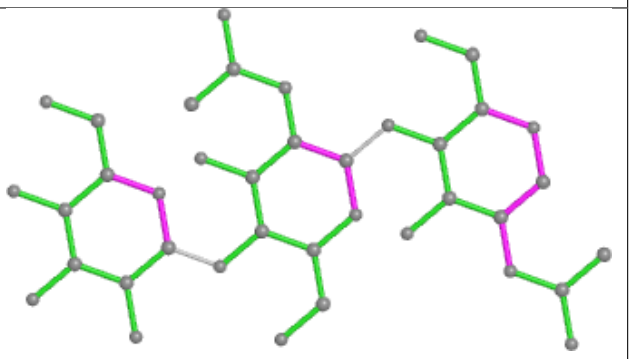


Rings

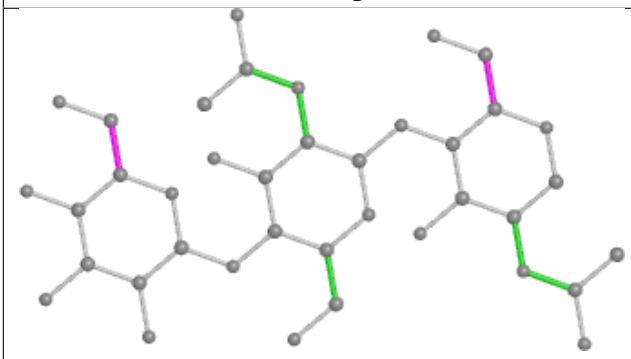
Oligosaccharide Chain H



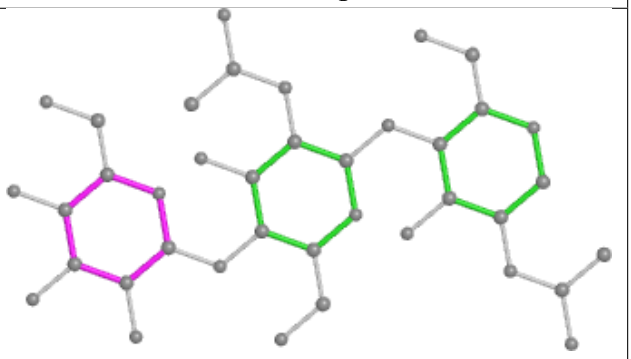
Bond lengths



Bond angles

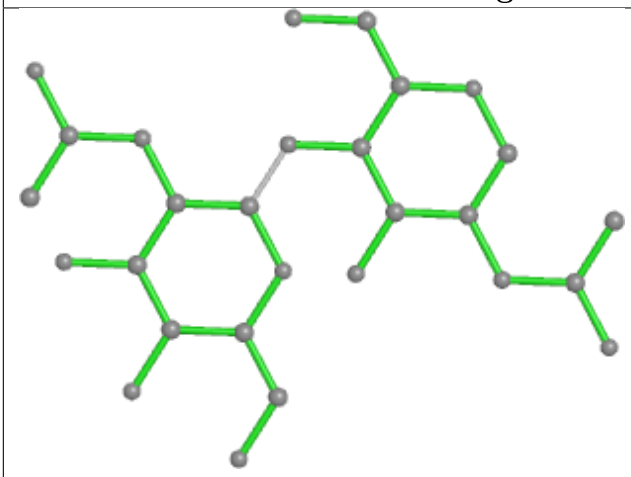


Torsions

