Full wwPDB X-ray Structure Validation Report (i)

Sep 25, 2023 – 10:39 PM EDT

PDB ID	:	6BMH
Title	:	Crystal structure of MHC-I like protein
Authors	:	Khandokar, Y.B.; Le Nours, J.; Rossjohn, J.
Deposited on	:	2017-11-14
Resolution	:	2.30 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:

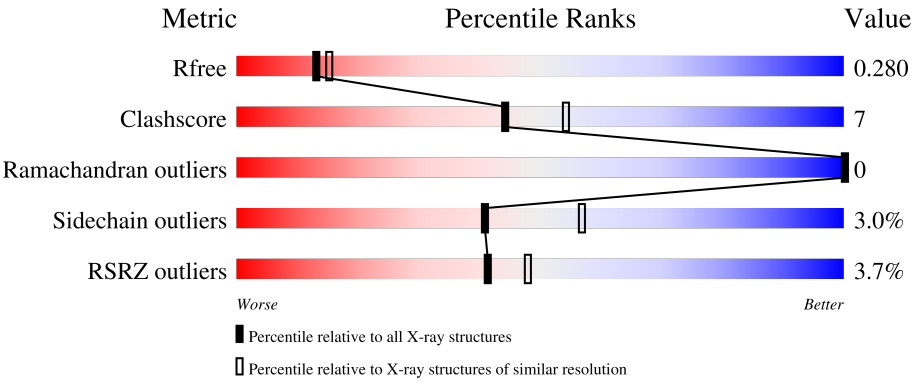
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	276	6% 78% 21%
1	C	276	8% 80% 19%
1	E	276	2% 81% 16%
1	G	276	3% 87% 11%
2	B	99	86% 13%

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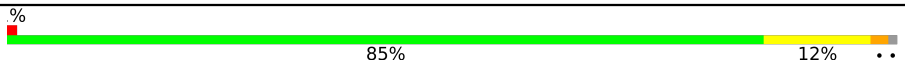
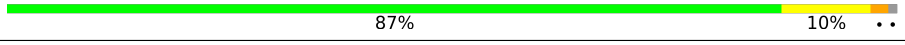
Mol	Chain	Length	Quality of chain
2	D	99	
2	F	99	
2	H	99	
3	I	2	
3	J	2	
3	K	2	
3	L	2	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12392 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 Antigen-presenting glycoprotein CD1d2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	7	2	0
			2138	1367	364	396	11			
1	C	273	Total	C	N	O	S	29	1	0
			2107	1349	358	389	11			
1	E	273	Total	C	N	O	S	11	2	0
			2146	1374	370	391	11			
1	G	273	Total	C	N	O	S	15	1	0
			2150	1375	368	396	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	46	ILE	THR	conflict	UNP P11610
C	46	ILE	THR	conflict	UNP P11610
E	46	ILE	THR	conflict	UNP P11610
G	46	ILE	THR	conflict	UNP P11610

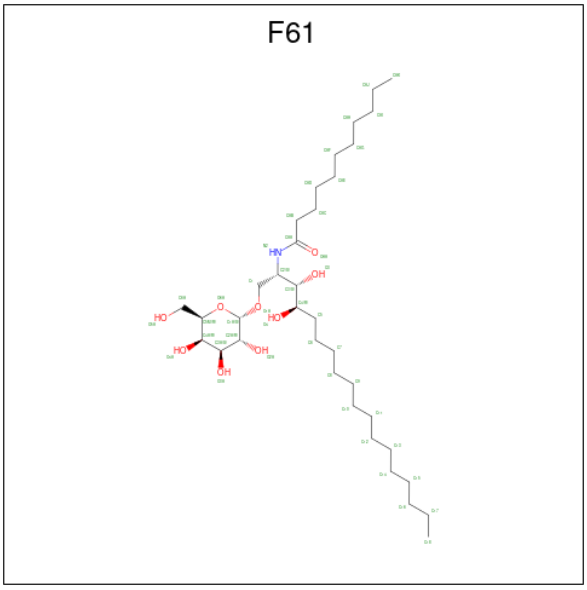
- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	98	Total	C	N	O	S	1	1	0
			800	512	137	144	7			
2	D	98	Total	C	N	O	S	0	0	0
			781	497	131	146	7			
2	F	98	Total	C	N	O	S	0	0	0
			805	515	137	146	7			
2	H	98	Total	C	N	O	S	0	0	0
			801	512	136	146	7			

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	I	2	Total C N O 28 16 2 10	0	0	0
3	J	2	Total C N O 28 16 2 10	0	0	0
3	K	2	Total C N O 28 16 2 10	0	0	0
3	L	2	Total C N O 28 16 2 10	0	0	0

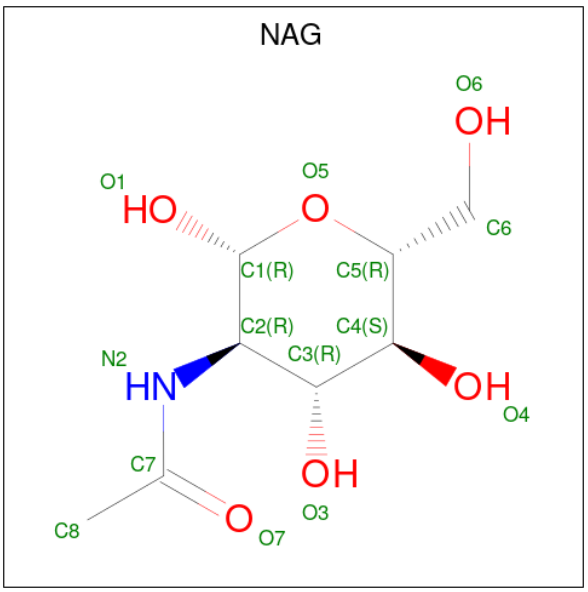
- Molecule 4 is N-[(2S,3S,4R)-1-(alpha-D-galactopyranosyloxy)-3,4-dihydroxyoctadecan-2-yl] undecanamide (three-letter code: F61) (formula: $C_{35}H_{69}NO_9$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 45 35 1 9	0	0
4	C	1	Total C N O 45 35 1 9	0	0
4	E	1	Total C N O 45 35 1 9	0	0
4	G	1	Total C N O 45 35 1 9	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:

$C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 14 8 1 5	0	0
5	C	1	Total C N O 14 8 1 5	0	0
5	E	1	Total C N O 14 8 1 5	0	0
5	G	1	Total C N O 14 8 1 5	0	0
5	G	1	Total C N O 15 8 1 6	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	35	Total O 35 35	0	0
6	B	32	Total O 32 32	0	0
6	C	56	Total O 56 56	0	0
6	D	29	Total O 29 29	0	0
6	E	37	Total O 37 37	0	0
6	F	33	Total O 33 33	0	0

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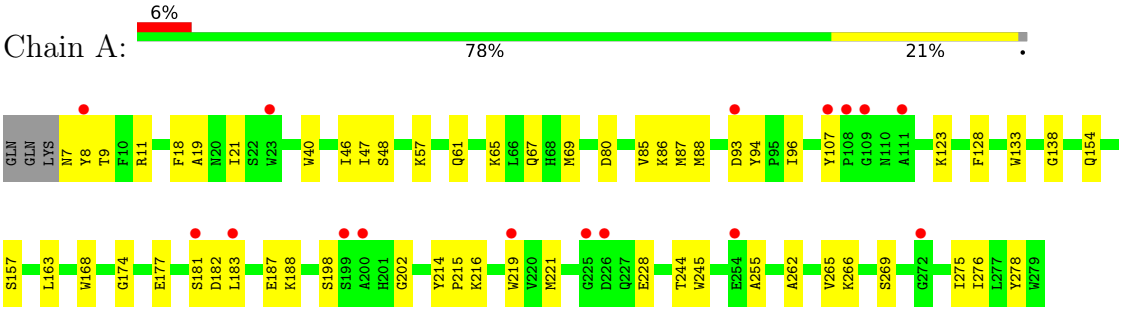
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	G	40	Total O 40 40	0	0
6	H	39	Total O 39 39	0	0

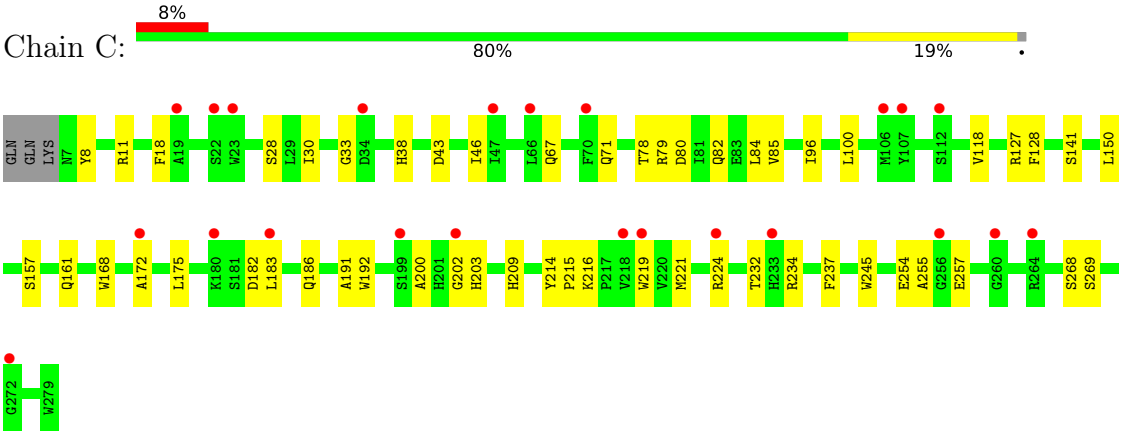
3 Residue-property plots (i)

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.

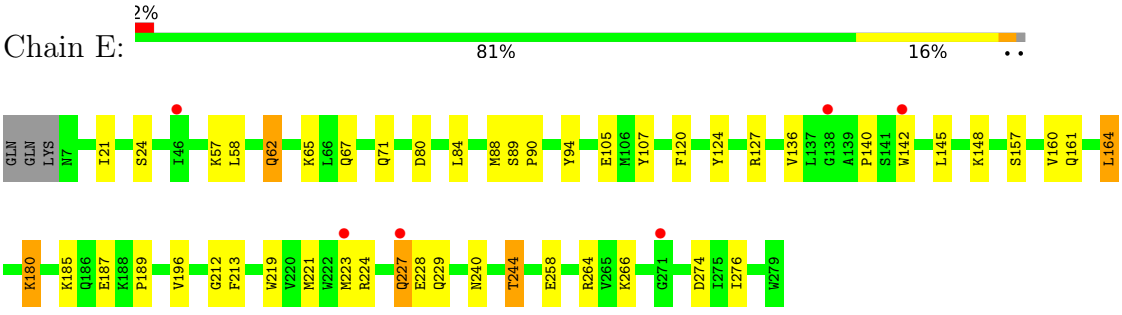
• Molecule 1: Antigen-presenting glycoprotein CD1d2



• Molecule 1: Antigen-presenting glycoprotein CD1d2

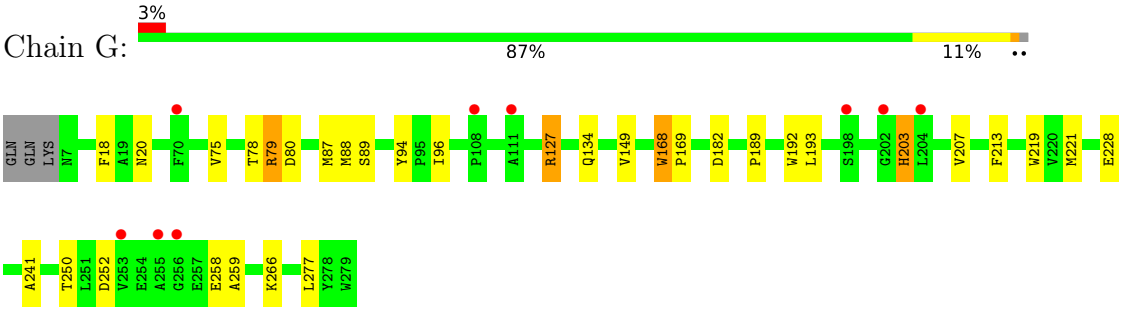


• Molecule 1: Antigen-presenting glycoprotein CD1d2



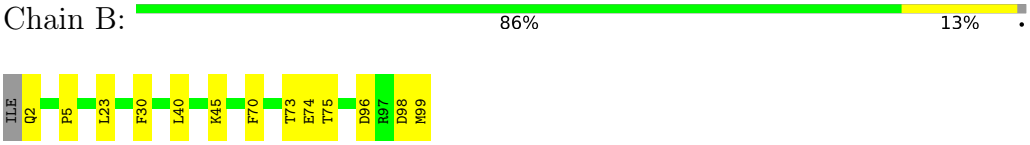
• Molecule 1: Antigen-presenting glycoprotein CD1d2

Chain G:



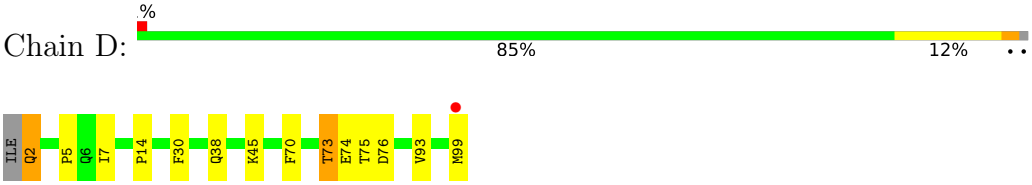
• Molecule 2: Beta-2-microglobulin

Chain B:



