



## Full wwPDB EM Validation Report ⓘ

Sep 8, 2025 – 06:49 PM EDT

PDB ID : 9N4R / pdb\_00009n4r  
EMDB ID : EMD-48903  
Title : Composite map for GluK2-0xNeto2 in the open state, in complex with the positive allosteric modulator BPAM344 and agonist kainate  
Authors : Gangwar, S.P.; Yelshanskaya, M.V.; Yen, L.Y.; Newton, T.P.; Sobolevsky, A.I.  
Deposited on : 2025-02-03  
Resolution : 3.48 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev126  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0rc1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.45.1

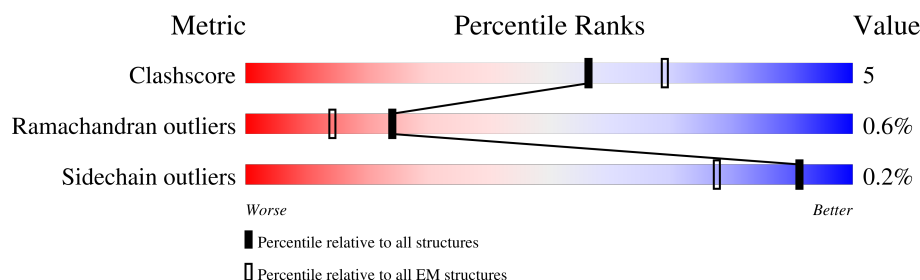
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.48 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 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  $\leq 5\%$ . 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	<div> <div>15%</div> <div>80%</div> <div>13%</div> <div>7%</div> </div>
1	B	908	<div> <div>15%</div> <div>79%</div> <div>13%</div> <div>7%</div> </div>
1	C	908	<div> <div>13%</div> <div>80%</div> <div>12%</div> <div>7%</div> </div>
1	D	908	<div> <div>13%</div> <div>79%</div> <div>14%</div> <div>7%</div> </div>
2	E	5	<div> <div>20%</div> <div>80%</div> </div>
2	G	5	<div> <div>100%</div> </div>
2	I	5	<div> <div>100%</div> </div>
2	K	5	<div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	2	<div><div></div><div>50%</div><div></div><div>50%</div></div>
3	J	2	<div><div></div><div>50%</div><div></div><div>50%</div></div>
4	H	4	<div><div></div><div>25%</div><div>75%</div><div></div><div>75%</div></div>
4	L	4	<div><div></div><div>25%</div><div>50%</div><div></div><div>75%</div></div>

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 28356 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.

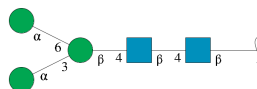
- Molecule 1 is a protein called Glutamate receptor ionotropic, kainate 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	842	Total	C	N	O	S	1	0
			6680	4280	1117	1243	40		
1	B	842	Total	C	N	O	S	1	0
			6680	4280	1117	1243	40		
1	C	842	Total	C	N	O	S	1	0
			6680	4280	1117	1243	40		
1	D	842	Total	C	N	O	S	1	0
			6680	4280	1117	1243	40		

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 alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
2	E	5	Total	C	N	O	0	0
			61	34	2	25		

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Mol	Chain	Residues	Atoms				AltConf	Trace
2	G	5	Total	C	N	O	0	0
			61	34	2	25		
2	I	5	Total	C	N	O	0	0
			61	34	2	25		
2	K	5	Total	C	N	O	0	0
			61	34	2	25		

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



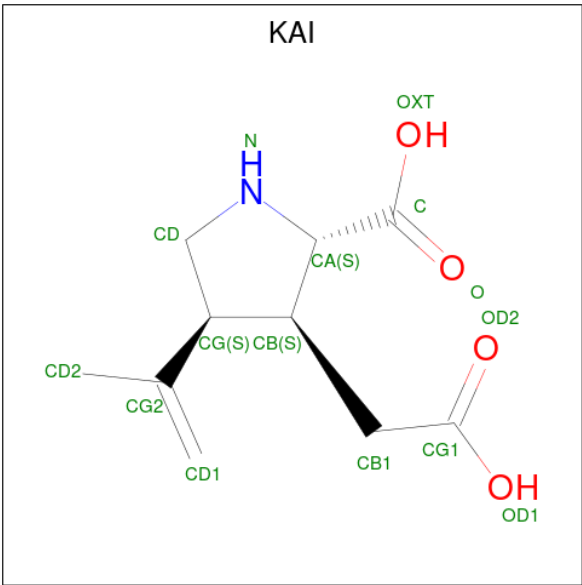
Mol	Chain	Residues	Atoms				AltConf	Trace
3	F	2	Total	C	N	O	0	0
			28	16	2	10		
3	J	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 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-glucopyranose.



