Full wwPDB EM Validation Report

Mar 6, 2026 – 10:14 AM UTC

PDB ID	:	8FWS / pdb_00008fws
EMDB ID	:	EMD-29517
Title	:	Structure of the ligand-binding and transmembrane domains of kainate receptor GluK2 in complex with the positive allosteric modulator BPAM344
Authors	:	Gangwar, S.P.; Yen, L.Y.; Yelshanskaya, M.V.; Sobolevsky, A.I.
Deposited on	:	2023-01-23
Resolution	:	3.23 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

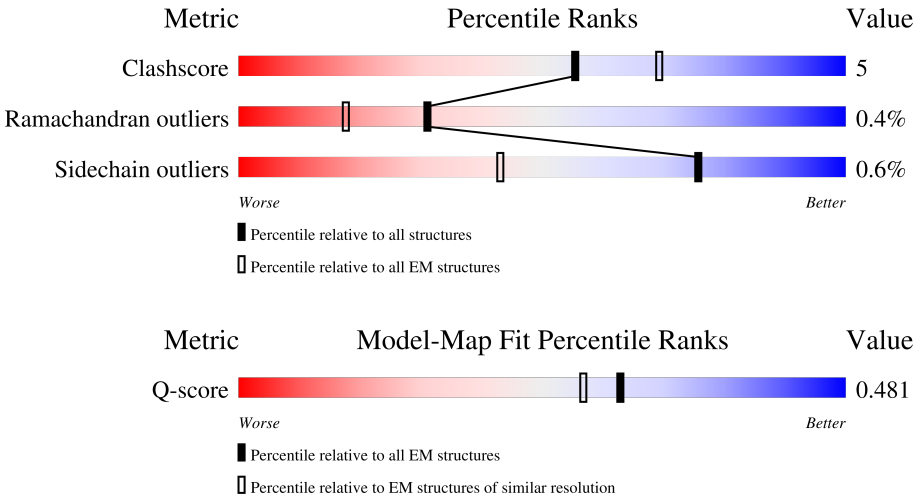
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.23 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.



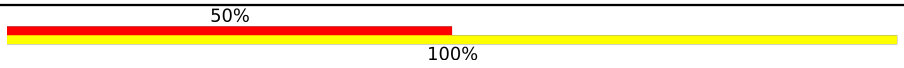
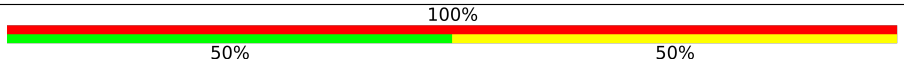
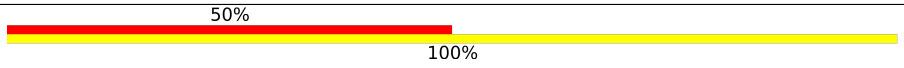
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14612 (2.73 - 3.73)

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	40% 6% 54%
1	B	908	40% 6% 54%
1	C	908	41% 5% 54%
1	D	908	40% 6% 54%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	E	2	
2	G	2	
2	H	2	
2	J	2	
3	F	4	
3	I	4	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 14416 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		

Continued on next page...

Continued from previous page...

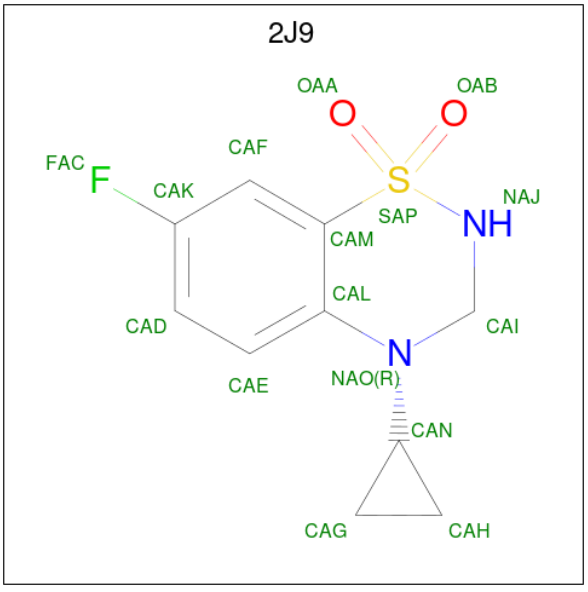
Mol	Chain	Residues	Atoms	AltConf	Trace
2	H	2	Total C N O 28 16 2 10	0	0
2	J	2	Total C N O 28 16 2 10	0	0

- 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 50 28 2 20	0	0
3	I	4	Total C N O 50 28 2 20	0	0

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



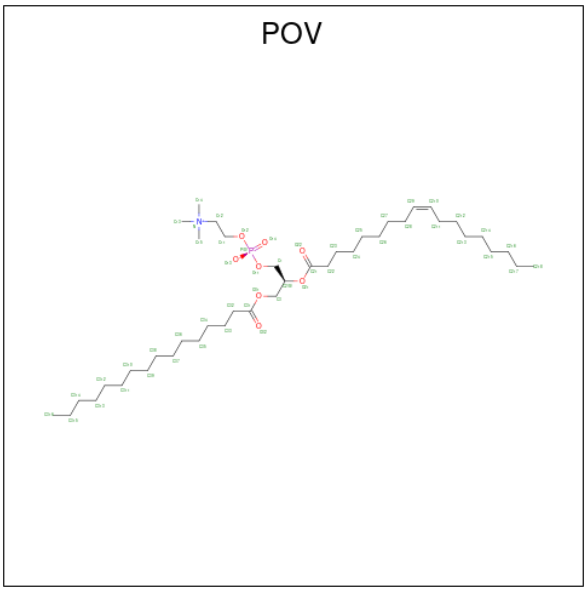
Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total C F N O S 16 10 1 2 2 1	0

Continued on next page...

Continued from previous page...

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

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



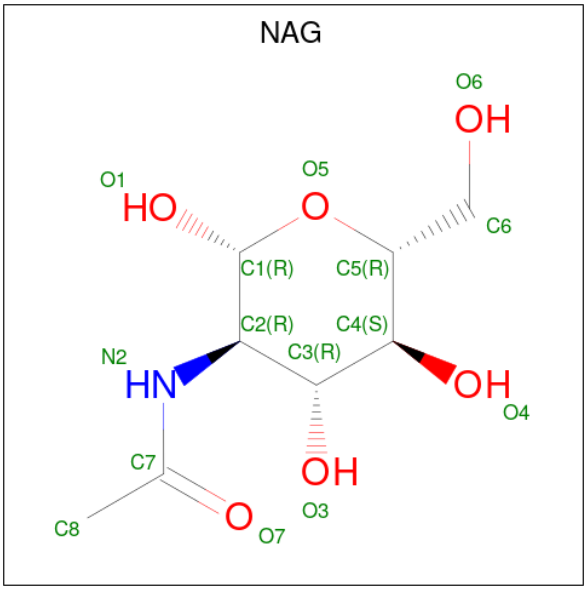
Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
5	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
5	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
5	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
5	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
5	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
5	B	1	Total	C	N	O	P	0
			52	42	1	8	1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

Continued on next page...

Continued from previous page...

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

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



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

- Molecule 7 is SODIUM ION (CCD ID: NA) (formula: Na) (labeled as "Ligand of Interest"

by depositor).

Mol	Chain	Residues	Atoms	AltConf
7	A	3	Total Na 3 3	0
7	B	1	Total Na 1 1	0
7	C	1	Total Na 1 1	0
7	D	1	Total Na 1 1	0

- Molecule 8 is CHLORIDE ION (CCD ID: 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

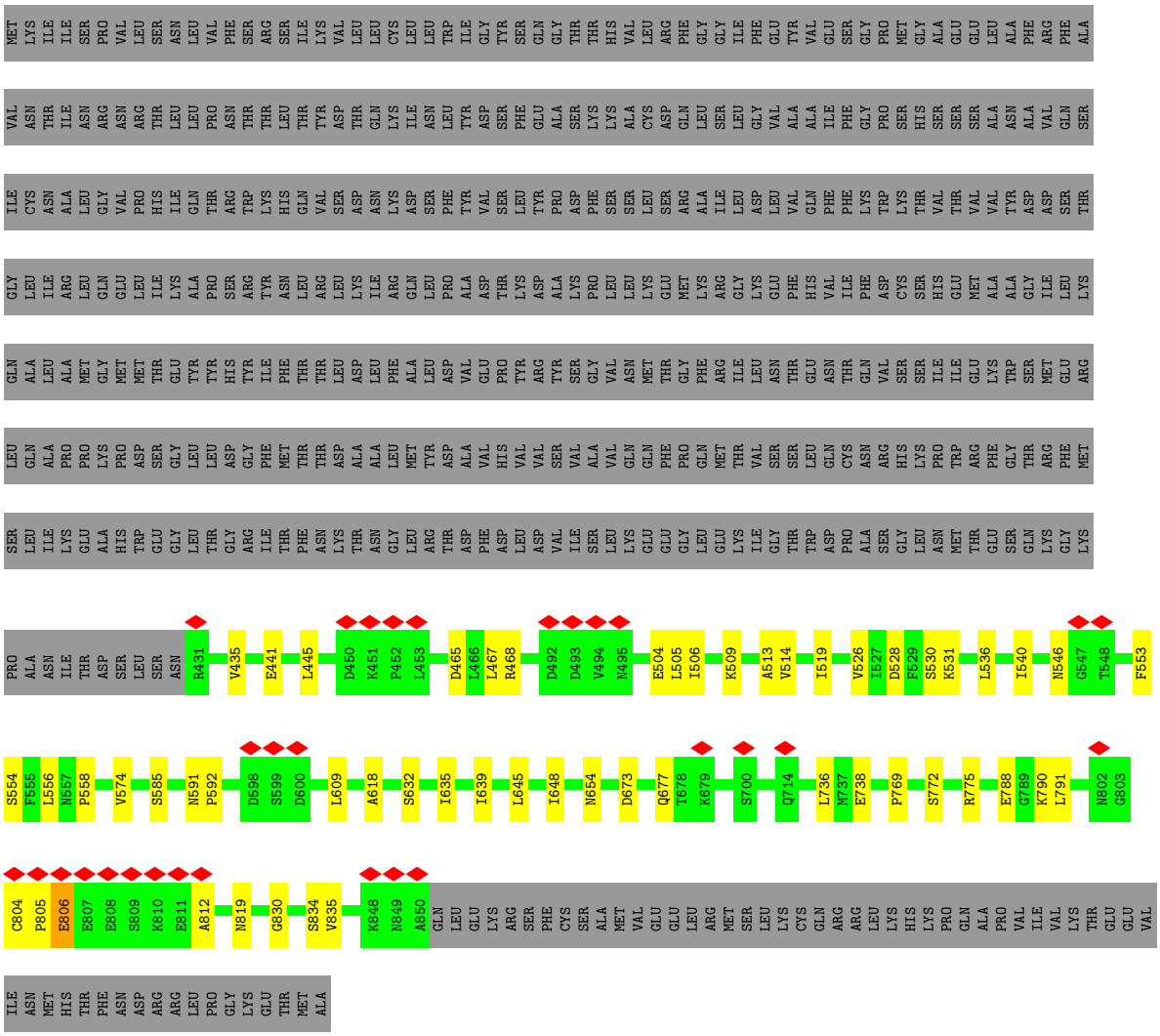
3 Residue-property plots (i)

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:

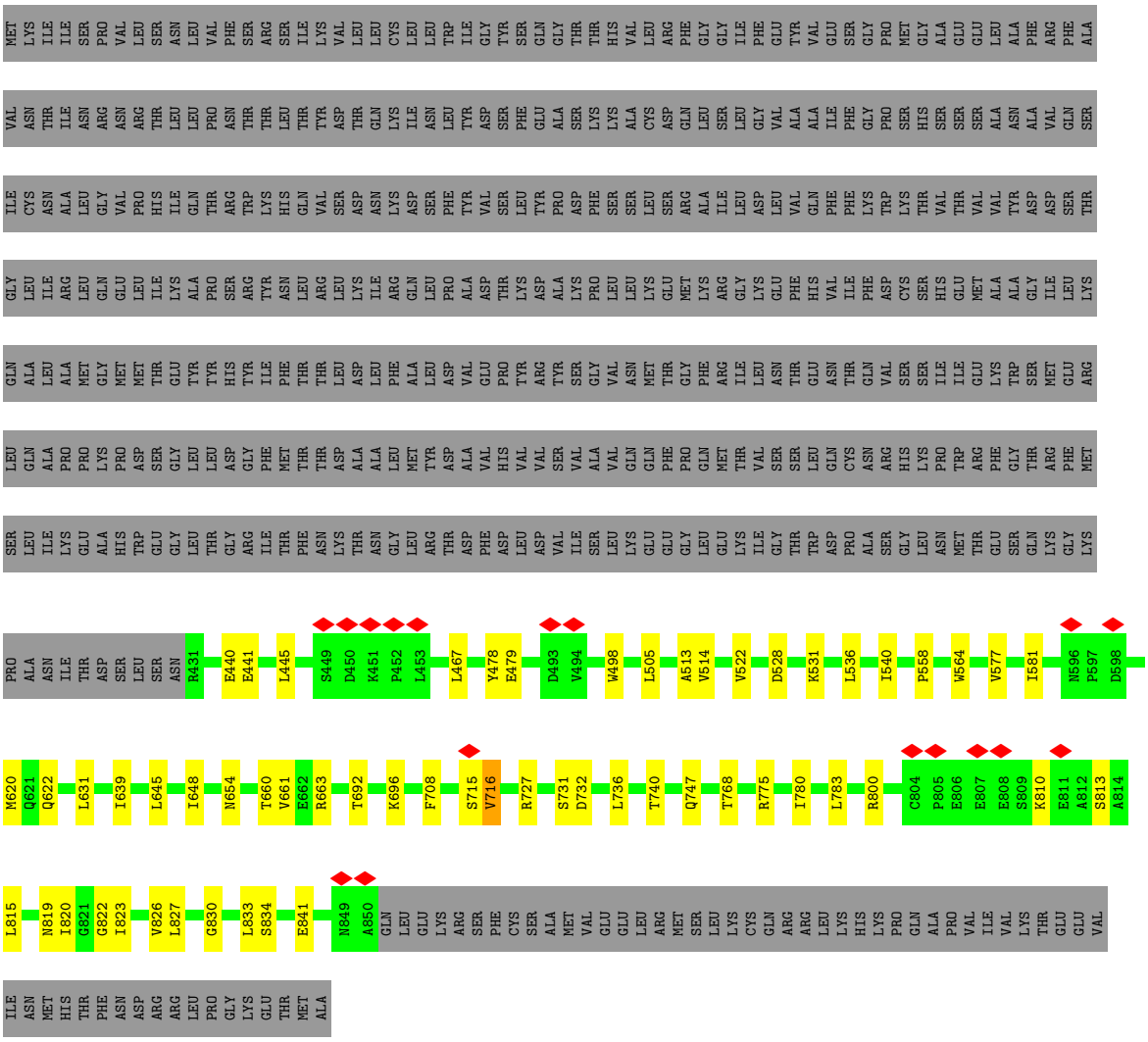




• Molecule 1: Glutamate receptor ionotropic, kainate 2

Chain B:

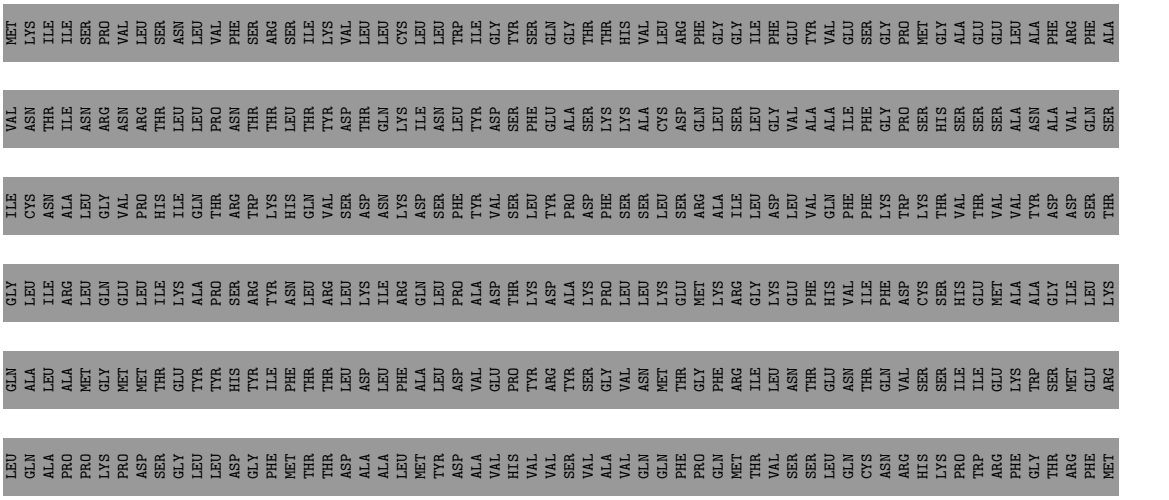


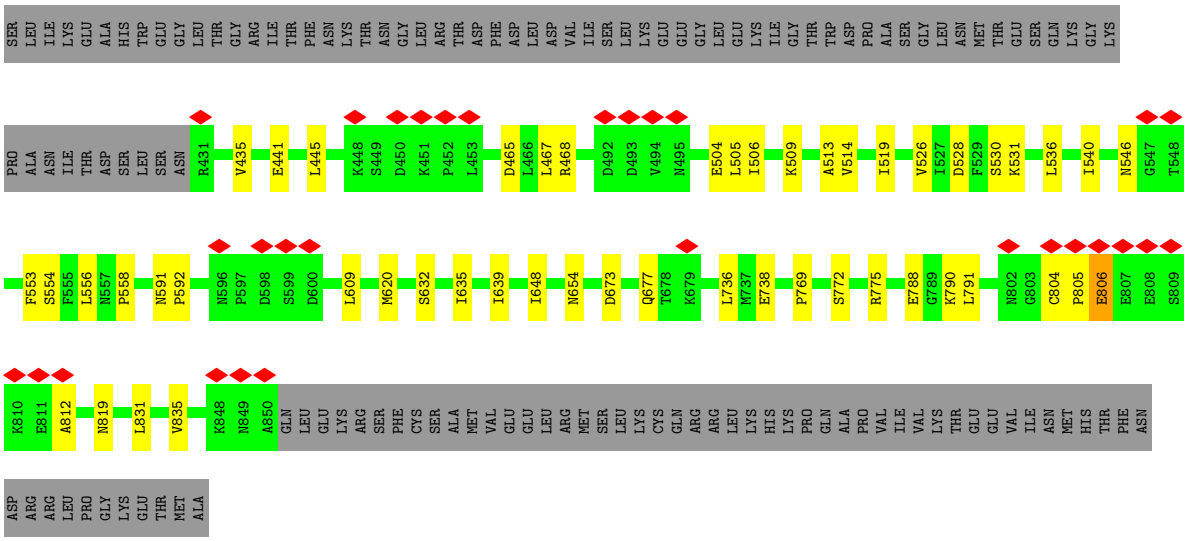


• Molecule 1: Glutamate receptor ionotropic, kainate 2

Chain C:



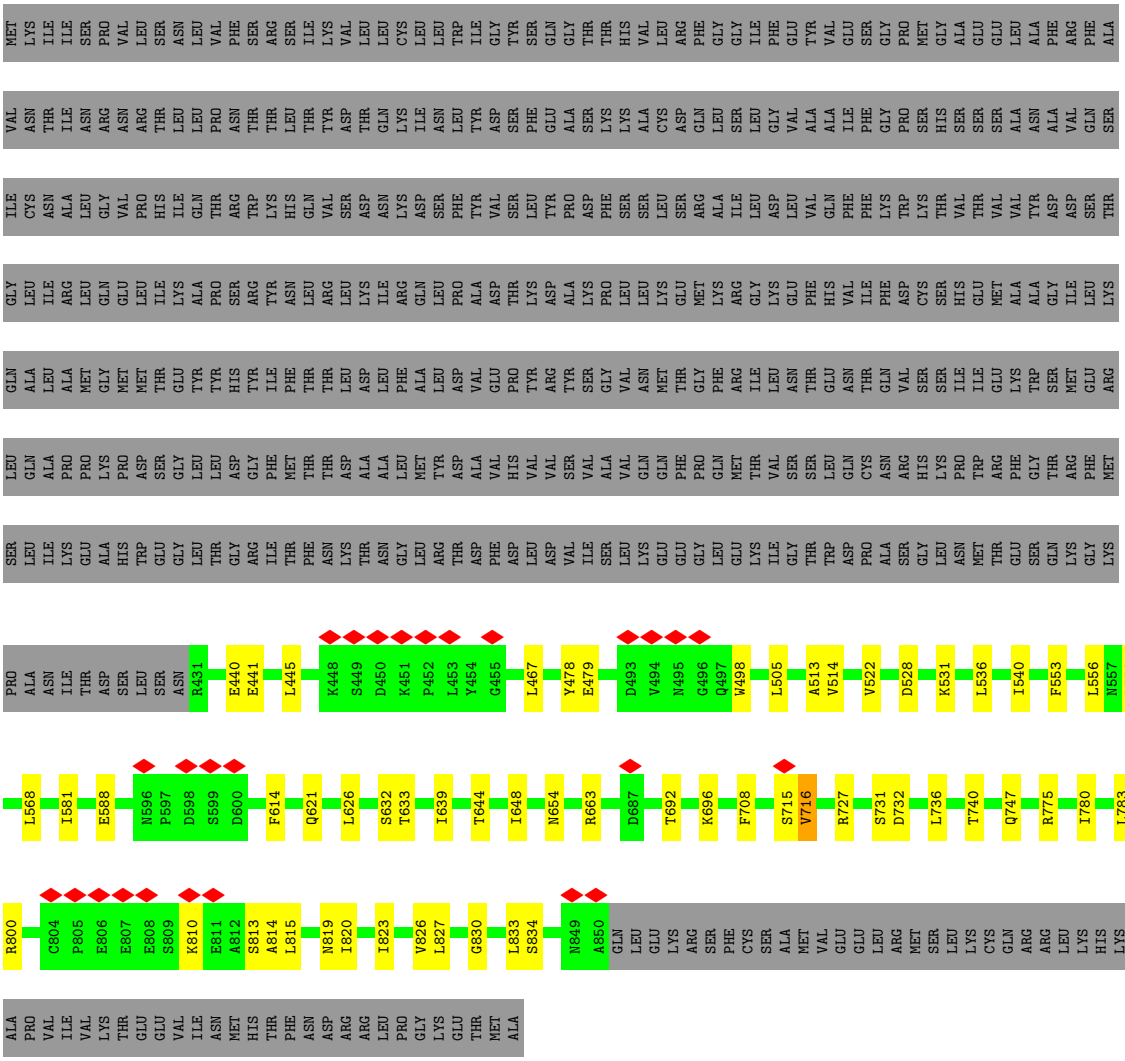




• Molecule 1: Glutamate receptor ionotropic, kainate 2

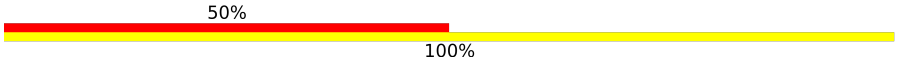
Chain D:





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

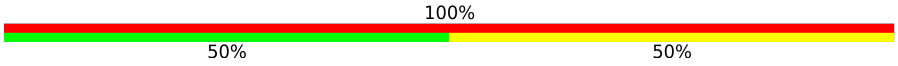
Chain E:





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

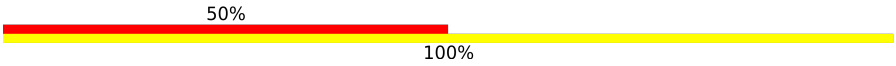
Chain G:





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

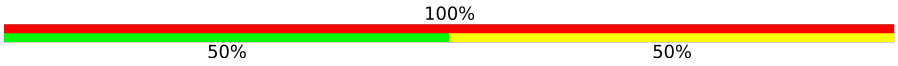
Chain H:





• 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:




NAG1
NAG2
BMA3
BMA4

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	125082	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	6.097	Depositor
Minimum map value	-3.915	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.085	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	355.2, 355.2, 355.2	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.925, 0.925, 0.925	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.29	0/3395	0.74	0/4600
1	B	0.29	1/3395 (0.0%)	0.72	0/4600
1	C	0.29	0/3395	0.74	0/4600
1	D	0.29	1/3395 (0.0%)	0.72	0/4600
All	All	0.29	2/13580 (0.0%)	0.73	0/18400

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	B	0	2
1	D	0	2
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	440	GLU	C-N	-5.09	1.23	1.33
1	B	440	GLU	C-N	-5.05	1.24	1.33

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	478	TYR	Peptide
1	B	716	VAL	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	D	478	TYR	Peptide
1	D	716	VAL	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	37	0
1	B	3318	0	3312	36	0
1	C	3318	0	3312	36	0
1	D	3318	0	3312	39	0
2	E	28	0	25	1	0
2	G	28	0	25	0	0
2	H	28	0	25	1	0
2	J	28	0	25	0	0
3	F	50	0	43	0	0
3	I	50	0	43	0	0
4	A	32	0	20	0	0
4	C	32	0	20	0	0
5	A	312	0	492	15	0
5	B	156	0	246	8	0
5	C	208	0	328	7	0
5	D	156	0	246	10	0
6	A	14	0	13	0	0
6	C	14	0	13	0	0
7	A	3	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
8	A	1	0	0	1	0
8	C	1	0	0	1	0
All	All	14416	0	14812	147	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 (147) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:531:LYS:NZ	8:C:1009:CL:CL	2.69	0.62
1:A:441:GLU:HG3	1:A:445:LEU:HD11	1.84	0.60
1:C:441:GLU:HG3	1:C:445:LEU:HD11	1.84	0.59
1:A:530:SER:O	1:D:531:LYS:NZ	2.36	0.58
1:C:639:ILE:HG13	1:D:830:GLY:HA3	1.85	0.57
1:B:528:ASP:HB3	1:B:775:ARG:HD3	1.86	0.57
1:C:505:LEU:HD21	1:C:513:ALA:HB2	1.85	0.56
1:A:505:LEU:HD21	1:A:513:ALA:HB2	1.85	0.56
1:D:528:ASP:HB3	1:D:775:ARG:HD3	1.86	0.56
1:B:815:LEU:HA	1:B:819:ASN:HD22	1.71	0.56
1:A:835:VAL:HG22	1:D:581:ILE:HD11	1.88	0.55
1:D:815:LEU:HA	1:D:819:ASN:HD22	1.71	0.55
1:B:692:THR:HG22	1:B:696:LYS:HE2	1.89	0.55
1:D:692:THR:HG22	1:D:696:LYS:HE2	1.89	0.55
1:A:528:ASP:HB3	1:A:775:ARG:HD2	1.90	0.55
1:A:812:ALA:HB3	1:D:663:ARG:HH22	1.72	0.55
1:C:528:ASP:HB3	1:C:775:ARG:HD2	1.89	0.55
1:B:531:LYS:NZ	1:C:530:SER:O	2.41	0.54
1:C:554:SER:OG	1:C:819:ASN:O	2.25	0.54
1:C:553:PHE:HB3	1:C:556:LEU:HD23	1.90	0.54
1:D:815:LEU:HD23	1:D:820:ILE:HG23	1.89	0.54
1:C:673:ASP:O	1:C:677:GLN:NE2	2.41	0.54
1:C:467:LEU:HD13	1:C:514:VAL:HG21	1.91	0.53
1:A:554:SER:OG	1:A:819:ASN:O	2.25	0.53
1:A:673:ASP:O	1:A:677:GLN:NE2	2.41	0.53
1:A:531:LYS:NZ	8:A:1013:CL:CL	2.79	0.53
5:C:1003:POV:H310	5:C:1004:POV:H31C	1.90	0.53
1:A:467:LEU:HD13	1:A:514:VAL:HG21	1.91	0.53
1:B:815:LEU:HD23	1:B:820:ILE:HG23	1.89	0.53
1:A:465:ASP:OD1	1:A:468:ARG:NH1	2.40	0.52
1:A:834:SER:OG	1:D:632:SER:O	2.27	0.52
1:A:618:ALA:O	1:B:622:GLN:NE2	2.42	0.52
1:A:553:PHE:HB3	1:A:556:LEU:HD23	1.90	0.52
1:C:465:ASP:OD1	1:C:468:ARG:NH1	2.40	0.52
1:D:823:ILE:HA	1:D:826:VAL:HG22	1.92	0.52
1:C:536:LEU:HD12	1:C:738:GLU:HB2	1.91	0.51
5:A:1003:POV:H37A	1:D:639:ILE:HD11	1.91	0.51
1:A:536:LEU:HD12	1:A:738:GLU:HB2	1.91	0.51
5:A:1007:POV:H37	1:B:833:LEU:HD23	1.91	0.51
1:B:823:ILE:HA	1:B:826:VAL:HG22	1.92	0.51
1:D:715:SER:O	1:D:727:ARG:NH2	2.41	0.51
1:C:635:ILE:HG23	5:D:1002:POV:H38A	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:564:TRP:HB3	5:D:1001:POV:H25	1.92	0.51
5:D:1001:POV:H33A	5:D:1002:POV:H32	1.93	0.51
1:D:833:LEU:HD23	5:D:1002:POV:H37	1.93	0.51
1:A:609:LEU:HD13	5:A:1005:POV:H310	1.93	0.50
1:A:435:VAL:HG21	1:A:467:LEU:HD21	1.94	0.49
1:B:631:LEU:HD13	1:C:609:LEU:HD11	1.93	0.49
1:A:645:LEU:HD11	1:B:620:MET:HA	1.94	0.49
1:B:715:SER:O	1:B:727:ARG:NH2	2.41	0.49
1:A:558:PRO:O	1:A:654:ASN:ND2	2.41	0.49
1:C:788:GLU:HG3	1:C:790:LYS:HG2	1.95	0.49
1:A:635:ILE:HG23	5:A:1007:POV:H38A	1.94	0.49
1:C:654:ASN:HD21	1:D:814:ALA:HA	1.77	0.49
1:B:577:VAL:HG21	1:C:831:LEU:HD23	1.95	0.48
1:C:632:SER:O	1:D:834:SER:OG	2.31	0.48
1:A:788:GLU:HG3	1:A:790:LYS:HG2	1.95	0.48
1:B:731:SER:OG	1:B:732:ASP:N	2.45	0.48
5:A:1007:POV:H21E	5:A:1007:POV:H38	1.96	0.48
1:C:435:VAL:HG21	1:C:467:LEU:HD21	1.94	0.48
1:D:731:SER:OG	1:D:732:ASP:N	2.45	0.48
1:B:467:LEU:HD13	1:B:514:VAL:HG21	1.96	0.48
5:A:1004:POV:H312	5:A:1004:POV:H39A	1.67	0.47
5:C:1005:POV:H312	5:C:1005:POV:H39A	1.66	0.47
1:A:504:GLU:HG2	1:A:509:LYS:HE2	1.96	0.47
1:B:810:LYS:NZ	1:B:813:SER:OG	2.47	0.47
1:D:467:LEU:HD13	1:D:514:VAL:HG21	1.96	0.47
1:A:830:GLY:HA3	1:D:639:ILE:HG13	1.96	0.47
1:B:645:LEU:HD11	1:C:620:MET:HA	1.97	0.47
1:D:558:PRO:HB3	1:D:654:ASN:HB3	1.97	0.47
5:D:1001:POV:H37A	5:D:1002:POV:H21A	1.97	0.47
1:A:519:ILE:HG22	1:D:783:LEU:HD21	1.95	0.47
1:B:558:PRO:HB3	1:B:654:ASN:HB3	1.98	0.46
1:B:708:PHE:HE2	1:B:716:VAL:HG21	1.80	0.46
5:D:1002:POV:H38	5:D:1002:POV:H21E	1.97	0.46
5:A:1007:POV:H32	5:B:1001:POV:H33A	1.97	0.46
1:D:708:PHE:HE2	1:D:716:VAL:HG21	1.80	0.46
5:A:1004:POV:H25A	5:A:1004:POV:H28A	1.62	0.46
1:D:810:LYS:NZ	1:D:813:SER:OG	2.47	0.46
5:A:1003:POV:H39A	1:D:639:ILE:HD11	1.97	0.46
1:C:506:ILE:HD12	1:C:526:VAL:HB	1.98	0.46
5:A:1007:POV:H21A	5:B:1001:POV:H37A	1.98	0.46
1:C:504:GLU:HG2	1:C:509:LYS:HE2	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:558:PRO:O	1:C:654:ASN:ND2	2.41	0.45
1:C:546:ASN:HB3	2:H:1:NAG:HN2	1.81	0.45
1:A:645:LEU:HD13	5:B:1001:POV:H21J	1.97	0.45
1:B:498:TRP:HH2	1:B:522:VAL:HG12	1.81	0.45
1:D:568:LEU:HG	5:D:1001:POV:H31G	1.98	0.45
1:A:804:CYS:O	1:A:806:GLU:N	2.45	0.45
1:B:581:ILE:HD11	1:C:835:VAL:HG22	1.98	0.45
1:A:506:ILE:HD12	1:A:526:VAL:HB	1.98	0.45
5:B:1003:POV:H310	1:C:609:LEU:HD13	1.98	0.45
1:C:639:ILE:HG22	1:D:827:LEU:HD12	1.98	0.45
1:D:441:GLU:HG3	1:D:445:LEU:HD11	1.99	0.45
5:A:1002:POV:H310	5:A:1003:POV:H31C	1.99	0.44
5:A:1008:POV:H28	5:A:1008:POV:H211	1.78	0.44
1:D:498:TRP:HH2	1:D:522:VAL:HG12	1.81	0.44
1:A:585:SER:OG	1:B:841:GLU:OE2	2.31	0.44
5:C:1005:POV:H37A	5:C:1005:POV:H34	1.59	0.43
5:A:1008:POV:H215	5:A:1008:POV:H212	1.84	0.43
1:B:528:ASP:O	1:B:768:THR:OG1	2.35	0.43
1:C:591:ASN:HD22	1:C:592:PRO:HD2	1.84	0.43
1:D:556:LEU:HD21	5:D:1001:POV:H24A	2.00	0.43
1:A:639:ILE:HG13	1:B:830:GLY:HA3	2.00	0.43
5:A:1005:POV:H36A	5:A:1005:POV:H39A	1.91	0.43
1:B:441:GLU:HG3	1:B:445:LEU:HD11	1.99	0.43
1:B:663:ARG:HH22	1:C:812:ALA:HB3	1.83	0.43
1:A:769:PRO:HG2	1:A:772:SER:HB2	2.00	0.43
1:B:540:ILE:HG12	1:B:736:LEU:HD23	2.01	0.43
1:D:540:ILE:HG12	1:D:736:LEU:HD23	2.01	0.42
1:B:536:LEU:HB3	1:B:740:THR:HG23	2.00	0.42
1:A:591:ASN:HD22	1:A:592:PRO:HD2	1.84	0.42
1:B:564:TRP:HB3	5:B:1001:POV:H25	2.00	0.42
1:C:769:PRO:HG2	1:C:772:SER:HB2	2.00	0.42
1:D:505:LEU:HD21	1:D:513:ALA:HB2	2.02	0.42
1:A:558:PRO:HB3	1:A:654:ASN:HB3	2.01	0.42
5:C:1005:POV:H28A	5:C:1005:POV:H25A	1.74	0.42
1:A:546:ASN:HB3	2:E:1:NAG:HN2	1.84	0.42
1:D:536:LEU:HB3	1:D:740:THR:HG23	2.01	0.42
1:B:820:ILE:O	1:B:822:GLY:N	2.49	0.42
5:B:1002:POV:H33	5:B:1002:POV:H36A	1.89	0.42
1:C:553:PHE:HE2	5:C:1004:POV:H1	1.84	0.42
1:C:558:PRO:HB3	1:C:654:ASN:HB3	2.02	0.41
1:B:783:LEU:HD21	1:C:519:ILE:HG22	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:804:CYS:O	1:C:806:GLU:N	2.45	0.41
1:A:632:SER:O	1:B:834:SER:OG	2.36	0.41
1:B:505:LEU:HD21	1:B:513:ALA:HB2	2.02	0.41
5:B:1001:POV:H31D	5:B:1001:POV:H31A	1.96	0.41
1:C:540:ILE:HG12	1:C:736:LEU:HD23	2.02	0.41
5:C:1007:POV:H211	5:C:1007:POV:H28	1.79	0.41
5:C:1007:POV:H21D	1:D:833:LEU:HD11	2.02	0.41
1:B:660:THR:HG23	1:B:661:VAL:HG23	2.03	0.41
1:C:639:ILE:HD13	1:C:639:ILE:HA	1.95	0.41
1:D:553:PHE:HB2	5:D:1001:POV:H11A	2.02	0.41
1:B:747:GLN:HG2	1:B:800:ARG:HA	2.03	0.41
5:D:1001:POV:H26	5:D:1001:POV:H36	2.02	0.41
1:B:639:ILE:HD13	1:B:639:ILE:HA	1.95	0.41
1:D:639:ILE:HD13	1:D:639:ILE:HA	1.95	0.41
1:A:574:VAL:HG21	1:B:827:LEU:HD11	2.02	0.40
1:D:614:PHE:HB2	1:D:626:LEU:HD12	2.03	0.40
1:D:747:GLN:HG2	1:D:800:ARG:HA	2.03	0.40
1:A:639:ILE:HD13	1:A:639:ILE:HA	1.95	0.40
1:D:621:GLN:HE21	1:D:644:THR:HG22	1.86	0.40
1:A:540:ILE:HG12	1:A:736:LEU:HD23	2.02	0.40
5:A:1004:POV:H37A	5:A:1004:POV:H34	1.85	0.40
5:B:1001:POV:H21D	5:B:1001:POV:H217	1.89	0.40
1:D:588:GLU:OE2	1:D:633:THR:OG1	2.39	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%)	385 (92%)	31 (7%)	2 (0%)	24	56
1	B	418/908 (46%)	377 (90%)	40 (10%)	1 (0%)	43	72

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	418/908 (46%)	385 (92%)	31 (7%)	2 (0%)	24 56
1	D	418/908 (46%)	377 (90%)	40 (10%)	1 (0%)	43 72
All	All	1672/3632 (46%)	1524 (91%)	142 (8%)	6 (0%)	31 60

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	479	GLU
1	D	479	GLU
1	A	806	GLU
1	C	806	GLU
1	A	805	PRO
1	C	805	PRO

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%)	360 (99%)	2 (1%)	78 83
1	B	362/794 (46%)	360 (99%)	2 (1%)	78 83
1	C	362/794 (46%)	360 (99%)	2 (1%)	78 83
1	D	362/794 (46%)	360 (99%)	2 (1%)	78 83
All	All	1448/3176 (46%)	1440 (99%)	8 (1%)	76 83

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	648	ILE
1	A	791	LEU
1	B	648	ILE
1	B	780	ILE
1	C	648	ILE
1	C	791	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	648	ILE
1	D	780	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	456	ASN
1	A	497	GLN
1	A	508	HIS
1	A	591	ASN
1	A	596	ASN
1	A	604	ASN
1	A	621	GLN
1	A	677	GLN
1	A	721	ASN
1	A	792	HIS
1	A	849	ASN
1	B	495	ASN
1	B	604	ASN
1	B	621	GLN
1	B	754	GLN
1	B	786	GLN
1	B	792	HIS
1	B	802	ASN
1	B	819	ASN
1	C	456	ASN
1	C	497	GLN
1	C	508	HIS
1	C	591	ASN
1	C	596	ASN
1	C	621	GLN
1	C	677	GLN
1	C	786	GLN
1	C	792	HIS
1	C	849	ASN
1	D	495	ASN
1	D	604	ASN
1	D	621	GLN
1	D	754	GLN
1	D	786	GLN
1	D	792	HIS
1	D	819	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	0.52	0	17,19,21	0.69	0
2	NAG	E	2	2	14,14,15	0.37	0	17,19,21	0.63	1 (5%)
3	NAG	F	1	3,1	14,14,15	0.39	0	17,19,21	0.44	0
3	NAG	F	2	3	14,14,15	0.61	0	17,19,21	0.77	0
3	BMA	F	3	3	11,11,12	1.23	3 (27%)	15,15,17	1.83	3 (20%)
3	BMA	F	4	3	11,11,12	0.82	0	15,15,17	1.03	1 (6%)
2	NAG	G	1	2,1	14,14,15	1.39	2 (14%)	17,19,21	1.83	2 (11%)
2	NAG	G	2	2	14,14,15	0.58	0	17,19,21	0.37	0
2	NAG	H	1	2,1	14,14,15	0.56	0	17,19,21	0.68	0
2	NAG	H	2	2	14,14,15	0.37	0	17,19,21	0.59	1 (5%)
3	NAG	I	1	3,1	14,14,15	0.40	0	17,19,21	0.43	0
3	NAG	I	2	3	14,14,15	0.58	0	17,19,21	0.77	0
3	BMA	I	3	3	11,11,12	1.25	3 (27%)	15,15,17	1.82	3 (20%)
3	BMA	I	4	3	11,11,12	0.84	0	15,15,17	1.04	1 (6%)
2	NAG	J	1	2,1	14,14,15	1.40	2 (14%)	17,19,21	1.84	3 (17%)
2	NAG	J	2	2	14,14,15	0.62	0	17,19,21	0.38	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	-	1/6/23/26	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	-	2/2/19/22	0/1/1/1
2	NAG	G	1	2,1	-	4/6/23/26	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	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	2/6/23/26	0/1/1/1
3	BMA	I	3	3	-	2/2/19/22	0/1/1/1
3	BMA	I	4	3	-	2/2/19/22	0/1/1/1
2	NAG	J	1	2,1	-	4/6/23/26	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	C1-C2	3.66	1.57	1.52
2	G	1	NAG	C1-C2	3.65	1.57	1.52
2	J	1	NAG	O5-C1	3.51	1.49	1.43
2	G	1	NAG	O5-C1	3.46	1.49	1.43
3	I	3	BMA	C1-C2	2.38	1.57	1.52
3	I	3	BMA	C2-C3	2.35	1.56	1.52
3	F	3	BMA	C1-C2	2.28	1.57	1.52
3	F	3	BMA	C2-C3	2.28	1.56	1.52
3	F	3	BMA	C4-C3	2.07	1.57	1.52
3	I	3	BMA	C4-C3	2.06	1.57	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	1	NAG	C1-O5-C5	6.15	120.43	112.19
2	J	1	NAG	C1-O5-C5	6.12	120.39	112.19
3	F	3	BMA	C1-C2-C3	4.23	115.81	109.64
3	I	3	BMA	C1-C2-C3	4.22	115.78	109.64
3	F	3	BMA	C2-C3-C4	3.66	117.30	110.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	3	BMA	C2-C3-C4	3.60	117.20	110.86
2	J	1	NAG	C2-N2-C7	2.84	126.70	122.90
3	F	3	BMA	O2-C2-C3	-2.82	104.32	110.15
2	G	1	NAG	C2-N2-C7	2.80	126.65	122.90
3	I	3	BMA	O2-C2-C3	-2.79	104.38	110.15
3	I	4	BMA	C1-O5-C5	2.69	115.79	112.19
3	F	4	BMA	C1-O5-C5	2.64	115.72	112.19
2	E	2	NAG	C1-O5-C5	2.21	115.15	112.19
2	J	1	NAG	C1-C2-N2	2.08	113.71	110.43
2	H	2	NAG	C1-O5-C5	2.02	114.89	112.19

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	4	BMA	O5-C5-C6-O6
2	J	1	NAG	O5-C5-C6-O6
3	F	3	BMA	O5-C5-C6-O6
3	F	4	BMA	O5-C5-C6-O6
2	G	1	NAG	O5-C5-C6-O6
3	F	4	BMA	C4-C5-C6-O6
2	H	1	NAG	O5-C5-C6-O6
3	F	3	BMA	C4-C5-C6-O6
3	I	4	BMA	C4-C5-C6-O6
2	J	1	NAG	C4-C5-C6-O6
3	I	3	BMA	C4-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
3	I	3	BMA	O5-C5-C6-O6
2	G	1	NAG	C4-C5-C6-O6
3	F	2	NAG	C8-C7-N2-C2
3	F	2	NAG	O7-C7-N2-C2
3	I	2	NAG	C8-C7-N2-C2
3	I	2	NAG	O7-C7-N2-C2
2	H	1	NAG	C4-C5-C6-O6
2	G	2	NAG	C4-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
2	J	2	NAG	C4-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
2	J	2	NAG	O5-C5-C6-O6
2	G	1	NAG	C1-C2-N2-C7
2	J	1	NAG	C1-C2-N2-C7

Continued on next page...

Continued from previous page...

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

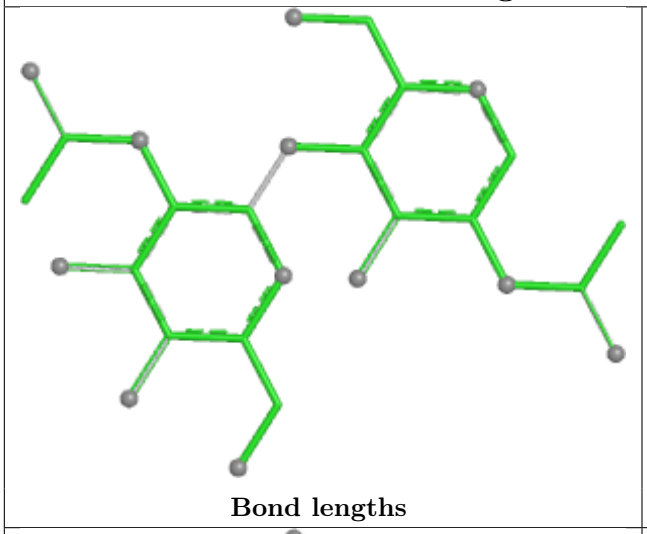
There are no ring outliers.

