Full wwPDB X-ray Structure Validation Report ⓘ

Nov 13, 2023 – 03:16 PM JST

PDB ID	:	5XF1
Title	:	Structure of the Full-length glucagon class B G protein-coupled receptor
Authors	:	Zhang, H.; Qiao, A.; Yang, D.; Yang, L.; Dai, A.; de Graaf, C.; Reedtz-Runge, S.; Dharmarajan, V.; Zhang, H.; Han, G.W.; Grant, T.; Sierra, R.; Weierstall, U.; Nelson, G.; Liu, W.; Wu, Y.; Ma, L.; Cai, X.; Lin, G.; Wu, X.; Geng, Z.; Dong, Y.; Song, G.; Griffin, P.; Lau, J.; Cherezov, V.; Yang, H.; Hanson, M.; Stevens, R.; Jiang, H.; Wang, M.; Zhao, Q.; Wu, B.
Deposited on	:	2017-04-06
Resolution	:	3.19 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:

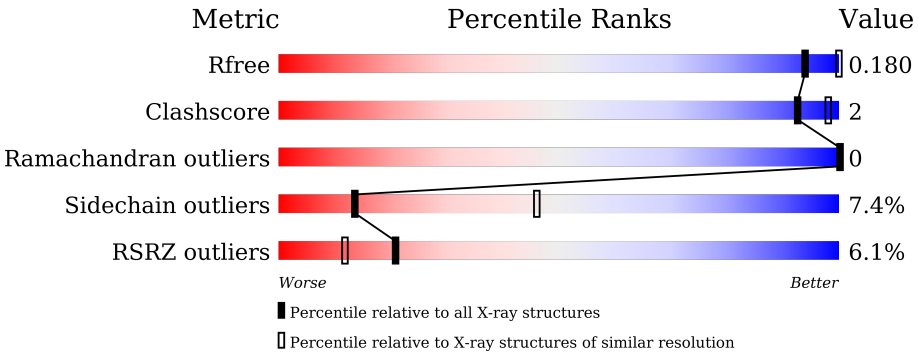
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)

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 3.19 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	574	8% 88% 7% 5%
1	B	574	11% 80% 5% 14%
2	C	231	% 91% 9%
2	H	231	% 82% 16%

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

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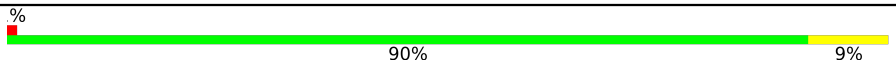
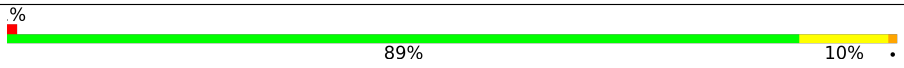
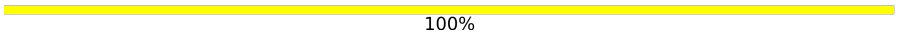
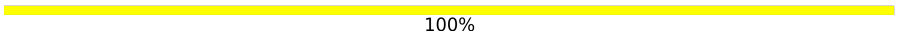
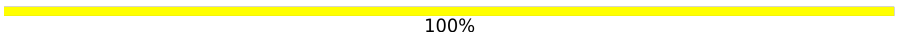
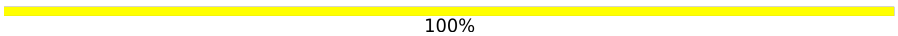
Mol	Chain	Length	Quality of chain
3	D	214	
3	L	214	
4	E	2	
4	F	2	
4	G	2	
4	I	2	
4	K	2	
5	J	3	

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 15041 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 Glucagon receptor,Endolysin,Glucagon receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	544	Total	C	N	O	S	0	0	0
			4222	2725	730	744	23			
1	B	496	Total	C	N	O	S	0	0	0
			3773	2434	653	664	22			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	GLY	-	expression tag	UNP P47871
A	25	ALA	-	expression tag	UNP P47871
A	26	PRO	-	expression tag	UNP P47871
A	1054	THR	CYS	engineered mutation	UNP D9IEF7
A	1097	ALA	CYS	engineered mutation	UNP D9IEF7
A	433	GLU	-	expression tag	UNP P47871
A	434	PHE	-	expression tag	UNP P47871
A	435	LEU	-	expression tag	UNP P47871
A	436	GLU	-	expression tag	UNP P47871
A	437	VAL	-	expression tag	UNP P47871
A	438	LEU	-	expression tag	UNP P47871
A	439	PHE	-	expression tag	UNP P47871
A	440	GLN	-	expression tag	UNP P47871
B	24	GLY	-	expression tag	UNP P47871
B	25	ALA	-	expression tag	UNP P47871
B	26	PRO	-	expression tag	UNP P47871
B	1054	THR	CYS	engineered mutation	UNP D9IEF7
B	1097	ALA	CYS	engineered mutation	UNP D9IEF7
B	433	GLU	-	expression tag	UNP P47871
B	434	PHE	-	expression tag	UNP P47871
B	435	LEU	-	expression tag	UNP P47871
B	436	GLU	-	expression tag	UNP P47871
B	437	VAL	-	expression tag	UNP P47871
B	438	LEU	-	expression tag	UNP P47871
B	439	PHE	-	expression tag	UNP P47871

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Chain	Residue	Modelled	Actual	Comment	Reference
B	440	GLN	-	expression tag	UNP P47871

- Molecule 2 is a protein called Antibody mAb1 Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	231	Total	C	N	O	S	0	0	0
			1756	1107	297	344	8			
2	H	231	Total	C	N	O	S	0	0	0
			1749	1103	296	342	8			

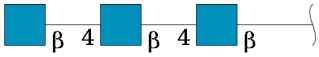
- Molecule 3 is a protein called Antibody mAb1 Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	214	Total	C	N	O	S	0	0	0
			1629	1013	280	330	6			
3	L	214	Total	C	N	O	S	0	0	0
			1633	1015	280	332	6			

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

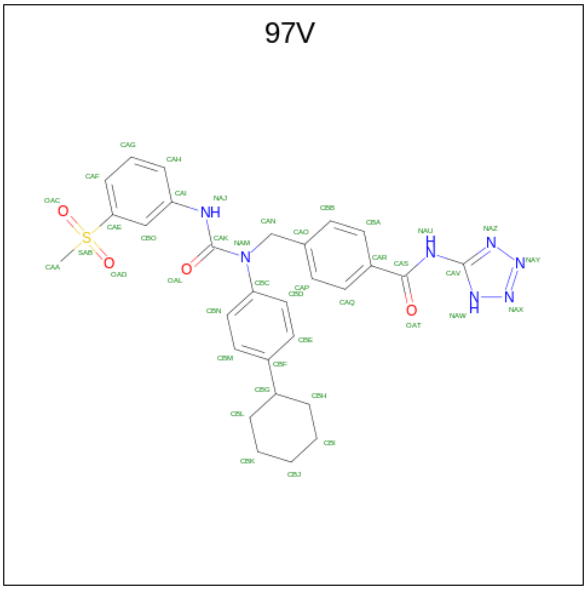
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	K	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



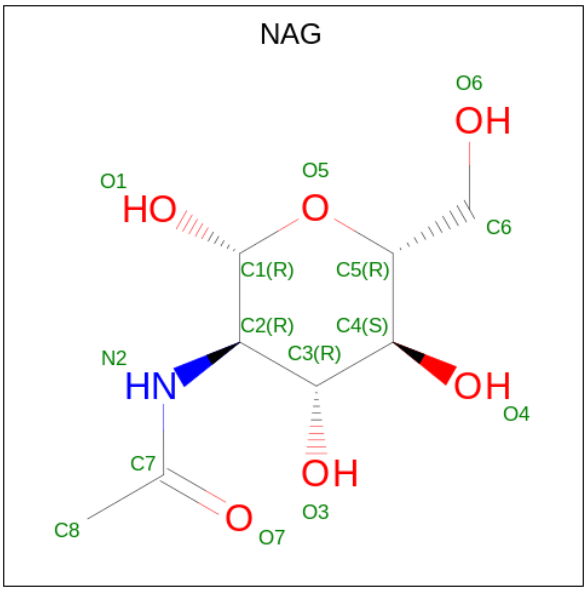
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	J	3	42	24	3	15	0	0	0

- Molecule 6 is 4-{[(4-cyclohexylphenyl){[3-(methylsulfonyl)phenyl]carbamoyl}amino]methyl }-N-(1H-tetrazol-5-yl)benzamide (three-letter code: 97V) (formula: $C_{29}H_{31}N_7O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
6	A	1	41	29	7	4	1	0	0
			Total	C	N	O	S		
6	B	1	41	29	7	4	1	0	0

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 8 is water.

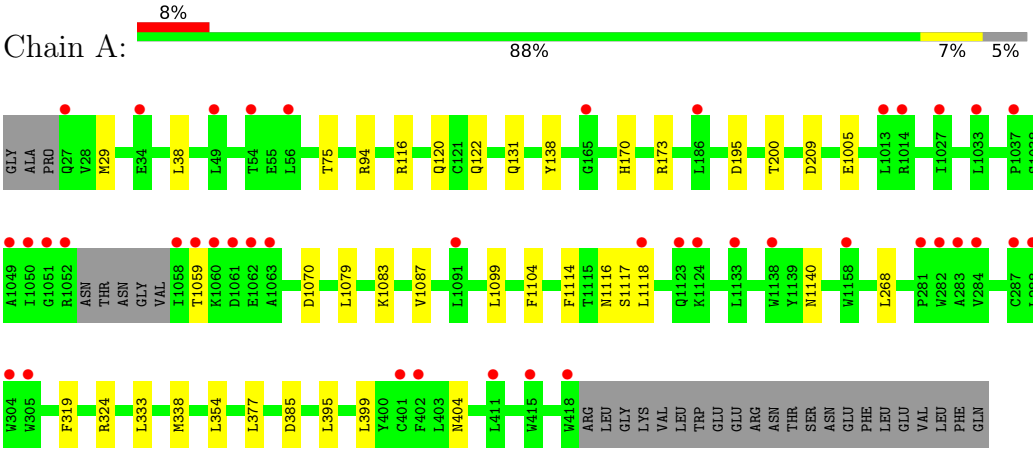
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total O 1 1	0	0

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.

