Full wwPDB EM Validation Report

Apr 11, 2023 – 04:36 PM EDT

PDB ID	:	8FWU
EMDB ID	:	EMD-29519
Title	:	Structure of the ligand-binding and transmembrane domains of kainate receptor GluK2 in complex with the positive allosteric modulator BPAM344 and competitive antagonist DNQX
Authors	:	Yen, L.Y.; Gangwar, S.P.; Yelshanskaya, M.V.; Sobolevsky, A.I.
Deposited on	:	2023-01-23
Resolution	:	3.18 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 (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 (1)) were used in the production of this report:

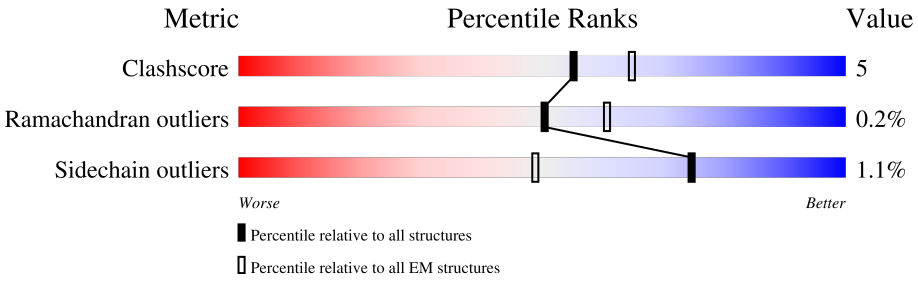
EMDB validation analysis	:	0.0.1.dev50
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

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 3.18 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	908	41% 5% 54%
1	B	908	38% 8% 54%
1	C	908	41% 6% 54%
1	D	908	39% 7% 54%
2	E	2	100%
2	G	2	50% 50% 50%
2	H	2	50% 100%
2	J	2	50% 50% 50%

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Mol	Chain	Length	Quality of chain
3	F	4	
3	I	4	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 14496 atoms, of which 0 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 Glutamate receptor ionotropic, kainate 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	420	Total	C	N	O	S	0	0
			3318	2146	538	615	19		
1	B	420	Total	C	N	O	S	0	0
			3318	2146	538	615	19		
1	C	420	Total	C	N	O	S	0	0
			3318	2146	538	615	19		
1	D	420	Total	C	N	O	S	0	0
			3318	2146	538	615	19		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	567	VAL	ILE	conflict	UNP P42260
A	571	CYS	TYR	conflict	UNP P42260
B	567	VAL	ILE	conflict	UNP P42260
B	571	CYS	TYR	conflict	UNP P42260
C	567	VAL	ILE	conflict	UNP P42260
C	571	CYS	TYR	conflict	UNP P42260
D	567	VAL	ILE	conflict	UNP P42260
D	571	CYS	TYR	conflict	UNP P42260

- 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	E	2	Total	C	N	O	0	0
			28	16	2	10		
2	G	2	Total	C	N	O	0	0
			28	16	2	10		

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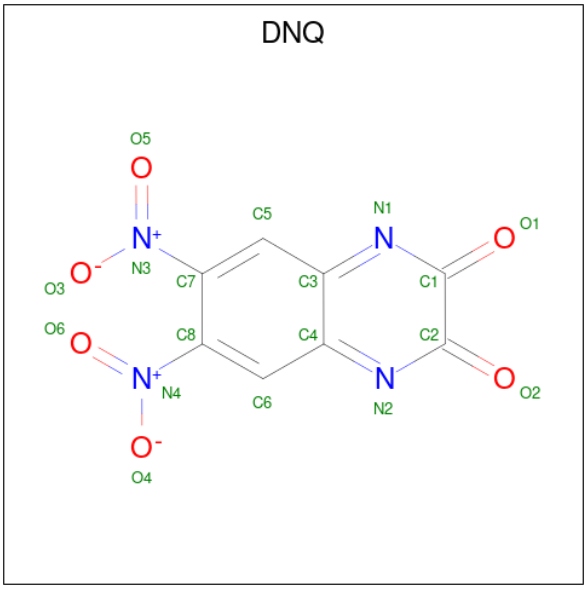
Mol	Chain	Residues	Atoms				AltConf	Trace
2	H	2	Total	C	N	O	0	0
			28	16	2	10		
2	J	2	Total	C	N	O	0	0
			28	16	2	10		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
3	F	4	Total	C	N	O	0	0
			50	28	2	20		
3	I	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 4 is 6,7-DINITROQUINOXALINE-2,3-DIONE (three-letter code: DNQ) (formula: $C_8H_2N_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			18	8	4	6	

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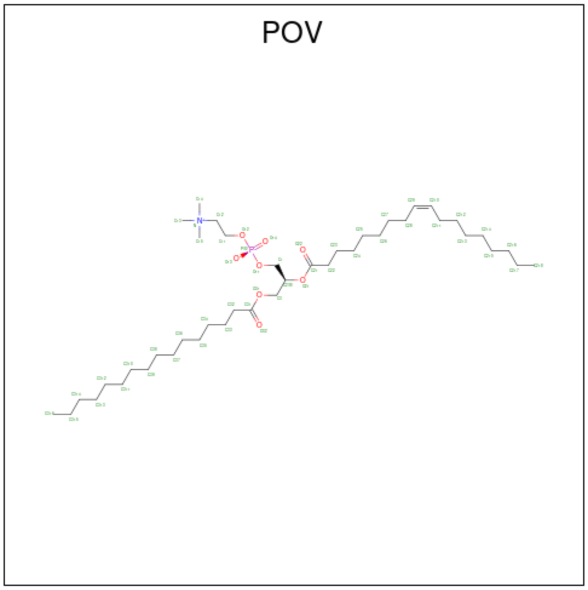
Mol	Chain	Residues	Atoms	AltConf
4	B	1	Total C N O 18 8 4 6	0
4	C	1	Total C N O 18 8 4 6	0
4	D	1	Total C N O 18 8 4 6	0

- Molecule 5 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (three-letter code: POV) (formula: $C_{42}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms	AltConf
5	A	1	Total C N O P 52 42 1 8 1	0
5	A	1	Total C N O P 52 42 1 8 1	0
5	A	1	Total C N O P 52 42 1 8 1	0
5	A	1	Total C N O P 52 42 1 8 1	0
5	A	1	Total C N O P 52 42 1 8 1	0
5	A	1	Total C N O P 52 42 1 8 1	0
5	B	1	Total C N O P 52 42 1 8 1	0
5	B	1	Total C N O P 52 42 1 8 1	0

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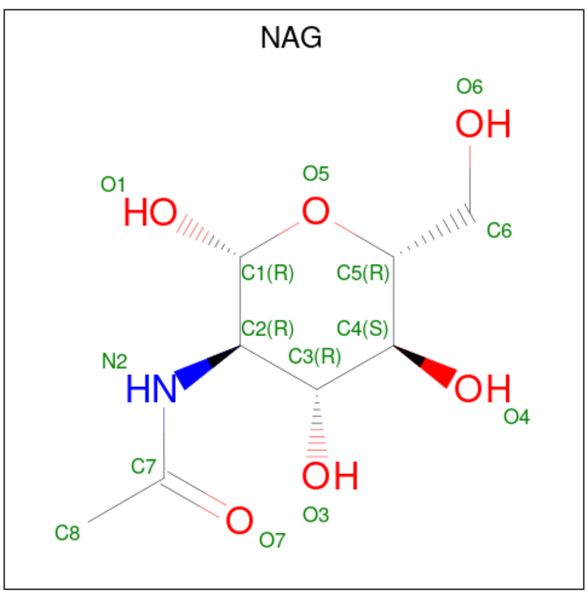
Mol	Chain	Residues	Atoms					AltConf
5	C	1	Total 52	C 42	N 1	O 8	P 1	0
5	C	1	Total 52	C 42	N 1	O 8	P 1	0
5	C	1	Total 52	C 42	N 1	O 8	P 1	0
5	C	1	Total 52	C 42	N 1	O 8	P 1	0
5	C	1	Total 52	C 42	N 1	O 8	P 1	0
5	C	1	Total 52	C 42	N 1	O 8	P 1	0
5	C	1	Total 52	C 42	N 1	O 8	P 1	0
5	D	1	Total 52	C 42	N 1	O 8	P 1	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 14	C 8	N 1	O 5	0
6	C	1	Total 14	C 8	N 1	O 5	0

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na) (labeled as "Ligand of

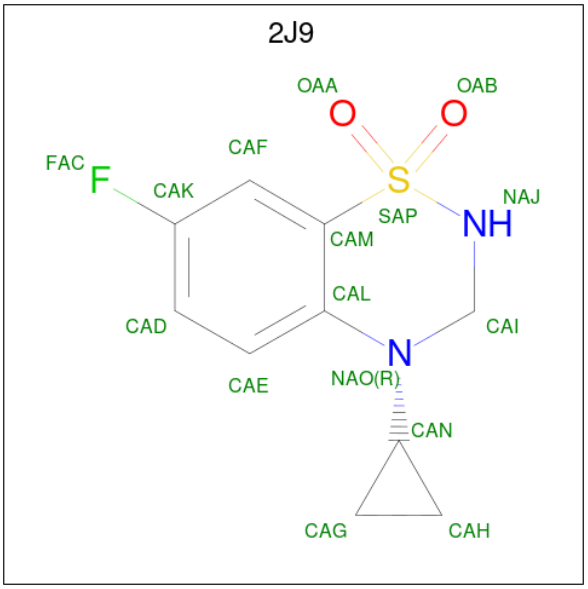
Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
7	A	4	Total Na 4 4	0
7	B	2	Total Na 2 2	0
7	C	1	Total Na 1 1	0
7	D	1	Total Na 1 1	0

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
8	A	1	Total Cl 1 1	0
8	C	1	Total Cl 1 1	0

- Molecule 9 is 4-cyclopropyl-7-fluoro-3,4-dihydro-2H-1,2,4-benzothiadiazine 1,1-dioxide (three-letter code: 2J9) (formula: $C_{10}H_{11}FN_2O_2S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
9	B	1	Total C F N O S 16 10 1 2 2 1	0

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Mol	Chain	Residues	Atoms						AltConf
9	B	1	Total	C	F	N	O	S	0
			16	10	1	2	2	1	
9	D	1	Total	C	F	N	O	S	0
			16	10	1	2	2	1	
9	D	1	Total	C	F	N	O	S	0
			16	10	1	2	2	1	

- Molecule 10 is water.

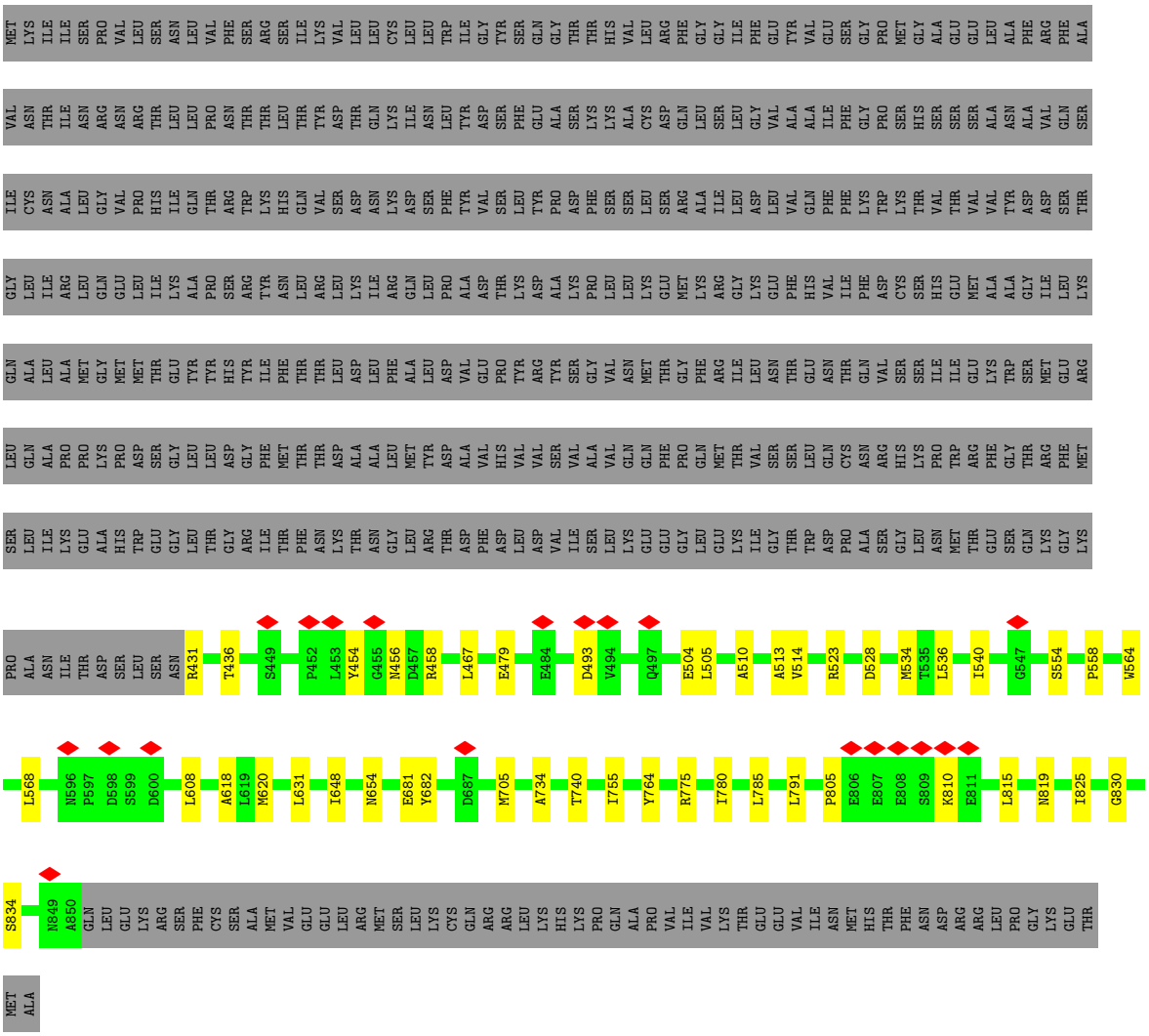
Mol	Chain	Residues	Atoms		AltConf
10	B	3	Total	O	0
			3	3	
10	C	1	Total	O	0
			1	1	
10	D	2	Total	O	0
			2	2	

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.

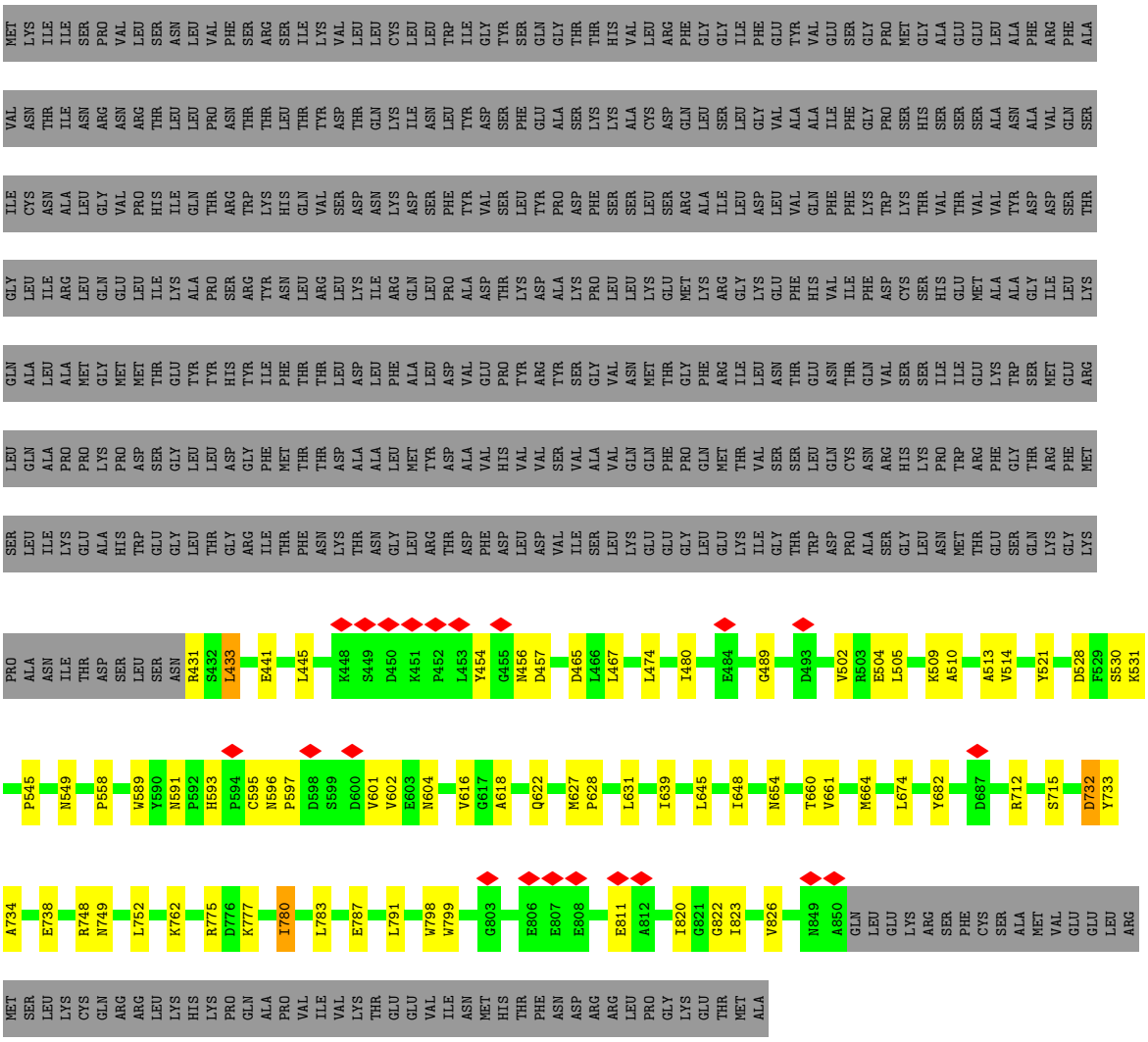
• Molecule 1: Glutamate receptor ionotropic, kainate 2

Chain A:



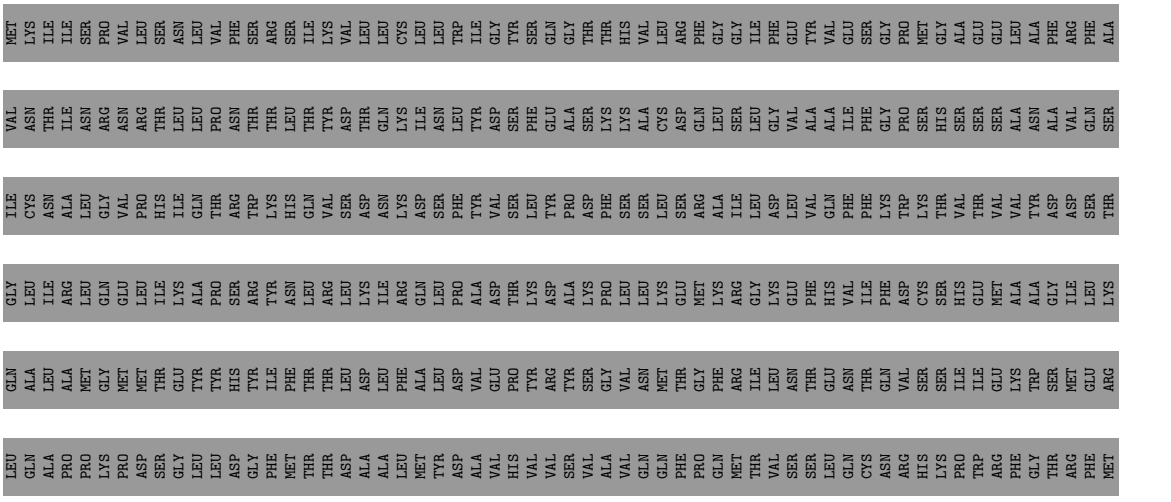
• Molecule 1: Glutamate receptor ionotropic, kainate 2

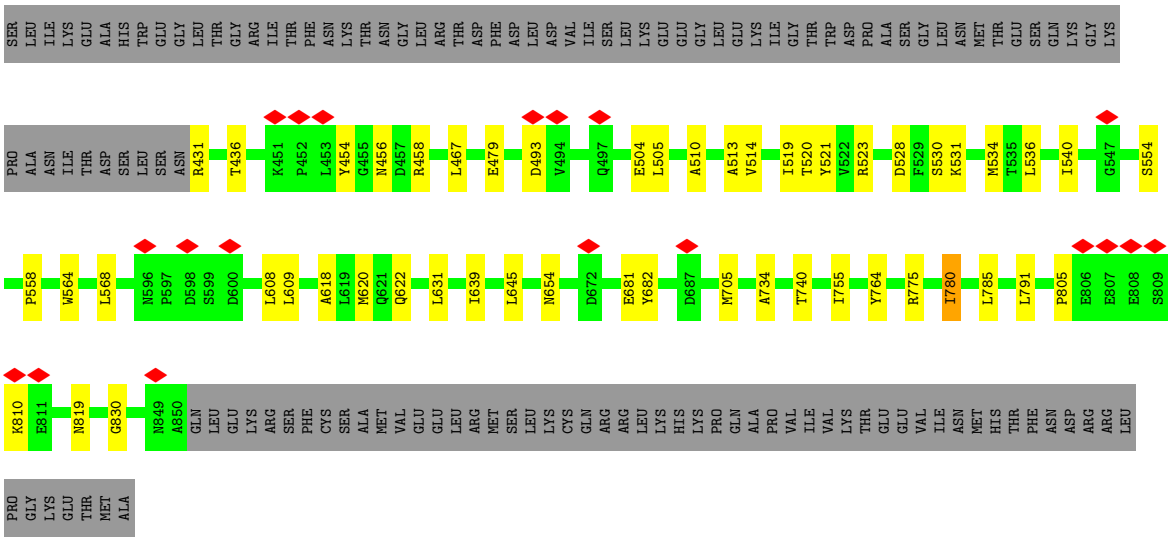
Chain B:



• Molecule 1: Glutamate receptor ionotropic, kainate 2

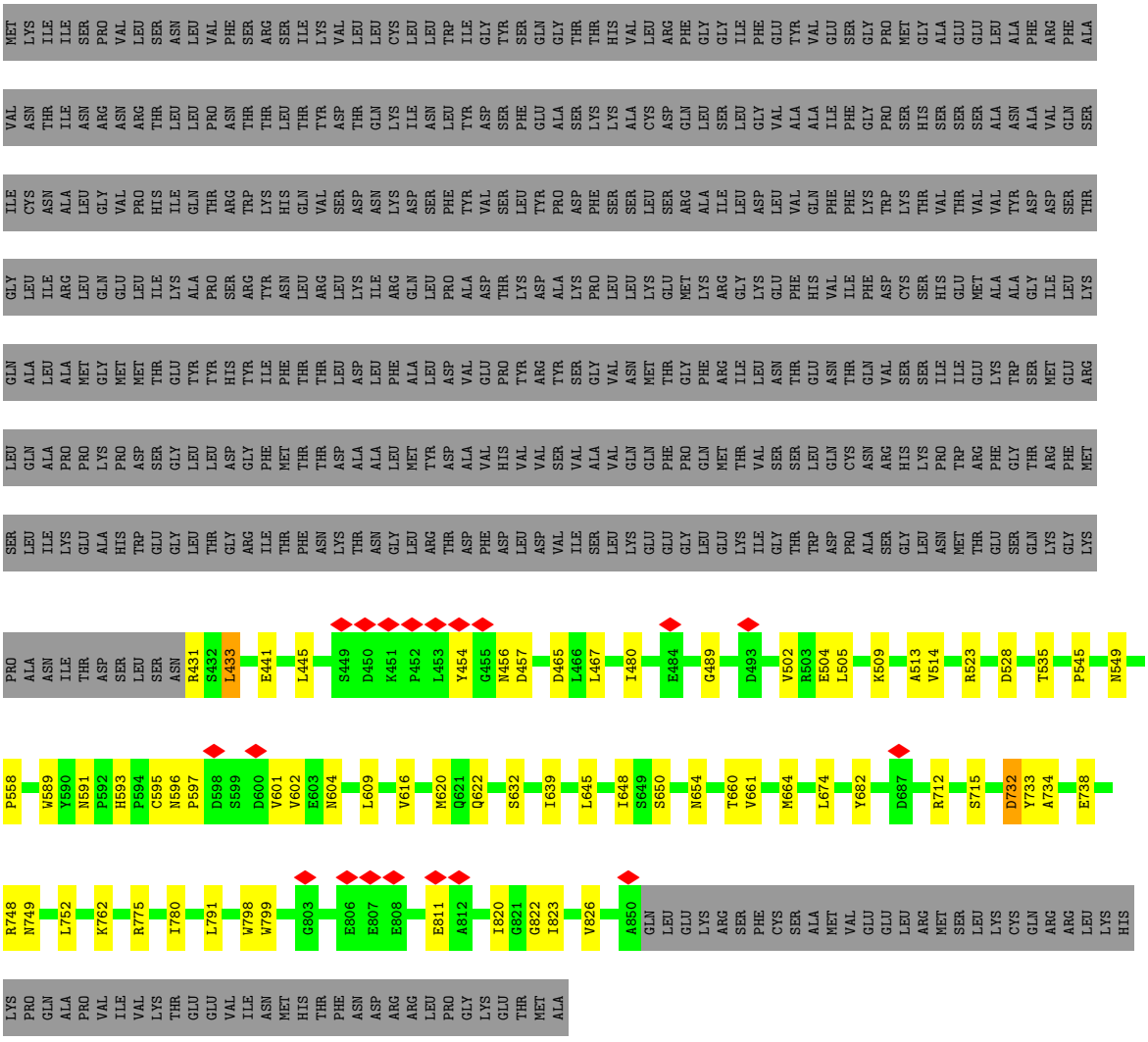
Chain C:





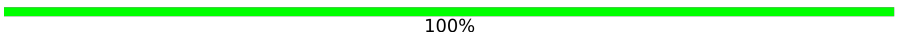
• Molecule 1: Glutamate receptor ionotropic, kainate 2

Chain D:



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

Chain E:

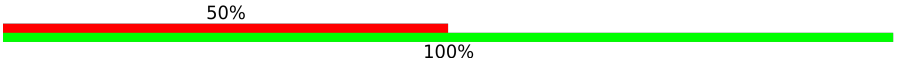


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 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 J:

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

Chain F:

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

Chain I:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	135549	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	57.9	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.256	Depositor
Minimum map value	-1.204	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.028	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	345.28, 345.28, 345.28	wwPDB
Map dimensions	416, 416, 416	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, 2J9, POV, DNQ, CL, BMA, NA

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	0.35	0/3395	0.61	1/4600 (0.0%)
1	B	0.35	0/3395	0.61	2/4600 (0.0%)
1	C	0.35	0/3395	0.61	1/4600 (0.0%)
1	D	0.35	0/3395	0.61	2/4600 (0.0%)
All	All	0.35	0/13580	0.61	6/18400 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
1	C	0	1
1	D	0	2
All	All	0	6