2 monomers are involved in 2 short contacts:

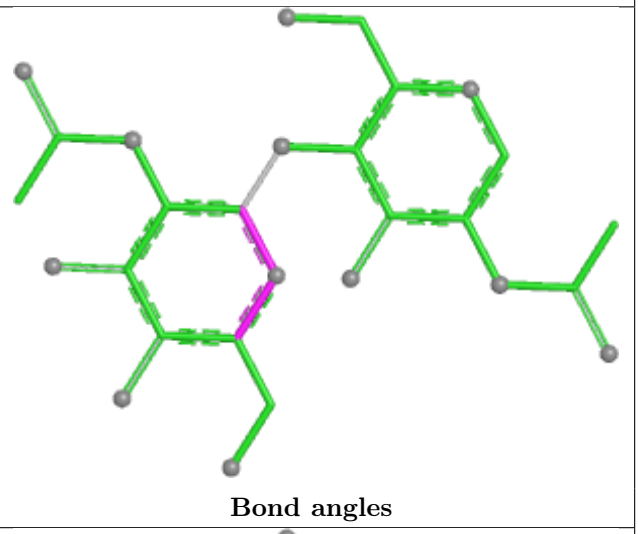
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1	NAG	1	0
2	H	1	NAG	1	0

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

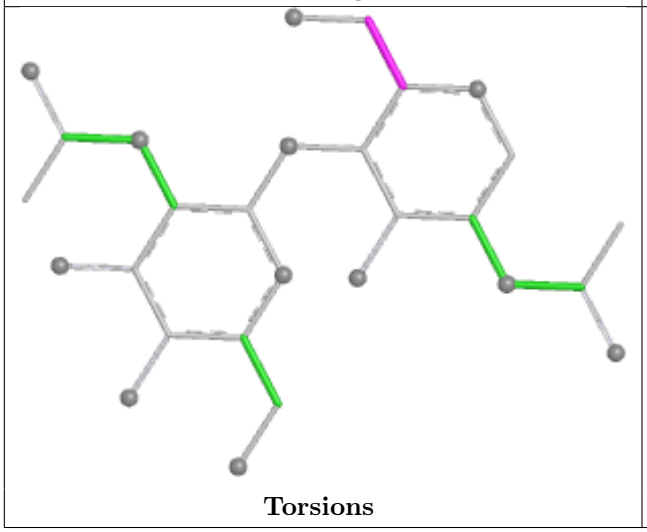
Oligosaccharide Chain E



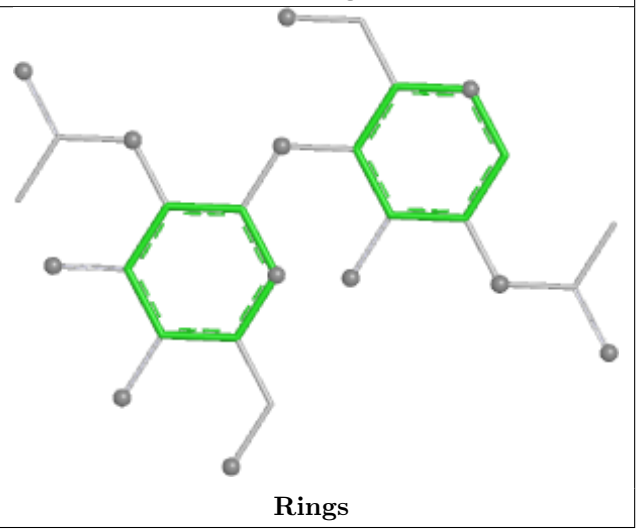
Bond lengths



Bond angles

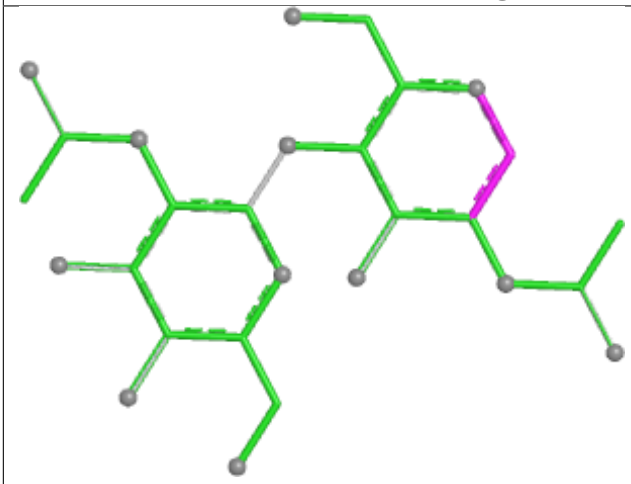


Torsions

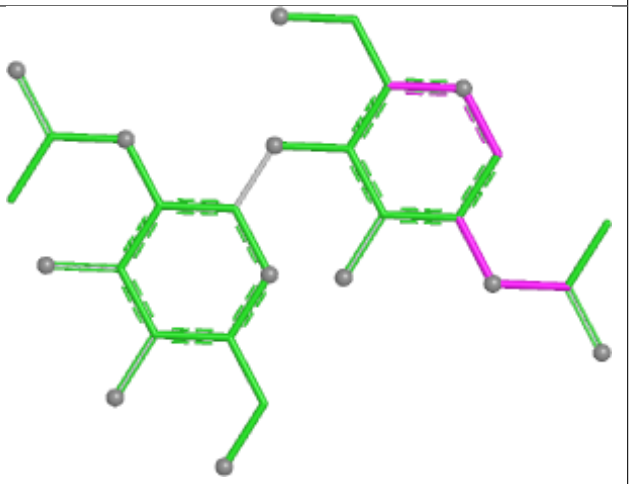


Rings

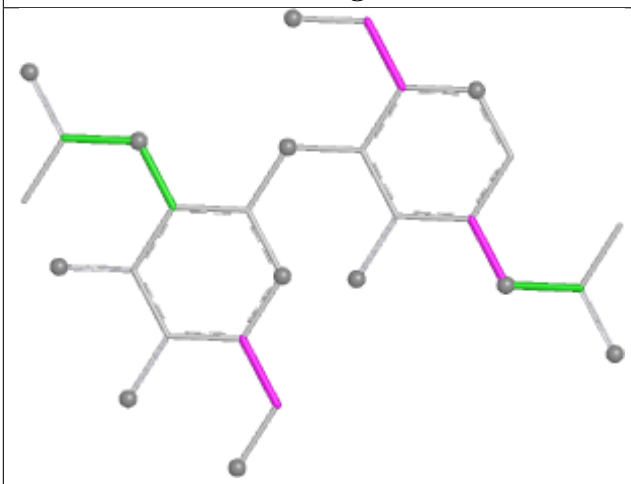
Oligosaccharide Chain G



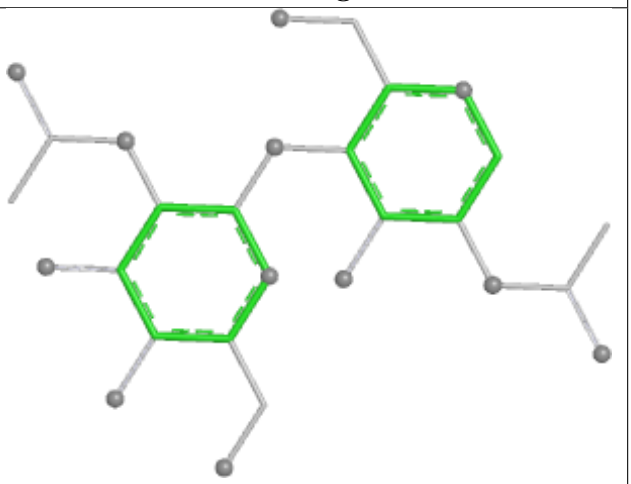
Bond lengths



Bond angles

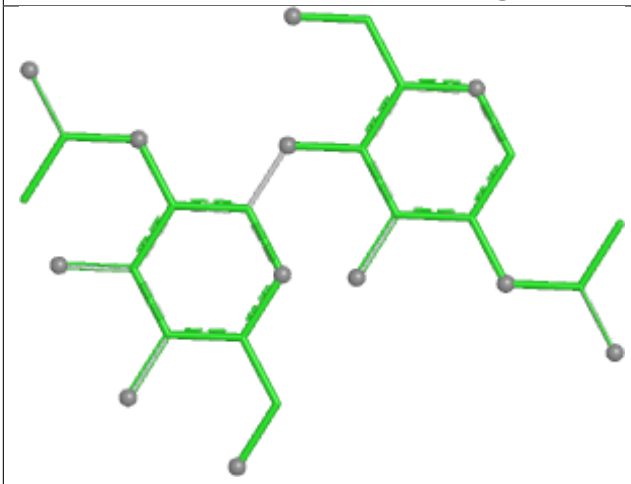


Torsions

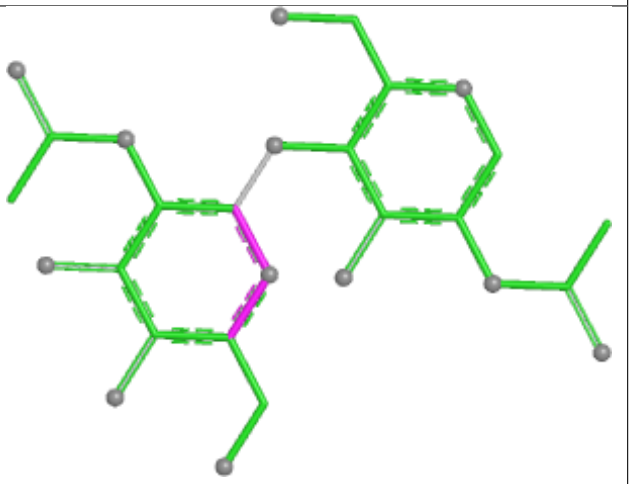


Rings

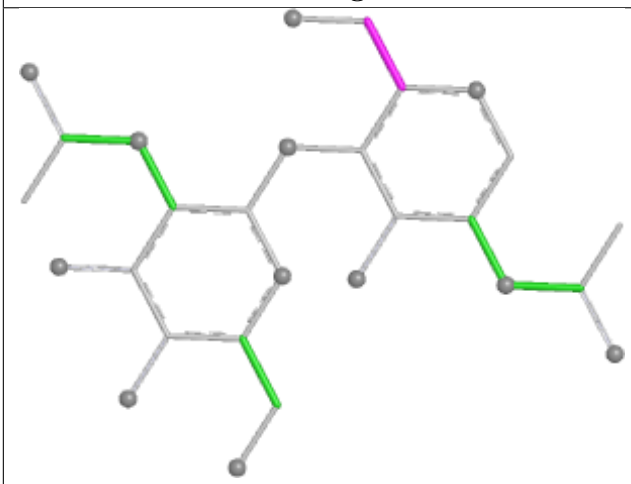
Oligosaccharide Chain H



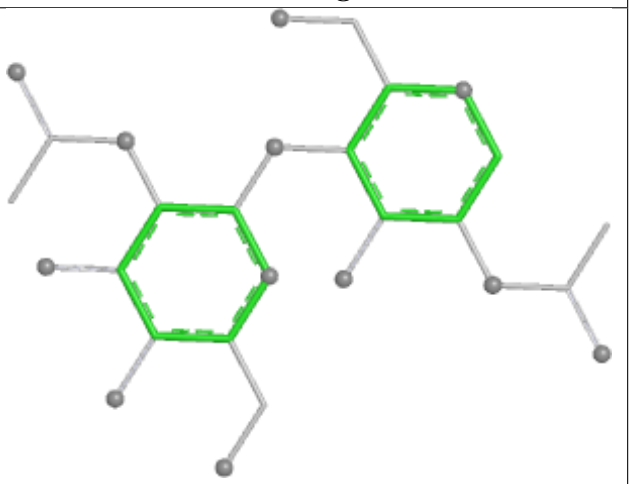
Bond lengths



Bond angles

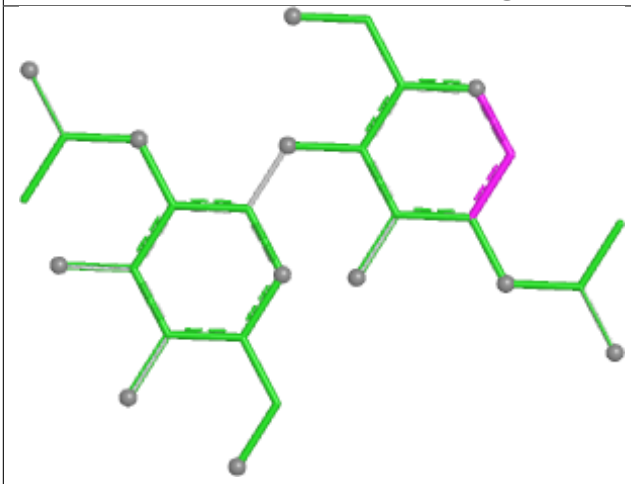


Torsions

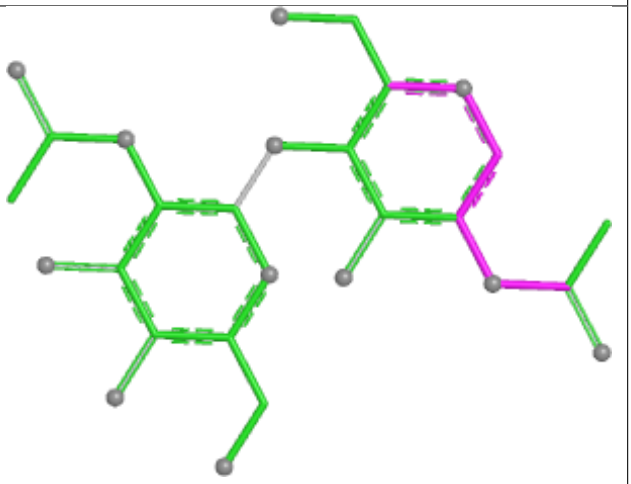


Rings

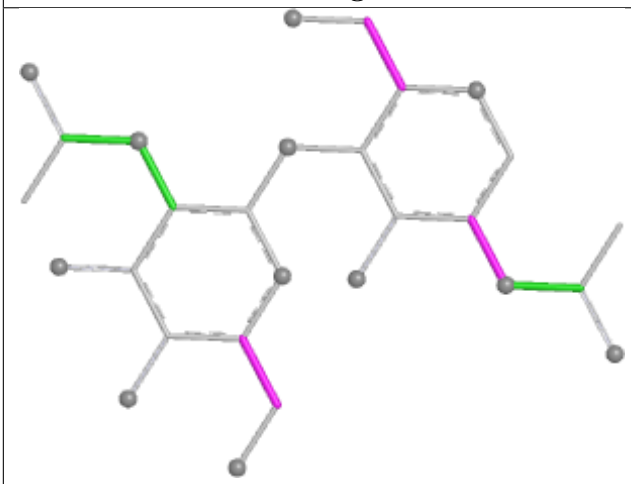
Oligosaccharide Chain J



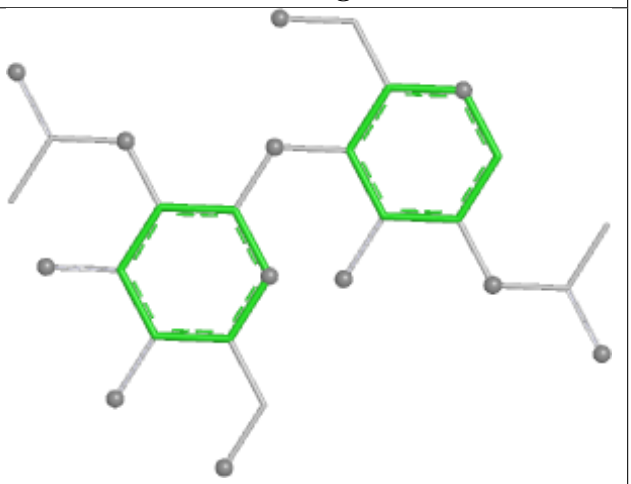
Bond lengths



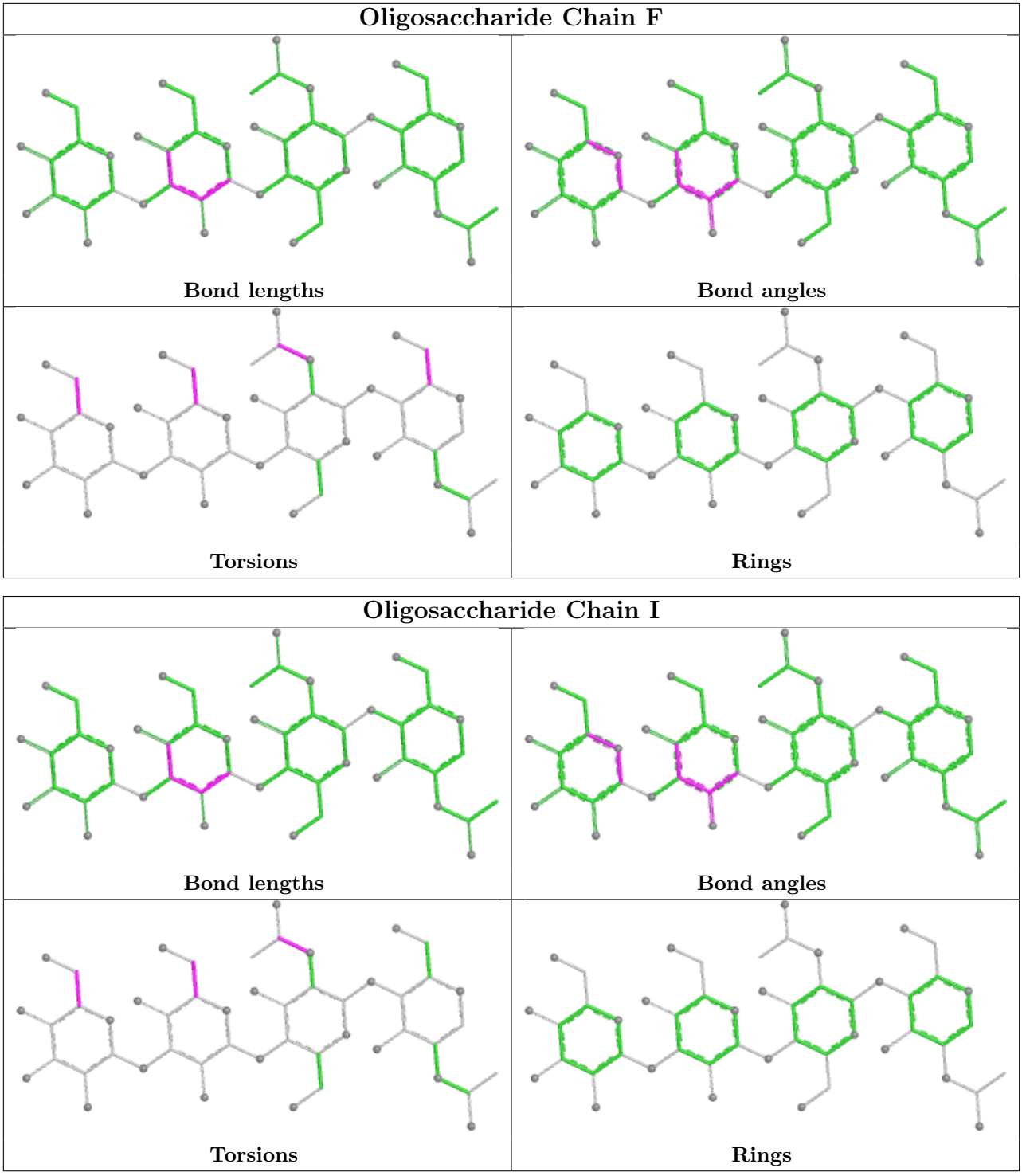
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

Of 30 ligands modelled in this entry, 8 are monoatomic - leaving 22 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	$\#\|Z\| > 2$
5	POV	D	1001	-	51,51,51	1.08	3 (5%)	57,59,59	1.12	4 (7%)
4	2J9	C	1002	-	17,18,18	7.11	8 (47%)	24,28,28	6.90	9 (37%)
4	2J9	A	1001	-	17,18,18	7.09	8 (47%)	24,28,28	6.93	9 (37%)
5	POV	A	1004	-	51,51,51	1.09	2 (3%)	57,59,59	0.99	3 (5%)
5	POV	A	1003	-	51,51,51	1.11	2 (3%)	57,59,59	0.97	3 (5%)
4	2J9	C	1001	-	17,18,18	7.12	8 (47%)	24,28,28	6.61	8 (33%)
5	POV	B	1002	-	51,51,51	1.09	3 (5%)	57,59,59	0.93	3 (5%)
4	2J9	A	1009	-	17,18,18	7.15	8 (47%)	24,28,28	6.60	8 (33%)
5	POV	A	1005	-	51,51,51	1.10	3 (5%)	57,59,59	0.96	3 (5%)
5	POV	D	1002	-	51,51,51	1.09	3 (5%)	57,59,59	0.97	3 (5%)
5	POV	B	1001	-	51,51,51	1.07	3 (5%)	57,59,59	1.07	3 (5%)
6	NAG	C	1006	1	14,14,15	1.14	2 (14%)	17,19,21	1.34	1 (5%)
5	POV	C	1003	-	51,51,51	1.08	3 (5%)	57,59,59	0.97	3 (5%)
5	POV	B	1003	-	51,51,51	1.10	3 (5%)	57,59,59	0.95	3 (5%)
5	POV	C	1007	-	51,51,51	1.07	2 (3%)	57,59,59	0.93	3 (5%)
5	POV	A	1002	-	51,51,51	1.08	3 (5%)	57,59,59	0.95	3 (5%)
5	POV	A	1008	-	51,51,51	1.07	2 (3%)	57,59,59	0.93	3 (5%)
5	POV	D	1003	-	51,51,51	1.09	3 (5%)	57,59,59	0.93	3 (5%)
5	POV	C	1005	-	51,51,51	1.09	2 (3%)	57,59,59	1.00	3 (5%)
6	NAG	A	1006	1	14,14,15	1.12	2 (14%)	17,19,21	1.33	1 (5%)
5	POV	A	1007	-	51,51,51	1.09	3 (5%)	57,59,59	0.97	3 (5%)
5	POV	C	1004	-	51,51,51	1.11	2 (3%)	57,59,59	0.97	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
5	POV	D	1001	-	-	23/55/55/55	-
4	2J9	C	1002	-	-	0/4/22/22	0/3/3/3
4	2J9	A	1001	-	-	2/4/22/22	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	POV	A	1004	-	-	25/55/55/55	-
5	POV	A	1003	-	-	24/55/55/55	-
4	2J9	C	1001	-	-	1/4/22/22	0/3/3/3
5	POV	B	1002	-	-	32/55/55/55	-
4	2J9	A	1009	-	-	1/4/22/22	0/3/3/3
5	POV	A	1005	-	-	32/55/55/55	-
5	POV	D	1002	-	-	23/55/55/55	-
5	POV	B	1001	-	-	25/55/55/55	-
6	NAG	C	1006	1	-	2/6/23/26	0/1/1/1
5	POV	C	1003	-	-	34/55/55/55	-
5	POV	B	1003	-	-	29/55/55/55	-
5	POV	C	1007	-	-	26/55/55/55	-
5	POV	A	1002	-	-	34/55/55/55	-
5	POV	A	1008	-	-	27/55/55/55	-
5	POV	D	1003	-	-	34/55/55/55	-
5	POV	C	1005	-	-	26/55/55/55	-
6	NAG	A	1006	1	-	2/6/23/26	0/1/1/1
5	POV	A	1007	-	-	22/55/55/55	-
5	POV	C	1004	-	-	25/55/55/55	-

All (78) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1001	2J9	OAA-SAP	19.34	1.65	1.43
4	C	1002	2J9	OAA-SAP	19.33	1.65	1.43
4	A	1009	2J9	OAA-SAP	19.32	1.65	1.43
4	A	1009	2J9	OAB-SAP	19.32	1.65	1.43
4	C	1001	2J9	OAA-SAP	19.29	1.65	1.43
4	C	1001	2J9	OAB-SAP	19.00	1.65	1.43
4	C	1002	2J9	OAB-SAP	18.83	1.65	1.43
4	A	1001	2J9	OAB-SAP	18.48	1.64	1.43
4	C	1001	2J9	CAL-NAO	6.50	1.55	1.40
4	A	1001	2J9	CAL-NAO	6.40	1.55	1.40
4	A	1009	2J9	CAL-NAO	6.33	1.55	1.40
4	C	1002	2J9	CAL-NAO	6.24	1.54	1.40
4	C	1002	2J9	CAH-CAN	-4.78	1.38	1.48
4	A	1001	2J9	CAH-CAN	-4.76	1.38	1.48
4	A	1001	2J9	CAM-SAP	-4.58	1.71	1.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1009	2J9	CAH-CAN	-4.55	1.39	1.48
4	C	1002	2J9	CAG-CAN	-4.52	1.39	1.48
4	C	1001	2J9	CAH-CAN	-4.52	1.39	1.48
4	A	1001	2J9	CAG-CAN	-4.52	1.39	1.48
4	A	1009	2J9	CAG-CAN	-4.50	1.39	1.48
4	C	1001	2J9	CAG-CAN	-4.50	1.39	1.48
4	A	1001	2J9	CAL-CAM	-4.10	1.34	1.40
4	C	1001	2J9	CAM-SAP	-3.98	1.72	1.75
4	C	1002	2J9	CAL-CAM	-3.95	1.35	1.40
4	C	1002	2J9	CAM-SAP	-3.88	1.72	1.75
4	A	1009	2J9	CAM-SAP	-3.72	1.72	1.75
6	C	1006	NAG	O5-C1	3.59	1.49	1.43
4	C	1001	2J9	CAL-CAM	-3.58	1.35	1.40
4	A	1009	2J9	CAL-CAM	-3.50	1.35	1.40
6	A	1006	NAG	O5-C1	3.49	1.49	1.43
5	C	1005	POV	O21-C21	3.13	1.43	1.34
5	A	1004	POV	O21-C21	3.11	1.43	1.34
5	A	1003	POV	O21-C21	3.11	1.43	1.34
5	D	1001	POV	O21-C21	3.10	1.43	1.34
5	A	1008	POV	O21-C21	3.09	1.43	1.34
5	C	1004	POV	O21-C21	3.08	1.43	1.34
5	C	1007	POV	O21-C21	3.06	1.42	1.34
5	B	1001	POV	O21-C21	3.06	1.42	1.34
5	A	1007	POV	O21-C21	2.90	1.42	1.34
5	B	1003	POV	O21-C21	2.89	1.42	1.34
5	D	1002	POV	O21-C21	2.88	1.42	1.34
5	A	1005	POV	O21-C21	2.86	1.42	1.34
5	D	1003	POV	O21-C21	2.84	1.42	1.34
5	C	1003	POV	O21-C21	2.84	1.42	1.34
5	C	1004	POV	O31-C31	2.84	1.41	1.33
5	A	1002	POV	O21-C21	2.83	1.42	1.34
5	B	1002	POV	O21-C21	2.83	1.42	1.34
5	A	1003	POV	O31-C31	2.81	1.41	1.33
5	C	1005	POV	O31-C31	2.80	1.41	1.33
5	A	1004	POV	O31-C31	2.78	1.41	1.33
4	A	1009	2J9	CAH-CAG	-2.78	1.38	1.48
4	C	1001	2J9	CAH-CAG	-2.77	1.38	1.48
5	D	1003	POV	O31-C31	2.77	1.41	1.33
5	B	1002	POV	O31-C31	2.76	1.41	1.33
4	A	1001	2J9	CAH-CAG	-2.76	1.39	1.48
5	B	1003	POV	O31-C31	2.76	1.41	1.33
4	C	1002	2J9	CAH-CAG	-2.76	1.39	1.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1005	POV	O31-C31	2.75	1.41	1.33
5	D	1002	POV	O31-C31	2.74	1.41	1.33
5	A	1002	POV	O31-C31	2.73	1.41	1.33
5	A	1007	POV	O31-C31	2.71	1.41	1.33
5	C	1003	POV	O31-C31	2.71	1.41	1.33
5	D	1001	POV	O31-C31	2.61	1.40	1.33
5	C	1007	POV	O31-C31	2.60	1.40	1.33
5	B	1001	POV	O31-C31	2.57	1.40	1.33
5	B	1002	POV	O21-C2	-2.57	1.40	1.46
5	D	1003	POV	O21-C2	-2.56	1.40	1.46
5	A	1008	POV	O31-C31	2.56	1.40	1.33
5	B	1003	POV	O21-C2	-2.54	1.40	1.46
5	A	1005	POV	O21-C2	-2.53	1.40	1.46
5	A	1007	POV	O21-C2	-2.51	1.40	1.46
5	D	1002	POV	O21-C2	-2.50	1.40	1.46
5	A	1002	POV	O21-C2	-2.42	1.40	1.46
5	C	1003	POV	O21-C2	-2.39	1.41	1.46
5	B	1001	POV	O21-C2	-2.28	1.41	1.46
5	D	1001	POV	O21-C2	-2.23	1.41	1.46
6	A	1006	NAG	C1-C2	2.19	1.55	1.52
6	C	1006	NAG	C1-C2	2.16	1.55	1.52