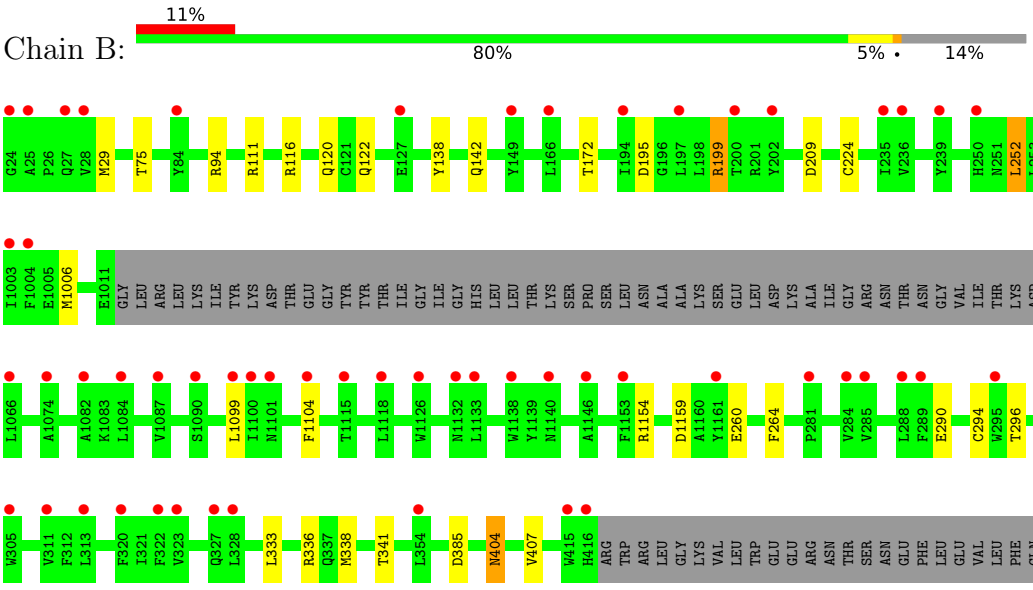
• Molecule 1: Glucagon receptor,Endolysin,Glucagon receptor

Chain A:



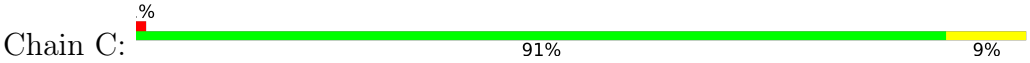
• Molecule 1: Glucagon receptor,Endolysin,Glucagon receptor

Chain B:

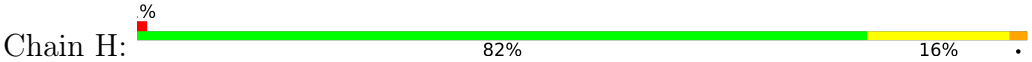


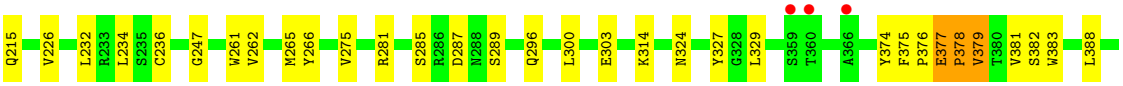
• Molecule 2: Antibody mAb1 Heavy chain

Chain C:

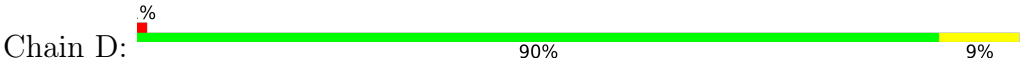


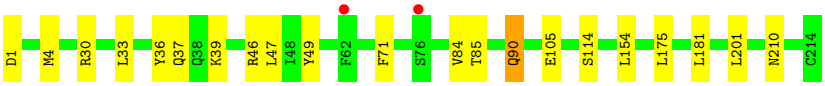
• Molecule 2: Antibody mAb1 Heavy chain



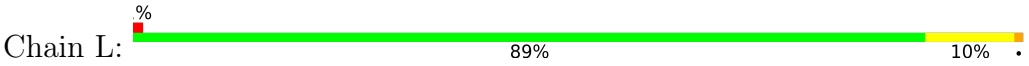


• Molecule 3: Antibody mAb1 Light chain





• Molecule 3: Antibody mAb1 Light chain



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

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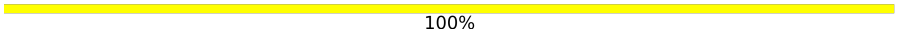
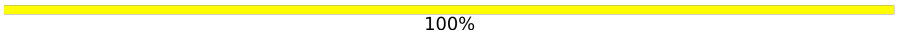
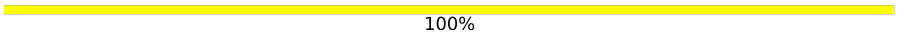
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I: 

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

Chain J: 

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	71.46Å 248.79Å 93.33Å 90.00° 90.16° 90.00°	Depositor
Resolution (Å)	46.92 – 3.19 46.92 – 3.19	Depositor EDS
% Data completeness (in resolution range)	94.1 (46.92-3.19) 98.5 (46.92-3.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.60 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.205 , 0.231 0.161 , 0.180	Depositor DCC
R_{free} test set	2648 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	96.6	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 49.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.109 for h,-k,-l	Xtriage
Reported twinning fraction	0.555 for H, K, L 0.445 for -h,-k,l	Depositor
Outliers	0 of 53171 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	15041	wwPDB-VP
Average B, all atoms (Å^2)	120.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% 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, 97V

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.48	0/4326	0.61	1/5886 (0.0%)
1	B	0.49	0/3869	0.61	2/5280 (0.0%)
2	C	0.62	0/1799	0.71	0/2448
2	H	0.68	0/1792	0.80	2/2440 (0.1%)
3	D	0.65	0/1662	0.68	0/2254
3	L	0.63	0/1666	0.69	0/2259
All	All	0.57	0/15114	0.66	5/20567 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	377	GLU	CB-CA-C	-7.48	95.44	110.40
1	B	111	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	A	173	ARG	NE-CZ-NH1	5.35	122.98	120.30
1	B	1154	ARG	NE-CZ-NH1	5.13	122.86	120.30
2	H	378	PRO	CA-N-CD	-5.08	104.39	111.50

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	4222	0	4075	5	0
1	B	3773	0	3553	7	0
2	C	1756	0	1704	1	1
2	H	1749	0	1691	19	1
3	D	1629	0	1586	6	0
3	L	1633	0	1590	9	0
4	E	28	0	25	0	0
4	F	28	0	25	0	0
4	G	28	0	25	0	0
4	I	28	0	25	0	0
4	K	28	0	25	0	0
5	J	42	0	37	0	0
6	A	41	0	0	0	0
6	B	41	0	0	0	0
7	B	14	0	13	0	0
8	A	1	0	0	0	0
All	All	15041	0	14374	44	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (44) 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)
2:H:375:PHE:CE1	2:H:376:PRO:HB3	2.09	0.88
1:B:256:ALA:HB3	1:B:1002:ASN:HA	1.84	0.59
2:H:375:PHE:CD1	2:H:376:PRO:HB3	2.37	0.58
2:H:444:SER:O	2:H:445:CYS:HB2	2.06	0.55
2:H:374:TYR:CE2	2:H:379:VAL:HG22	2.42	0.54
2:H:374:TYR:CZ	2:H:379:VAL:CG2	2.90	0.54
2:H:226:VAL:HG11	2:H:300:LEU:HD13	1.90	0.53
2:C:226:VAL:HG11	2:C:300:LEU:HD13	1.89	0.52
1:B:256:ALA:N	1:B:1002:ASN:HB2	2.25	0.51
2:H:374:TYR:CZ	2:H:379:VAL:HG22	2.45	0.51
1:A:94:ARG:HB3	1:A:120:GLN:HB3	1.93	0.51
1:A:354:LEU:HD11	1:A:399:LEU:HD11	1.93	0.50
3:D:46:ARG:HD3	3:D:49:TYR:HB3	1.94	0.49
2:H:375:PHE:CD1	2:H:376:PRO:N	2.80	0.49
1:B:94:ARG:HB3	1:B:120:GLN:HB3	1.94	0.49
2:H:375:PHE:CD1	2:H:375:PHE:C	2.86	0.49
1:B:404:ASN:HB3	1:B:407:VAL:HG22	1.96	0.48
2:H:383:TRP:HB3	2:H:388:LEU:HD23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:46:ARG:HD3	3:L:49:TYR:HB3	1.95	0.48
2:H:287:ASP:OD1	2:H:289:SER:OG	2.28	0.48
1:B:252:LEU:HG	1:B:260:GLU:HG2	1.95	0.48
3:D:36:TYR:CE1	3:D:46:ARG:HB2	2.49	0.48
3:L:103:LYS:HE3	3:L:105:GLU:HB3	1.97	0.47
2:H:375:PHE:CD1	2:H:376:PRO:CA	2.98	0.47
2:H:261:TRP:O	2:H:275:VAL:HG21	2.16	0.46
3:L:36:TYR:CE1	3:L:46:ARG:HB2	2.50	0.46
3:D:4:MET:HE1	3:D:90:GLN:HB2	1.97	0.45
3:L:191:VAL:HA	3:L:210:ASN:HA	1.98	0.45
2:H:247:GLY:HA3	2:H:266:TYR:CE1	2.52	0.45
2:H:327:TYR:O	3:L:46:ARG:NH2	2.50	0.45
1:A:1114:PHE:HB3	1:A:1117:SER:HB2	1.99	0.45
1:B:172:THR:CB	1:B:1159:ASP:OD1	2.65	0.45
1:A:1087:VAL:HG21	1:A:1118:LEU:HB3	2.00	0.44
3:L:4:MET:HE1	3:L:90:GLN:HB2	1.99	0.43
1:A:395:LEU:O	1:A:399:LEU:HG	2.18	0.43
2:H:381:VAL:HG12	2:H:382:SER:N	2.31	0.43
3:D:33:LEU:HD13	3:D:71:PHE:CG	2.54	0.43
2:H:375:PHE:CD1	2:H:376:PRO:CB	3.01	0.43
2:H:329:LEU:HD13	3:L:89:LEU:HD21	2.01	0.43
3:L:33:LEU:HD13	3:L:71:PHE:CG	2.54	0.42
3:D:37:GLN:HB2	3:D:47:LEU:HD11	2.02	0.41
1:B:142:GLN:OE1	1:B:199:ARG:NH1	2.54	0.40
3:D:39:LYS:HG2	3:D:84:VAL:HG11	2.03	0.40
2:H:410:VAL:HG11	3:L:135:LEU:CD2	2.51	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:385:SER:OG	2:H:287:ASP:OD2[1_455]	2.19	0.01

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	540/574 (94%)	509 (94%)	31 (6%)	0	100	100
1	B	492/574 (86%)	470 (96%)	22 (4%)	0	100	100
2	C	229/231 (99%)	213 (93%)	16 (7%)	0	100	100
2	H	229/231 (99%)	210 (92%)	19 (8%)	0	100	100
3	D	212/214 (99%)	202 (95%)	10 (5%)	0	100	100
3	L	212/214 (99%)	200 (94%)	12 (6%)	0	100	100
All	All	1914/2038 (94%)	1804 (94%)	110 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	426/493 (86%)	398 (93%)	28 (7%)	16	51
1	B	369/493 (75%)	346 (94%)	23 (6%)	18	53
2	C	196/196 (100%)	179 (91%)	17 (9%)	10	37
2	H	194/196 (99%)	172 (89%)	22 (11%)	6	25
3	D	186/187 (100%)	175 (94%)	11 (6%)	19	54
3	L	187/187 (100%)	173 (92%)	14 (8%)	13	45
All	All	1558/1752 (89%)	1443 (93%)	115 (7%)	13	46

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	MET
1	A	38	LEU
1	A	75	THR
1	A	116	ARG

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Mol	Chain	Res	Type
1	A	122	GLN
1	A	131	GLN
1	A	138	TYR
1	A	170	HIS
1	A	195	ASP
1	A	200	THR
1	A	209	ASP
1	A	1005	GLU
1	A	1059	THR
1	A	1070	ASP
1	A	1079	LEU
1	A	1083	LYS
1	A	1099	LEU
1	A	1104	PHE
1	A	1116	ASN
1	A	1140	ASN
1	A	268	LEU
1	A	319	PHE
1	A	324	ARG
1	A	333	LEU
1	A	338	MET
1	A	377	LEU
1	A	385	ASP
1	A	404	ASN
1	B	29	MET
1	B	75	THR
1	B	116	ARG
1	B	122	GLN
1	B	138	TYR
1	B	195	ASP
1	B	199	ARG
1	B	209	ASP
1	B	224	CYS
1	B	252	LEU
1	B	1006	MET
1	B	1099	LEU
1	B	1104	PHE
1	B	264	PHE
1	B	290	GLU
1	B	294	CYS
1	B	296	THR
1	B	333	LEU