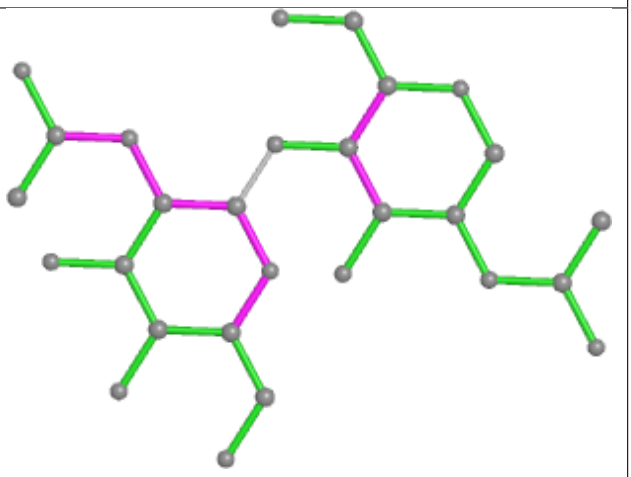


Rings

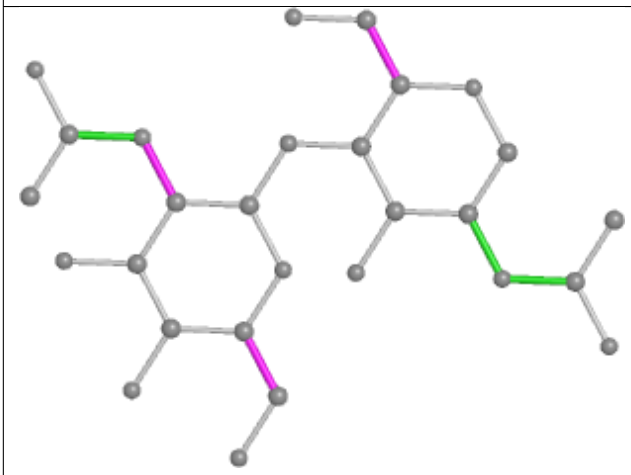
Oligosaccharide Chain E



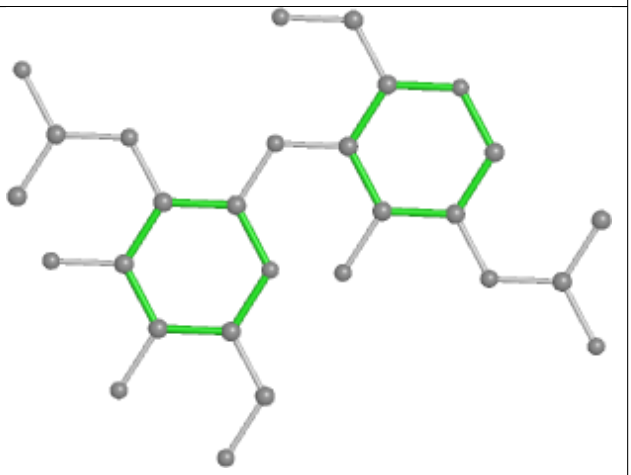
Bond lengths



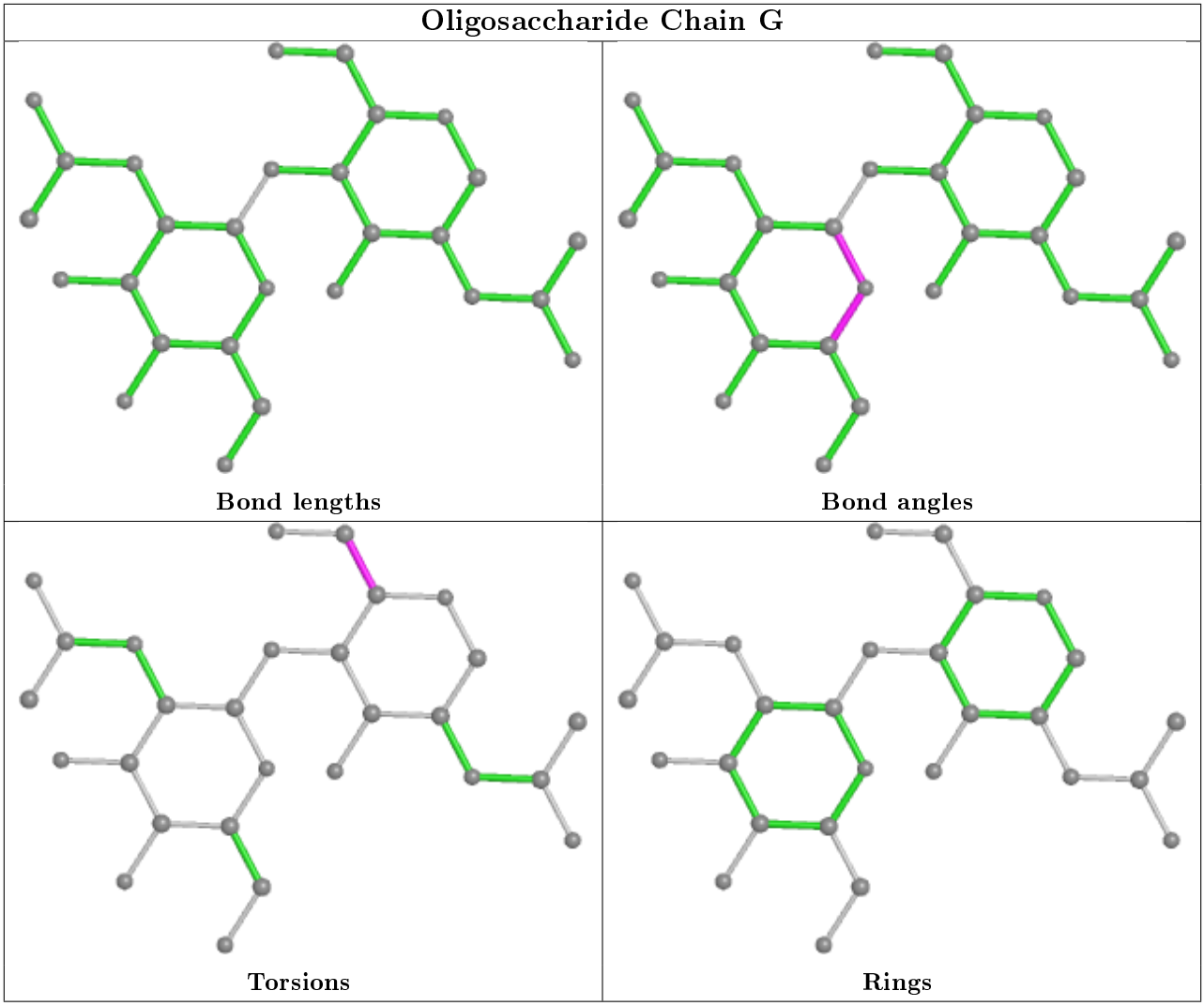
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