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	1002	2J9	CAI-NAO-CAL	18.86	121.33	110.17
4	A	1001	2J9	CAI-NAO-CAL	18.45	121.08	110.17
4	A	1001	2J9	CAG-CAN-NAO	16.71	150.74	118.82
4	A	1009	2J9	CAI-NAO-CAL	16.69	120.04	110.17
4	A	1009	2J9	CAH-CAN-NAO	16.61	150.56	118.82
4	C	1001	2J9	CAH-CAN-NAO	16.46	150.26	118.82
4	C	1002	2J9	CAG-CAN-NAO	16.44	150.23	118.82
4	C	1001	2J9	CAI-NAO-CAL	16.32	119.82	110.17
4	C	1001	2J9	CAG-CAN-NAO	16.26	149.89	118.82
4	C	1002	2J9	CAH-CAN-NAO	16.19	149.75	118.82
4	A	1009	2J9	CAG-CAN-NAO	16.11	149.59	118.82
4	A	1001	2J9	CAH-CAN-NAO	15.93	149.25	118.82
4	A	1001	2J9	CAM-SAP-NAJ	10.55	110.80	102.40
4	C	1002	2J9	CAM-SAP-NAJ	10.38	110.66	102.40
4	A	1009	2J9	CAM-SAP-NAJ	9.80	110.21	102.40
4	C	1001	2J9	CAM-SAP-NAJ	9.77	110.18	102.40
4	C	1001	2J9	OAB-SAP-OAA	-8.88	109.40	118.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1009	2J9	OAB-SAP-OAA	-8.57	109.72	118.44
4	C	1002	2J9	OAB-SAP-OAA	-8.27	110.02	118.44
4	A	1001	2J9	OAB-SAP-OAA	-8.25	110.04	118.44
4	A	1001	2J9	OAB-SAP-NAJ	6.54	113.94	107.92
4	C	1002	2J9	CAK-CAF-CAM	5.50	120.21	116.92
4	C	1001	2J9	OAB-SAP-NAJ	5.37	112.87	107.92
6	C	1006	NAG	C1-O5-C5	5.30	119.29	112.19
6	A	1006	NAG	C1-O5-C5	5.26	119.23	112.19
5	D	1001	POV	O21-C21-C22	5.23	122.79	111.48
4	C	1002	2J9	OAB-SAP-NAJ	5.10	112.62	107.92
4	A	1001	2J9	CAK-CAF-CAM	5.00	119.91	116.92
4	A	1009	2J9	CAK-CAF-CAM	4.99	119.90	116.92
5	B	1001	POV	O21-C21-C22	4.95	122.19	111.48
4	C	1001	2J9	CAK-CAF-CAM	4.78	119.78	116.92
5	A	1003	POV	O21-C21-C22	4.28	120.73	111.48
5	C	1005	POV	O21-C21-C22	4.25	120.67	111.48
5	C	1004	POV	O21-C21-C22	4.23	120.64	111.48
5	A	1004	POV	O21-C21-C22	4.17	120.50	111.48
5	D	1002	POV	O21-C21-C22	4.17	120.49	111.48
4	A	1009	2J9	OAB-SAP-NAJ	4.15	111.74	107.92
5	A	1007	POV	O21-C21-C22	4.13	120.41	111.48
5	C	1003	POV	O21-C21-C22	4.11	120.38	111.48
5	A	1002	POV	O21-C21-C22	3.99	120.11	111.48
5	A	1005	POV	O21-C21-C22	3.89	119.89	111.48
5	B	1003	POV	O21-C21-C22	3.89	119.89	111.48
5	D	1003	POV	O21-C21-C22	3.84	119.78	111.48
5	B	1002	POV	O21-C21-C22	3.82	119.74	111.48
5	A	1008	POV	O21-C21-C22	3.78	119.67	111.48
5	C	1007	POV	O21-C21-C22	3.73	119.54	111.48
4	A	1001	2J9	CAD-CAK-CAF	-3.06	119.19	123.23
4	A	1001	2J9	OAB-SAP-CAM	-3.06	105.48	109.30
5	C	1005	POV	O31-C31-C32	2.95	120.84	111.83
4	C	1002	2J9	CAD-CAK-CAF	-2.83	119.49	123.23
5	C	1004	POV	O31-C31-C32	2.82	120.43	111.83
5	A	1003	POV	O31-C31-C32	2.81	120.39	111.83
5	A	1004	POV	O31-C31-C32	2.76	120.26	111.83
5	B	1003	POV	O31-C31-C32	2.76	120.25	111.83
5	D	1001	POV	O31-C31-C32	2.75	120.23	111.83
5	A	1005	POV	O31-C31-C32	2.75	120.21	111.83
5	B	1002	POV	O31-C31-C32	2.74	120.18	111.83
5	D	1003	POV	O31-C31-C32	2.71	120.11	111.83
5	D	1002	POV	O31-C31-C32	2.71	120.11	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1009	2J9	CAD-CAK-CAF	-2.70	119.66	123.23
4	C	1001	2J9	CAD-CAK-CAF	-2.70	119.67	123.23
5	C	1003	POV	O31-C31-C32	2.68	120.02	111.83
5	A	1007	POV	O31-C31-C32	2.67	119.98	111.83
5	A	1002	POV	C14-N-C12	2.66	120.50	109.91
5	A	1002	POV	O31-C31-C32	2.66	119.94	111.83
5	B	1001	POV	C14-N-C12	2.65	120.43	109.91
5	B	1001	POV	O31-C31-C32	2.64	119.90	111.83
5	C	1003	POV	C14-N-C12	2.64	120.41	109.91
5	D	1001	POV	C14-N-C12	2.57	120.11	109.91
5	D	1003	POV	C14-N-C12	2.54	119.99	109.91
5	B	1002	POV	C14-N-C12	2.51	119.90	109.91
5	A	1003	POV	C14-N-C12	2.37	119.31	109.91
5	C	1004	POV	C14-N-C12	2.36	119.31	109.91
5	A	1005	POV	C14-N-C12	2.36	119.29	109.91
5	B	1003	POV	C14-N-C12	2.33	119.17	109.91
5	A	1007	POV	C14-N-C12	2.30	119.05	109.91
5	C	1007	POV	O31-C31-C32	2.30	118.85	111.83
5	D	1002	POV	C14-N-C12	2.29	119.01	109.91
5	A	1008	POV	O31-C31-C32	2.27	118.74	111.83
5	C	1007	POV	C14-N-C12	2.22	118.74	109.91
5	A	1008	POV	C14-N-C12	2.21	118.68	109.91
5	A	1004	POV	C14-N-C12	2.19	118.63	109.91
5	C	1005	POV	C14-N-C12	2.17	118.54	109.91
4	C	1002	2J9	OAB-SAP-CAM	-2.12	106.65	109.30
5	D	1001	POV	O21-C21-O22	-2.06	118.89	123.70

There are no chirality outliers.

All (449) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1001	2J9	CAH-CAN-NAO-CAI
4	C	1001	2J9	CAG-CAN-NAO-CAL
5	A	1002	POV	C1-O11-P-O14
5	A	1002	POV	C11-O12-P-O11
5	A	1002	POV	C11-O12-P-O13
5	A	1002	POV	C11-O12-P-O14
5	A	1002	POV	C22-C21-O21-C2
5	A	1002	POV	O22-C21-O21-C2
5	A	1003	POV	O11-C1-C2-O21
5	A	1003	POV	O12-C11-C12-N
5	A	1003	POV	C22-C21-O21-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	A	1004	POV	C11-O12-P-O11
5	A	1004	POV	C22-C21-O21-C2
5	A	1004	POV	C32-C31-O31-C3
5	A	1005	POV	C1-O11-P-O12
5	A	1005	POV	C1-O11-P-O13
5	A	1005	POV	C11-O12-P-O11
5	A	1005	POV	C11-O12-P-O14
5	A	1005	POV	O12-C11-C12-N
5	A	1007	POV	C1-O11-P-O12
5	A	1007	POV	O12-C11-C12-N
5	A	1008	POV	C1-O11-P-O12
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	A	1008	POV	C22-C21-O21-C2
5	B	1001	POV	C1-O11-P-O12
5	B	1001	POV	C1-O11-P-O14
5	B	1001	POV	C11-O12-P-O11
5	B	1001	POV	C11-O12-P-O13
5	B	1001	POV	O12-C11-C12-N
5	B	1001	POV	C22-C21-O21-C2
5	B	1001	POV	O22-C21-O21-C2
5	B	1002	POV	C1-O11-P-O12
5	B	1002	POV	C1-O11-P-O13
5	B	1002	POV	C11-O12-P-O11
5	B	1002	POV	C11-O12-P-O13
5	B	1002	POV	C22-C21-O21-C2
5	B	1002	POV	O22-C21-O21-C2
5	B	1003	POV	C1-O11-P-O12
5	B	1003	POV	C1-O11-P-O13
5	B	1003	POV	C11-O12-P-O11
5	B	1003	POV	C11-O12-P-O14
5	B	1003	POV	O12-C11-C12-N
5	C	1003	POV	C1-O11-P-O14
5	C	1003	POV	C11-O12-P-O11
5	C	1003	POV	C11-O12-P-O13
5	C	1003	POV	C11-O12-P-O14
5	C	1003	POV	O22-C21-O21-C2
5	C	1004	POV	O11-C1-C2-O21
5	C	1004	POV	O12-C11-C12-N
5	C	1004	POV	C22-C21-O21-C2
5	C	1005	POV	C11-O12-P-O11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	C	1005	POV	C22-C21-O21-C2
5	C	1005	POV	C32-C31-O31-C3
5	C	1005	POV	O32-C31-O31-C3
5	C	1007	POV	C1-O11-P-O12
5	C	1007	POV	C1-O11-P-O13
5	C	1007	POV	C1-O11-P-O14
5	C	1007	POV	O12-C11-C12-N
5	C	1007	POV	C22-C21-O21-C2
5	D	1001	POV	C1-O11-P-O12
5	D	1001	POV	C1-O11-P-O14
5	D	1001	POV	C11-O12-P-O11
5	D	1001	POV	C11-O12-P-O13
5	D	1001	POV	O12-C11-C12-N
5	D	1001	POV	C22-C21-O21-C2
5	D	1001	POV	O22-C21-O21-C2
5	D	1002	POV	C1-O11-P-O12
5	D	1002	POV	C1-O11-P-O14
5	D	1002	POV	O12-C11-C12-N
5	D	1003	POV	C1-O11-P-O12
5	D	1003	POV	C1-O11-P-O13
5	D	1003	POV	C11-O12-P-O11
5	D	1003	POV	C11-O12-P-O13
5	D	1003	POV	C22-C21-O21-C2
5	A	1004	POV	O32-C31-O31-C3
5	B	1002	POV	O32-C31-O31-C3
5	A	1003	POV	O32-C31-O31-C3
5	C	1004	POV	O32-C31-O31-C3
5	D	1003	POV	O32-C31-O31-C3
5	A	1003	POV	O22-C21-O21-C2
5	A	1004	POV	O22-C21-O21-C2
5	A	1008	POV	O22-C21-O21-C2
5	C	1004	POV	O22-C21-O21-C2
5	C	1005	POV	O22-C21-O21-C2
5	C	1007	POV	O22-C21-O21-C2
5	D	1003	POV	O22-C21-O21-C2
5	B	1002	POV	C32-C31-O31-C3
5	D	1003	POV	C32-C31-O31-C3
5	C	1003	POV	C22-C21-O21-C2
5	A	1003	POV	C32-C31-O31-C3
5	B	1001	POV	C32-C31-O31-C3
5	C	1004	POV	C32-C31-O31-C3
5	D	1001	POV	C32-C31-O31-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	B	1001	POV	O32-C31-O31-C3
5	D	1001	POV	O32-C31-O31-C3
5	C	1003	POV	C32-C31-O31-C3
5	A	1002	POV	C32-C31-O31-C3
5	C	1003	POV	O32-C31-O31-C3
6	A	1006	NAG	C4-C5-C6-O6
5	C	1005	POV	C34-C35-C36-C37
5	A	1002	POV	O32-C31-O31-C3
5	A	1005	POV	C32-C31-O31-C3
5	B	1003	POV	C32-C31-O31-C3
5	D	1003	POV	C311-C310-C39-C38
5	B	1002	POV	C311-C310-C39-C38
5	A	1004	POV	C25-C26-C27-C28
5	A	1008	POV	C31-C32-C33-C34
5	B	1002	POV	C21-C22-C23-C24
6	C	1006	NAG	C4-C5-C6-O6
5	D	1001	POV	C31-C32-C33-C34
5	B	1001	POV	C31-C32-C33-C34
6	A	1006	NAG	O5-C5-C6-O6
5	A	1005	POV	O32-C31-O31-C3
4	A	1001	2J9	CAG-CAN-NAO-CAL
5	A	1005	POV	C21-C22-C23-C24
5	B	1003	POV	C21-C22-C23-C24
5	C	1007	POV	C31-C32-C33-C34
5	D	1003	POV	C21-C22-C23-C24
5	B	1003	POV	O32-C31-O31-C3
5	C	1007	POV	C21-C22-C23-C24
5	A	1008	POV	C32-C31-O31-C3
5	A	1007	POV	C21-C22-C23-C24
5	B	1002	POV	C31-C32-C33-C34
5	C	1007	POV	C32-C31-O31-C3
5	D	1002	POV	C21-C22-C23-C24
5	C	1005	POV	C39-C310-C311-C312
5	C	1003	POV	C310-C311-C312-C313
6	C	1006	NAG	O5-C5-C6-O6
5	A	1003	POV	C3-C2-O21-C21
5	A	1008	POV	C3-C2-O21-C21
5	C	1004	POV	C3-C2-O21-C21
5	C	1007	POV	C3-C2-O21-C21
5	A	1005	POV	C213-C214-C215-C216
5	B	1003	POV	C213-C214-C215-C216
5	A	1008	POV	O32-C31-O31-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	A	1002	POV	C310-C311-C312-C313
5	A	1004	POV	C22-C23-C24-C25
5	A	1008	POV	C37-C38-C39-C310
5	B	1003	POV	C22-C23-C24-C25
5	C	1007	POV	C33-C34-C35-C36
5	A	1008	POV	C33-C34-C35-C36
5	D	1002	POV	C25-C26-C27-C28
5	A	1005	POV	C22-C23-C24-C25
5	B	1002	POV	C213-C214-C215-C216
5	A	1007	POV	C39-C310-C311-C312
5	C	1004	POV	C22-C23-C24-C25
5	D	1003	POV	C213-C214-C215-C216
5	D	1003	POV	C32-C33-C34-C35
5	A	1003	POV	C22-C23-C24-C25
5	A	1007	POV	C25-C26-C27-C28
5	C	1003	POV	C24-C25-C26-C27
5	A	1008	POV	C21-C22-C23-C24
5	C	1005	POV	C311-C310-C39-C38
5	D	1001	POV	C25-C26-C27-C28
5	A	1004	POV	C36-C37-C38-C39
5	A	1003	POV	C310-C311-C312-C313
5	D	1003	POV	C25-C26-C27-C28
5	C	1007	POV	O32-C31-O31-C3
5	A	1008	POV	C311-C310-C39-C38
5	D	1001	POV	C33-C34-C35-C36
5	B	1002	POV	C36-C37-C38-C39
5	C	1003	POV	C37-C38-C39-C310
5	C	1005	POV	C22-C23-C24-C25
5	C	1007	POV	C24-C25-C26-C27
5	D	1002	POV	C311-C310-C39-C38
5	D	1003	POV	C212-C213-C214-C215
5	D	1003	POV	C36-C37-C38-C39
5	A	1005	POV	C214-C215-C216-C217
5	B	1002	POV	C211-C212-C213-C214
5	A	1004	POV	C311-C310-C39-C38
5	B	1003	POV	C214-C215-C216-C217
5	A	1008	POV	C24-C25-C26-C27
5	B	1002	POV	C32-C33-C34-C35
5	A	1002	POV	C24-C25-C26-C27
5	B	1002	POV	C25-C26-C27-C28
5	C	1005	POV	C36-C37-C38-C39
5	D	1003	POV	C31-C32-C33-C34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	A	1002	POV	C22-C23-C24-C25
5	B	1002	POV	C24-C25-C26-C27
5	A	1005	POV	C24-C25-C26-C27
5	C	1007	POV	C311-C310-C39-C38
5	D	1002	POV	C310-C311-C312-C313
4	A	1009	2J9	CAG-CAN-NAO-CAL
5	D	1003	POV	C24-C25-C26-C27
5	B	1003	POV	C312-C313-C314-C315
5	B	1003	POV	C24-C25-C26-C27
5	D	1002	POV	C23-C24-C25-C26
5	C	1003	POV	C311-C310-C39-C38
5	C	1005	POV	C25-C26-C27-C28
5	D	1002	POV	C39-C310-C311-C312
5	A	1005	POV	C33-C34-C35-C36
5	A	1005	POV	C312-C313-C314-C315
5	B	1001	POV	C33-C34-C35-C36
5	B	1003	POV	C33-C34-C35-C36
5	A	1007	POV	C22-C21-O21-C2
5	C	1004	POV	C311-C310-C39-C38
5	C	1003	POV	C35-C36-C37-C38
5	C	1004	POV	C21-C22-C23-C24
5	D	1003	POV	C39-C310-C311-C312
5	A	1007	POV	C23-C24-C25-C26
5	B	1002	POV	C39-C310-C311-C312
5	A	1007	POV	C311-C310-C39-C38
5	B	1003	POV	C311-C310-C39-C38
5	C	1007	POV	C211-C212-C213-C214
5	A	1004	POV	C39-C310-C311-C312
5	A	1003	POV	C21-C22-C23-C24
5	A	1007	POV	C24-C25-C26-C27
5	A	1008	POV	C211-C212-C213-C214
5	B	1003	POV	C23-C24-C25-C26
5	C	1005	POV	C35-C36-C37-C38
5	C	1007	POV	C312-C313-C314-C315
5	A	1007	POV	C210-C211-C212-C213
5	C	1003	POV	C210-C211-C212-C213
5	C	1003	POV	C34-C35-C36-C37
5	A	1007	POV	C37-C38-C39-C310
5	C	1004	POV	C24-C25-C26-C27
5	B	1002	POV	C212-C213-C214-C215
5	A	1003	POV	C24-C25-C26-C27
5	C	1005	POV	C24-C25-C26-C27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	C	1004	POV	C310-C311-C312-C313
5	A	1008	POV	C311-C312-C313-C314
5	C	1007	POV	C37-C38-C39-C310
5	D	1002	POV	C22-C21-O21-C2
5	D	1003	POV	C211-C212-C213-C214
5	A	1002	POV	C210-C211-C212-C213
5	D	1002	POV	C210-C211-C212-C213
5	A	1003	POV	O11-C1-C2-C3
5	C	1007	POV	C311-C312-C313-C314
5	B	1001	POV	C25-C26-C27-C28
5	C	1003	POV	C21-C22-C23-C24
5	A	1005	POV	C23-C24-C25-C26
5	C	1005	POV	C23-C24-C25-C26
5	A	1002	POV	C1-C2-C3-O31
5	A	1002	POV	C37-C38-C39-C310
5	D	1002	POV	C311-C312-C313-C314
5	B	1002	POV	C26-C27-C28-C29
5	D	1003	POV	C26-C27-C28-C29
5	B	1003	POV	C36-C37-C38-C39
5	C	1003	POV	C25-C26-C27-C28
5	D	1002	POV	C24-C25-C26-C27
5	A	1005	POV	C311-C312-C313-C314
5	B	1001	POV	C2-C1-O11-P
5	A	1004	POV	C24-C25-C26-C27
5	A	1005	POV	C212-C213-C214-C215
5	A	1004	POV	C1-C2-O21-C21
5	C	1005	POV	C1-C2-O21-C21
5	A	1008	POV	C22-C23-C24-C25
5	C	1003	POV	C33-C34-C35-C36
5	C	1005	POV	C310-C311-C312-C313
5	D	1003	POV	O11-C1-C2-O21
5	A	1004	POV	C23-C24-C25-C26
5	A	1008	POV	C39-C310-C311-C312
5	C	1003	POV	C22-C23-C24-C25
5	C	1007	POV	C39-C310-C311-C312
5	C	1007	POV	C22-C23-C24-C25
5	A	1005	POV	C36-C37-C38-C39
5	A	1007	POV	C310-C311-C312-C313
5	B	1002	POV	C310-C311-C312-C313
5	C	1004	POV	C25-C26-C27-C28
5	A	1003	POV	C39-C310-C311-C312
5	B	1002	POV	C22-C23-C24-C25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	C	1004	POV	C212-C213-C214-C215
5	A	1002	POV	C34-C35-C36-C37
5	B	1003	POV	C212-C213-C214-C215
5	A	1008	POV	C312-C313-C314-C315
5	D	1003	POV	C310-C311-C312-C313
5	A	1004	POV	C37-C38-C39-C310
5	A	1007	POV	O22-C21-O21-C2
5	B	1001	POV	C27-C28-C29-C210
5	D	1001	POV	C2-C1-O11-P
5	A	1007	POV	C311-C312-C313-C314
5	D	1001	POV	C312-C313-C314-C315
5	C	1004	POV	O11-C1-C2-C3
5	B	1002	POV	C23-C24-C25-C26
5	A	1003	POV	C25-C26-C27-C28
5	D	1001	POV	C22-C23-C24-C25
5	A	1005	POV	C1-C2-C3-O31
5	B	1002	POV	C1-C2-C3-O31
5	B	1003	POV	C1-C2-C3-O31
5	C	1003	POV	C1-C2-C3-O31
5	D	1003	POV	C1-C2-C3-O31
5	A	1002	POV	C311-C312-C313-C314
5	A	1002	POV	C311-C310-C39-C38
5	B	1002	POV	O11-C1-C2-O21
5	D	1002	POV	C37-C38-C39-C310
5	A	1007	POV	O21-C2-C3-O31
5	C	1004	POV	C311-C312-C313-C314
5	D	1003	POV	C23-C24-C25-C26
5	D	1003	POV	C22-C23-C24-C25
5	A	1002	POV	C21-C22-C23-C24
5	B	1001	POV	C210-C211-C212-C213
5	A	1002	POV	C35-C36-C37-C38
5	C	1005	POV	C37-C38-C39-C310
5	A	1003	POV	C37-C38-C39-C310
5	A	1008	POV	C36-C37-C38-C39
5	D	1002	POV	O22-C21-O21-C2
5	A	1002	POV	C33-C34-C35-C36
5	D	1001	POV	C27-C28-C29-C210
5	A	1002	POV	C12-C11-O12-P
5	B	1001	POV	C12-C11-O12-P
5	C	1003	POV	C12-C11-O12-P
5	D	1001	POV	C12-C11-O12-P
5	B	1001	POV	C39-C310-C311-C312