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	433	LEU	CA-CB-CG	8.80	135.53	115.30
1	B	433	LEU	CA-CB-CG	8.79	135.51	115.30
1	C	493	ASP	CB-CG-OD1	7.66	125.20	118.30
1	A	493	ASP	CB-CG-OD1	7.66	125.19	118.30
1	D	674	LEU	CA-CB-CG	5.55	128.06	115.30
1	B	674	LEU	CA-CB-CG	5.54	128.05	115.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	805	PRO	Peptide
1	B	732	ASP	Peptide
1	B	811	GLU	Peptide
1	C	805	PRO	Peptide
1	D	732	ASP	Peptide
1	D	811	GLU	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3318	0	3312	28	0
1	B	3318	0	3312	42	0
1	C	3318	0	3312	36	0
1	D	3318	0	3312	39	0
2	E	28	0	25	0	0
2	G	28	0	25	0	0
2	H	28	0	25	0	0
2	J	28	0	25	0	0
3	F	50	0	43	0	0
3	I	50	0	43	0	0
4	A	18	0	2	4	0
4	B	18	0	2	0	0
4	C	18	0	2	4	0
4	D	18	0	2	1	0
5	A	312	0	492	14	0
5	B	104	0	164	9	0
5	C	364	0	574	21	0
5	D	52	0	82	1	0
6	A	14	0	13	0	0
6	C	14	0	13	0	0
7	A	4	0	0	0	0
7	B	2	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
8	A	1	0	0	0	0
8	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	B	32	0	20	0	0
9	D	32	0	20	1	0
10	B	3	0	0	0	0
10	C	1	0	0	0	0
10	D	2	0	0	0	0
All	All	14496	0	14820	155	0

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

All (155) 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:B:505:LEU:HD21	1:B:513:ALA:HB2	1.78	0.66
1:D:505:LEU:HD21	1:D:513:ALA:HB2	1.78	0.64
1:C:523:ARG:NH1	4:C:1001:DNQ:O2	2.31	0.62
1:D:456:ASN:ND2	1:D:480:ILE:O	2.33	0.61
1:B:456:ASN:ND2	1:B:480:ILE:O	2.33	0.61
1:A:523:ARG:NH1	4:A:1001:DNQ:O2	2.33	0.61
1:B:467:LEU:HD13	1:B:514:VAL:HG21	1.84	0.60
1:A:830:GLY:HA3	1:D:639:ILE:HG13	1.82	0.60
1:B:521:TYR:HE1	1:C:780:ILE:HG23	1.67	0.60
1:C:523:ARG:NH2	4:C:1001:DNQ:O1	2.35	0.60
1:D:467:LEU:HD13	1:D:514:VAL:HG21	1.83	0.59
1:D:441:GLU:HG3	1:D:445:LEU:HD11	1.85	0.58
1:B:441:GLU:HG3	1:B:445:LEU:HD11	1.85	0.58
1:A:618:ALA:O	1:B:622:GLN:NE2	2.36	0.56
1:B:631:LEU:HD13	1:C:609:LEU:HD11	1.87	0.56
1:B:531:LYS:HD3	1:C:519:ILE:HG21	1.88	0.55
1:D:748:ARG:NH1	1:D:799:TRP:O	2.40	0.55
1:C:618:ALA:O	1:D:622:GLN:NE2	2.40	0.55
1:A:534:MET:HB3	1:A:764:TYR:HB2	1.89	0.55
1:B:530:SER:O	1:C:531:LYS:NZ	2.40	0.55
1:B:748:ARG:NH1	1:B:799:TRP:O	2.40	0.54
5:A:1003:POV:H37A	1:D:639:ILE:HD11	1.89	0.54
1:C:534:MET:HB3	1:C:764:TYR:HB2	1.89	0.54
1:D:489:GLY:HA3	1:D:502:VAL:HG22	1.90	0.53
1:B:489:GLY:HA3	1:B:502:VAL:HG22	1.90	0.53
1:B:531:LYS:NZ	1:C:530:SER:O	2.42	0.53
5:C:1007:POV:H21J	1:D:648:ILE:HG13	1.91	0.52
1:B:738:GLU:OE1	1:B:762:LYS:NZ	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:528:ASP:HB3	1:B:775:ARG:HD3	1.93	0.51
1:A:568:LEU:HD11	5:A:1003:POV:H211	1.93	0.51
1:D:528:ASP:HB3	1:D:775:ARG:HD3	1.93	0.50
1:D:712:ARG:HB3	1:D:715:SER:HB3	1.92	0.50
1:D:738:GLU:OE1	1:D:762:LYS:NZ	2.41	0.50
1:B:712:ARG:HB3	1:B:715:SER:HB3	1.92	0.50
1:D:660:THR:HG23	1:D:661:VAL:HG23	1.94	0.50
1:C:564:TRP:HB3	5:C:1002:POV:H28	1.92	0.50
1:C:608:LEU:HD23	5:C:1005:POV:H37A	1.94	0.50
1:B:648:ILE:HG13	5:B:1003:POV:H21J	1.93	0.49
1:A:467:LEU:HD13	1:A:514:VAL:HG21	1.94	0.49
1:A:554:SER:OG	1:A:819:ASN:O	2.29	0.49
4:A:1001:DNQ:O3	4:A:1001:DNQ:O4	2.31	0.49
1:B:749:ASN:HD22	1:B:752:LEU:HD12	1.77	0.49
1:C:467:LEU:HD13	1:C:514:VAL:HG21	1.94	0.49
1:D:749:ASN:HD22	1:D:752:LEU:HD12	1.78	0.49
1:C:639:ILE:HD13	5:C:1008:POV:H37A	1.95	0.49
1:C:785:LEU:HB3	1:C:791:LEU:HD13	1.94	0.49
1:A:785:LEU:HB3	1:A:791:LEU:HD13	1.94	0.48
1:A:523:ARG:NH2	4:A:1001:DNQ:O1	2.46	0.48
1:C:528:ASP:HB3	1:C:775:ARG:HD2	1.96	0.48
1:A:558:PRO:O	1:A:654:ASN:ND2	2.45	0.48
1:B:660:THR:HG23	1:B:661:VAL:HG23	1.94	0.48
1:B:545:PRO:HB2	1:B:664:MET:HB3	1.95	0.48
1:B:823:ILE:HA	1:B:826:VAL:HG22	1.96	0.48
1:D:545:PRO:HB2	1:D:664:MET:HB3	1.95	0.48
1:B:787:GLU:OE2	1:C:520:THR:OG1	2.25	0.48
1:A:528:ASP:HB3	1:A:775:ARG:HD2	1.96	0.48
1:A:536:LEU:HB3	1:A:740:THR:HG23	1.96	0.48
1:B:504:GLU:HG3	1:B:509:LYS:HG3	1.96	0.48
1:A:648:ILE:HG13	5:A:1002:POV:H21J	1.95	0.47
5:B:1004:POV:H31E	5:B:1004:POV:H31B	1.67	0.47
1:C:536:LEU:HB3	1:C:740:THR:HG23	1.96	0.47
4:C:1001:DNQ:O3	4:C:1001:DNQ:O4	2.32	0.47
1:B:595:CYS:HB2	1:D:595:CYS:HB2	1.95	0.47
5:A:1008:POV:H31H	5:B:1003:POV:H315	1.96	0.47
5:C:1007:POV:H217	5:C:1007:POV:H21D	1.71	0.47
1:D:523:ARG:NH2	4:D:1003:DNQ:O1	2.46	0.47
1:D:504:GLU:HG3	1:D:509:LYS:HG3	1.96	0.47
1:B:465:ASP:OD2	1:B:798:TRP:NE1	2.43	0.46
1:D:823:ILE:HA	1:D:826:VAL:HG22	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:554:SER:OG	1:C:819:ASN:O	2.29	0.46
1:A:608:LEU:HD23	5:A:1005:POV:H37A	1.98	0.46
1:B:645:LEU:HD11	1:C:620:MET:HA	1.96	0.46
1:B:783:LEU:HD21	1:C:519:ILE:HG22	1.98	0.45
1:A:620:MET:HA	1:D:645:LEU:HD11	1.97	0.45
5:C:1007:POV:H24A	5:C:1007:POV:H3A	1.99	0.45
1:A:456:ASN:HD22	1:A:479:GLU:HA	1.82	0.45
1:D:558:PRO:HB3	1:D:654:ASN:HB3	1.99	0.45
5:A:1002:POV:H316	5:A:1005:POV:H315	1.99	0.45
1:B:558:PRO:HB3	1:B:654:ASN:HB3	1.99	0.45
1:B:596:ASN:HA	1:B:597:PRO:HD3	1.84	0.45
1:C:456:ASN:HD22	1:C:479:GLU:HA	1.82	0.45
1:D:465:ASP:OD2	1:D:798:TRP:NE1	2.43	0.45
1:D:596:ASN:HA	1:D:597:PRO:HD3	1.84	0.45
5:A:1002:POV:H31A	5:A:1002:POV:H21A	1.99	0.44
1:D:431:ARG:HG2	1:D:433:LEU:H	1.83	0.44
1:A:505:LEU:HD11	1:A:513:ALA:HB2	1.99	0.44
1:B:593:HIS:CE1	1:B:601:VAL:HG21	2.53	0.44
1:C:568:LEU:HD11	5:C:1003:POV:H211	1.99	0.44
1:B:682:TYR:HA	1:B:734:ALA:HB3	2.00	0.44
5:C:1007:POV:H314	1:D:616:VAL:HG22	1.99	0.44
1:B:454:TYR:HB3	1:B:457:ASP:HB3	2.00	0.44
1:C:505:LEU:HD11	1:C:513:ALA:HB2	1.99	0.44
1:C:609:LEU:HD13	5:C:1005:POV:H31A	2.00	0.44
1:D:589:TRP:HB3	1:D:602:VAL:HG13	1.99	0.44
1:A:454:TYR:CG	1:A:458:ARG:HB3	2.53	0.44
1:A:564:TRP:HB3	5:A:1002:POV:H28	1.98	0.44
1:C:454:TYR:CG	1:C:458:ARG:HB3	2.53	0.44
1:C:558:PRO:O	1:C:654:ASN:ND2	2.45	0.44
1:D:454:TYR:HB3	1:D:457:ASP:HB3	2.00	0.44
1:B:589:TRP:HB3	1:B:602:VAL:HG13	1.99	0.43
1:B:616:VAL:HG22	5:B:1003:POV:H314	1.99	0.43
1:A:825:ILE:HD11	5:A:1004:POV:H1A	1.99	0.43
4:C:1001:DNQ:O4	4:C:1001:DNQ:N3	2.51	0.43
1:B:431:ARG:HG2	1:B:433:LEU:H	1.82	0.43
1:B:618:ALA:O	1:C:622:GLN:NE2	2.37	0.43
5:B:1003:POV:H21D	5:B:1003:POV:H217	1.81	0.43
1:B:820:ILE:O	1:B:822:GLY:N	2.50	0.43
1:C:631:LEU:HD13	1:D:609:LEU:HD11	2.01	0.43
1:D:593:HIS:CE1	1:D:601:VAL:HG21	2.53	0.43
1:A:834:SER:OG	1:D:632:SER:O	2.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:436:THR:HG21	1:C:504:GLU:HG3	2.01	0.43
5:B:1003:POV:H24A	5:B:1003:POV:H3A	2.01	0.43
1:C:645:LEU:HD11	1:D:620:MET:HA	1.99	0.43
1:B:639:ILE:HD11	5:C:1003:POV:H37A	2.00	0.43
5:C:1002:POV:H316	5:C:1005:POV:H315	2.00	0.43
5:C:1002:POV:H27	5:C:1002:POV:H34A	2.01	0.42
5:C:1007:POV:H315	5:C:1009:POV:H31H	2.02	0.42
1:D:682:TYR:HA	1:D:734:ALA:HB3	2.00	0.42
5:D:1004:POV:H31B	5:D:1004:POV:H31E	1.68	0.42
1:A:505:LEU:HD12	1:A:510:ALA:HB3	2.01	0.42
1:B:780:ILE:HG23	1:C:521:TYR:HE1	1.85	0.42
5:C:1009:POV:H13B	5:C:1009:POV:H11	1.77	0.42
1:D:593:HIS:HE1	1:D:601:VAL:HG11	1.85	0.42
1:A:436:THR:HG21	1:A:504:GLU:HG3	2.01	0.42
5:B:1004:POV:H39	5:B:1004:POV:H36A	1.86	0.42
1:A:681:GLU:O	1:A:734:ALA:N	2.48	0.41
4:A:1001:DNQ:O4	4:A:1001:DNQ:N3	2.53	0.41
5:A:1005:POV:H26A	5:A:1005:POV:H23A	1.66	0.41
1:C:505:LEU:HD12	1:C:510:ALA:HB3	2.01	0.41
5:C:1007:POV:H310	5:C:1008:POV:H39	2.02	0.41
1:D:752:LEU:HD23	1:D:752:LEU:HA	1.94	0.41
5:A:1007:POV:H213	5:A:1007:POV:H210	1.70	0.41
5:B:1003:POV:H31D	5:B:1003:POV:H31A	1.96	0.41
5:C:1007:POV:H35	5:C:1007:POV:H38A	1.94	0.41
1:A:631:LEU:HD22	5:A:1008:POV:H32	2.03	0.41
5:A:1005:POV:H28A	5:A:1005:POV:H211	1.83	0.41
5:C:1009:POV:H33A	1:D:609:LEU:HB2	2.03	0.41
1:A:815:LEU:HD13	1:D:650:SER:HB3	2.03	0.41
5:B:1004:POV:H31G	5:B:1004:POV:H313	1.86	0.41
5:C:1009:POV:H21D	5:C:1009:POV:H211	1.77	0.41
1:A:682:TYR:HE2	1:A:705:MET:HA	1.86	0.41
1:C:540:ILE:HB	1:C:755:ILE:HG13	2.03	0.41
5:A:1008:POV:H39	5:A:1008:POV:H31C	1.81	0.41
5:C:1007:POV:H31G	5:C:1007:POV:H31D	1.87	0.41
1:A:540:ILE:HB	1:A:755:ILE:HG13	2.03	0.41
1:B:504:GLU:HG2	1:B:510:ALA:HB2	2.03	0.41
1:B:627:MET:HA	1:B:628:PRO:HD3	1.96	0.40
1:B:474:LEU:HD11	1:B:777:LYS:HB3	2.04	0.40
1:B:639:ILE:HG13	1:C:830:GLY:HA3	2.04	0.40
5:C:1005:POV:H28A	5:C:1005:POV:H211	1.82	0.40
5:C:1008:POV:H213	5:C:1008:POV:H210	1.66	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:535:THR:HG23	9:D:1001:2J9:H10	2.02	0.40
1:D:820:ILE:O	1:D:822:GLY:N	2.50	0.40
1:C:681:GLU:O	1:C:734:ALA:N	2.48	0.40
1:C:682:TYR:HE2	1:C:705:MET:HA	1.86	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	418/908 (46%)	383 (92%)	35 (8%)	0	100	100
1	B	418/908 (46%)	374 (90%)	42 (10%)	2 (0%)	29	66
1	C	418/908 (46%)	383 (92%)	35 (8%)	0	100	100
1	D	418/908 (46%)	374 (90%)	42 (10%)	2 (0%)	29	66
All	All	1672/3632 (46%)	1514 (91%)	154 (9%)	4 (0%)	50	78

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	733	TYR
1	D	733	TYR
1	B	732	ASP
1	D	732	ASP

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	362/794 (46%)	359 (99%)	3 (1%)	81 92
1	B	362/794 (46%)	357 (99%)	5 (1%)	67 85
1	C	362/794 (46%)	359 (99%)	3 (1%)	81 92
1	D	362/794 (46%)	357 (99%)	5 (1%)	67 85
All	All	1448/3176 (46%)	1432 (99%)	16 (1%)	74 88

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	431	ARG
1	A	780	ILE
1	A	810	LYS
1	B	549	ASN
1	B	591	ASN
1	B	604	ASN
1	B	780	ILE
1	B	791	LEU
1	C	431	ARG
1	C	780	ILE
1	C	810	LYS
1	D	549	ASN
1	D	591	ASN
1	D	604	ASN
1	D	780	ILE
1	D	791	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	604	ASN
1	B	549	ASN
1	B	591	ASN
1	B	593	HIS
1	B	604	ASN
1	B	721	ASN
1	C	604	ASN
1	D	549	ASN
1	D	591	ASN

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Mol	Chain	Res	Type
1	D	593	HIS
1	D	604	ASN
1	D	721	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

16 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	E	1	2,1	14,14,15	0.47	0	17,19,21	0.85	0
2	NAG	E	2	2	14,14,15	0.26	0	17,19,21	0.55	0
3	NAG	F	1	3,1	14,14,15	0.40	0	17,19,21	0.42	0
3	NAG	F	2	3	14,14,15	0.30	0	17,19,21	0.68	1 (5%)
3	BMA	F	3	3	11,11,12	1.44	3 (27%)	15,15,17	1.89	3 (20%)
3	BMA	F	4	3	11,11,12	0.87	0	15,15,17	0.90	0
2	NAG	G	1	2,1	14,14,15	1.63	2 (14%)	17,19,21	1.76	2 (11%)
2	NAG	G	2	2	14,14,15	0.58	0	17,19,21	0.42	0
2	NAG	H	1	2,1	14,14,15	0.46	0	17,19,21	0.81	0
2	NAG	H	2	2	14,14,15	0.29	0	17,19,21	0.56	0
3	NAG	I	1	3,1	14,14,15	0.41	0	17,19,21	0.41	0
3	NAG	I	2	3	14,14,15	0.31	0	17,19,21	0.67	1 (5%)
3	BMA	I	3	3	11,11,12	1.44	3 (27%)	15,15,17	1.89	3 (20%)
3	BMA	I	4	3	11,11,12	0.88	0	15,15,17	0.91	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	J	1	2,1	14,14,15	1.64	2 (14%)	17,19,21	1.77	2 (11%)
2	NAG	J	2	2	14,14,15	0.58	0	17,19,21	0.42	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	E	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
3	NAG	F	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	BMA	F	3	3	-	2/2/19/22	0/1/1/1
3	BMA	F	4	3	-	1/2/19/22	0/1/1/1
2	NAG	G	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
2	NAG	H	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	H	2	2	-	0/6/23/26	0/1/1/1
3	NAG	I	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	I	2	3	-	1/6/23/26	0/1/1/1
3	BMA	I	3	3	-	2/2/19/22	0/1/1/1
3	BMA	I	4	3	-	1/2/19/22	0/1/1/1
2	NAG	J	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	1	NAG	O5-C1	4.48	1.50	1.43
2	G	1	NAG	O5-C1	4.39	1.50	1.43
2	G	1	NAG	C1-C2	4.08	1.58	1.52
2	J	1	NAG	C1-C2	4.04	1.58	1.52
3	I	3	BMA	C4-C3	2.85	1.59	1.52
3	F	3	BMA	C4-C3	2.79	1.59	1.52
3	F	3	BMA	C1-C2	2.67	1.58	1.52
3	I	3	BMA	C1-C2	2.67	1.58	1.52
3	F	3	BMA	C2-C3	2.30	1.55	1.52
3	I	3	BMA	C2-C3	2.26	1.55	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	1	NAG	C1-O5-C5	5.78	120.03	112.19
2	G	1	NAG	C1-O5-C5	5.75	119.98	112.19
3	F	3	BMA	C1-C2-C3	4.74	115.49	109.67
3	I	3	BMA	C1-C2-C3	4.69	115.43	109.67
3	F	3	BMA	C2-C3-C4	3.51	116.98	110.89
3	I	3	BMA	C2-C3-C4	3.51	116.97	110.89
2	J	1	NAG	C2-N2-C7	3.03	127.22	122.90
2	G	1	NAG	C2-N2-C7	3.03	127.21	122.90
3	I	3	BMA	O2-C2-C3	-2.56	105.02	110.14
3	F	3	BMA	O2-C2-C3	-2.51	105.10	110.14
3	F	2	NAG	C1-O5-C5	2.34	115.37	112.19
3	I	2	NAG	C1-O5-C5	2.30	115.31	112.19

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	1	NAG	C4-C5-C6-O6
2	H	1	NAG	C4-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
2	J	2	NAG	O5-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
2	G	1	NAG	O5-C5-C6-O6
2	H	1	NAG	O5-C5-C6-O6
2	J	1	NAG	O5-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
2	G	2	NAG	C4-C5-C6-O6
2	J	2	NAG	C4-C5-C6-O6
3	I	1	NAG	C4-C5-C6-O6
3	F	3	BMA	C4-C5-C6-O6
2	G	1	NAG	C4-C5-C6-O6
3	F	3	BMA	O5-C5-C6-O6
2	J	1	NAG	C4-C5-C6-O6
3	I	3	BMA	O5-C5-C6-O6
3	I	3	BMA	C4-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
3	I	4	BMA	O5-C5-C6-O6
3	F	4	BMA	O5-C5-C6-O6
3	I	2	NAG	C4-C5-C6-O6

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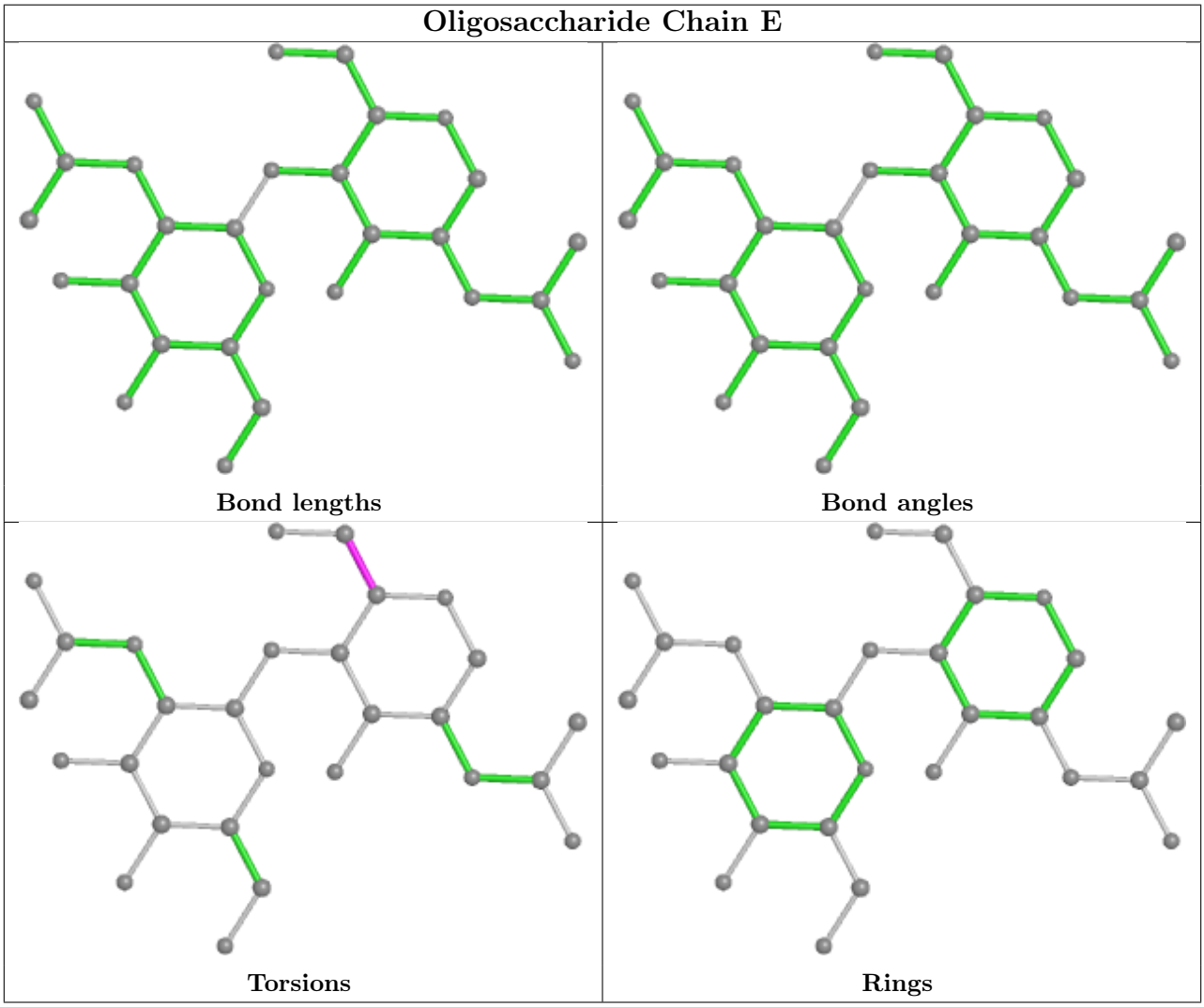
Mol	Chain	Res	Type	Atoms
3	F	2	NAG	O5-C5-C6-O6
2	G	1	NAG	C3-C2-N2-C7
2	J	1	NAG	C3-C2-N2-C7

There are no ring outliers.

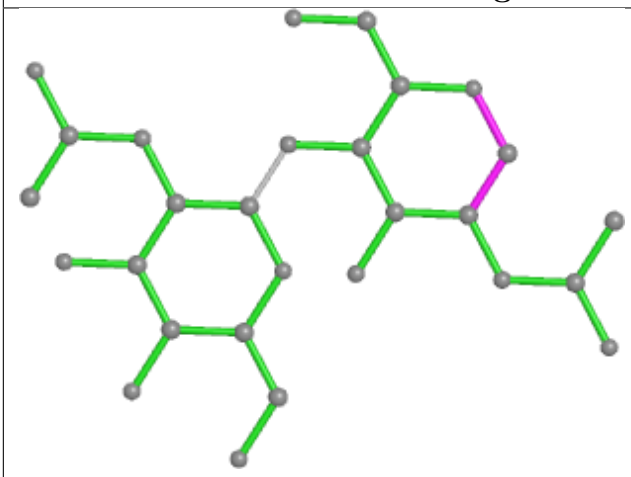
No monomer is involved in short contacts.