4 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	$\#\|Z\| > 2$
6	NAG	C	208	2	14,14,15	0.28	0	17,19,21	0.57	0
5	PTY	B	200	-	49,49,49	0.47	0	52,54,54	0.58	1 (1%)
6	NAG	C	204	2	14,14,15	0.42	0	17,19,21	1.45	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	PTY	C	201	-	49,49,49	0.32	0	52,54,54	0.46	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
6	NAG	C	208	2	-	0/6/23/26	0/1/1/1
5	PTY	B	200	-	-	24/53/53/53	-
6	NAG	C	204	2	-	1/6/23/26	0/1/1/1
5	PTY	C	201	-	-	36/53/53/53	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	204	NAG	C1-O5-C5	5.12	119.12	112.19
5	B	200	PTY	O11-P1-O13	2.65	119.41	109.07
6	C	204	NAG	O5-C1-C2	2.64	115.45	111.29

There are no chirality outliers.

All (61) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	200	PTY	N1-C2-C3-O11
5	C	201	PTY	N1-C2-C3-O11
5	C	201	PTY	C11-C8-O7-C6
5	C	201	PTY	C5-O14-P1-O12
5	C	201	PTY	C5-O14-P1-O13
5	C	201	PTY	O10-C8-O7-C6
5	C	201	PTY	C31-C30-O4-C1
5	C	201	PTY	O30-C30-O4-C1
5	C	201	PTY	C8-C11-C12-C13
5	C	201	PTY	C5-O14-P1-O11
5	C	201	PTY	C24-C25-C26-C27
5	B	200	PTY	C8-C11-C12-C13
5	B	200	PTY	C16-C17-C18-C19
5	B	200	PTY	C38-C39-C40-C41
5	C	201	PTY	C33-C34-C35-C36
5	B	200	PTY	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
5	C	201	PTY	C25-C26-C27-C28
5	B	200	PTY	C15-C16-C17-C18
5	C	201	PTY	C14-C15-C16-C17
5	C	201	PTY	C37-C38-C39-C40
5	C	201	PTY	C13-C14-C15-C16
5	B	200	PTY	C31-C32-C33-C34
5	C	201	PTY	C20-C21-C22-C23
5	C	201	PTY	C11-C12-C13-C14
5	C	201	PTY	C22-C23-C24-C25
5	B	200	PTY	C14-C15-C16-C17
5	B	200	PTY	C37-C38-C39-C40
5	C	201	PTY	C16-C17-C18-C19
5	C	201	PTY	C35-C36-C37-C38
5	B	200	PTY	C39-C40-C41-C42
5	C	201	PTY	C34-C35-C36-C37
5	B	200	PTY	C19-C20-C21-C22
5	C	201	PTY	C31-C32-C33-C34
5	B	200	PTY	O14-C5-C6-C1
5	C	201	PTY	O14-C5-C6-C1
5	C	201	PTY	C39-C40-C41-C42
6	C	204	NAG	O5-C5-C6-O6
5	B	200	PTY	C24-C25-C26-C27
5	B	200	PTY	C11-C12-C13-C14
5	C	201	PTY	C19-C20-C21-C22
5	C	201	PTY	C36-C37-C38-C39
5	C	201	PTY	C6-C5-O14-P1
5	B	200	PTY	O10-C8-O7-C6
5	C	201	PTY	C17-C18-C19-C20
5	C	201	PTY	C12-C13-C14-C15
5	B	200	PTY	C36-C37-C38-C39
5	C	201	PTY	O14-C5-C6-O7
5	C	201	PTY	C15-C16-C17-C18
5	B	200	PTY	C11-C8-O7-C6
5	B	200	PTY	C23-C24-C25-C26
5	B	200	PTY	C40-C41-C42-C43
5	B	200	PTY	O14-C5-C6-O7
5	B	200	PTY	C3-O11-P1-O14
5	C	201	PTY	C3-O11-P1-O14
5	B	200	PTY	O4-C1-C6-C5
5	B	200	PTY	O4-C1-C6-O7
5	B	200	PTY	C20-C21-C22-C23
5	C	201	PTY	C26-C27-C28-C29