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	C	1003	POV	O21-C2-C3-O31
5	D	1002	POV	O21-C2-C3-O31
5	A	1004	POV	C310-C311-C312-C313
5	A	1005	POV	C39-C310-C311-C312
5	A	1003	POV	C311-C310-C39-C38
5	A	1002	POV	O12-C11-C12-N
5	A	1004	POV	O12-C11-C12-N
5	B	1002	POV	O12-C11-C12-N
5	C	1003	POV	O12-C11-C12-N
5	C	1005	POV	O12-C11-C12-N
5	D	1003	POV	O12-C11-C12-N
5	C	1007	POV	C26-C27-C28-C29
5	A	1002	POV	C11-C12-N-C14
5	C	1004	POV	C36-C37-C38-C39
5	C	1003	POV	C313-C314-C315-C316
5	C	1003	POV	C39-C310-C311-C312
5	C	1003	POV	C311-C312-C313-C314
5	A	1005	POV	O11-C1-C2-O21
5	B	1003	POV	O11-C1-C2-O21
5	D	1003	POV	C11-C12-N-C14
5	A	1008	POV	C215-C216-C217-C218
5	C	1007	POV	C215-C216-C217-C218
5	A	1002	POV	O21-C2-C3-O31
5	A	1005	POV	O21-C2-C3-O31
5	B	1002	POV	O21-C2-C3-O31
5	B	1003	POV	O21-C2-C3-O31
5	D	1003	POV	O21-C2-C3-O31
5	A	1007	POV	C1-C2-C3-O31
5	D	1002	POV	C1-C2-C3-O31
5	A	1002	POV	C313-C314-C315-C316
5	A	1004	POV	C11-O12-P-O14
5	A	1007	POV	C1-O11-P-O14
5	C	1003	POV	C11-C12-N-C14
5	C	1005	POV	C11-O12-P-O14
5	A	1003	POV	C36-C37-C38-C39
5	A	1005	POV	O31-C31-C32-C33
5	A	1002	POV	C2-C1-O11-P
5	C	1003	POV	C2-C1-O11-P
5	D	1001	POV	C310-C311-C312-C313
5	A	1002	POV	C11-C12-N-C13
5	A	1004	POV	C35-C36-C37-C38
5	A	1002	POV	C39-C310-C311-C312

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	B	1003	POV	C311-C312-C313-C314
5	C	1004	POV	C211-C212-C213-C214
5	A	1004	POV	C211-C212-C213-C214
5	A	1007	POV	C26-C27-C28-C29
5	A	1008	POV	C26-C27-C28-C29
5	D	1002	POV	C26-C27-C28-C29
5	B	1003	POV	O31-C31-C32-C33
5	A	1007	POV	C214-C215-C216-C217
5	A	1003	POV	C27-C28-C29-C210
5	A	1005	POV	C313-C314-C315-C316
5	B	1001	POV	C312-C313-C314-C315
5	D	1003	POV	C11-C12-N-C13
5	A	1002	POV	C25-C26-C27-C28
5	C	1005	POV	C29-C210-C211-C212
5	A	1003	POV	C212-C213-C214-C215
5	D	1002	POV	C214-C215-C216-C217
5	A	1002	POV	C36-C37-C38-C39
5	C	1004	POV	C33-C34-C35-C36
5	A	1003	POV	C213-C214-C215-C216
5	A	1008	POV	C313-C314-C315-C316
5	C	1003	POV	C32-C33-C34-C35
5	A	1002	POV	C11-C12-N-C15
5	B	1001	POV	C11-C12-N-C14
5	D	1003	POV	C11-C12-N-C15
5	A	1005	POV	C34-C35-C36-C37
5	A	1003	POV	C211-C212-C213-C214
5	B	1003	POV	C313-C314-C315-C316
5	C	1005	POV	C211-C212-C213-C214
5	A	1005	POV	C37-C38-C39-C310
5	C	1003	POV	C11-C12-N-C15
5	B	1001	POV	C310-C311-C312-C313
5	B	1003	POV	C34-C35-C36-C37
5	C	1004	POV	C34-C35-C36-C37
5	D	1002	POV	C27-C28-C29-C210
5	A	1008	POV	O21-C2-C3-O31
5	C	1007	POV	O21-C2-C3-O31
5	D	1001	POV	C210-C211-C212-C213
5	C	1003	POV	C215-C216-C217-C218
5	D	1001	POV	C39-C310-C311-C312
5	A	1005	POV	C311-C310-C39-C38
5	A	1004	POV	C29-C210-C211-C212
5	A	1007	POV	C215-C216-C217-C218

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	C	1003	POV	C11-C12-N-C13
5	B	1001	POV	C36-C37-C38-C39
5	C	1007	POV	C212-C213-C214-C215
5	A	1005	POV	O11-C1-C2-C3
5	B	1003	POV	O11-C1-C2-C3
5	D	1003	POV	O11-C1-C2-C3
5	A	1005	POV	C27-C28-C29-C210
5	B	1003	POV	C27-C28-C29-C210
5	C	1004	POV	C27-C28-C29-C210
5	C	1004	POV	C35-C36-C37-C38
5	D	1001	POV	C29-C210-C211-C212
5	D	1002	POV	C29-C210-C211-C212
5	C	1007	POV	C313-C314-C315-C316
5	B	1002	POV	C311-C312-C313-C314
5	C	1007	POV	C25-C26-C27-C28
5	B	1001	POV	C21-C22-C23-C24
5	D	1002	POV	C215-C216-C217-C218
5	C	1003	POV	C29-C210-C211-C212
5	C	1005	POV	C33-C34-C35-C36
5	A	1003	POV	C311-C312-C313-C314
5	A	1002	POV	C32-C33-C34-C35
5	A	1002	POV	C29-C210-C211-C212
5	A	1003	POV	C29-C210-C211-C212
5	A	1007	POV	C27-C28-C29-C210
5	B	1002	POV	O11-C1-C2-C3
5	B	1001	POV	C11-C12-N-C15
5	B	1002	POV	C11-C12-N-C14
5	C	1005	POV	O21-C21-C22-C23
5	B	1001	POV	C29-C210-C211-C212
5	C	1004	POV	C29-C210-C211-C212
5	A	1002	POV	C211-C212-C213-C214
5	B	1002	POV	O31-C31-C32-C33
5	A	1004	POV	O21-C21-C22-C23
5	A	1005	POV	C215-C216-C217-C218
5	D	1003	POV	O31-C31-C32-C33
5	D	1001	POV	C35-C36-C37-C38
5	B	1001	POV	C11-C12-N-C13
5	A	1007	POV	C29-C210-C211-C212
5	A	1004	POV	C214-C215-C216-C217
5	C	1003	POV	C211-C212-C213-C214
5	C	1004	POV	C31-C32-C33-C34
5	C	1004	POV	C213-C214-C215-C216

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	D	1003	POV	C311-C312-C313-C314
5	A	1008	POV	C25-C26-C27-C28
5	A	1004	POV	C26-C27-C28-C29
5	A	1005	POV	C2-C1-O11-P
5	C	1005	POV	O22-C21-C22-C23
5	A	1003	POV	C312-C313-C314-C315
5	D	1001	POV	C214-C215-C216-C217
5	B	1003	POV	C215-C216-C217-C218
5	B	1002	POV	O32-C31-C32-C33
5	C	1005	POV	C214-C215-C216-C217
5	A	1004	POV	C31-C32-C33-C34
5	B	1003	POV	O22-C21-O21-C2
5	D	1003	POV	O32-C31-C32-C33
5	A	1004	POV	O22-C21-C22-C23
5	C	1005	POV	C212-C213-C214-C215
5	A	1005	POV	O22-C21-O21-C2
5	D	1002	POV	C313-C314-C315-C316
5	A	1008	POV	C212-C213-C214-C215

There are no ring outliers.

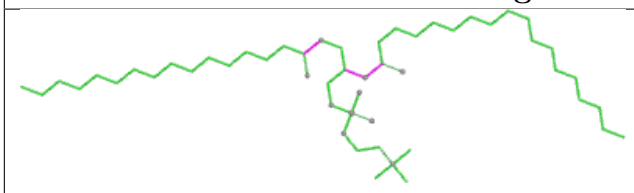
15 monomers are involved in 38 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	1001	POV	7	0
5	A	1004	POV	3	0
5	A	1003	POV	3	0
5	B	1002	POV	1	0
5	A	1005	POV	2	0
5	D	1002	POV	5	0
5	B	1001	POV	6	0
5	C	1003	POV	1	0
5	B	1003	POV	1	0
5	C	1007	POV	2	0
5	A	1002	POV	1	0
5	A	1008	POV	2	0
5	C	1005	POV	3	0
5	A	1007	POV	5	0
5	C	1004	POV	2	0

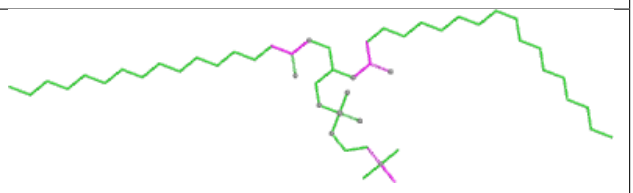
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