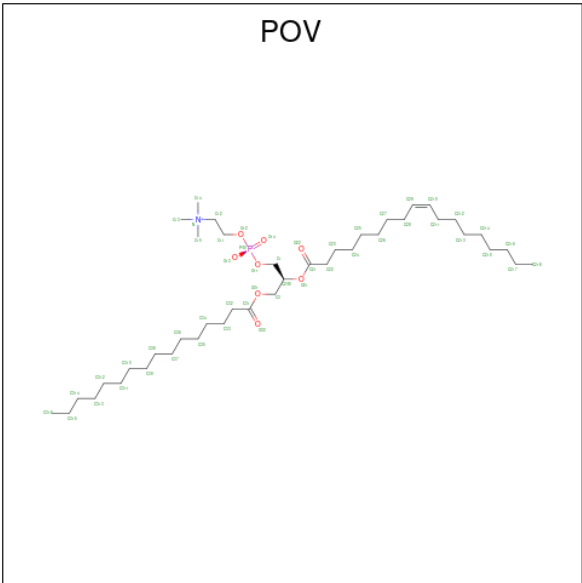
Mol	Chain	Residues	Atoms				AltConf	Trace
4	H	4	Total	C	N	O	0	0
			50	28	2	20		
4	L	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 5 is 3-(CARBOXYMETHYL)-4-ISOPROPENYLPROLINE (CCD ID: KAI) (formula: C<sub>10</sub>H<sub>15</sub>NO<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			15	10	1	4	
5	B	1	Total	C	N	O	0
			15	10	1	4	
5	C	1	Total	C	N	O	0
			15	10	1	4	
5	D	1	Total	C	N	O	0
			15	10	1	4	

- Molecule 6 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylamm onio)ethyl phosphate (CCD ID: POV) (formula: C<sub>42</sub>H<sub>82</sub>NO<sub>8</sub>P).



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

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



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

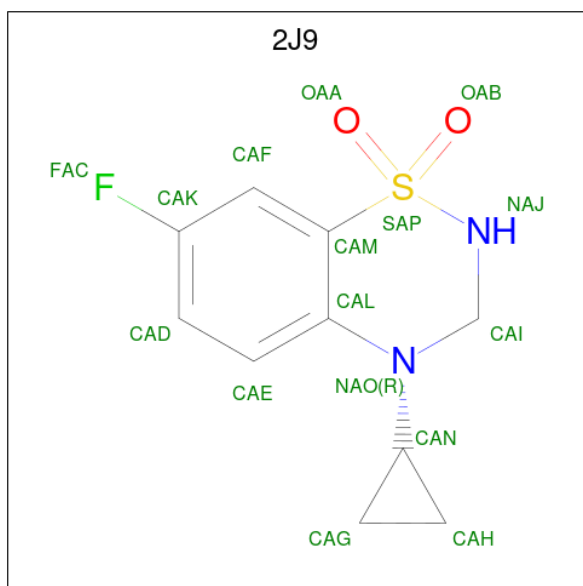
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Mol	Chain	Residues	Atoms				AltConf
7	C	1	Total	C	N	O	0
			14	8	1	5	
7	C	1	Total	C	N	O	0
			14	8	1	5	
7	D	1	Total	C	N	O	0
			14	8	1	5	
7	D	1	Total	C	N	O	0
			14	8	1	5	
7	D	1	Total	C	N	O	0
			14	8	1	5	
7	D	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 8 is 4-cyclopropyl-7-fluoro-3,4-dihydro-2H-1,2,4-benzothiadiazine 1,1-dioxide (CCD ID: 2J9) (formula: C<sub>10</sub>H<sub>11</sub>FN<sub>2</sub>O<sub>2</sub>S) (labeled as "Ligand of Interest" by depositor).

