Full wwPDB EM Validation Report ⓘ

Nov 13, 2022 – 06:02 AM EST

PDB ID	:	6U9V
EMDB ID	:	EMD-20702
Title	:	Cryo electron microscopy structure of the ATP-gated rat P2X7 ion channel in the apo, closed state
Authors	:	Mansoor, S.E.; McCarthy, A.E.
Deposited on	:	2019-09-09
Resolution	:	2.90 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp
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:

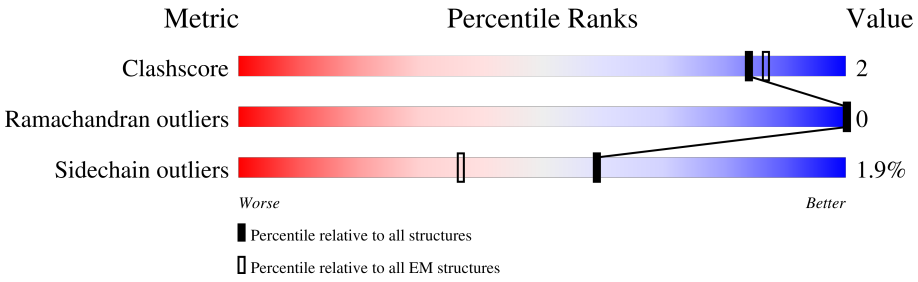
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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.



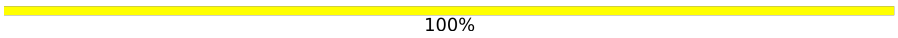
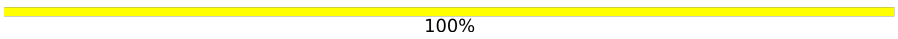
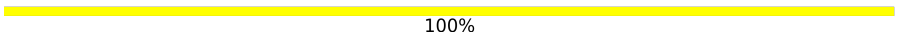
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	609	7% 85% 6% 8%
1	B	609	8% 85% 7% 8%
1	C	609	8% 85% 7% 8%
2	D	2	50% 50% 50%
2	E	2	50% 50% 50%
2	F	2	100%
2	G	2	50% 50%
2	H	2	50% 100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	I	2	
3	J	2	
3	K	2	
3	L	2	

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 27529 atoms, of which 13462 are hydrogens and 0 are deuteriums.

In the tables below, 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 P2X purinoceptor 7.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	560	Total	C	H	N	O	S	0	0
			8625	2829	4213	754	791	38		
1	B	560	Total	C	H	N	O	S	0	0
			8623	2829	4211	754	791	38		
1	C	560	Total	C	H	N	O	S	0	0
			8622	2829	4210	754	791	38		

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	596	SER	-	expression tag	UNP Q64663
A	597	ASN	-	expression tag	UNP Q64663
A	598	SER	-	expression tag	UNP Q64663
A	599	ALA	-	expression tag	UNP Q64663
A	600	VAL	-	expression tag	UNP Q64663
A	601	ASP	-	expression tag	UNP Q64663
A	602	ALA	-	expression tag	UNP Q64663
A	603	GLY	-	expression tag	UNP Q64663
A	604	LEU	-	expression tag	UNP Q64663
A	605	GLU	-	expression tag	UNP Q64663
A	606	VAL	-	expression tag	UNP Q64663
A	607	LEU	-	expression tag	UNP Q64663
A	608	PHE	-	expression tag	UNP Q64663
A	609	GLN	-	expression tag	UNP Q64663
B	596	SER	-	expression tag	UNP Q64663
B	597	ASN	-	expression tag	UNP Q64663
B	598	SER	-	expression tag	UNP Q64663
B	599	ALA	-	expression tag	UNP Q64663
B	600	VAL	-	expression tag	UNP Q64663
B	601	ASP	-	expression tag	UNP Q64663
B	602	ALA	-	expression tag	UNP Q64663
B	603	GLY	-	expression tag	UNP Q64663
B	604	LEU	-	expression tag	UNP Q64663
B	605	GLU	-	expression tag	UNP Q64663

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	606	VAL	-	expression tag	UNP Q64663
B	607	LEU	-	expression tag	UNP Q64663
B	608	PHE	-	expression tag	UNP Q64663
B	609	GLN	-	expression tag	UNP Q64663
C	596	SER	-	expression tag	UNP Q64663
C	597	ASN	-	expression tag	UNP Q64663
C	598	SER	-	expression tag	UNP Q64663
C	599	ALA	-	expression tag	UNP Q64663
C	600	VAL	-	expression tag	UNP Q64663
C	601	ASP	-	expression tag	UNP Q64663
C	602	ALA	-	expression tag	UNP Q64663
C	603	GLY	-	expression tag	UNP Q64663
C	604	LEU	-	expression tag	UNP Q64663
C	605	GLU	-	expression tag	UNP Q64663
C	606	VAL	-	expression tag	UNP Q64663
C	607	LEU	-	expression tag	UNP Q64663
C	608	PHE	-	expression tag	UNP Q64663
C	609	GLN	-	expression tag	UNP Q64663

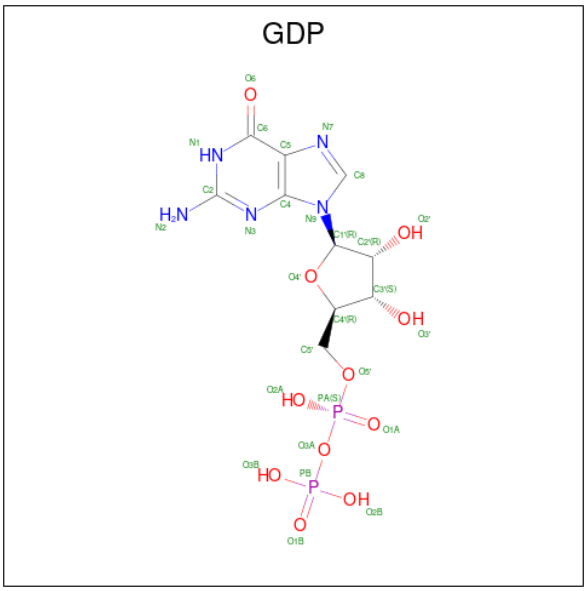
- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
2	E	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
2	F	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
2	G	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
2	H	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
2	I	2	Total	C	H	N	O	0	0
			53	16	25	2	10		

- Molecule 3 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	J	2	Total	C	H	O	0	0
			44	12	21	11		
3	K	2	Total	C	H	O	0	0
			44	12	21	11		
3	L	2	Total	C	H	O	0	0
			44	12	21	11		

- Molecule 4 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$) (labeled as "Ligand of Interest" by depositor).

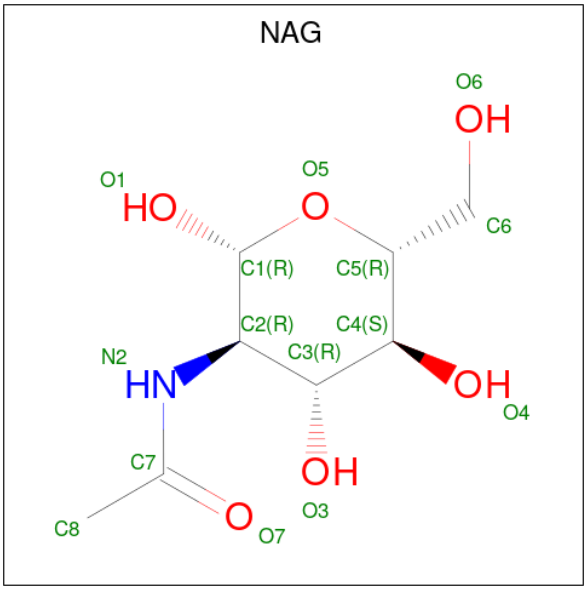


Mol	Chain	Residues	Atoms						AltConf
4	A	1	Total	C	H	N	O	P	0
			40	10	12	5	11	2	
4	B	1	Total	C	H	N	O	P	0
			40	10	12	5	11	2	
4	C	1	Total	C	H	N	O	P	0
			40	10	12	5	11	2	

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
5	A	2	Total Zn 2 2	0
5	B	2	Total Zn 2 2	0
5	C	2	Total Zn 2 2	0

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



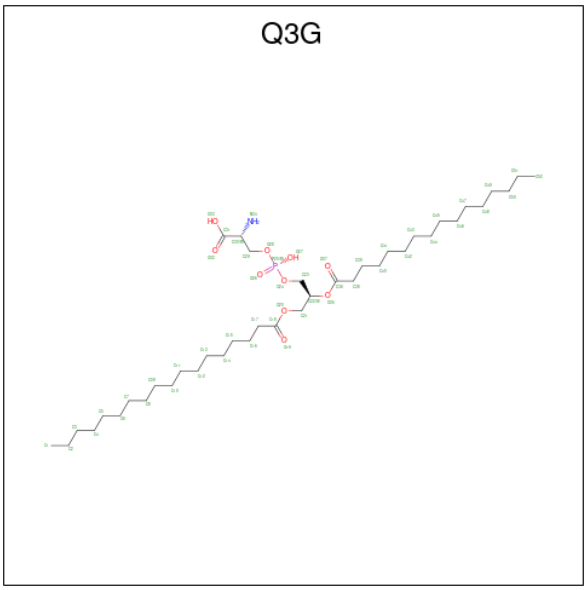
Mol	Chain	Residues	Atoms	AltConf
6	A	1	Total C H N O 81 24 39 3 15	0
6	A	1	Total C H N O 81 24 39 3 15	0
6	A	1	Total C H N O 81 24 39 3 15	0
6	B	1	Total C H N O 81 24 39 3 15	0
6	B	1	Total C H N O 81 24 39 3 15	0
6	B	1	Total C H N O 81 24 39 3 15	0
6	C	1	Total C H N O 81 24 39 3 15	0
6	C	1	Total C H N O 81 24 39 3 15	0

Continued on next page...

Continued from previous page...

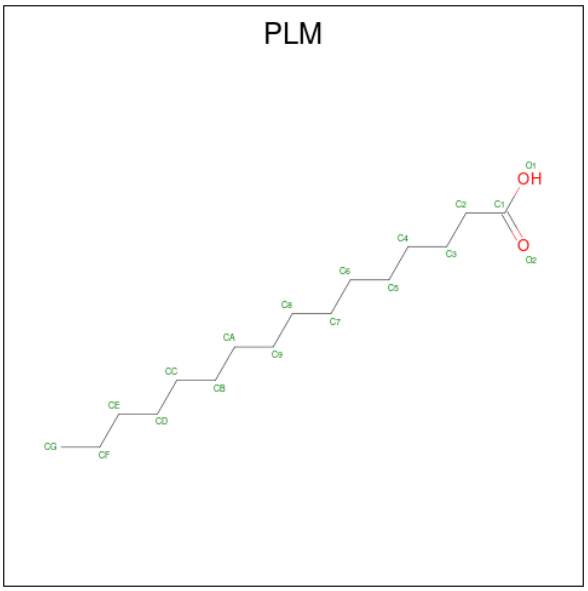
Mol	Chain	Residues	Atoms					AltConf
6	C	1	Total	C	H	N	O	0
			81	24	39	3	15	

- Molecule 7 is O-[(R)-[(2S)-2-(hexadecanoyloxy)-3-(octadecanoyloxy)propoxy](hydroxy)phosphoryl]-D-serine (three-letter code: Q3G) (formula: $C_{40}H_{78}NO_{10}P$).



Mol	Chain	Residues	Atoms					AltConf
7	A	1	Total	C	N	O	P	0
			37	25	1	10	1	
7	B	1	Total	C	N	O	P	0
			37	25	1	10	1	
7	C	1	Total	C	N	O	P	0
			37	25	1	10	1	

- Molecule 8 is PALMITIC ACID (three-letter code: PLM) (formula: $C_{16}H_{32}O_2$).



Mol	Chain	Residues	Atoms				AltConf
8	A	1	Total	C	H	O	0
			243	83	154	6	
8	A	1	Total	C	H	O	0
			243	83	154	6	
8	A	1	Total	C	H	O	0
			243	83	154	6	
8	A	1	Total	C	H	O	0
			243	83	154	6	
8	A	1	Total	C	H	O	0
			243	83	154	6	
8	A	1	Total	C	H	O	0
			243	83	154	6	
8	B	1	Total	C	H	O	0
			243	83	154	6	
8	B	1	Total	C	H	O	0
			243	83	154	6	
8	B	1	Total	C	H	O	0
			243	83	154	6	
8	B	1	Total	C	H	O	0
			243	83	154	6	
8	B	1	Total	C	H	O	0
			243	83	154	6	
8	B	1	Total	C	H	O	0
			243	83	154	6	
8	C	1	Total	C	H	O	0
			243	83	154	6	
8	C	1	Total	C	H	O	0
			243	83	154	6	

Continued on next page...

Continued from previous page...

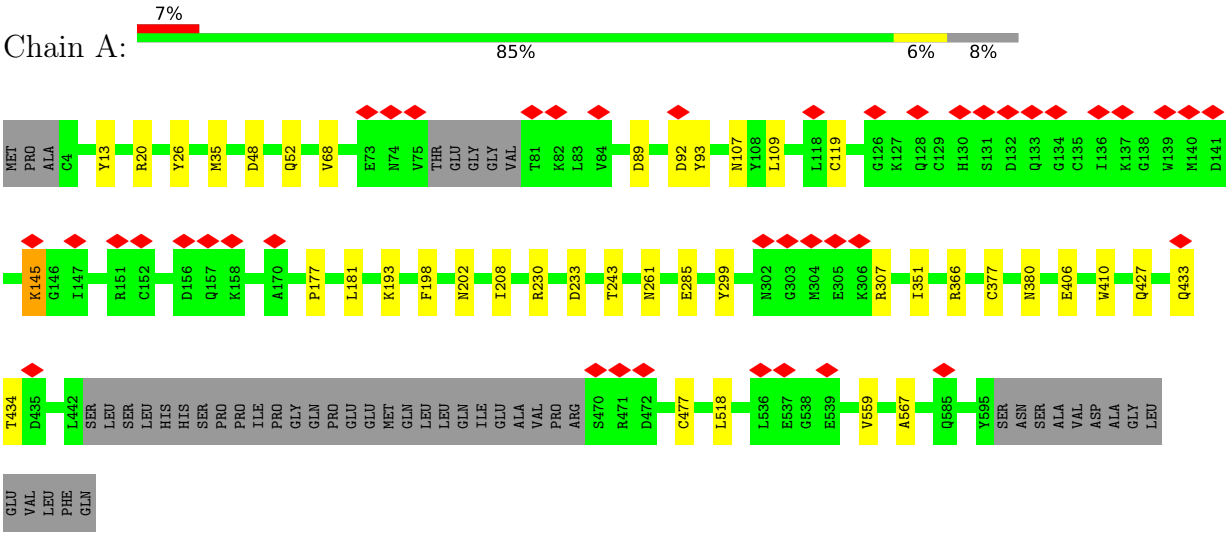
Mol	Chain	Residues	Atoms				AltConf
8	C	1	Total	C	H	O	0
			243	83	154	6	
8	C	1	Total	C	H	O	0
			243	83	154	6	
8	C	1	Total	C	H	O	0
			243	83	154	6	
8	C	1	Total	C	H	O	0
			243	83	154	6	

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

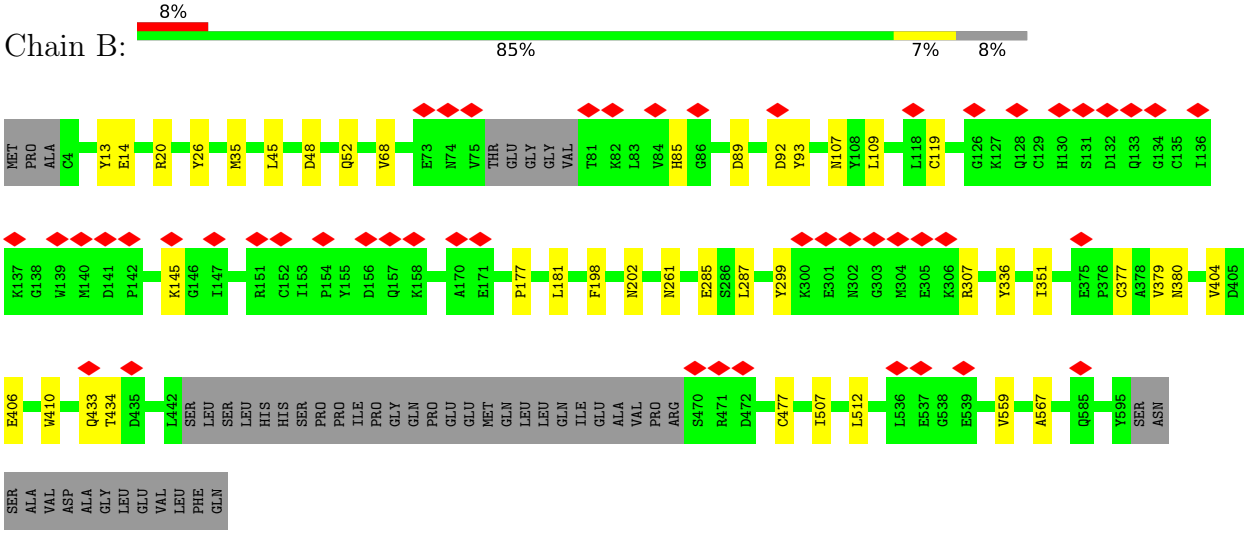
• Molecule 1: P2X purinoceptor 7

Chain A:



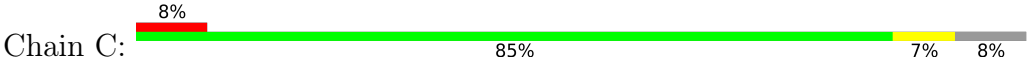
• Molecule 1: P2X purinoceptor 7

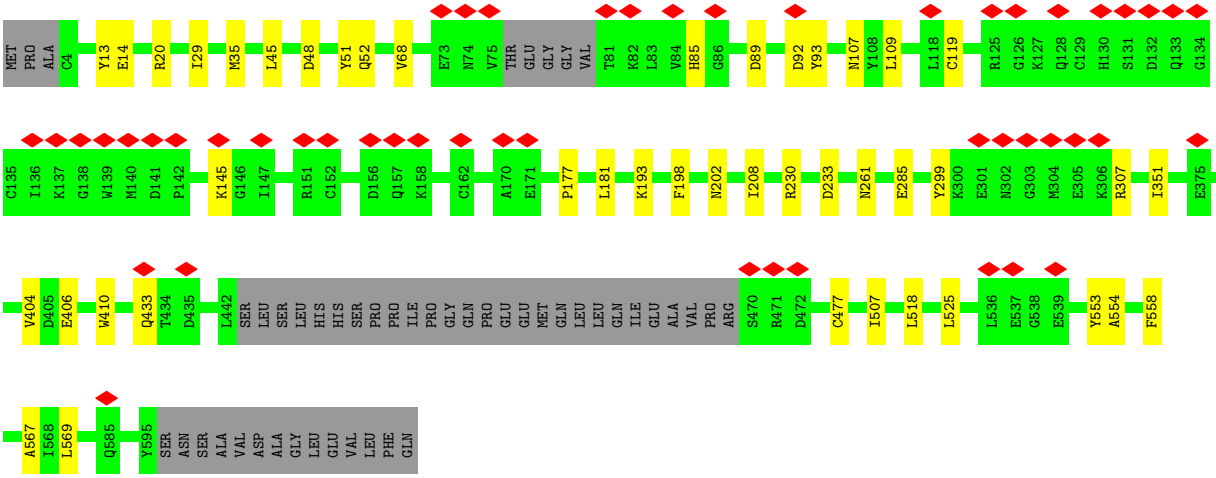
Chain B:



• Molecule 1: P2X purinoceptor 7

Chain C:





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

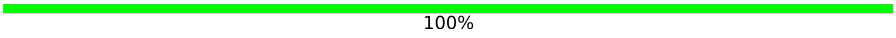
Chain D:

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

Chain E:

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

Chain F:

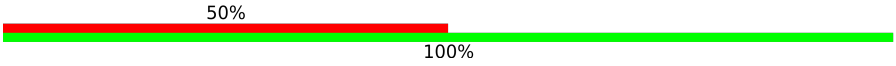


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:

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

Chain H:

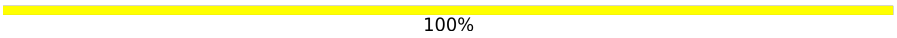


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

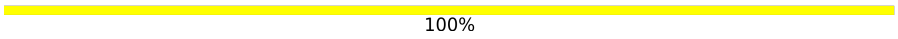
• Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain J:



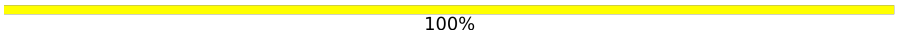
• Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain K:



• Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain L:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	77697	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	27	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.276	Depositor
Minimum map value	-0.156	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0349	Depositor
Map size (Å)	334.4, 334.4, 334.4	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.045, 1.045, 1.045	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GLC, Q3G, NAG, GDP, PLM, ZN

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	0.25	0/4528	0.48	0/6143
1	B	0.26	0/4528	0.48	0/6143
1	C	0.25	0/4528	0.48	0/6143
All	All	0.25	0/13584	0.48	0/18429

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	4412	4213	4213	22	0
1	B	4412	4211	4213	23	0
1	C	4412	4210	4213	25	0
2	D	28	25	25	1	0
2	E	28	25	25	1	0
2	F	28	25	25	0	0
2	G	28	25	25	1	0
2	H	28	25	25	0	0
2	I	28	25	25	1	0
3	J	23	21	20	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	K	23	21	20	0	0
3	L	23	21	20	0	0
4	A	28	12	11	1	0
4	B	28	12	11	1	0
4	C	28	12	11	1	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	C	2	0	0	0	0
6	A	42	39	39	0	0
6	B	42	39	39	0	0
6	C	42	39	39	0	0
7	A	37	0	0	0	0
7	B	37	0	0	0	0
7	C	37	0	0	0	0
8	A	89	154	154	0	0
8	B	89	154	154	0	0
8	C	89	154	154	0	0
All	All	14067	13462	13461	62	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 2.