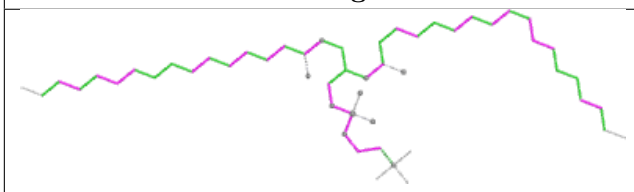
Ligand POV D 1001



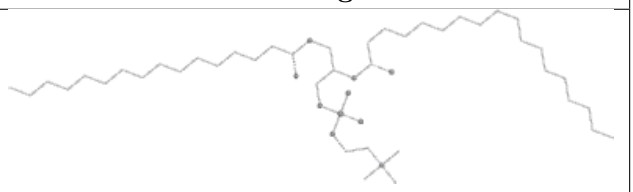
Bond lengths



Bond angles

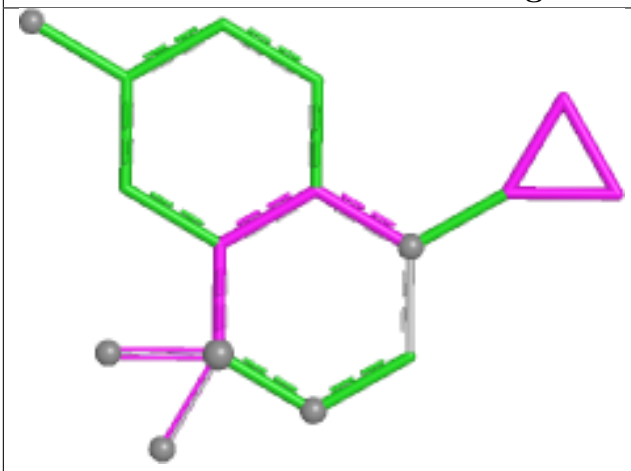


Torsions

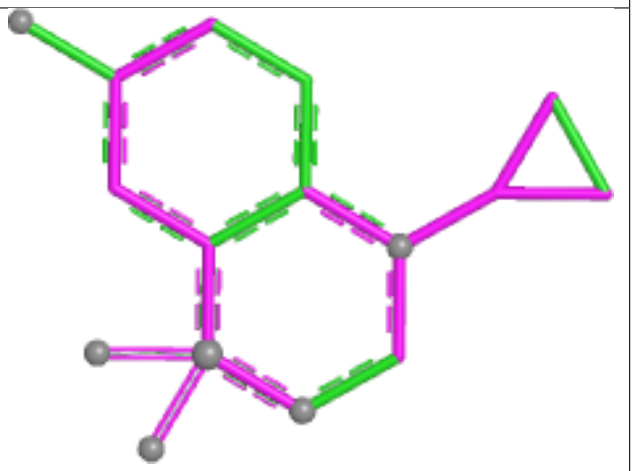


Rings

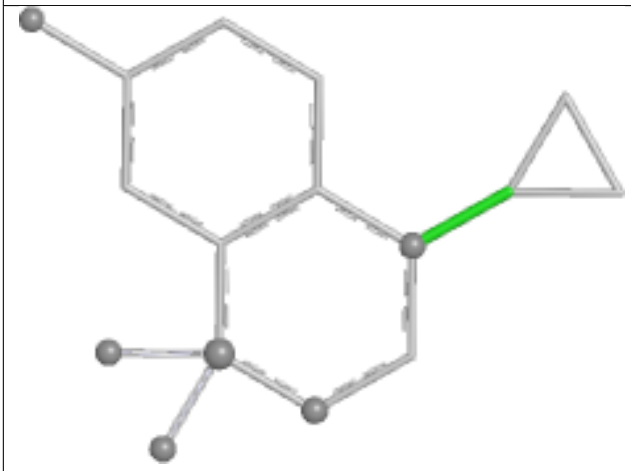
Ligand 2J9 C 1002



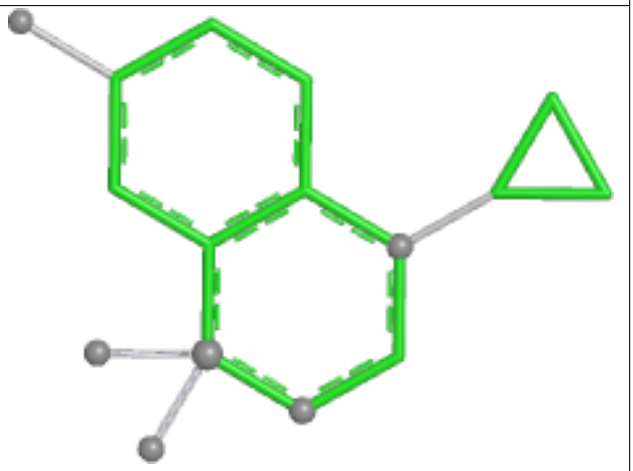
Bond lengths



Bond angles

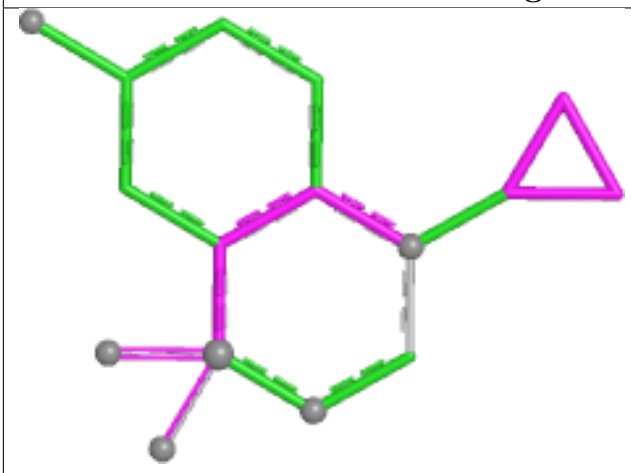


Torsions

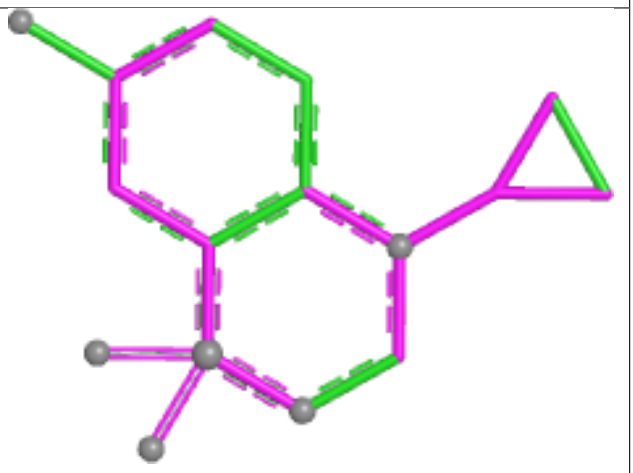


Rings

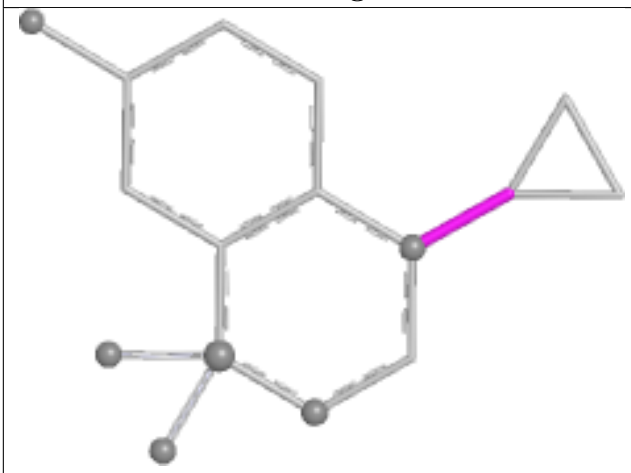
Ligand 2J9 A 1001



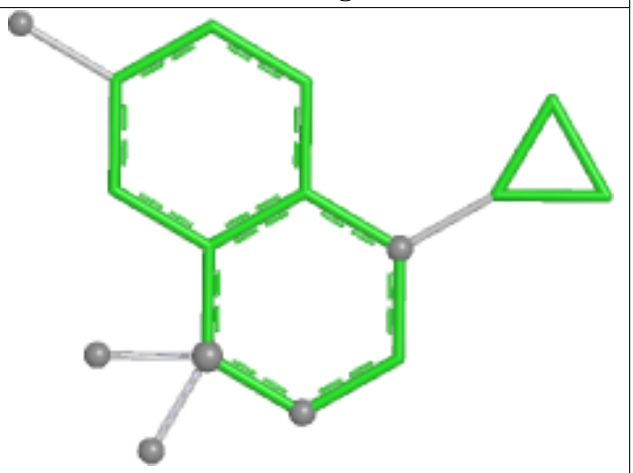
Bond lengths



Bond angles

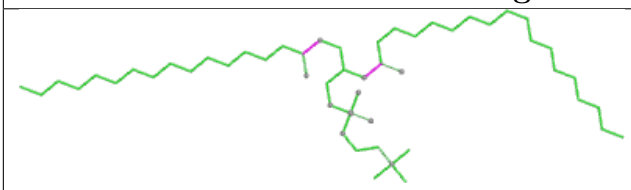


Torsions

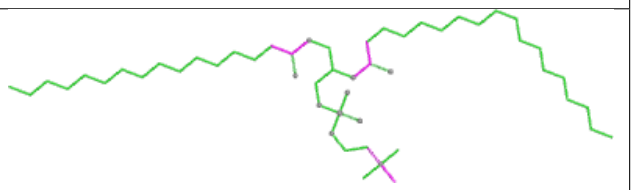


Rings

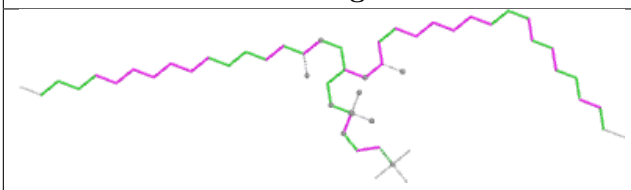
Ligand POV A 1004



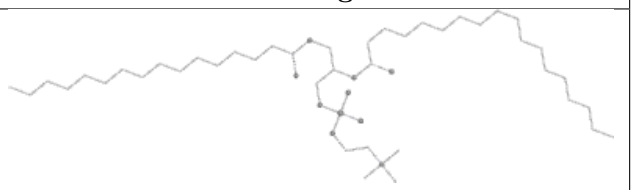
Bond lengths



Bond angles

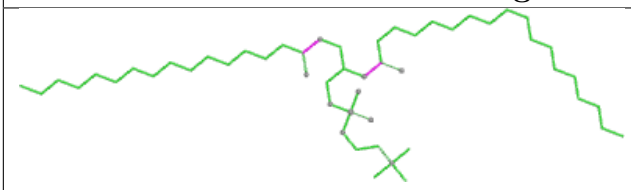


Torsions

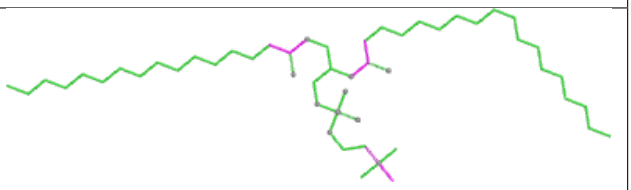


Rings

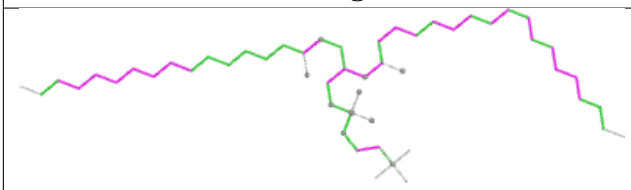
Ligand POV A 1003



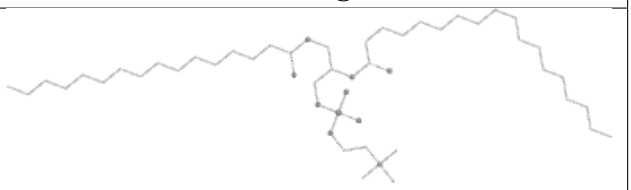
Bond lengths



Bond angles

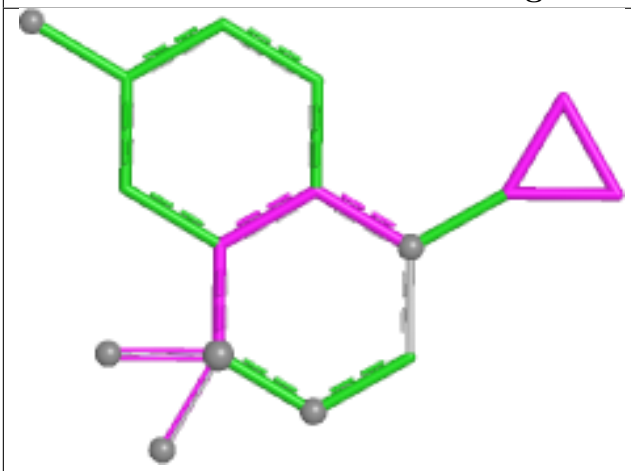


Torsions

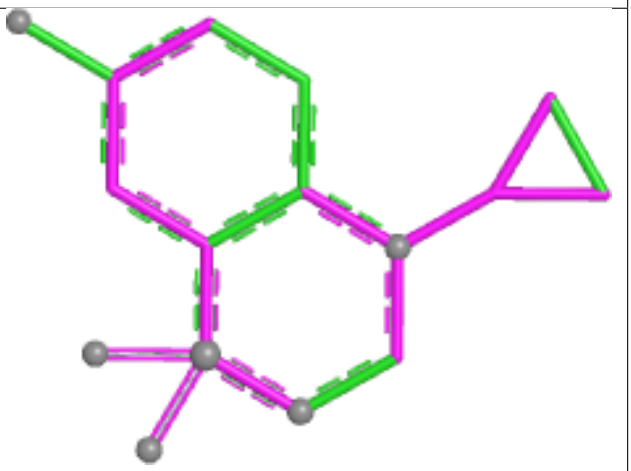


Rings

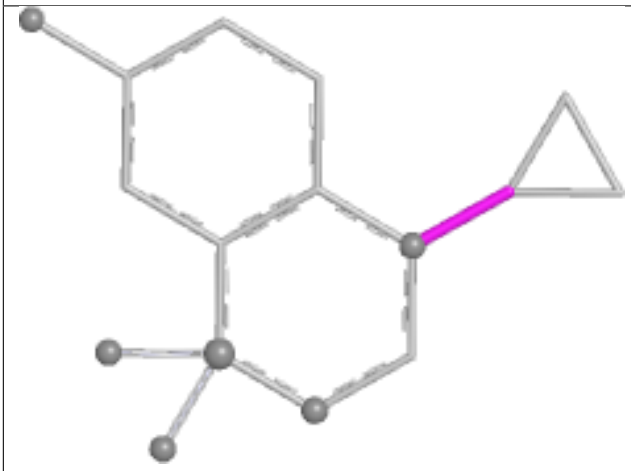
Ligand 2J9 C 1001



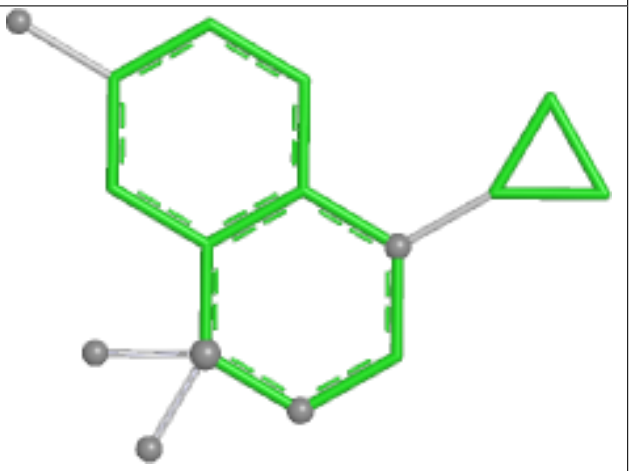
Bond lengths



Bond angles

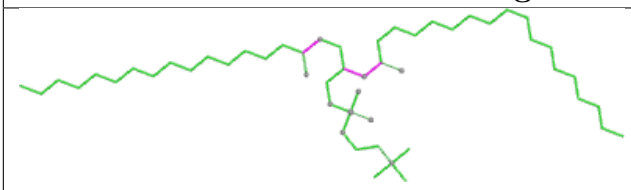


Torsions

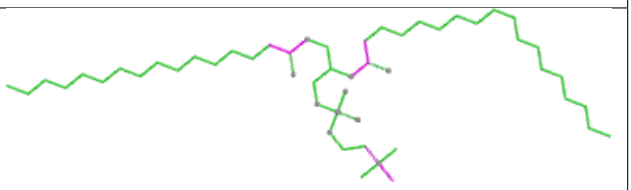


Rings

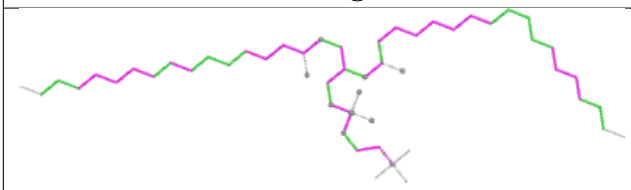
Ligand POV B 1002



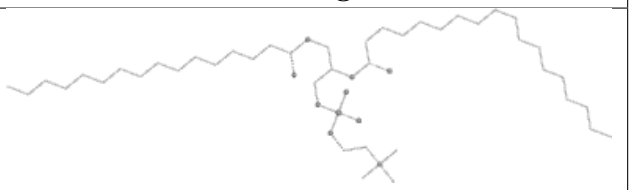
Bond lengths



Bond angles

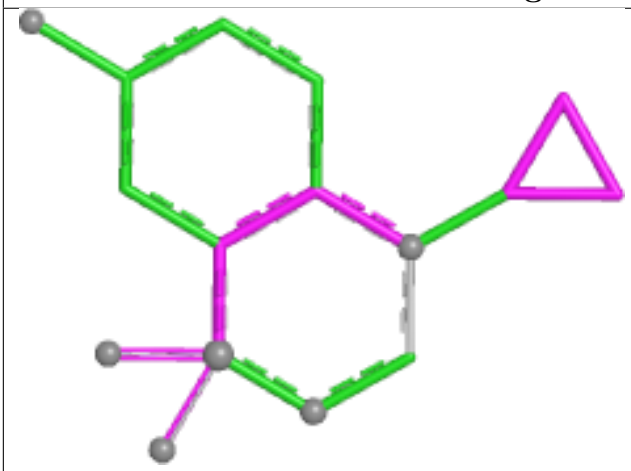


Torsions

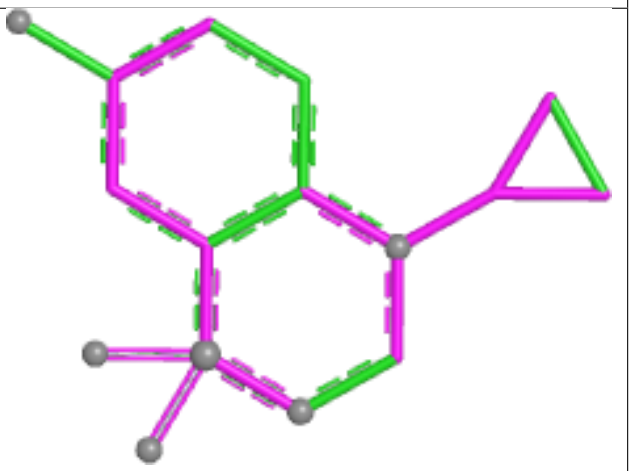


Rings

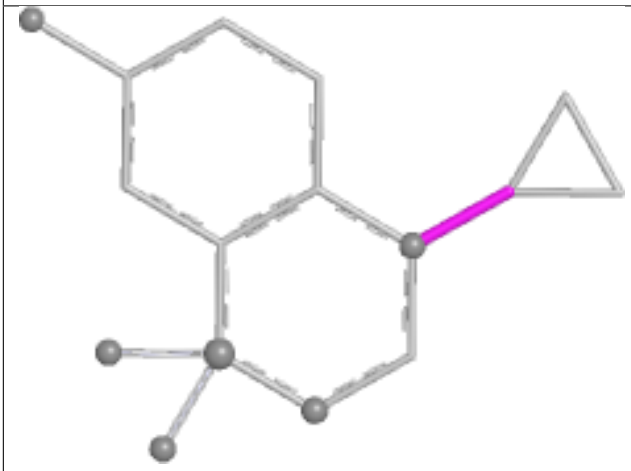
Ligand 2J9 A 1009



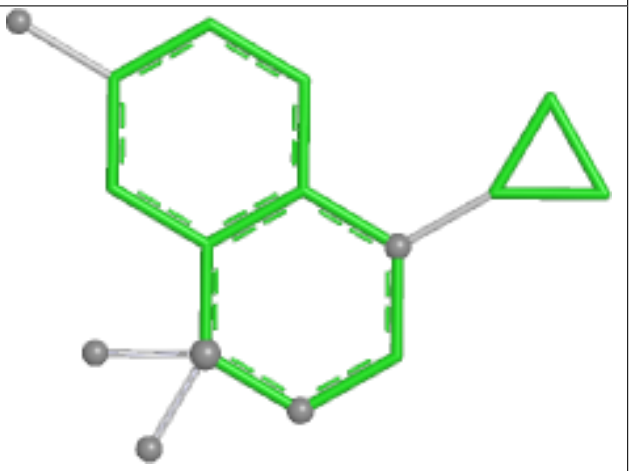
Bond lengths



Bond angles

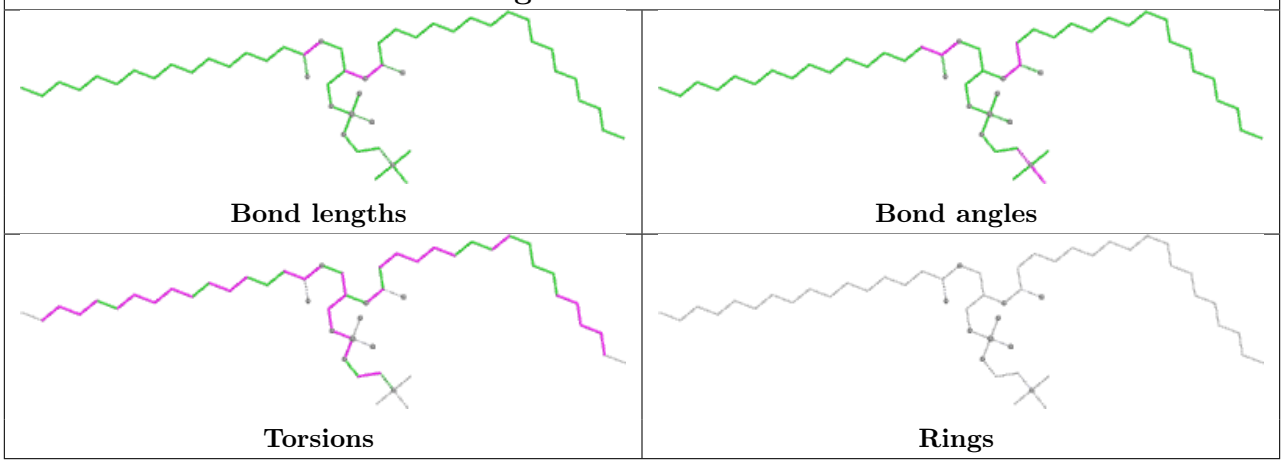


Torsions

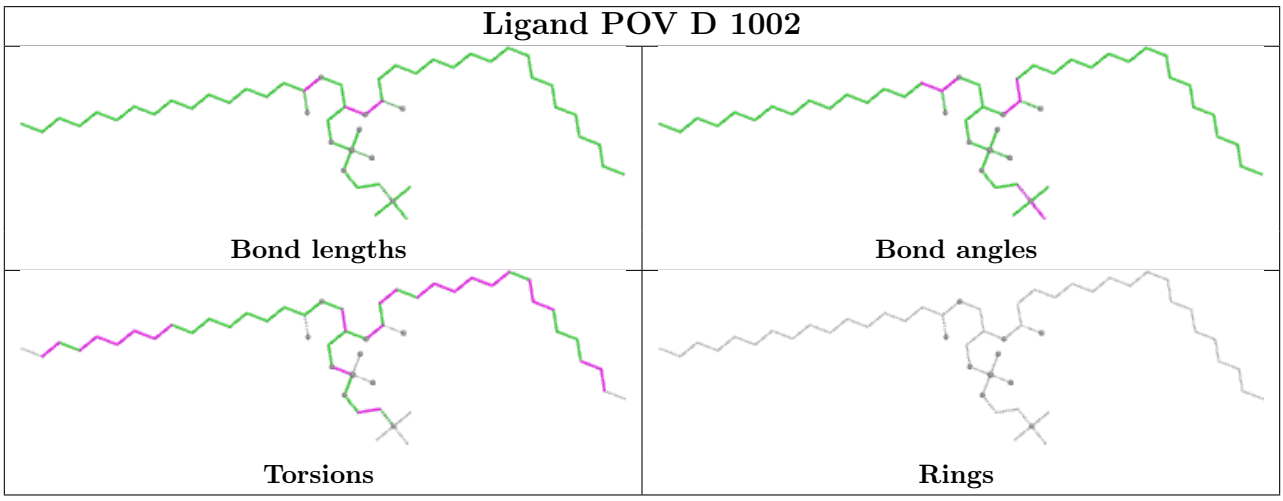


Rings

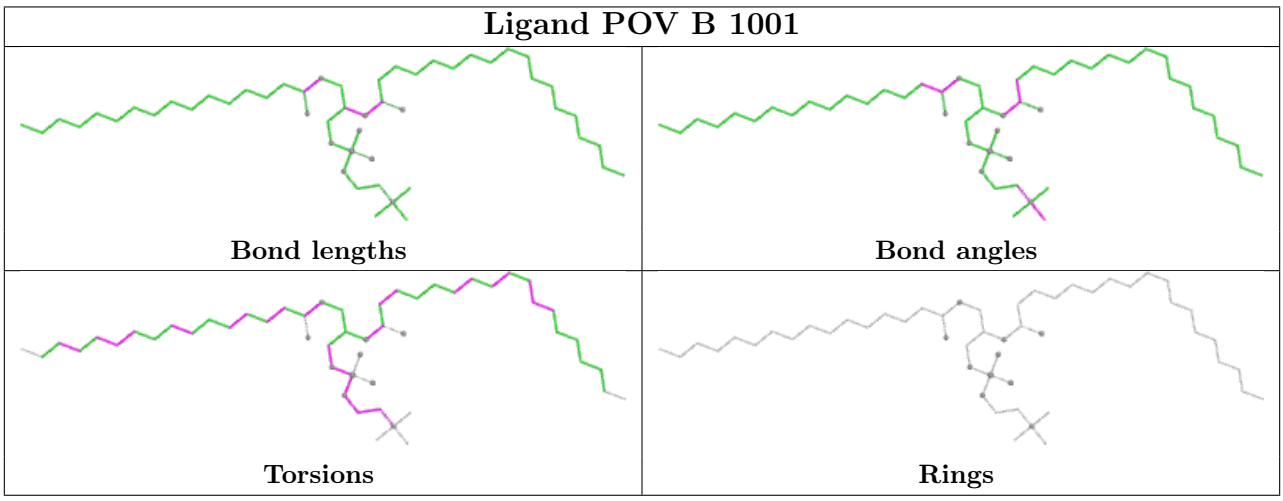
Ligand POV A 1005



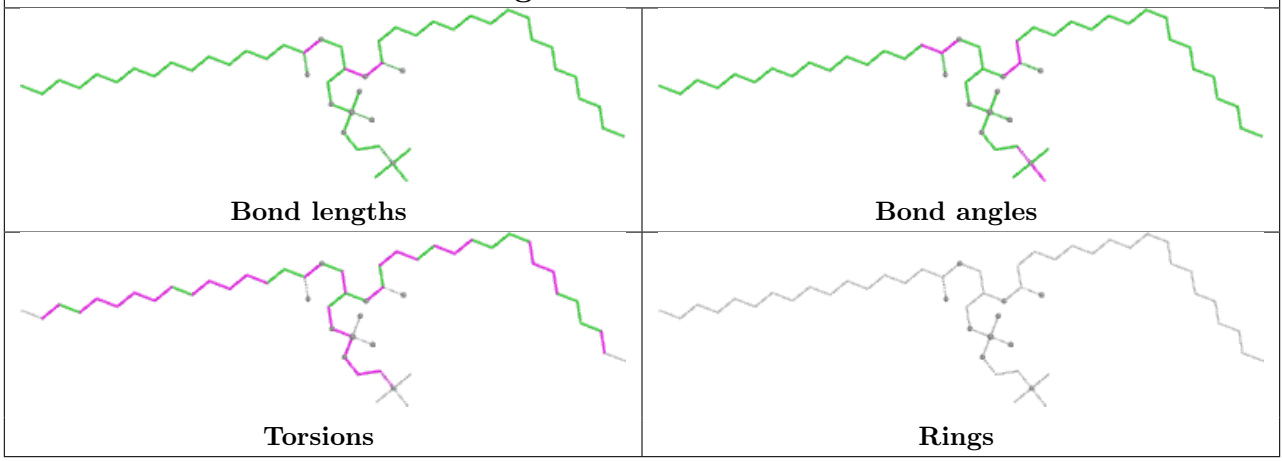
Ligand POV D 1002



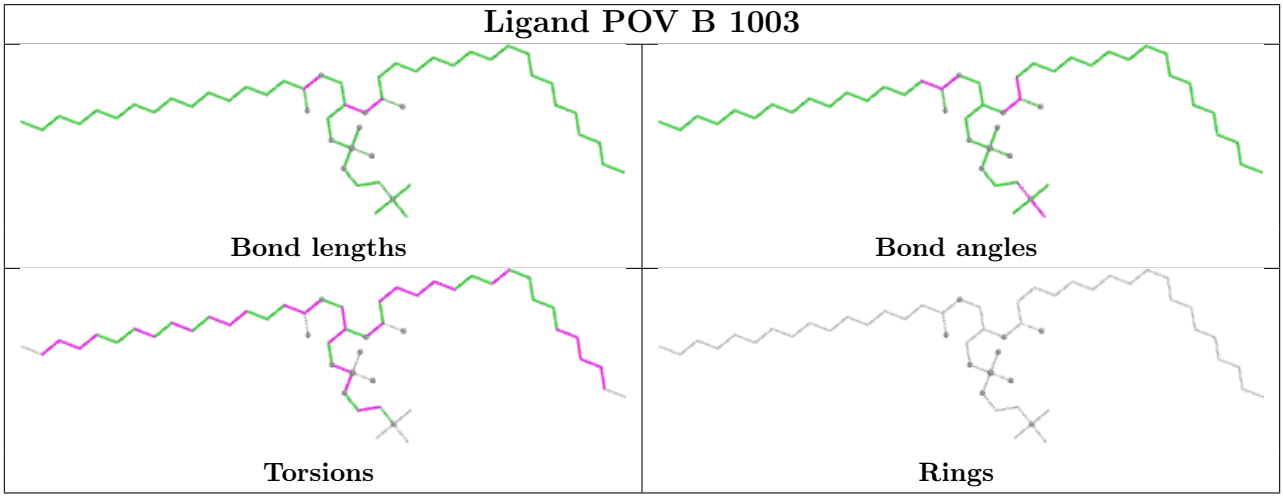
Ligand POV B 1001



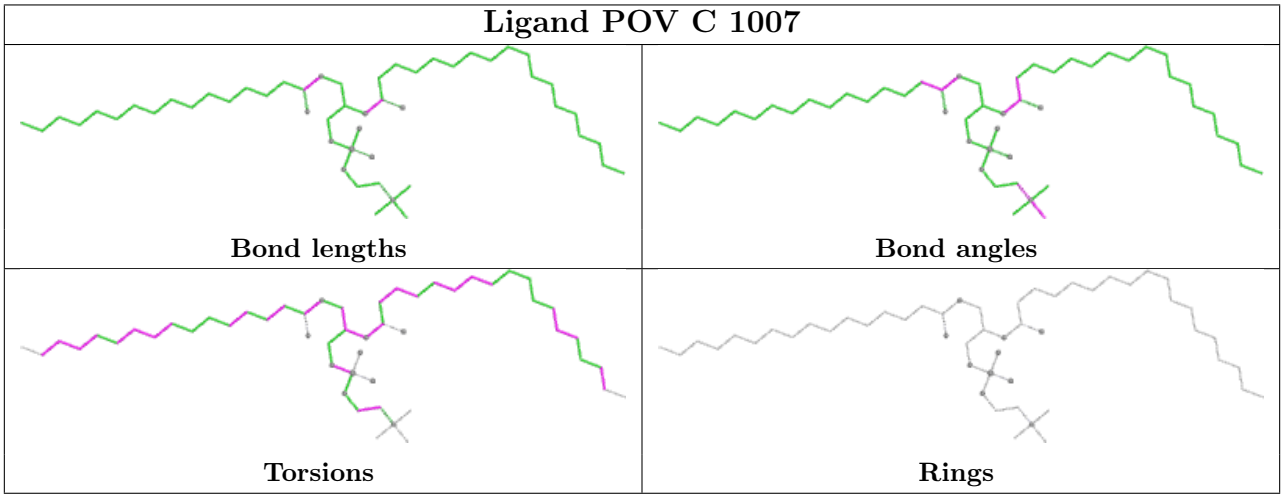
Ligand POV C 1003



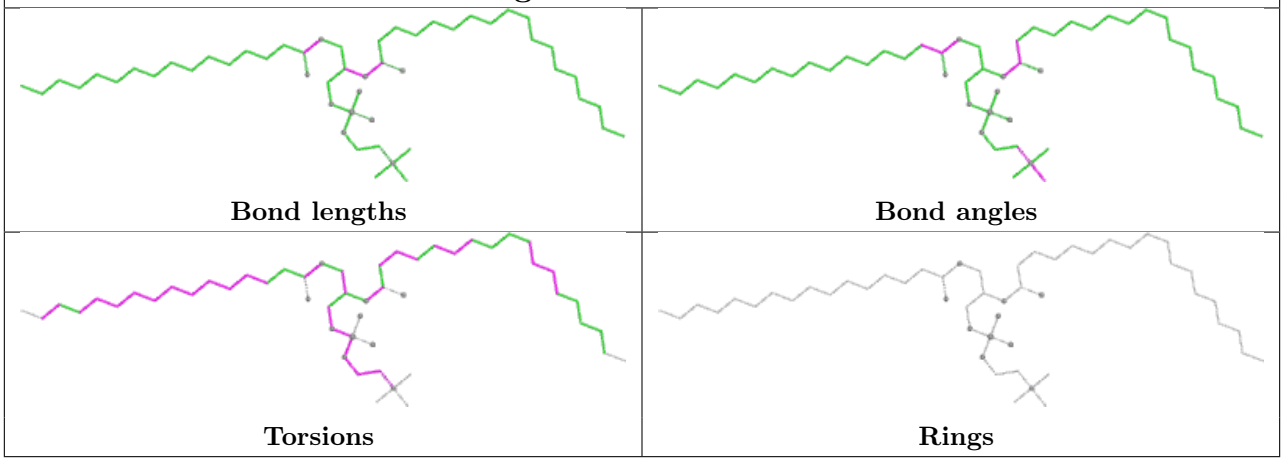
Ligand POV B 1003



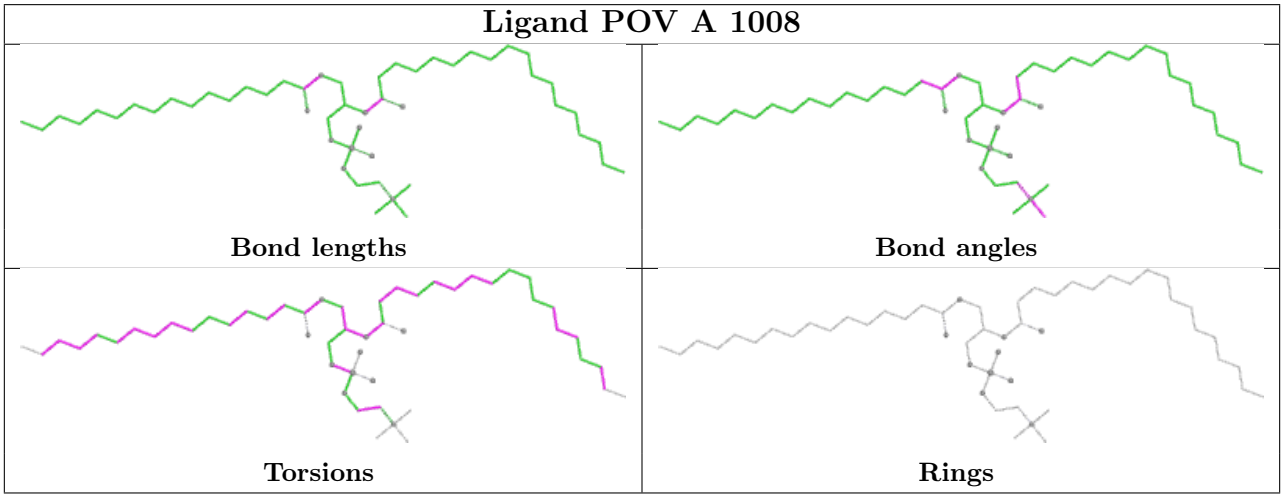
Ligand POV C 1007



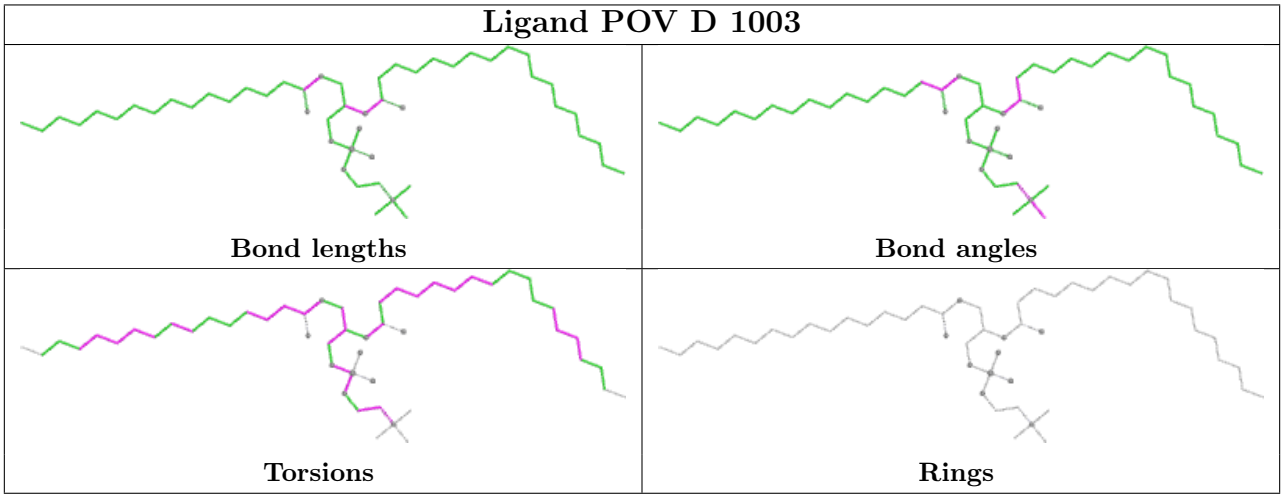
Ligand POV A 1002