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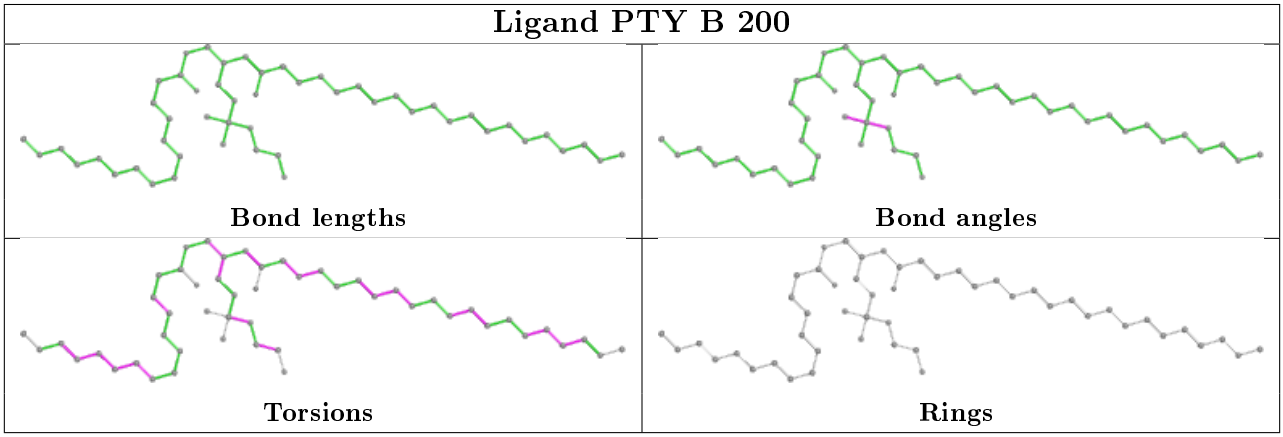
Mol	Chain	Res	Type	Atoms
5	C	201	PTY	C18-C19-C20-C21
5	C	201	PTY	C12-C11-C8-O7
5	C	201	PTY	C12-C11-C8-O10

There are no ring outliers.

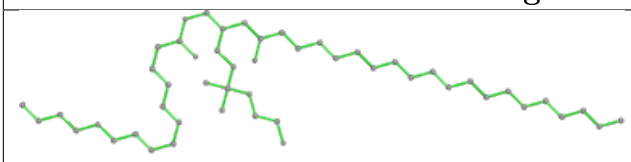
1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	200	PTY	5	0

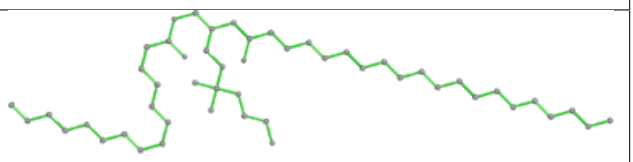
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



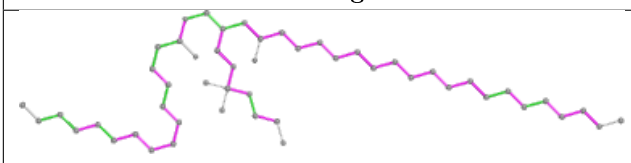
Ligand PTY C 201



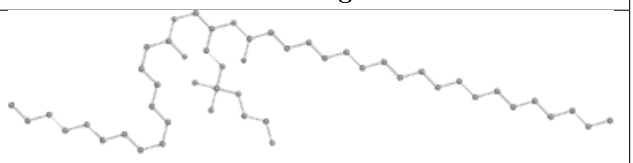
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	107/124 (86%)	0.87	18 (16%) 1 1	98, 162, 222, 239	0
2	B	169/193 (87%)	0.26	4 (2%) 59 37	73, 111, 156, 206	0
2	C	169/193 (87%)	0.45	8 (4%) 31 14	73, 113, 173, 232	0
All	All	445/510 (87%)	0.48	30 (6%) 17 7	73, 118, 202, 239	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	105	PRO	6.8
1	A	27	GLU	4.8
1	A	113	GLU	4.6
1	A	28	ALA	4.0
1	A	49	TRP	3.8
1	A	26	LYS	3.6
2	C	104	PRO	3.2
1	A	30	LYS	3.1
2	B	106	GLU	3.1
2	C	106	GLU	3.0
1	A	33	LYS	2.9
1	A	116	GLU	2.8
1	A	23	GLU	2.7
2	C	165	LEU	2.6
2	C	9	GLN	2.5
1	A	111	ILE	2.5
1	A	17	TYR	2.4
2	C	103	LEU	2.4
2	B	47	ASN	2.4
1	A	24	LEU	2.4
2	C	89	LEU	2.3
1	A	31	ALA	2.3
1	A	108	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	52	ARG	2.2
2	C	173	VAL	2.1
2	B	157	THR	2.1
1	A	56	LEU	2.1
1	A	32	ARG	2.1
1	A	3	TRP	2.0
2	B	108	SER	2.0

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

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

6.3 Carbohydrates (i)

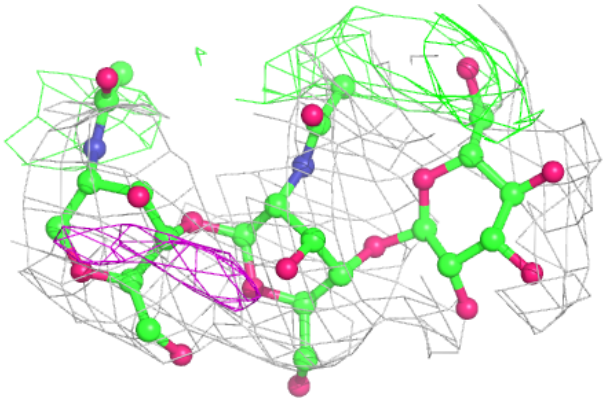
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