All (62) 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:C:52:GLN:OE1	1:C:261:ASN:ND2	2.24	0.71
1:A:26:TYR:OH	1:A:380:ASN:OD1	2.09	0.68
1:B:26:TYR:OH	1:B:380:ASN:OD1	2.09	0.68
1:A:52:GLN:OE1	1:A:261:ASN:ND2	2.30	0.64
1:B:377:CYS:O	1:B:380:ASN:ND2	2.30	0.64
1:A:377:CYS:O	1:A:380:ASN:ND2	2.31	0.64
1:B:52:GLN:OE1	1:B:261:ASN:ND2	2.32	0.62
1:B:434:THR:HA	1:B:559:VAL:HG11	1.83	0.60
1:A:434:THR:HA	1:A:559:VAL:HG11	1.85	0.58
1:C:68:VAL:HG12	1:C:89:ASP:HA	1.85	0.57
1:B:68:VAL:HG12	1:B:89:ASP:HA	1.90	0.54
1:A:68:VAL:HG12	1:A:89:ASP:HA	1.90	0.54
1:A:107:ASN:OD1	1:A:181:LEU:N	2.41	0.53
1:C:285:GLU:N	1:C:285:GLU:OE1	2.42	0.53
1:A:285:GLU:N	1:A:285:GLU:OE1	2.42	0.53
1:C:107:ASN:OD1	1:C:181:LEU:N	2.43	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:ASN:OD1	1:B:181:LEU:N	2.42	0.52
1:B:68:VAL:HG11	1:C:145:LYS:O	2.10	0.52
1:B:285:GLU:N	1:B:285:GLU:OE1	2.42	0.52
1:B:45:LEU:HD13	1:B:336:TYR:CD2	2.44	0.51
1:A:20:ARG:NH2	1:C:14:GLU:OE2	2.44	0.51
1:A:145:LYS:O	1:C:68:VAL:HG11	2.11	0.50
1:B:406:GLU:OE1	1:B:410:TRP:NE1	2.44	0.50
1:B:567:ALA:O	4:B:701:GDP:N1	2.45	0.50
1:A:208:ILE:HD13	1:B:287:LEU:CD2	2.41	0.49
1:A:567:ALA:O	4:A:701:GDP:N1	2.42	0.49
1:C:45:LEU:HD11	1:C:51:TYR:HB3	1.95	0.48
1:C:92:ASP:OD1	1:C:93:TYR:N	2.47	0.48
1:A:92:ASP:OD1	1:A:93:TYR:N	2.46	0.48
2:E:1:NAG:H83	2:E:1:NAG:H3	1.96	0.48
1:B:92:ASP:OD1	1:B:93:TYR:N	2.46	0.48
2:G:1:NAG:H83	2:G:1:NAG:H3	1.95	0.48
1:A:68:VAL:HG11	1:B:145:LYS:O	2.14	0.47
2:I:1:NAG:H3	2:I:1:NAG:H83	1.96	0.47
1:A:433:GLN:N	1:A:433:GLN:OE1	2.47	0.47
1:C:567:ALA:O	4:C:701:GDP:N1	2.48	0.47
1:C:406:GLU:OE1	1:C:410:TRP:NE1	2.46	0.47
1:B:14:GLU:OE2	1:C:20:ARG:NH2	2.48	0.47
1:A:243:THR:CG2	2:D:1:NAG:O6	2.63	0.46
1:C:554:ALA:O	1:C:558:PHE:N	2.46	0.46
1:A:406:GLU:OE1	1:A:410:TRP:NE1	2.46	0.46
1:C:198:PHE:O	1:C:202:ASN:N	2.48	0.46
1:B:433:GLN:N	1:B:433:GLN:OE1	2.49	0.46
1:C:433:GLN:N	1:C:433:GLN:OE1	2.49	0.45
1:A:198:PHE:O	1:A:202:ASN:N	2.50	0.44
1:B:109:LEU:HD11	1:B:177:PRO:HD3	1.99	0.44
1:C:193:LYS:HG2	1:C:208:ILE:HD12	2.00	0.44
1:A:13:TYR:CE2	1:B:351:ILE:HG21	2.53	0.43
1:B:13:TYR:CE2	1:C:351:ILE:HG21	2.53	0.43
1:A:351:ILE:HG21	1:C:13:TYR:CE2	2.54	0.43
1:B:198:PHE:O	1:B:202:ASN:N	2.51	0.42
1:A:193:LYS:HG2	1:A:208:ILE:HD12	2.01	0.42
1:A:109:LEU:HD11	1:A:177:PRO:HD3	2.01	0.42
1:B:512:LEU:HD21	1:C:525:LEU:HG	2.02	0.42
1:C:230:ARG:NH1	1:C:233:ASP:OD1	2.50	0.42
1:C:29:ILE:HD11	1:C:351:ILE:HG12	2.02	0.41
1:A:230:ARG:NH1	1:A:233:ASP:OD1	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:404:VAL:CG1	1:B:507:ILE:HD12	2.50	0.41
1:B:379:VAL:HG13	1:C:394:PRO:HG2	2.03	0.41
1:C:404:VAL:CG1	1:C:507:ILE:HD12	2.51	0.41
1:C:553:TYR:HD2	1:C:569:LEU:HD22	1.85	0.40
1:C:109:LEU:HD11	1:C:177:PRO:HD3	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 PDB entries followed by that with respect to all EM entries.

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	554/609 (91%)	524 (95%)	30 (5%)	0	100	100
1	B	554/609 (91%)	529 (96%)	25 (4%)	0	100	100
1	C	554/609 (91%)	528 (95%)	26 (5%)	0	100	100
All	All	1662/1827 (91%)	1581 (95%)	81 (5%)	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 PDB entries followed by that with respect to all EM entries.

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	467/546 (86%)	457 (98%)	10 (2%)	53	81
1	B	467/546 (86%)	459 (98%)	8 (2%)	60	86

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	467/546 (86%)	459 (98%)	8 (2%)	60 86
All	All	1401/1638 (86%)	1375 (98%)	26 (2%)	59 84

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	MET
1	A	48	ASP
1	A	119	CYS
1	A	145	LYS
1	A	299	TYR
1	A	307	ARG
1	A	366	ARG
1	A	427	GLN
1	A	477	CYS
1	A	518	LEU
1	B	20	ARG
1	B	35	MET
1	B	48	ASP
1	B	85	HIS
1	B	119	CYS
1	B	299	TYR
1	B	307	ARG
1	B	477	CYS
1	C	35	MET
1	C	48	ASP
1	C	85	HIS
1	C	119	CYS
1	C	299	TYR
1	C	307	ARG
1	C	477	CYS
1	C	518	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	GLN
1	A	207	ASN
1	A	261	ASN
1	B	52	GLN
1	B	207	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	261	ASN
1	C	52	GLN
1	C	207	ASN
1	C	261	ASN

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)

18 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	$\#\|Z\| > 2$
2	NAG	D	1	2,1	14,14,15	0.30	0	17,19,21	0.61	0
2	NAG	D	2	2	14,14,15	0.20	0	17,19,21	0.41	0
2	NAG	E	1	2,1	14,14,15	0.28	0	17,19,21	1.37	2 (11%)
2	NAG	E	2	2	14,14,15	0.37	0	17,19,21	0.75	1 (5%)
2	NAG	F	1	2,1	14,14,15	0.19	0	17,19,21	0.42	0
2	NAG	F	2	2	14,14,15	0.22	0	17,19,21	0.41	0
2	NAG	G	1	2,1	14,14,15	0.27	0	17,19,21	1.37	2 (11%)
2	NAG	G	2	2	14,14,15	0.34	0	17,19,21	0.39	0
2	NAG	H	1	2,1	14,14,15	0.21	0	17,19,21	0.42	0
2	NAG	H	2	2	14,14,15	0.22	0	17,19,21	0.41	0
2	NAG	I	1	2,1	14,14,15	0.26	0	17,19,21	1.37	2 (11%)
2	NAG	I	2	2	14,14,15	0.35	0	17,19,21	0.40	0
3	GLC	J	1	3	12,12,12	1.39	1 (8%)	17,17,17	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	GLC	J	2	3	11,11,12	1.80	3 (27%)	15,15,17	0.94	0
3	GLC	K	1	3	12,12,12	1.39	1 (8%)	17,17,17	0.79	0
3	GLC	K	2	3	11,11,12	1.80	3 (27%)	15,15,17	0.94	0
3	GLC	L	1	3	12,12,12	1.40	1 (8%)	17,17,17	0.78	0
3	GLC	L	2	3	11,11,12	1.78	3 (27%)	15,15,17	0.94	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
2	NAG	D	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	1/6/23/26	0/1/1/1
2	NAG	E	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	E	2	2	-	1/6/23/26	0/1/1/1
2	NAG	F	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	1/6/23/26	0/1/1/1
2	NAG	G	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	G	2	2	-	1/6/23/26	0/1/1/1
2	NAG	H	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	1/6/23/26	0/1/1/1
2	NAG	I	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	I	2	2	-	1/6/23/26	0/1/1/1
3	GLC	J	1	3	-	0/2/22/22	0/1/1/1
3	GLC	J	2	3	-	2/2/19/22	0/1/1/1
3	GLC	K	1	3	-	0/2/22/22	0/1/1/1
3	GLC	K	2	3	-	2/2/19/22	0/1/1/1
3	GLC	L	1	3	-	0/2/22/22	0/1/1/1
3	GLC	L	2	3	-	2/2/19/22	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	2	GLC	O5-C1	4.58	1.51	1.43
3	J	2	GLC	O5-C1	4.55	1.51	1.43
3	L	2	GLC	O5-C1	4.53	1.50	1.43
3	L	1	GLC	O5-C1	3.70	1.52	1.42
3	J	1	GLC	O5-C1	3.69	1.52	1.42
3	K	1	GLC	O5-C1	3.67	1.52	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	2	GLC	C2-C3	-2.24	1.49	1.52
3	J	2	GLC	C2-C3	-2.23	1.49	1.52
3	L	2	GLC	C2-C3	-2.21	1.49	1.52
3	K	2	GLC	O5-C5	2.09	1.47	1.43
3	J	2	GLC	O5-C5	2.08	1.47	1.43
3	L	2	GLC	O5-C5	2.04	1.47	1.43

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	1	NAG	C2-N2-C7	4.46	129.25	122.90
2	I	1	NAG	C2-N2-C7	4.46	129.25	122.90
2	E	1	NAG	C2-N2-C7	4.45	129.24	122.90
2	E	1	NAG	C1-C2-N2	2.19	114.23	110.49
2	I	1	NAG	C1-C2-N2	2.16	114.19	110.49
2	G	1	NAG	C1-C2-N2	2.15	114.16	110.49
2	E	2	NAG	C3-C4-C5	2.01	113.82	110.24

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	K	2	GLC	O5-C5-C6-O6
3	L	2	GLC	O5-C5-C6-O6
3	J	2	GLC	O5-C5-C6-O6
2	E	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2
2	G	1	NAG	C8-C7-N2-C2
2	G	1	NAG	O7-C7-N2-C2
2	I	1	NAG	C8-C7-N2-C2
2	I	1	NAG	O7-C7-N2-C2
3	K	2	GLC	C4-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
2	I	2	NAG	O5-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6
3	L	2	GLC	C4-C5-C6-O6
3	J	2	GLC	C4-C5-C6-O6
2	E	1	NAG	C3-C2-N2-C7
2	G	1	NAG	C3-C2-N2-C7

Continued on next page...

Continued from previous page...

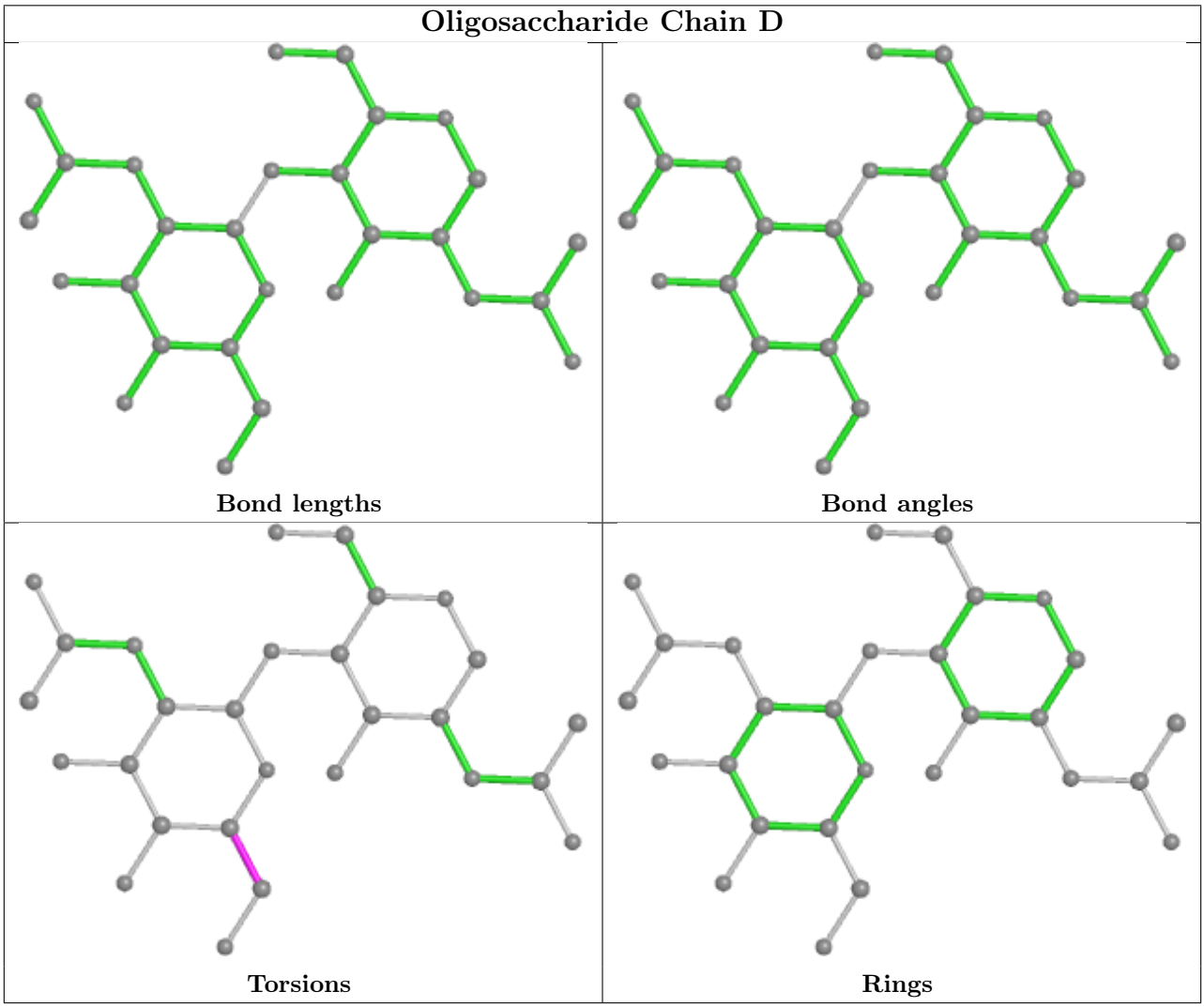
Mol	Chain	Res	Type	Atoms
2	I	1	NAG	C3-C2-N2-C7

There are no ring outliers.

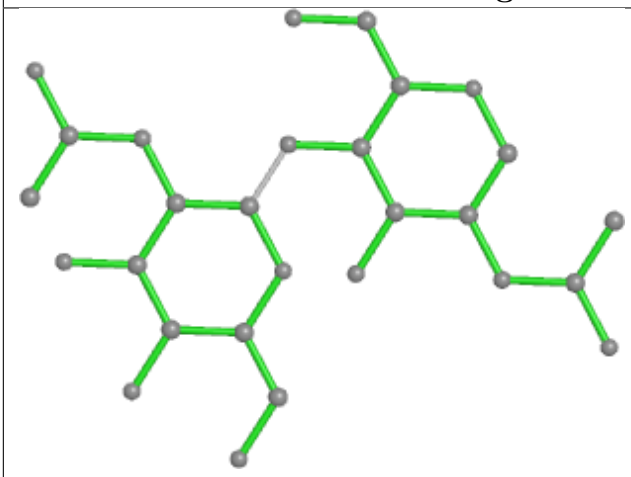
4 monomers are involved in 4 short contacts:

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

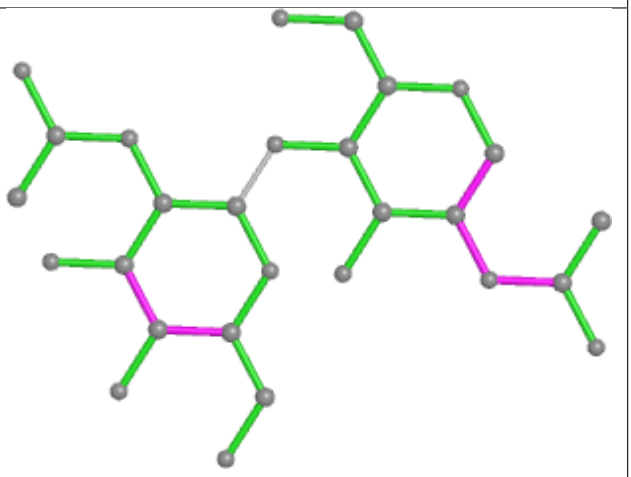
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