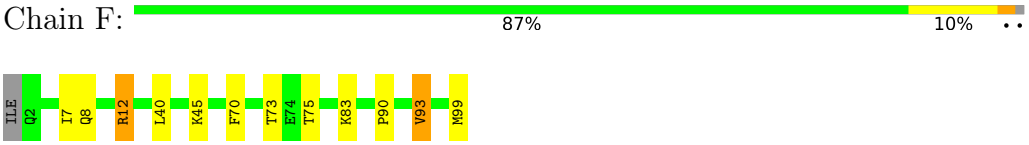
• Molecule 2: Beta-2-microglobulin

Chain D:



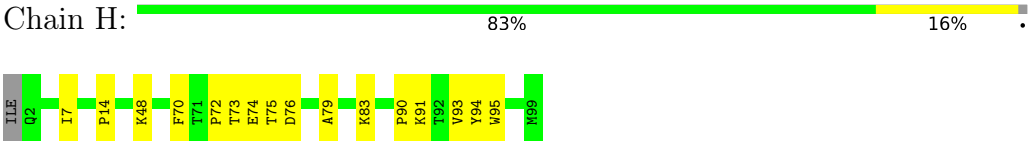
• Molecule 2: Beta-2-microglobulin

Chain F:



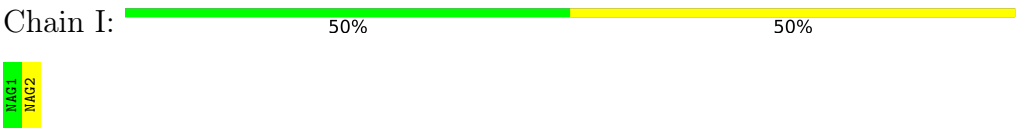
• Molecule 2: Beta-2-microglobulin

Chain H:



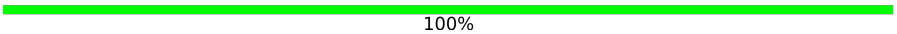
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:



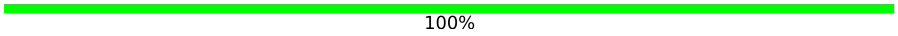
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:



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

Chain K:



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

Chain L:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	105.95Å 74.23Å 117.59Å 90.00° 102.94° 90.00°	Depositor
Resolution (Å)	45.93 – 2.30 45.93 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (45.93-2.30) 99.7 (45.93-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.01 (at 2.29Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.230 , 0.280 0.230 , 0.280	Depositor DCC
R_{free} test set	4000 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	36.2	Xtriage
Anisotropy	0.539	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 47.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	12392	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 63.27 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.9236e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, F61

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	0.30	0/2204	0.51	0/3007
1	C	0.34	0/2172	0.51	0/2967
1	E	0.29	0/2211	0.49	0/3012
1	G	0.29	0/2215	0.49	0/3016
2	B	0.29	0/830	0.47	0/1130
2	D	0.35	0/807	0.52	0/1104
2	F	0.29	0/831	0.47	0/1128
2	H	0.28	0/827	0.48	0/1124
All	All	0.31	0/12097	0.50	0/16488

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	2138	0	1993	37	0
1	C	2107	0	1954	33	0
1	E	2146	0	2028	32	0
1	G	2150	0	2036	20	0
2	B	800	0	760	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	781	0	713	12	0
2	F	805	0	779	6	0
2	H	801	0	768	12	0
3	I	28	0	25	1	0
3	J	28	0	25	0	0
3	K	28	0	25	0	0
3	L	28	0	25	1	0
4	A	45	0	0	1	0
4	C	45	0	0	1	0
4	E	45	0	0	1	0
4	G	45	0	0	1	0
5	A	14	0	13	0	0
5	C	14	0	13	0	0
5	E	14	0	13	0	0
5	G	29	0	27	0	0
6	A	35	0	0	3	0
6	B	32	0	0	2	0
6	C	56	0	0	2	0
6	D	29	0	0	1	0
6	E	37	0	0	0	0
6	F	33	0	0	1	0
6	G	40	0	0	3	0
6	H	39	0	0	0	0
All	All	12392	0	11197	152	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 7.

All (152) 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:G:80:ASP:OD1	4:G:301:F61:O4	1.61	1.17
1:G:79:ARG:NH2	6:G:401:HOH:O	1.77	1.13
1:E:80:ASP:OD2	4:E:301:F61:O4	1.84	0.95
1:E:196:VAL:HG11	2:F:99:MET:HG2	1.58	0.85
1:A:80:ASP:OD2	4:A:301:F61:O4	1.97	0.82
1:C:221:MET:SD	1:C:232:THR:HG21	2.24	0.77
1:A:40:TRP:HB2	1:A:47:ILE:HD13	1.71	0.72
1:E:223:MET:HE1	1:E:228:GLU:HA	1.71	0.70
1:G:75:VAL:O	1:G:79:ARG:HG2	1.92	0.70
1:E:21:ILE:HD12	1:E:94:TYR:CE2	2.27	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:186:GLN:NE2	1:C:268:SER:OG	2.26	0.69
1:A:57:LYS:HD3	1:A:177:GLU:OE2	1.92	0.69
2:D:73:THR:HG22	2:D:75:THR:H	1.58	0.68
6:G:402:HOH:O	3:L:1:NAG:O7	2.10	0.67
1:E:264:ARG:NH1	1:E:274:ASP:OD1	2.28	0.67
1:A:187:GLU:OE1	1:A:244:THR:HG22	1.95	0.67
1:A:48:SER:OG	6:A:401:HOH:O	2.13	0.66
1:E:62:GLN:HE21	2:H:74:GLU:HG2	1.61	0.66
1:C:172:ALA:HA	1:C:175:LEU:HB2	1.77	0.65
1:G:241:ALA:O	6:G:403:HOH:O	2.15	0.65
2:D:2:GLN:N	6:D:101:HOH:O	2.30	0.65
1:A:85:VAL:HG11	1:A:96:ILE:HD11	1.78	0.64
1:C:224:ARG:NH1	6:C:404:HOH:O	2.30	0.63
2:F:73:THR:HG22	2:F:75:THR:H	1.63	0.62
2:F:83:LYS:HG2	2:F:90:PRO:HG3	1.79	0.62
1:A:187:GLU:OE1	1:A:244:THR:CG2	2.49	0.60
2:F:12:ARG:NH2	6:F:101:HOH:O	2.24	0.60
2:B:2:GLN:N	6:B:103:HOH:O	2.32	0.60
1:A:202:GLY:O	1:A:255:ALA:N	2.33	0.60
1:C:18:PHE:HB2	1:C:96:ILE:HB	1.84	0.59
2:B:96:ASP:HB3	2:B:99:MET:HG2	1.85	0.59
1:A:7:ASN:OD1	1:A:107:TYR:HA	2.04	0.58
1:G:78:THR:HB	1:G:79:ARG:HE	1.68	0.58
1:E:240:ASN:HB2	1:E:244:THR:HG22	1.86	0.58
2:H:7:ILE:HD12	2:H:91:LYS:HD2	1.85	0.58
1:A:47:ILE:HB	1:A:67:GLN:HE21	1.69	0.57
1:C:78:THR:O	1:C:82:GLN:HG3	2.05	0.56
6:A:402:HOH:O	3:I:2:NAG:O4	2.18	0.56
1:G:203:HIS:NE2	1:G:252:ASP:OD1	2.39	0.55
1:C:202:GLY:O	1:C:255:ALA:N	2.37	0.55
1:E:189:PRO:HB3	1:E:213:PHE:HB3	1.89	0.55
1:E:212:GLY:HA2	1:E:244:THR:HG21	1.89	0.55
1:A:262:ALA:HB2	1:A:278:TYR:CD2	2.42	0.54
1:C:186:GLN:HE22	1:C:268:SER:CB	2.20	0.54
1:E:84:LEU:O	1:E:88:MET:HG2	2.07	0.54
1:C:216:LYS:HD3	1:C:245:TRP:CE2	2.43	0.54
1:E:140:PRO:HB2	1:E:142:TRP:CD1	2.43	0.54
1:A:216:LYS:HD3	1:A:245:TRP:CE2	2.43	0.54
1:A:21:ILE:HA	1:A:94:TYR:CZ	2.43	0.53
1:C:219:TRP:CZ2	1:C:221:MET:HG3	2.44	0.53
2:H:73:THR:HG23	2:H:75:THR:H	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:100:LEU:HD21	1:C:118:VAL:HG22	1.91	0.53
1:G:127:ARG:HD2	1:G:134:GLN:HB2	1.90	0.52
1:C:141:SER:HB2	2:H:48:LYS:HD2	1.91	0.52
1:C:254:GLU:O	1:C:257:GLU:HG3	2.10	0.52
1:A:11:ARG:NH1	6:A:403:HOH:O	2.31	0.51
2:D:73:THR:CG2	2:D:74:GLU:N	2.73	0.51
1:E:62:GLN:HE22	2:H:73:THR:HG23	1.74	0.51
1:C:11:ARG:NH2	1:C:33:GLY:O	2.29	0.51
1:A:128:PHE:HB2	1:A:133:TRP:CZ3	2.46	0.51
1:A:265:VAL:HB	1:A:275:ILE:HB	1.93	0.51
1:A:47:ILE:HB	1:A:67:GLN:NE2	2.25	0.51
2:H:73:THR:HG22	2:H:76:ASP:HB2	1.92	0.51
2:B:73:THR:HG22	2:B:75:THR:H	1.76	0.51
1:A:123:LYS:NZ	1:A:138:GLY:O	2.45	0.50
1:A:9:THR:HG22	1:A:11:ARG:HG3	1.92	0.50
1:E:21:ILE:HD12	1:E:94:TYR:CD2	2.46	0.50
1:A:18:PHE:HB2	1:A:96:ILE:HB	1.93	0.50
1:A:219:TRP:HB3	1:A:266:LYS:HB2	1.92	0.50
1:C:8:TYR:CE1	1:C:183:LEU:HD23	2.46	0.50
1:G:18:PHE:HB2	1:G:96:ILE:HB	1.94	0.50
1:A:61:GLN:O	1:A:65:LYS:HG3	2.13	0.49
1:C:157:SER:O	1:C:161:GLN:HG3	2.13	0.49
2:B:5:PRO:HB3	2:B:30:PHE:HB3	1.95	0.48
1:E:219:TRP:CH2	1:E:221:MET:HB2	2.48	0.48
1:E:105:GLU:HG2	1:E:107:TYR:CZ	2.48	0.48
1:E:157:SER:O	1:E:161:GLN:HG3	2.13	0.48
1:E:185:LYS:HD3	1:E:187:GLU:OE2	2.13	0.48
1:G:219:TRP:HB3	1:G:266:LYS:HB2	1.95	0.48
1:A:86:LYS:HA	1:A:93:ASP:CG	2.35	0.47
1:G:193:LEU:CD1	1:G:277:LEU:HD22	2.44	0.47
1:G:20:ASN:HA	1:G:94:TYR:CG	2.49	0.47
1:A:69:MET:CE	1:A:163:LEU:HD11	2.45	0.47
1:A:87:MET:HG2	1:A:88:MET:HG2	1.97	0.46
1:A:154:GLN:HA	1:A:157:SER:HB3	1.97	0.46
1:C:30:ILE:HB	1:C:38:HIS:HB2	1.97	0.46
1:C:100:LEU:CD2	1:C:118:VAL:HG22	2.46	0.46
1:E:88:MET:SD	1:E:145:LEU:HD22	2.55	0.46
1:G:87:MET:HE1	1:G:149:VAL:HG21	1.97	0.46
1:C:85:VAL:HG11	1:C:96:ILE:HD11	1.97	0.46
2:D:73:THR:CG2	2:D:75:THR:H	2.25	0.46
2:D:5:PRO:HB3	2:D:30:PHE:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:264:ARG:NE	1:E:276:ILE:HD11	2.31	0.46
1:E:62:GLN:HE22	2:H:73:THR:CG2	2.29	0.46
1:C:67:GLN:O	1:C:71:GLN:HG3	2.15	0.46
1:G:168:TRP:HB2	1:G:169:PRO:HD3	1.98	0.46
1:C:46:ILE:HD11	1:C:67:GLN:CD	2.36	0.45
1:A:57:LYS:HE2	1:A:174:GLY:CA	2.47	0.45
2:D:73:THR:HG22	2:D:76:ASP:H	1.80	0.45
1:E:67:GLN:O	1:E:71:GLN:HG3	2.17	0.44
2:H:83:LYS:HG2	2:H:90:PRO:HB3	2.00	0.44
1:C:79:ARG:NH2	6:C:405:HOH:O	2.40	0.44
1:C:191:ALA:HA	1:C:209:HIS:O	2.17	0.44
1:E:120:PHE:CE2	1:E:142:TRP:HZ2	2.36	0.44
1:A:21:ILE:HA	1:A:94:TYR:OH	2.17	0.44
1:A:214:TYR:CG	1:A:215:PRO:HA	2.52	0.44
1:C:214:TYR:CG	1:C:215:PRO:HA	2.53	0.44
2:D:38:GLN:OE1	2:D:45:LYS:HE3	2.17	0.44
1:C:234:ARG:NH2	1:C:237:PHE:CE1	2.86	0.44
1:C:186:GLN:OE1	1:C:269:SER:HA	2.18	0.43
2:B:73:THR:HG22	2:B:74:GLU:N	2.34	0.43
1:E:89:SER:HA	1:E:90:PRO:HA	1.59	0.43
1:G:20:ASN:HA	1:G:94:TYR:CB	2.48	0.43
1:G:207:VAL:HG12	1:G:250:THR:HG22	2.00	0.43
2:B:23:LEU:HB2	2:B:70:PHE:CD1	2.53	0.43
1:E:221:MET:HE2	1:E:228:GLU:HB3	2.00	0.43
1:A:276:ILE:HD12	1:G:259:ALA:HB3	2.01	0.43
1:E:219:TRP:CE3	1:E:266:LYS:HD2	2.54	0.43
1:G:189:PRO:HB3	1:G:213:PHE:HB3	2.00	0.43
2:B:40:LEU:HD23	2:B:45:LYS:HA	2.01	0.43
2:D:73:THR:HG23	2:D:74:GLU:N	2.34	0.43
1:C:80:ASP:OD2	4:C:301:F61:O4	2.37	0.43
1:C:209:HIS:HE1	2:D:99:MET:O	2.02	0.43
1:E:180:LYS:HB3	1:E:180:LYS:HE3	1.62	0.43
1:A:19:ALA:O	1:A:94:TYR:HB3	2.19	0.42
2:B:98:ASP:OD2	6:B:101:HOH:O	2.21	0.42
1:E:160:VAL:O	1:E:164:LEU:HD22	2.20	0.42
1:G:193:LEU:HG	1:G:277:LEU:HD22	2.00	0.42
1:G:221:MET:HE2	1:G:228:GLU:HB3	2.01	0.42
2:H:79:ALA:HB2	2:H:94:TYR:CD2	2.54	0.42
1:A:46:ILE:HG13	1:A:67:GLN:NE2	2.35	0.42
2:F:7:ILE:HB	2:F:93:VAL:HG11	2.01	0.42
2:F:40:LEU:HD23	2:F:45:LYS:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:65:LYS:HA	1:E:65:LYS:HD2	1.64	0.42
1:C:175:LEU:HD23	1:C:175:LEU:HA	1.87	0.41
1:E:58:LEU:HD21	2:H:74:GLU:OE2	2.20	0.41
1:C:127:ARG:HG2	1:C:128:PHE:N	2.36	0.41
2:D:73:THR:HG23	2:D:74:GLU:H	1.84	0.41
1:A:221:MET:HE2	1:A:228:GLU:HB3	2.03	0.41
1:A:46:ILE:HD12	1:A:46:ILE:HA	1.80	0.41
1:A:86:LYS:HA	1:A:93:ASP:OD2	2.21	0.41
1:A:188:LYS:HA	1:A:269:SER:OG	2.21	0.41
1:C:192:TRP:CE3	2:D:14:PRO:HG3	2.55	0.41
1:A:8:TYR:CE1	1:A:183:LEU:HD22	2.55	0.41
1:E:224:ARG:HB2	1:E:227:GLN:HG2	2.02	0.41
1:C:46:ILE:HD12	1:C:46:ILE:HA	1.75	0.40
2:D:7:ILE:HB	2:D:93:VAL:HG11	2.03	0.40
1:E:124:TYR:CZ	1:E:136:VAL:HG11	2.55	0.40
1:G:192:TRP:CE3	2:H:14:PRO:HG3	2.56	0.40
1:E:224:ARG:HE	1:E:229:GLN:NE2	2.20	0.40
2:H:72:PRO:HB3	2:H:95:TRP:CH2	2.57	0.40
1:C:200:ALA:HB3	1:C:203:HIS:HB2	2.03	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	273/276 (99%)	268 (98%)	5 (2%)	0	100	100
1	C	272/276 (99%)	262 (96%)	10 (4%)	0	100	100
1	E	273/276 (99%)	264 (97%)	9 (3%)	0	100	100
1	G	272/276 (99%)	263 (97%)	9 (3%)	0	100	100
2	B	97/99 (98%)	96 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	96/99 (97%)	96 (100%)	0	0	100	100
2	F	96/99 (97%)	95 (99%)	1 (1%)	0	100	100
2	H	96/99 (97%)	96 (100%)	0	0	100	100
All	All	1475/1500 (98%)	1440 (98%)	35 (2%)	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	222/240 (92%)	218 (98%)	4 (2%)	59	75
1	C	216/240 (90%)	210 (97%)	6 (3%)	43	60
1	E	223/240 (93%)	213 (96%)	10 (4%)	27	39
1	G	226/240 (94%)	218 (96%)	8 (4%)	36	50
2	B	89/93 (96%)	89 (100%)	0	100	100
2	D	85/93 (91%)	82 (96%)	3 (4%)	36	50
2	F	91/93 (98%)	87 (96%)	4 (4%)	28	39
2	H	90/93 (97%)	88 (98%)	2 (2%)	52	69
All	All	1242/1332 (93%)	1205 (97%)	37 (3%)	41	57