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Mol	Chain	Res	Type
1	B	336	ARG
1	B	338	MET
1	B	341	THR
1	B	385	ASP
1	B	404	ASN
2	C	215	GLN
2	C	232	LEU
2	C	234	LEU
2	C	236	CYS
2	C	268	ASP
2	C	273	ASP
2	C	281	ARG
2	C	285	SER
2	C	296	GLN
2	C	303	GLU
2	C	377	GLU
2	C	412	THR
2	C	421	GLN
2	C	425	CYS
2	C	432	SER
2	C	433	ASN
2	C	438	LYS
3	D	1	ASP
3	D	30	ARG
3	D	85	THR
3	D	90	GLN
3	D	105	GLU
3	D	114	SER
3	D	154	LEU
3	D	175	LEU
3	D	181	LEU
3	D	201	LEU
3	D	210	ASN
2	H	215	GLN
2	H	232	LEU
2	H	234	LEU
2	H	236	CYS
2	H	262	VAL
2	H	265	MET
2	H	281	ARG
2	H	285	SER
2	H	296	GLN

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Mol	Chain	Res	Type
2	H	303	GLU
2	H	314	LYS
2	H	324	ASN
2	H	377	GLU
2	H	378	PRO
2	H	379	VAL
2	H	412	THR
2	H	421	GLN
2	H	425	CYS
2	H	432	SER
2	H	433	ASN
2	H	438	LYS
2	H	444	SER
3	L	1	ASP
3	L	30	ARG
3	L	56	SER
3	L	85	THR
3	L	90	GLN
3	L	105	GLU
3	L	114	SER
3	L	145	LYS
3	L	154	LEU
3	L	181	LEU
3	L	201	LEU
3	L	210	ASN
3	L	213	GLU
3	L	214	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1132	ASN
2	H	421	GLN

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)

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	$\#\|Z\|>2$
4	NAG	E	1	4,1	14,14,15	0.77	1 (7%)	17,19,21	1.73	2 (11%)
4	NAG	E	2	4	14,14,15	0.42	0	17,19,21	1.58	2 (11%)
4	NAG	F	1	4,1	14,14,15	0.64	0	17,19,21	1.50	3 (17%)
4	NAG	F	2	4	14,14,15	0.42	0	17,19,21	0.66	0
4	NAG	G	1	4,1	14,14,15	0.69	0	17,19,21	1.78	4 (23%)
4	NAG	G	2	4	14,14,15	0.31	0	17,19,21	1.00	0
4	NAG	I	1	4,1	14,14,15	0.55	0	17,19,21	1.56	2 (11%)
4	NAG	I	2	4	14,14,15	0.52	0	17,19,21	1.13	1 (5%)
5	NAG	J	1	5,1	14,14,15	0.84	1 (7%)	17,19,21	1.79	2 (11%)
5	NAG	J	2	5	14,14,15	0.77	1 (7%)	17,19,21	1.28	3 (17%)
5	NAG	J	3	5	14,14,15	1.17	1 (7%)	17,19,21	1.38	2 (11%)
4	NAG	K	1	4,1	14,14,15	0.70	0	17,19,21	1.48	3 (17%)
4	NAG	K	2	4	14,14,15	0.96	1 (7%)	17,19,21	1.14	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
4	NAG	E	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	3/6/23/26	0/1/1/1
4	NAG	F	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	G	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	G	2	4	-	0/6/23/26	0/1/1/1
4	NAG	I	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	I	2	4	-	2/6/23/26	0/1/1/1
5	NAG	J	1	5,1	-	1/6/23/26	0/1/1/1
5	NAG	J	2	5	-	0/6/23/26	0/1/1/1
5	NAG	J	3	5	-	0/6/23/26	0/1/1/1
4	NAG	K	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	K	2	4	-	0/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	3	NAG	C1-C2	3.83	1.58	1.52
4	K	2	NAG	C1-C2	2.73	1.56	1.52
5	J	2	NAG	O4-C4	2.48	1.48	1.43
5	J	1	NAG	O5-C1	-2.45	1.39	1.43
4	E	1	NAG	C1-C2	2.11	1.55	1.52

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	1	NAG	C1-O5-C5	5.75	119.98	112.19
5	J	1	NAG	C1-O5-C5	5.36	119.45	112.19
4	E	2	NAG	C1-O5-C5	4.94	118.88	112.19
5	J	3	NAG	O5-C1-C2	-4.20	104.66	111.29
4	G	1	NAG	O5-C1-C2	-3.88	105.17	111.29
4	G	1	NAG	C1-O5-C5	3.72	117.23	112.19
4	I	1	NAG	O5-C1-C2	-3.71	105.43	111.29
4	F	1	NAG	O5-C1-C2	-3.32	106.04	111.29
4	E	2	NAG	C2-N2-C7	3.20	127.47	122.90
4	K	1	NAG	C1-O5-C5	3.10	116.39	112.19
4	K	1	NAG	C1-C2-N2	3.04	115.68	110.49
4	K	2	NAG	O5-C1-C2	-3.01	106.54	111.29
4	F	1	NAG	O5-C5-C6	2.99	111.90	107.20
5	J	2	NAG	O4-C4-C3	2.94	117.15	110.35
5	J	2	NAG	C1-O5-C5	2.82	116.01	112.19
4	G	1	NAG	C1-C2-N2	2.79	115.25	110.49
5	J	1	NAG	C2-N2-C7	2.76	126.83	122.90
4	E	1	NAG	O4-C4-C5	2.66	115.91	109.30
4	I	2	NAG	C2-N2-C7	2.64	126.67	122.90
4	K	1	NAG	C2-N2-C7	2.61	126.62	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	J	3	NAG	C1-C2-N2	2.44	114.65	110.49
5	J	2	NAG	O3-C3-C2	-2.38	104.54	109.47
4	I	1	NAG	C1-C2-N2	2.31	114.44	110.49
4	G	1	NAG	C3-C4-C5	2.24	114.23	110.24
4	F	1	NAG	C3-C4-C5	2.16	114.10	110.24

There are no chirality outliers.

All (10) torsion outliers are listed below:

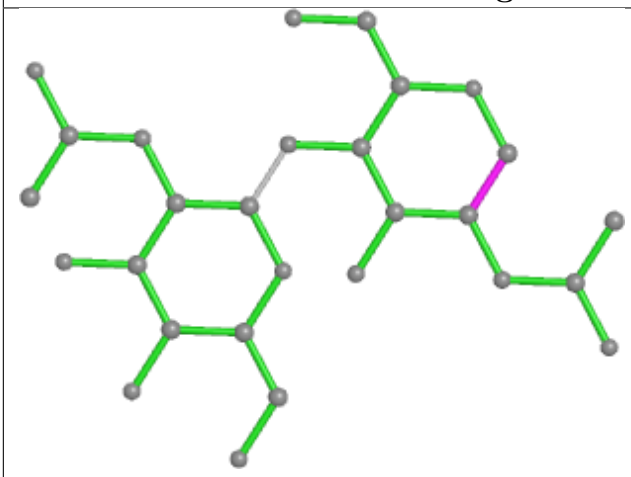
Mol	Chain	Res	Type	Atoms
4	E	2	NAG	O5-C5-C6-O6
4	E	2	NAG	C4-C5-C6-O6
4	E	2	NAG	C3-C2-N2-C7
5	J	1	NAG	C3-C2-N2-C7
4	I	2	NAG	C3-C2-N2-C7
4	I	1	NAG	C1-C2-N2-C7
4	G	1	NAG	C3-C2-N2-C7
4	I	1	NAG	C3-C2-N2-C7
4	K	1	NAG	C3-C2-N2-C7
4	I	2	NAG	C1-C2-N2-C7

There are no ring outliers.

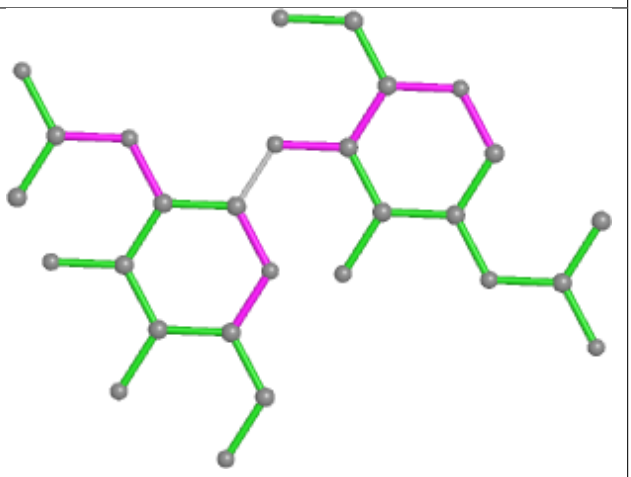
No monomer is involved in short contacts.