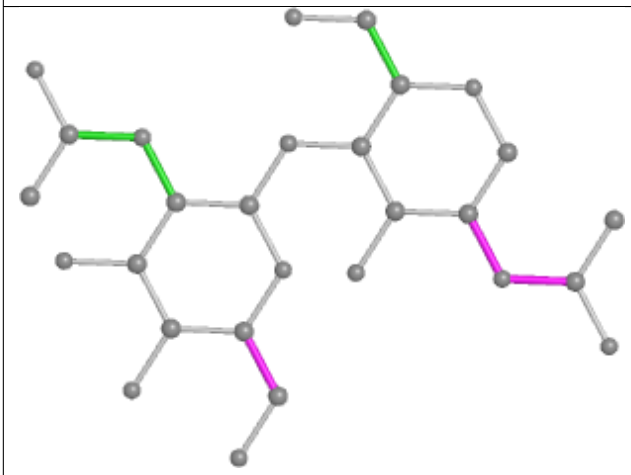
Oligosaccharide Chain E



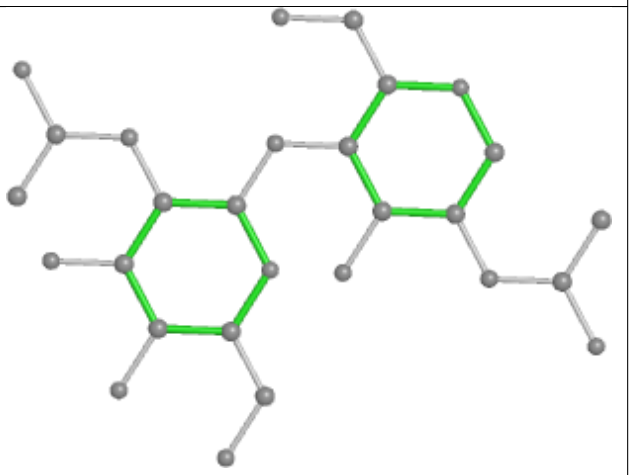
Bond lengths



Bond angles

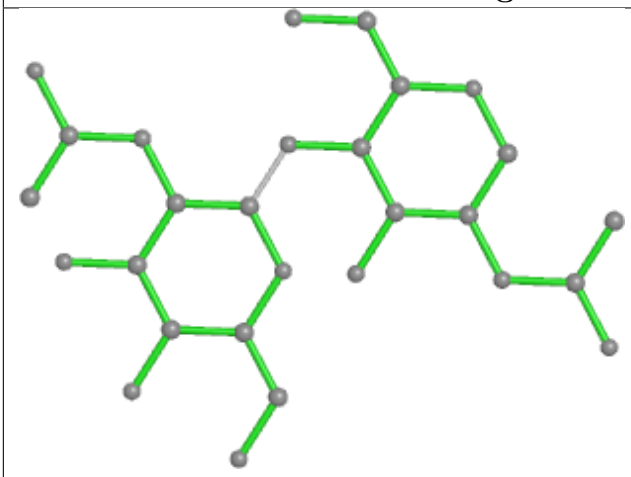


Torsions

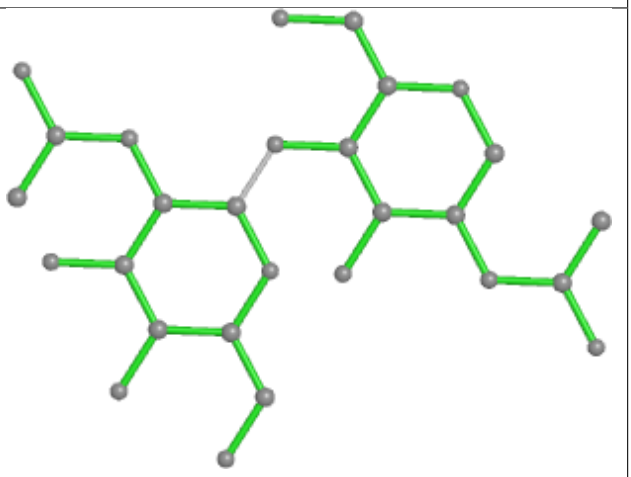


Rings

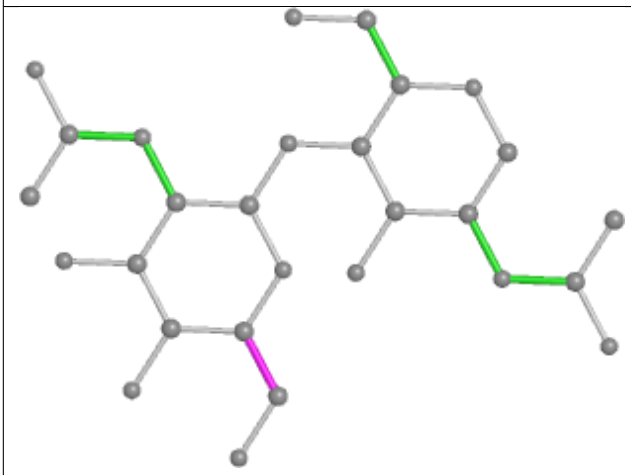
Oligosaccharide Chain F



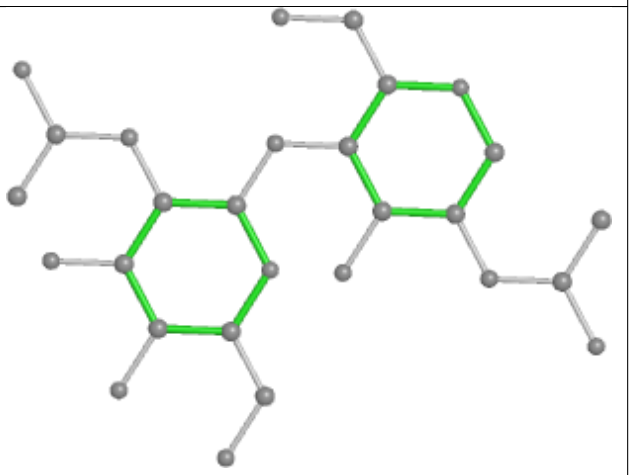
Bond lengths



Bond angles

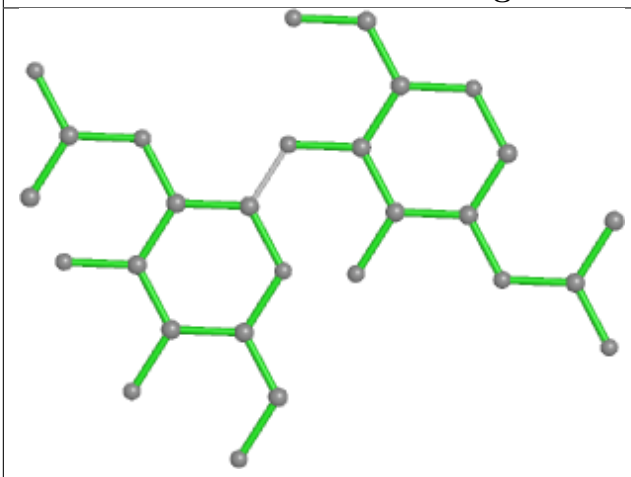


Torsions

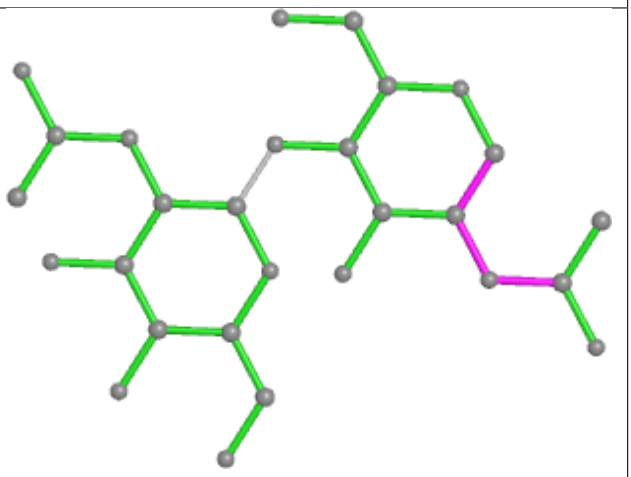


Rings

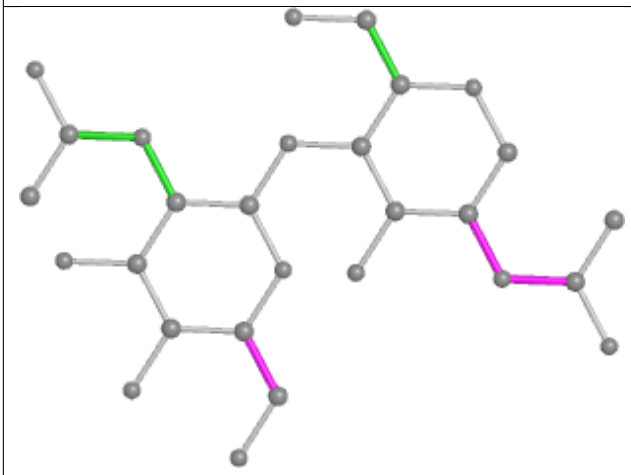
Oligosaccharide Chain G



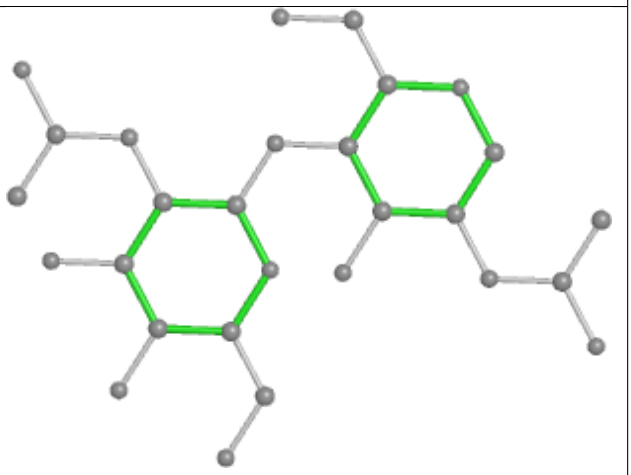
Bond lengths



Bond angles

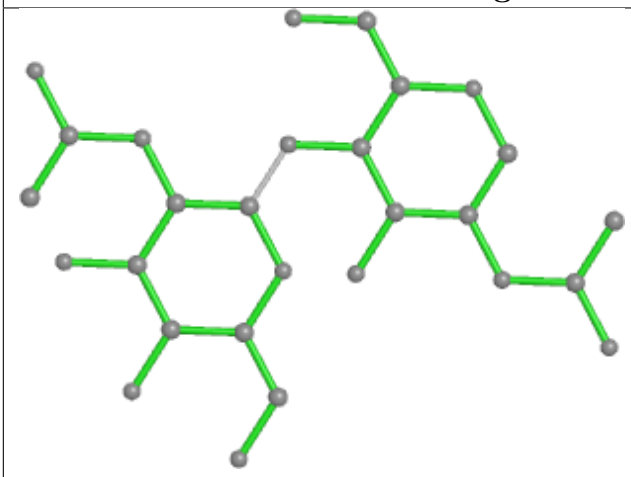


Torsions

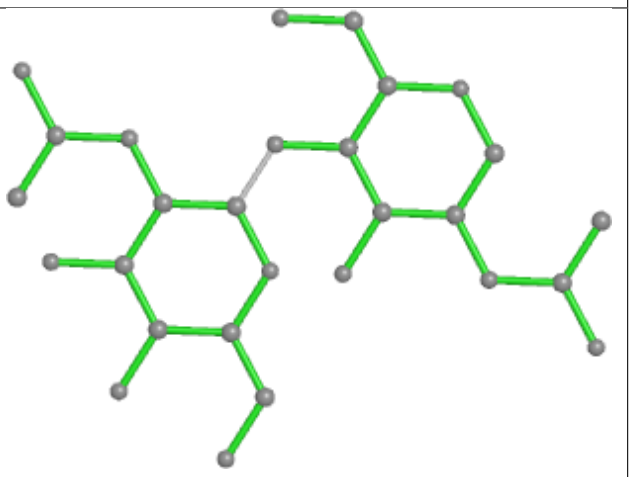


Rings

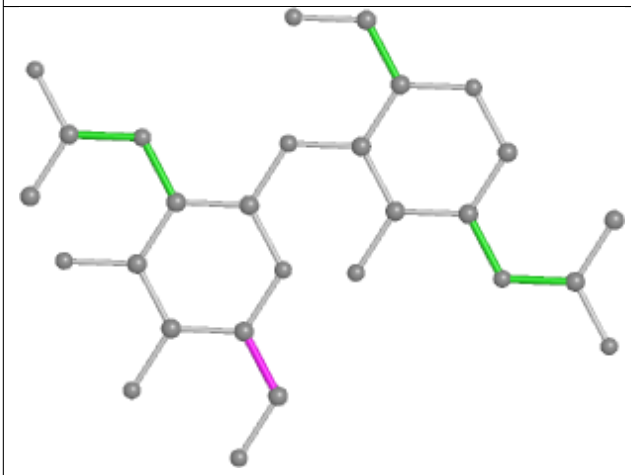
Oligosaccharide Chain H



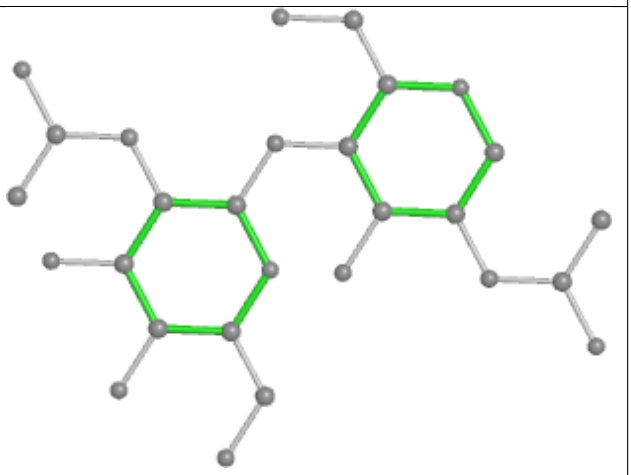
Bond lengths



Bond angles

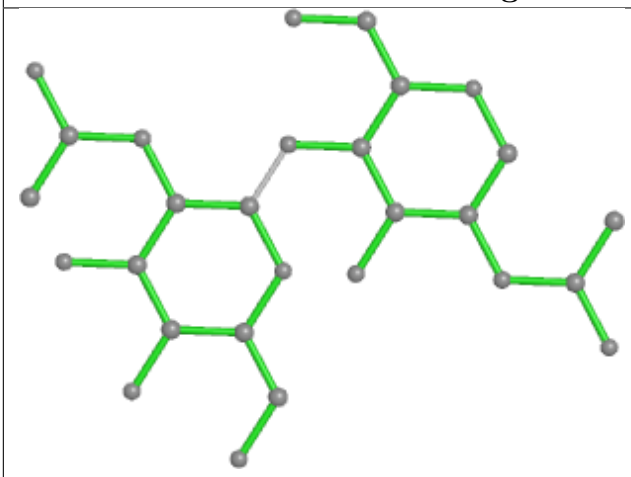


Torsions

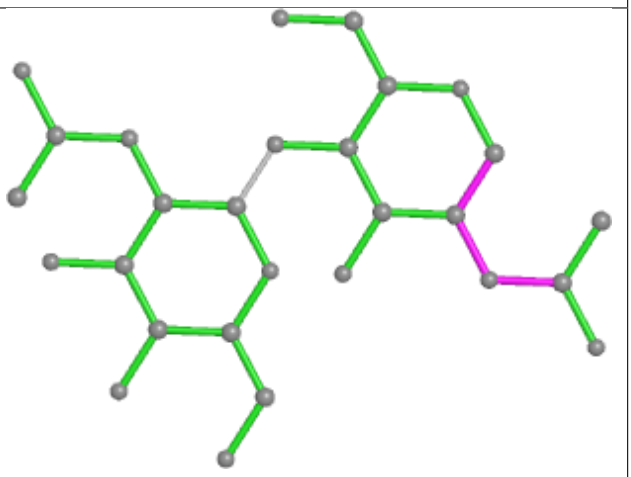


Rings

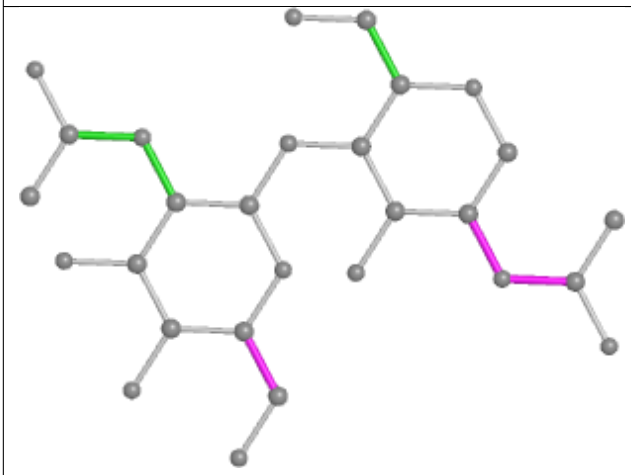
Oligosaccharide Chain I



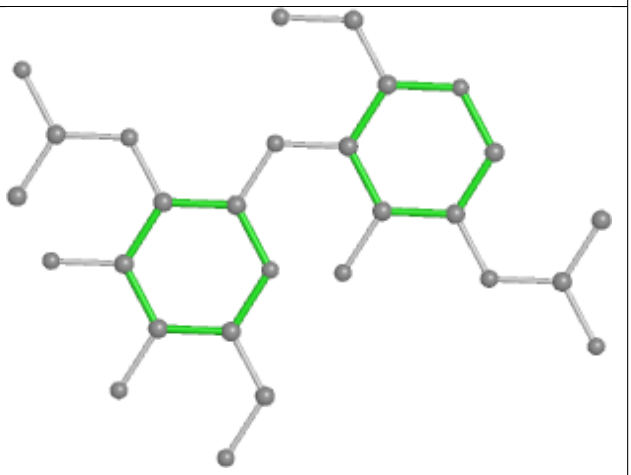
Bond lengths



Bond angles

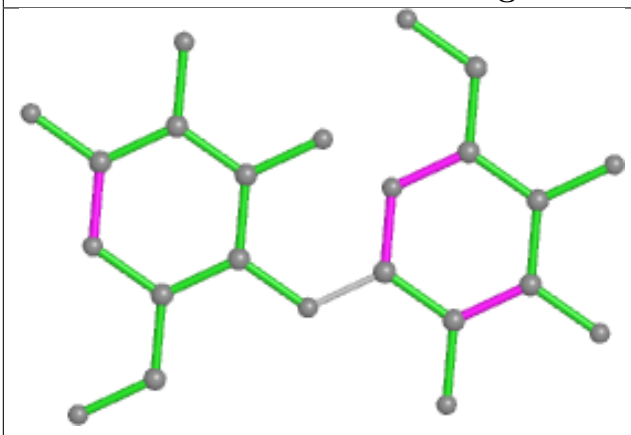


Torsions

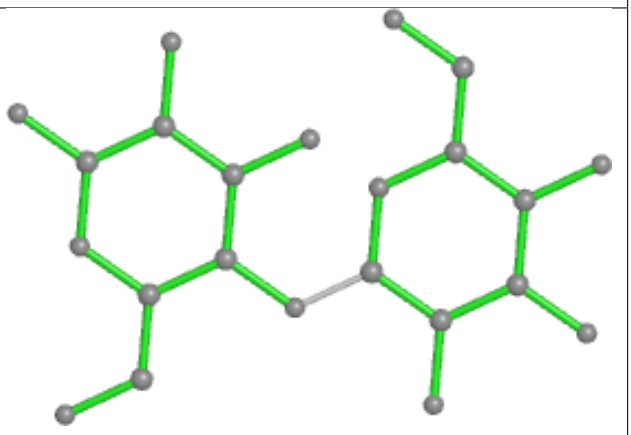


Rings

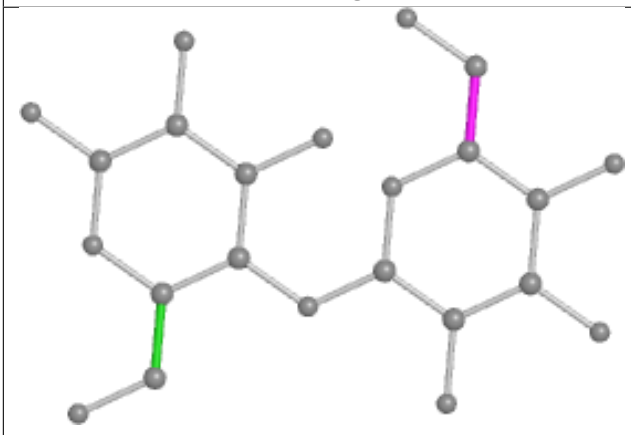
Oligosaccharide Chain J



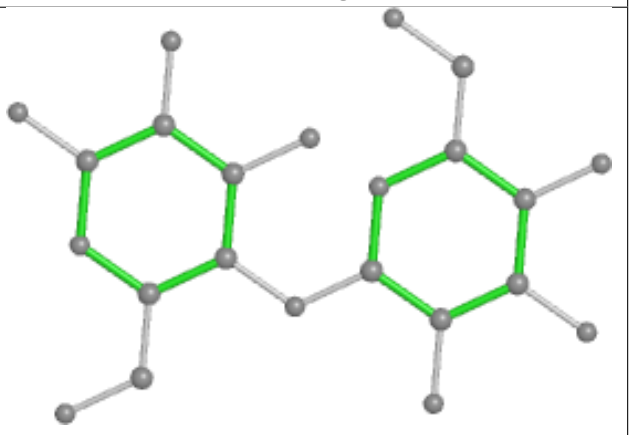
Bond lengths



Bond angles

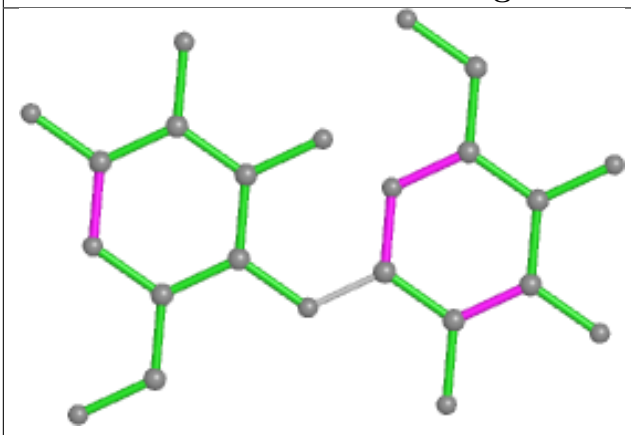


Torsions

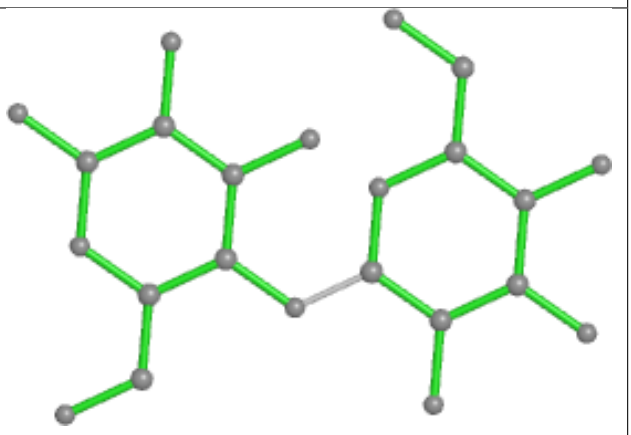


Rings

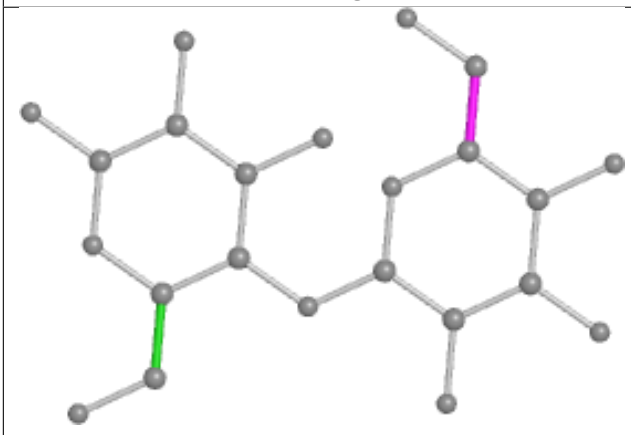
Oligosaccharide Chain K



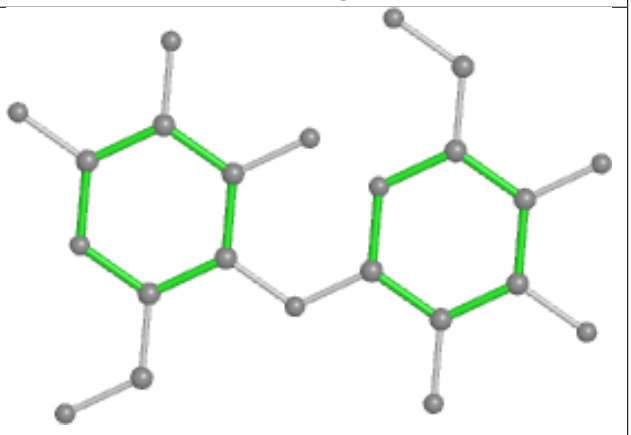
Bond lengths



Bond angles

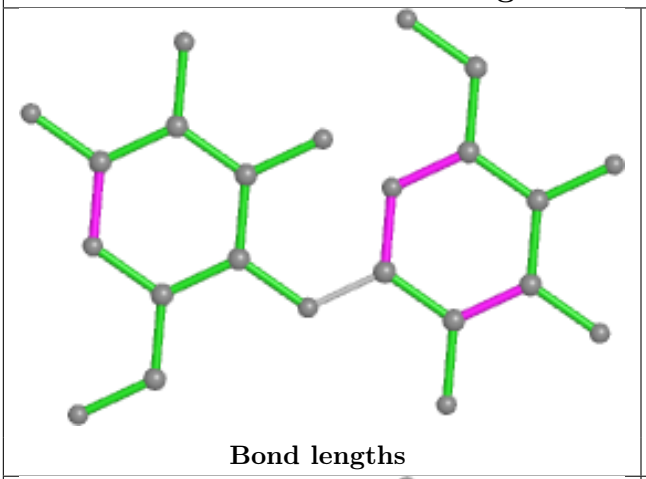


Torsions

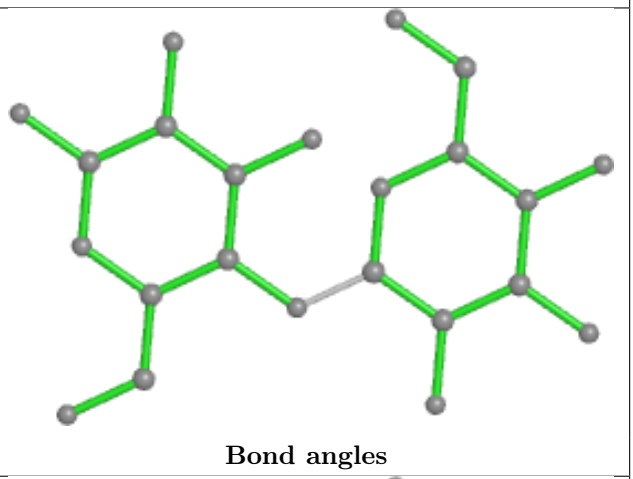


Rings

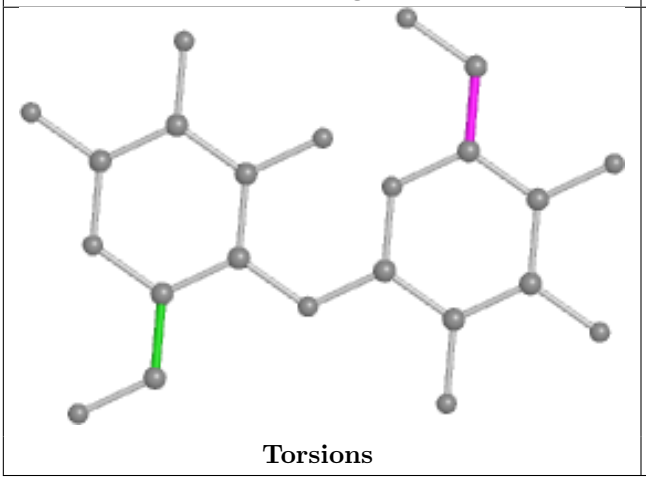
Oligosaccharide Chain L



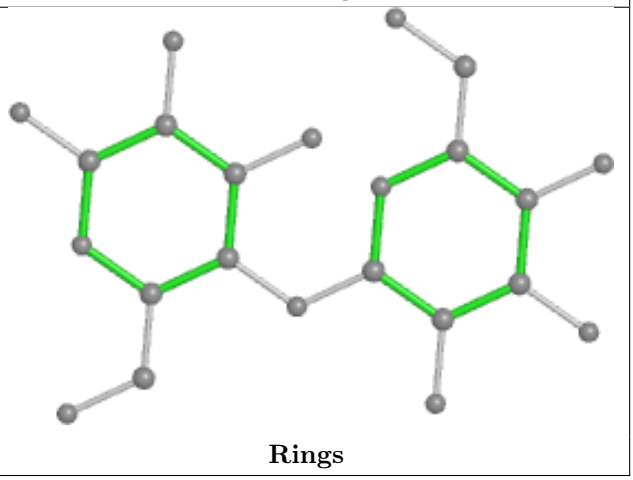
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

Of 39 ligands modelled in this entry, 6 are monoatomic - leaving 33 for Mogul analysis.

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	$\#\|Z\| > 2$
7	Q3G	C	711	-	35,36,51	1.12	5 (14%)	39,43,58	1.05	2 (5%)
8	PLM	A	713	1	16,16,17	0.20	0	15,15,17	0.55	0
6	NAG	B	710	1	14,14,15	0.18	0	17,19,21	0.77	1 (5%)
8	PLM	B	713	1	16,16,17	0.21	0	15,15,17	0.55	0
8	PLM	C	713	1	16,16,17	0.21	0	15,15,17	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	PLM	A	716	1	16,16,17	0.21	0	15,15,17	0.47	0
4	GDP	C	701	-	24,30,30	3.70	13 (54%)	30,47,47	1.47	6 (20%)
8	PLM	C	716	1	16,16,17	0.22	0	15,15,17	0.47	0
8	PLM	B	714	1	16,16,17	0.21	0	15,15,17	0.47	0
8	PLM	C	718	1	16,16,17	0.21	0	15,15,17	0.49	0
4	GDP	B	701	-	24,30,30	3.70	13 (54%)	30,47,47	1.47	6 (20%)
8	PLM	C	715	1	6,6,17	0.34	0	5,5,17	0.36	0
8	PLM	A	717	1	13,13,17	0.24	0	12,12,17	0.54	0
6	NAG	B	705	1	14,14,15	0.52	0	17,19,21	0.81	1 (5%)
8	PLM	A	718	1	16,16,17	0.21	0	15,15,17	0.49	0
8	PLM	A	715	1	6,6,17	0.34	0	5,5,17	0.36	0
8	PLM	A	714	1	16,16,17	0.22	0	15,15,17	0.47	0
8	PLM	B	715	1	6,6,17	0.34	0	5,5,17	0.36	0
8	PLM	B	718	1	16,16,17	0.21	0	15,15,17	0.49	0
8	PLM	C	717	1	13,13,17	0.24	0	12,12,17	0.53	0
6	NAG	B	704	-	14,14,15	0.37	0	17,19,21	0.75	1 (5%)
6	NAG	C	704	-	14,14,15	0.37	0	17,19,21	0.75	1 (5%)
6	NAG	C	705	1	14,14,15	0.46	0	17,19,21	0.81	1 (5%)
8	PLM	B	717	1	13,13,17	0.24	0	12,12,17	0.54	0
8	PLM	C	714	1	16,16,17	0.21	0	15,15,17	0.47	0
7	Q3G	A	711	-	35,36,51	1.13	5 (14%)	39,43,58	1.06	2 (5%)
4	GDP	A	701	-	24,30,30	3.69	13 (54%)	30,47,47	1.48	6 (20%)
6	NAG	C	710	1	14,14,15	0.17	0	17,19,21	0.77	1 (5%)
6	NAG	A	704	-	14,14,15	0.38	0	17,19,21	0.75	1 (5%)
6	NAG	A	705	1	14,14,15	0.52	0	17,19,21	0.80	1 (5%)
6	NAG	A	710	1	14,14,15	0.18	0	17,19,21	0.77	1 (5%)
7	Q3G	B	711	-	35,36,51	1.13	5 (14%)	39,43,58	1.06	2 (5%)
8	PLM	B	716	1	16,16,17	0.21	0	15,15,17	0.48	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
7	Q3G	C	711	-	-	16/42/42/57	-
8	PLM	A	713	1	-	1/13/14/15	-
6	NAG	B	710	1	-	2/6/23/26	0/1/1/1
8	PLM	B	713	1	-	1/13/14/15	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	PLM	C	713	1	-	1/13/14/15	-
8	PLM	A	716	1	-	5/13/14/15	-
4	GDP	C	701	-	-	3/12/32/32	0/3/3/3
8	PLM	C	716	1	-	4/13/14/15	-
8	PLM	B	714	1	-	5/13/14/15	-
8	PLM	C	718	1	-	5/13/14/15	-
4	GDP	B	701	-	-	3/12/32/32	0/3/3/3
8	PLM	C	715	1	-	0/3/4/15	-