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	168	TRP
1	A	181	SER
1	A	182	ASP
1	A	198	SER
1	C	28	SER
1	C	43	ASP
1	C	84	LEU
1	C	150	LEU

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Mol	Chain	Res	Type
1	C	168	TRP
1	C	182	ASP
2	D	2	GLN
2	D	70	PHE
2	D	73	THR
1	E	24	SER
1	E	57	LYS
1	E	62	GLN
1	E	127	ARG
1	E	148	LYS
1	E	164	LEU
1	E	180	LYS
1	E	227	GLN
1	E	244	THR
1	E	258	GLU
2	F	8	GLN
2	F	12	ARG
2	F	70	PHE
2	F	93	VAL
1	G	79	ARG
1	G	88	MET
1	G	89	SER
1	G	127	ARG
1	G	168	TRP
1	G	182	ASP
1	G	203	HIS
1	G	258	GLU
2	H	70	PHE
2	H	93	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	GLN
1	C	67	GLN
1	C	186	GLN
1	E	62	GLN
1	E	229	GLN
1	G	134	GLN
2	H	38	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)

8 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	I	1	1,3	14,14,15	0.23	0	17,19,21	0.53	0
3	NAG	I	2	3	14,14,15	0.20	0	17,19,21	0.40	0
3	NAG	J	1	1,3	14,14,15	0.24	0	17,19,21	0.41	0
3	NAG	J	2	3	14,14,15	0.26	0	17,19,21	0.56	0
3	NAG	K	1	3	14,14,15	0.25	0	17,19,21	0.55	0
3	NAG	K	2	3	14,14,15	0.17	0	17,19,21	0.37	0
3	NAG	L	1	1,3	14,14,15	0.27	0	17,19,21	0.35	0
3	NAG	L	2	3	14,14,15	0.20	0	17,19,21	0.63	0

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	L	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	L	2	3	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	L	2	NAG	O5-C5-C6-O6
3	K	2	NAG	C4-C5-C6-O6
3	K	1	NAG	C4-C5-C6-O6
3	L	2	NAG	C4-C5-C6-O6
3	K	1	NAG	O5-C5-C6-O6
3	K	2	NAG	O5-C5-C6-O6
3	L	1	NAG	C4-C5-C6-O6
3	J	2	NAG	O5-C5-C6-O6
3	L	1	NAG	O5-C5-C6-O6

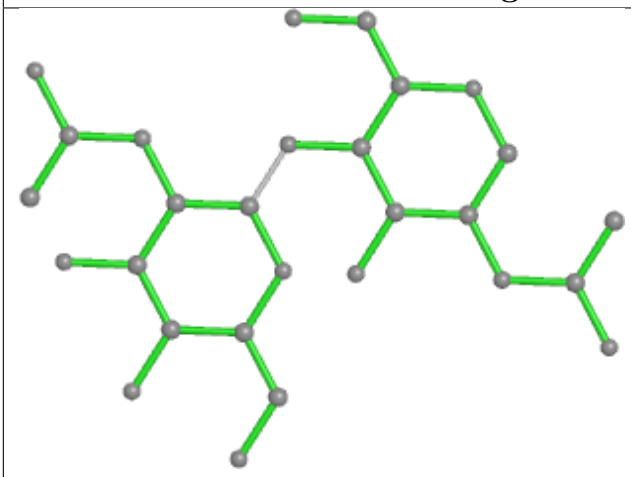
There are no ring outliers.

2 monomers are involved in 2 short contacts:

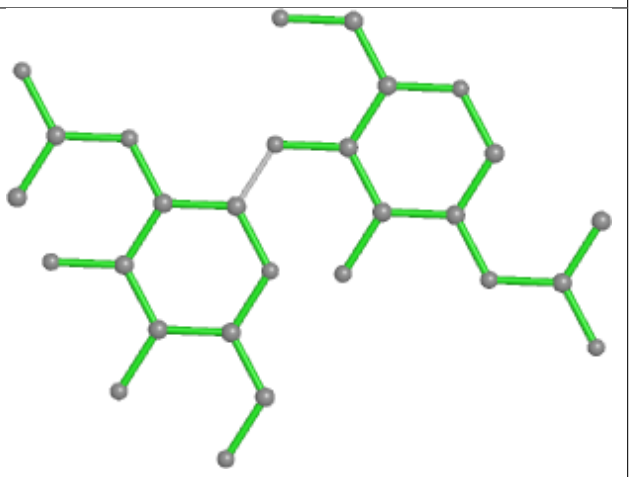
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L	1	NAG	1	0
3	I	2	NAG	1	0