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

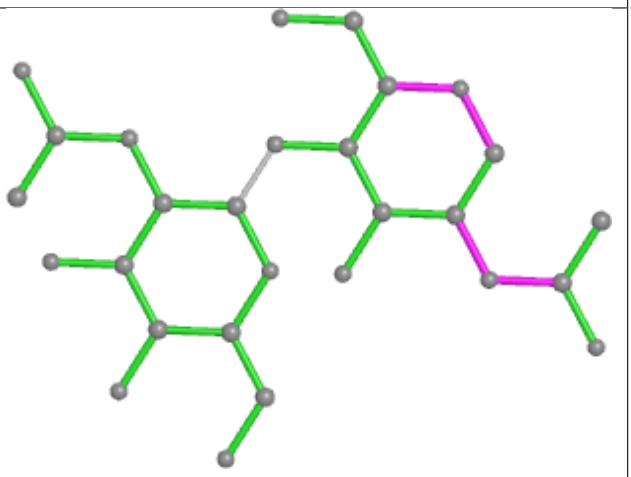
Oligosaccharide Chain E



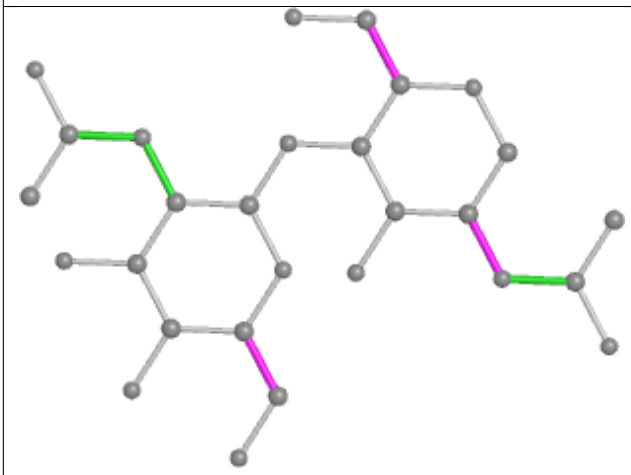
Oligosaccharide Chain G



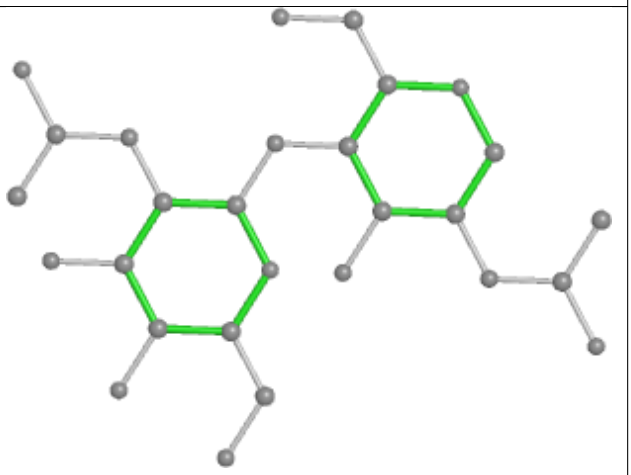
Bond lengths



Bond angles

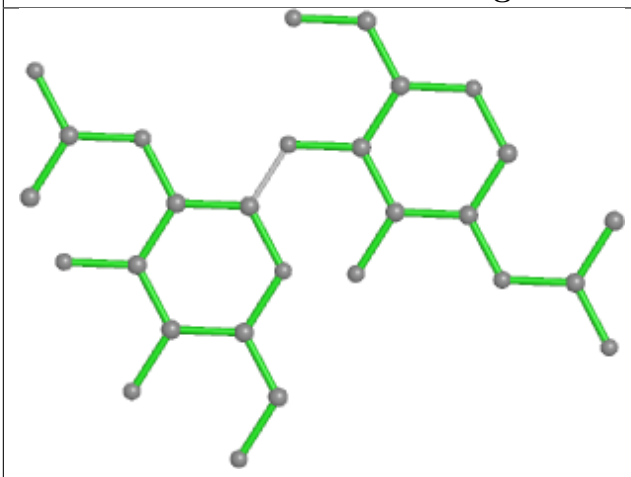


Torsions

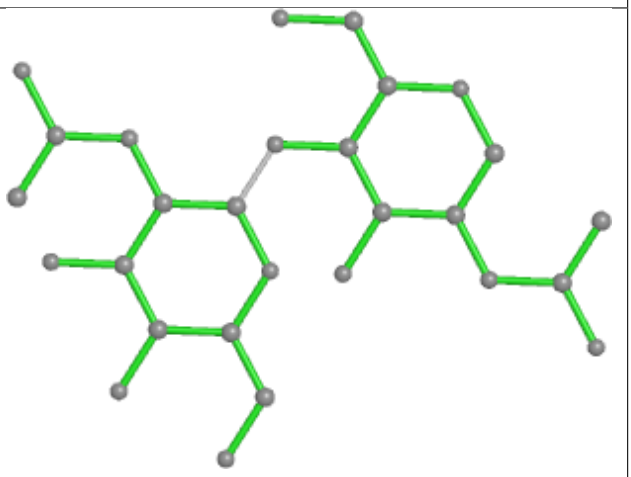


Rings

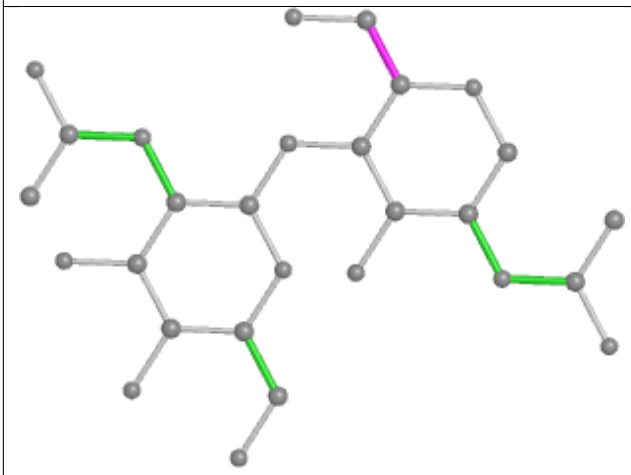
Oligosaccharide Chain H



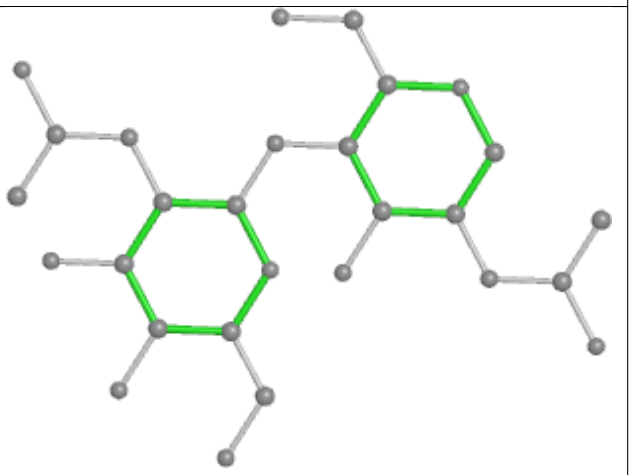
Bond lengths



Bond angles

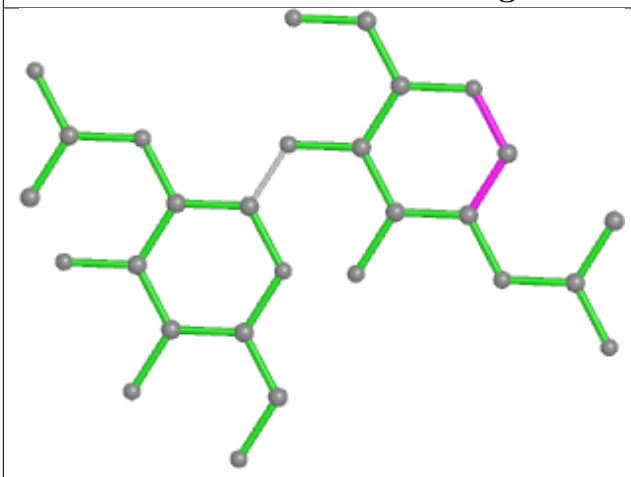


Torsions

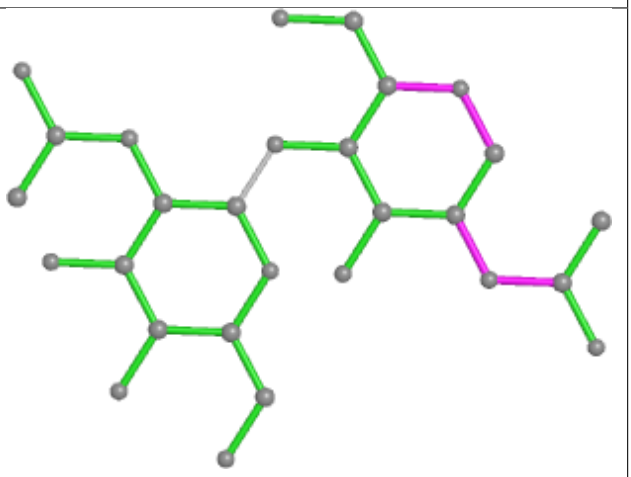


Rings

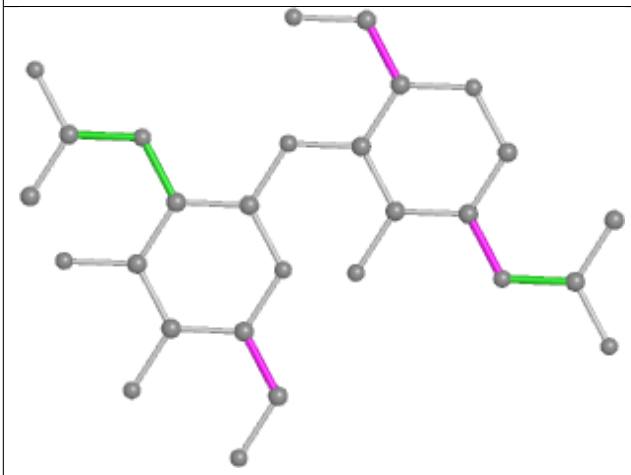
Oligosaccharide Chain J



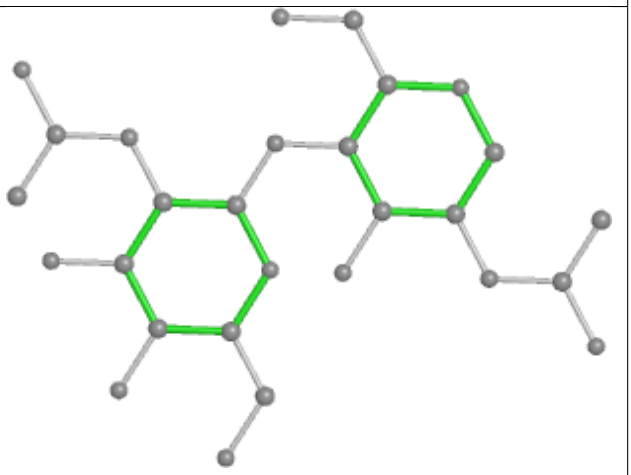
Bond lengths



Bond angles

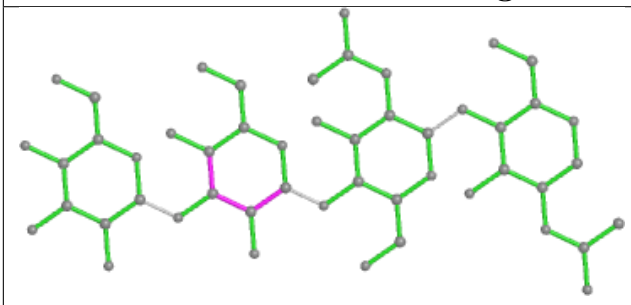


Torsions

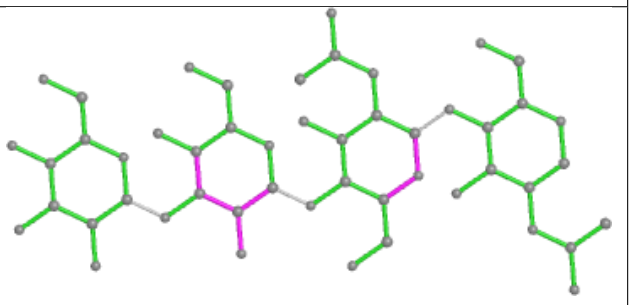


Rings

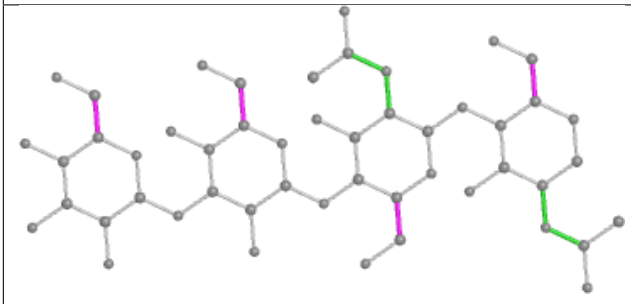
Oligosaccharide Chain F



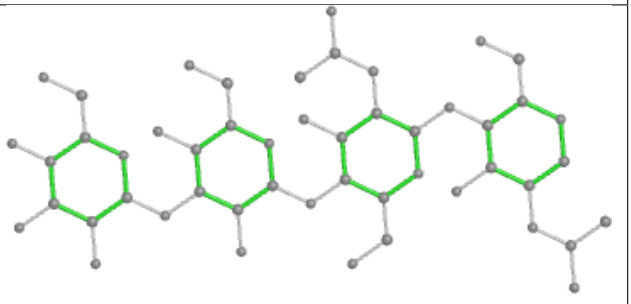
Bond lengths



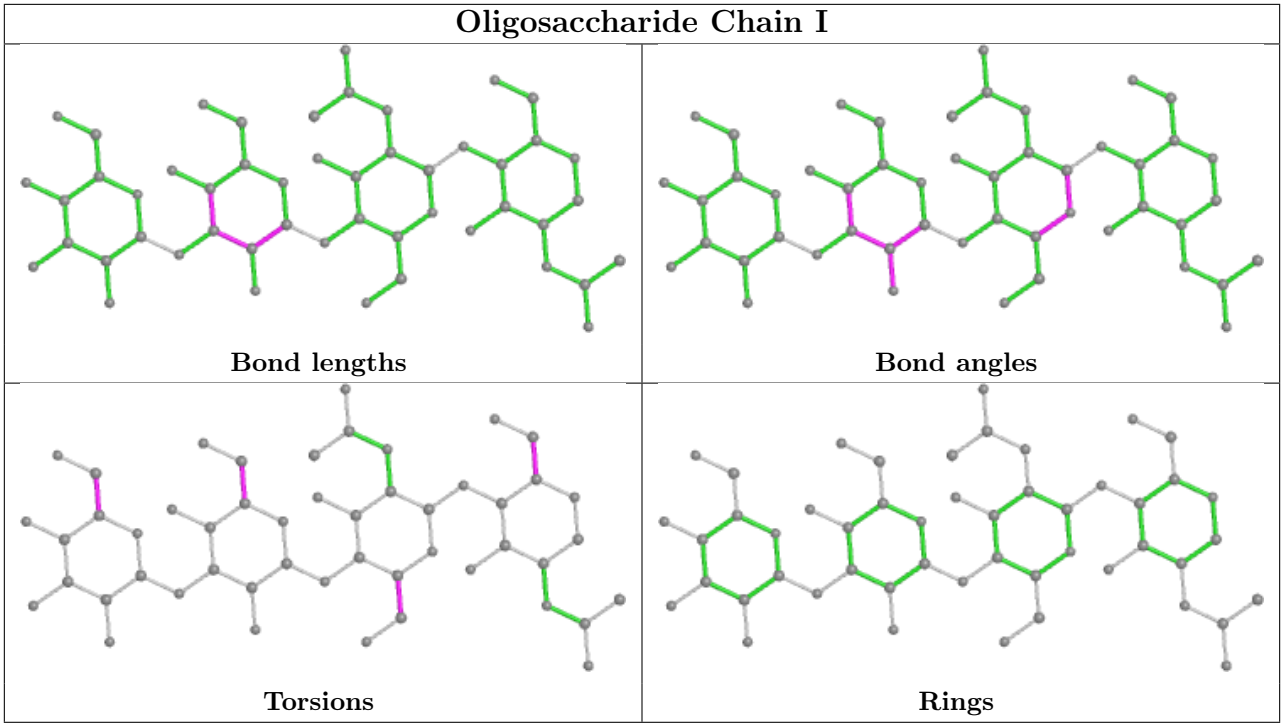
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

Of 36 ligands modelled in this entry, 10 are monoatomic - leaving 26 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	$\#\|Z\| > 2$
4	DNQ	C	1001	-	17,19,19	5.86	13 (76%)	10,28,28	1.15	1 (10%)
5	POV	A	1003	-	51,51,51	1.07	3 (5%)	57,59,59	0.87	3 (5%)
5	POV	B	1004	-	51,51,51	1.07	3 (5%)	57,59,59	0.93	3 (5%)
5	POV	A	1005	-	51,51,51	1.06	3 (5%)	57,59,59	0.96	3 (5%)
5	POV	A	1008	-	51,51,51	1.06	3 (5%)	57,59,59	0.84	3 (5%)
5	POV	A	1002	-	51,51,51	1.08	2 (3%)	57,59,59	0.95	3 (5%)
6	NAG	A	1006	1	14,14,15	1.15	1 (7%)	17,19,21	1.31	1 (5%)
5	POV	C	1007	-	51,51,51	1.06	3 (5%)	57,59,59	1.12	4 (7%)
5	POV	A	1004	-	51,51,51	1.05	3 (5%)	57,59,59	0.91	3 (5%)
9	2J9	D	1002	-	17,18,18	7.22	8 (47%)	23,28,28	5.85	6 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	DNQ	B	1002	-	17,19,19	5.89	13 (76%)	10,28,28	1.19	1 (10%)
4	DNQ	A	1001	-	17,19,19	5.88	13 (76%)	10,28,28	1.13	1 (10%)
5	POV	C	1004	-	51,51,51	1.06	3 (5%)	57,59,59	0.93	3 (5%)
5	POV	C	1002	-	51,51,51	1.07	2 (3%)	57,59,59	0.91	3 (5%)
5	POV	D	1004	-	51,51,51	1.07	3 (5%)	57,59,59	0.92	3 (5%)
5	POV	C	1008	-	51,51,51	1.06	3 (5%)	57,59,59	0.92	3 (5%)
9	2J9	B	1005	-	17,18,18	7.15	8 (47%)	23,28,28	6.15	8 (34%)
5	POV	C	1003	-	51,51,51	1.07	3 (5%)	57,59,59	0.86	3 (5%)
9	2J9	D	1001	-	17,18,18	7.16	8 (47%)	23,28,28	6.07	7 (30%)
4	DNQ	D	1003	-	17,19,19	5.88	13 (76%)	10,28,28	1.19	1 (10%)
5	POV	B	1003	-	51,51,51	1.06	3 (5%)	57,59,59	1.05	3 (5%)
9	2J9	B	1001	-	17,18,18	7.22	8 (47%)	23,28,28	5.86	7 (30%)
6	NAG	C	1006	1	14,14,15	1.14	1 (7%)	17,19,21	1.29	1 (5%)
5	POV	C	1009	-	51,51,51	1.06	2 (3%)	57,59,59	0.86	3 (5%)
5	POV	C	1005	-	51,51,51	1.06	3 (5%)	57,59,59	0.95	3 (5%)
5	POV	A	1007	-	51,51,51	1.07	3 (5%)	57,59,59	0.92	3 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	DNQ	C	1001	-	-	2/4/20/20	0/2/2/2
5	POV	A	1003	-	-	24/55/55/55	-
5	POV	B	1004	-	-	30/55/55/55	-
5	POV	A	1005	-	-	30/55/55/55	-
5	POV	A	1008	-	-	31/55/55/55	-
5	POV	A	1002	-	-	35/55/55/55	-
6	NAG	A	1006	1	-	2/6/23/26	0/1/1/1
5	POV	C	1007	-	-	33/55/55/55	-
5	POV	A	1004	-	-	25/55/55/55	-
9	2J9	D	1002	-	-	2/4/22/22	0/3/3/3
4	DNQ	B	1002	-	-	3/4/20/20	0/2/2/2
4	DNQ	A	1001	-	-	2/4/20/20	0/2/2/2
5	POV	C	1004	-	-	24/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	POV	C	1002	-	-	35/55/55/55	-
5	POV	D	1004	-	-	28/55/55/55	-
5	POV	C	1008	-	-	29/55/55/55	-
9	2J9	B	1005	-	-	2/4/22/22	0/3/3/3
5	POV	C	1003	-	-	27/55/55/55	-
9	2J9	D	1001	-	-	2/4/22/22	0/3/3/3
4	DNQ	D	1003	-	-	3/4/20/20	0/2/2/2
5	POV	B	1003	-	-	30/55/55/55	-
9	2J9	B	1001	-	-	2/4/22/22	0/3/3/3
6	NAG	C	1006	1	-	2/6/23/26	0/1/1/1
5	POV	C	1009	-	-	31/55/55/55	-
5	POV	C	1005	-	-	30/55/55/55	-
5	POV	A	1007	-	-	32/55/55/55	-

All (131) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	1005	2J9	OAA-SAP	19.81	1.66	1.43
9	B	1001	2J9	OAA-SAP	19.79	1.66	1.43
9	D	1002	2J9	OAA-SAP	19.72	1.65	1.43
9	D	1001	2J9	OAA-SAP	19.56	1.65	1.43
9	D	1002	2J9	OAB-SAP	19.05	1.65	1.43
9	B	1001	2J9	OAB-SAP	18.84	1.64	1.43
9	D	1001	2J9	OAB-SAP	18.73	1.64	1.43
9	B	1005	2J9	OAB-SAP	18.29	1.64	1.43
4	B	1002	DNQ	O5-N3	13.14	1.45	1.22
4	C	1001	DNQ	O5-N3	13.12	1.45	1.22
4	A	1001	DNQ	O5-N3	13.10	1.45	1.22
4	D	1003	DNQ	O5-N3	13.09	1.45	1.22
4	A	1001	DNQ	O1-C1	11.21	1.42	1.23
4	B	1002	DNQ	O2-C2	11.11	1.42	1.23
4	C	1001	DNQ	O1-C1	11.08	1.41	1.23
4	D	1003	DNQ	O2-C2	11.07	1.41	1.23
4	B	1002	DNQ	O1-C1	11.01	1.41	1.23
4	D	1003	DNQ	O1-C1	11.01	1.41	1.23
4	A	1001	DNQ	O2-C2	10.95	1.41	1.23
4	C	1001	DNQ	O2-C2	10.95	1.41	1.23
4	B	1002	DNQ	O6-N4	8.83	1.37	1.22
4	D	1003	DNQ	O6-N4	8.82	1.37	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1001	DNQ	O6-N4	8.74	1.37	1.22
4	C	1001	DNQ	O6-N4	8.67	1.37	1.22
9	D	1001	2J9	CAL-NAO	6.07	1.55	1.40
9	D	1002	2J9	CAL-NAO	6.02	1.55	1.40
9	B	1001	2J9	CAL-NAO	5.99	1.55	1.40
9	B	1005	2J9	CAL-NAO	5.94	1.54	1.40
4	D	1003	DNQ	C1-C2	-5.53	1.40	1.52
4	B	1002	DNQ	C1-C2	-5.49	1.40	1.52
4	A	1001	DNQ	C1-C2	-5.49	1.40	1.52
4	C	1001	DNQ	C1-C2	-5.46	1.40	1.52
9	B	1005	2J9	CAL-CAM	-5.30	1.34	1.40
9	B	1001	2J9	CAL-CAM	-5.01	1.35	1.40
9	D	1001	2J9	CAL-CAM	-4.95	1.35	1.40
9	B	1001	2J9	CAH-CAN	-4.83	1.38	1.48
9	B	1005	2J9	CAH-CAN	-4.74	1.38	1.48
9	D	1001	2J9	CAH-CAN	-4.74	1.38	1.48
9	D	1002	2J9	CAH-CAN	-4.72	1.38	1.48
9	D	1002	2J9	CAL-CAM	-4.70	1.35	1.40
9	B	1005	2J9	CAM-SAP	-4.61	1.71	1.75
9	B	1005	2J9	CAG-CAN	-4.53	1.39	1.48
9	D	1002	2J9	CAG-CAN	-4.50	1.39	1.48
9	D	1001	2J9	CAG-CAN	-4.49	1.39	1.48
9	B	1001	2J9	CAG-CAN	-4.42	1.39	1.48
9	B	1001	2J9	CAM-SAP	-4.39	1.71	1.75
9	D	1001	2J9	CAM-SAP	-4.21	1.72	1.75
9	D	1002	2J9	CAM-SAP	-4.15	1.72	1.75
4	D	1003	DNQ	C3-N1	3.79	1.38	1.33
6	A	1006	NAG	O5-C1	3.74	1.49	1.43
4	B	1002	DNQ	C3-N1	3.71	1.38	1.33
6	C	1006	NAG	O5-C1	3.70	1.49	1.43
4	A	1001	DNQ	C3-N1	3.65	1.37	1.33
4	C	1001	DNQ	C3-N1	3.58	1.37	1.33
5	A	1002	POV	O21-C21	3.29	1.43	1.34
5	C	1002	POV	O21-C21	3.26	1.43	1.34
4	C	1001	DNQ	C1-N1	-3.13	1.32	1.38
5	C	1007	POV	O21-C21	3.11	1.43	1.34
4	A	1001	DNQ	C1-N1	-3.10	1.32	1.38
4	D	1003	DNQ	C1-N1	-3.08	1.32	1.38
5	C	1009	POV	O21-C21	3.07	1.43	1.34
4	B	1002	DNQ	C1-N1	-3.03	1.32	1.38
5	A	1008	POV	O21-C21	3.03	1.42	1.34
5	B	1003	POV	O21-C21	3.00	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1003	POV	O21-C21	2.88	1.42	1.34
5	A	1003	POV	O21-C21	2.87	1.42	1.34
4	C	1001	DNQ	C2-N2	-2.87	1.32	1.38
5	B	1004	POV	O31-C31	2.83	1.41	1.33
5	D	1004	POV	O31-C31	2.80	1.41	1.33
4	A	1001	DNQ	C2-N2	-2.80	1.33	1.38
4	B	1002	DNQ	C2-N2	-2.79	1.33	1.38
5	A	1007	POV	O21-C21	2.79	1.42	1.34
5	B	1003	POV	O31-C31	2.78	1.41	1.33
5	C	1008	POV	O21-C21	2.77	1.42	1.34
5	C	1005	POV	O21-C21	2.77	1.42	1.34
5	C	1004	POV	O21-C21	2.76	1.42	1.34
4	D	1003	DNQ	C2-N2	-2.76	1.33	1.38
5	A	1005	POV	O21-C21	2.75	1.42	1.34
5	C	1005	POV	O31-C31	2.74	1.41	1.33
4	C	1001	DNQ	C3-C4	-2.74	1.36	1.42
5	C	1007	POV	O31-C31	2.74	1.41	1.33
5	A	1004	POV	O21-C21	2.73	1.42	1.34
5	A	1002	POV	O31-C31	2.72	1.41	1.33
5	A	1005	POV	O31-C31	2.72	1.41	1.33
5	C	1002	POV	O31-C31	2.71	1.41	1.33
4	A	1001	DNQ	C3-C4	-2.69	1.36	1.42
5	C	1008	POV	O31-C31	2.68	1.41	1.33
5	A	1007	POV	O31-C31	2.68	1.41	1.33
5	A	1004	POV	O31-C31	2.67	1.41	1.33
5	D	1004	POV	O21-C21	2.66	1.41	1.34
9	D	1001	2J9	CAH-CAG	-2.65	1.38	1.48
5	C	1004	POV	O31-C31	2.65	1.41	1.33
4	D	1003	DNQ	C3-C4	-2.64	1.36	1.42
9	B	1005	2J9	CAH-CAG	-2.64	1.38	1.48
5	B	1004	POV	O21-C21	2.63	1.41	1.34
9	D	1002	2J9	CAH-CAG	-2.62	1.38	1.48
5	A	1003	POV	O31-C31	2.62	1.41	1.33
9	B	1001	2J9	CAH-CAG	-2.61	1.38	1.48
4	B	1002	DNQ	C6-C4	2.61	1.43	1.40
5	C	1003	POV	O31-C31	2.61	1.40	1.33
5	A	1008	POV	O31-C31	2.60	1.40	1.33
4	B	1002	DNQ	C3-C4	-2.60	1.37	1.42
5	B	1004	POV	O21-C2	-2.56	1.40	1.46
5	D	1004	POV	O21-C2	-2.55	1.40	1.46
5	C	1009	POV	O31-C31	2.54	1.40	1.33
4	A	1001	DNQ	C6-C4	2.53	1.43	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1005	POV	O21-C2	-2.53	1.40	1.46
5	C	1005	POV	O21-C2	-2.53	1.40	1.46
4	D	1003	DNQ	C4-N2	2.51	1.36	1.33
4	D	1003	DNQ	C6-C4	2.48	1.43	1.40
4	B	1002	DNQ	C4-N2	2.47	1.36	1.33
5	C	1004	POV	O21-C2	-2.47	1.40	1.46
5	A	1004	POV	O21-C2	-2.45	1.40	1.46
5	A	1007	POV	O21-C2	-2.45	1.40	1.46
5	C	1008	POV	O21-C2	-2.43	1.40	1.46
4	A	1001	DNQ	C4-N2	2.43	1.36	1.33
4	C	1001	DNQ	C6-C4	2.42	1.43	1.40
4	C	1001	DNQ	C4-N2	2.37	1.36	1.33
5	C	1003	POV	O21-C2	-2.36	1.40	1.46
5	A	1003	POV	O21-C2	-2.34	1.40	1.46
4	B	1002	DNQ	C5-C3	2.33	1.43	1.40
4	D	1003	DNQ	C5-C3	2.29	1.43	1.40
4	C	1001	DNQ	C5-C3	2.27	1.43	1.40
4	C	1001	DNQ	C6-C8	-2.27	1.37	1.40
5	B	1003	POV	O21-C2	-2.24	1.41	1.46
4	A	1001	DNQ	C5-C3	2.23	1.43	1.40
4	B	1002	DNQ	C6-C8	-2.23	1.37	1.40
4	D	1003	DNQ	C6-C8	-2.22	1.37	1.40
5	C	1007	POV	O21-C2	-2.15	1.41	1.46
4	A	1001	DNQ	C6-C8	-2.12	1.37	1.40
5	A	1008	POV	O21-C2	-2.01	1.41	1.46