8	PLM	A	717	1	-	1/10/11/15	-
6	NAG	B	705	1	-	1/6/23/26	0/1/1/1
8	PLM	A	718	1	-	5/13/14/15	-
8	PLM	A	715	1	-	0/3/4/15	-
8	PLM	A	714	1	-	5/13/14/15	-
8	PLM	B	715	1	-	0/3/4/15	-
8	PLM	B	718	1	-	5/13/14/15	-
8	PLM	C	717	1	-	1/10/11/15	-
6	NAG	B	704	-	-	2/6/23/26	0/1/1/1
6	NAG	C	704	-	-	2/6/23/26	0/1/1/1
6	NAG	C	705	1	-	2/6/23/26	0/1/1/1
8	PLM	B	717	1	-	1/10/11/15	-
8	PLM	C	714	1	-	5/13/14/15	-
7	Q3G	A	711	-	-	16/42/42/57	-
4	GDP	A	701	-	-	3/12/32/32	0/3/3/3
6	NAG	C	710	1	-	2/6/23/26	0/1/1/1
6	NAG	A	704	-	-	2/6/23/26	0/1/1/1
6	NAG	A	705	1	-	1/6/23/26	0/1/1/1
6	NAG	A	710	1	-	2/6/23/26	0/1/1/1
7	Q3G	B	711	-	-	16/42/42/57	-
8	PLM	B	716	1	-	5/13/14/15	-

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	701	GDP	C3'-C4'	-8.55	1.31	1.53
4	B	701	GDP	C3'-C4'	-8.55	1.31	1.53
4	A	701	GDP	C3'-C4'	-8.54	1.31	1.53
4	B	701	GDP	O4'-C4'	7.77	1.62	1.45
4	A	701	GDP	O4'-C4'	7.75	1.62	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	701	GDP	O4'-C4'	7.74	1.62	1.45
4	B	701	GDP	O4'-C1'	-7.18	1.31	1.41
4	C	701	GDP	O4'-C1'	-7.14	1.31	1.41
4	A	701	GDP	O4'-C1'	-7.08	1.31	1.41
4	C	701	GDP	C2-N3	5.48	1.46	1.33
4	A	701	GDP	C2-N3	5.47	1.46	1.33
4	B	701	GDP	C2-N3	5.45	1.46	1.33
4	B	701	GDP	C4-N3	5.03	1.49	1.37
4	C	701	GDP	C4-N3	5.00	1.49	1.37
4	A	701	GDP	C4-N3	4.97	1.49	1.37
4	C	701	GDP	C2-N2	4.74	1.45	1.34
4	B	701	GDP	C2-N2	4.73	1.45	1.34
4	A	701	GDP	C2-N2	4.73	1.45	1.34
4	A	701	GDP	C6-N1	3.74	1.43	1.37
4	C	701	GDP	C6-N1	3.73	1.43	1.37
4	B	701	GDP	C6-N1	3.71	1.43	1.37
4	B	701	GDP	C5-C6	3.12	1.53	1.47
4	C	701	GDP	C5-C6	3.11	1.53	1.47
4	A	701	GDP	C5-C6	3.06	1.53	1.47
4	A	701	GDP	O3'-C3'	3.01	1.50	1.43
4	B	701	GDP	O3'-C3'	2.99	1.50	1.43
4	C	701	GDP	O3'-C3'	2.97	1.50	1.43
4	B	701	GDP	O2'-C2'	-2.94	1.36	1.43
4	C	701	GDP	O2'-C2'	-2.93	1.36	1.43
4	A	701	GDP	O2'-C2'	-2.92	1.36	1.43
4	C	701	GDP	C2-N1	2.82	1.44	1.37
4	B	701	GDP	C2-N1	2.82	1.44	1.37
4	A	701	GDP	C2-N1	2.79	1.44	1.37
7	A	711	Q3G	O35-C22	-2.53	1.40	1.46
4	B	701	GDP	C5-C4	-2.51	1.36	1.43
7	B	711	Q3G	O35-C22	-2.51	1.40	1.46
7	C	711	Q3G	O35-C22	-2.50	1.40	1.46
4	C	701	GDP	C5-C4	-2.50	1.36	1.43
4	A	701	GDP	C5-C4	-2.48	1.36	1.43
7	C	711	Q3G	O20-C18	2.39	1.40	1.33
7	B	711	Q3G	O20-C18	2.39	1.40	1.33
7	A	711	Q3G	O20-C18	2.37	1.40	1.33
7	A	711	Q3G	C09-C10	-2.18	1.32	1.49
7	C	711	Q3G	C09-C10	-2.17	1.32	1.49
7	B	711	Q3G	C09-C10	-2.17	1.32	1.49
4	C	701	GDP	O6-C6	-2.16	1.18	1.23
7	A	711	Q3G	O35-C36	2.15	1.40	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	711	Q3G	O35-C36	2.15	1.40	1.34
4	B	701	GDP	O6-C6	-2.15	1.18	1.23
4	A	701	GDP	O6-C6	-2.14	1.18	1.23
7	A	711	Q3G	O20-C21	-2.14	1.40	1.45
7	C	711	Q3G	O35-C36	2.13	1.40	1.34
7	B	711	Q3G	O20-C21	-2.12	1.40	1.45
7	C	711	Q3G	O20-C21	-2.11	1.40	1.45

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	711	Q3G	O35-C36-C38	3.94	120.00	111.50
7	B	711	Q3G	O35-C36-C38	3.92	119.95	111.50
7	C	711	Q3G	O35-C36-C38	3.88	119.87	111.50
4	A	701	GDP	C5-C6-N1	3.40	119.96	113.95
4	B	701	GDP	C5-C6-N1	3.40	119.96	113.95
4	C	701	GDP	C5-C6-N1	3.38	119.92	113.95
4	A	701	GDP	C2-N1-C6	-2.89	119.77	125.10
4	B	701	GDP	C2-N1-C6	-2.89	119.78	125.10
4	C	701	GDP	C2-N1-C6	-2.88	119.80	125.10
4	B	701	GDP	C8-N7-C5	2.81	108.34	102.99
4	A	701	GDP	C8-N7-C5	2.80	108.33	102.99
4	C	701	GDP	C8-N7-C5	2.79	108.31	102.99
4	A	701	GDP	C3'-C2'-C1'	2.74	105.11	100.98
4	A	701	GDP	PA-O3A-PB	-2.73	123.45	132.83
4	B	701	GDP	PA-O3A-PB	-2.73	123.47	132.83
4	C	701	GDP	PA-O3A-PB	-2.72	123.48	132.83
4	C	701	GDP	C3'-C2'-C1'	2.70	105.05	100.98
6	C	705	NAG	C1-O5-C5	2.65	115.79	112.19
4	B	701	GDP	C3'-C2'-C1'	2.63	104.93	100.98
6	B	705	NAG	C1-O5-C5	2.57	115.67	112.19
7	B	711	Q3G	O20-C18-C17	2.56	119.95	111.91
6	A	705	NAG	C1-O5-C5	2.55	115.65	112.19
7	A	711	Q3G	O20-C18-C17	2.55	119.91	111.91
7	C	711	Q3G	O20-C18-C17	2.54	119.87	111.91
6	A	710	NAG	C2-N2-C7	2.52	126.49	122.90
6	C	710	NAG	C2-N2-C7	2.47	126.42	122.90
6	B	710	NAG	C2-N2-C7	2.47	126.41	122.90
4	B	701	GDP	O6-C6-C5	-2.27	119.93	124.37
4	A	701	GDP	O6-C6-C5	-2.27	119.95	124.37
4	C	701	GDP	O6-C6-C5	-2.24	120.01	124.37
6	B	704	NAG	C3-C4-C5	2.04	113.88	110.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	704	NAG	C3-C4-C5	2.03	113.85	110.24
6	A	704	NAG	C3-C4-C5	2.01	113.83	110.24

There are no chirality outliers.