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

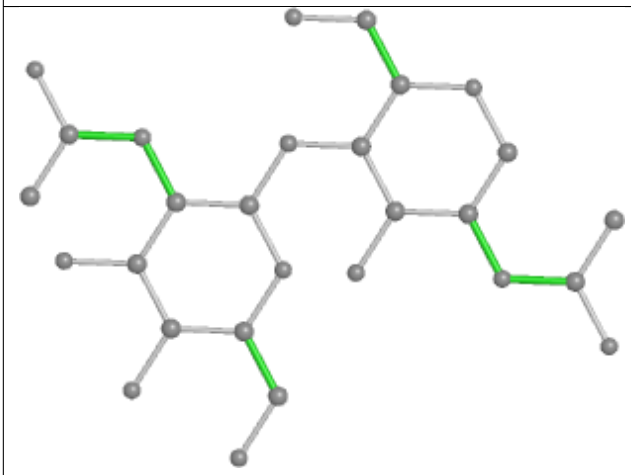
Oligosaccharide Chain I



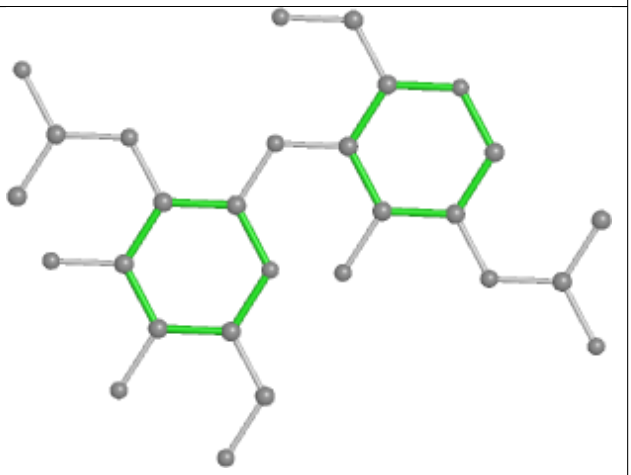
Bond lengths



Bond angles

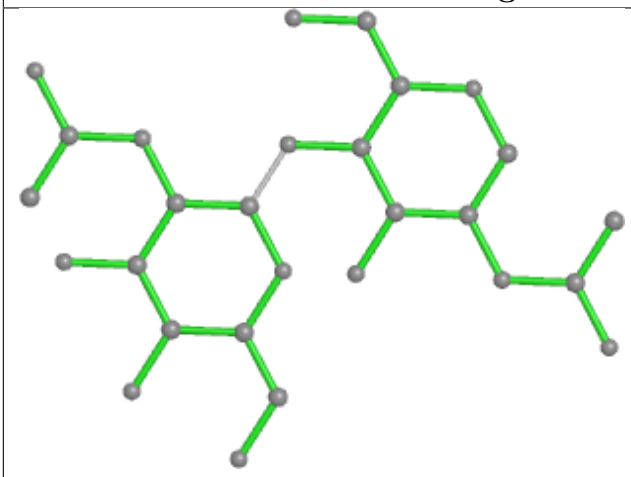


Torsions

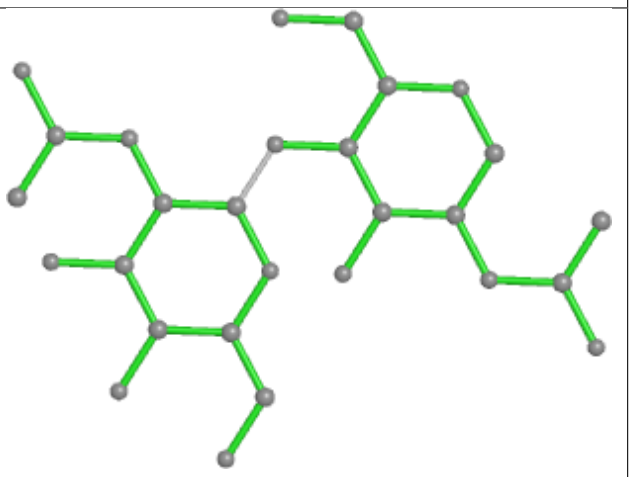


Rings

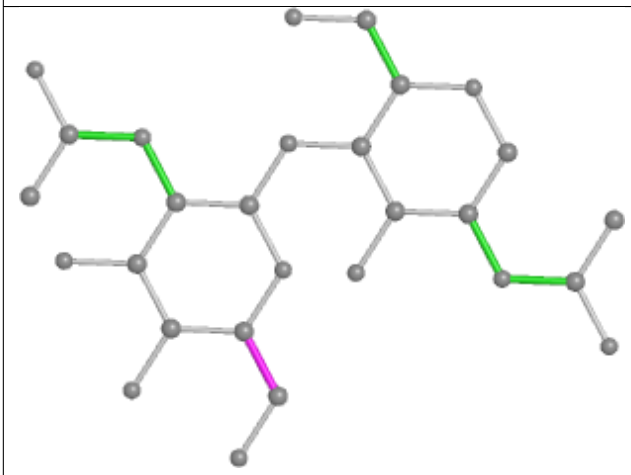
Oligosaccharide Chain J



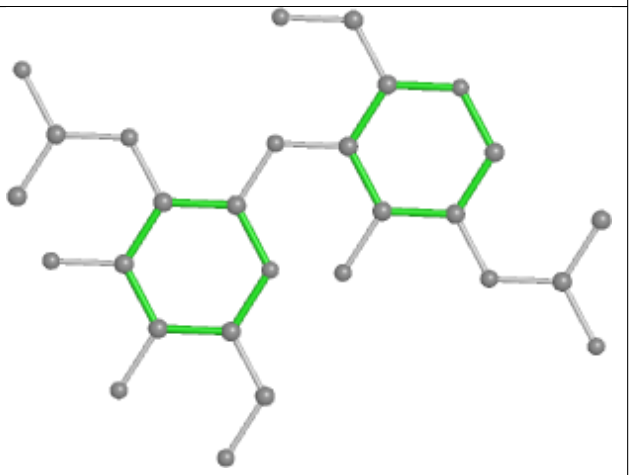
Bond lengths



Bond angles

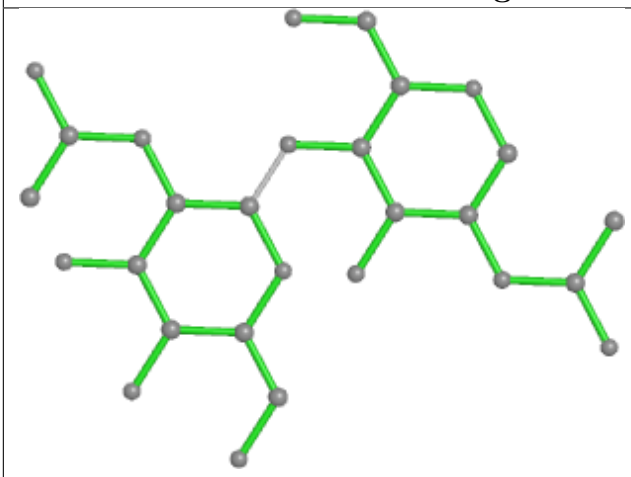


Torsions

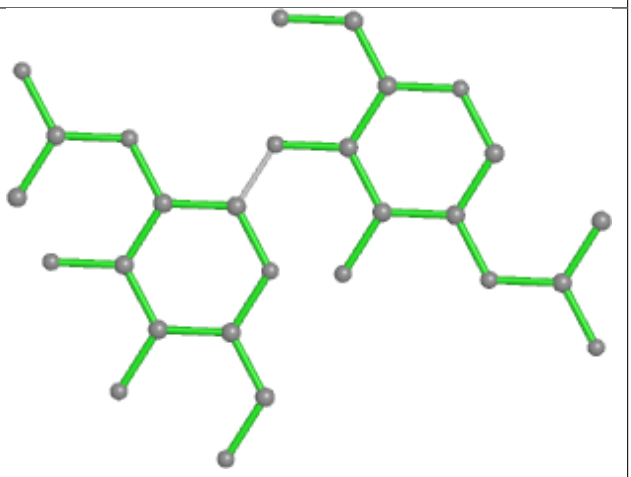


Rings

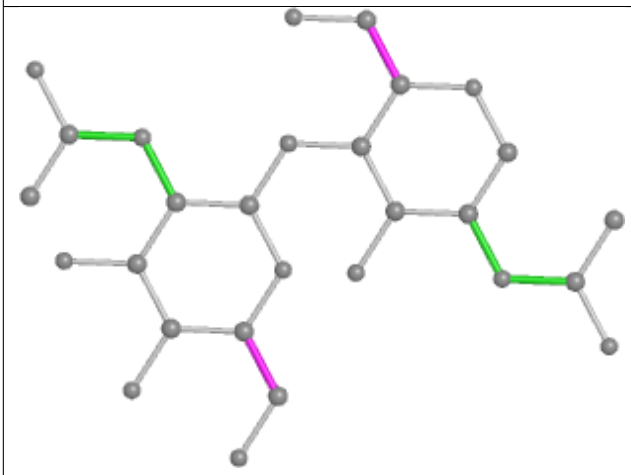
Oligosaccharide Chain K



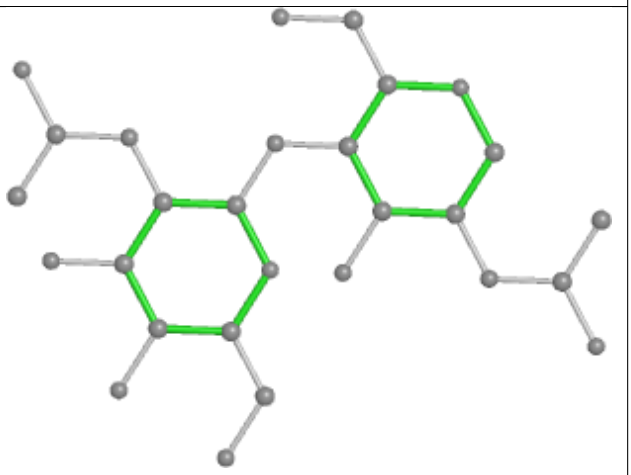
Bond lengths



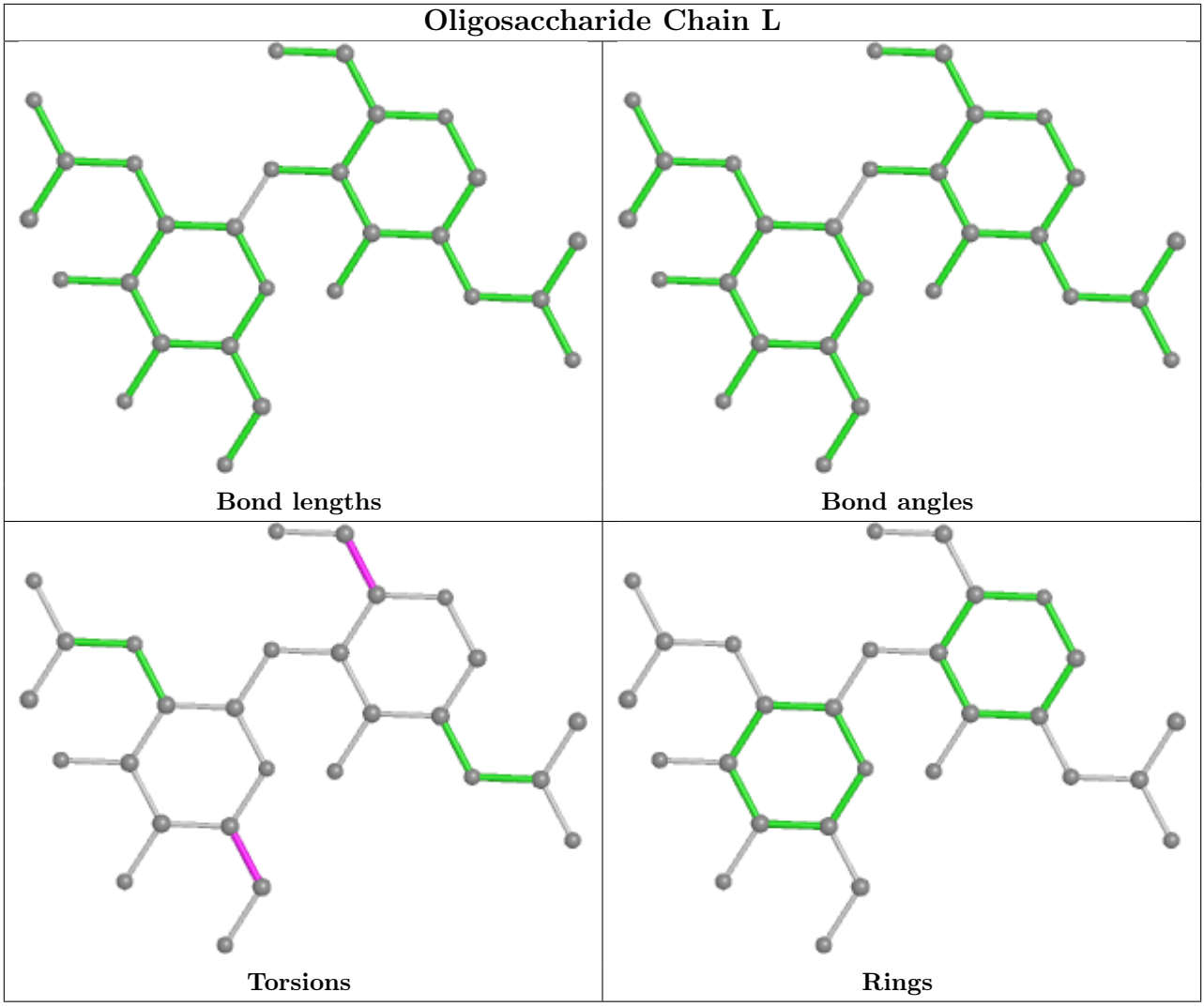
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

9 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	NAG	G	302	1	14,14,15	0.22	0	17,19,21	0.43	0
5	NAG	C	302	1	14,14,15	0.38	0	17,19,21	0.43	0
5	NAG	E	302	1	14,14,15	0.34	0	17,19,21	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	F61	G	301	-	45,45,45	1.49	7 (15%)	50,54,54	1.77	12 (24%)
5	NAG	A	302	1	14,14,15	0.32	0	17,19,21	0.47	0
4	F61	A	301	-	45,45,45	1.47	7 (15%)	50,54,54	1.28	7 (14%)
4	F61	C	301	-	45,45,45	1.60	5 (11%)	50,54,54	1.29	6 (12%)
5	NAG	G	305	-	15,15,15	1.72	3 (20%)	21,21,21	2.38	7 (33%)
4	F61	E	301	-	45,45,45	1.52	8 (17%)	50,54,54	1.67	13 (26%)

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	NAG	G	302	1	-	0/6/23/26	0/1/1/1
5	NAG	C	302	1	-	0/6/23/26	0/1/1/1
5	NAG	E	302	1	-	2/6/23/26	0/1/1/1
4	F61	G	301	-	-	20/43/63/63	0/1/1/1
5	NAG	A	302	1	-	2/6/23/26	0/1/1/1
4	F61	A	301	-	-	11/43/63/63	0/1/1/1
4	F61	C	301	-	-	4/43/63/63	0/1/1/1
5	NAG	G	305	-	-	1/6/26/26	0/1/1/1
4	F61	E	301	-	-	13/43/63/63	0/1/1/1

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	301	F61	CAA-N2	7.27	1.49	1.34
4	G	301	F61	CAA-N2	5.92	1.46	1.34
4	A	301	F61	CAA-N2	5.34	1.45	1.34
4	E	301	F61	CAA-N2	5.33	1.45	1.34
4	E	301	F61	O1A-C1	-4.09	1.36	1.43
4	A	301	F61	OAA-CAA	-3.98	1.15	1.23
4	A	301	F61	O1A-C1	-3.97	1.36	1.43
4	E	301	F61	OAA-CAA	-3.83	1.15	1.23
4	G	301	F61	OAA-CAA	-3.70	1.15	1.23
5	G	305	NAG	C7-N2	3.50	1.46	1.34
4	C	301	F61	CAB-CAA	3.30	1.57	1.51
4	G	301	F61	O1A-C1	-3.20	1.37	1.43
5	G	305	NAG	O5-C1	2.81	1.49	1.42
4	C	301	F61	O1A-C1	-2.77	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	305	NAG	C2-N2	2.73	1.50	1.45
4	C	301	F61	O6A-C1A	2.63	1.48	1.41
4	A	301	F61	O1A-C1A	-2.56	1.35	1.40
4	E	301	F61	O4-C4	-2.48	1.38	1.43
4	E	301	F61	O1A-C1A	-2.43	1.36	1.40
4	G	301	F61	O1A-C1A	-2.38	1.36	1.40
4	E	301	F61	O6A-C1A	2.37	1.47	1.41
4	A	301	F61	C2A-C3A	-2.33	1.46	1.52
4	G	301	F61	C2A-C3A	-2.33	1.46	1.52
4	G	301	F61	O4-C4	-2.31	1.38	1.43
4	C	301	F61	OAA-CAA	-2.16	1.18	1.23
4	A	301	F61	O6A-C1A	2.15	1.47	1.41
4	E	301	F61	O3-C3	-2.11	1.38	1.43
4	A	301	F61	O4-C4	-2.11	1.38	1.43
4	G	301	F61	CAB-CAA	2.07	1.55	1.51
4	E	301	F61	C3A-C4A	-2.04	1.47	1.52