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

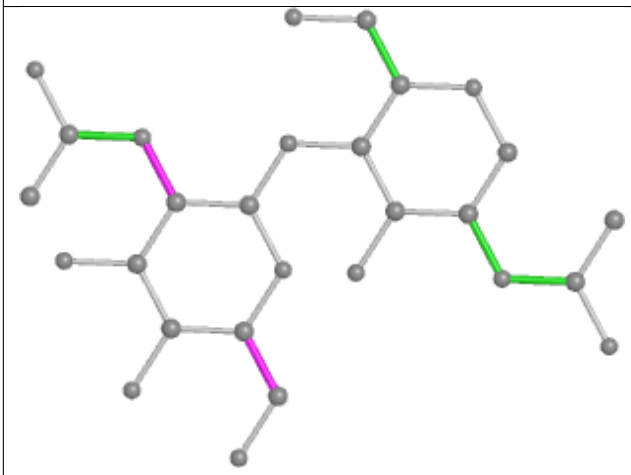
Oligosaccharide Chain E



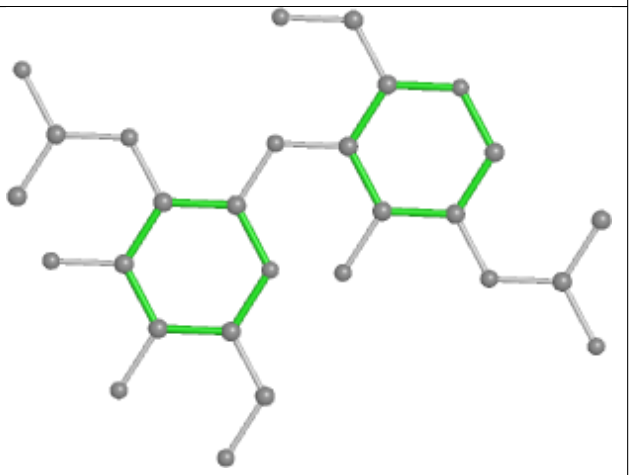
Bond lengths



Bond angles

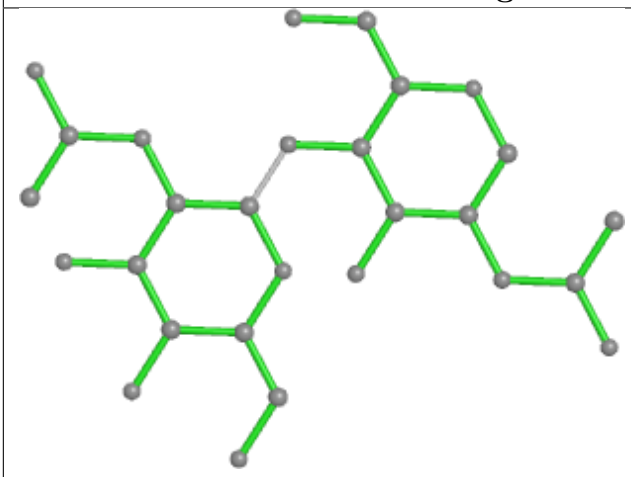


Torsions

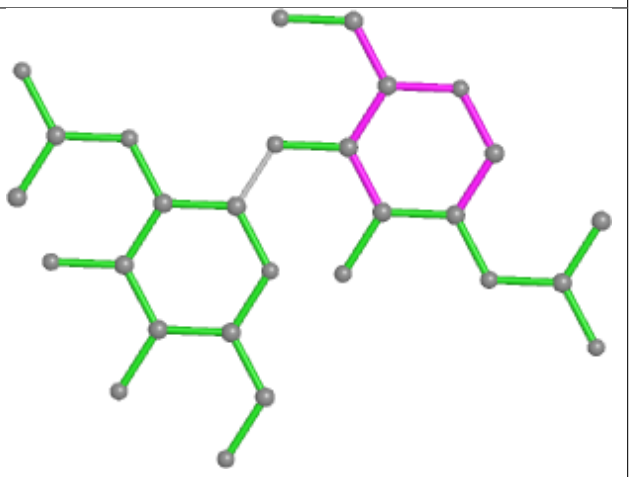


Rings

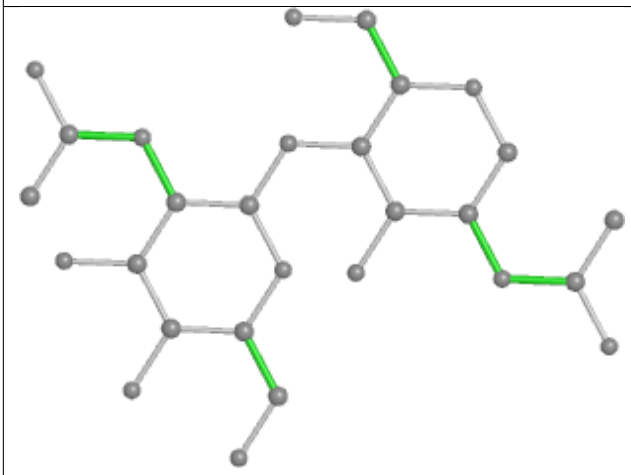
Oligosaccharide Chain F



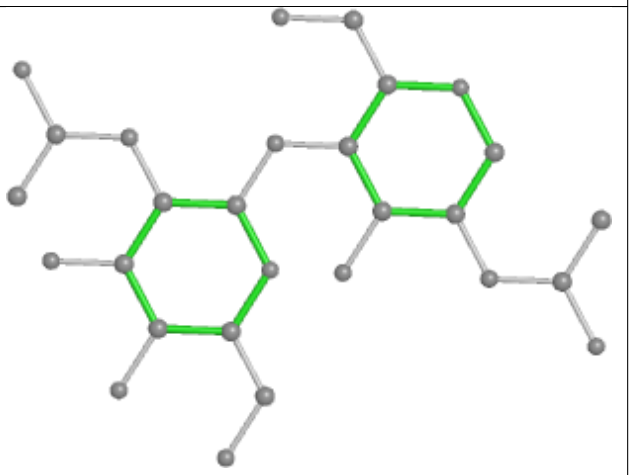
Bond lengths



Bond angles

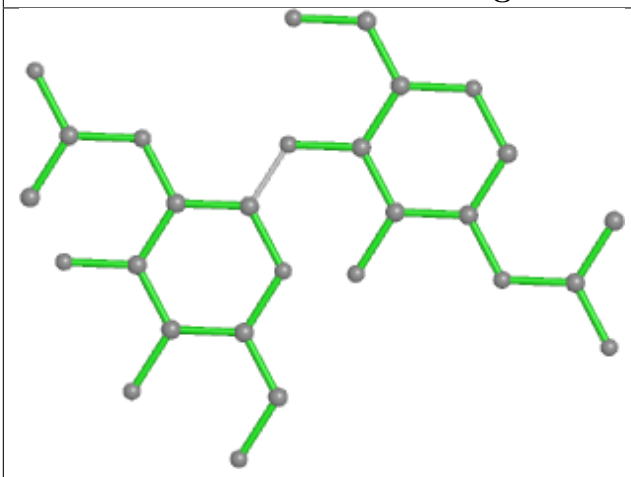


Torsions

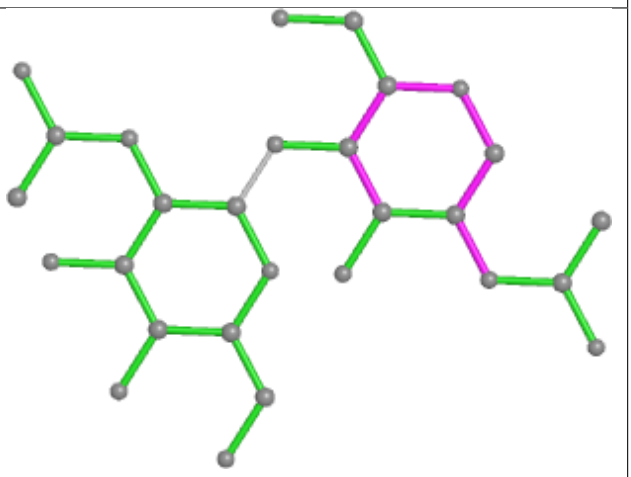


Rings

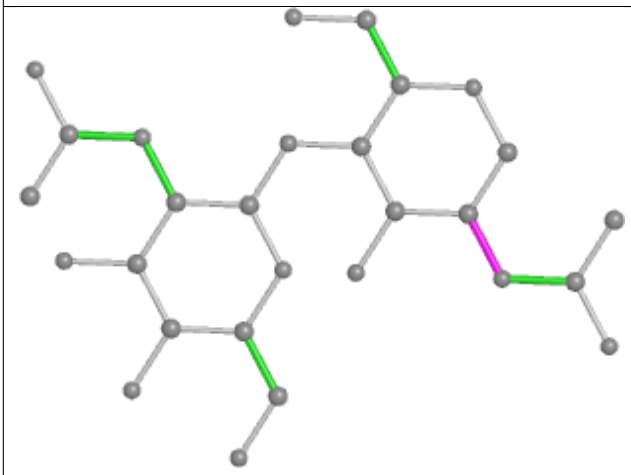
Oligosaccharide Chain G



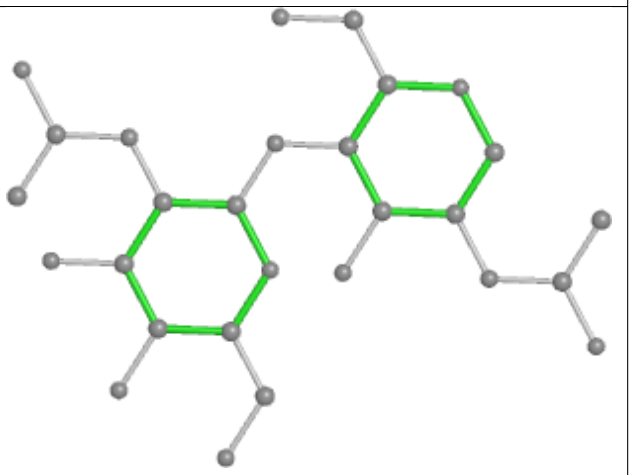
Bond lengths



Bond angles

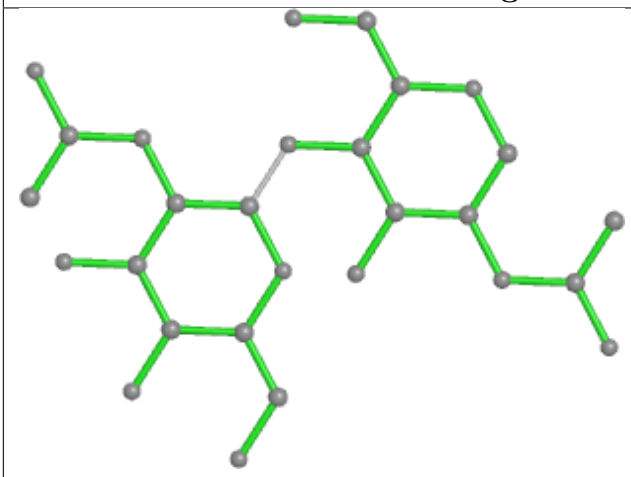


Torsions

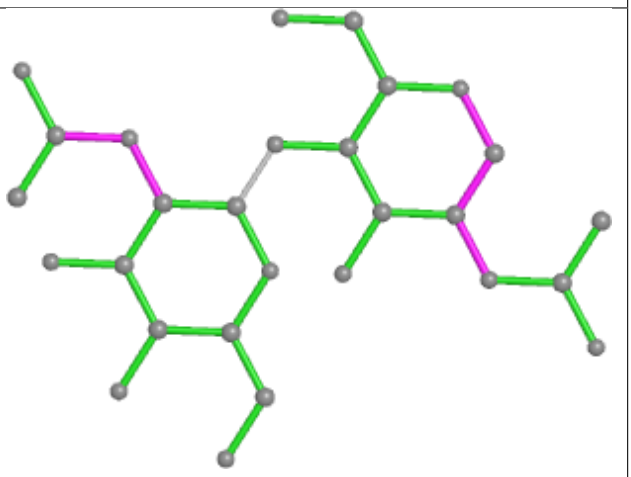


Rings

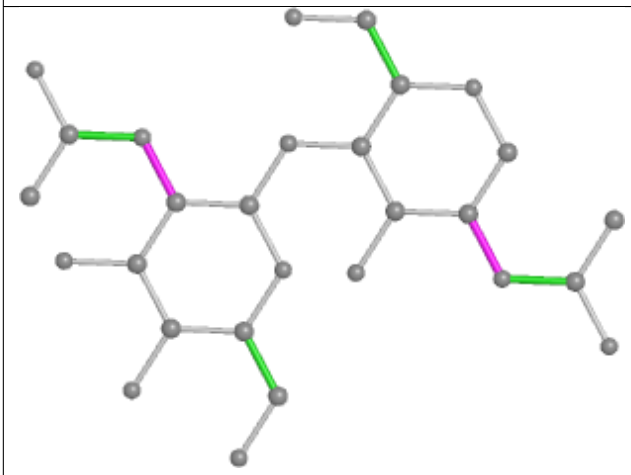
Oligosaccharide Chain I



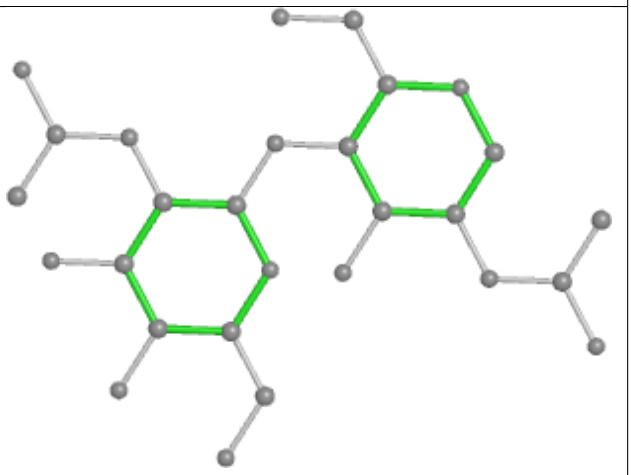
Bond lengths



Bond angles

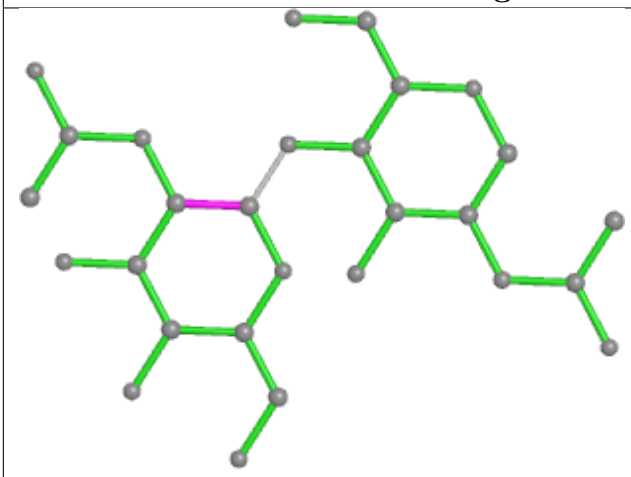


Torsions

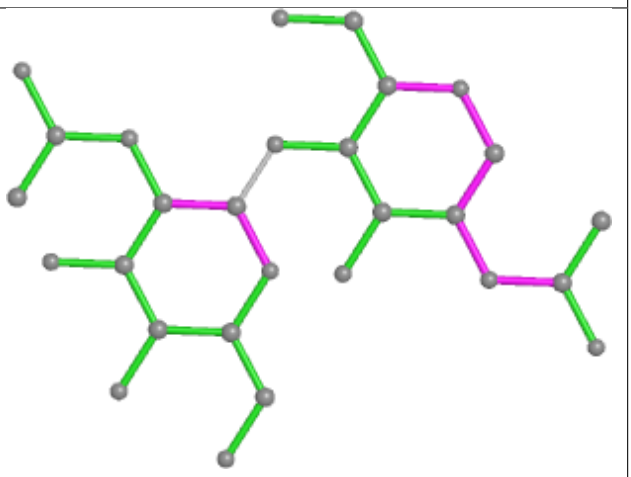


Rings

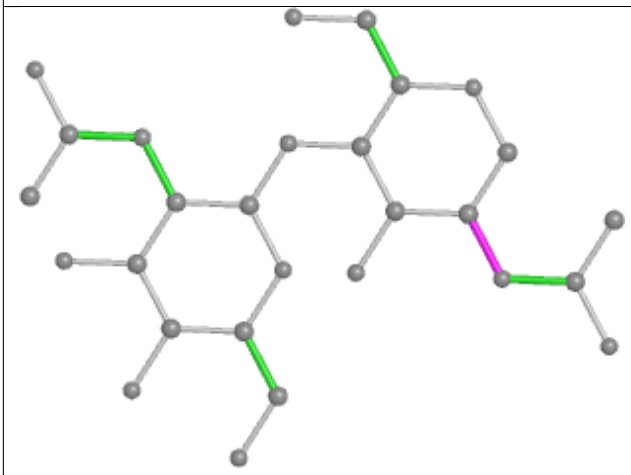
Oligosaccharide Chain K



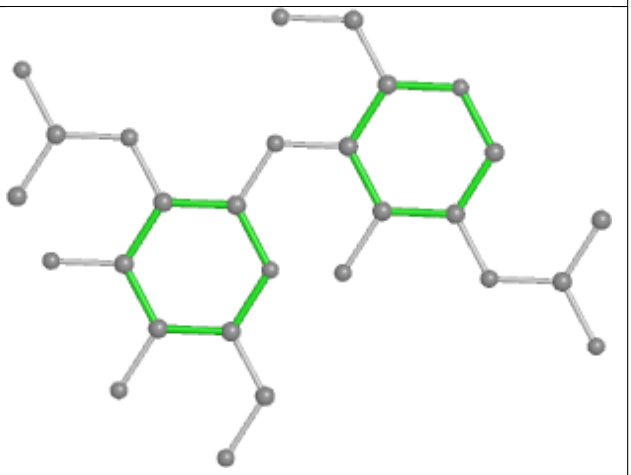
Bond lengths



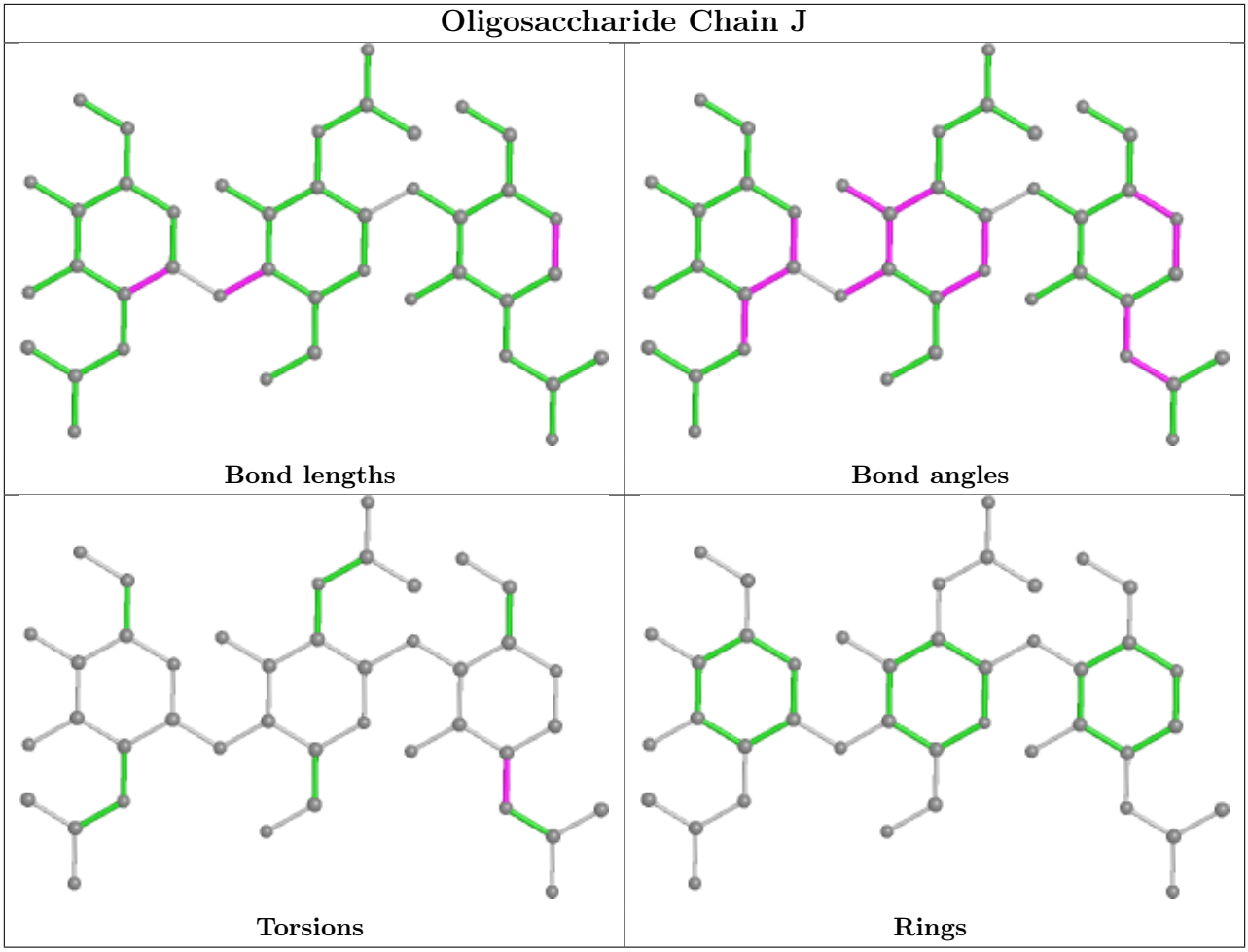
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

3 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	97V	A	1207	-	43,45,45	1.93	8 (18%)	55,63,63	1.43	7 (12%)
6	97V	B	1209	-	43,45,45	1.90	8 (18%)	55,63,63	1.58	8 (14%)
7	NAG	B	1206	1	14,14,15	0.31	0	17,19,21	1.37	2 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	97V	A	1207	-	-	10/32/42/42	0/5/5/5
6	97V	B	1209	-	-	12/32/42/42	0/5/5/5
7	NAG	B	1206	1	-	2/6/23/26	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1209	97V	CAN-CAO	-5.62	1.41	1.51
6	A	1207	97V	CAN-CAO	-5.55	1.41	1.51
6	A	1207	97V	CAR-CAS	-5.07	1.39	1.50
6	B	1209	97V	CAR-CAS	-5.02	1.39	1.50
6	B	1209	97V	CBF-CBG	-4.94	1.42	1.52
6	A	1207	97V	CBF-CBG	-4.79	1.42	1.52
6	A	1207	97V	CBC-NAM	-3.97	1.35	1.43
6	A	1207	97V	CAV-NAU	-3.80	1.33	1.38