All (123) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	701	GDP	C5'-O5'-PA-O3A
4	A	701	GDP	C5'-O5'-PA-O2A
4	B	701	GDP	C5'-O5'-PA-O3A
4	B	701	GDP	C5'-O5'-PA-O2A
4	C	701	GDP	C5'-O5'-PA-O3A
4	C	701	GDP	C5'-O5'-PA-O2A
7	A	711	Q3G	O20-C21-C22-O35
7	A	711	Q3G	C29-O28-P25-O24
7	B	711	Q3G	O20-C21-C22-O35
7	B	711	Q3G	C29-O28-P25-O24
7	C	711	Q3G	O20-C21-C22-O35
8	A	717	PLM	C1-C2-C3-C4
8	A	718	PLM	C1-C2-C3-C4
8	B	717	PLM	C1-C2-C3-C4
8	B	718	PLM	C1-C2-C3-C4
8	C	717	PLM	C1-C2-C3-C4
8	C	718	PLM	C1-C2-C3-C4
7	B	711	Q3G	C15-C16-C17-C18
6	C	705	NAG	O5-C5-C6-O6
7	A	711	Q3G	C15-C16-C17-C18
6	C	705	NAG	C4-C5-C6-O6
7	C	711	Q3G	C15-C16-C17-C18
6	A	710	NAG	C8-C7-N2-C2
6	A	710	NAG	O7-C7-N2-C2
6	B	710	NAG	C8-C7-N2-C2
6	B	710	NAG	O7-C7-N2-C2
6	C	710	NAG	C8-C7-N2-C2
6	C	710	NAG	O7-C7-N2-C2
8	B	718	PLM	CB-CC-CD-CE
8	C	716	PLM	C6-C7-C8-C9
8	C	718	PLM	CB-CC-CD-CE
8	A	716	PLM	C6-C7-C8-C9
8	A	718	PLM	CB-CC-CD-CE
8	B	716	PLM	C6-C7-C8-C9
8	C	716	PLM	C2-C3-C4-C5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	A	718	PLM	C6-C7-C8-C9
8	B	718	PLM	C6-C7-C8-C9
8	C	718	PLM	C6-C7-C8-C9
8	B	714	PLM	CB-CC-CD-CE
7	B	711	Q3G	C41-C42-C43-C44
6	B	705	NAG	O5-C5-C6-O6
7	C	711	Q3G	C41-C42-C43-C44
7	A	711	Q3G	C41-C42-C43-C44
8	A	716	PLM	C2-C3-C4-C5
8	A	714	PLM	CB-CC-CD-CE
8	B	716	PLM	C2-C3-C4-C5
6	A	705	NAG	O5-C5-C6-O6
8	C	714	PLM	CB-CC-CD-CE
7	B	711	Q3G	C11-C12-C13-C14
7	A	711	Q3G	C11-C12-C13-C14
8	C	714	PLM	C5-C6-C7-C8
8	A	714	PLM	C5-C6-C7-C8
7	B	711	Q3G	C13-C14-C15-C16
7	A	711	Q3G	C13-C14-C15-C16
7	C	711	Q3G	C11-C12-C13-C14
7	A	711	Q3G	O20-C21-C22-C23
7	B	711	Q3G	O20-C21-C22-C23
7	C	711	Q3G	O20-C21-C22-C23
7	C	711	Q3G	C38-C39-C40-C41
7	B	711	Q3G	C38-C39-C40-C41
7	C	711	Q3G	C13-C14-C15-C16
7	A	711	Q3G	C40-C41-C42-C43
8	A	718	PLM	C3-C4-C5-C6
8	B	718	PLM	C3-C4-C5-C6
8	C	718	PLM	C3-C4-C5-C6
8	C	716	PLM	C8-C9-CA-CB
8	B	716	PLM	C8-C9-CA-CB
7	C	711	Q3G	C29-O28-P25-O24
6	A	704	NAG	C4-C5-C6-O6
6	B	704	NAG	C4-C5-C6-O6
6	C	704	NAG	C4-C5-C6-O6
8	A	718	PLM	C8-C9-CA-CB
8	B	714	PLM	C5-C6-C7-C8
8	C	718	PLM	C8-C9-CA-CB
8	A	716	PLM	C8-C9-CA-CB
8	B	718	PLM	C8-C9-CA-CB
8	B	714	PLM	C7-C8-C9-CA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	C	714	PLM	C3-C4-C5-C6
7	B	711	Q3G	C21-C22-C23-O24
7	B	711	Q3G	C40-C41-C42-C43
8	A	714	PLM	C3-C4-C5-C6
8	B	716	PLM	CD-CE-CF-CG
8	B	714	PLM	C3-C4-C5-C6
8	A	714	PLM	CD-CE-CF-CG
7	C	711	Q3G	C40-C41-C42-C43
8	C	716	PLM	CD-CE-CF-CG
4	A	701	GDP	C5'-O5'-PA-O1A
4	B	701	GDP	C5'-O5'-PA-O1A
4	C	701	GDP	C5'-O5'-PA-O1A
8	A	716	PLM	CD-CE-CF-CG
7	A	711	Q3G	C21-C22-C23-O24
7	C	711	Q3G	C21-C22-C23-O24
8	C	714	PLM	CD-CE-CF-CG
7	A	711	Q3G	O35-C22-C23-O24
7	B	711	Q3G	O35-C22-C23-O24
7	C	711	Q3G	O35-C22-C23-O24
8	A	713	PLM	C1-C2-C3-C4
8	B	713	PLM	C1-C2-C3-C4
8	C	713	PLM	C1-C2-C3-C4
8	C	714	PLM	C7-C8-C9-CA
8	A	714	PLM	C7-C8-C9-CA
7	B	711	Q3G	C39-C40-C41-C42
7	A	711	Q3G	C38-C39-C40-C41
7	A	711	Q3G	C22-C23-O24-P25
7	B	711	Q3G	C22-C23-O24-P25
6	C	704	NAG	O5-C5-C6-O6
6	A	704	NAG	O5-C5-C6-O6
6	B	704	NAG	O5-C5-C6-O6
7	C	711	Q3G	C39-C40-C41-C42
8	B	714	PLM	CD-CE-CF-CG
7	C	711	Q3G	C22-C23-O24-P25
7	A	711	Q3G	C39-C40-C41-C42
7	C	711	Q3G	C16-C17-C18-O20
7	A	711	Q3G	C16-C17-C18-O20
7	B	711	Q3G	C16-C17-C18-O20
7	C	711	Q3G	C10-C11-C12-C13
7	A	711	Q3G	C16-C17-C18-O19
7	A	711	Q3G	C23-O24-P25-O26
7	B	711	Q3G	C23-O24-P25-O26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	C	711	Q3G	C16-C17-C18-O19
8	A	716	PLM	C7-C8-C9-CA
7	B	711	Q3G	C16-C17-C18-O19
8	B	716	PLM	C7-C8-C9-CA

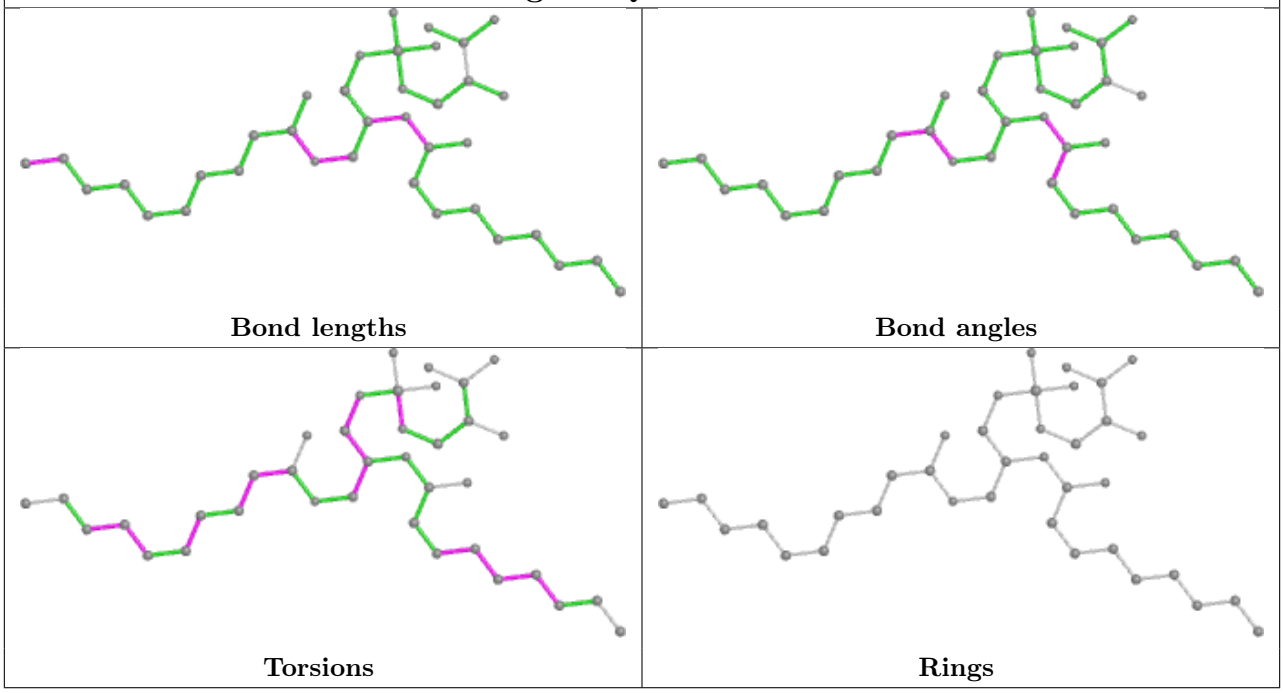
There are no ring outliers.

3 monomers are involved in 3 short contacts:

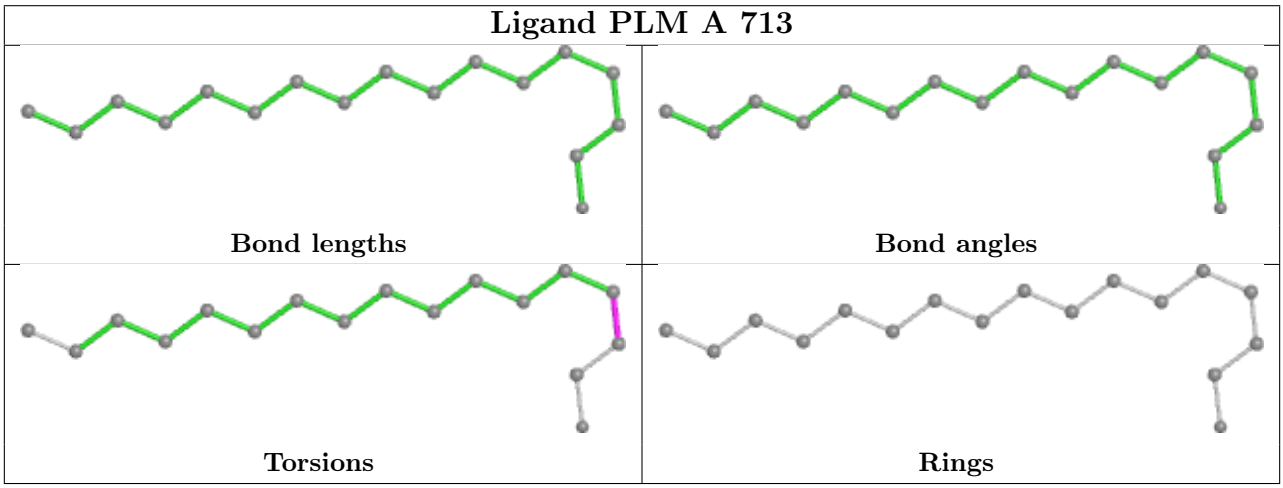
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	701	GDP	1	0
4	B	701	GDP	1	0
4	A	701	GDP	1	0

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.