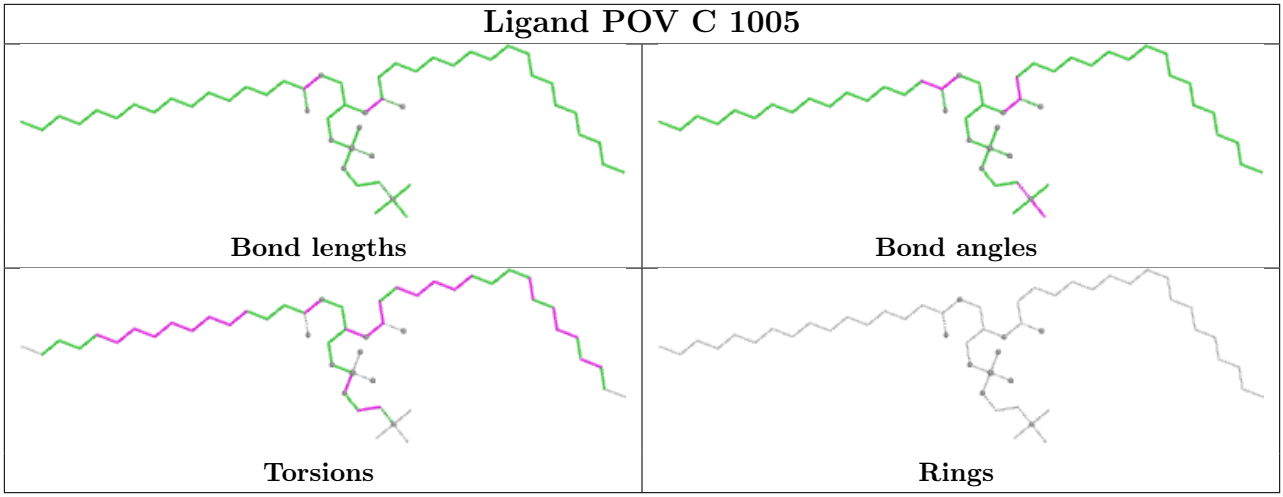


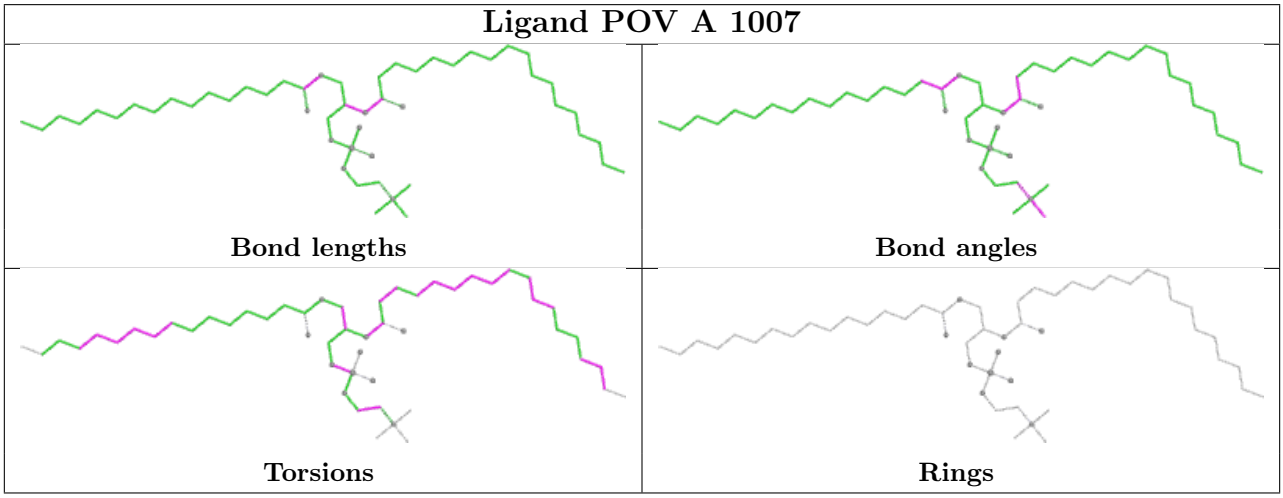
Ligand POV A 1008

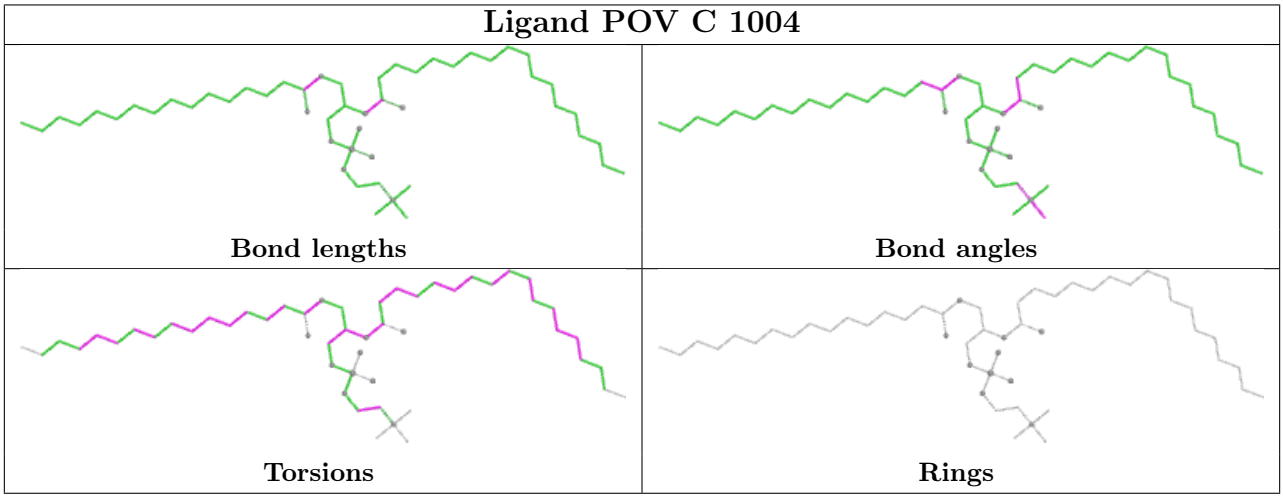


Ligand POV D 1003









5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

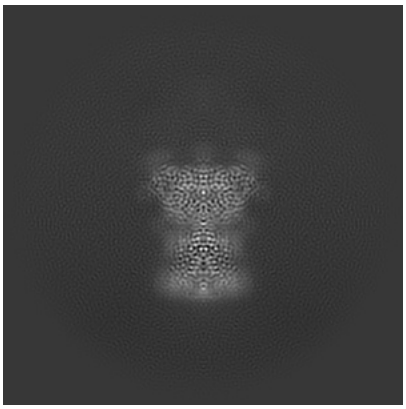
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-29517. These allow visual inspection of the internal detail of the map and identification of artifacts.

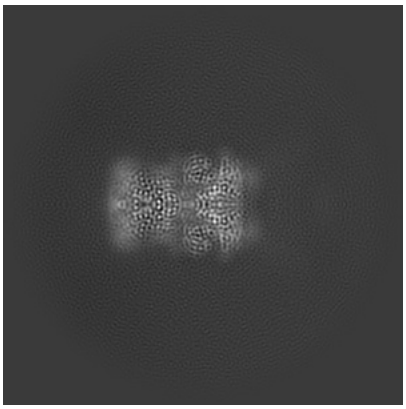
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

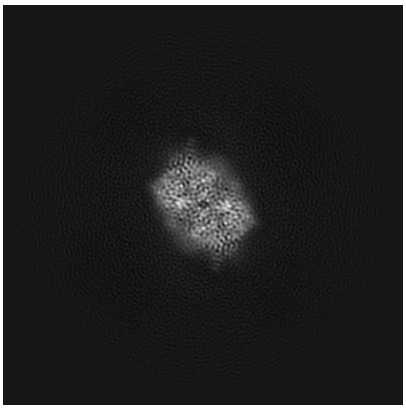
6.1.1 Primary map



X

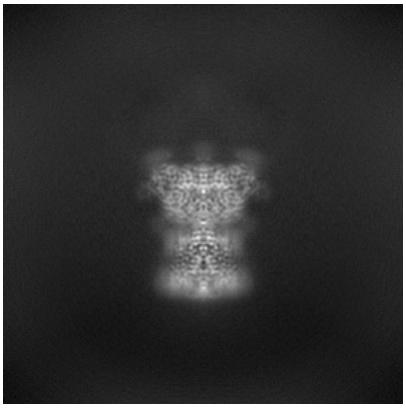


Y

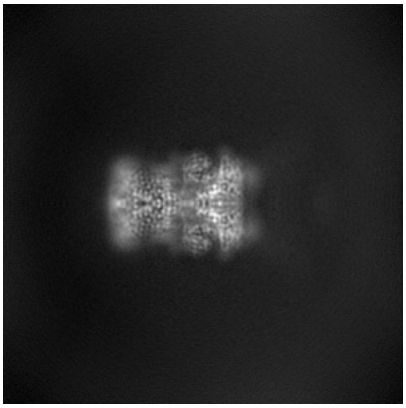


Z

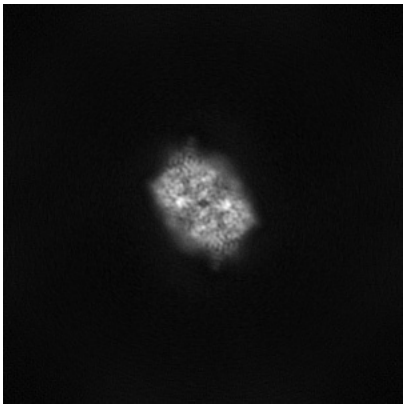
6.1.2 Raw map



X



Y

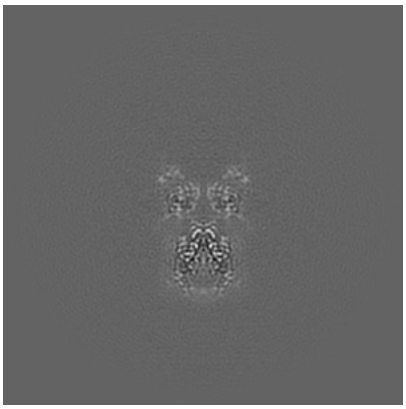


Z

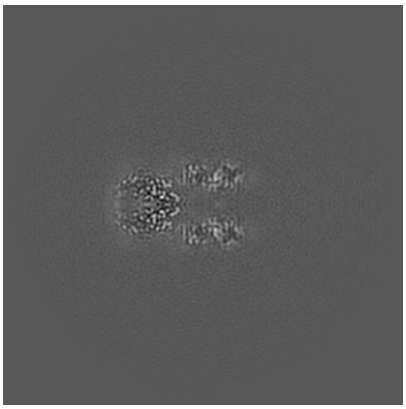
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

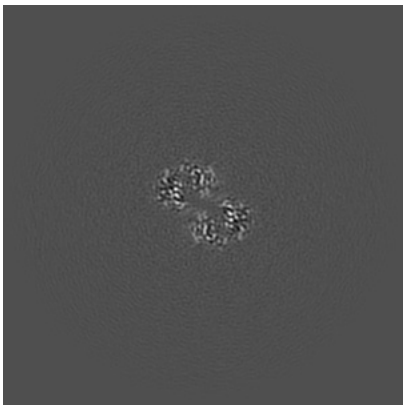
6.2.1 Primary map



X Index: 192

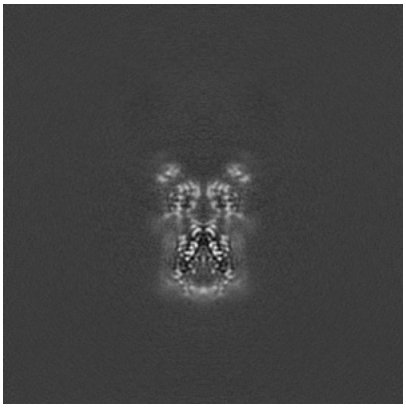


Y Index: 192

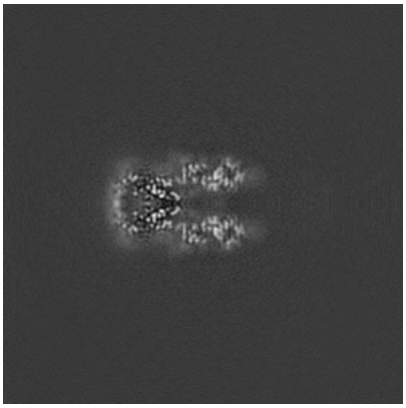


Z Index: 192

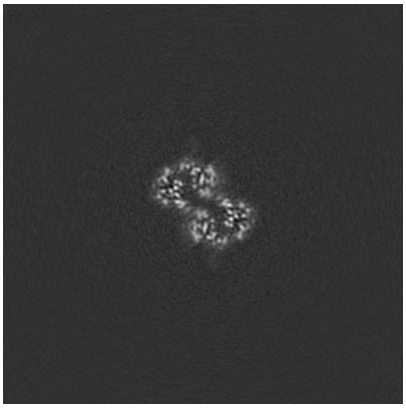
6.2.2 Raw map



X Index: 192



Y Index: 192

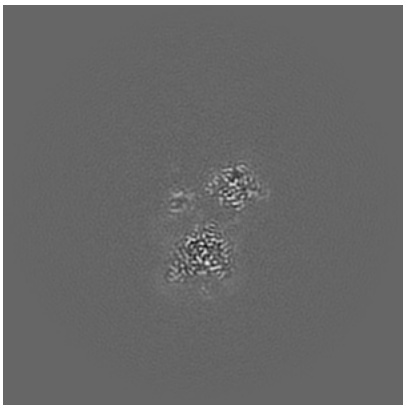


Z Index: 192

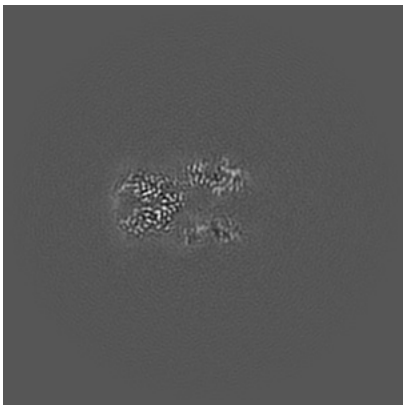
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

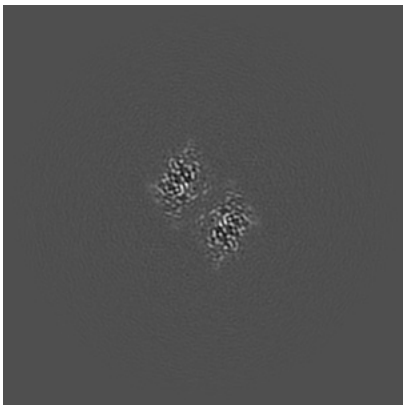
6.3.1 Primary map



X Index: 182

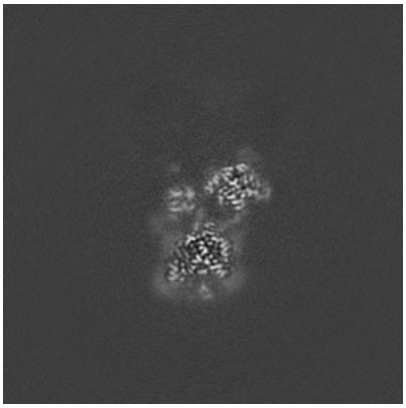


Y Index: 189

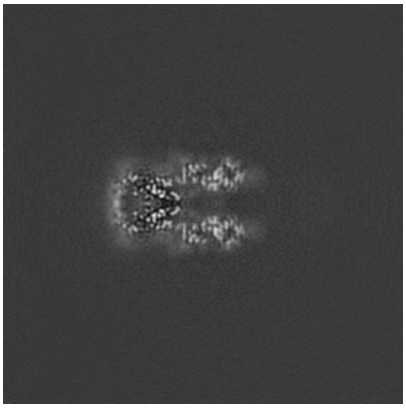


Z Index: 211

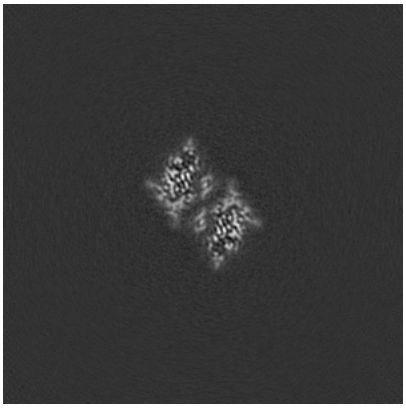
6.3.2 Raw map



X Index: 182



Y Index: 192

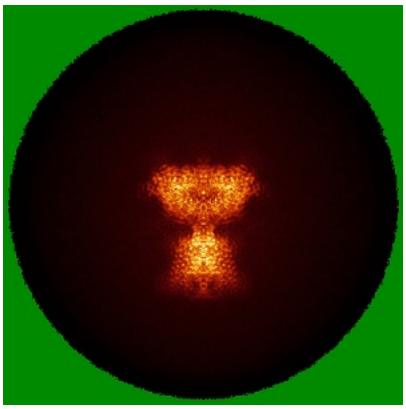


Z Index: 209

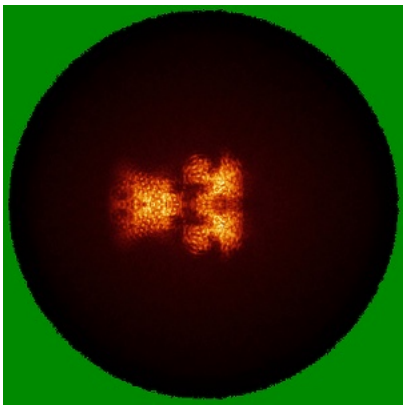
The images above show the largest variance slices of the map in three orthogonal directions.

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

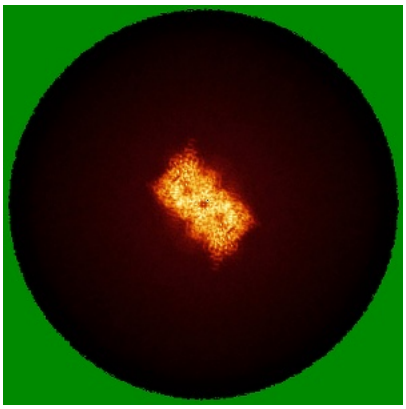
6.4.1 Primary map



X

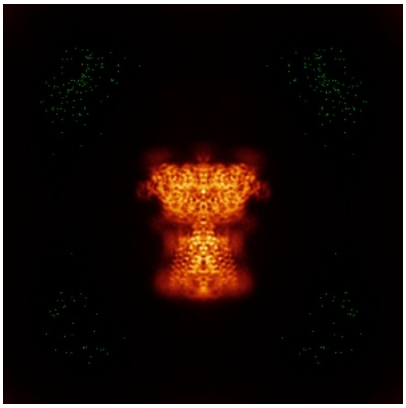


Y

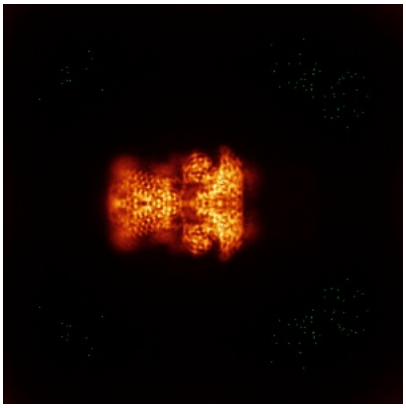


Z

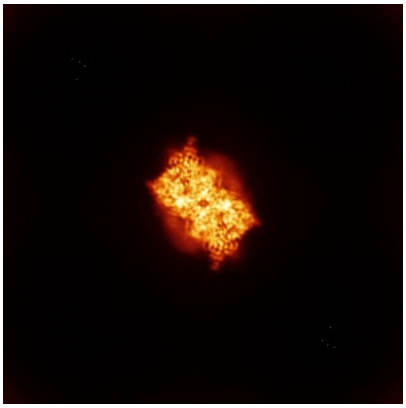
6.4.2 Raw map



X



Y

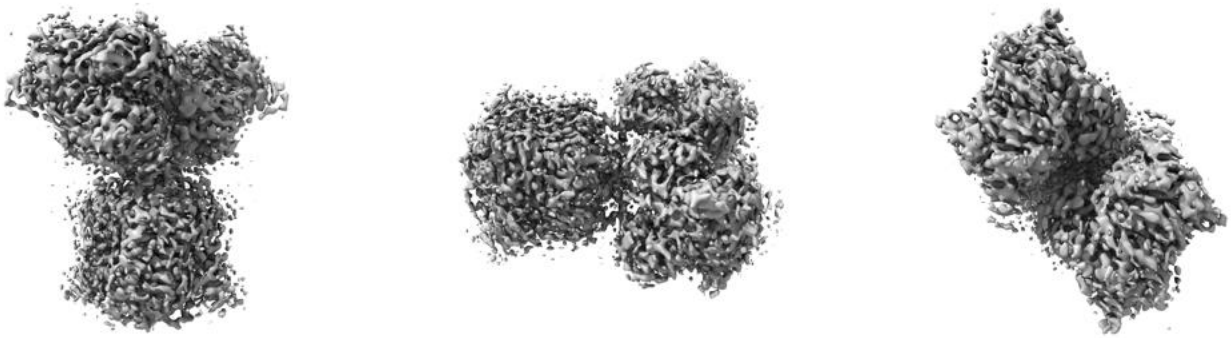


Z

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)

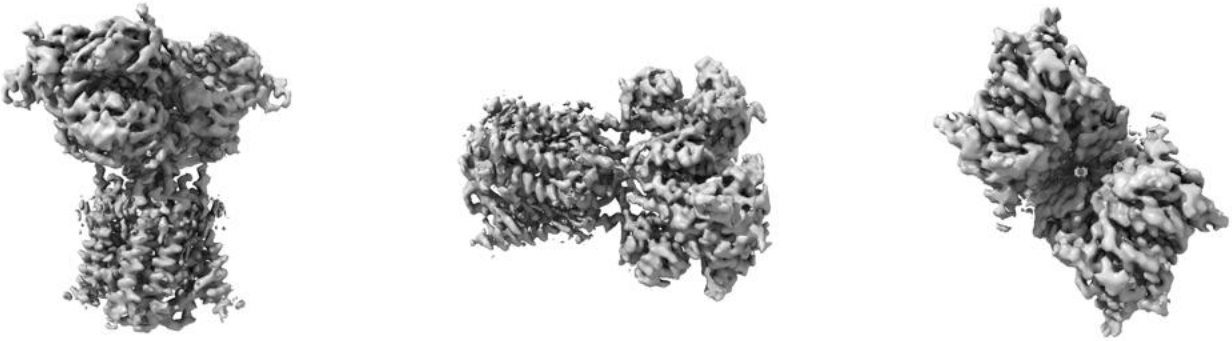
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.5. 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.