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	B	1005	2J9	CAI-NAO-CAL	24.47	121.20	110.25
9	D	1001	2J9	CAI-NAO-CAL	24.32	121.13	110.25
9	D	1002	2J9	CAI-NAO-CAL	23.93	120.96	110.25
9	B	1001	2J9	CAI-NAO-CAL	23.61	120.81	110.25
9	D	1001	2J9	CAM-SAP-NAJ	10.96	111.05	102.37
9	B	1005	2J9	CAM-SAP-NAJ	10.38	110.58	102.37
9	D	1002	2J9	CAM-SAP-NAJ	9.51	109.90	102.37
9	B	1001	2J9	CAM-SAP-NAJ	9.14	109.61	102.37
9	B	1005	2J9	OAB-SAP-OAA	-8.17	110.13	118.46
9	B	1001	2J9	OAB-SAP-OAA	-8.08	110.22	118.46
9	D	1002	2J9	OAB-SAP-OAA	-7.97	110.33	118.46
9	D	1001	2J9	OAB-SAP-OAA	-7.95	110.34	118.46
9	B	1001	2J9	OAB-SAP-NAJ	6.18	113.69	107.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	B	1005	2J9	OAB-SAP-NAJ	5.74	113.27	107.92
6	A	1006	NAG	C1-O5-C5	5.24	119.29	112.19
5	C	1007	POV	O21-C21-C22	5.20	122.71	111.50
9	D	1001	2J9	OAB-SAP-NAJ	5.15	112.73	107.92
6	C	1006	NAG	C1-O5-C5	5.14	119.16	112.19
9	D	1002	2J9	OAB-SAP-NAJ	5.13	112.71	107.92
9	B	1005	2J9	CAK-CAF-CAM	4.86	120.17	116.86
5	B	1003	POV	O21-C21-C22	4.72	121.67	111.50
9	B	1001	2J9	CAK-CAF-CAM	4.42	119.87	116.86
9	D	1001	2J9	CAK-CAF-CAM	4.42	119.87	116.86
5	A	1005	POV	O21-C21-C22	4.00	120.12	111.50
5	C	1004	POV	O21-C21-C22	3.98	120.09	111.50
5	C	1005	POV	O21-C21-C22	3.89	119.89	111.50
5	A	1004	POV	O21-C21-C22	3.89	119.87	111.50
5	B	1004	POV	O21-C21-C22	3.86	119.81	111.50
5	A	1007	POV	O21-C21-C22	3.85	119.80	111.50
5	C	1008	POV	O21-C21-C22	3.83	119.75	111.50
5	D	1004	POV	O21-C21-C22	3.82	119.72	111.50
9	D	1002	2J9	CAK-CAF-CAM	3.75	119.42	116.86
9	B	1005	2J9	OAB-SAP-CAM	-3.68	104.75	109.29
5	A	1003	POV	O21-C21-C22	3.64	119.34	111.50
5	C	1003	POV	O21-C21-C22	3.61	119.29	111.50
5	C	1002	POV	O21-C21-C22	3.53	119.12	111.50
5	A	1002	POV	O21-C21-C22	3.53	119.10	111.50
9	B	1005	2J9	CAD-CAK-CAF	-3.35	118.94	123.29
5	A	1008	POV	O21-C21-C22	3.23	118.47	111.50
5	C	1009	POV	O21-C21-C22	3.20	118.40	111.50
9	D	1001	2J9	CAD-CAK-CAF	-2.89	119.54	123.29
5	B	1003	POV	O31-C31-C32	2.88	120.93	111.91
5	A	1002	POV	O31-C31-C32	2.85	120.86	111.91
5	B	1003	POV	C14-N-C12	2.85	121.57	109.92
5	C	1007	POV	O31-C31-C32	2.84	120.81	111.91
9	B	1001	2J9	CAD-CAK-CAF	-2.83	119.62	123.29
5	C	1007	POV	C14-N-C12	2.80	121.38	109.92
5	C	1002	POV	O31-C31-C32	2.66	120.25	111.91
5	C	1005	POV	O31-C31-C32	2.64	120.18	111.91
5	B	1004	POV	O31-C31-C32	2.60	120.05	111.91
5	A	1005	POV	O31-C31-C32	2.57	119.97	111.91
5	D	1004	POV	O31-C31-C32	2.56	119.93	111.91
5	C	1008	POV	O31-C31-C32	2.54	119.87	111.91
5	C	1003	POV	O31-C31-C32	2.53	119.84	111.91
5	A	1003	POV	O31-C31-C32	2.52	119.81	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	D	1001	2J9	OAB-SAP-CAM	-2.51	106.19	109.29
5	A	1007	POV	O31-C31-C32	2.51	119.78	111.91
9	D	1002	2J9	CAD-CAK-CAF	-2.46	120.10	123.29
5	D	1004	POV	C14-N-C12	2.43	119.87	109.92
5	C	1004	POV	O31-C31-C32	2.42	119.49	111.91
5	B	1004	POV	C14-N-C12	2.40	119.73	109.92
5	A	1004	POV	O31-C31-C32	2.39	119.41	111.91
4	B	1002	DNQ	C1-N1-C3	2.37	120.41	116.92
4	D	1003	DNQ	C1-N1-C3	2.35	120.38	116.92
4	A	1001	DNQ	C1-N1-C3	2.35	120.38	116.92
4	C	1001	DNQ	C1-N1-C3	2.34	120.38	116.92
5	A	1007	POV	C14-N-C12	2.33	119.45	109.92
9	B	1005	2J9	CAE-CAD-CAK	2.33	120.77	118.36
5	C	1008	POV	C14-N-C12	2.32	119.42	109.92
5	A	1005	POV	C14-N-C12	2.31	119.36	109.92
5	C	1005	POV	C14-N-C12	2.29	119.30	109.92
5	C	1009	POV	C14-N-C12	2.28	119.25	109.92
5	A	1003	POV	C14-N-C12	2.27	119.19	109.92
5	C	1003	POV	C14-N-C12	2.27	119.19	109.92
5	A	1008	POV	C14-N-C12	2.27	119.19	109.92
5	C	1004	POV	C14-N-C12	2.24	119.08	109.92
5	A	1004	POV	C14-N-C12	2.22	119.01	109.92
9	B	1001	2J9	CAM-CAL-NAO	-2.14	119.80	121.57
5	C	1007	POV	O21-C21-O22	-2.11	118.60	123.70
5	A	1008	POV	O31-C31-C32	2.11	118.52	111.91
5	C	1002	POV	C14-N-C12	2.08	118.42	109.92
5	C	1009	POV	O31-C31-C32	2.06	118.37	111.91
5	A	1002	POV	C14-N-C12	2.04	118.28	109.92

There are no chirality outliers.

All (496) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1001	DNQ	C5-C7-N3-O5
4	A	1001	DNQ	C8-C7-N3-O5
4	B	1002	DNQ	C6-C8-N4-O6
4	B	1002	DNQ	C7-C8-N4-O6
4	C	1001	DNQ	C5-C7-N3-O5
4	C	1001	DNQ	C8-C7-N3-O5
4	D	1003	DNQ	C6-C8-N4-O6
4	D	1003	DNQ	C7-C8-N4-O6
5	A	1002	POV	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
5	A	1002	POV	C1-O11-P-O14
5	A	1002	POV	C11-O12-P-O11
5	A	1002	POV	C11-O12-P-O14
5	A	1003	POV	C1-O11-P-O12
5	A	1003	POV	C1-O11-P-O13
5	A	1003	POV	C1-O11-P-O14
5	A	1003	POV	C11-O12-P-O11
5	A	1003	POV	C11-O12-P-O13
5	A	1003	POV	C11-O12-P-O14
5	A	1003	POV	O11-C1-C2-O21
5	A	1004	POV	C1-O11-P-O12
5	A	1004	POV	C1-O11-P-O13
5	A	1004	POV	C11-O12-P-O14
5	A	1004	POV	O12-C11-C12-N
5	A	1004	POV	O32-C31-O31-C3
5	A	1005	POV	C1-O11-P-O13
5	A	1005	POV	C1-O11-P-O14
5	A	1005	POV	C11-O12-P-O14
5	A	1005	POV	O12-C11-C12-N
5	A	1007	POV	C1-O11-P-O13
5	A	1007	POV	C1-O11-P-O14
5	A	1007	POV	C11-O12-P-O11
5	A	1007	POV	C11-O12-P-O14
5	A	1007	POV	O21-C2-C3-O31
5	A	1008	POV	C1-O11-P-O13
5	A	1008	POV	C1-O11-P-O14
5	A	1008	POV	O12-C11-C12-N
5	B	1003	POV	C1-O11-P-O14
5	B	1003	POV	C11-O12-P-O13
5	B	1003	POV	C22-C21-O21-C2
5	B	1003	POV	O22-C21-O21-C2
5	B	1003	POV	C32-C31-O31-C3
5	B	1003	POV	O32-C31-O31-C3
5	B	1004	POV	O12-C11-C12-N
5	C	1002	POV	C1-O11-P-O13
5	C	1002	POV	C1-O11-P-O14
5	C	1002	POV	C11-O12-P-O11
5	C	1002	POV	C11-O12-P-O14
5	C	1003	POV	C1-O11-P-O12
5	C	1003	POV	C1-O11-P-O13
5	C	1003	POV	C1-O11-P-O14
5	C	1003	POV	C11-O12-P-O11

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Mol	Chain	Res	Type	Atoms
5	C	1003	POV	C11-O12-P-O13
5	C	1003	POV	C11-O12-P-O14
5	C	1003	POV	O11-C1-C2-O21
5	C	1004	POV	C11-O12-P-O14
5	C	1004	POV	O12-C11-C12-N
5	C	1004	POV	O32-C31-O31-C3
5	C	1005	POV	C1-O11-P-O13
5	C	1005	POV	C1-O11-P-O14
5	C	1005	POV	C11-O12-P-O14
5	C	1005	POV	O12-C11-C12-N
5	C	1007	POV	C1-O11-P-O14
5	C	1007	POV	C11-O12-P-O13
5	C	1007	POV	C22-C21-O21-C2
5	C	1007	POV	O22-C21-O21-C2
5	C	1007	POV	C32-C31-O31-C3
5	C	1008	POV	C1-O11-P-O13
5	C	1008	POV	C1-O11-P-O14
5	C	1008	POV	C11-O12-P-O11
5	C	1008	POV	C11-O12-P-O14
5	C	1008	POV	O21-C2-C3-O31
5	C	1008	POV	C210-C211-C212-C213
5	C	1009	POV	C1-O11-P-O12
5	C	1009	POV	C1-O11-P-O13
5	C	1009	POV	C1-O11-P-O14
5	C	1009	POV	O12-C11-C12-N
5	D	1004	POV	O21-C2-C3-O31
5	D	1004	POV	O12-C11-C12-N
9	B	1001	2J9	CAG-CAN-NAO-CAL
9	B	1001	2J9	CAH-CAN-NAO-CAI
9	D	1001	2J9	CAG-CAN-NAO-CAL
9	D	1001	2J9	CAH-CAN-NAO-CAI
5	C	1007	POV	O32-C31-O31-C3
5	A	1005	POV	O32-C31-O31-C3
5	B	1004	POV	O32-C31-O31-C3
5	C	1005	POV	O32-C31-O31-C3
5	A	1004	POV	C32-C31-O31-C3
5	A	1005	POV	C32-C31-O31-C3
5	C	1004	POV	C32-C31-O31-C3
5	C	1005	POV	C32-C31-O31-C3
5	C	1003	POV	O32-C31-O31-C3
5	B	1004	POV	C32-C31-O31-C3
6	A	1006	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	C	1006	NAG	O5-C5-C6-O6
5	A	1003	POV	O32-C31-O31-C3
5	D	1004	POV	O32-C31-O31-C3
5	C	1003	POV	C32-C31-O31-C3
5	C	1009	POV	C211-C212-C213-C214
5	A	1007	POV	C210-C211-C212-C213
5	A	1003	POV	C32-C31-O31-C3
5	D	1004	POV	C32-C31-O31-C3
6	A	1006	NAG	C4-C5-C6-O6
5	A	1008	POV	C211-C212-C213-C214
5	A	1002	POV	C11-C12-N-C13
5	C	1007	POV	C11-C12-N-C14
5	B	1004	POV	C24-C25-C26-C27
5	D	1004	POV	C24-C25-C26-C27
5	B	1004	POV	O11-C1-C2-O21
5	C	1007	POV	C33-C34-C35-C36
6	C	1006	NAG	C4-C5-C6-O6
5	C	1004	POV	C31-C32-C33-C34
5	C	1008	POV	C21-C22-C23-C24
5	A	1004	POV	O21-C2-C3-O31
5	A	1004	POV	C31-C32-C33-C34
5	A	1005	POV	C31-C32-C33-C34
5	A	1002	POV	C21-C22-C23-C24
5	A	1003	POV	C21-C22-C23-C24
5	C	1002	POV	C21-C22-C23-C24
5	C	1003	POV	C21-C22-C23-C24
5	B	1004	POV	C311-C312-C313-C314
5	A	1002	POV	C11-C12-N-C14
5	A	1007	POV	C21-C22-C23-C24
5	D	1004	POV	C311-C312-C313-C314
5	A	1005	POV	C36-C37-C38-C39
5	A	1008	POV	C22-C21-O21-C2
5	A	1004	POV	C311-C310-C39-C38
5	A	1002	POV	C1-O11-P-O12
5	A	1005	POV	C1-O11-P-O12
5	A	1005	POV	C11-O12-P-O11
5	A	1007	POV	C1-O11-P-O12
5	A	1008	POV	C1-O11-P-O12
5	B	1003	POV	C1-O11-P-O12
5	B	1003	POV	C11-O12-P-O11
5	B	1004	POV	C11-O12-P-O11
5	C	1002	POV	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
5	C	1004	POV	C1-O11-P-O12
5	C	1005	POV	C1-O11-P-O12
5	C	1005	POV	C11-O12-P-O11
5	C	1007	POV	C1-O11-P-O12
5	C	1007	POV	C11-O12-P-O11
5	C	1008	POV	C1-O11-P-O12
5	D	1004	POV	C11-O12-P-O11
5	C	1005	POV	C31-C32-C33-C34
5	C	1009	POV	C32-C31-O31-C3
5	A	1008	POV	C21-C22-C23-C24
5	A	1008	POV	O22-C21-O21-C2
5	C	1007	POV	C35-C36-C37-C38
5	B	1003	POV	C11-C12-N-C13
5	B	1003	POV	C11-C12-N-C14
5	C	1002	POV	C11-C12-N-C14
5	C	1007	POV	C11-C12-N-C13
5	C	1007	POV	C11-C12-N-C15
5	B	1003	POV	C33-C34-C35-C36
5	C	1005	POV	C214-C215-C216-C217
5	C	1009	POV	C22-C23-C24-C25
5	C	1002	POV	C22-C21-O21-C2
5	C	1009	POV	C22-C21-O21-C2
5	A	1005	POV	C214-C215-C216-C217
5	A	1008	POV	C213-C214-C215-C216
5	A	1008	POV	C22-C23-C24-C25
5	B	1004	POV	C312-C313-C314-C315
5	C	1002	POV	C311-C312-C313-C314
5	C	1007	POV	C25-C26-C27-C28
5	C	1008	POV	C310-C311-C312-C313
5	C	1009	POV	C311-C312-C313-C314
5	C	1009	POV	C212-C213-C214-C215
5	D	1004	POV	C312-C313-C314-C315
5	A	1002	POV	C311-C312-C313-C314
5	A	1008	POV	C33-C34-C35-C36
5	B	1003	POV	C312-C313-C314-C315
5	C	1009	POV	C213-C214-C215-C216
5	C	1002	POV	O22-C21-O21-C2
5	C	1009	POV	O22-C21-O21-C2
5	A	1003	POV	C31-C32-C33-C34
5	A	1005	POV	C25-C26-C27-C28
5	C	1005	POV	C311-C312-C313-C314
5	A	1007	POV	C214-C215-C216-C217

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Mol	Chain	Res	Type	Atoms
5	A	1008	POV	C311-C312-C313-C314
5	C	1007	POV	C312-C313-C314-C315
5	C	1009	POV	C33-C34-C35-C36
5	D	1004	POV	C214-C215-C216-C217
5	A	1002	POV	C33-C34-C35-C36
5	C	1004	POV	C34-C35-C36-C37
5	C	1005	POV	C25-C26-C27-C28
5	A	1004	POV	C34-C35-C36-C37
5	B	1004	POV	C214-C215-C216-C217
5	C	1008	POV	C34-C35-C36-C37
5	A	1008	POV	C37-C38-C39-C310
5	C	1009	POV	C37-C38-C39-C310
5	A	1008	POV	C311-C310-C39-C38
5	C	1002	POV	C33-C34-C35-C36
5	A	1002	POV	O22-C21-O21-C2
5	B	1004	POV	O22-C21-O21-C2
5	A	1007	POV	C22-C21-O21-C2
5	B	1004	POV	C22-C21-O21-C2
5	A	1003	POV	C22-C23-C24-C25
5	C	1004	POV	C35-C36-C37-C38
5	C	1007	POV	C214-C215-C216-C217
5	B	1003	POV	C210-C211-C212-C213
5	C	1007	POV	C210-C211-C212-C213
5	A	1005	POV	C21-C22-C23-C24
5	C	1005	POV	C21-C22-C23-C24
5	A	1002	POV	C312-C313-C314-C315
5	A	1004	POV	C25-C26-C27-C28
5	A	1007	POV	C34-C35-C36-C37
5	A	1008	POV	C212-C213-C214-C215
5	B	1003	POV	C36-C37-C38-C39
5	C	1003	POV	C22-C23-C24-C25
5	C	1004	POV	C25-C26-C27-C28
5	C	1008	POV	C214-C215-C216-C217
5	B	1003	POV	C11-C12-N-C15
5	A	1004	POV	C35-C36-C37-C38
5	B	1003	POV	C25-C26-C27-C28
5	A	1005	POV	C311-C312-C313-C314
5	C	1003	POV	C23-C24-C25-C26
5	A	1008	POV	C36-C37-C38-C39
5	C	1004	POV	C311-C310-C39-C38
5	C	1007	POV	C36-C37-C38-C39
5	C	1009	POV	O32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
5	A	1007	POV	O22-C21-O21-C2
5	A	1003	POV	C23-C24-C25-C26
5	B	1003	POV	C35-C36-C37-C38
5	C	1002	POV	C24-C25-C26-C27
5	C	1003	POV	C31-C32-C33-C34
5	A	1002	POV	C22-C21-O21-C2
5	C	1008	POV	C22-C21-O21-C2
5	D	1004	POV	C22-C21-O21-C2
5	A	1003	POV	C32-C33-C34-C35
5	C	1009	POV	C311-C310-C39-C38
5	C	1004	POV	C210-C211-C212-C213
5	B	1004	POV	C21-C22-C23-C24
5	C	1009	POV	C25-C26-C27-C28
5	A	1007	POV	C312-C313-C314-C315
5	A	1007	POV	C310-C311-C312-C313
5	C	1008	POV	O22-C21-O21-C2
5	D	1004	POV	O22-C21-O21-C2
5	C	1009	POV	C214-C215-C216-C217
5	B	1004	POV	C39-C310-C311-C312
5	A	1002	POV	C11-C12-N-C15
5	C	1002	POV	C11-C12-N-C13
5	C	1002	POV	C11-C12-N-C15
5	C	1004	POV	C211-C212-C213-C214
5	A	1004	POV	C211-C212-C213-C214
5	B	1004	POV	C210-C211-C212-C213
5	C	1009	POV	C210-C211-C212-C213
5	D	1004	POV	C210-C211-C212-C213
5	D	1004	POV	C21-C22-C23-C24
5	A	1008	POV	C214-C215-C216-C217
5	C	1009	POV	C39-C310-C311-C312
5	D	1004	POV	C39-C310-C311-C312
5	C	1003	POV	C32-C33-C34-C35
5	C	1009	POV	C36-C37-C38-C39
5	D	1004	POV	O11-C1-C2-O21
5	C	1007	POV	C21-C22-C23-C24
5	D	1004	POV	C211-C212-C213-C214
5	C	1004	POV	O21-C2-C3-O31
9	D	1002	2J9	CAG-CAN-NAO-CAL
5	A	1008	POV	C25-C26-C27-C28
5	A	1008	POV	C210-C211-C212-C213
5	A	1002	POV	C24-C25-C26-C27
5	C	1007	POV	C313-C314-C315-C316

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Mol	Chain	Res	Type	Atoms
5	B	1003	POV	C21-C22-C23-C24
5	A	1008	POV	C32-C31-O31-C3
5	C	1002	POV	C312-C313-C314-C315
5	C	1009	POV	C31-C32-C33-C34
5	C	1004	POV	C22-C23-C24-C25
5	C	1002	POV	C25-C26-C27-C28
5	A	1004	POV	C210-C211-C212-C213
5	B	1003	POV	C26-C27-C28-C29
5	A	1004	POV	C22-C23-C24-C25
5	A	1007	POV	C36-C37-C38-C39
5	B	1003	POV	C313-C314-C315-C316
5	A	1002	POV	C1-C2-C3-O31
5	A	1008	POV	C39-C310-C311-C312
5	B	1004	POV	C1-C2-C3-O31
5	C	1002	POV	C1-C2-C3-O31
5	B	1004	POV	C310-C311-C312-C313
5	C	1002	POV	C215-C216-C217-C218
5	A	1004	POV	C313-C314-C315-C316
5	A	1007	POV	C33-C34-C35-C36
5	C	1004	POV	C313-C314-C315-C316
5	C	1008	POV	C215-C216-C217-C218
5	C	1007	POV	C215-C216-C217-C218
5	A	1002	POV	C31-C32-C33-C34
5	B	1004	POV	C211-C212-C213-C214
5	C	1008	POV	C33-C34-C35-C36
5	A	1002	POV	C215-C216-C217-C218
5	A	1002	POV	C25-C26-C27-C28
5	C	1007	POV	C39-C310-C311-C312
5	C	1007	POV	C211-C212-C213-C214
5	C	1002	POV	C32-C31-O31-C3
5	A	1008	POV	O32-C31-O31-C3
5	A	1007	POV	C215-C216-C217-C218
5	B	1004	POV	O21-C2-C3-O31
5	A	1005	POV	C23-C24-C25-C26
5	C	1002	POV	C213-C214-C215-C216
5	A	1002	POV	C211-C212-C213-C214
5	D	1004	POV	C310-C311-C312-C313
5	A	1008	POV	C31-C32-C33-C34
5	A	1003	POV	C213-C214-C215-C216
5	A	1002	POV	C32-C31-O31-C3
5	C	1002	POV	C31-C32-C33-C34
5	A	1007	POV	C211-C212-C213-C214

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Mol	Chain	Res	Type	Atoms
5	C	1002	POV	C32-C33-C34-C35
5	B	1004	POV	O11-C1-C2-C3
5	D	1004	POV	O11-C1-C2-C3
5	C	1008	POV	C31-C32-C33-C34
5	A	1002	POV	C22-C23-C24-C25
5	C	1005	POV	C39-C310-C311-C312
5	C	1007	POV	C37-C38-C39-C310
9	B	1005	2J9	CAG-CAN-NAO-CAL
5	A	1008	POV	C215-C216-C217-C218
5	C	1003	POV	C213-C214-C215-C216
5	B	1003	POV	C211-C212-C213-C214
5	A	1004	POV	C1-C2-C3-O31
5	A	1005	POV	C1-C2-C3-O31
5	C	1004	POV	C1-C2-C3-O31
5	C	1005	POV	C1-C2-C3-O31
5	C	1008	POV	C1-C2-C3-O31
5	D	1004	POV	C1-C2-C3-O31
5	D	1004	POV	C34-C35-C36-C37
5	B	1003	POV	C215-C216-C217-C218
5	C	1002	POV	O32-C31-O31-C3
5	C	1008	POV	C312-C313-C314-C315
5	C	1009	POV	C215-C216-C217-C218
5	A	1005	POV	C24-C25-C26-C27
5	A	1007	POV	C31-C32-C33-C34
5	B	1004	POV	C34-C35-C36-C37
5	A	1002	POV	O32-C31-O31-C3
5	C	1007	POV	C24-C25-C26-C27
5	B	1004	POV	C313-C314-C315-C316
5	A	1007	POV	C311-C310-C39-C38
5	C	1008	POV	C36-C37-C38-C39
5	D	1004	POV	C313-C314-C315-C316
5	C	1005	POV	C22-C21-O21-C2
5	C	1005	POV	C24-C25-C26-C27
5	A	1003	POV	O11-C1-C2-C3
5	C	1003	POV	O11-C1-C2-C3
5	C	1005	POV	C37-C38-C39-C310
5	A	1008	POV	C1-C2-O21-C21
5	C	1009	POV	C1-C2-O21-C21
5	A	1005	POV	C34-C35-C36-C37
5	C	1005	POV	C36-C37-C38-C39
5	A	1007	POV	C1-C2-C3-O31
5	A	1002	POV	O11-C1-C2-O21