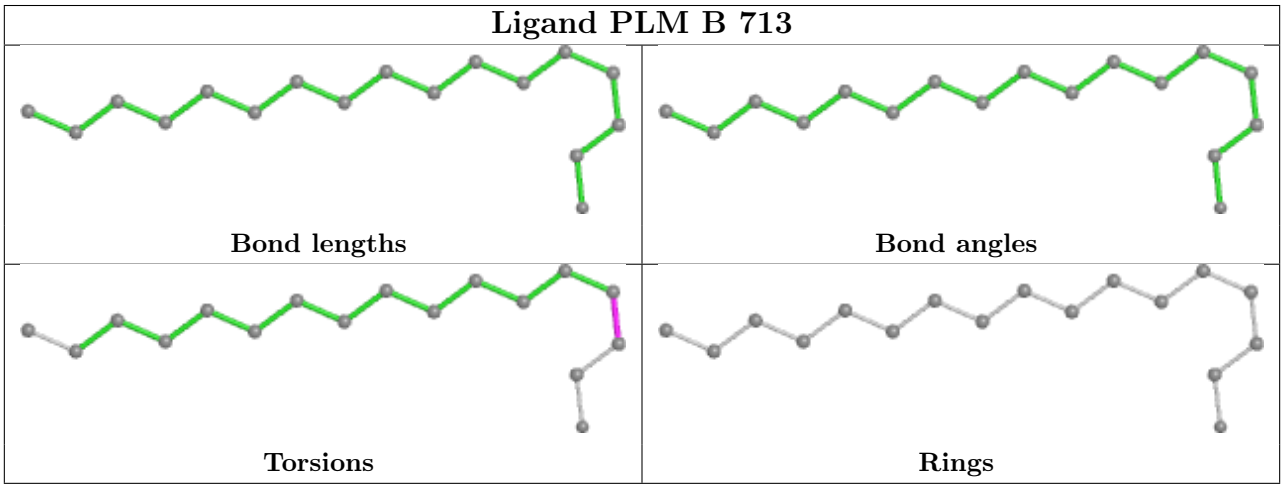
Ligand Q3G C 711



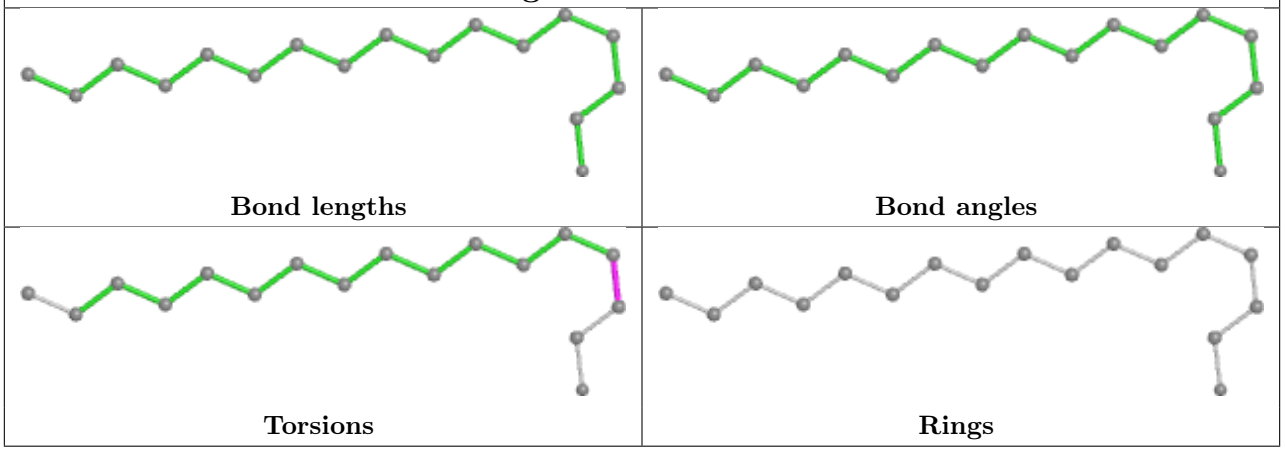
Ligand PLM A 713



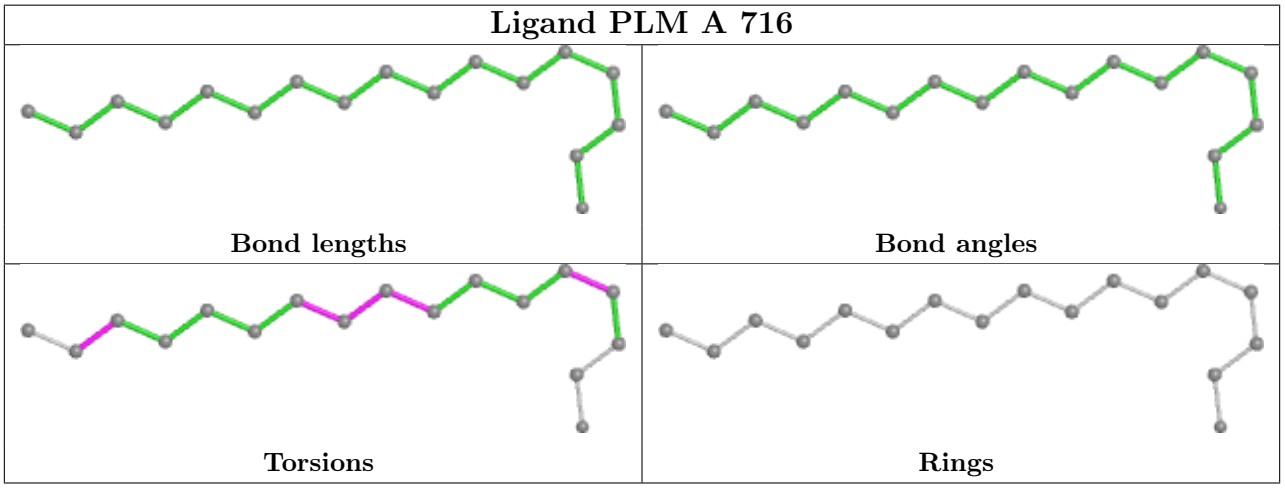
Ligand PLM B 713



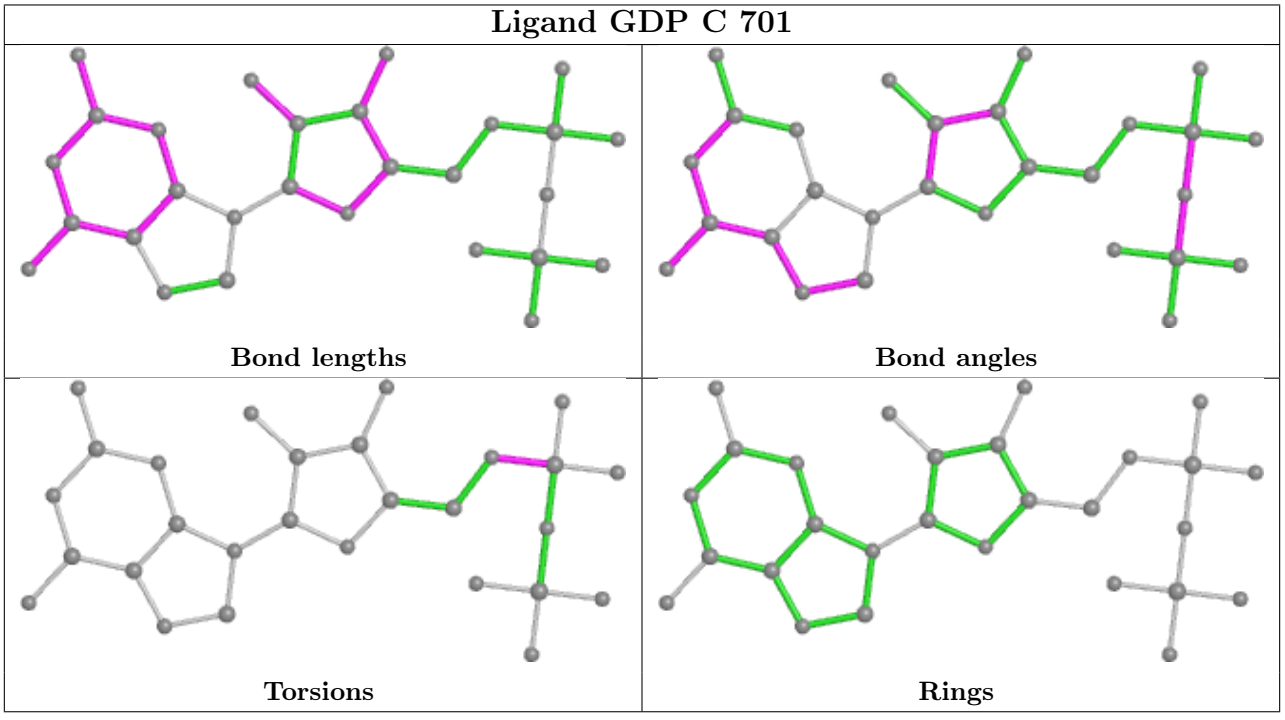
Ligand PLM C 713



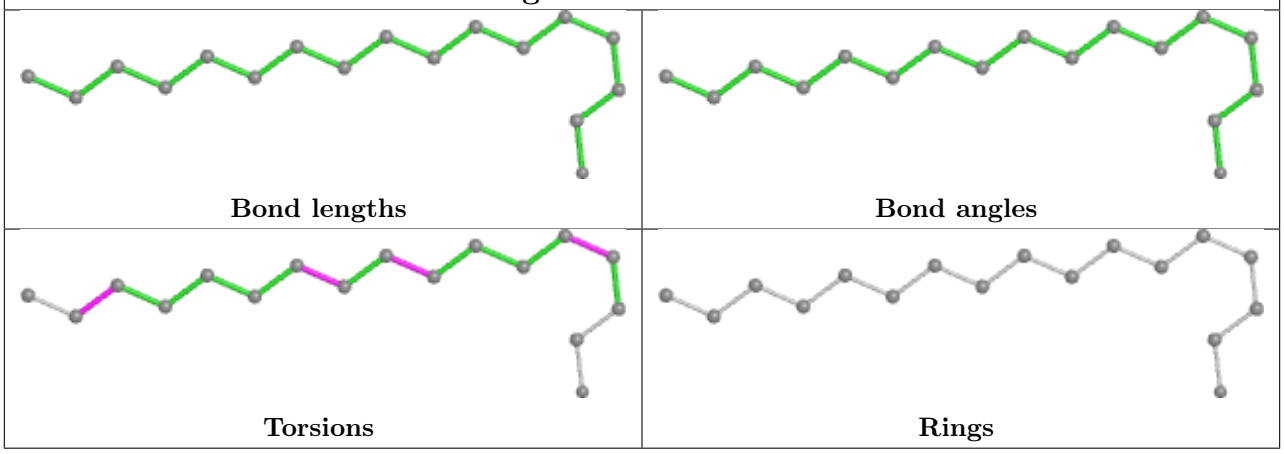
Ligand PLM A 716



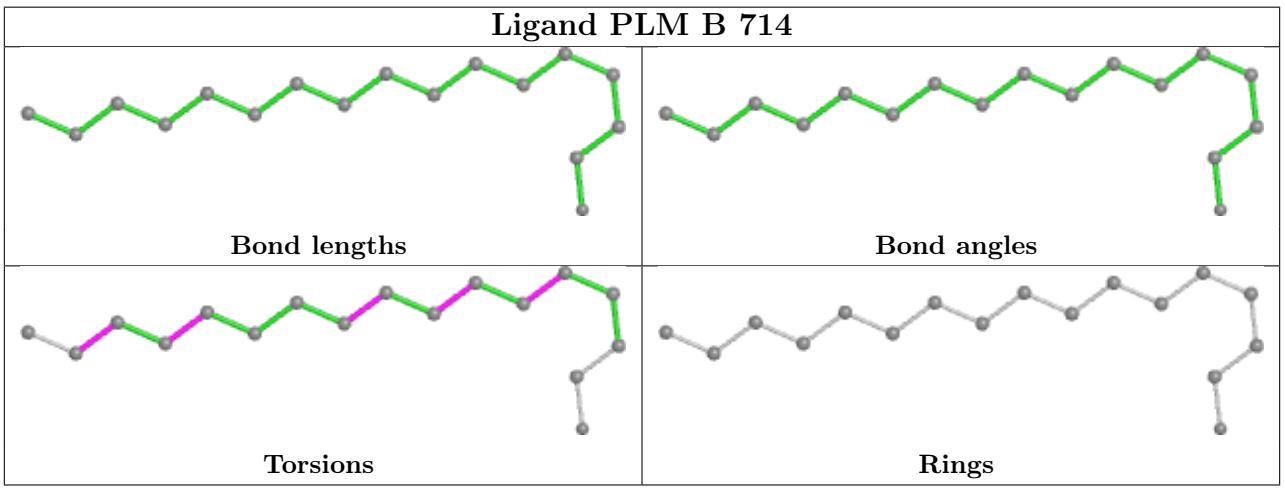
Ligand GDP C 701



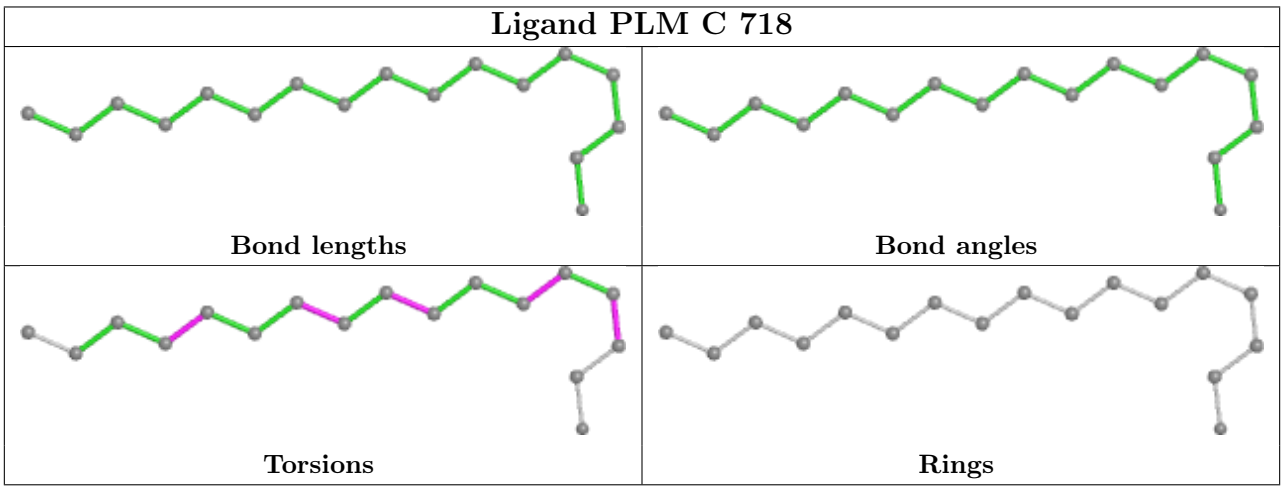
Ligand PLM C 716



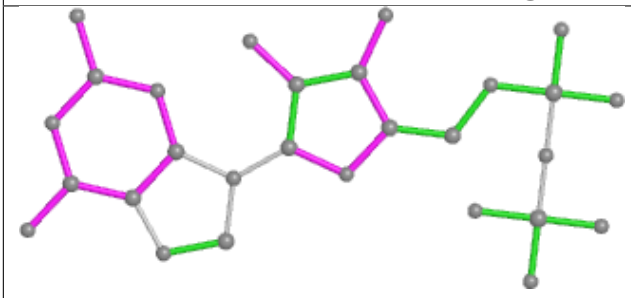
Ligand PLM B 714



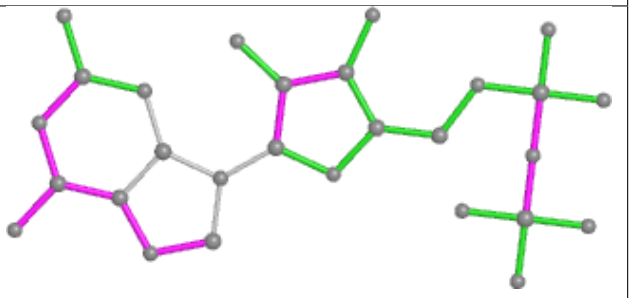
Ligand PLM C 718



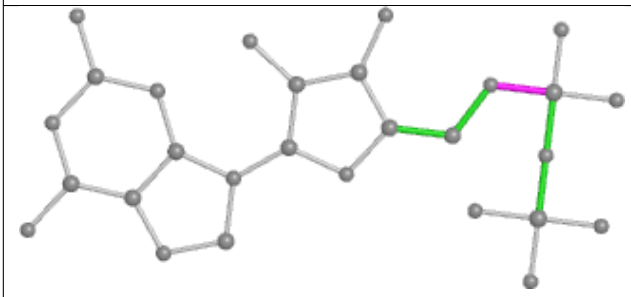
Ligand GDP B 701



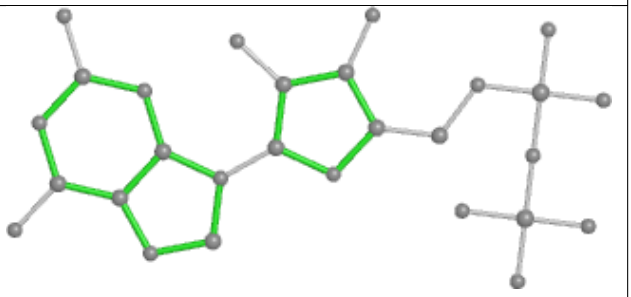
Bond lengths



Bond angles

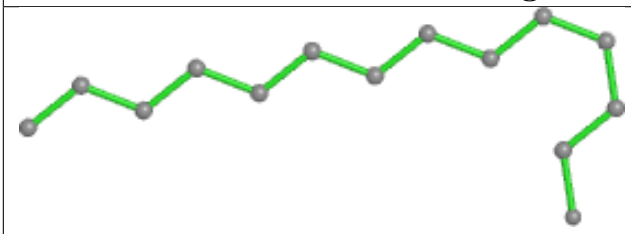


Torsions

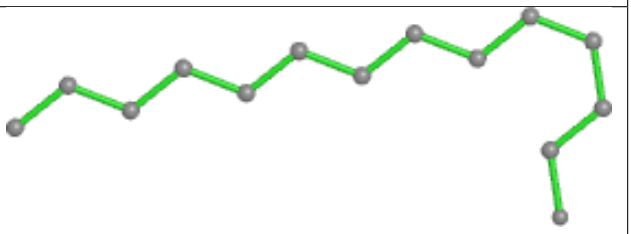


Rings

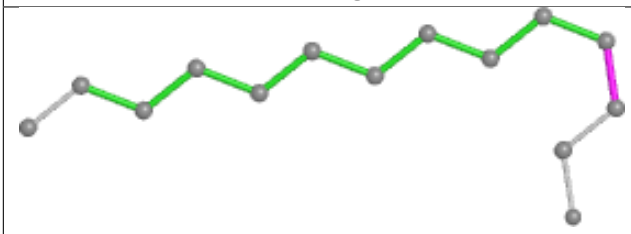
Ligand PLM A 717



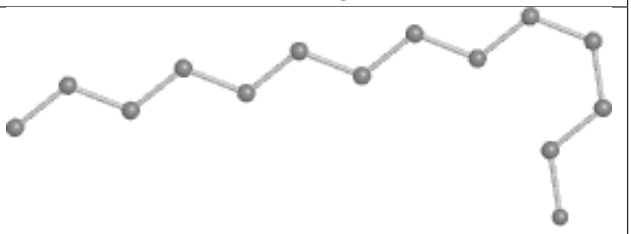
Bond lengths



Bond angles

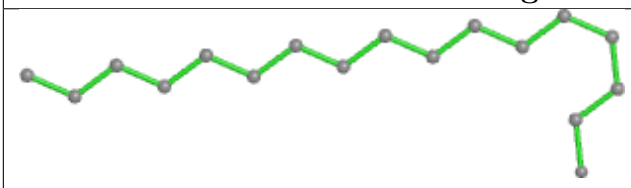


Torsions

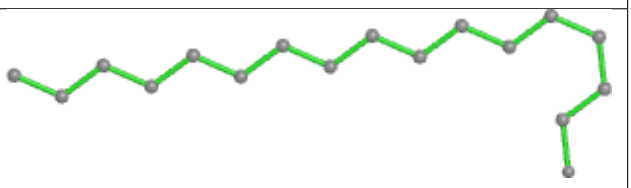


Rings

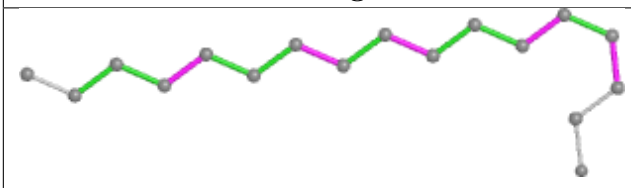
Ligand PLM A 718



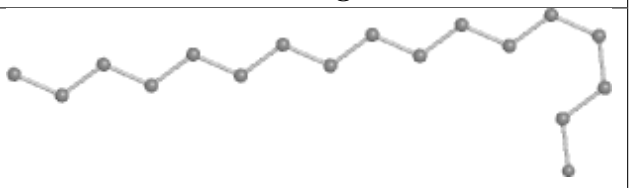
Bond lengths



Bond angles

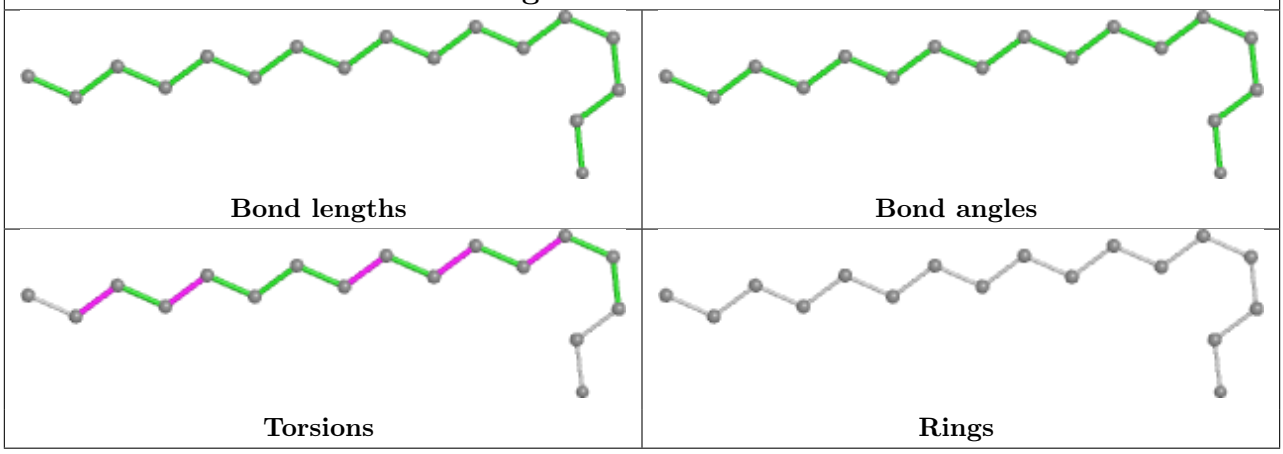


Torsions

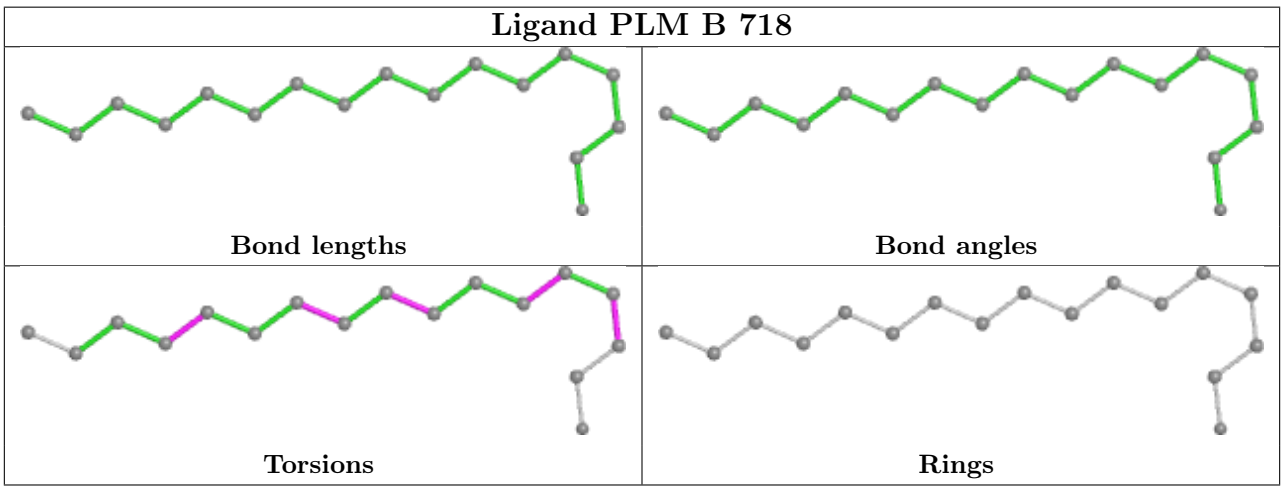


Rings

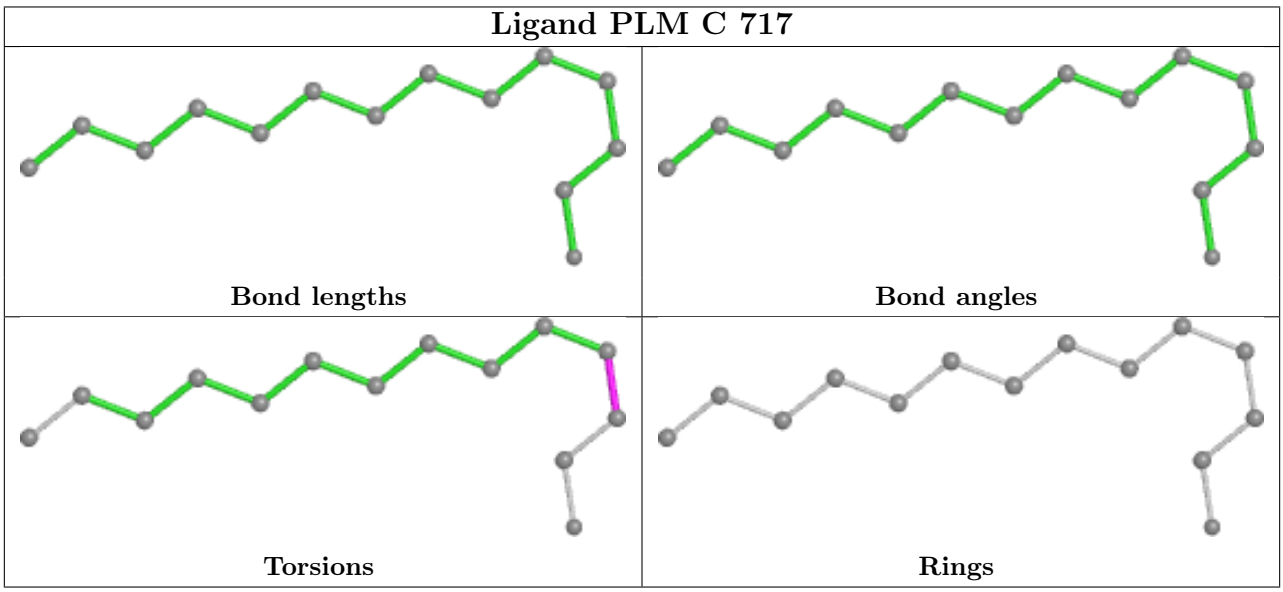
Ligand PLM A 714



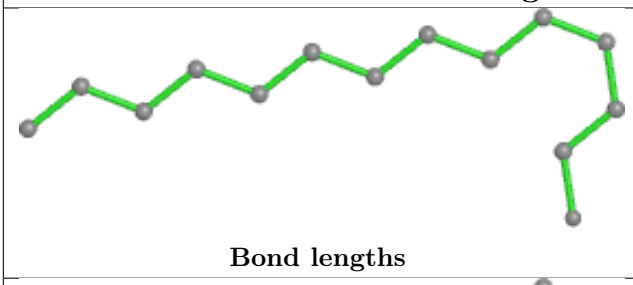
Ligand PLM B 718



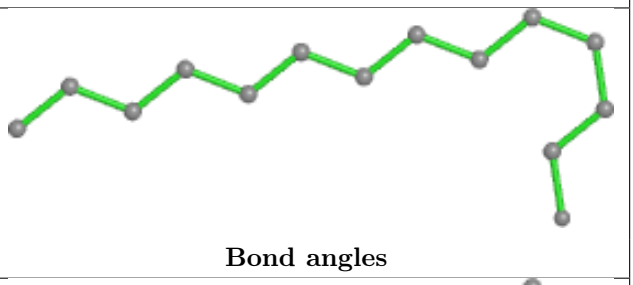
Ligand PLM C 717



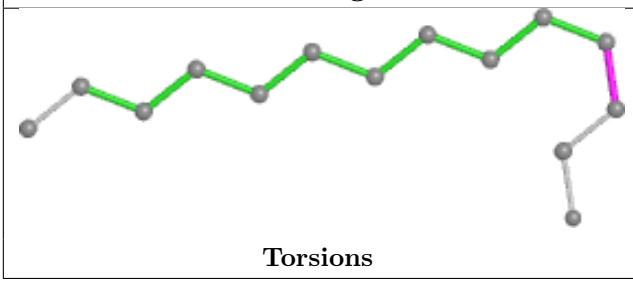
Ligand PLM B 717



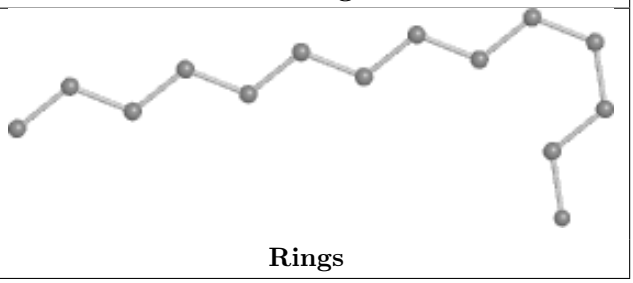
Bond lengths



Bond angles