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	G	305	NAG	O5-C5-C4	5.35	119.40	109.69
5	G	305	NAG	C4-C3-C2	4.77	117.33	110.34
4	G	301	F61	C1-C2-N2	-4.67	102.73	109.61
5	G	305	NAG	O5-C1-C2	4.52	114.06	109.52
4	G	301	F61	C1-C2-C3	-3.92	105.01	112.71
5	G	305	NAG	C3-C4-C5	3.90	117.19	110.24
4	G	301	F61	CAB-CAA-N2	3.74	122.32	115.83
4	E	301	F61	C6-C5-C4	-3.49	108.44	114.18
4	E	301	F61	C1-C2-N2	-3.42	104.58	109.61
4	G	301	F61	C6-C5-C4	-3.31	108.75	114.18
4	E	301	F61	O6A-C5M-C6A	3.23	114.48	106.44
5	G	305	NAG	O5-C5-C6	3.20	114.39	106.44
4	E	301	F61	C2A-C3A-C4A	3.08	116.21	110.82
4	C	301	F61	C6-C5-C4	-2.99	109.26	114.18
4	E	301	F61	C1-O1A-C1A	2.98	119.56	113.74
4	G	301	F61	O5A-C6A-C5M	-2.92	101.28	111.29
4	G	301	F61	O4-C4-C3	-2.83	102.21	109.10
4	G	301	F61	C8-C7-C6	-2.78	100.32	114.42
4	E	301	F61	CAB-CAA-N2	2.74	120.58	115.83
4	A	301	F61	CAB-CAA-N2	2.56	120.27	115.83
4	E	301	F61	C2-N2-CAA	-2.51	119.24	123.48
4	C	301	F61	C1-C2-C3	-2.48	107.83	112.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	301	F61	OAA-CAA-N2	-2.39	118.92	122.95
4	E	301	F61	CAD-CAC-CAB	-2.37	104.66	113.19
4	C	301	F61	CAB-CAA-N2	2.34	119.89	115.83
5	G	305	NAG	C1-C2-N2	-2.32	108.03	110.73
4	G	301	F61	O2A-C2A-C3A	-2.31	105.02	110.35
4	G	301	F61	O6A-C1A-C2A	-2.27	105.54	110.35
4	E	301	F61	O3A-C3A-C2A	-2.27	105.11	110.35
4	A	301	F61	C6-C5-C4	-2.21	110.54	114.18
5	G	305	NAG	C8-C7-N2	2.20	119.82	116.10
4	C	301	F61	C1-O1A-C1A	2.19	118.02	113.74
4	A	301	F61	CAC-CAB-CAA	-2.18	107.14	113.26
4	C	301	F61	OAA-CAA-N2	-2.15	119.32	122.95
4	E	301	F61	C7-C6-C5	-2.15	106.02	113.62
4	A	301	F61	OAA-CAA-N2	-2.13	119.35	122.95
4	C	301	F61	C2-N2-CAA	-2.13	119.90	123.48
4	E	301	F61	O4-C4-C5	-2.09	104.61	109.15
4	G	301	F61	C8-C9-C10	-2.07	103.94	114.42
4	E	301	F61	C1A-O6A-C5M	-2.06	109.64	113.69
4	A	301	F61	CAD-CAC-CAB	-2.03	105.88	113.19
4	G	301	F61	O1A-C1A-C2A	2.02	111.46	108.30
4	A	301	F61	C1-O1A-C1A	2.01	117.67	113.74
4	E	301	F61	OAA-CAA-N2	-2.01	119.56	122.95
4	A	301	F61	C8-C9-C10	-2.01	104.23	114.42

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	301	F61	C2-C3-C4-C5
4	G	301	F61	O3-C3-C4-C5
4	G	301	F61	O3-C3-C4-O4
4	A	301	F61	CAA-CAB-CAC-CAD
5	A	302	NAG	O5-C5-C6-O6
5	G	305	NAG	C4-C5-C6-O6
5	A	302	NAG	C4-C5-C6-O6
4	G	301	F61	C2-C3-C4-O4
4	A	301	F61	C13-C14-C15-C16
4	G	301	F61	CAF-CAG-CAH-CAI
4	E	301	F61	C6-C7-C8-C9
4	E	301	F61	CAA-CAB-CAC-CAD
4	C	301	F61	O6A-C5M-C6A-O5A
4	E	301	F61	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
4	G	301	F61	C7-C8-C9-C10
4	A	301	F61	C6-C7-C8-C9
4	G	301	F61	CAD-CAE-CAF-CAG
4	A	301	F61	CAF-CAG-CAH-CAI
4	G	301	F61	C13-C14-C15-C16
4	E	301	F61	CAF-CAG-CAH-CAI
4	E	301	F61	C11-C12-C13-C14
4	C	301	F61	C9-C10-C11-C12
4	G	301	F61	C9-C10-C11-C12
4	C	301	F61	C6-C7-C8-C9
4	G	301	F61	C11-C10-C9-C8
4	E	301	F61	CAG-CAH-CAI-CAJ
4	A	301	F61	CAB-CAC-CAD-CAE
4	A	301	F61	CAC-CAD-CAE-CAF
5	E	302	NAG	C4-C5-C6-O6
4	G	301	F61	CAC-CAD-CAE-CAF
4	E	301	F61	C11-C10-C9-C8
4	E	301	F61	CAC-CAD-CAE-CAF
4	G	301	F61	CAE-CAF-CAG-CAH
5	E	302	NAG	O5-C5-C6-O6
4	A	301	F61	O6A-C1A-O1A-C1
4	G	301	F61	O6A-C5M-C6A-O5A
4	G	301	F61	C10-C11-C12-C13
4	A	301	F61	C11-C12-C13-C14
4	C	301	F61	CAB-CAC-CAD-CAE
4	G	301	F61	C6-C7-C8-C9
4	A	301	F61	CAG-CAH-CAI-CAJ
4	E	301	F61	C9-C10-C11-C12
4	A	301	F61	C11-C10-C9-C8
4	E	301	F61	CAD-CAE-CAF-CAG
4	E	301	F61	O6A-C1A-O1A-C1
4	E	301	F61	C2A-C1A-O1A-C1
4	G	301	F61	O6A-C1A-O1A-C1
4	G	301	F61	C4A-C5M-C6A-O5A
4	G	301	F61	OAA-CAA-CAB-CAC
4	G	301	F61	C12-C13-C14-C15
4	G	301	F61	N2-CAA-CAB-CAC
4	A	301	F61	CAD-CAE-CAF-CAG
4	E	301	F61	C15-C16-C17-C18

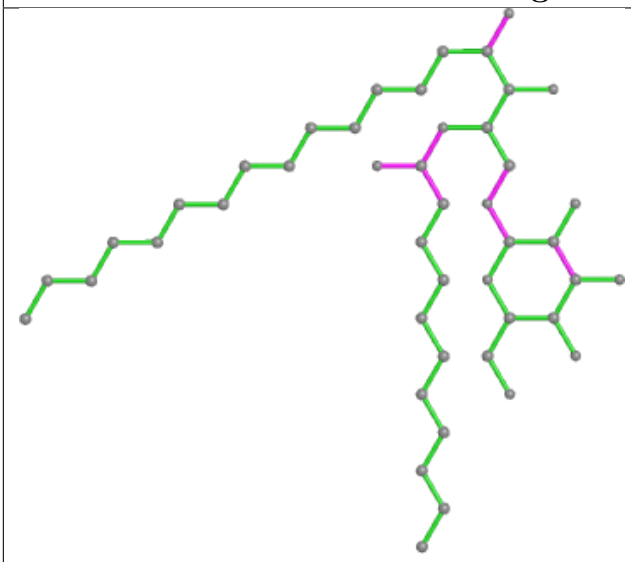
There are no ring outliers.

4 monomers are involved in 4 short contacts:

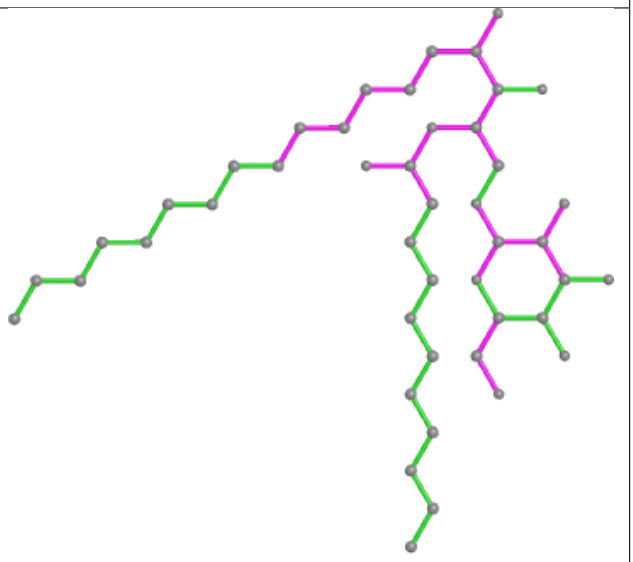
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	301	F61	1	0
4	A	301	F61	1	0
4	C	301	F61	1	0
4	E	301	F61	1	0