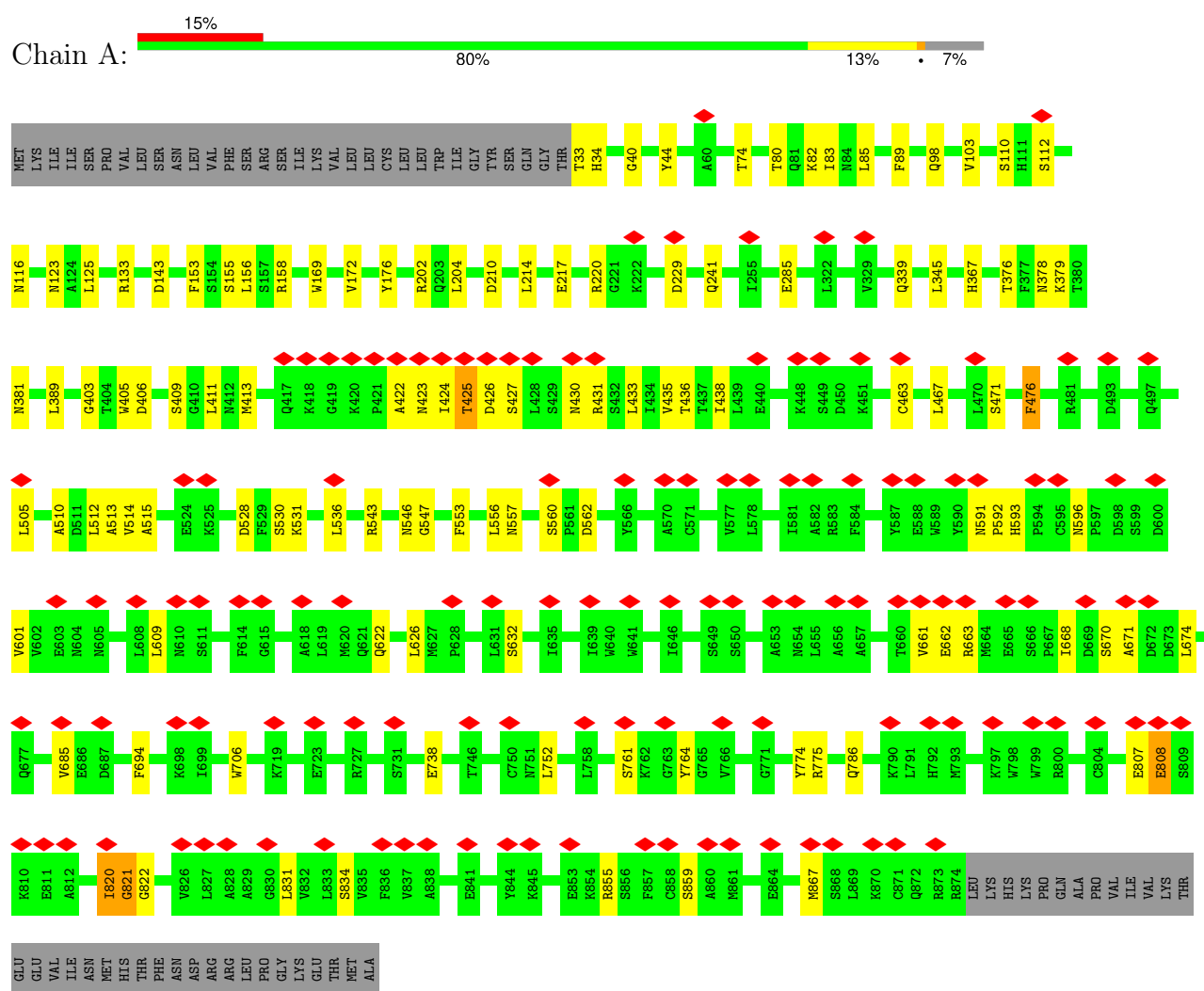


Mol	Chain	Residues	Atoms						AltConf
8	A	1	Total	C	F	N	O	S	0
			16	10	1	2	2	1	
8	B	1	Total	C	F	N	O	S	0
			16	10	1	2	2	1	
8	B	1	Total	C	F	N	O	S	0
			16	10	1	2	2	1	
8	D	1	Total	C	F	N	O	S	0
			16	10	1	2	2	1	