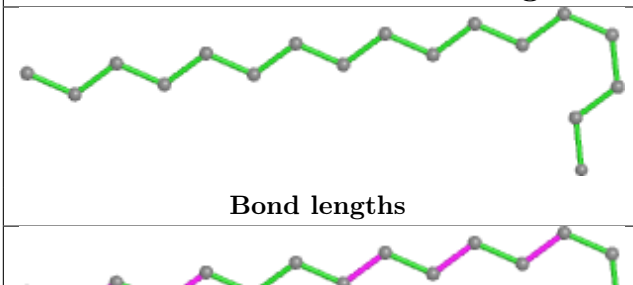


Torsions

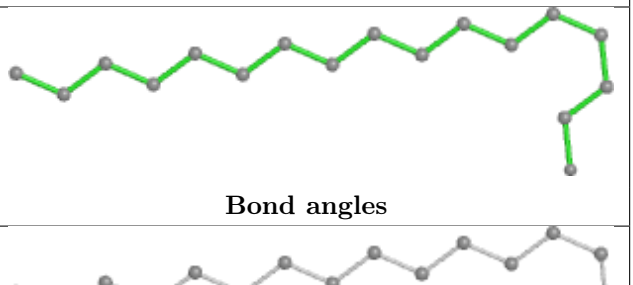


Rings

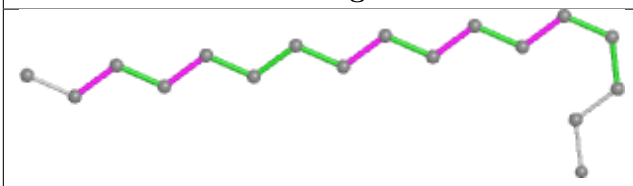
Ligand PLM C 714



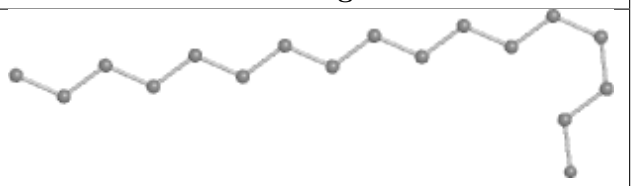
Bond lengths



Bond angles

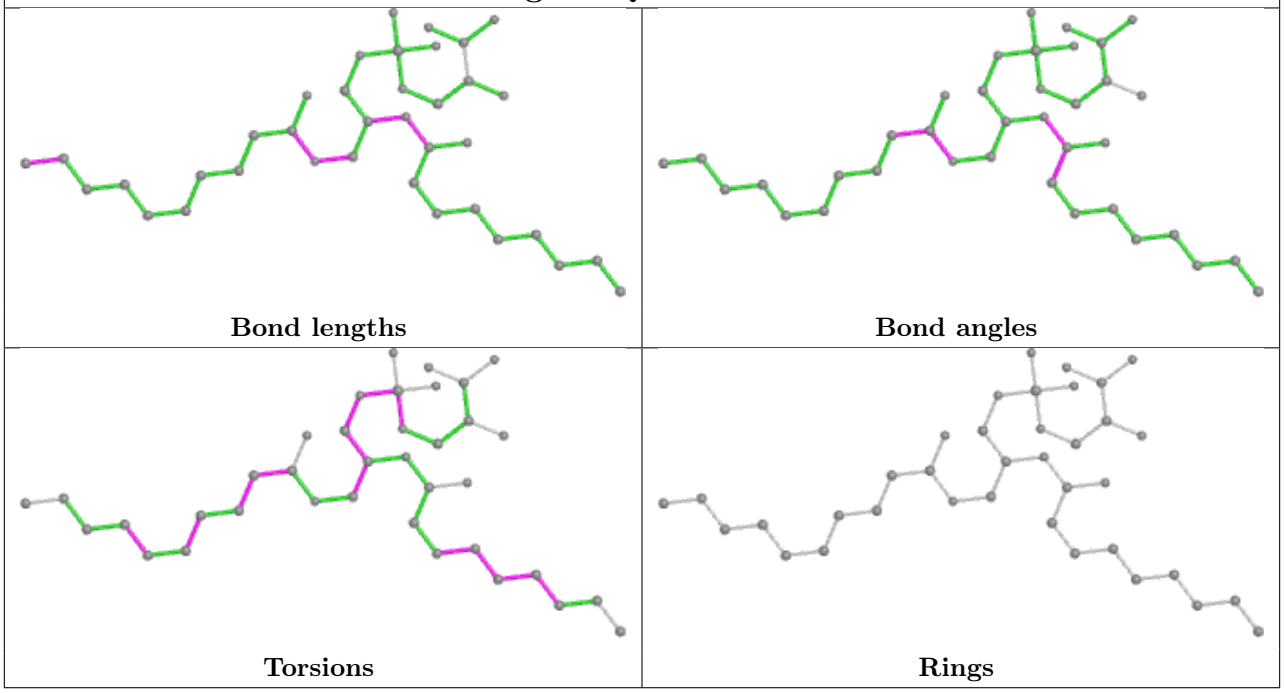


Torsions

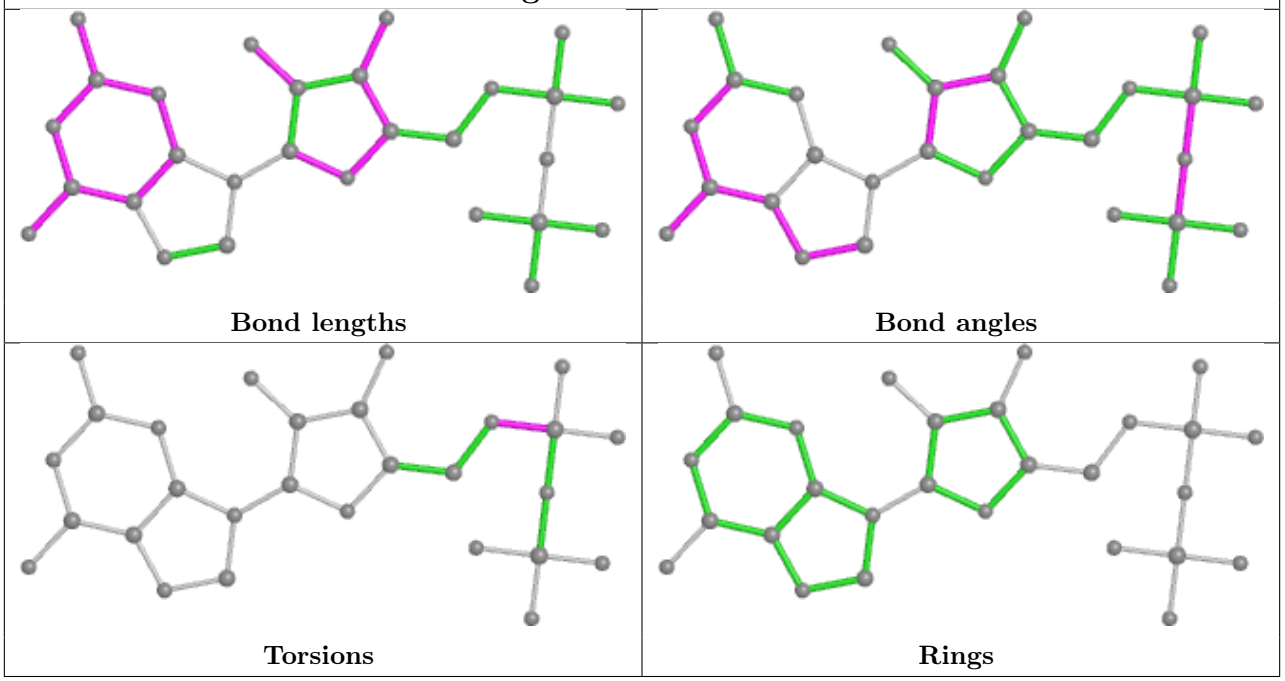


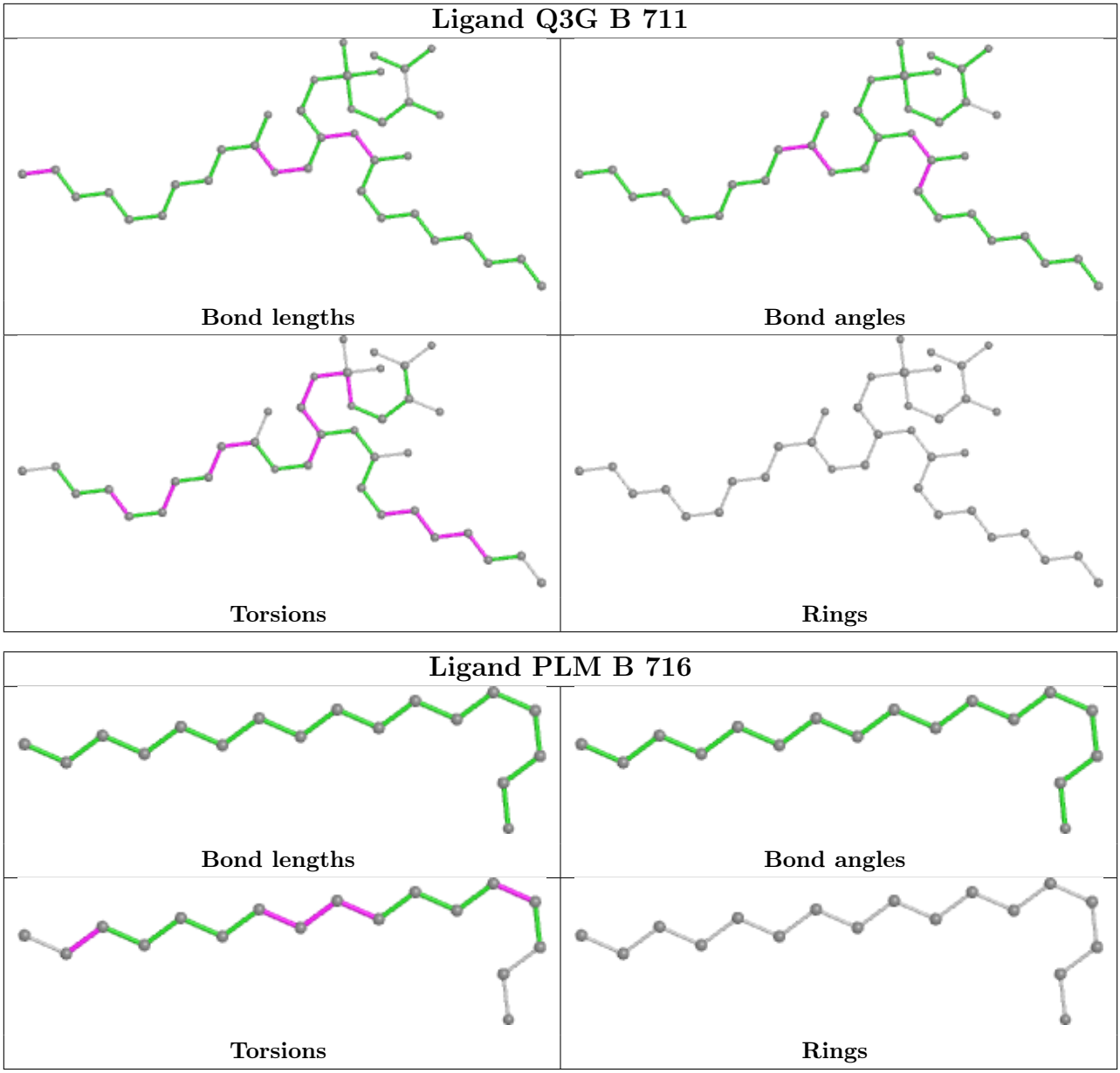
Rings

Ligand Q3G A 711



Ligand GDP A 701





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.

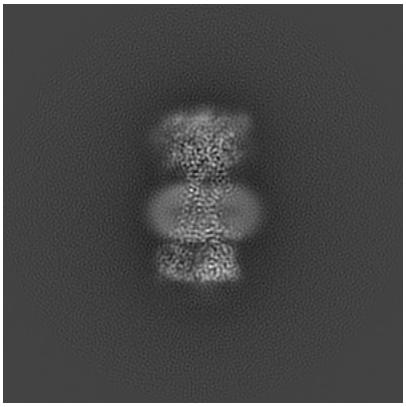
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-20702. These allow visual inspection of the internal detail of the map and identification of artifacts.

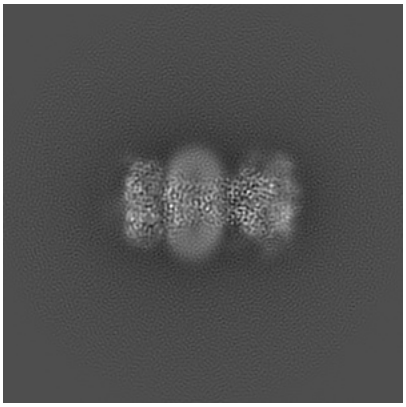
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

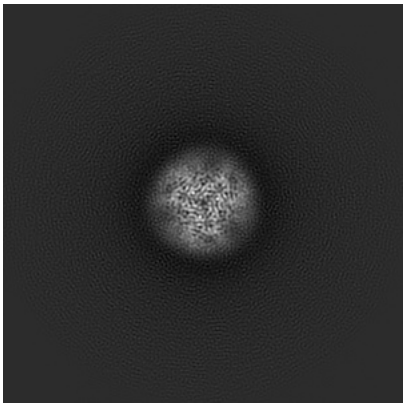
6.1.1 Primary map



X



Y

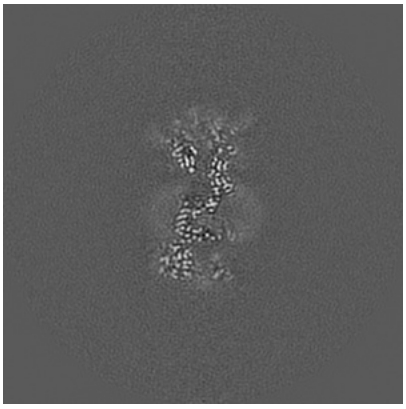


Z

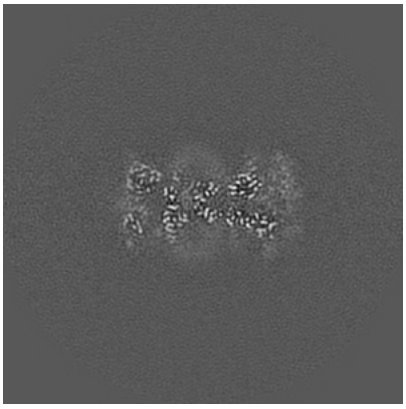
The images above show the map projected in three orthogonal directions.

6.2 Central slices

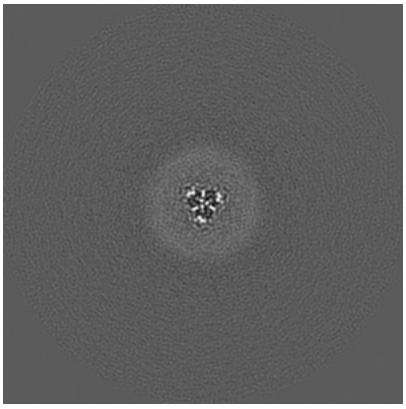
6.2.1 Primary map



X Index: 160



Y Index: 160

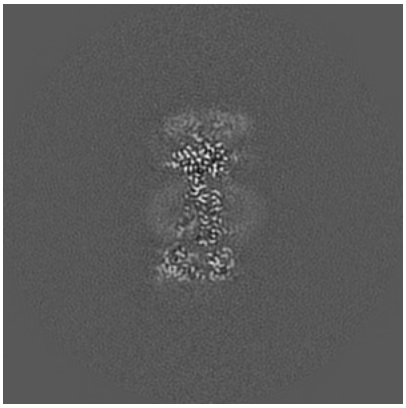


Z Index: 160

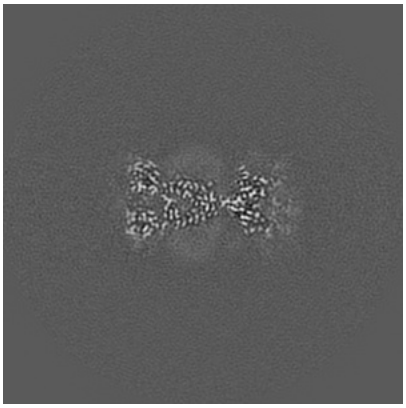
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

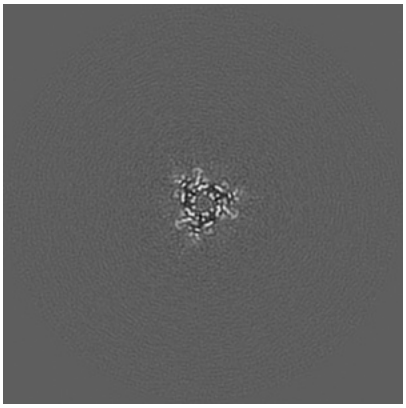
6.3.1 Primary map



X Index: 151



Y Index: 167



Z Index: 193

The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.0349. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

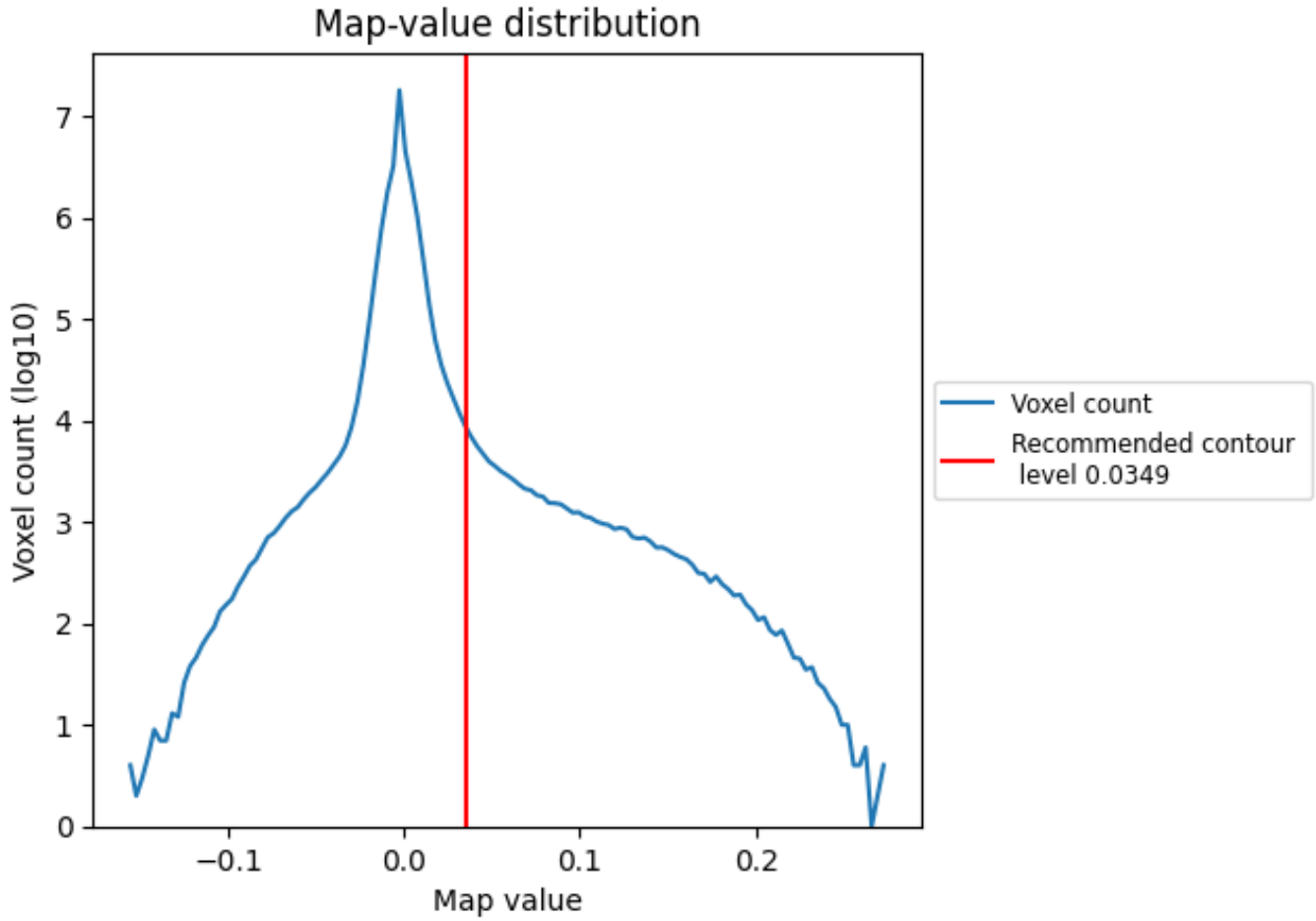
6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