6	B	1209	97V	CBC-NAM	-3.73	1.35	1.43
6	B	1209	97V	OAD-SAB	3.39	1.53	1.44
6	B	1209	97V	CAV-NAU	-3.37	1.34	1.38
6	A	1207	97V	OAC-SAB	3.35	1.53	1.44
6	A	1207	97V	OAD-SAB	3.33	1.53	1.44
6	B	1209	97V	OAC-SAB	3.13	1.52	1.44
6	A	1207	97V	CAI-NAJ	-2.66	1.36	1.41
6	B	1209	97V	CAI-NAJ	-2.15	1.37	1.41

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	1209	97V	OAD-SAB-OAC	-5.73	108.05	117.92
6	A	1207	97V	OAD-SAB-OAC	-5.15	109.04	117.92
6	B	1209	97V	CAA-SAB-CAE	4.60	110.02	104.58
6	A	1207	97V	CAA-SAB-CAE	4.46	109.85	104.58
6	B	1209	97V	CAI-CBO-CAE	4.18	122.04	118.89
7	B	1206	NAG	O5-C1-C2	-4.07	104.87	111.29
6	A	1207	97V	CAI-CBO-CAE	3.84	121.79	118.89
6	A	1207	97V	OAC-SAB-CAE	2.84	110.56	108.25
6	B	1209	97V	CAH-CAI-CBO	-2.76	116.38	119.65
6	B	1209	97V	CBJ-CBI-CBH	-2.55	106.22	111.42
6	B	1209	97V	NAW-NAX-NAY	-2.48	107.91	109.53
6	A	1207	97V	NAW-NAX-NAY	-2.45	107.93	109.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	1207	97V	CBJ-CBI-CBH	-2.28	106.76	111.42
6	A	1207	97V	CBI-CBH-CBG	-2.14	107.28	111.47
6	B	1209	97V	CAH-CAI-NAJ	2.12	127.55	120.40
7	B	1206	NAG	C1-C2-N2	2.10	114.08	110.49
6	B	1209	97V	NAZ-NAY-NAX	-2.02	108.21	109.53

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1207	97V	NAJ-CAK-NAM-CAN
6	A	1207	97V	OAL-CAK-NAM-CAN
6	B	1209	97V	NAJ-CAK-NAM-CAN
6	B	1209	97V	OAL-CAK-NAM-CAN
6	A	1207	97V	CAQ-CAR-CAS-NAU
6	A	1207	97V	CAQ-CAR-CAS-OAT
6	A	1207	97V	CBA-CAR-CAS-OAT
6	A	1207	97V	CBA-CAR-CAS-NAU
6	B	1209	97V	CBA-CAR-CAS-OAT
6	B	1209	97V	CBA-CAR-CAS-NAU
6	B	1209	97V	CAQ-CAR-CAS-NAU
6	B	1209	97V	CAQ-CAR-CAS-OAT
6	B	1209	97V	CBO-CAE-SAB-OAC
7	B	1206	NAG	C4-C5-C6-O6
6	B	1209	97V	CAF-CAE-SAB-OAC
7	B	1206	NAG	O5-C5-C6-O6
6	A	1207	97V	OAL-CAK-NAM-CBC
6	B	1209	97V	CBO-CAE-SAB-CAA
6	A	1207	97V	NAJ-CAK-NAM-CBC
6	A	1207	97V	CBO-CAE-SAB-OAD
6	A	1207	97V	CAF-CAE-SAB-OAD
6	B	1209	97V	CAF-CAE-SAB-CAA
6	B	1209	97V	OAL-CAK-NAM-CBC
6	B	1209	97V	NAJ-CAK-NAM-CBC

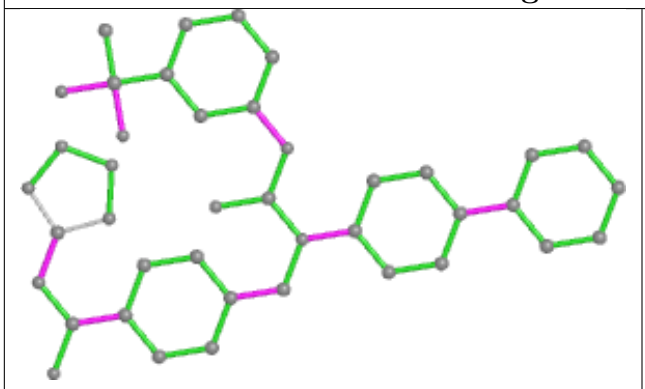
There are no ring outliers.