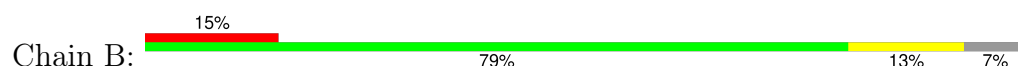
### 3 Residue-property plots

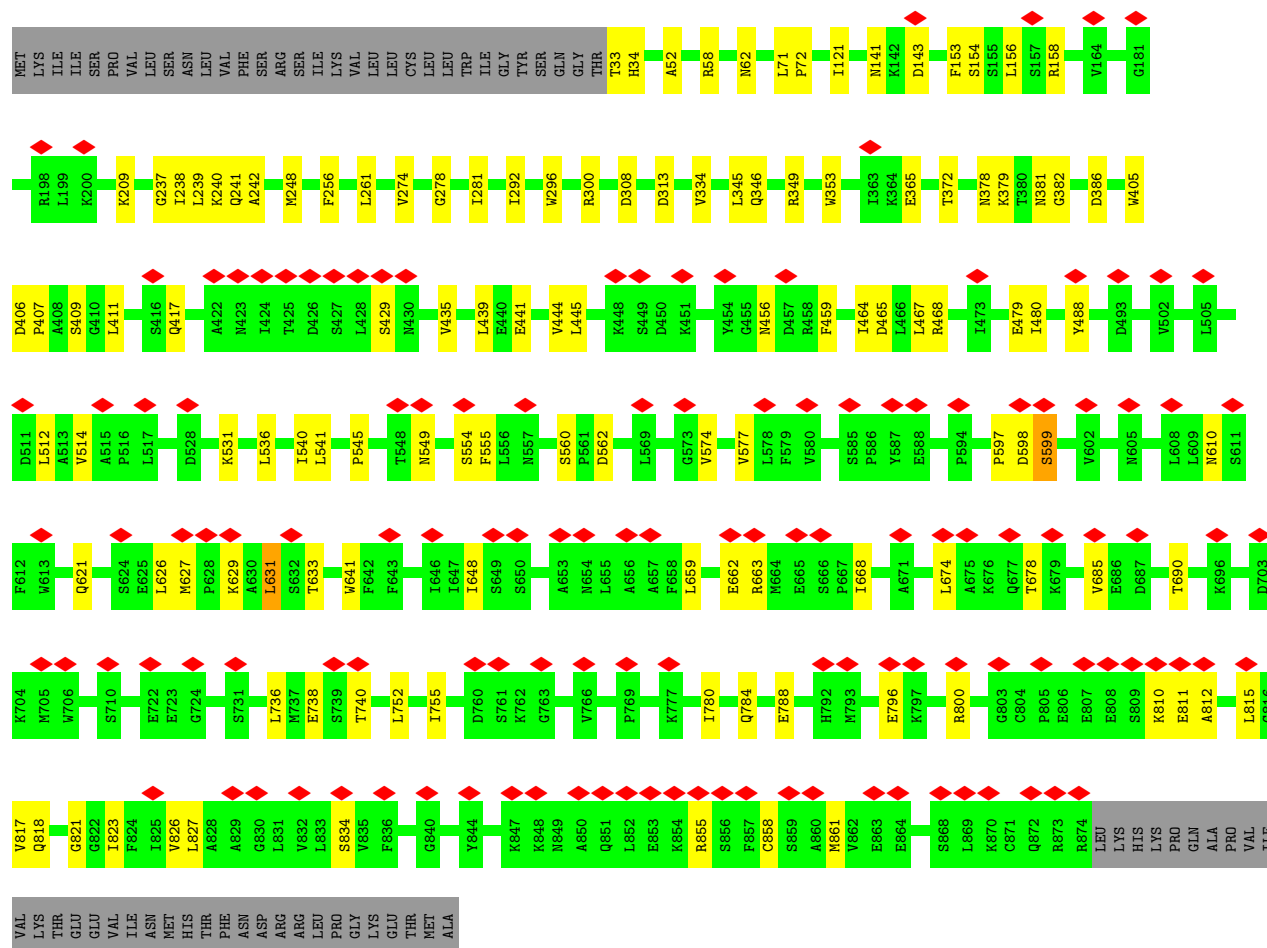
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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