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Mol	Chain	Res	Type	Atoms
5	C	1002	POV	O11-C1-C2-O21
5	C	1005	POV	O22-C21-O21-C2
5	A	1008	POV	O21-C2-C3-O31
5	C	1009	POV	O21-C2-C3-O31
5	A	1005	POV	C22-C23-C24-C25
5	A	1004	POV	C33-C34-C35-C36
5	C	1002	POV	C310-C311-C312-C313
5	C	1005	POV	C211-C212-C213-C214
5	A	1005	POV	C22-C21-O21-C2
5	C	1007	POV	C26-C27-C28-C29
5	C	1003	POV	C311-C310-C39-C38
5	A	1005	POV	O22-C21-O21-C2
5	D	1004	POV	C36-C37-C38-C39
5	C	1005	POV	C22-C23-C24-C25
5	A	1004	POV	C11-O12-P-O11
5	C	1004	POV	C11-O12-P-O11
5	D	1004	POV	C1-O11-P-O12
5	C	1008	POV	C211-C212-C213-C214
5	C	1005	POV	C23-C24-C25-C26
5	A	1004	POV	C1-O11-P-O14
5	B	1003	POV	C1-O11-P-O13
5	B	1004	POV	C11-O12-P-O13
5	C	1004	POV	C1-O11-P-O14
5	C	1007	POV	C1-O11-P-O13
5	C	1007	POV	C11-O12-P-O14
5	D	1004	POV	C11-O12-P-O13
5	A	1007	POV	O11-C1-C2-C3
5	C	1008	POV	O11-C1-C2-C3
5	C	1004	POV	C33-C34-C35-C36
5	B	1003	POV	C310-C311-C312-C313
5	B	1003	POV	C12-C11-O12-P
5	C	1007	POV	C12-C11-O12-P
5	C	1004	POV	C24-C25-C26-C27
5	B	1003	POV	C214-C215-C216-C217
5	C	1002	POV	C211-C212-C213-C214
5	A	1007	POV	O11-C1-C2-O21
5	C	1008	POV	O11-C1-C2-O21
5	A	1008	POV	C24-C25-C26-C27
5	C	1005	POV	C33-C34-C35-C36
5	C	1008	POV	C212-C213-C214-C215
5	C	1008	POV	C313-C314-C315-C316
5	A	1003	POV	O12-C11-C12-N

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Mol	Chain	Res	Type	Atoms
5	A	1007	POV	O12-C11-C12-N
5	C	1003	POV	O12-C11-C12-N
5	C	1008	POV	O12-C11-C12-N
5	A	1005	POV	O21-C2-C3-O31
5	C	1005	POV	O21-C2-C3-O31
5	A	1004	POV	C24-C25-C26-C27
5	C	1002	POV	C210-C211-C212-C213
5	A	1004	POV	C39-C310-C311-C312
5	B	1003	POV	C311-C310-C39-C38
5	A	1005	POV	C37-C38-C39-C310
5	A	1008	POV	C23-C24-C25-C26
5	A	1005	POV	C33-C34-C35-C36
5	B	1004	POV	C36-C37-C38-C39
5	A	1002	POV	C3-C2-O21-C21
5	C	1002	POV	C3-C2-O21-C21
5	C	1005	POV	C34-C35-C36-C37
5	A	1005	POV	C35-C36-C37-C38
5	A	1002	POV	C32-C33-C34-C35
5	A	1002	POV	C29-C210-C211-C212
5	C	1002	POV	C29-C210-C211-C212
5	C	1003	POV	O21-C2-C3-O31
5	B	1004	POV	C1-O11-P-O12
5	C	1003	POV	C35-C36-C37-C38
5	C	1002	POV	C22-C23-C24-C25
5	B	1004	POV	C22-C23-C24-C25
5	A	1003	POV	C36-C37-C38-C39
5	C	1007	POV	C27-C28-C29-C210
5	B	1003	POV	C39-C310-C311-C312
5	A	1004	POV	C310-C311-C312-C313
5	A	1005	POV	C26-C27-C28-C29
5	C	1004	POV	C310-C311-C312-C313
5	C	1008	POV	C29-C210-C211-C212
5	C	1004	POV	C39-C310-C311-C312
5	D	1004	POV	C22-C23-C24-C25
5	B	1004	POV	C213-C214-C215-C216
9	B	1005	2J9	CAH-CAN-NAO-CAI
9	D	1002	2J9	CAH-CAN-NAO-CAI
5	C	1007	POV	C29-C210-C211-C212
5	A	1002	POV	C210-C211-C212-C213
5	A	1003	POV	C311-C312-C313-C314
5	A	1002	POV	C310-C311-C312-C313
5	A	1005	POV	C212-C213-C214-C215

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Mol	Chain	Res	Type	Atoms
5	A	1003	POV	O21-C2-C3-O31
5	D	1004	POV	C27-C28-C29-C210
5	C	1005	POV	C311-C310-C39-C38
5	A	1005	POV	C211-C212-C213-C214
5	C	1003	POV	C1-C2-C3-O31
5	C	1007	POV	C311-C310-C39-C38
5	C	1005	POV	C212-C213-C214-C215
5	A	1002	POV	C27-C28-C29-C210
5	A	1003	POV	C27-C28-C29-C210
5	C	1003	POV	C27-C28-C29-C210
5	A	1005	POV	C311-C310-C39-C38
5	A	1007	POV	C313-C314-C315-C316
5	C	1002	POV	C27-C28-C29-C210
5	A	1005	POV	C39-C310-C311-C312
5	C	1005	POV	C32-C33-C34-C35
5	A	1002	POV	C34-C35-C36-C37
4	B	1002	DNQ	C5-C7-N3-O5
4	D	1003	DNQ	C5-C7-N3-O5
5	C	1005	POV	C26-C27-C28-C29
5	A	1007	POV	C29-C210-C211-C212
5	B	1004	POV	C27-C28-C29-C210
5	C	1009	POV	C29-C210-C211-C212
5	A	1007	POV	C212-C213-C214-C215
5	D	1004	POV	O31-C31-C32-C33
5	A	1003	POV	C215-C216-C217-C218
5	B	1003	POV	C37-C38-C39-C310
5	C	1003	POV	C39-C310-C311-C312
5	C	1003	POV	C311-C312-C313-C314
5	A	1003	POV	C29-C210-C211-C212
5	B	1003	POV	C27-C28-C29-C210
5	C	1008	POV	C26-C27-C28-C29
5	C	1008	POV	C22-C23-C24-C25
5	A	1002	POV	O11-C1-C2-C3
5	A	1004	POV	C213-C214-C215-C216
5	A	1007	POV	C22-C23-C24-C25
5	B	1004	POV	O31-C31-C32-C33
5	C	1009	POV	C11-C12-N-C14
5	C	1002	POV	C37-C38-C39-C310
5	C	1009	POV	C313-C314-C315-C316
5	A	1008	POV	C29-C210-C211-C212
5	C	1003	POV	C29-C210-C211-C212
5	B	1004	POV	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
5	D	1004	POV	O32-C31-C32-C33
5	A	1003	POV	C1-C2-C3-O31
5	C	1009	POV	C21-C22-C23-C24
5	C	1004	POV	C23-C24-C25-C26
5	C	1002	POV	O11-C1-C2-C3
5	A	1002	POV	C213-C214-C215-C216
5	B	1004	POV	O32-C31-C32-C33
5	A	1007	POV	C25-C26-C27-C28
5	C	1007	POV	C311-C312-C313-C314
5	C	1002	POV	C12-C11-O12-P
5	C	1009	POV	C12-C11-O12-P
5	A	1007	POV	O32-C31-O31-C3
5	A	1004	POV	C214-C215-C216-C217
5	C	1003	POV	C37-C38-C39-C310
5	C	1003	POV	C215-C216-C217-C218
5	A	1008	POV	O21-C21-C22-C23
5	A	1002	POV	C37-C38-C39-C310
5	C	1002	POV	C34-C35-C36-C37
5	C	1004	POV	C214-C215-C216-C217
5	A	1007	POV	C32-C31-O31-C3
5	A	1007	POV	C26-C27-C28-C29
5	C	1008	POV	C311-C310-C39-C38
5	A	1008	POV	C313-C314-C315-C316
5	C	1009	POV	C11-C12-N-C13
5	A	1002	POV	C35-C36-C37-C38

There are no ring outliers.

19 monomers are involved in 54 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1001	DNQ	4	0
5	A	1003	POV	2	0
5	B	1004	POV	3	0
5	A	1005	POV	4	0
5	A	1008	POV	3	0
5	A	1002	POV	4	0
5	C	1007	POV	8	0
5	A	1004	POV	1	0
4	A	1001	DNQ	4	0
5	C	1002	POV	3	0
5	D	1004	POV	1	0
5	C	1008	POV	3	0

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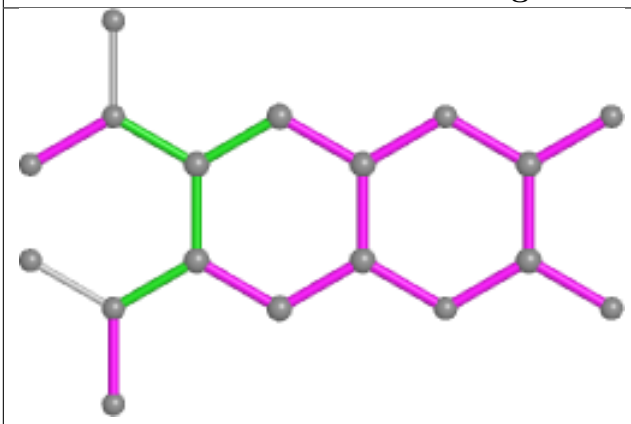
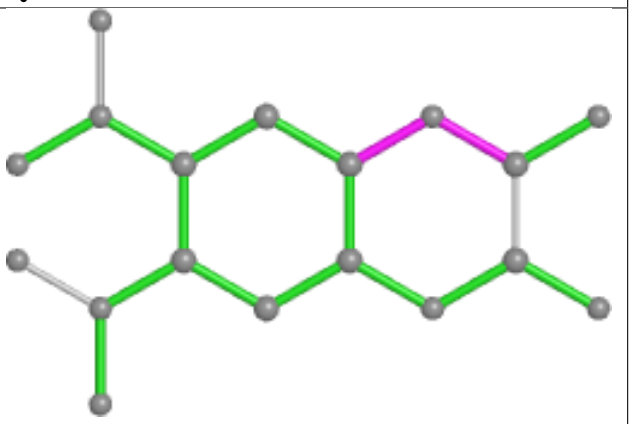
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1003	POV	2	0
9	D	1001	2J9	1	0
4	D	1003	DNQ	1	0
5	B	1003	POV	6	0
5	C	1009	POV	4	0
5	C	1005	POV	4	0
5	A	1007	POV	1	0

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.

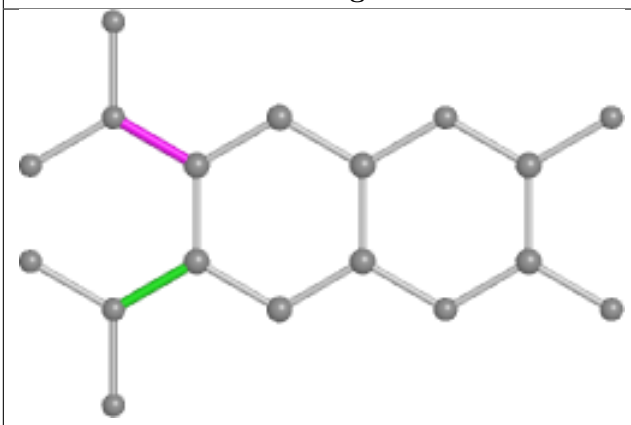
Ligand DNQ C 1001



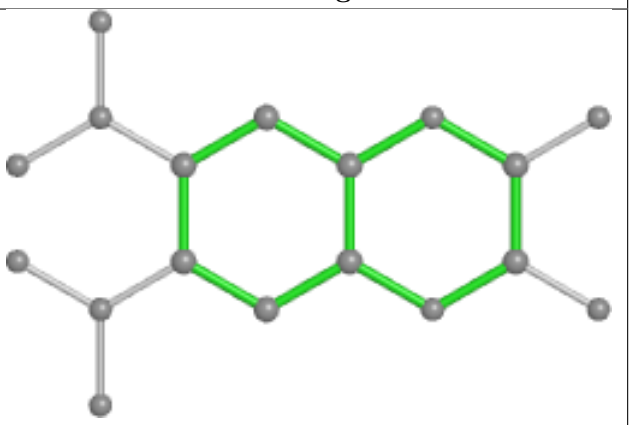
Bond lengths



Bond angles

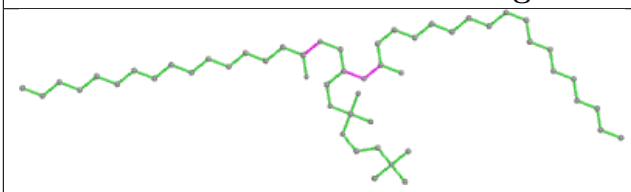


Torsions

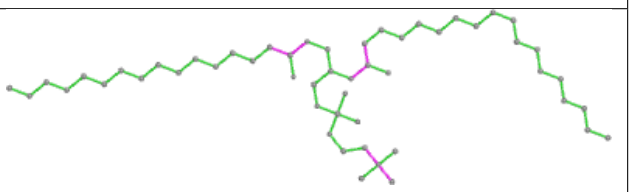


Rings

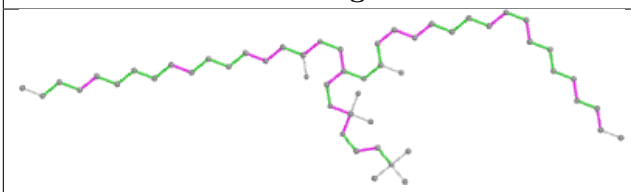
Ligand POV A 1003



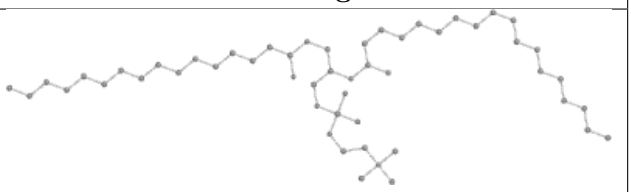
Bond lengths



Bond angles

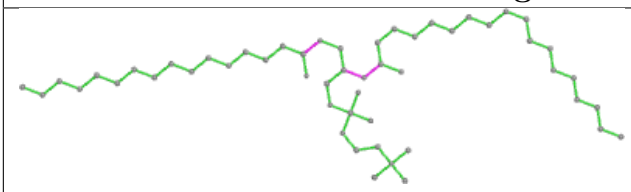


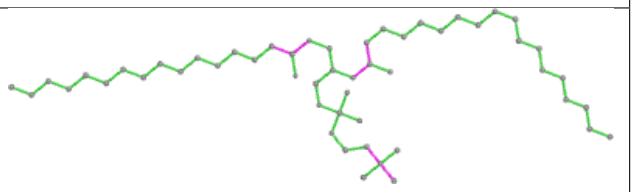
Torsions

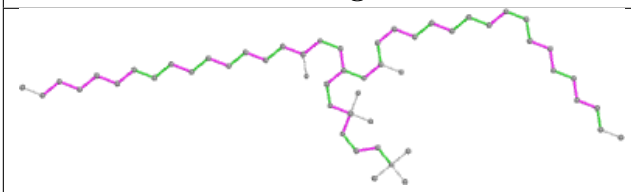


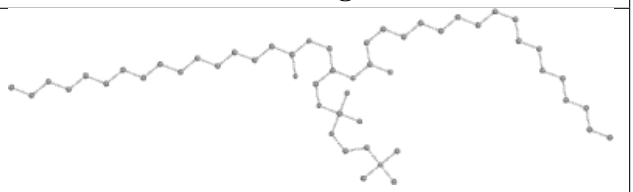
Rings

Ligand POV B 1004

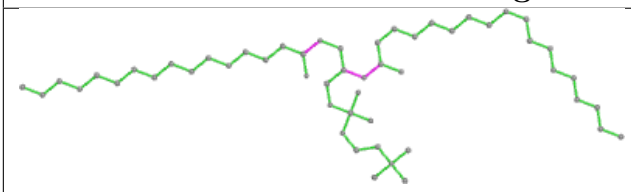

Bond lengths


Bond angles


Torsions


Rings

Ligand POV A 1005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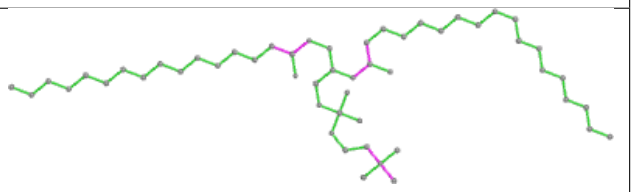
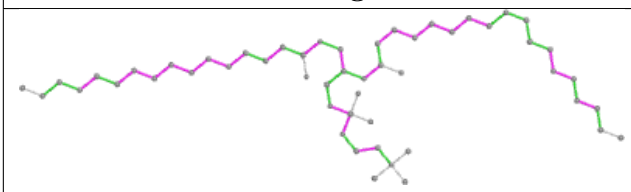
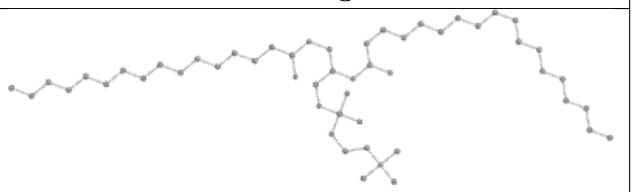
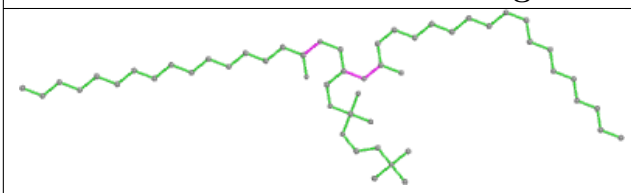

Bond angles


Torsions


Rings

Ligand POV A 1008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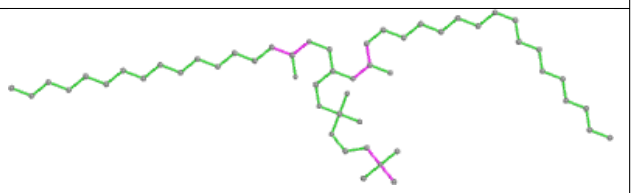
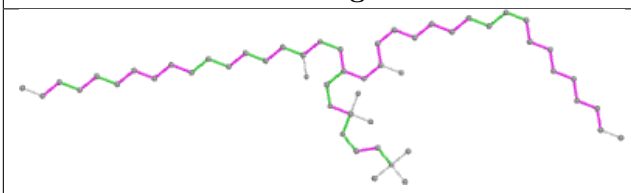
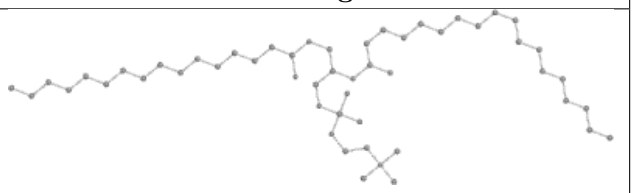
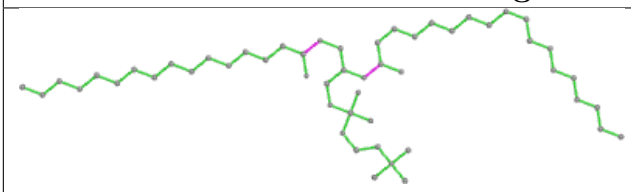

Bond angles


Torsions


Rings

Ligand POV A 1002



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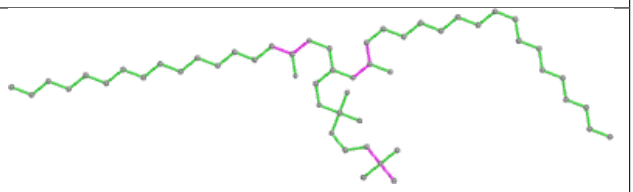
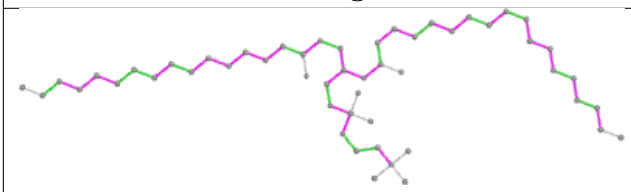


Bond angles



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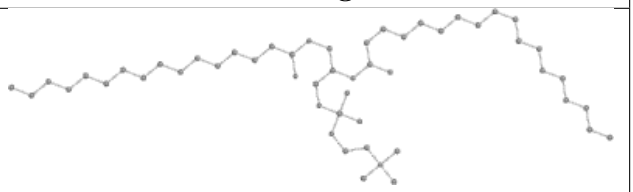
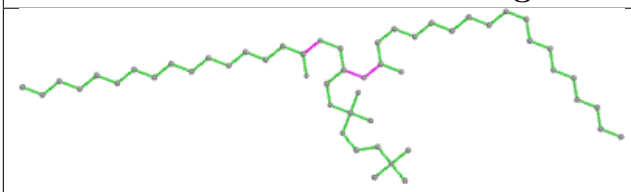
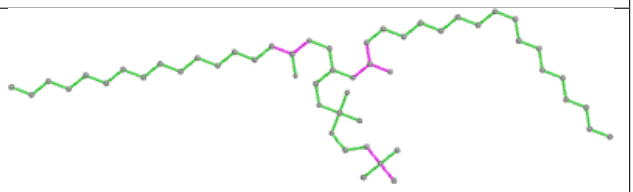


Rings

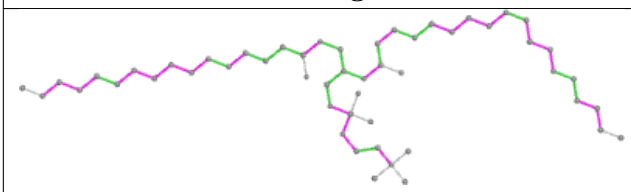
Ligand POV C 1007



Bond lengths



Bond angles



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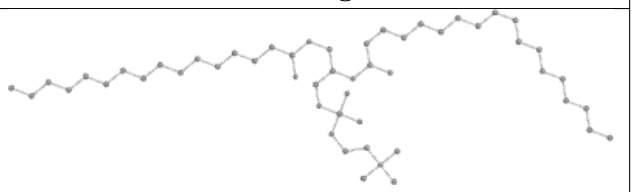
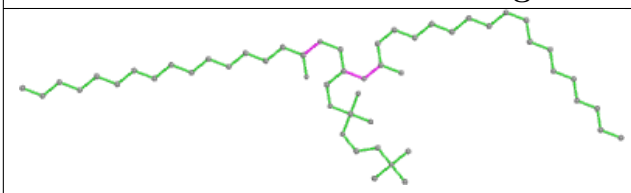


Rings

Ligand POV A 1004



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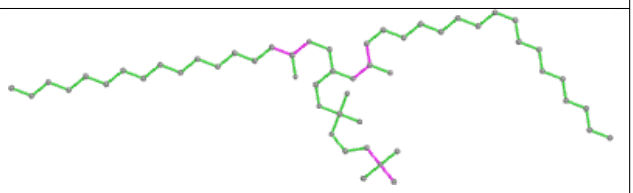
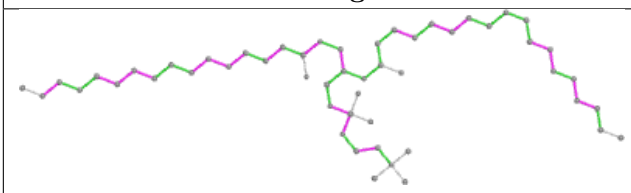


Bond angles



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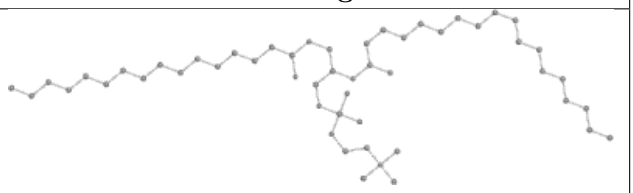
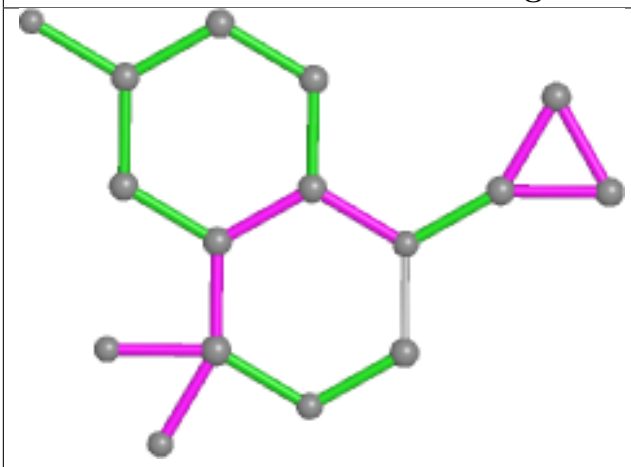


Rings

Ligand 2J9 D 1002



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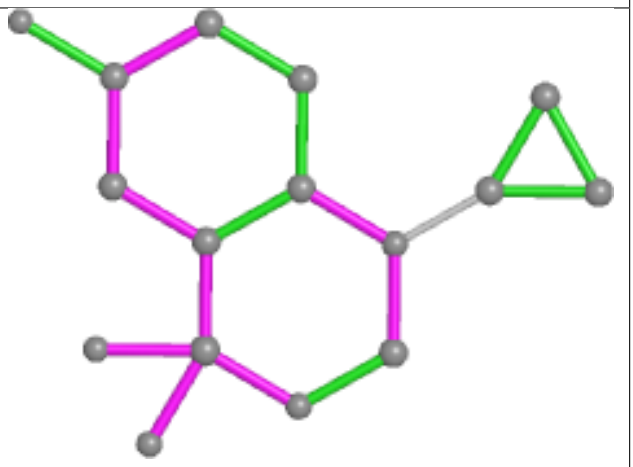
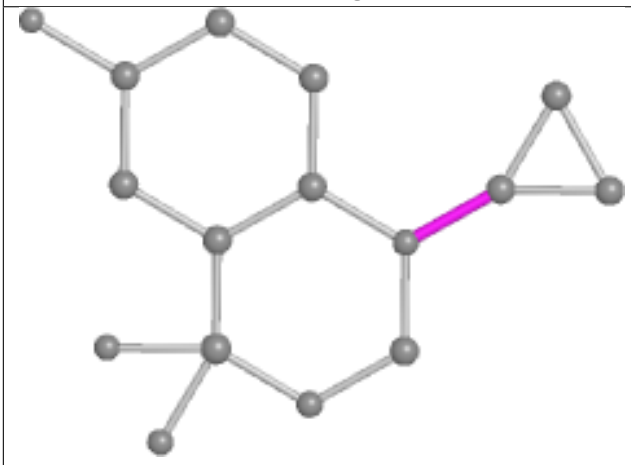