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

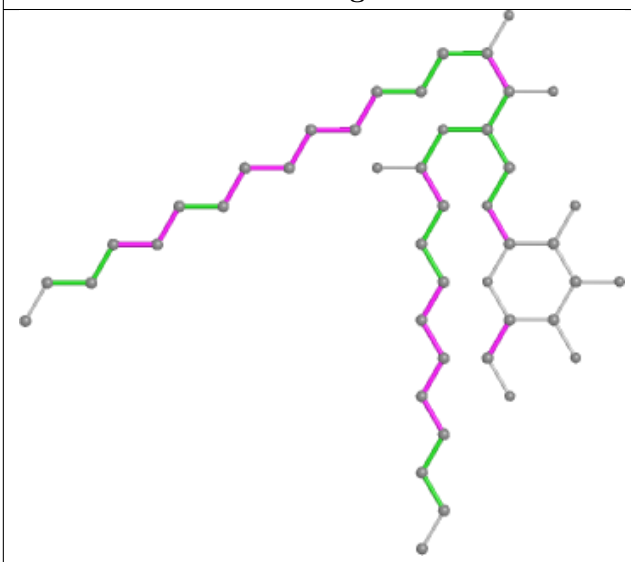
Ligand F61 G 301



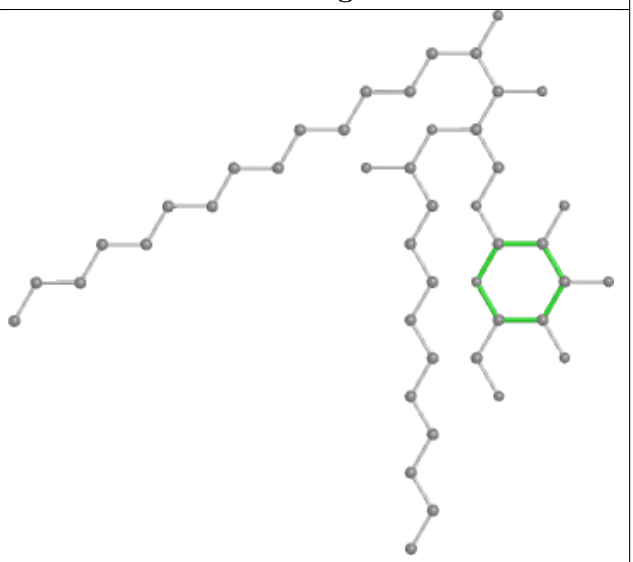
Bond lengths



Bond angles

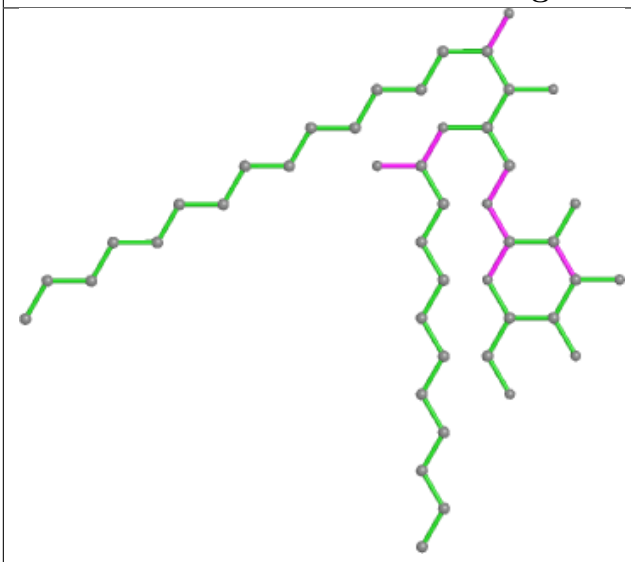


Torsions

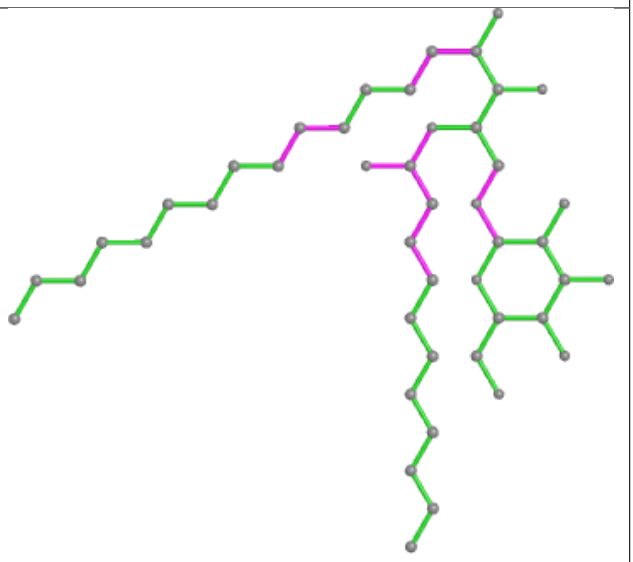


Rings

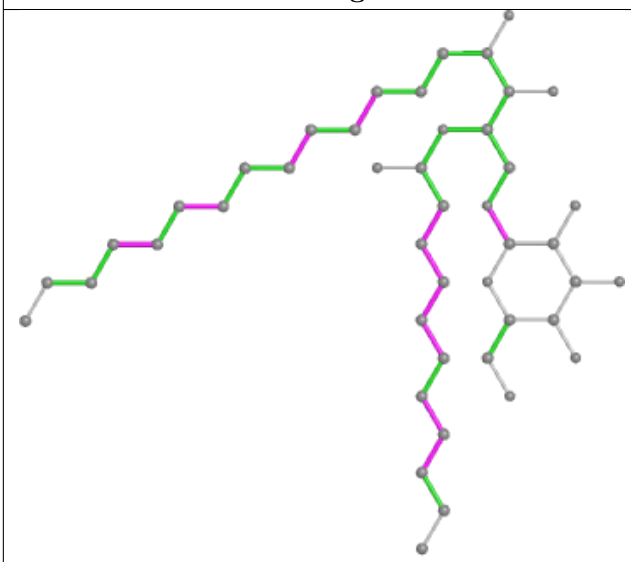
Ligand F61 A 301



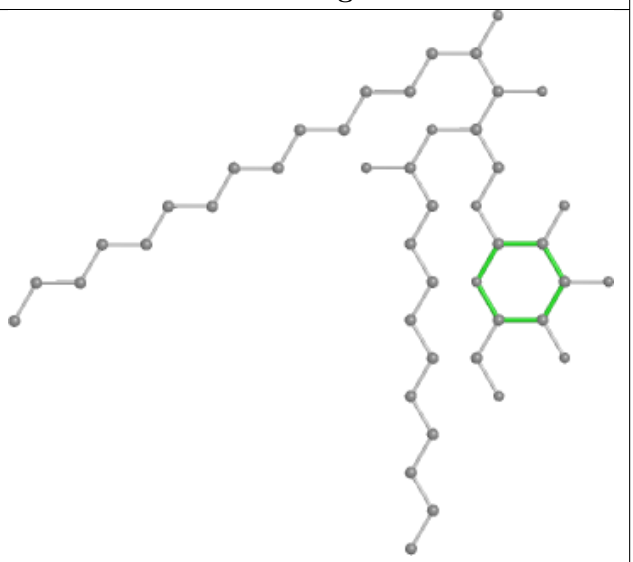
Bond lengths



Bond angles

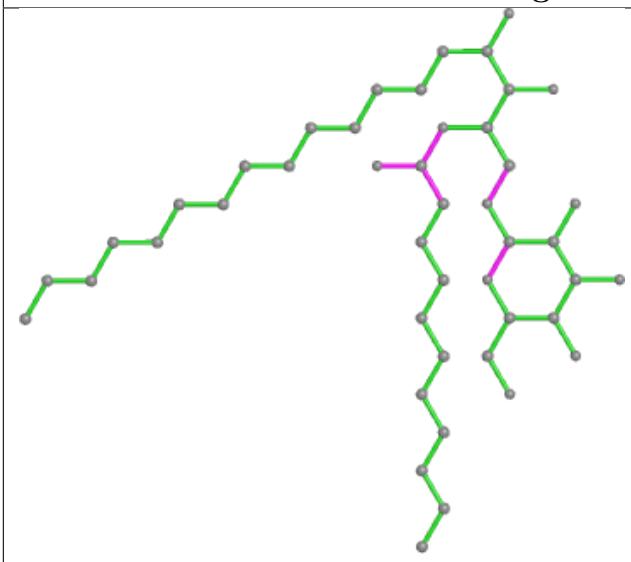


Torsions

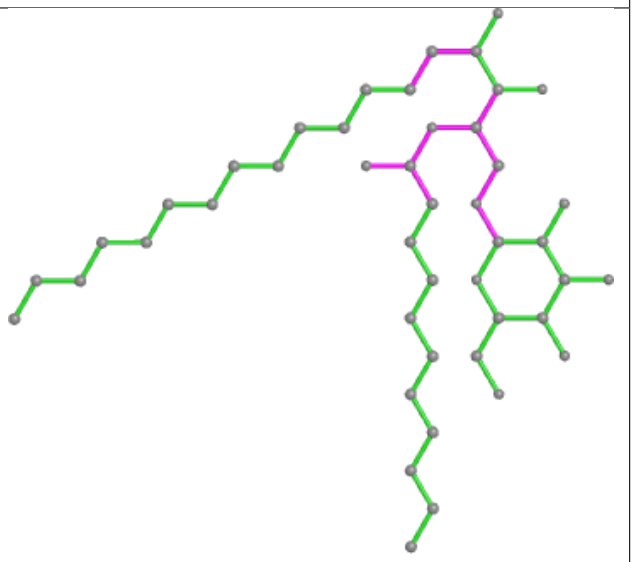


Rings

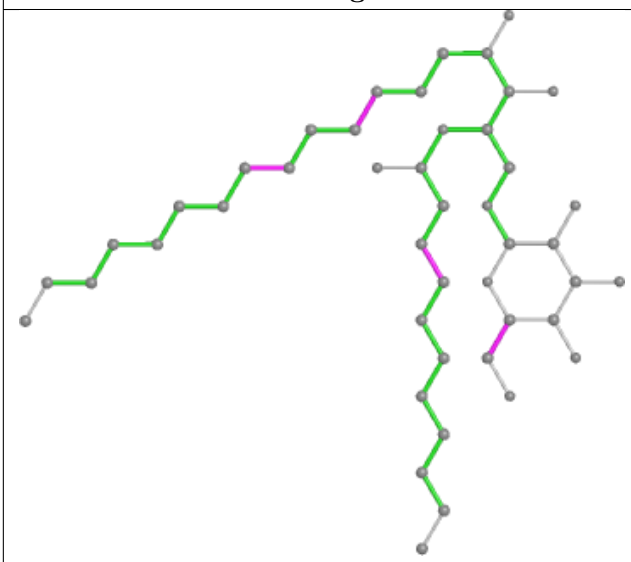
Ligand F61 C 301



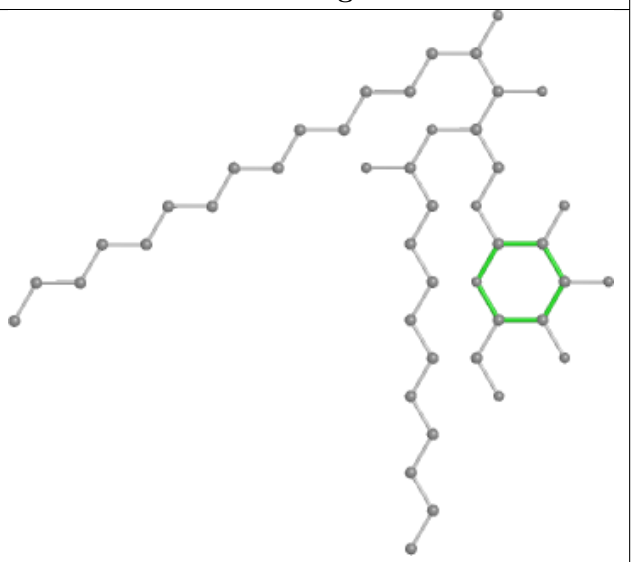
Bond lengths



Bond angles

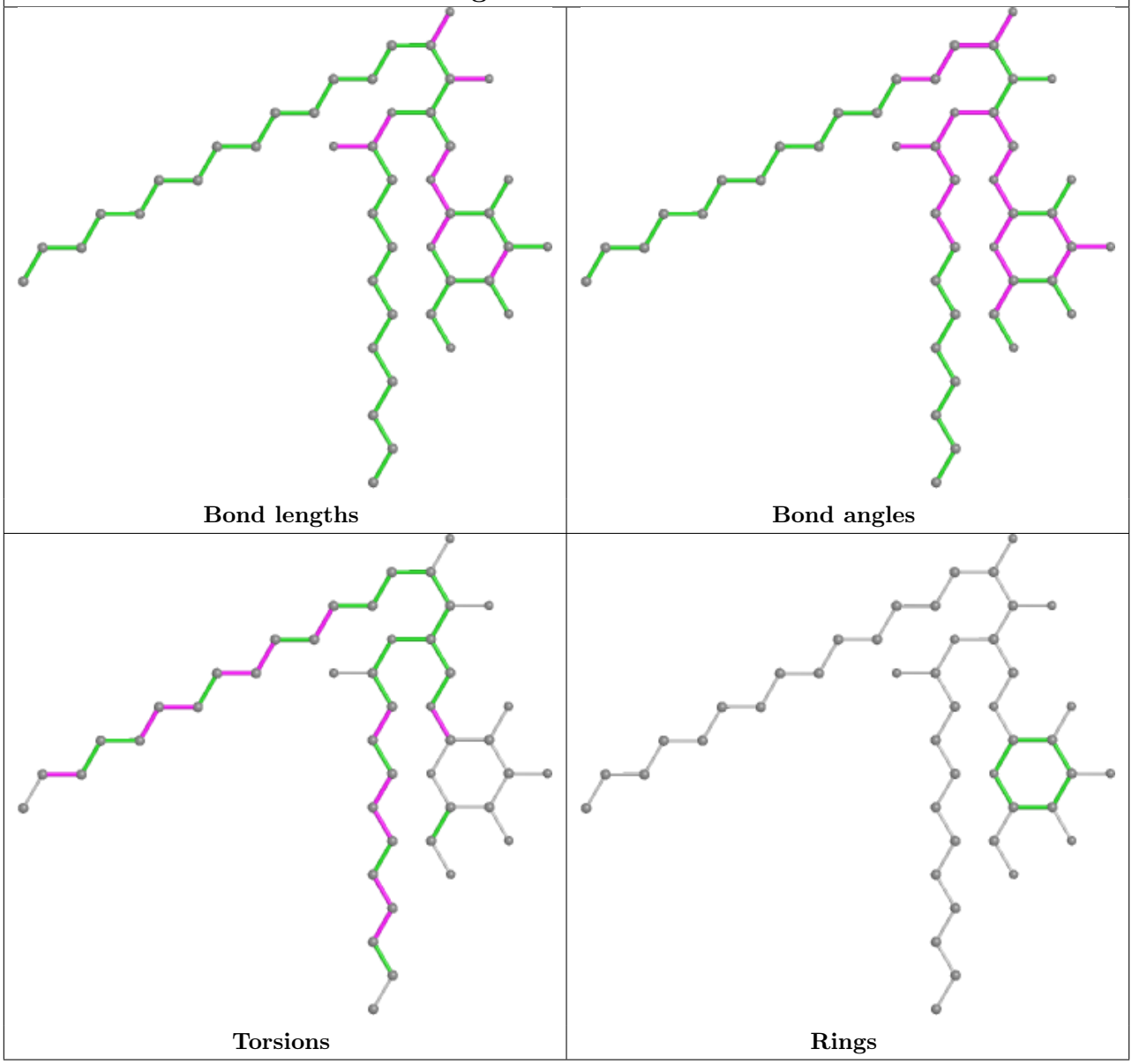


Torsions



Rings

Ligand F61 E 301



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	272/276 (98%)	0.53	16 (5%) 22 28	23, 39, 68, 92	3 (1%)
1	C	268/276 (97%)	0.67	23 (8%) 10 14	25, 43, 71, 100	1 (0%)
1	E	271/276 (98%)	0.36	6 (2%) 62 69	24, 40, 64, 80	2 (0%)
1	G	270/276 (97%)	0.43	9 (3%) 46 53	23, 39, 62, 85	1 (0%)
2	B	98/99 (98%)	0.09	0 100 100	22, 33, 48, 53	1 (1%)
2	D	98/99 (98%)	0.08	1 (1%) 82 86	25, 38, 52, 56	0
2	F	98/99 (98%)	0.16	0 100 100	21, 34, 52, 58	0
2	H	98/99 (98%)	0.07	0 100 100	22, 32, 48, 57	0
All	All	1473/1500 (98%)	0.39	55 (3%) 41 48	21, 39, 64, 100	8 (0%)

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	202	GLY	9.5
1	A	109	GLY	5.2
1	C	107	TYR	4.4
1	A	226	ASP	4.3
1	A	107	TYR	4.3
1	A	23	TRP	3.8
1	A	111	ALA	3.8
1	C	219	TRP	3.8
1	C	47	ILE	3.7
1	A	108	PRO	3.6
1	A	93	ASP	3.5
1	C	112	SER	3.2
1	G	256	GLY	3.1
1	A	225	GLY	2.9
1	E	271	GLY	2.9
1	A	200	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	183	LEU	2.8
1	C	199	SER	2.6
1	C	23	TRP	2.6
1	C	172	ALA	2.6
1	E	46	ILE	2.6
1	C	70	PHE	2.6
1	C	22	SER	2.6
2	D	99	MET	2.6
1	A	8	TYR	2.6
1	A	272	GLY	2.4
1	G	70	PHE	2.4
1	A	181	SER	2.4
1	C	256	GLY	2.3
1	A	219	TRP	2.3
1	G	108	PRO	2.3
1	C	180	LYS	2.3
1	C	66	LEU	2.3
1	E	223	MET	2.2
1	E	138	GLY	2.2
1	C	264	ARG	2.2
1	G	198	SER	2.2
1	A	183	LEU	2.2
1	C	260	GLY	2.2
1	C	224	ARG	2.2
1	C	19	ALA	2.2
1	E	227	GLN	2.2
1	G	111	ALA	2.1
1	E	142	TRP	2.1
1	G	204	LEU	2.1
1	G	255	ALA	2.1
1	C	202	GLY	2.1
1	C	106	MET	2.1
1	C	218	VAL	2.1
1	G	253	VAL	2.1
1	C	34	ASP	2.1
1	C	233	HIS	2.0
1	A	199	SER	2.0
1	C	272	GLY	2.0
1	A	254	GLU	2.0