No monomer is involved in short contacts.

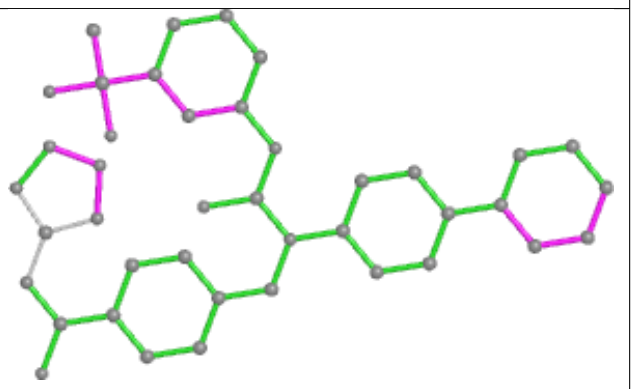
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

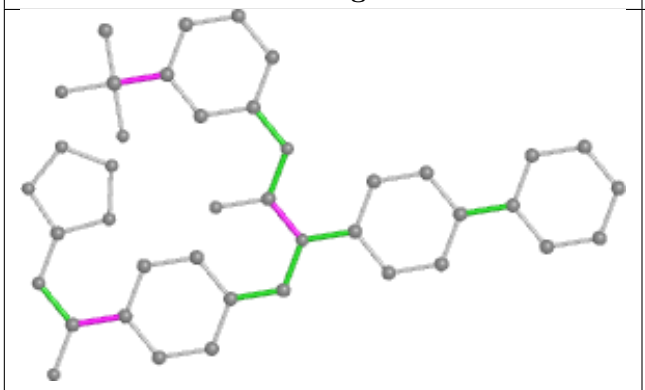
Ligand 97V A 1207



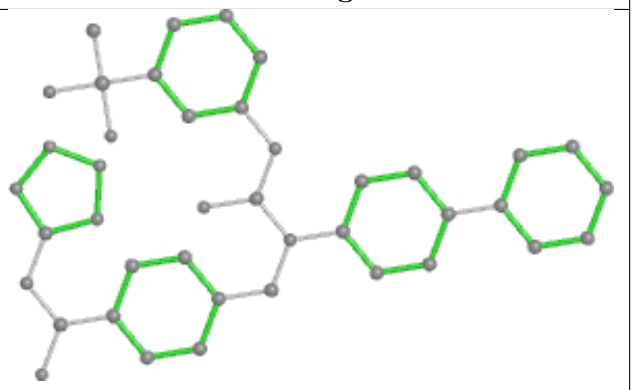
Bond lengths



Bond angles

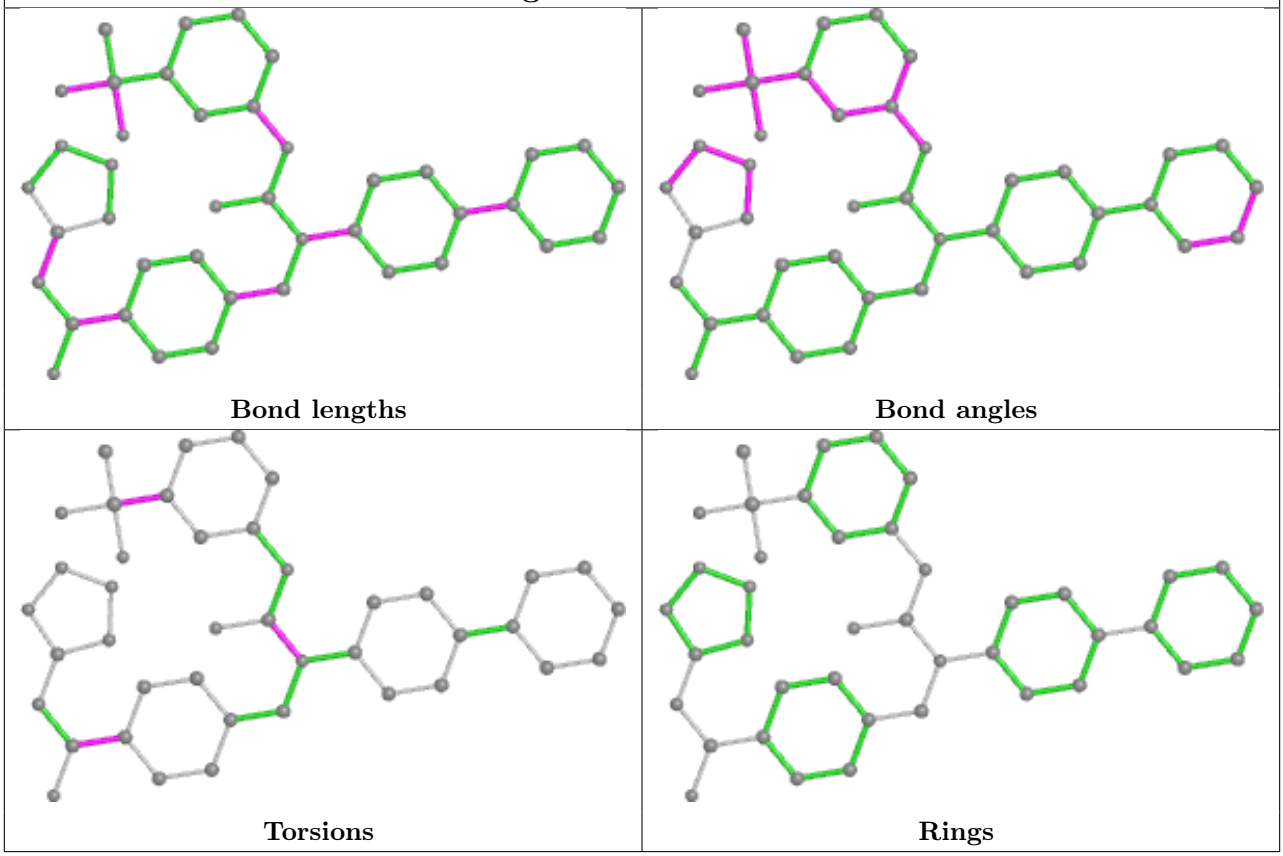


Torsions



Rings

Ligand 97V B 1209



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	544/574 (94%)	0.42	47 (8%) 10 5	71, 143, 197, 259	0
1	B	496/574 (86%)	0.52	61 (12%) 4 2	69, 152, 197, 231	0
2	C	231/231 (100%)	-0.13	3 (1%) 77 65	62, 89, 123, 183	0
2	H	231/231 (100%)	-0.16	3 (1%) 77 65	53, 83, 118, 193	0
3	D	214/214 (100%)	-0.10	2 (0%) 84 75	58, 83, 112, 143	0
3	L	214/214 (100%)	-0.20	2 (0%) 84 75	58, 80, 119, 173	0
All	All	1930/2038 (94%)	0.18	118 (6%) 21 12	53, 114, 188, 259	0

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	359	SER	9.8
1	A	305	TRP	7.5
2	C	359	SER	7.0
1	A	1049	ALA	6.7
1	B	25	ALA	6.0
1	B	289	PHE	5.8
1	A	1058	ILE	5.7
1	A	402	PHE	5.2
1	A	295	TRP	5.2
1	B	202	TYR	5.2
1	B	305	TRP	5.0
1	B	1099	LEU	4.9
1	B	416	HIS	4.8
1	A	165	GLY	4.7
1	A	1059	THR	4.6
1	A	1051	GLY	4.4
1	B	1153	PHE	4.4
1	A	1033	LEU	4.4
1	B	285	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	250	HIS	4.0
1	A	1013	LEU	4.0
1	B	200	THR	4.0
1	B	1003	ILE	3.9
1	B	281	PRO	3.9
1	B	256	ALA	3.9
1	A	288	LEU	3.8
1	B	1138	TRP	3.8
1	A	54	THR	3.8
1	A	1052	ARG	3.8
1	A	1039	LEU	3.7
1	B	288	LEU	3.7
1	B	1087	VAL	3.6
1	B	255	LEU	3.4
1	B	320	PHE	3.4
1	B	1084	LEU	3.4
1	B	1004	PHE	3.3
1	B	323	VAL	3.3
1	A	1062	GLU	3.3
1	B	28	VAL	3.2
1	A	1050	ILE	3.2
1	A	1061	ASP	3.1
2	H	366	ALA	3.1
2	C	360	THR	3.1
1	B	235	ILE	3.1
1	B	284	VAL	3.1
1	A	284	VAL	3.0
1	A	1048	LYS	3.0
1	A	418	TRP	3.0
2	C	358	LYS	2.9
1	A	1063	ALA	2.9
1	A	411	LEU	2.9
1	A	304	TRP	2.9
1	B	1100	ILE	2.9
1	B	1126	TRP	2.9
1	B	84	TYR	2.9
2	H	360	THR	2.9
1	B	239	TYR	2.8
1	B	1132	ASN	2.8
1	A	56	LEU	2.8
1	B	24	GLY	2.8
1	B	1066	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	186	LEU	2.8
1	B	1133	LEU	2.8
1	B	194	ILE	2.7
1	A	34	GLU	2.7
1	B	166	LEU	2.7
1	B	322	PHE	2.7
1	B	295	TRP	2.7
3	D	62	PHE	2.7
1	B	27	GLN	2.7
1	B	1101	ASN	2.6
1	B	127	GLU	2.6
1	A	1138	TRP	2.6
1	B	304	TRP	2.5
1	B	1090	SER	2.5
1	A	1123	GLN	2.5
3	L	129	THR	2.5
1	B	328	LEU	2.5
1	B	1140	ASN	2.5
1	B	301	MET	2.5
1	B	300	ASN	2.4
3	D	76	SER	2.4
1	B	354	LEU	2.4
1	A	1118	LEU	2.4
1	A	1133	LEU	2.4
1	A	401	CYS	2.4
1	B	197	LEU	2.4
1	A	1091	LEU	2.3
1	A	1014	ARG	2.3
1	B	1115	THR	2.3
1	B	254	GLY	2.3
1	A	1124	LYS	2.3
1	A	1037	PRO	2.3
1	B	1161	TYR	2.3
1	A	49	LEU	2.2
1	A	287	CYS	2.2
1	B	1118	LEU	2.2
1	A	283	ALA	2.2
1	A	1060	LYS	2.2
3	L	184	ALA	2.2
1	A	1027	ILE	2.2
1	A	27	GLN	2.2
1	A	415	TRP	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	149	TYR	2.1
1	B	1082	ALA	2.1
1	B	1146	ALA	2.1
1	B	236	VAL	2.1
1	B	327	GLN	2.1
1	A	1047	ASP	2.1
1	B	311	VAL	2.1
1	B	1074	ALA	2.1
1	A	1158	TRP	2.0
1	B	1104	PHE	2.0
1	A	289	PHE	2.0
1	A	282	TRP	2.0
1	B	313	LEU	2.0
1	A	281	PRO	2.0
1	B	415	TRP	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)