Bond angles



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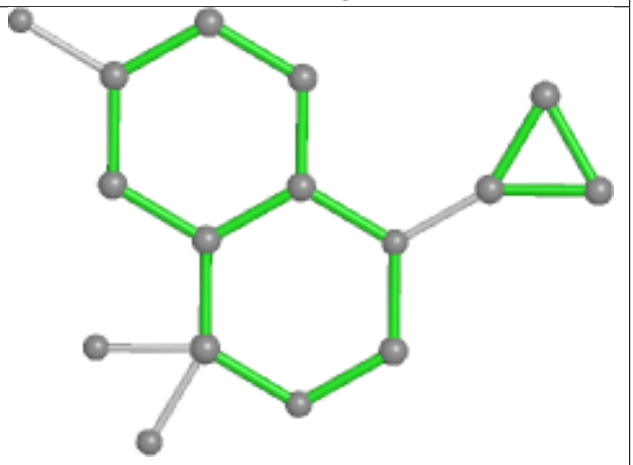
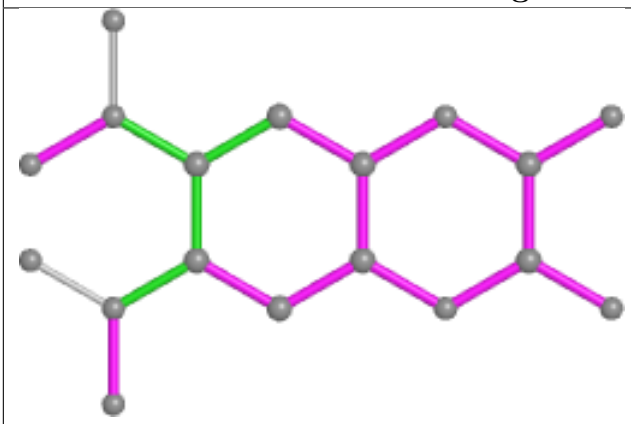


Rings

Ligand DNQ B 1002



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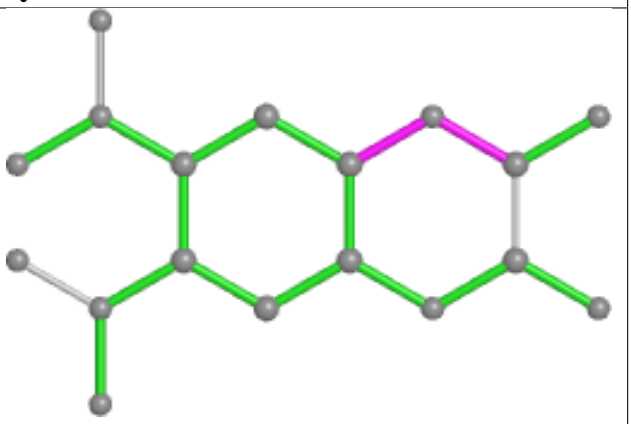
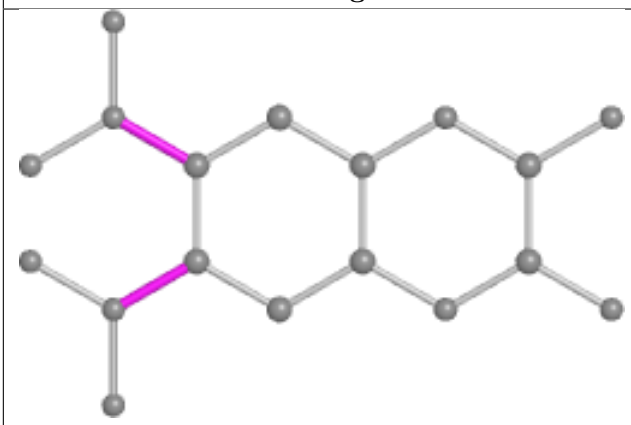


Bond angles



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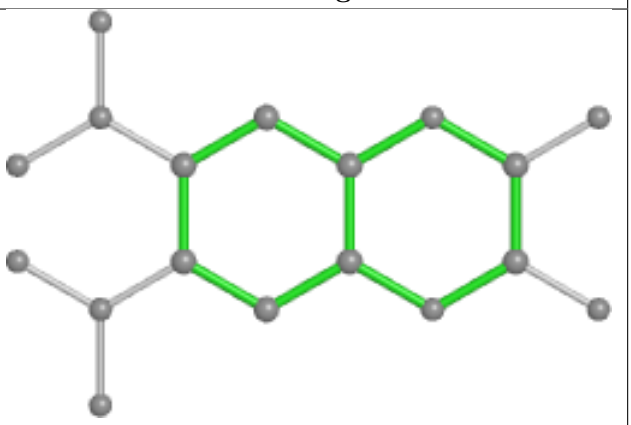
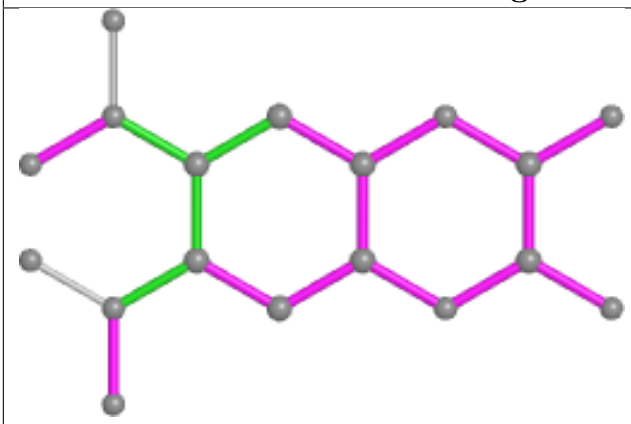
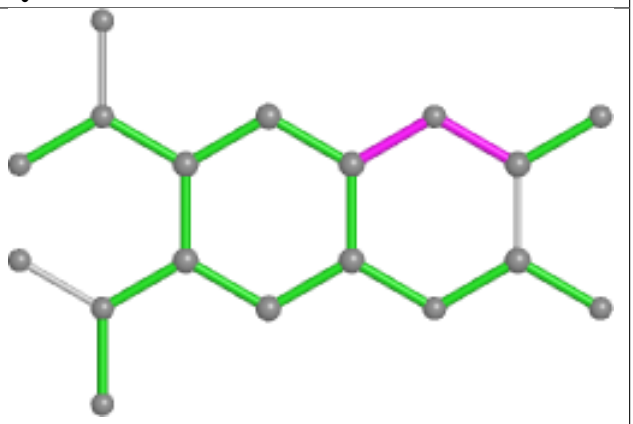