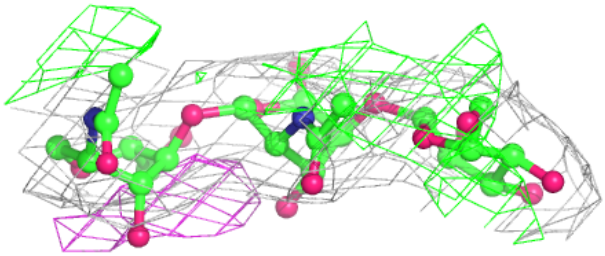
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	E	1	14/15	-	-	80,83,85,87	14
4	NAG	G	2	14/15	0.78	0.22	160,175,183,184	0
3	MAN	H	3	11/12	-	-	180,187,193,194	11
4	NAG	E	2	14/15	-	-	82,86,93,97	14
3	NAG	F	1	14/15	-0.07	0.39	144,150,164,166	13
4	NAG	G	1	14/15	0.39	0.33	126,138,147,159	13
3	MAN	D	3	11/12	0.68	0.18	211,219,223,229	0
3	MAN	F	3	11/12	0.73	0.23	211,221,230,235	0
3	NAG	D	1	14/15	0.79	0.32	158,174,189,190	0
3	NAG	F	2	14/15	0.83	0.28	175,184,198,207	0
3	NAG	D	2	14/15	0.85	0.24	187,196,203,204	0
3	NAG	H	1	14/15	0.92	0.21	123,138,152,152	0
3	NAG	H	2	14/15	-	-	155,160,171,177	14

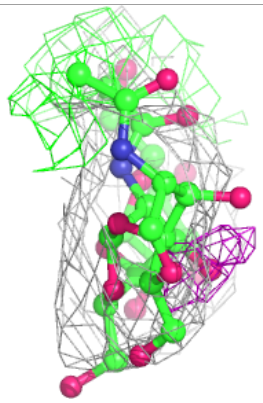
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain D:

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

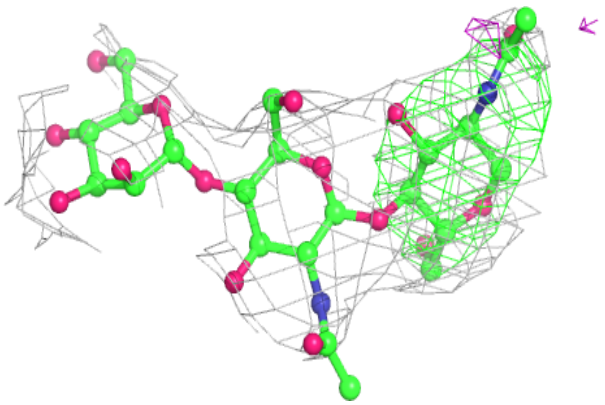


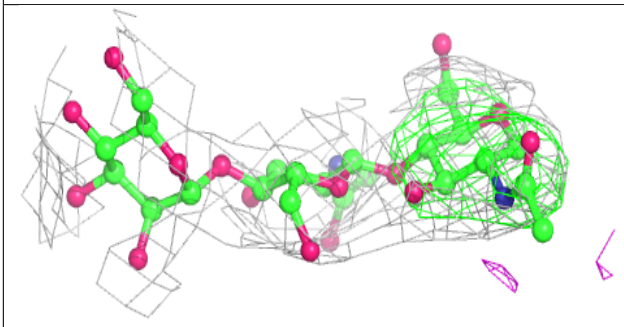


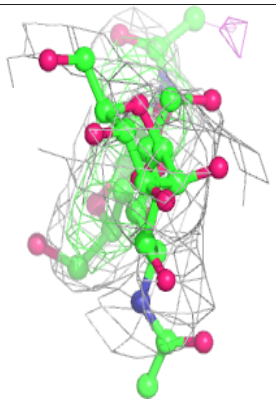


Electron density around Chain F:

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

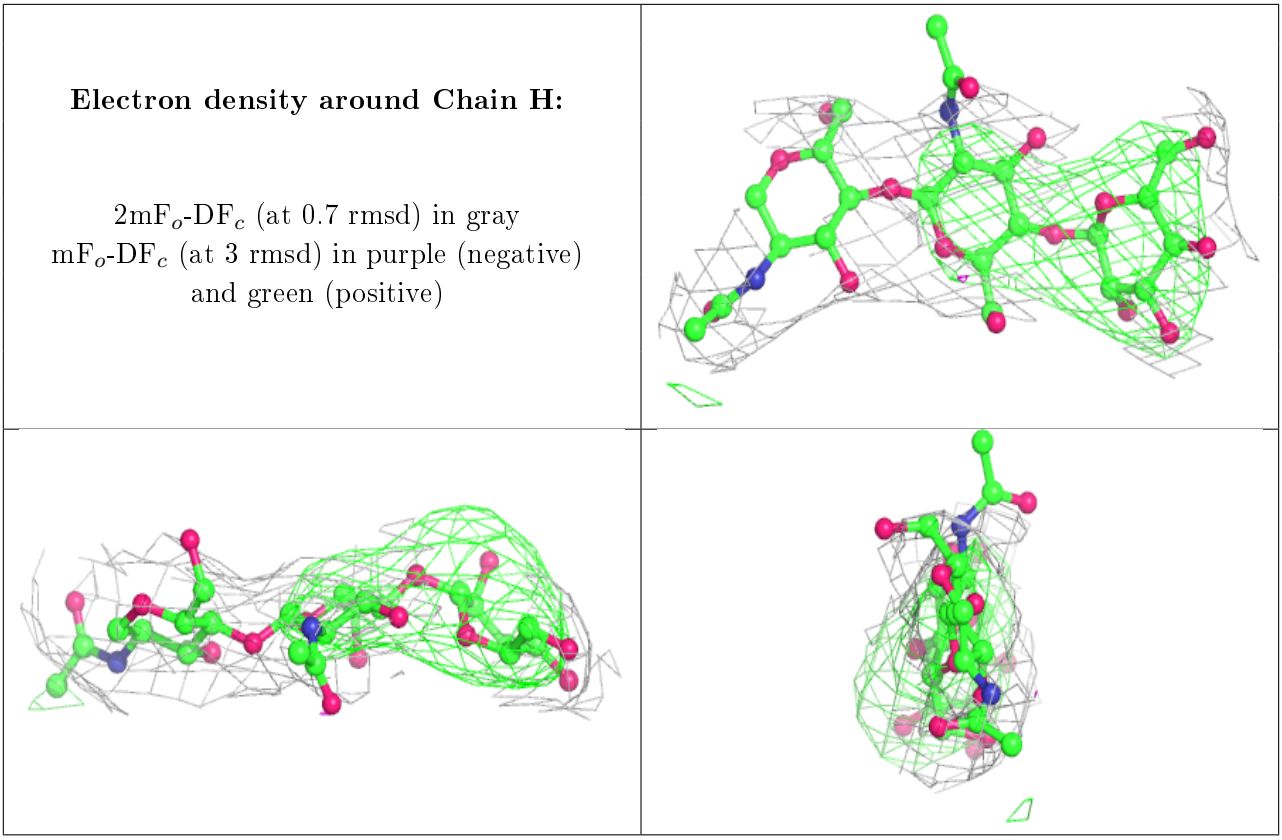






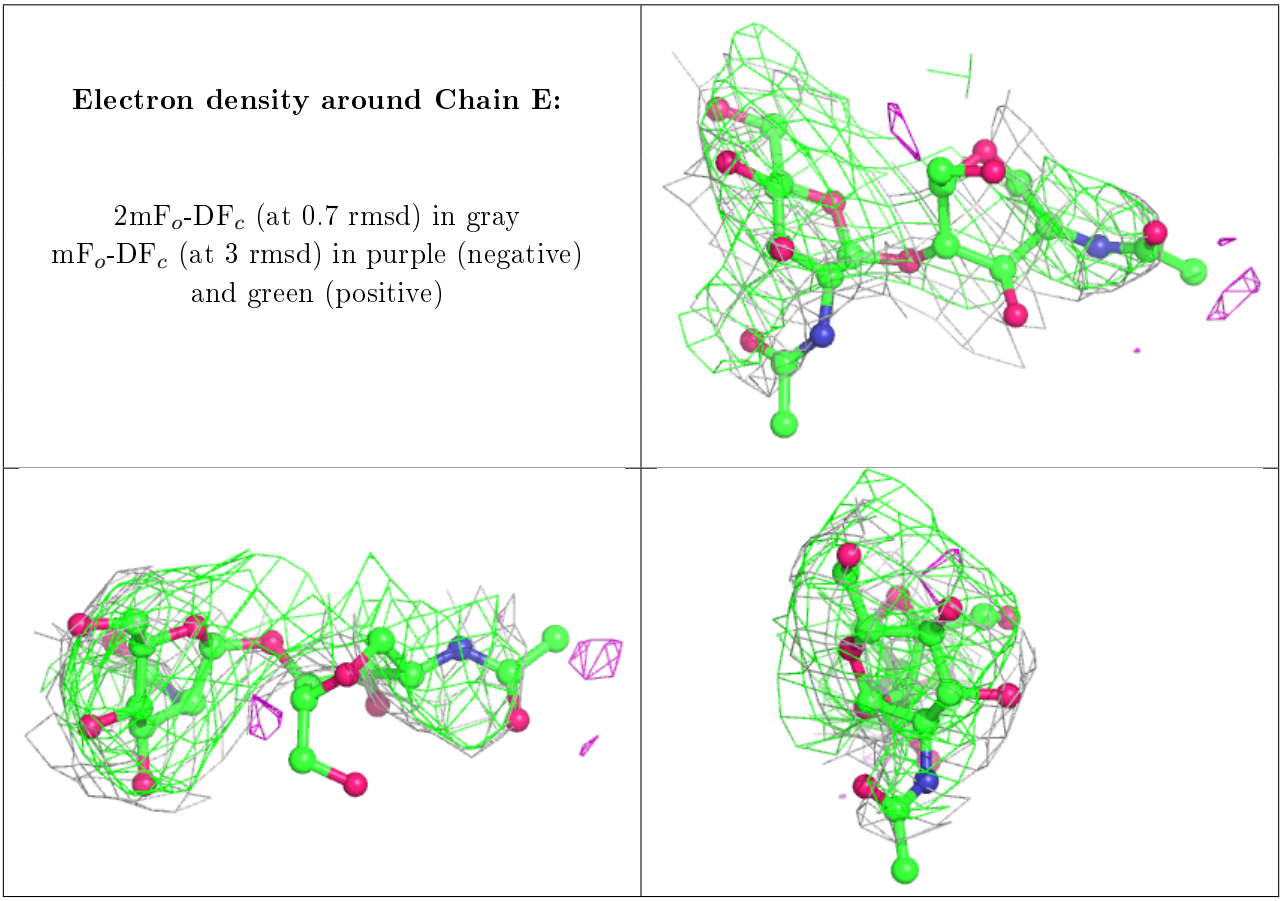
Electron density around Chain H:

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



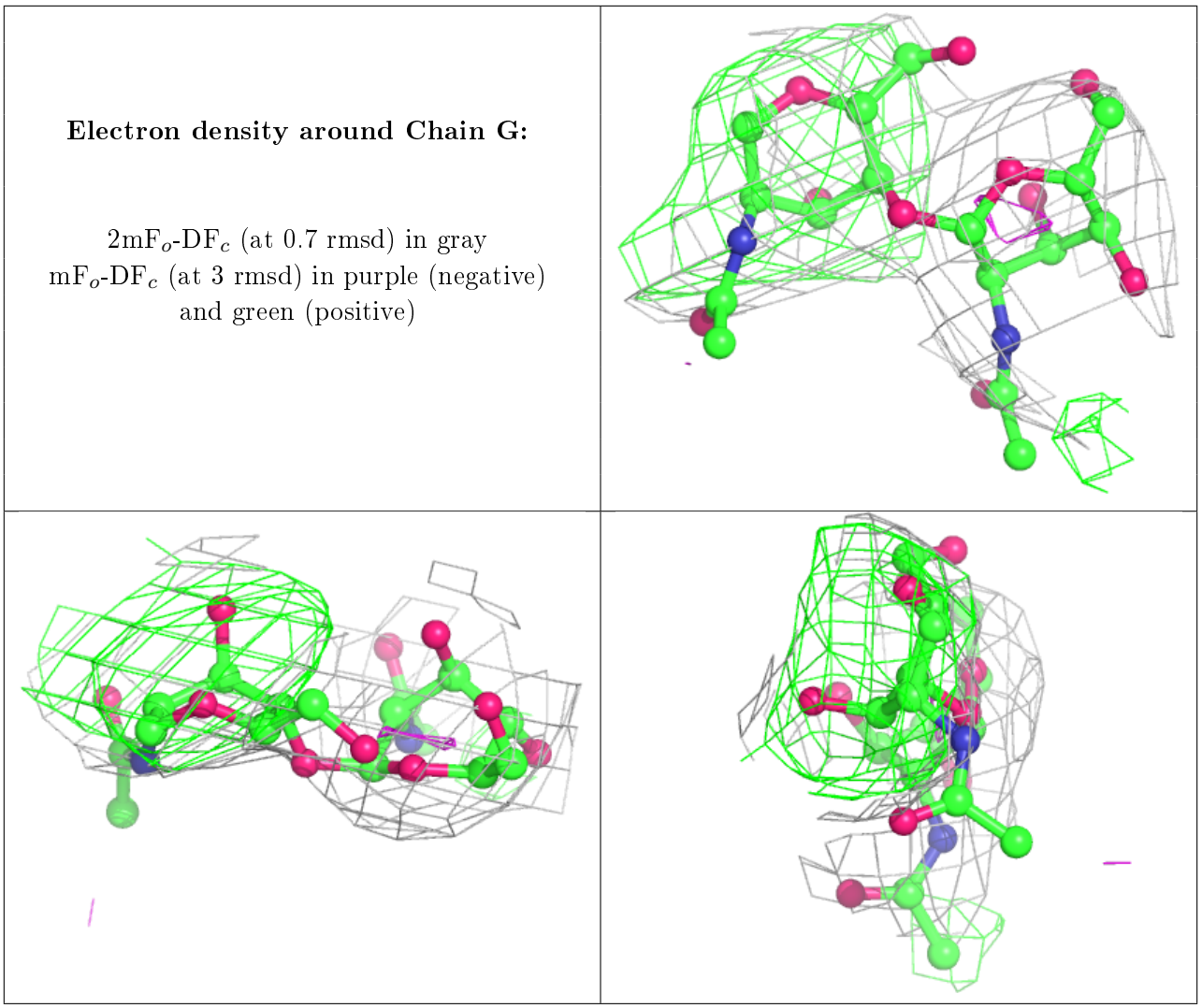
Electron density around Chain E:

$2mF_o$-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)



6.4 Ligands

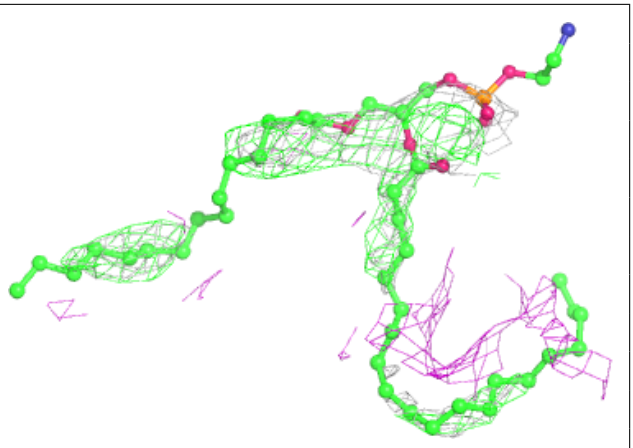
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