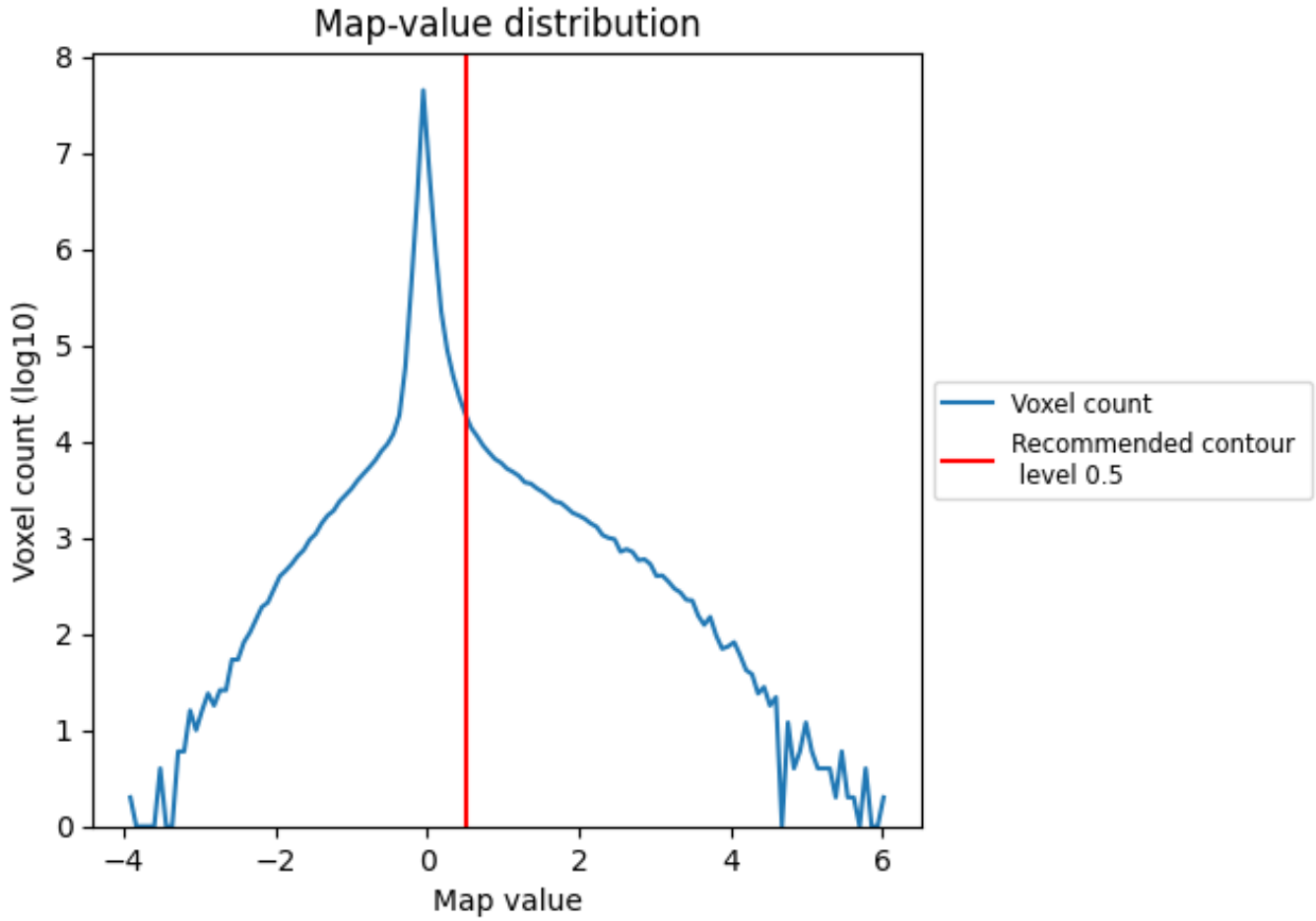
6.6 Mask visualisation (i)

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

7 Map analysis

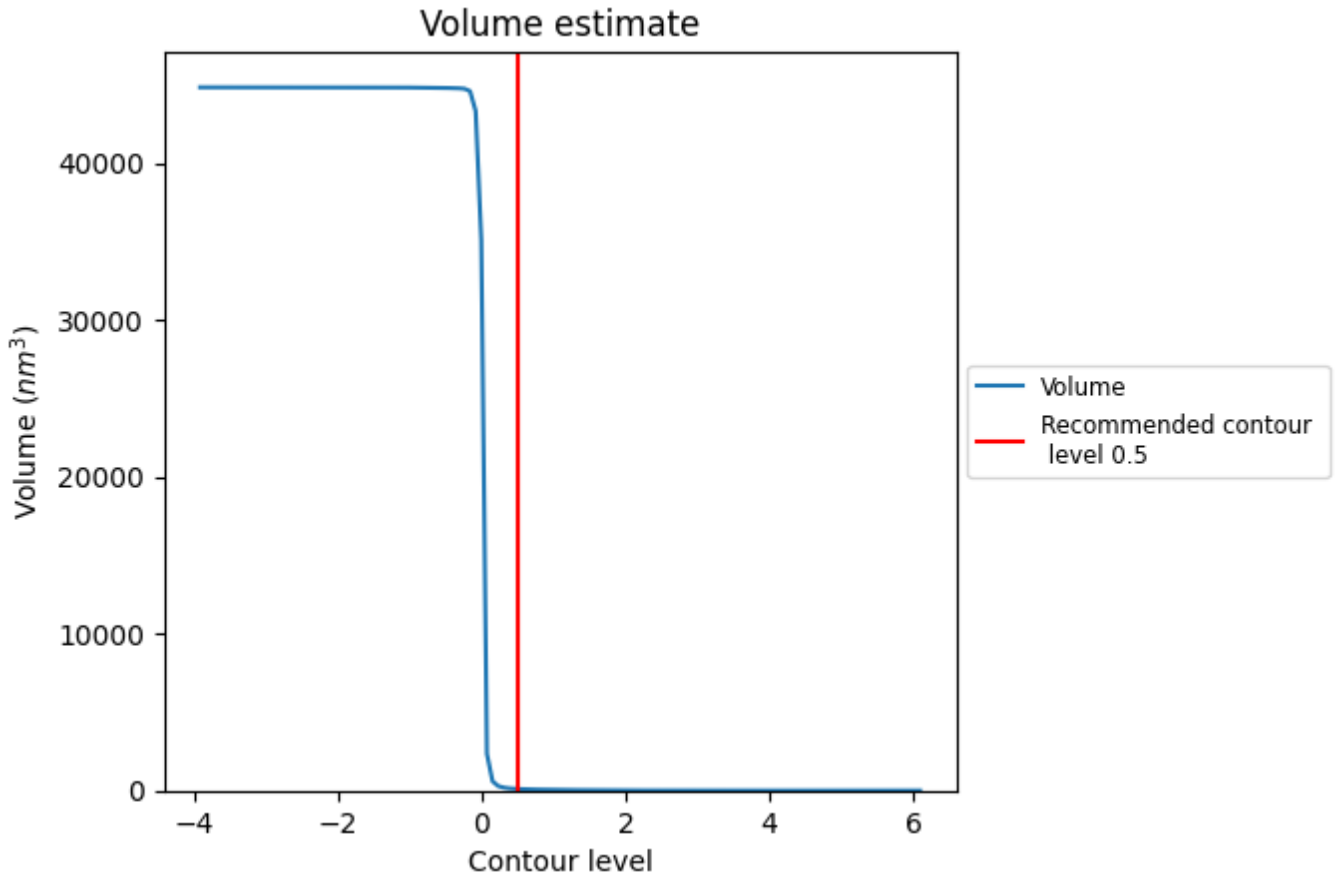
This section contains the results of statistical analysis of the map.

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.

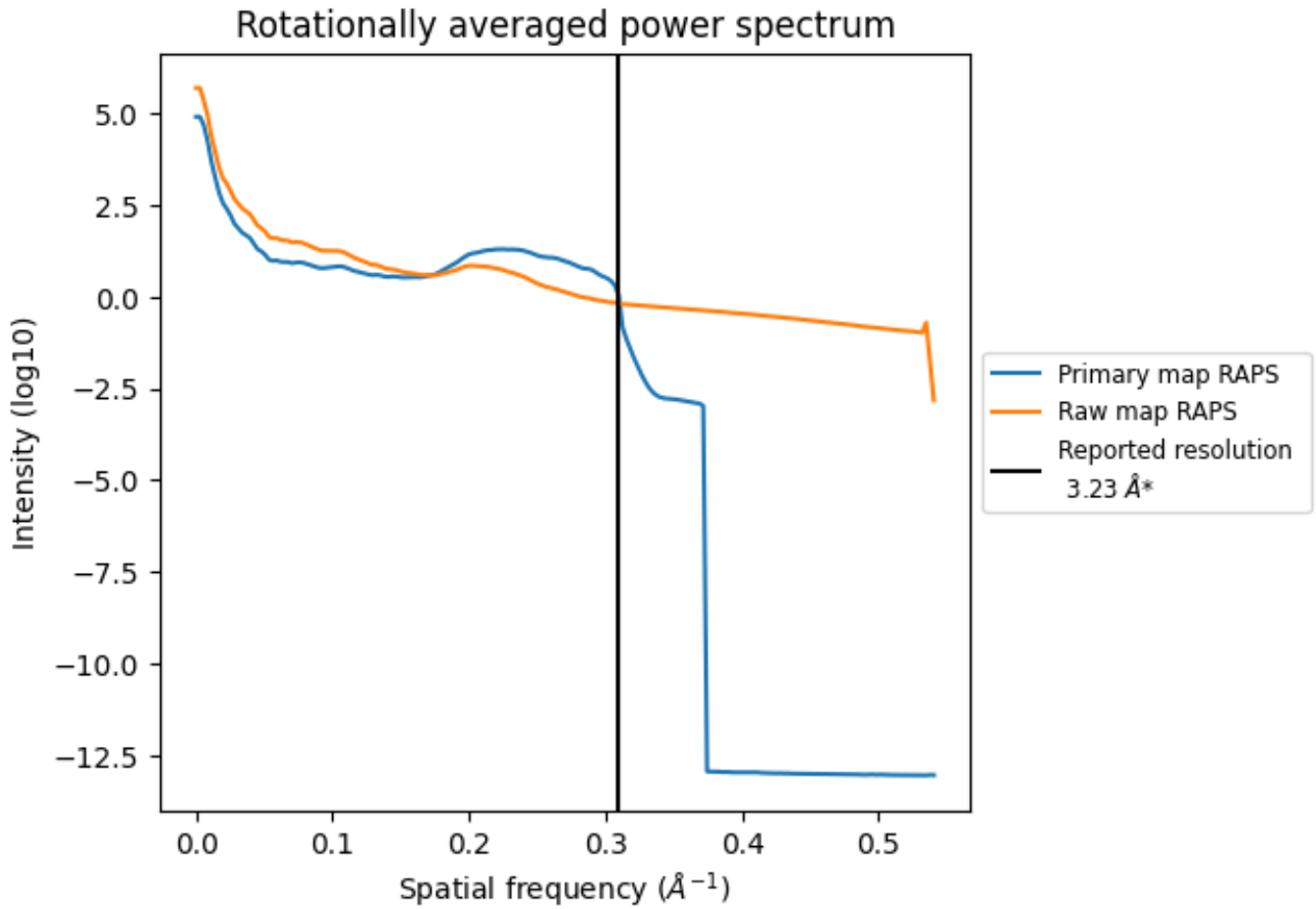
7.2 Volume estimate



The volume at the recommended contour level is 103 nm^3; this corresponds to an approximate mass of 93 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)

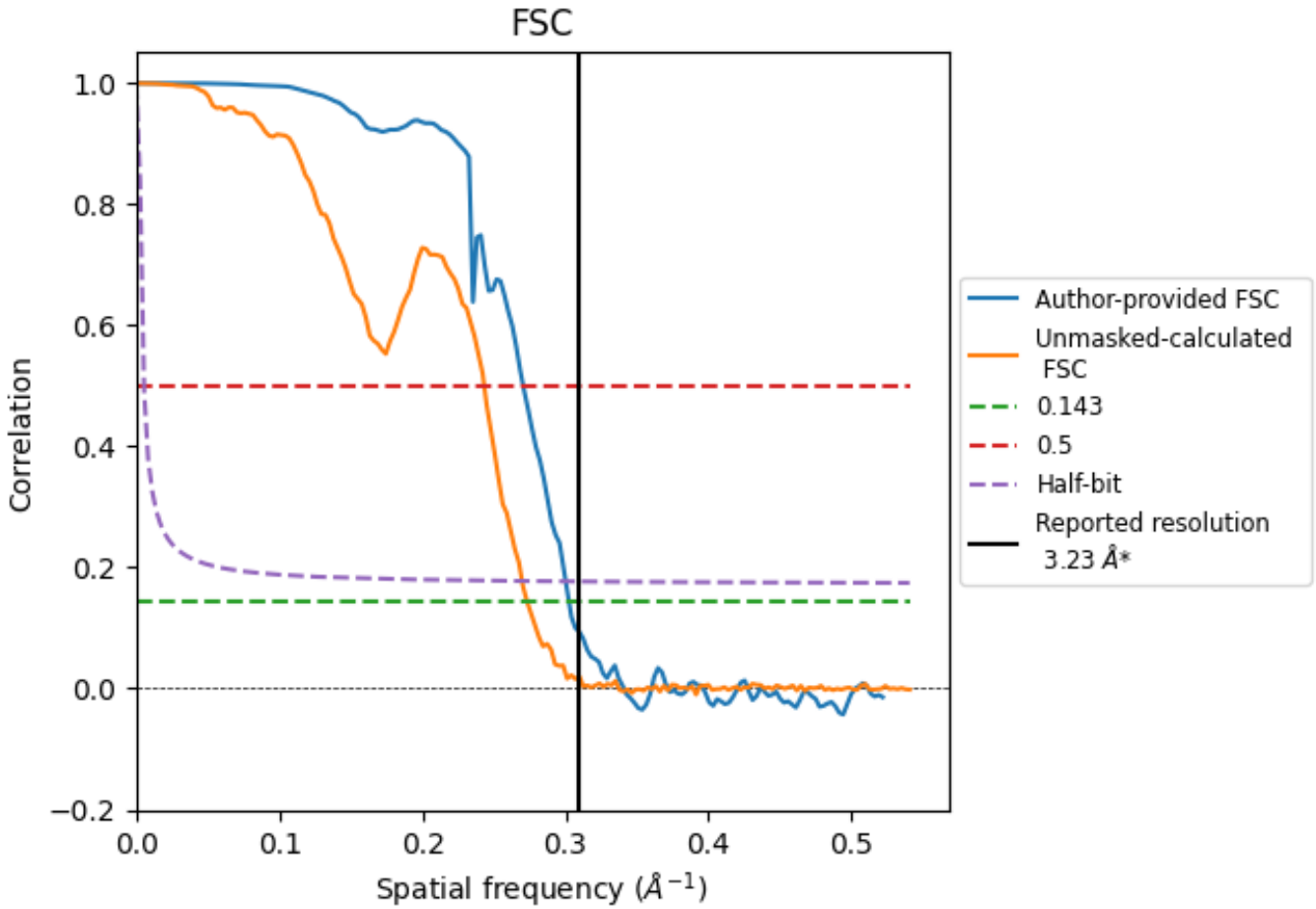


*Reported resolution corresponds to spatial frequency of 0.310 $Å^{-1}$

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 0.310 Å^{-1}

8.2 Resolution estimates (i)

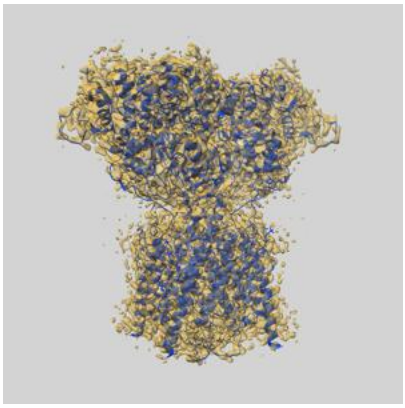
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.23	-	-
Author-provided FSC curve	3.31	3.70	3.33
Unmasked-calculated*	3.66	4.11	3.71

*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 3.66 differs from the reported value 3.23 by more than 10 %

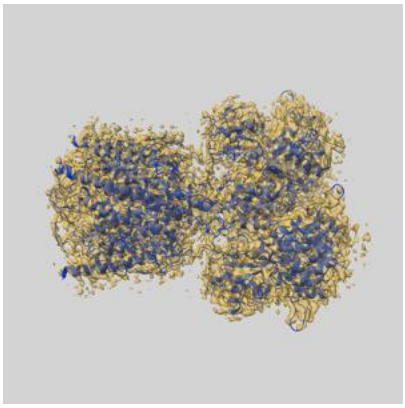
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-29517 and PDB model 8FWS. Per-residue inclusion information can be found in section 3 on page 9.

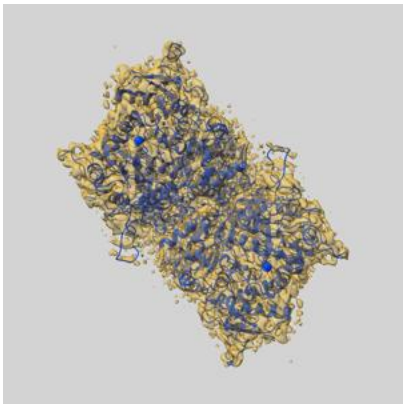
9.1 Map-model overlay



X



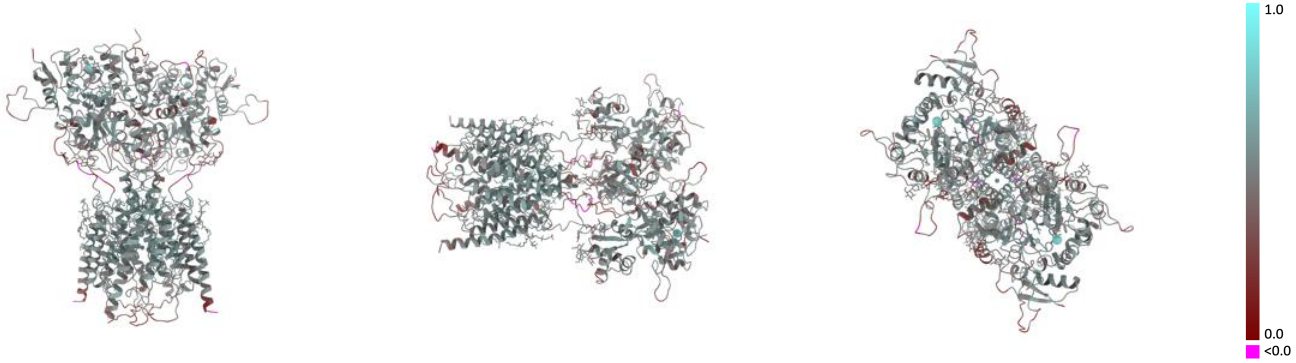
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.5 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.

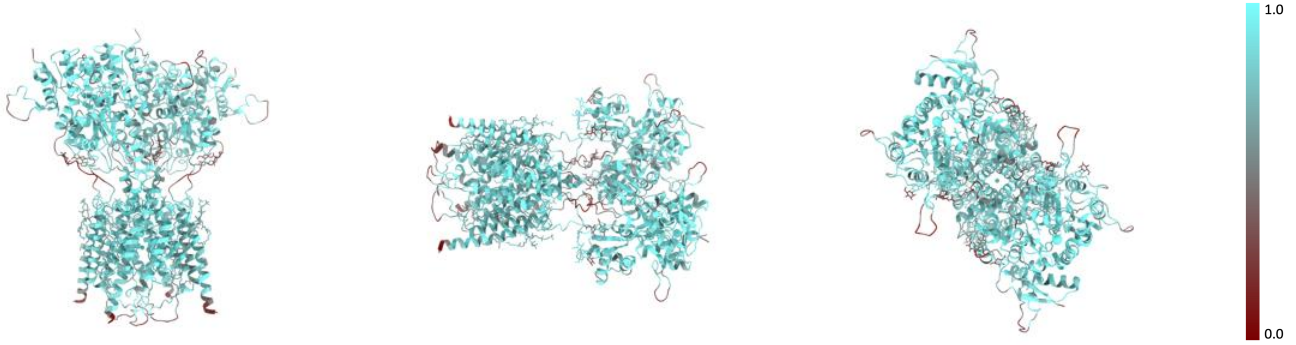
9.2 Q-score mapped to coordinate model (i)



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.

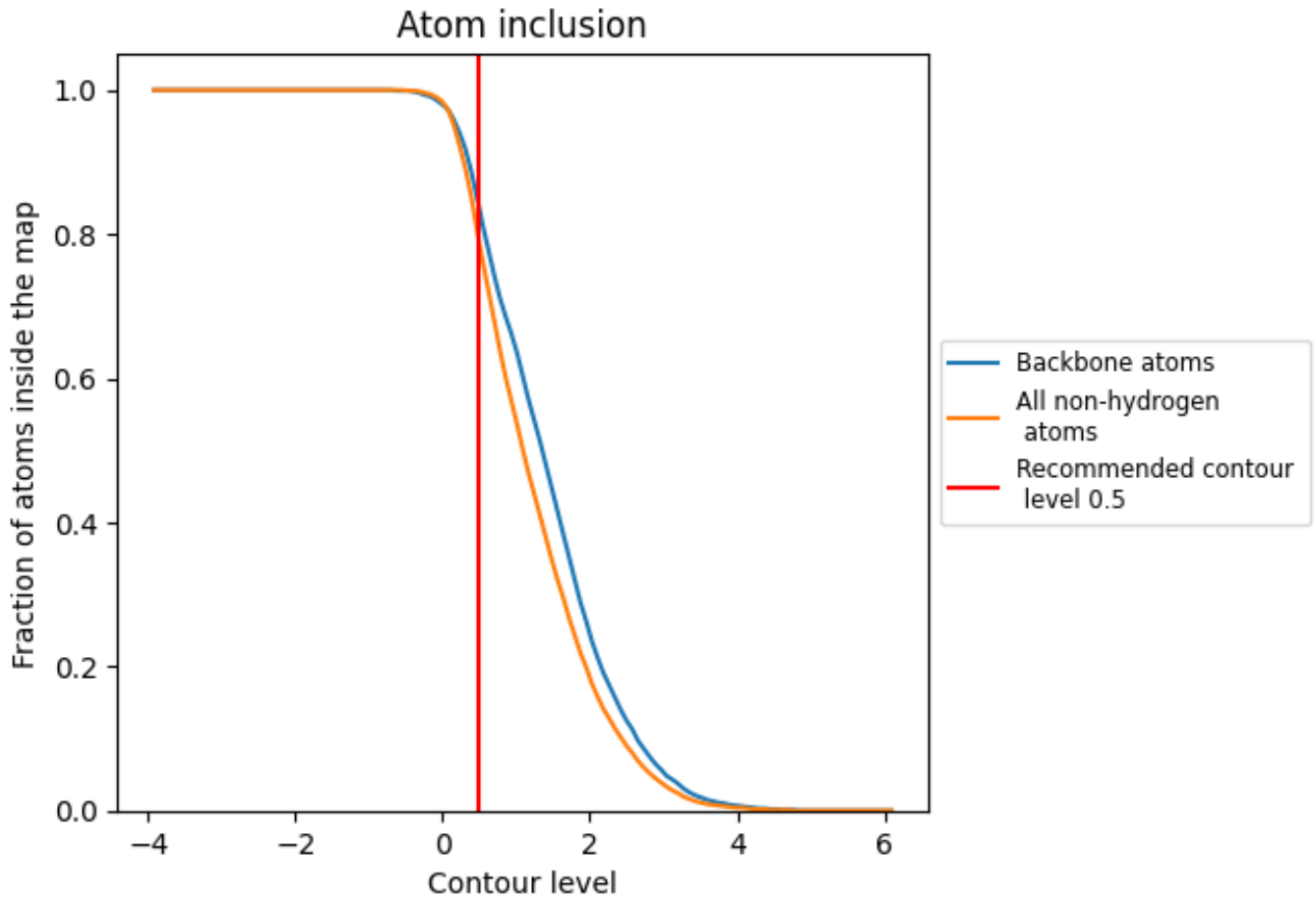
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.5).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 79% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7870	0.4810
A	0.7810	0.4780
B	0.8040	0.4900
C	0.7800	0.4740
D	0.7980	0.4880
E	0.4640	0.3760
F	0.8000	0.4700
G	0.2140	0.2690
H	0.3930	0.4010
I	0.7600	0.4700
J	0.2500	0.2870