Rings

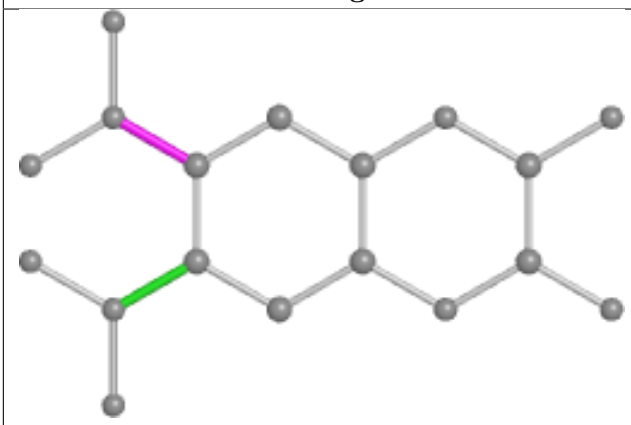
Ligand DNQ A 1001



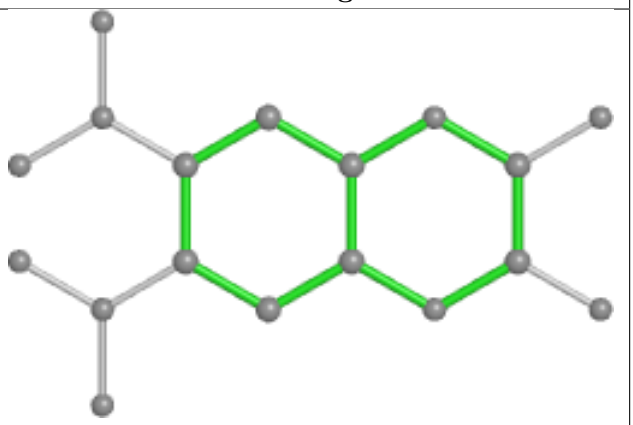
Bond lengths



Bond angles

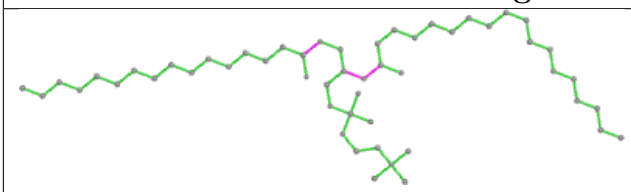


Torsions

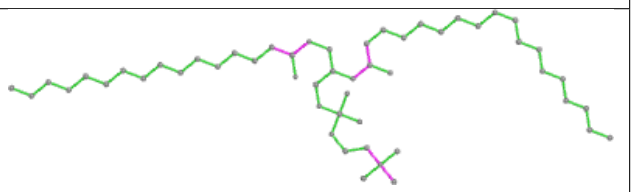


Rings

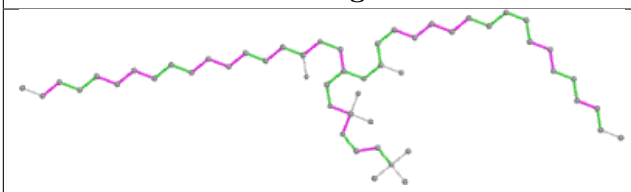
Ligand POV C 1004



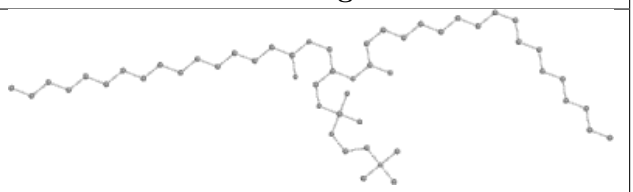
Bond lengths



Bond angles

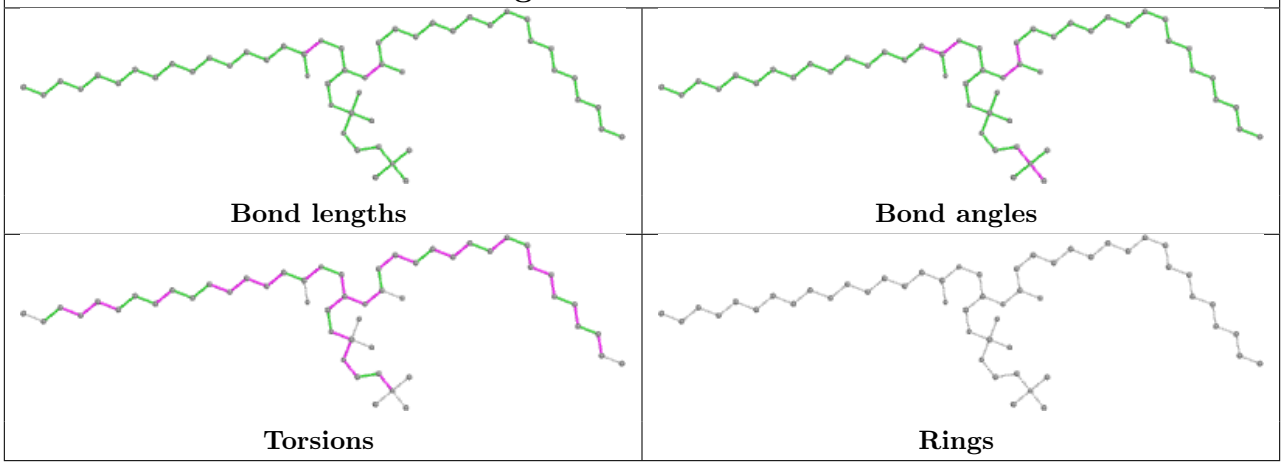


Torsions

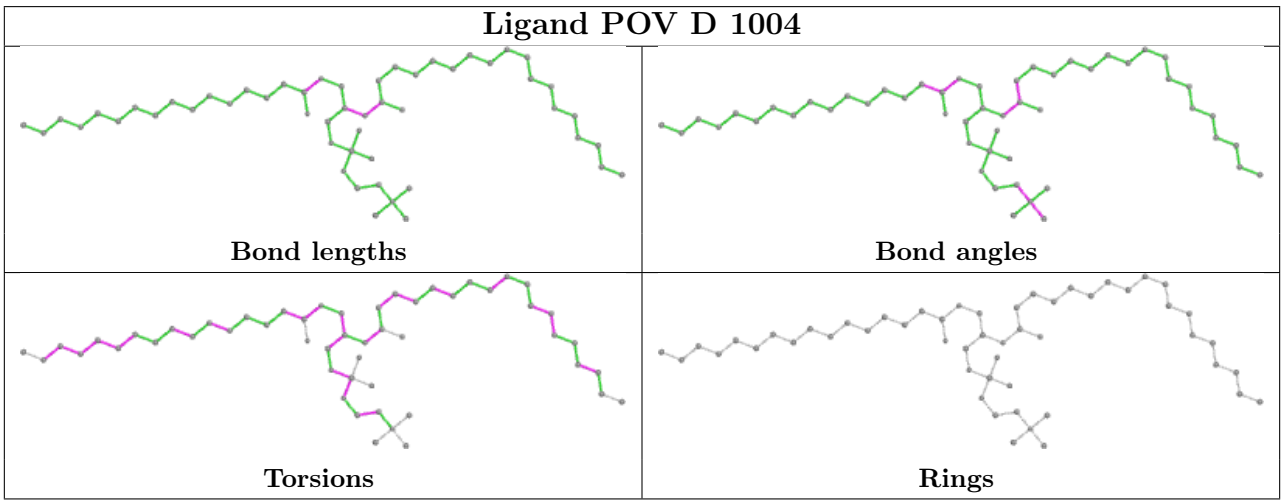


Rings

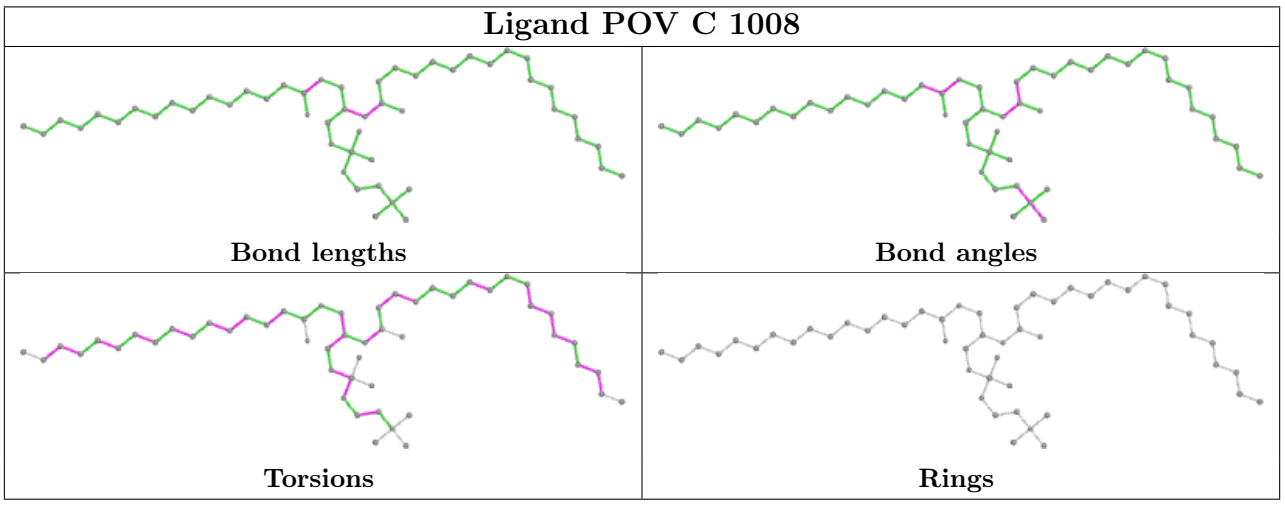
Ligand POV C 1002



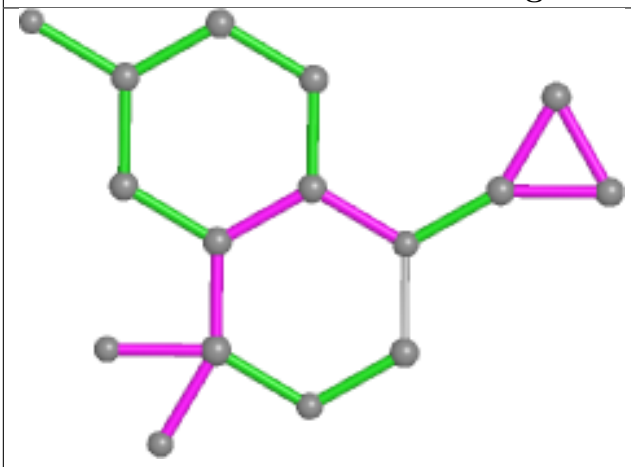
Ligand POV D 1004



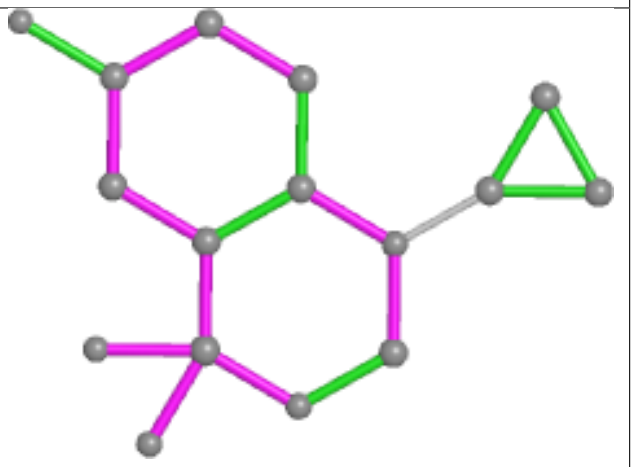
Ligand POV C 1008



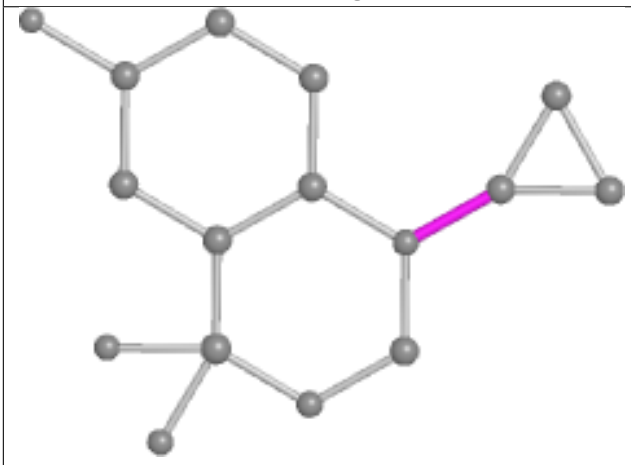
Ligand 2J9 B 1005



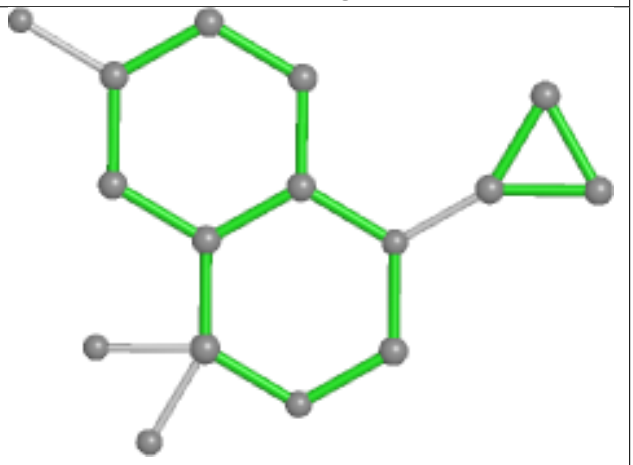
Bond lengths



Bond angles

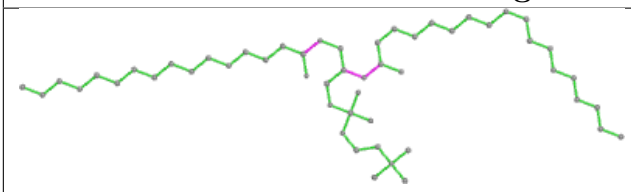


Torsions

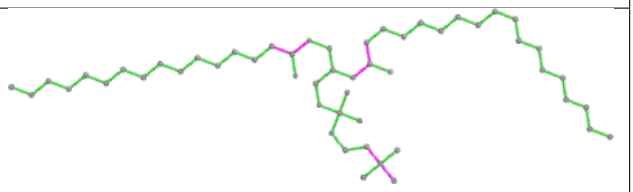


Rings

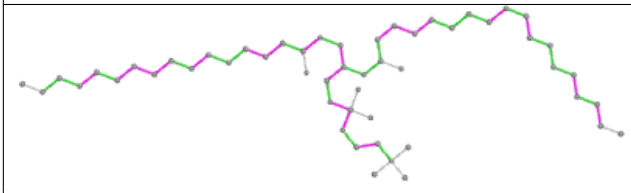
Ligand POV C 1003



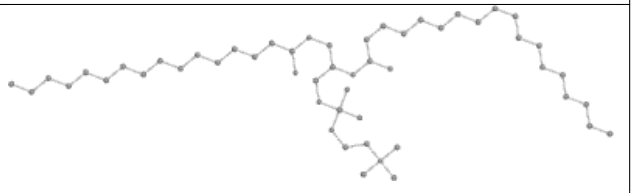
Bond lengths



Bond angles

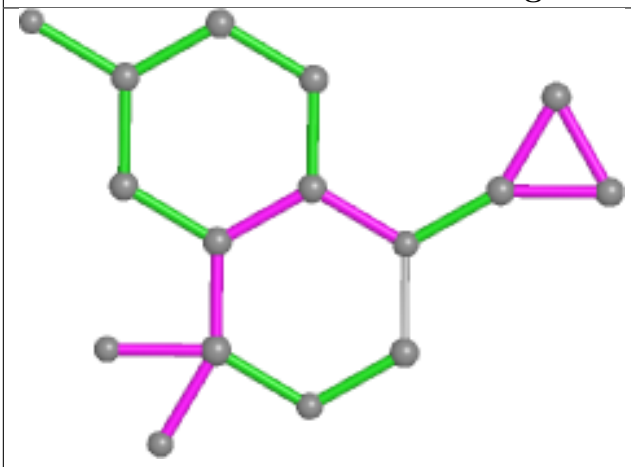


Torsions

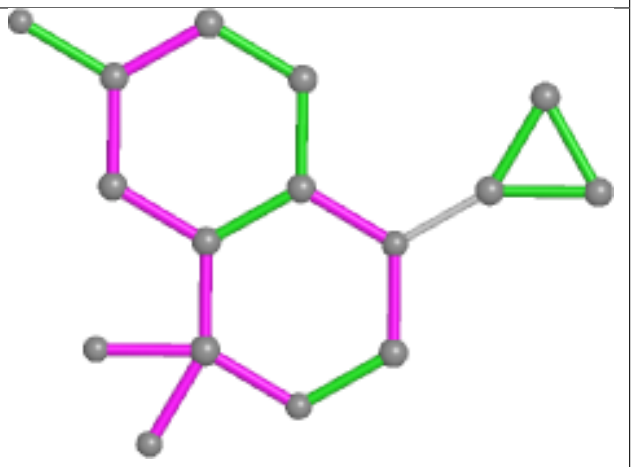


Rings

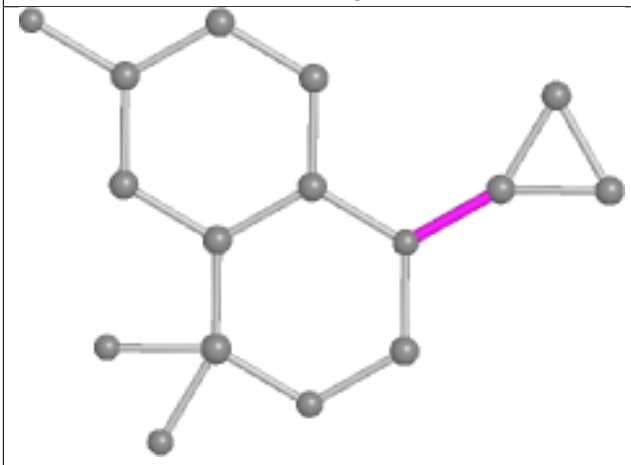
Ligand 2J9 D 1001



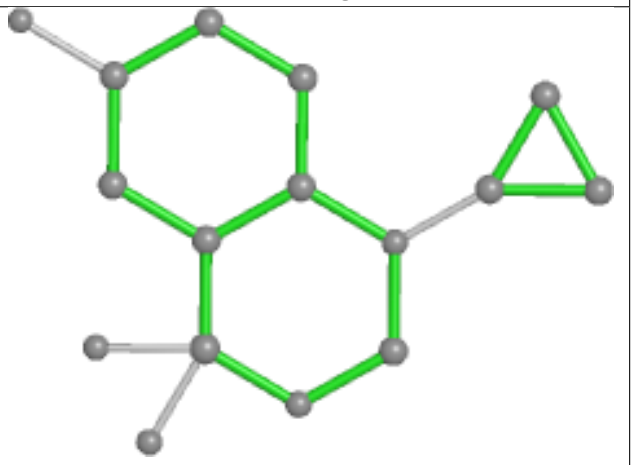
Bond lengths



Bond angles

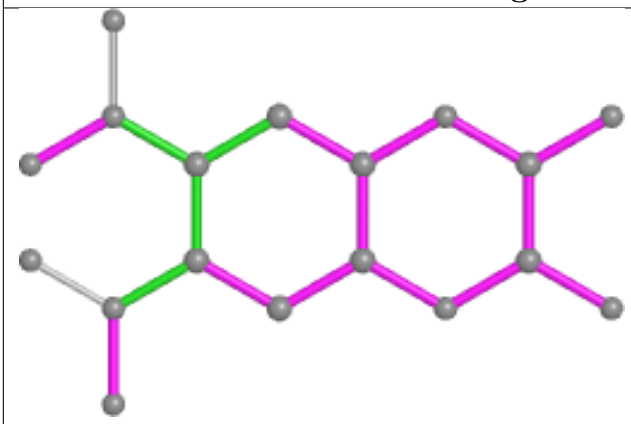


Torsions

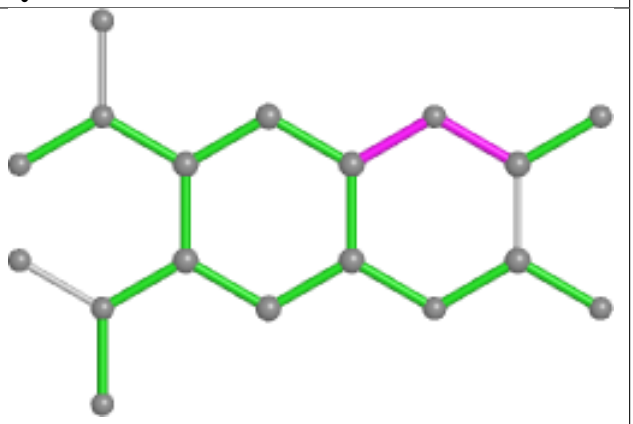


Rings

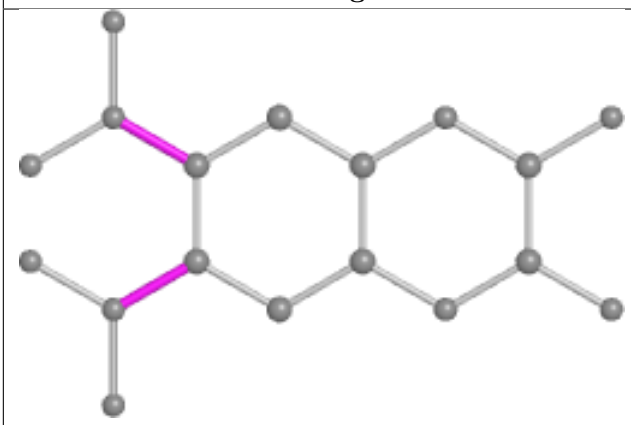
Ligand DNQ D 1003



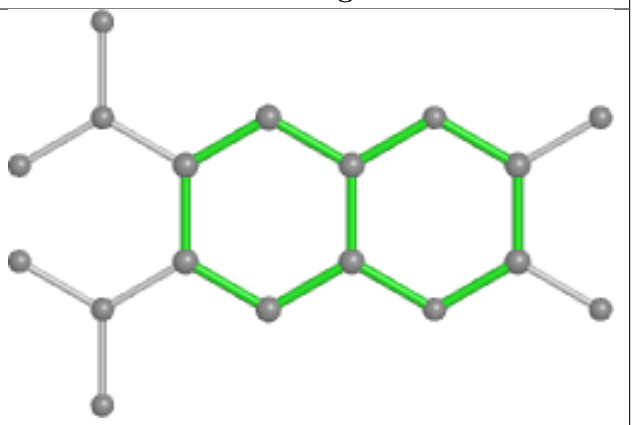
Bond lengths



Bond angles

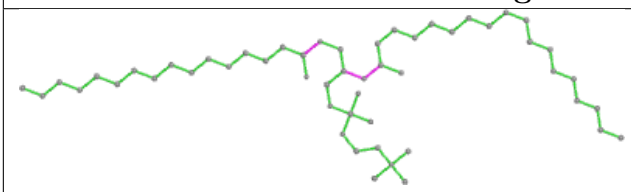


Torsions

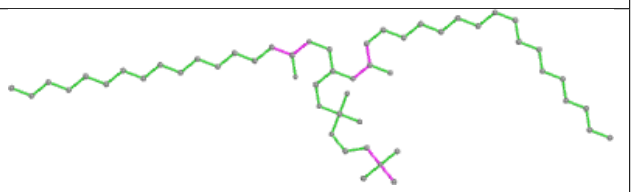


Rings

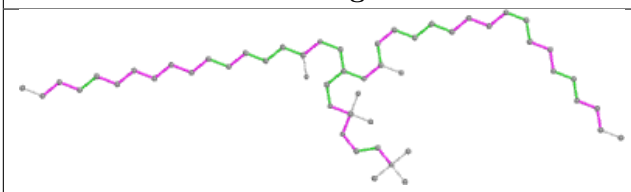
Ligand POV B 1003



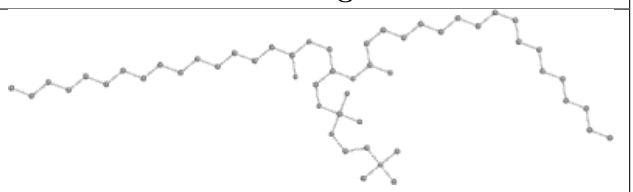
Bond lengths



Bond angles

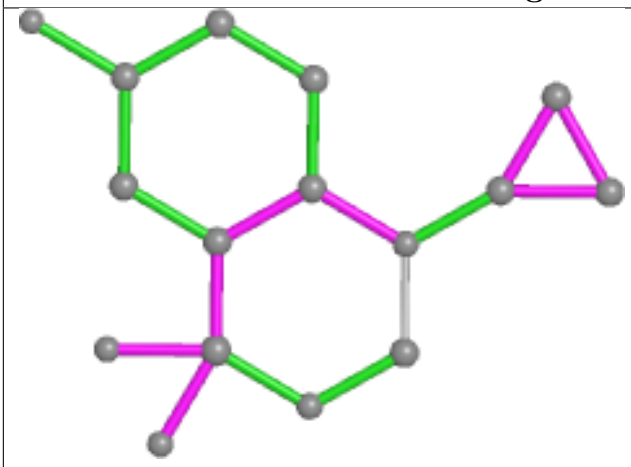


Torsions

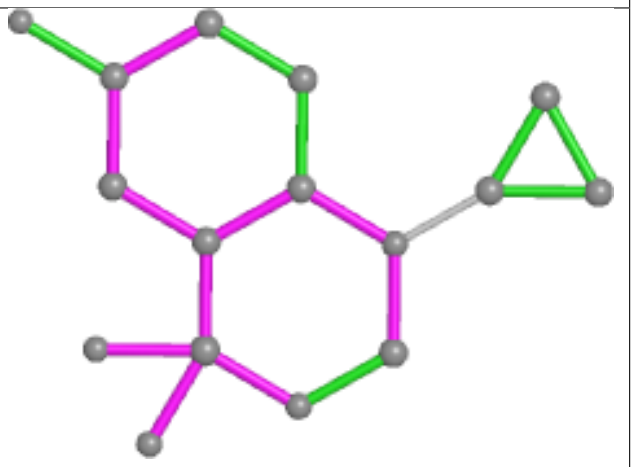


Rings

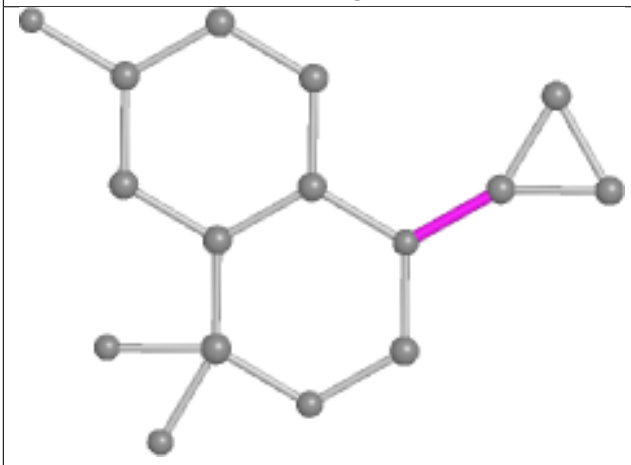
Ligand 2J9 B 1001



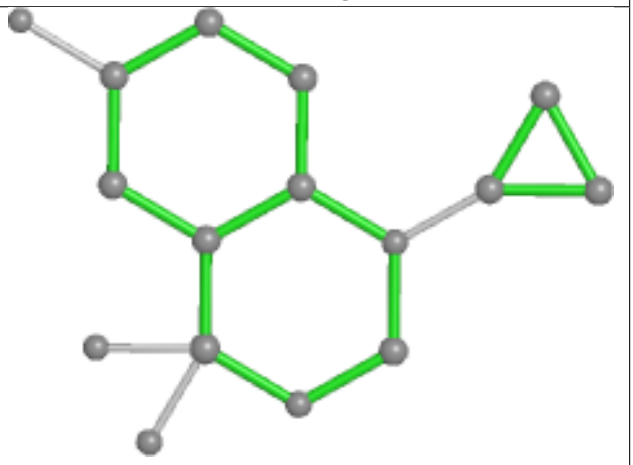
Bond lengths



Bond angles

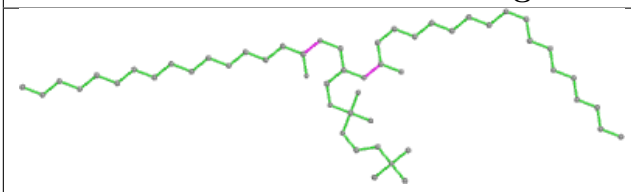


Torsions

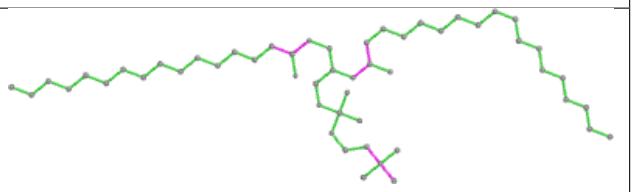


Rings

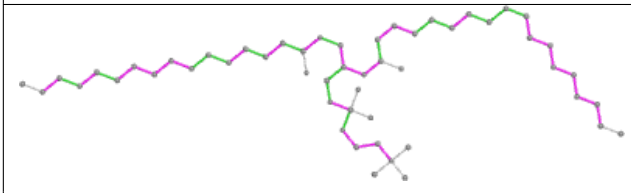
Ligand POV C 1009



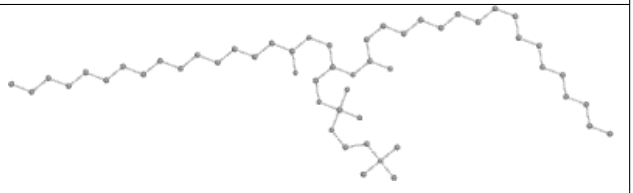
Bond lengths



Bond angles

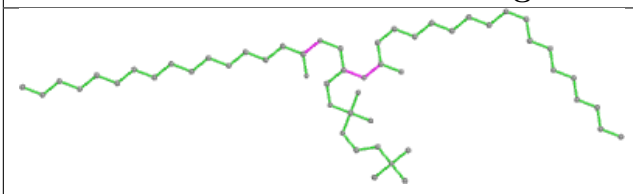


Torsions

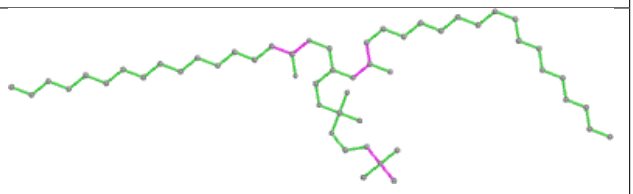


Rings

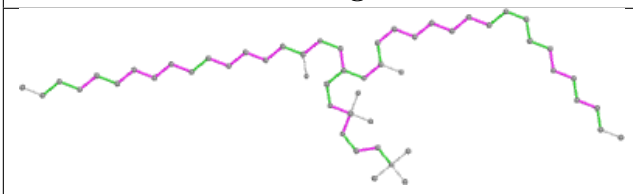
Ligand POV C 1005



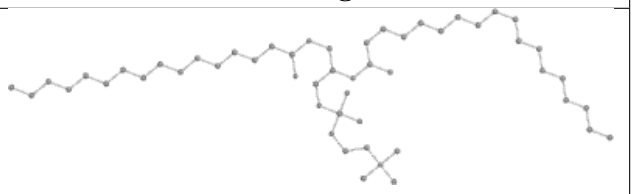
Bond lengths



Bond angles

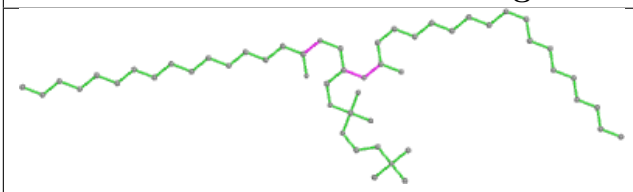


Torsions

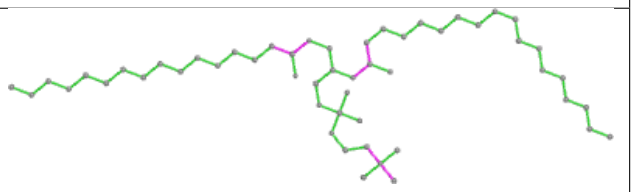


Rings

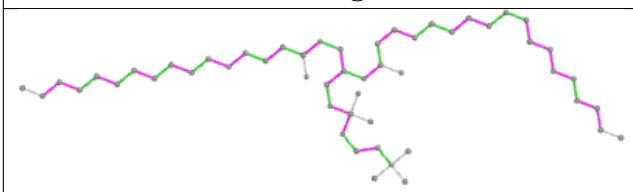
Ligand POV A 1007



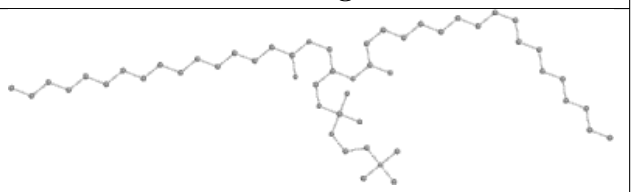
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

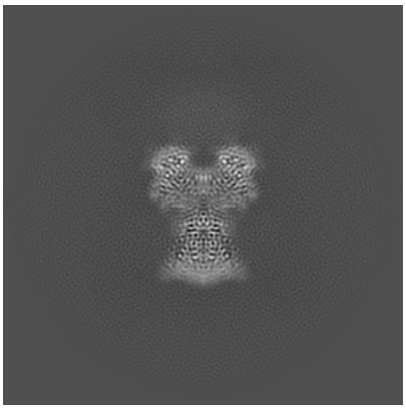
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-29519. These allow visual inspection of the internal detail of the map and identification of artifacts.

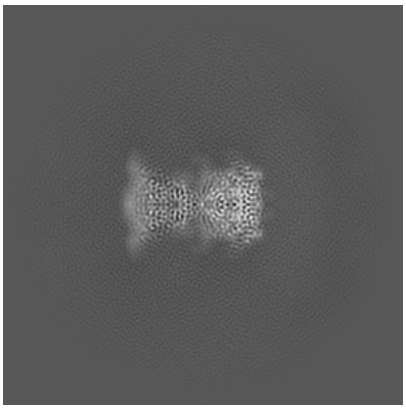
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

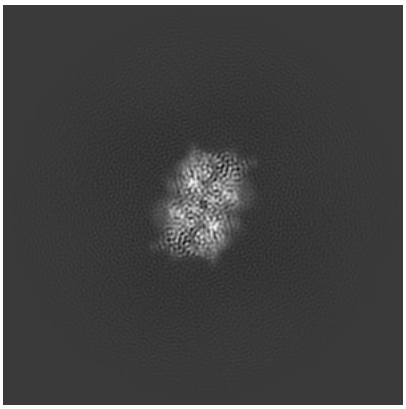
6.1.1 Primary map



X

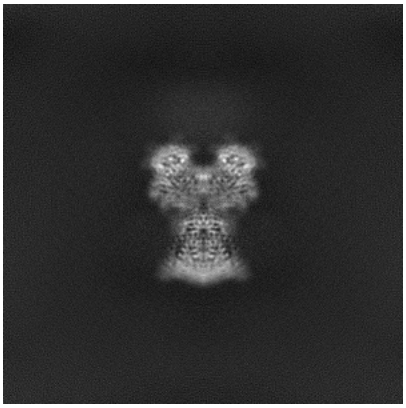


Y

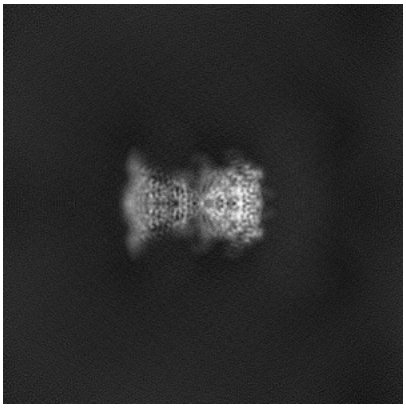


Z

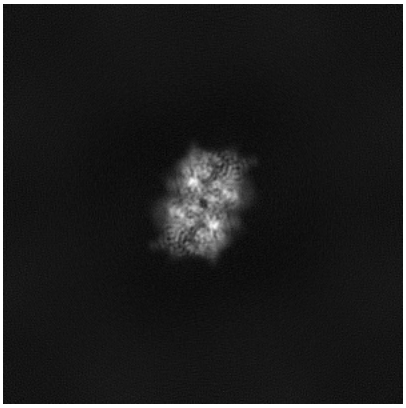
6.1.2 Raw map



X



Y

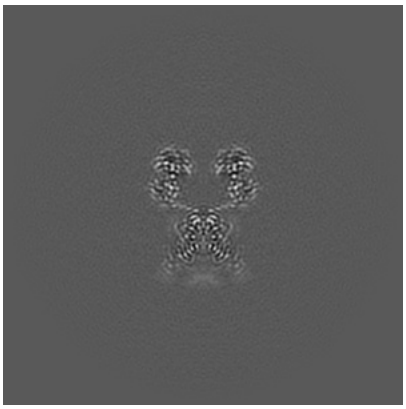


Z

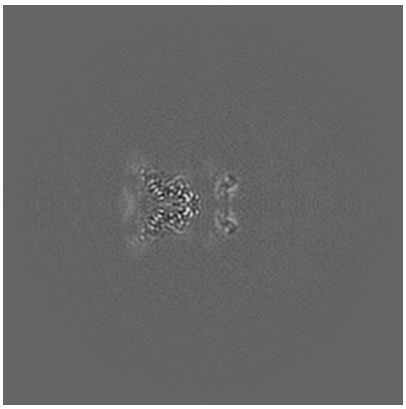
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

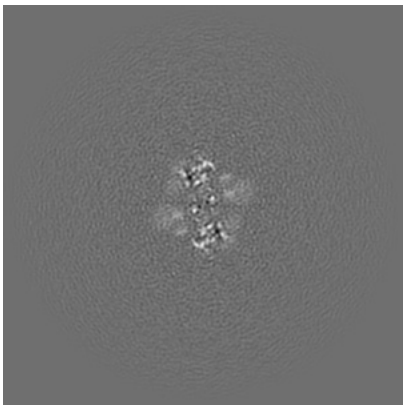
6.2.1 Primary map



X Index: 208

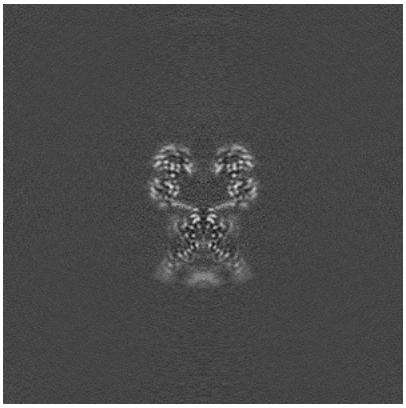


Y Index: 208

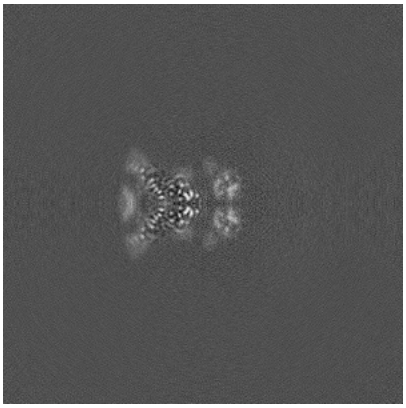


Z Index: 208

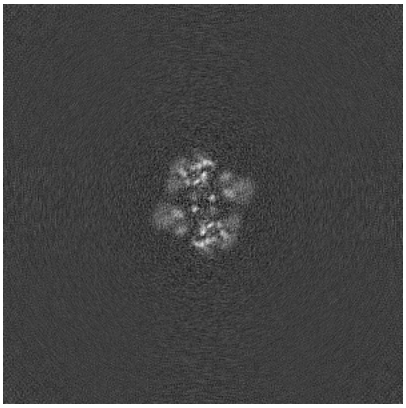
6.2.2 Raw map



X Index: 208



Y Index: 208

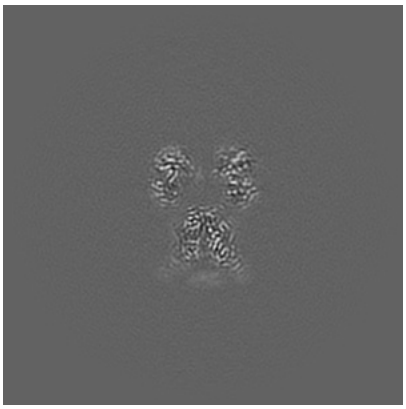


Z Index: 208

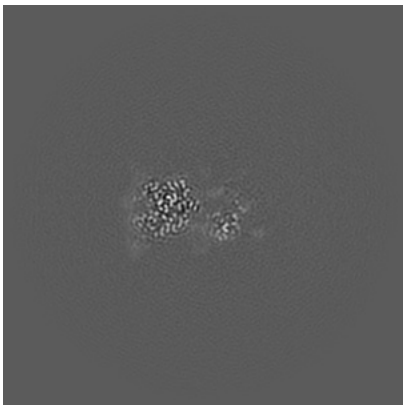
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

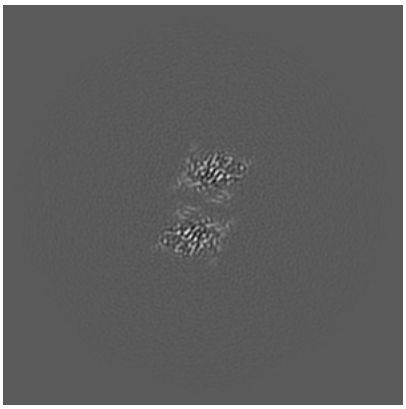
6.3.1 Primary map



X Index: 205

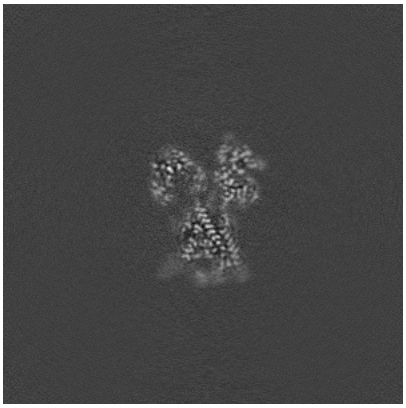


Y Index: 197

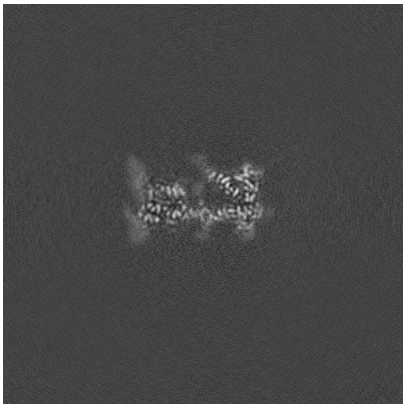


Z Index: 245

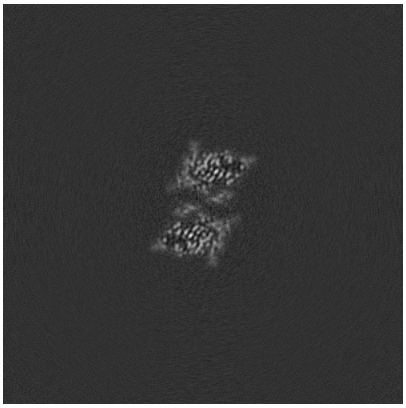
6.3.2 Raw map



X Index: 200



Y Index: 230

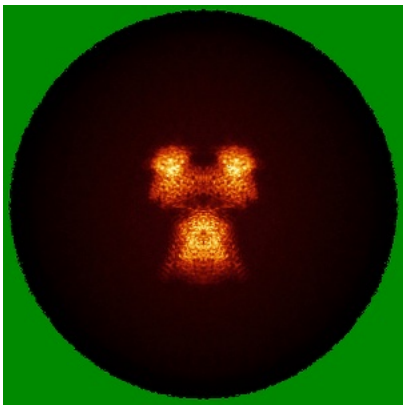


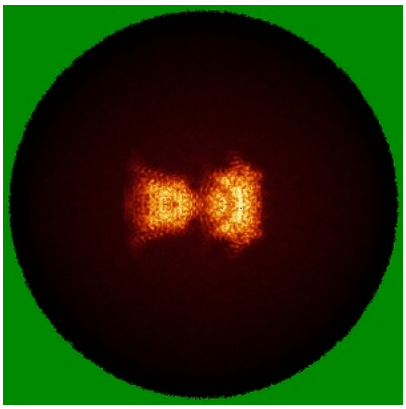
Z Index: 246

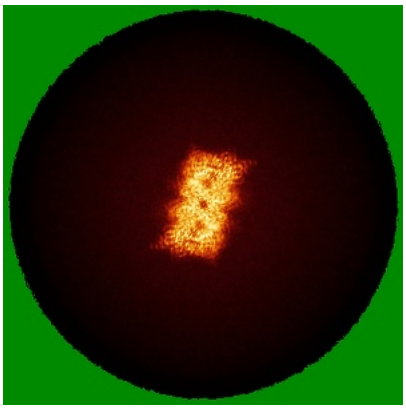
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