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

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

6.3 Carbohydrates (i)

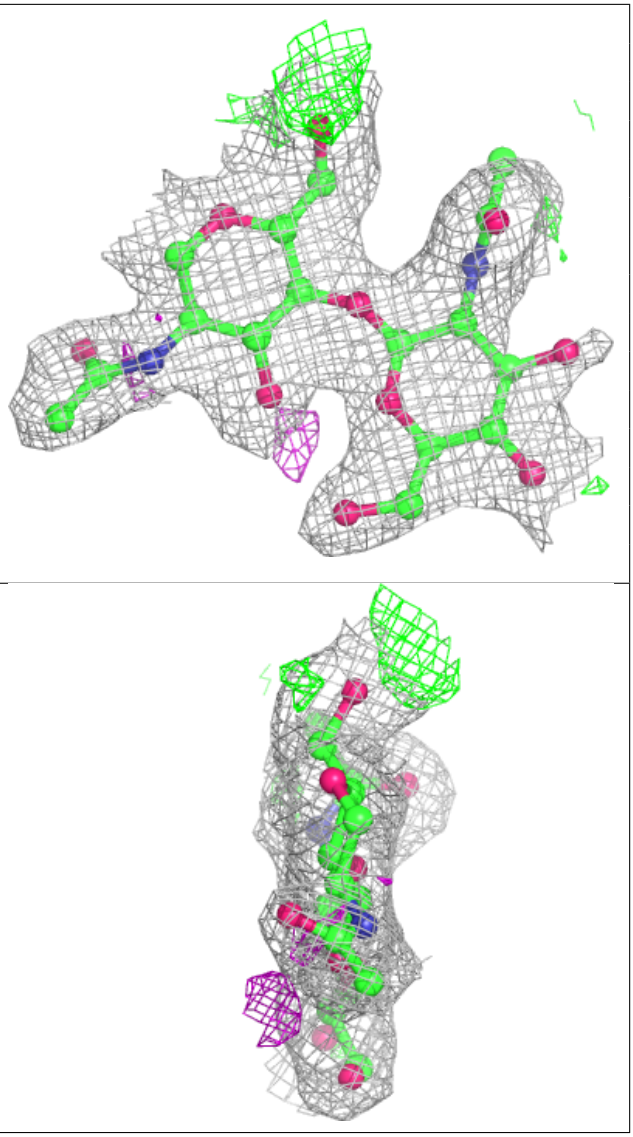
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	J	2	14/15	0.67	0.28	48,66,73,83	0
3	NAG	L	2	14/15	0.73	0.30	53,66,77,80	0
3	NAG	I	2	14/15	0.81	0.17	43,51,62,62	0
3	NAG	L	1	14/15	0.82	0.18	31,45,54,61	0
3	NAG	I	1	14/15	0.83	0.19	30,37,50,51	0
3	NAG	K	2	14/15	0.83	0.23	45,52,58,58	0
3	NAG	K	1	14/15	0.88	0.17	23,38,46,52	0
3	NAG	J	1	14/15	0.92	0.13	27,38,47,50	0

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

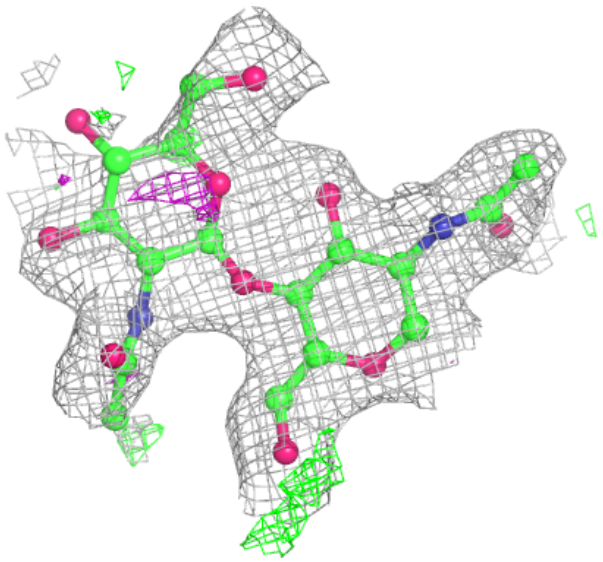
Electron density around Chain I:

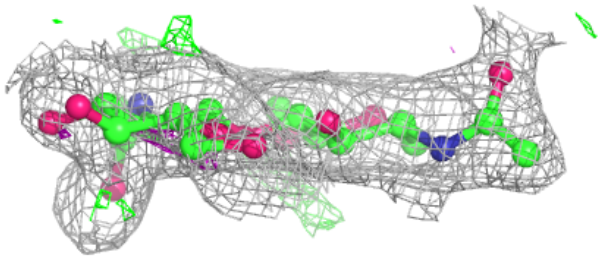
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

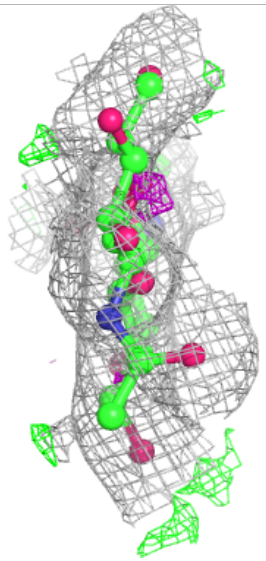


Electron density around Chain J:

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

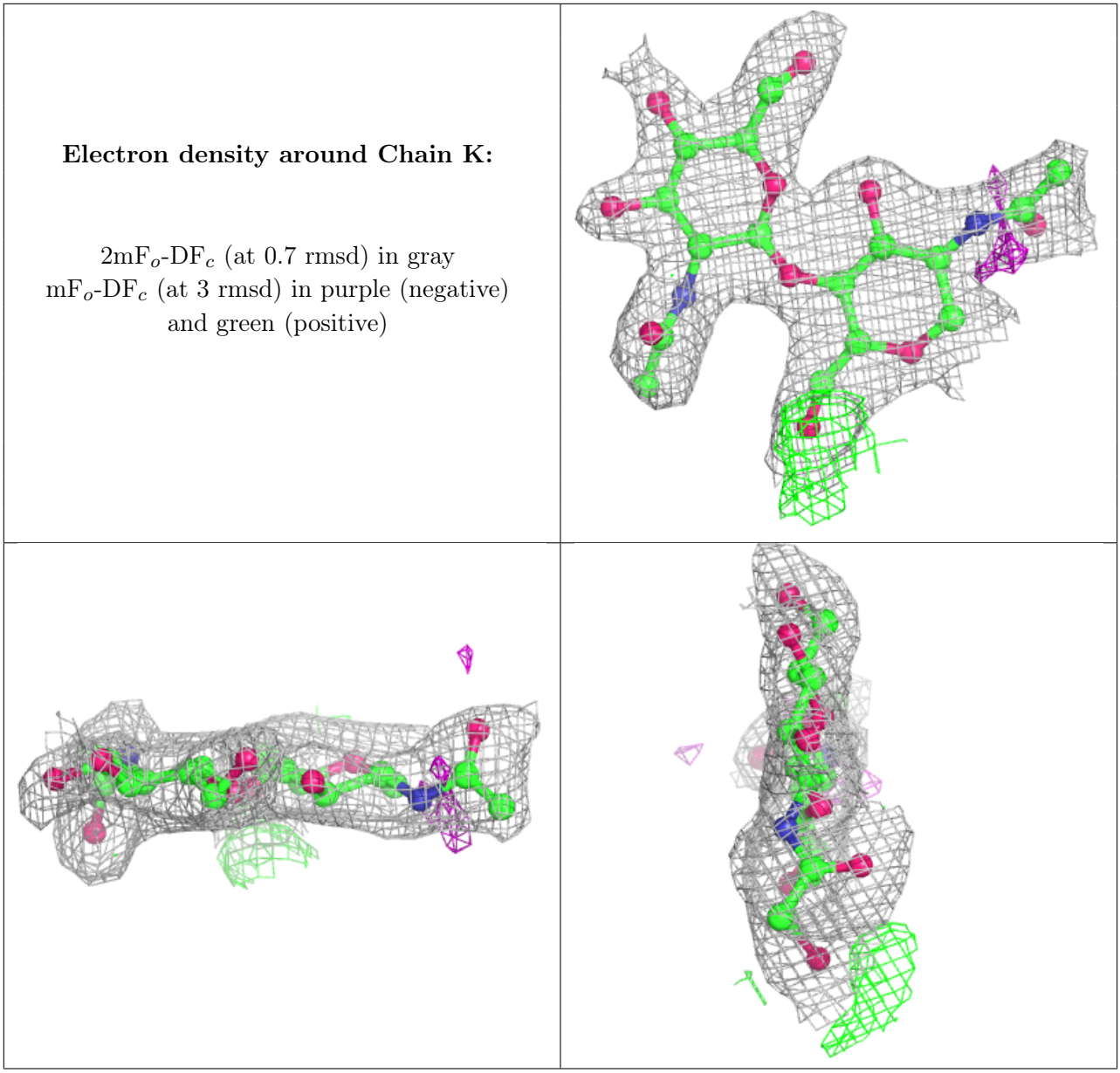






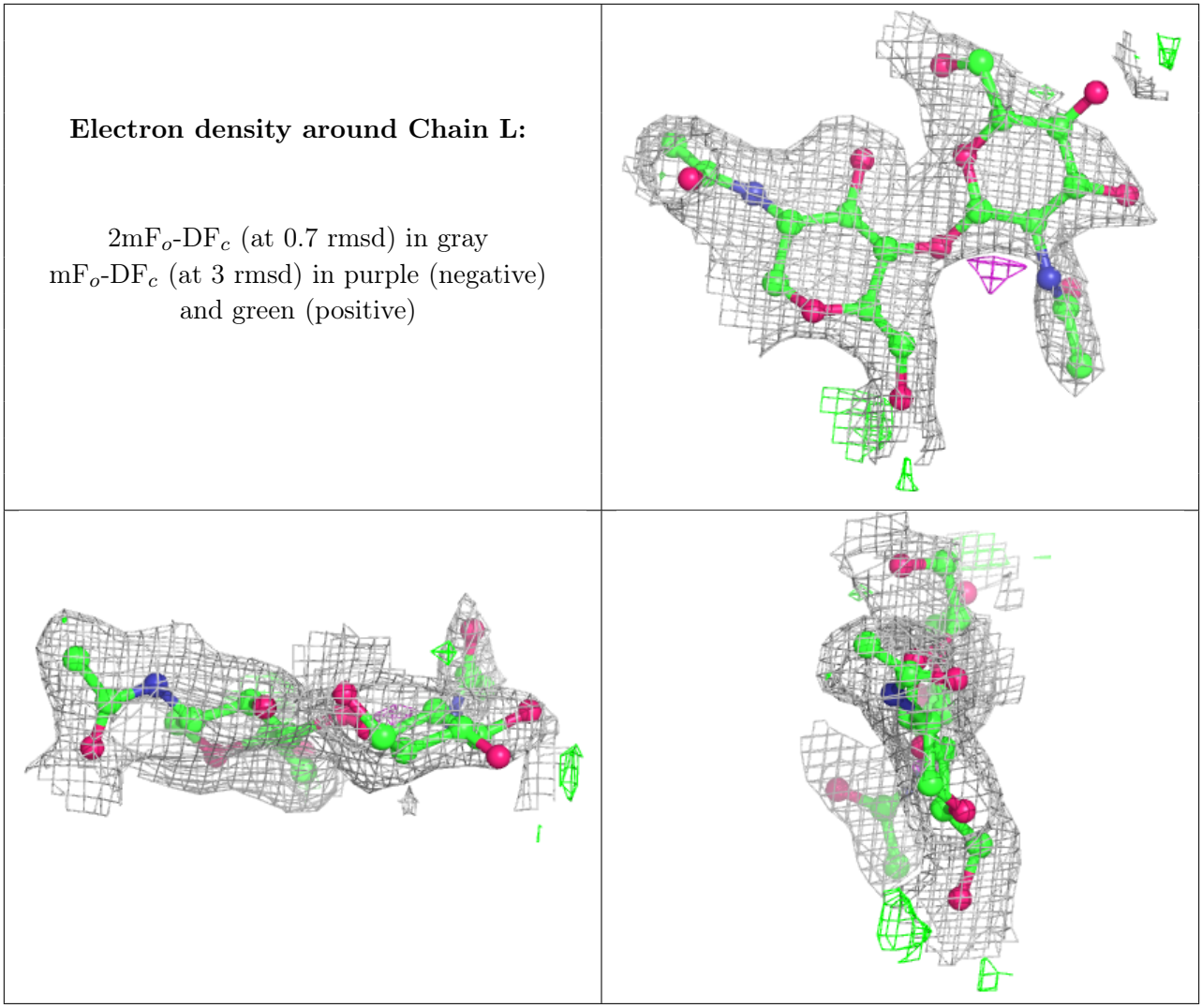
Electron density around Chain K:

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



Electron density around Chain L:

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



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	NAG	G	305	15/15	0.82	0.28	42,57,62,63	0
5	NAG	C	302	14/15	0.84	0.16	51,60,66,66	0
4	F61	E	301	45/45	0.87	0.17	32,47,56,59	0
5	NAG	G	302	14/15	0.87	0.13	32,42,48,49	0
4	F61	G	301	45/45	0.87	0.21	34,50,64,70	0
5	NAG	A	302	14/15	0.89	0.14	44,49,52,55	0
4	F61	C	301	45/45	0.90	0.21	29,44,54,55	0
4	F61	A	301	45/45	0.92	0.14	35,45,53,55	0