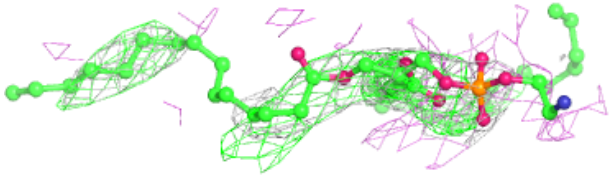
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	PTY	C	201	50/50	-	-	16,20,28,29	50
6	NAG	C	204	14/15	-	-	112,117,121,122	14
5	PTY	B	200	50/50	0.88	0.62	86,94,134,137	0
6	NAG	C	208	14/15	-	-	129,135,143,146	14

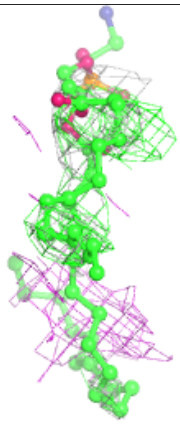
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PTY C 201:

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

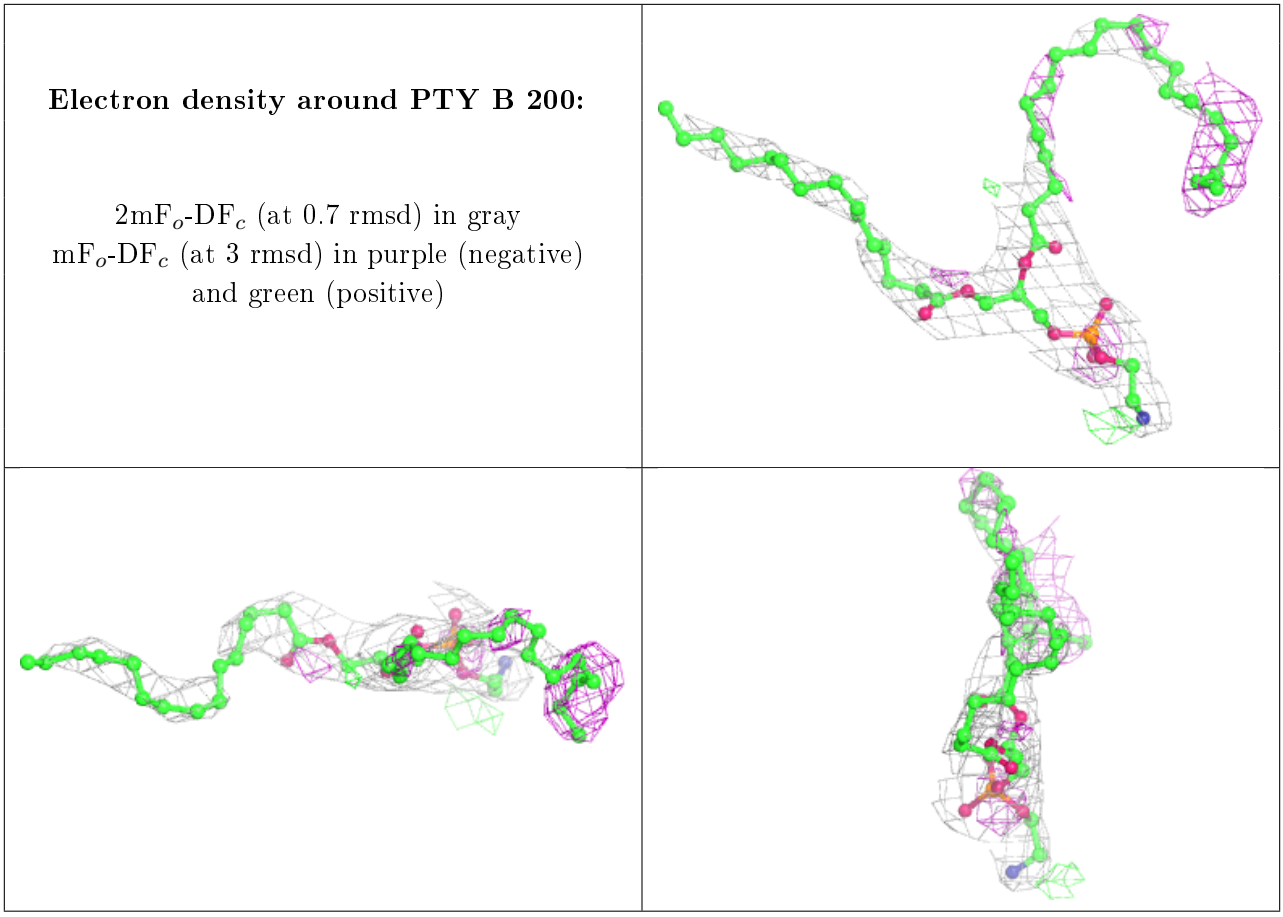






Electron density around PTY B 200:

$2mF_o$-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

There are no such residues in this entry.