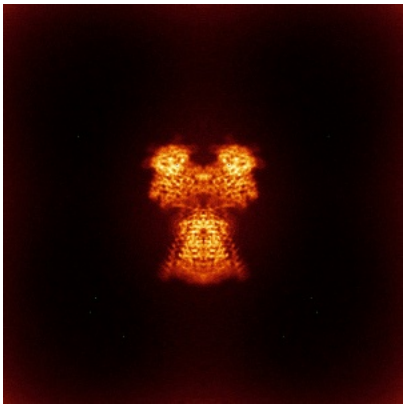
6.4.1 Primary map

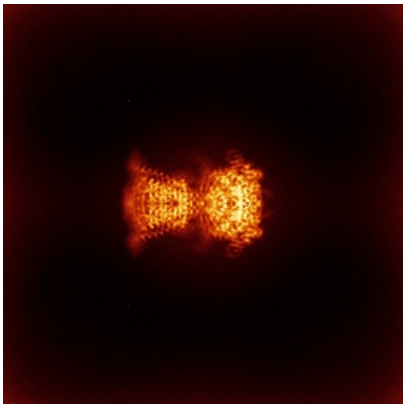

X

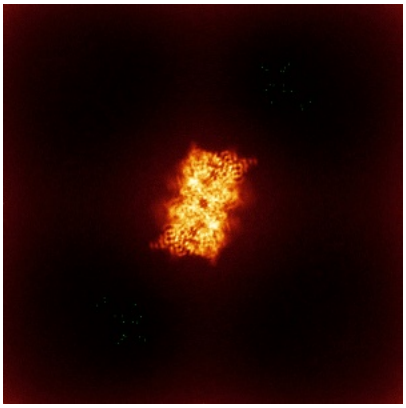

Y


Z

6.4.2 Raw map


X

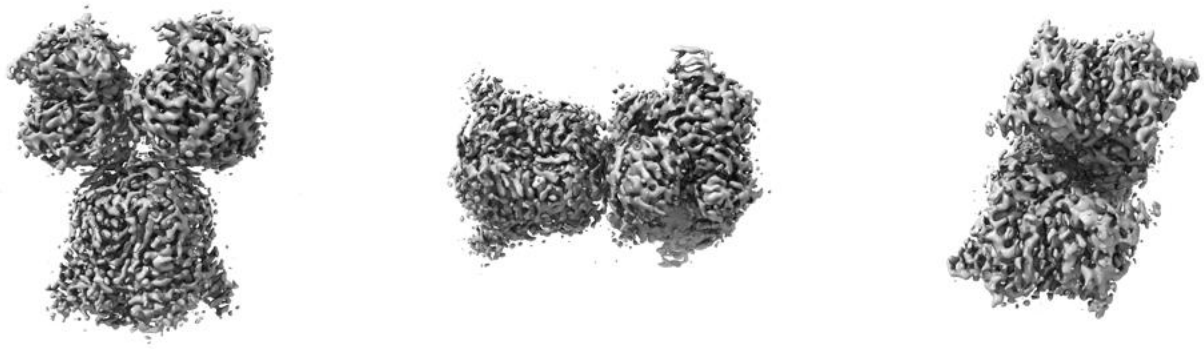

Y


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

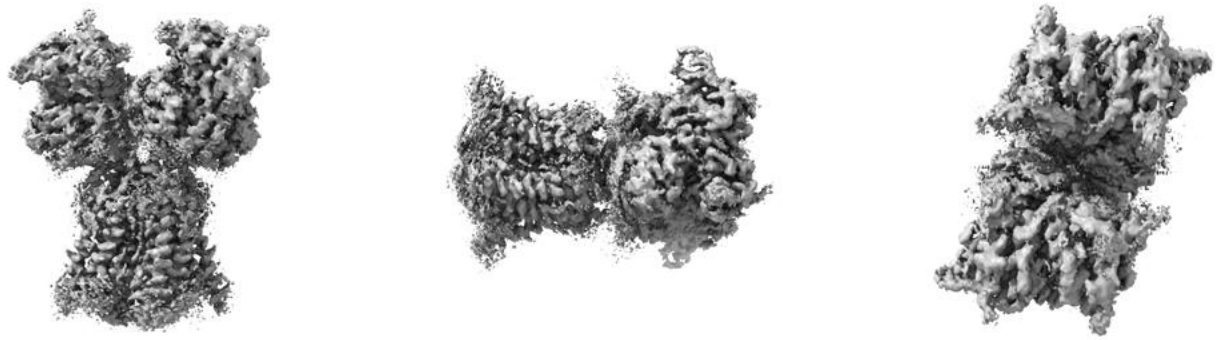
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

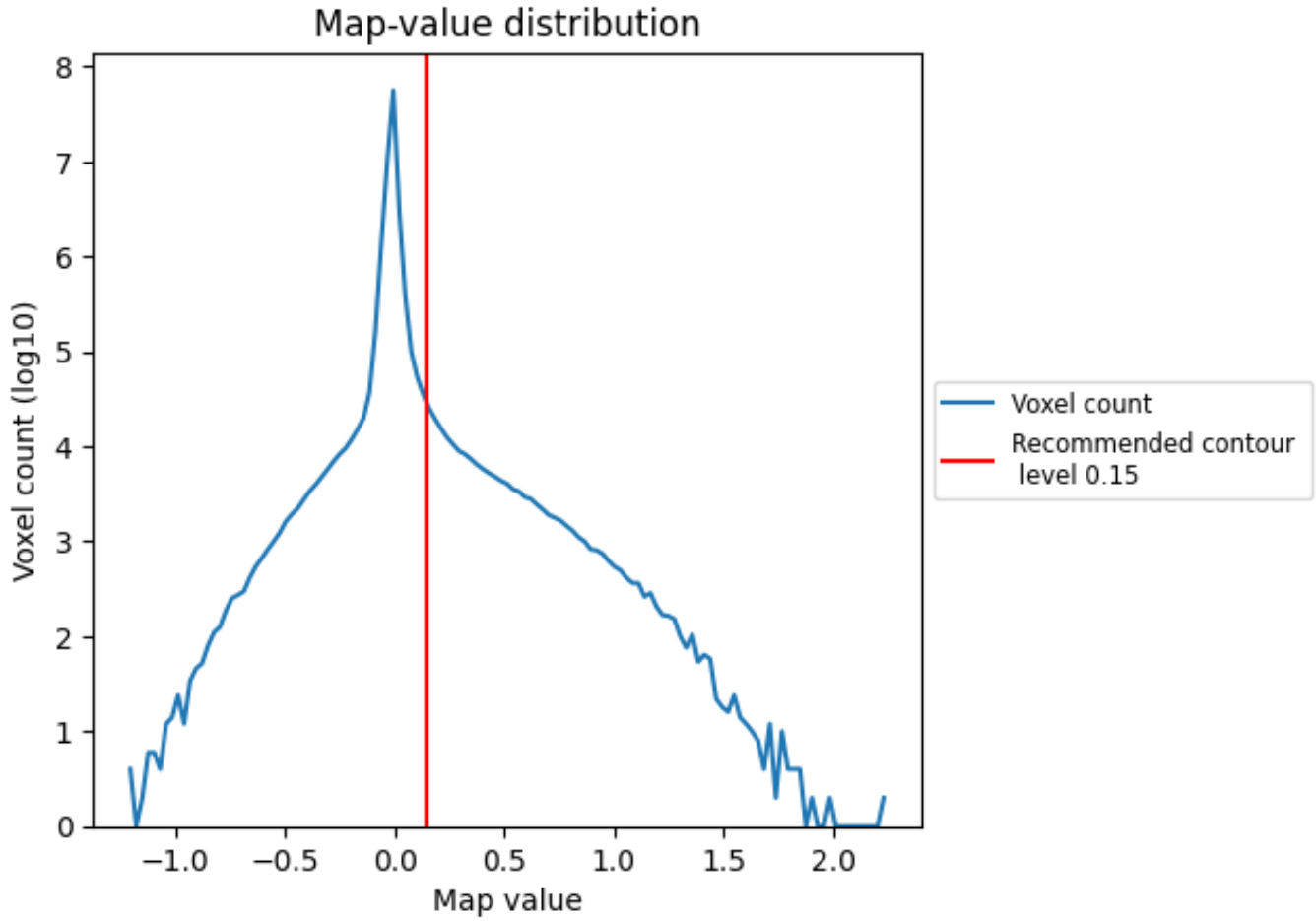
6.6 Mask visualisation (i)

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

7 Map analysis

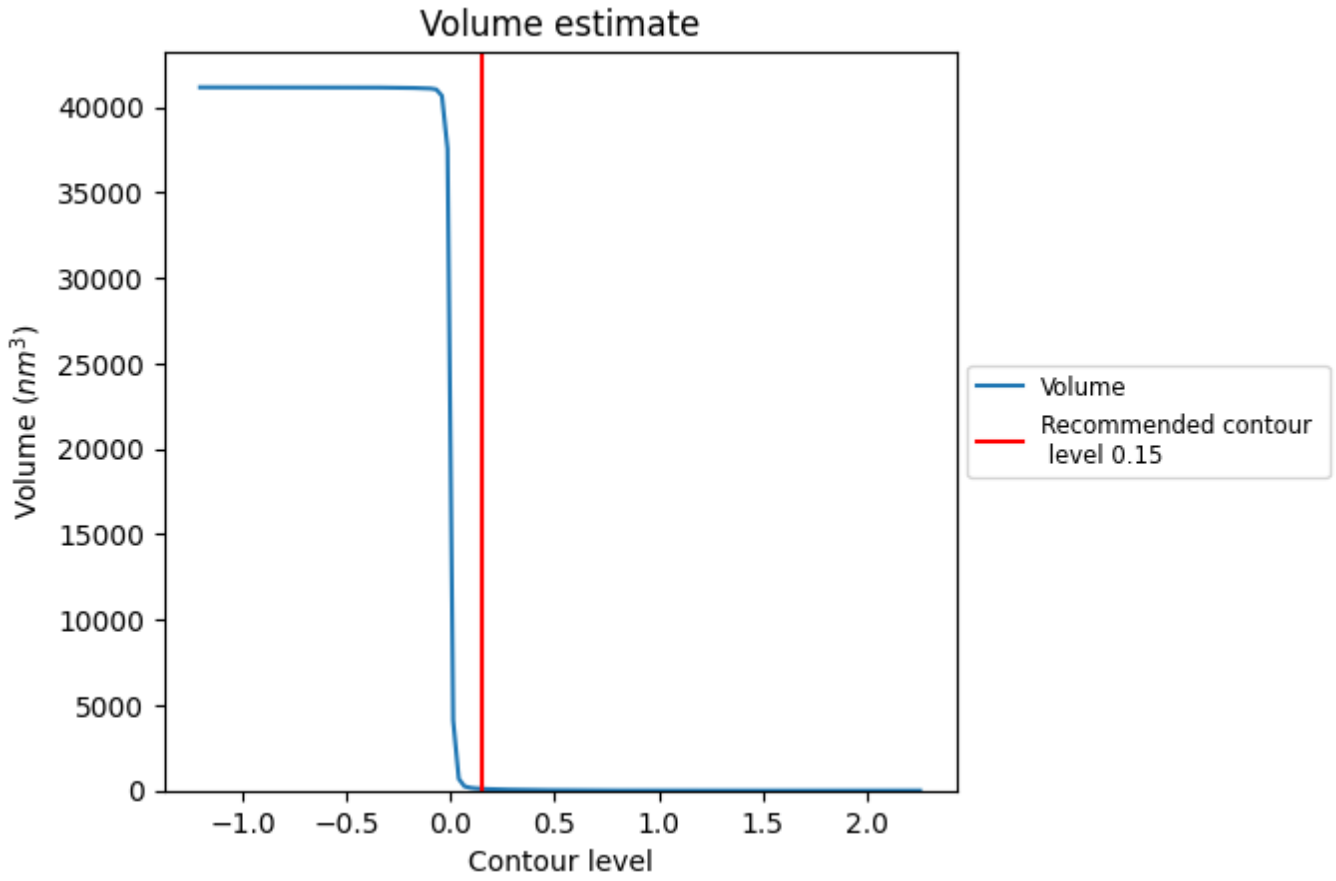
This section contains the results of statistical analysis of the map.

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.

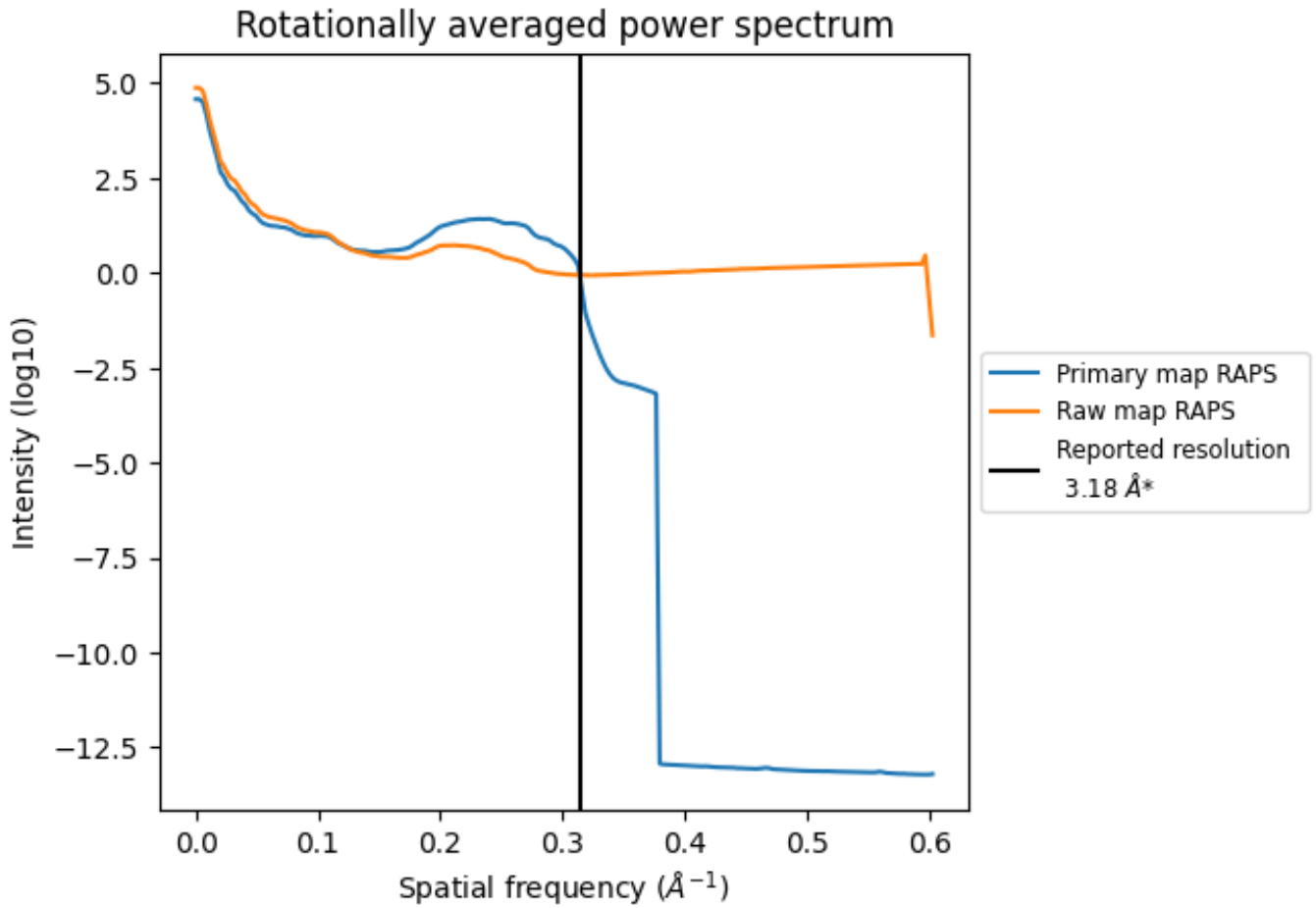
7.2 Volume estimate



The volume at the recommended contour level is 104 nm^3; this corresponds to an approximate mass of 94 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)

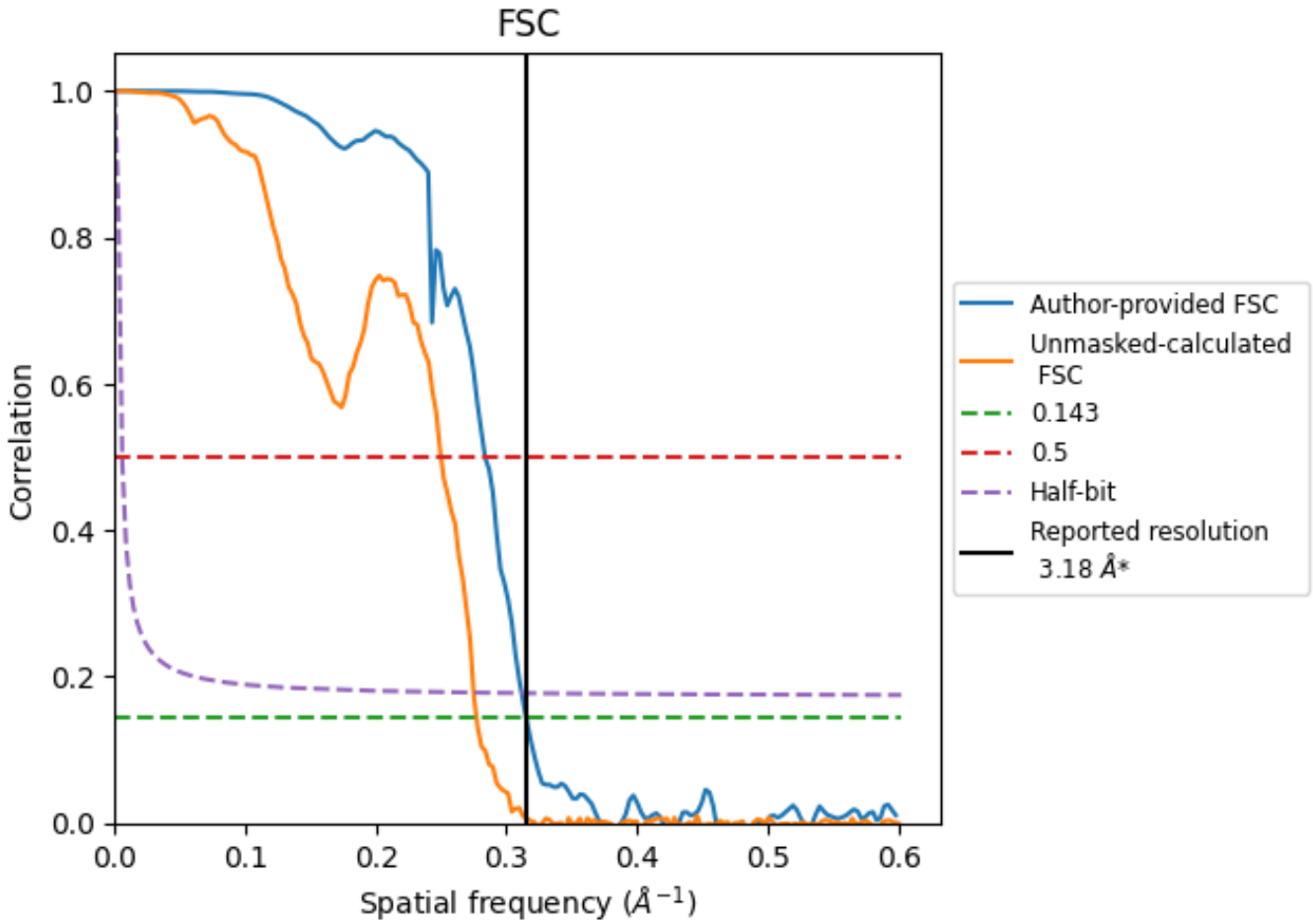


*Reported resolution corresponds to spatial frequency of 0.314 $Å^{-1}$

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 0.314 Å^{-1}

8.2 Resolution estimates (i)

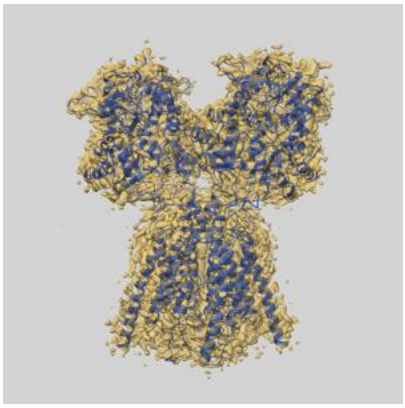
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.18	-	-
Author-provided FSC curve	3.17	3.53	3.21
Unmasked-calculated*	3.61	4.00	3.64

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.61 differs from the reported value 3.18 by more than 10 %

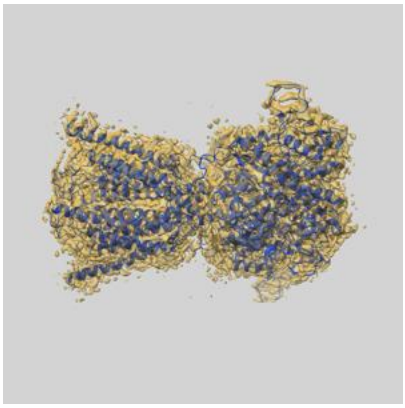
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-29519 and PDB model 8FWU. Per-residue inclusion information can be found in section 3 on page 10.

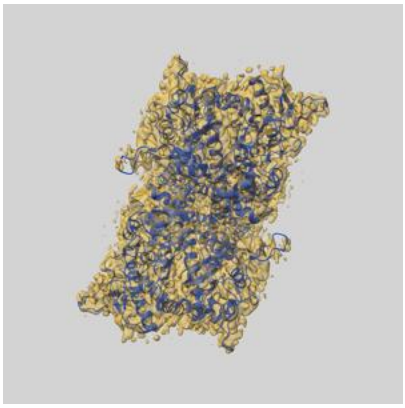
9.1 Map-model overlay



X



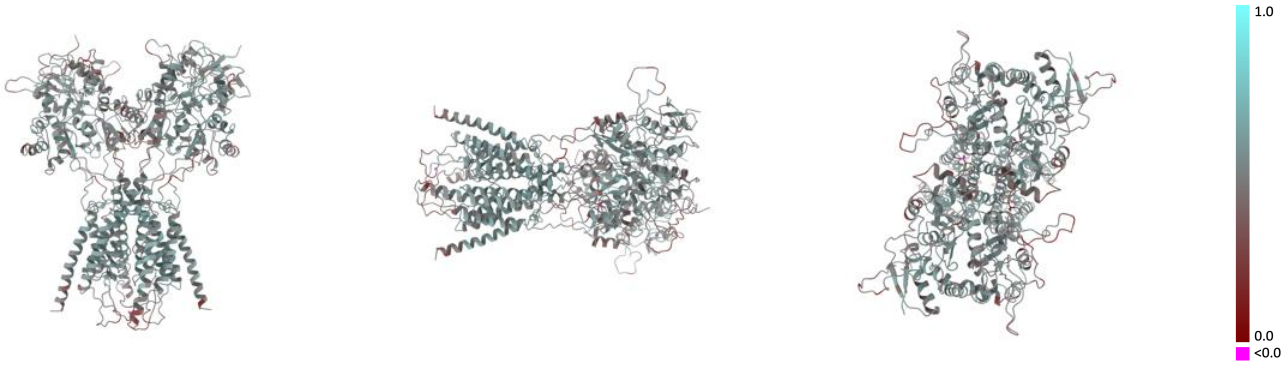
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.15 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.

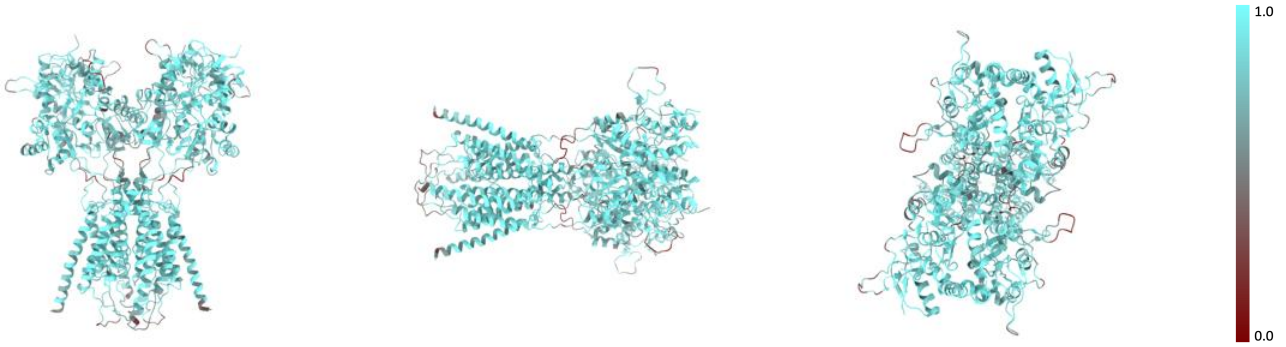
9.2 Q-score mapped to coordinate model (i)



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.

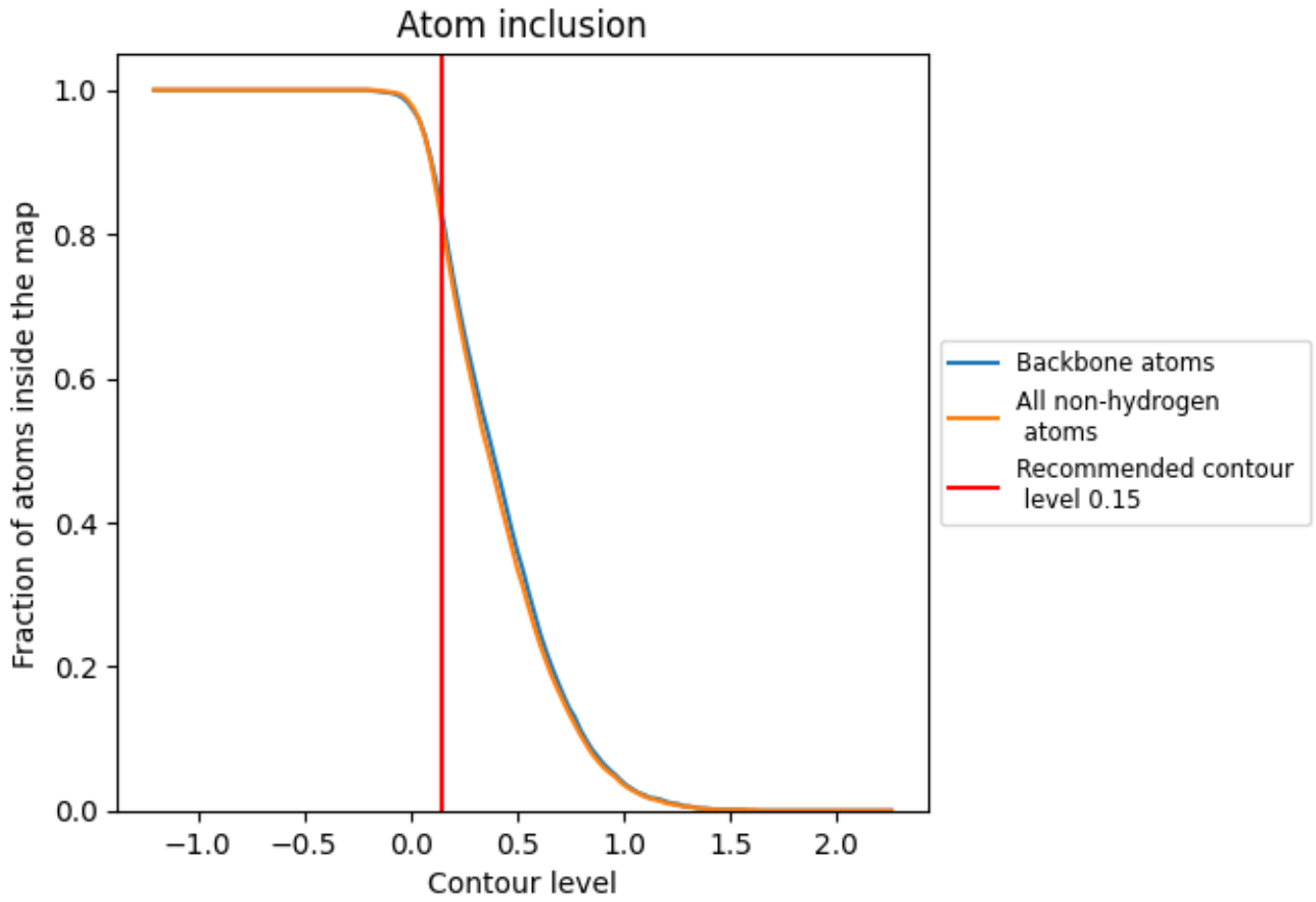
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.15).

9.4 Atom inclusion (i)



At the recommended contour level, 82% of all backbone atoms, 81% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8080	0.4990
A	0.8050	0.5030
B	0.8240	0.5010
C	0.8090	0.5050
D	0.8210	0.4940
E	0.5000	0.4180
F	0.7200	0.4420
G	0.2860	0.1570
H	0.4640	0.4230
I	0.7200	0.4420
J	0.2860	0.1450