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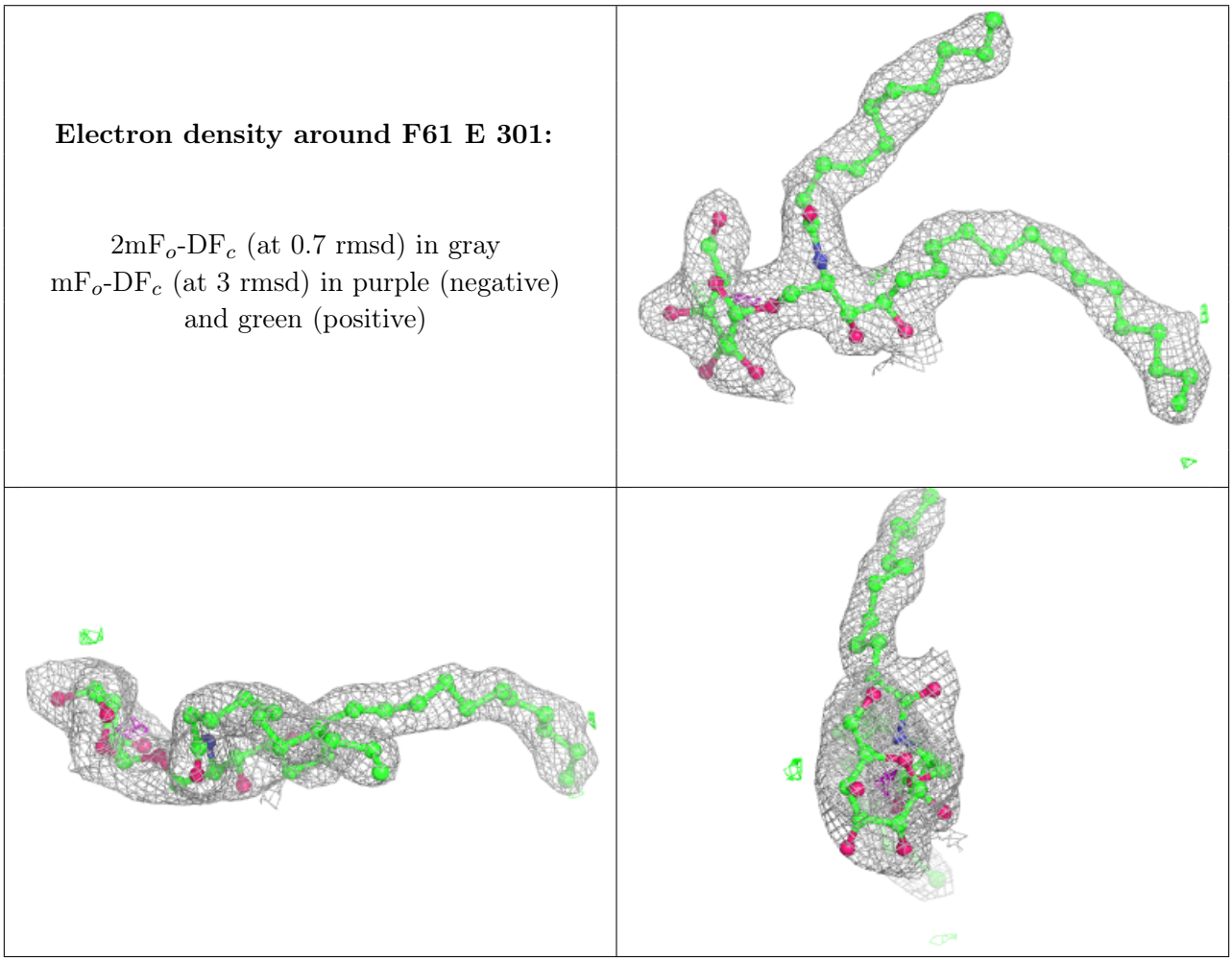
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NAG	E	302	14/15	0.92	0.13	35,40,55,57	0

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.

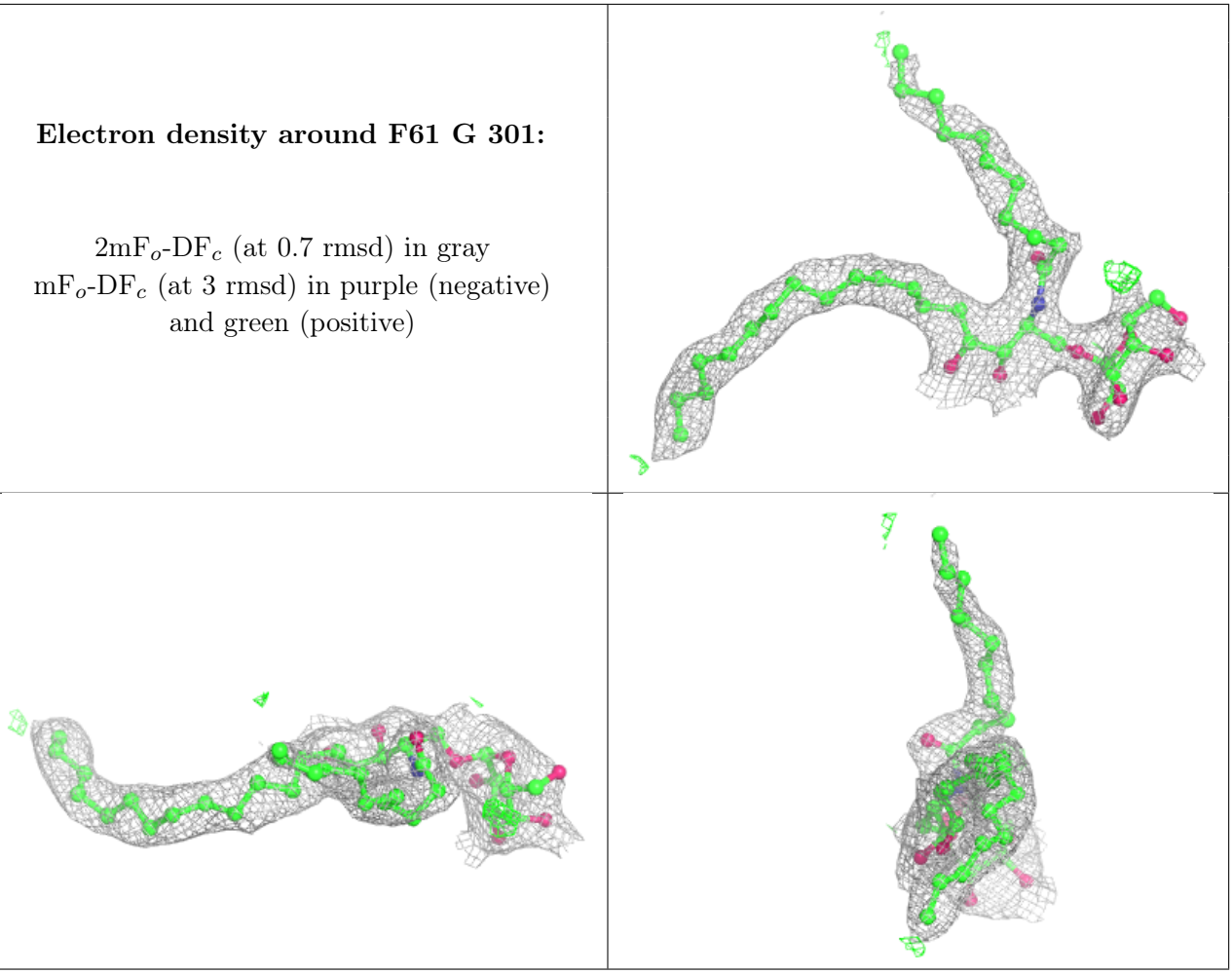
Electron density around F61 E 301:

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



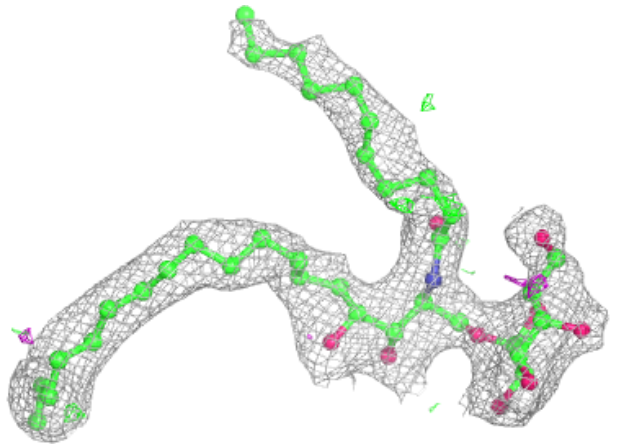
Electron density around F61 G 301:

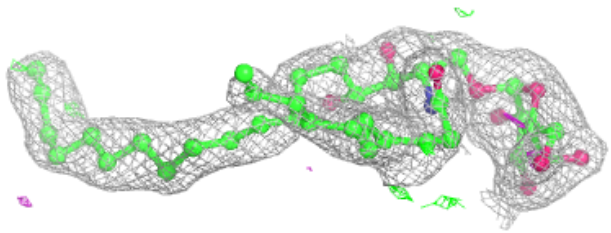
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

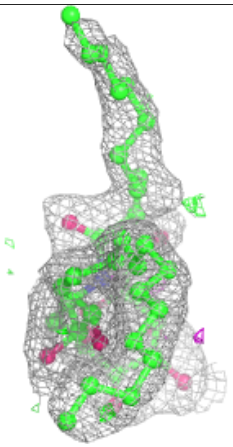


Electron density around F61 C 301:

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

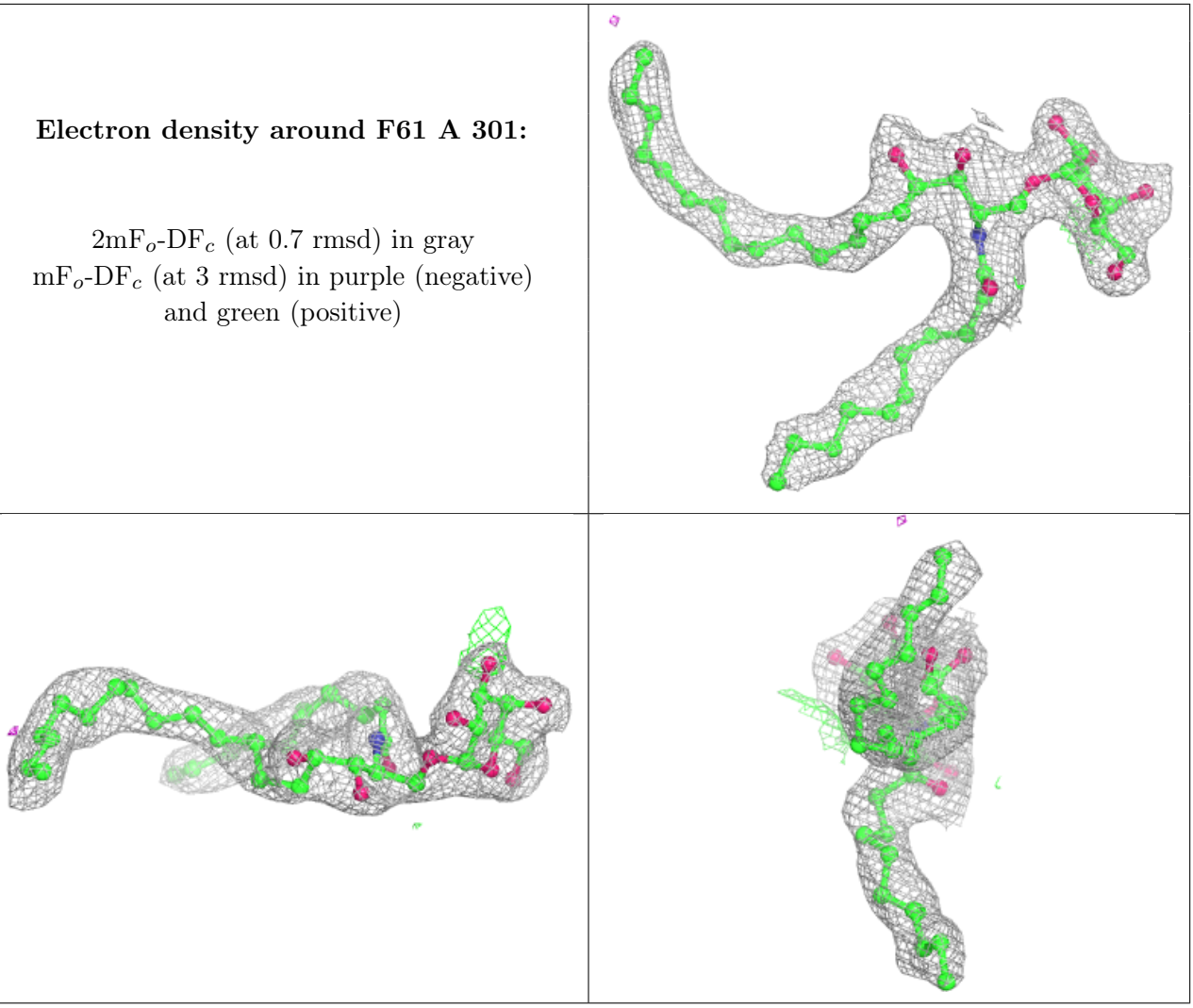






Electron density around F61 A 301:

$2mF_o$-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.