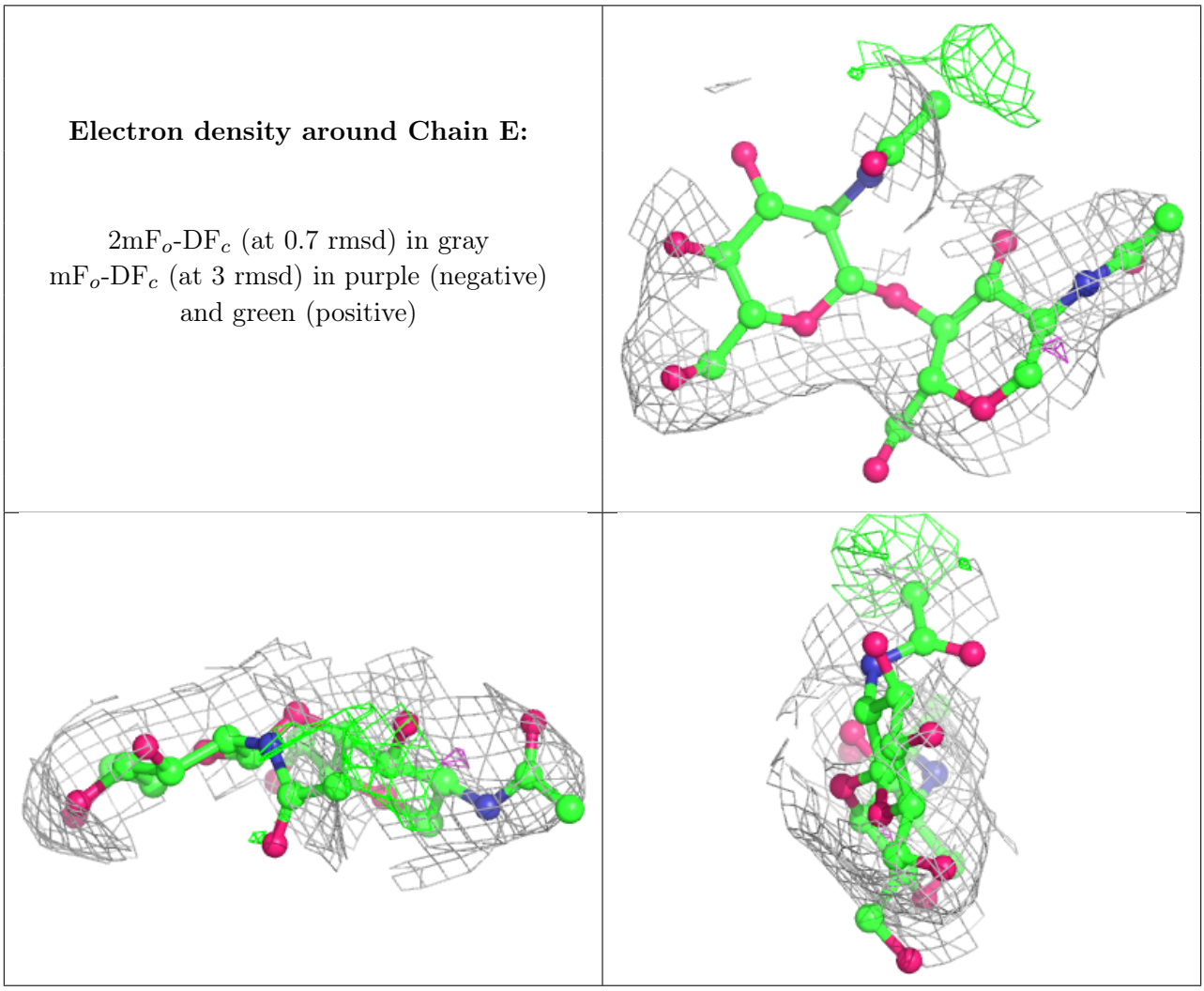
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	G	2	14/15	0.82	0.37	179,190,204,204	0
4	NAG	K	2	14/15	0.82	0.26	137,148,154,157	0
4	NAG	E	1	14/15	0.84	0.21	146,166,182,190	0
4	NAG	E	2	14/15	0.84	0.12	144,163,172,174	0
5	NAG	J	3	14/15	0.87	0.15	167,174,182,183	0
4	NAG	F	1	14/15	0.88	0.14	119,141,146,146	0
4	NAG	I	2	14/15	0.89	0.18	139,150,156,160	0
4	NAG	F	2	14/15	0.90	0.15	137,149,154,156	0
4	NAG	K	1	14/15	0.90	0.16	118,133,137,142	0
5	NAG	J	2	14/15	0.91	0.15	146,162,192,204	0
4	NAG	G	1	14/15	0.91	0.14	157,161,180,182	0
5	NAG	J	1	14/15	0.93	0.18	119,132,143,148	0
4	NAG	I	1	14/15	0.95	0.20	145,157,166,168	0

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

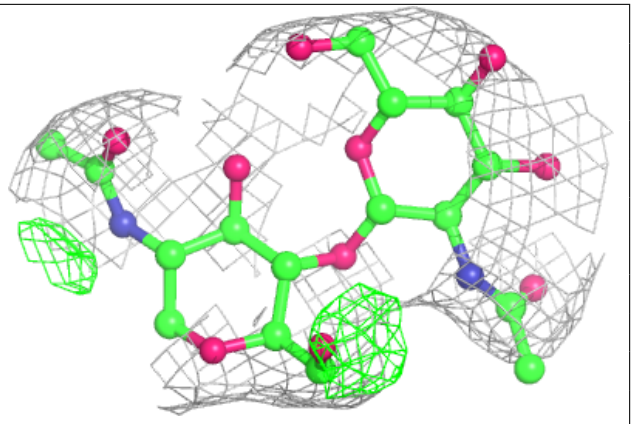
Electron density around Chain E:

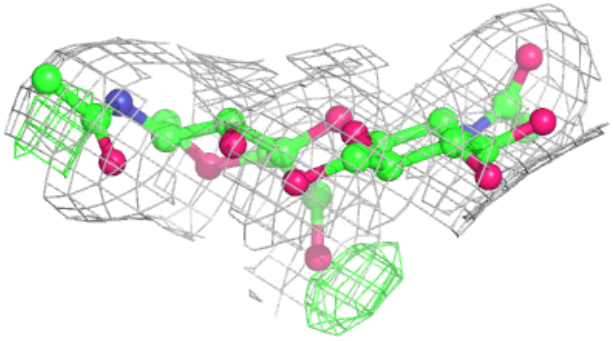
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

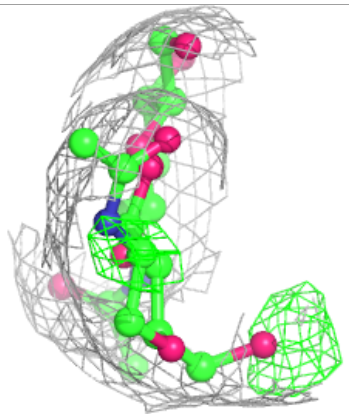


Electron density around Chain F:

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

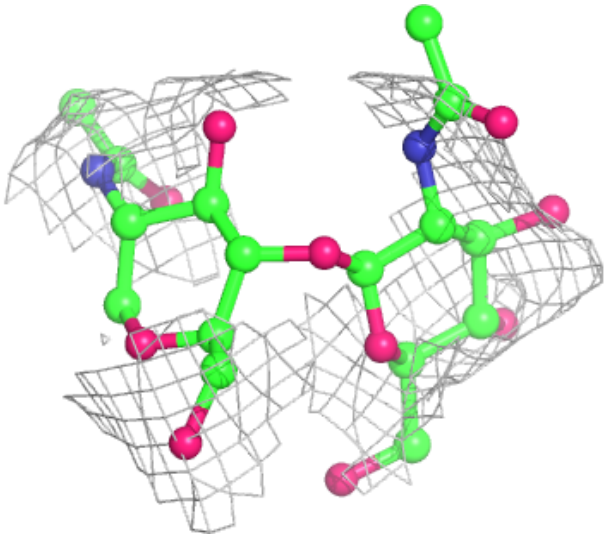


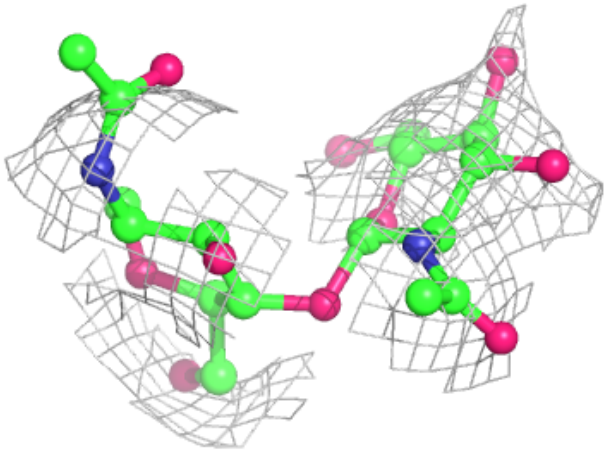


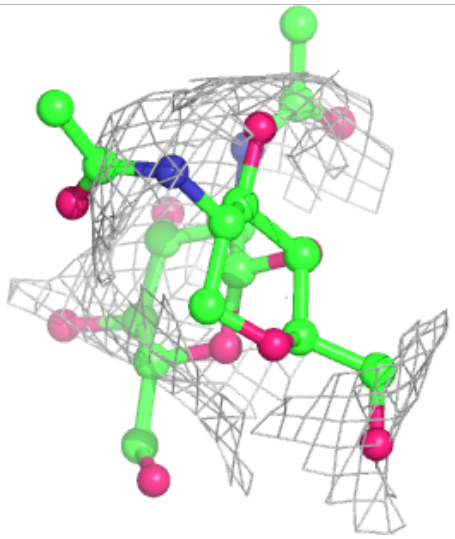


Electron density around Chain G:

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

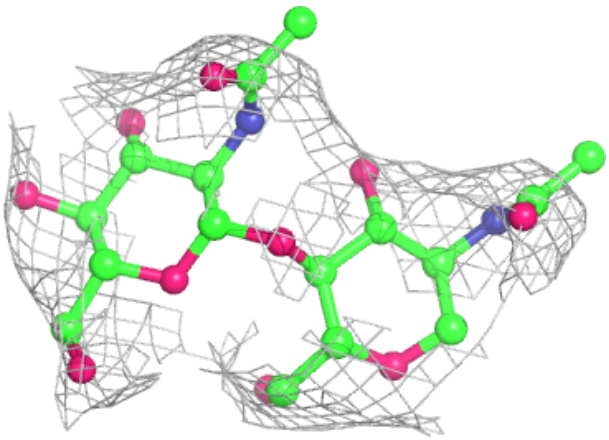


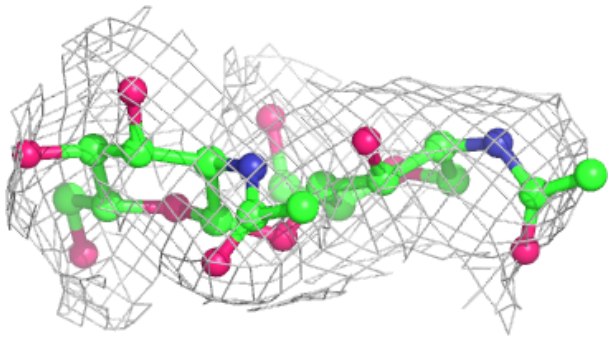


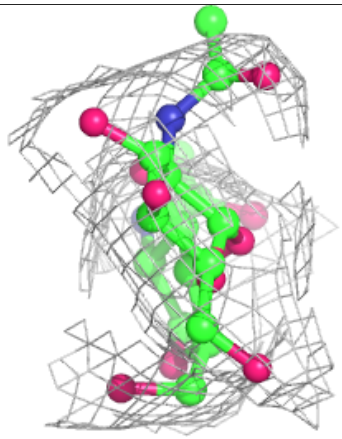


Electron density around Chain I:

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

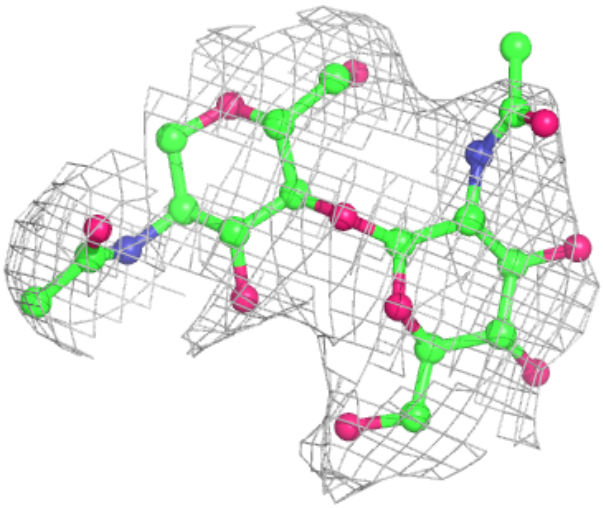


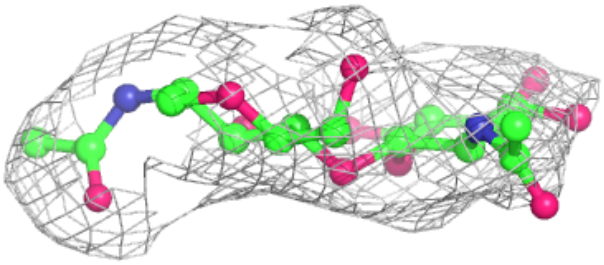


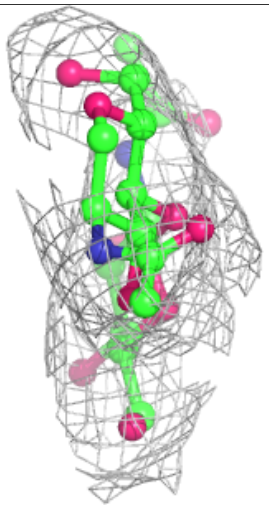


Electron density around Chain K:

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

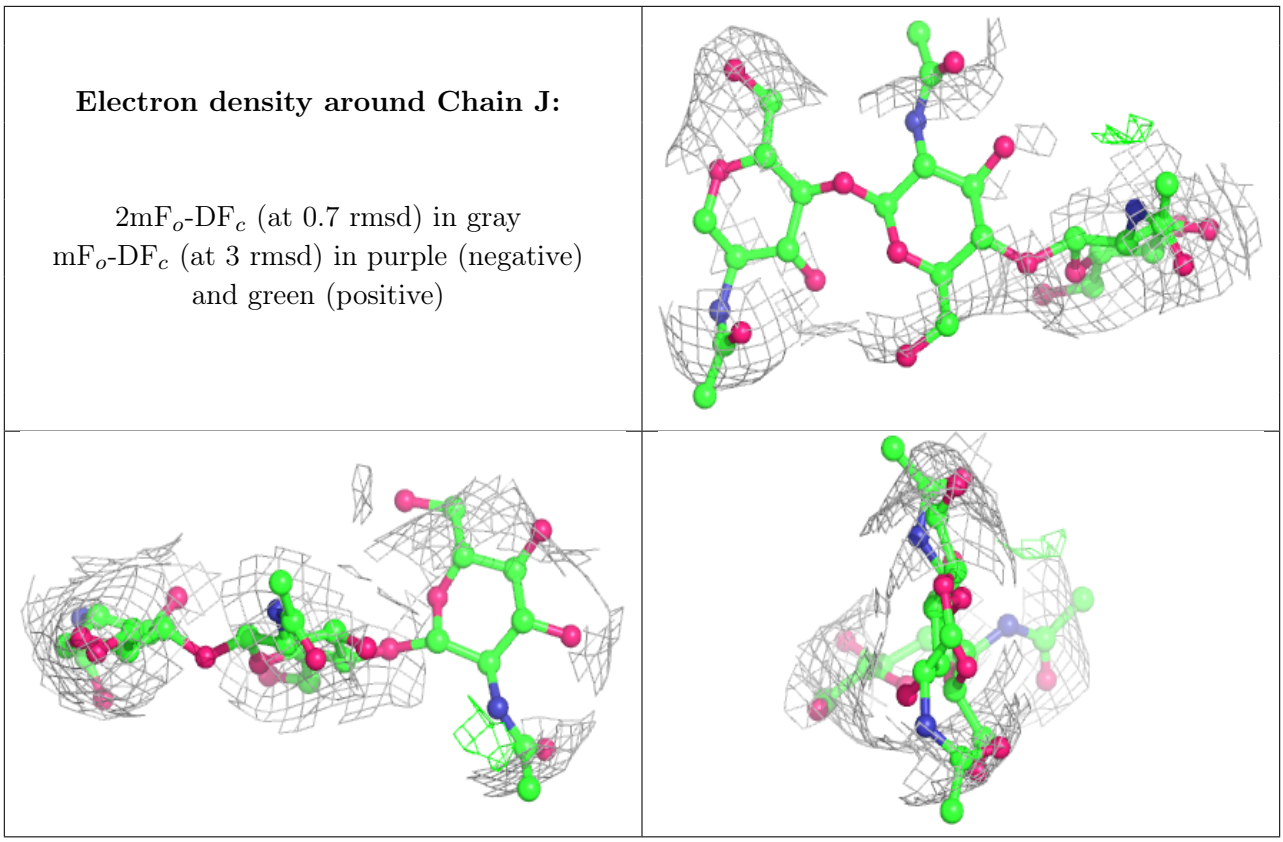






Electron density around Chain J:

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



6.4 Ligands

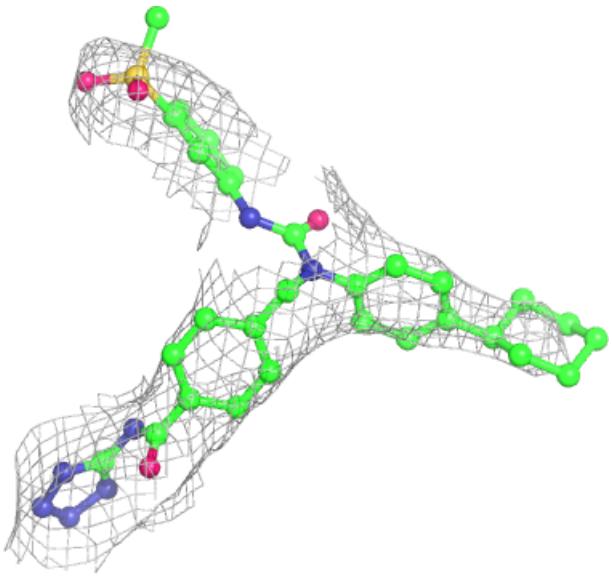
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

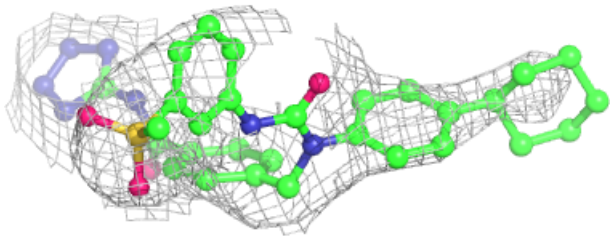
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	97V	A	1207	41/41	0.86	0.26	155,176,191,195	0
7	NAG	B	1206	14/15	0.90	0.17	123,131,137,149	0
6	97V	B	1209	41/41	0.91	0.23	157,173,187,188	0

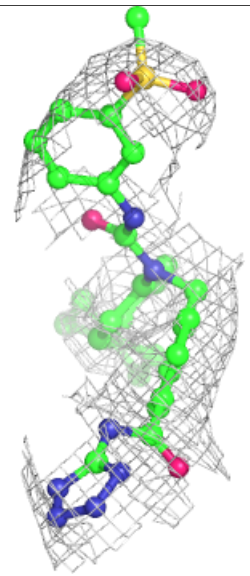
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 97V A 1207:

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

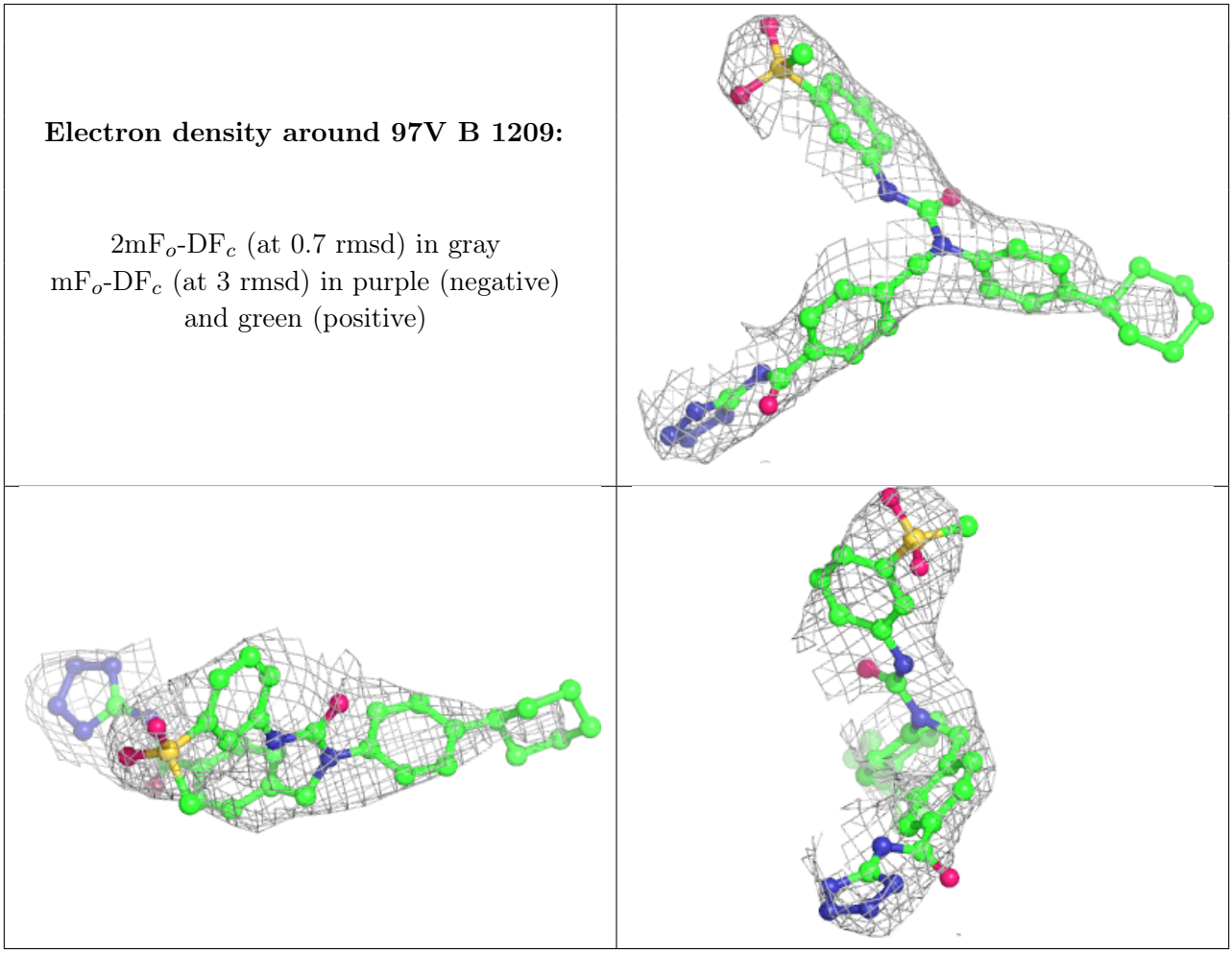






Electron density around 97V B 1209:

$2mF_o$-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.