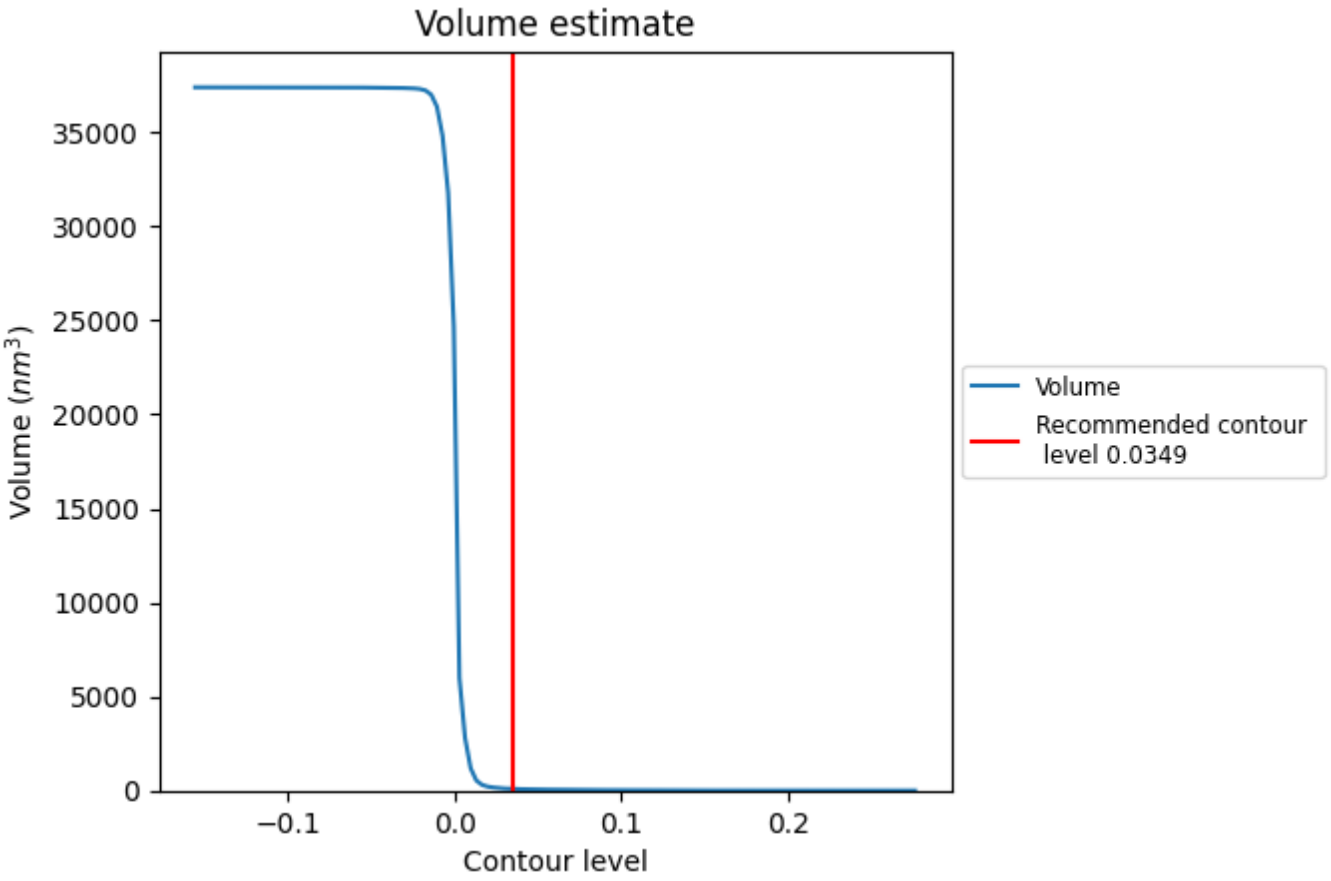
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

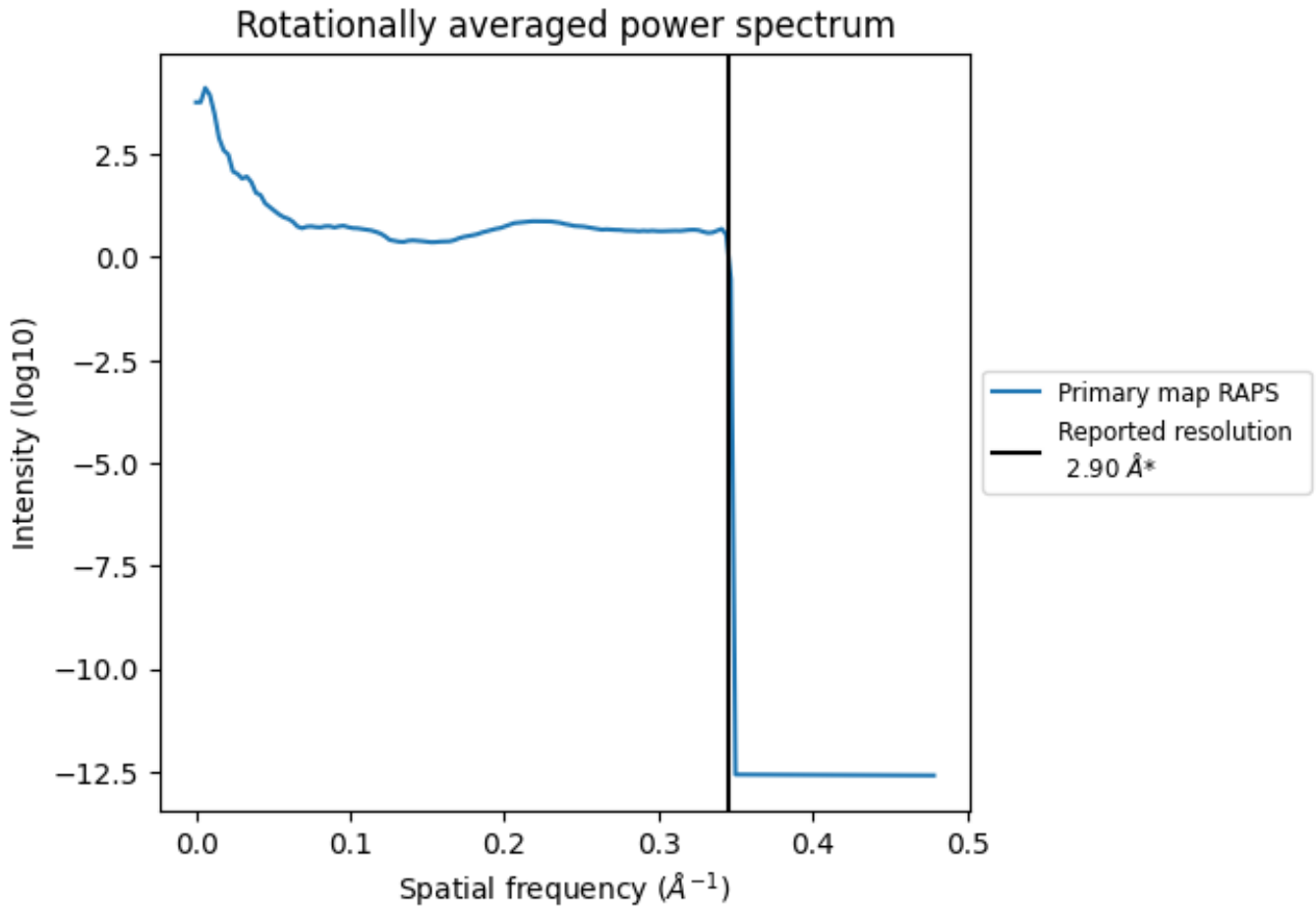
7.2 Volume estimate



The volume at the recommended contour level is 89 nm^3; this corresponds to an approximate mass of 80 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

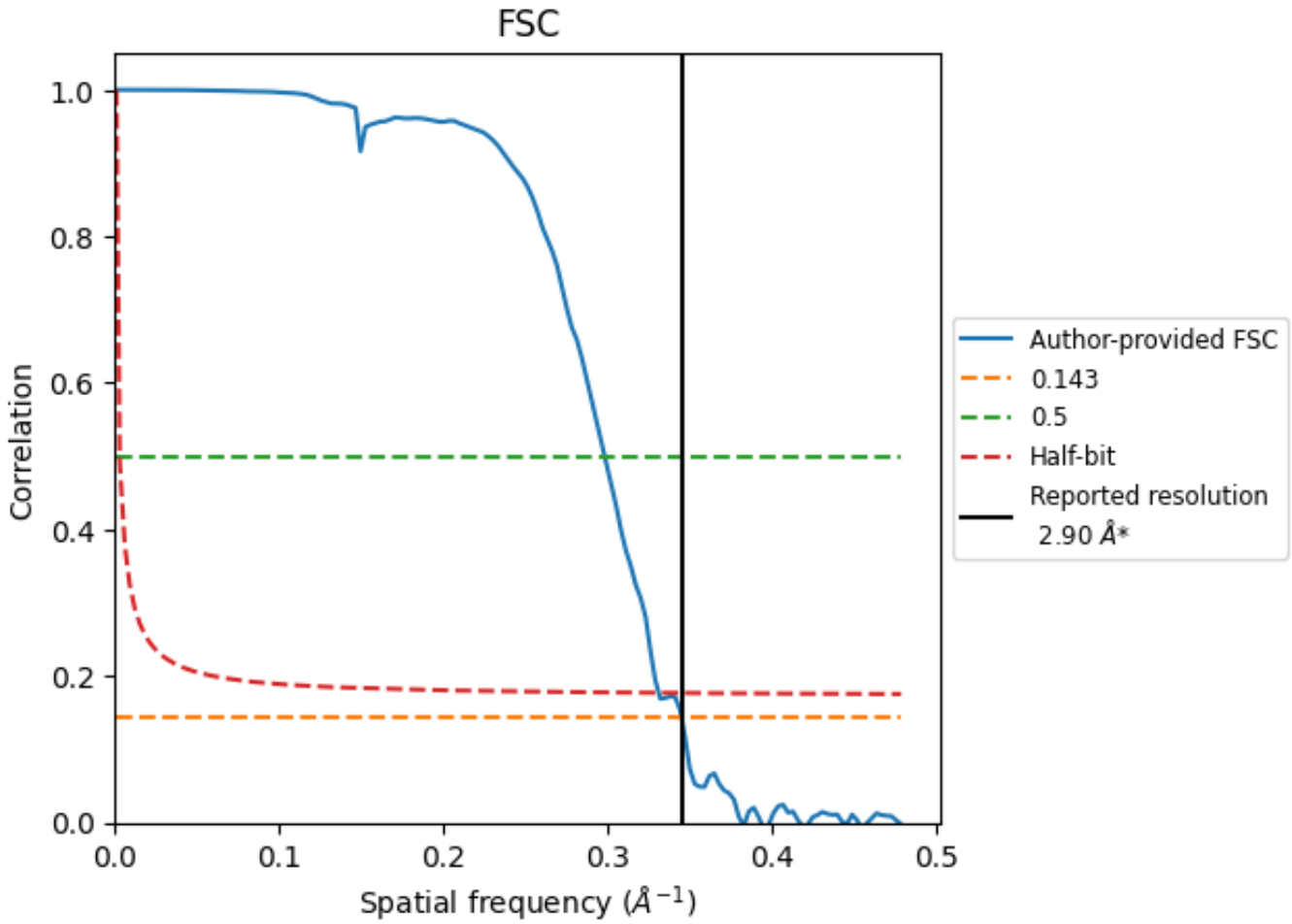


*Reported resolution corresponds to spatial frequency of 0.345 $Å^{-1}$

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.345 Å^{-1}

8.2 Resolution estimates (i)

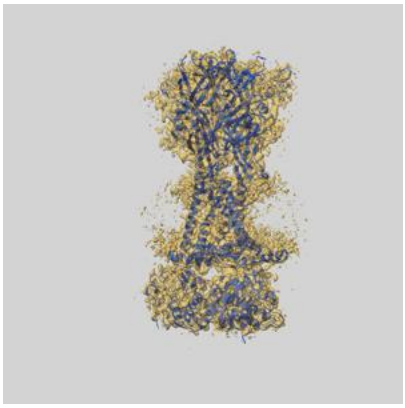
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.90	3.35	3.02
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

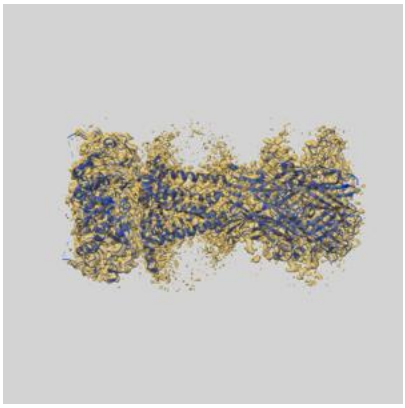
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-20702 and PDB model 6U9V. Per-residue inclusion information can be found in section 3 on page 11.

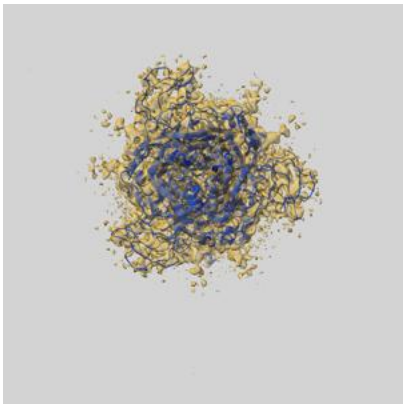
9.1 Map-model overlay



X



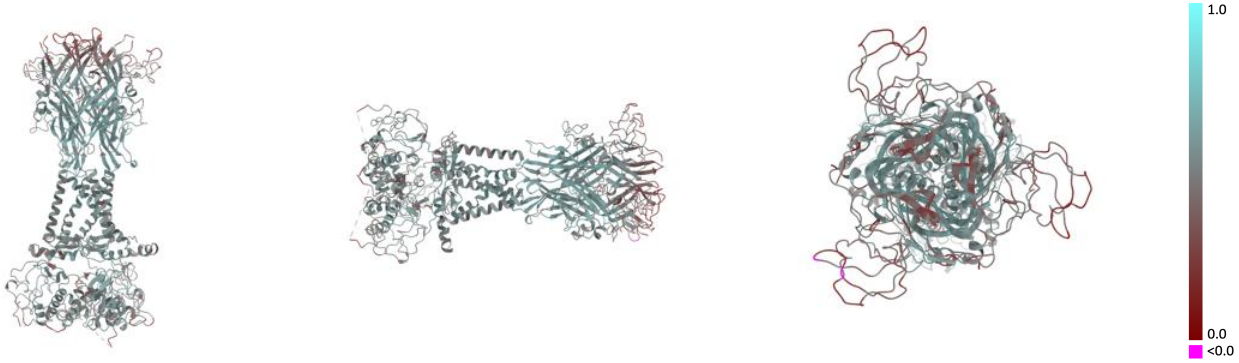
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0349 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

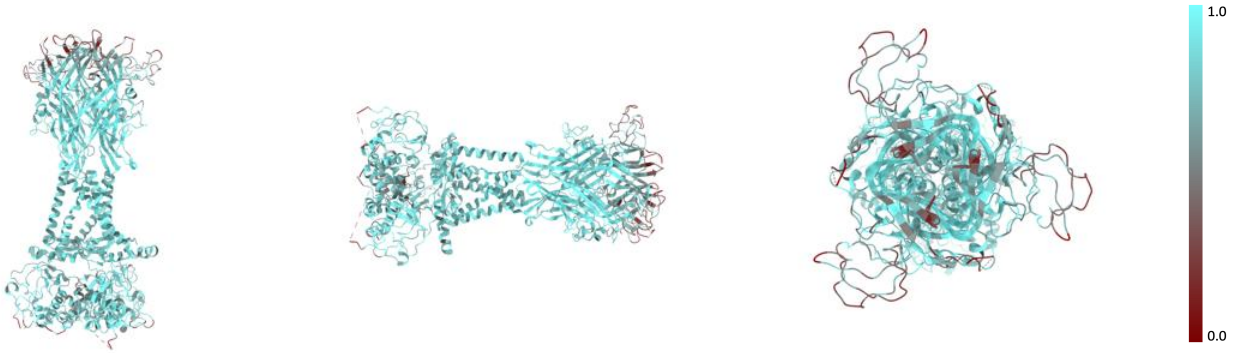
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

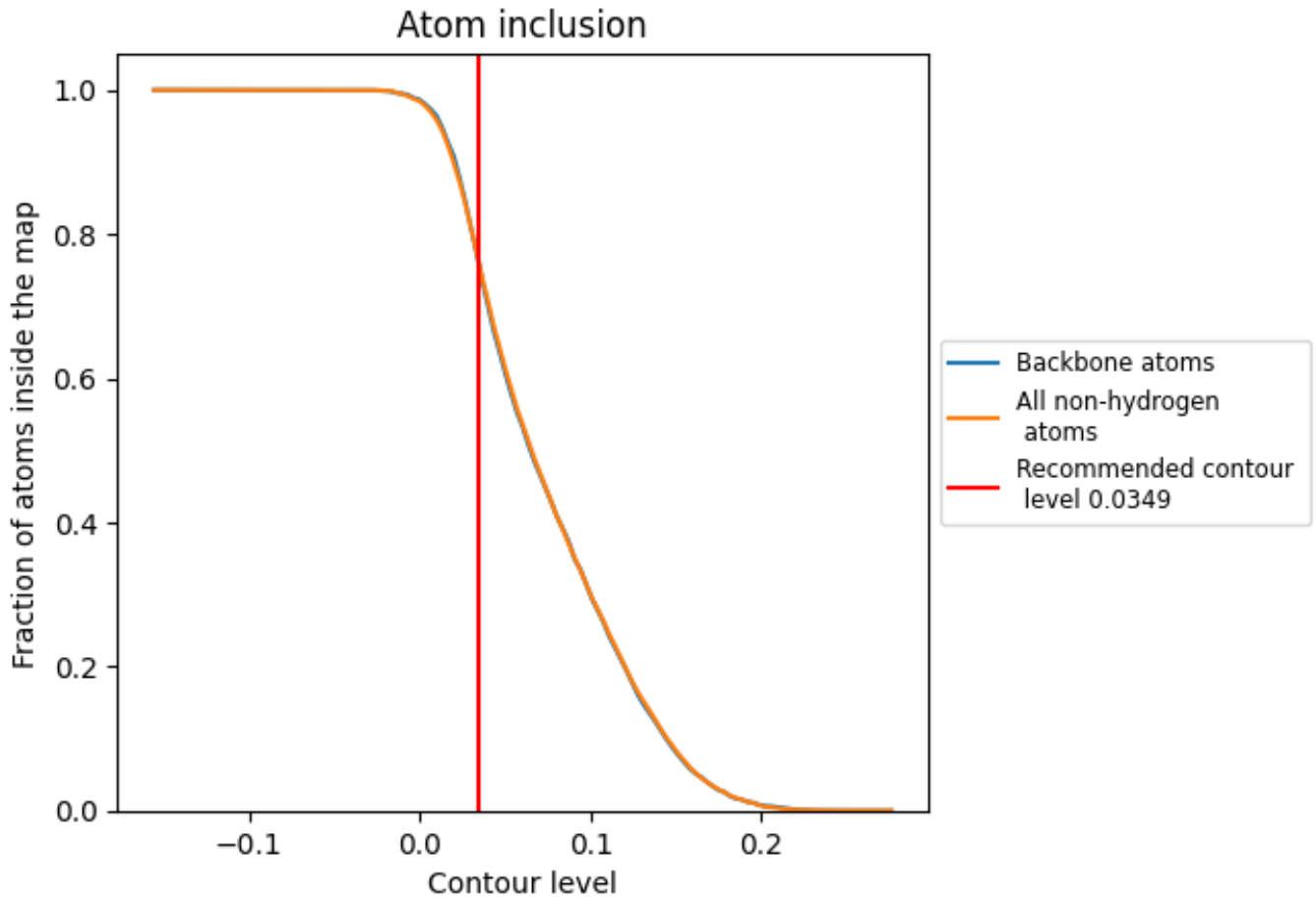
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0349).

9.4 Atom inclusion (i)



At the recommended contour level, 76% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0349) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7569	0.5030
A	0.7698	0.5040
B	0.7707	0.5040
C	0.7669	0.5040
D	0.5357	0.4150
E	0.5714	0.4170
F	0.6071	0.4480
G	0.7143	0.5070
H	0.6071	0.4510
I	0.7143	0.4870
J	0.5652	0.3570
K	0.5217	0.3690
L	0.5652	0.3680