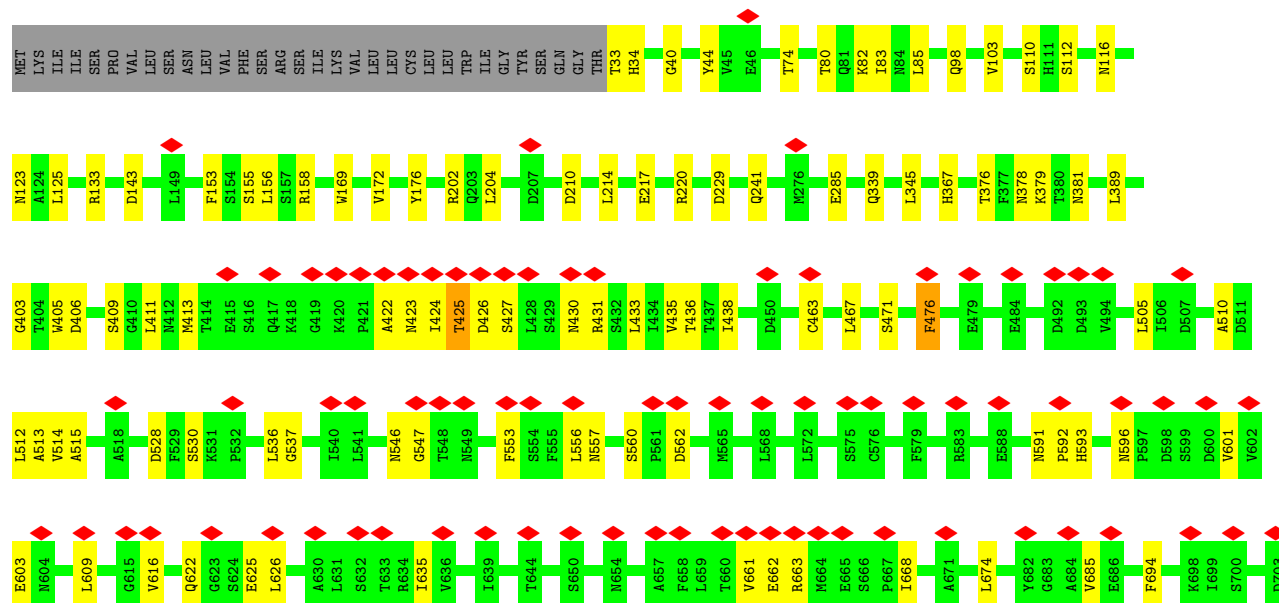
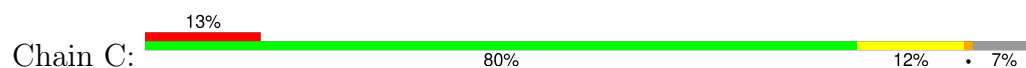


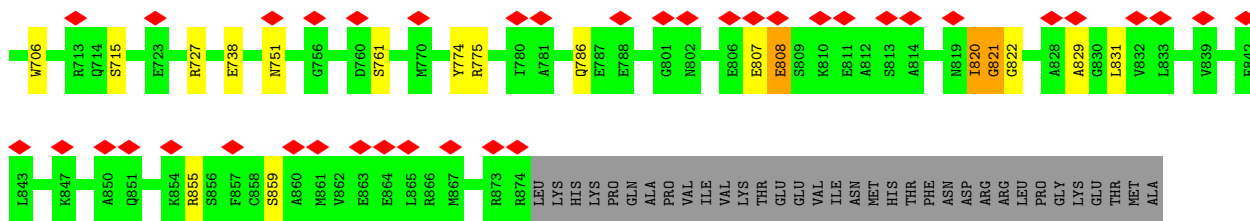
- Molecule 1: Glutamate receptor ionotropic, kainate 2



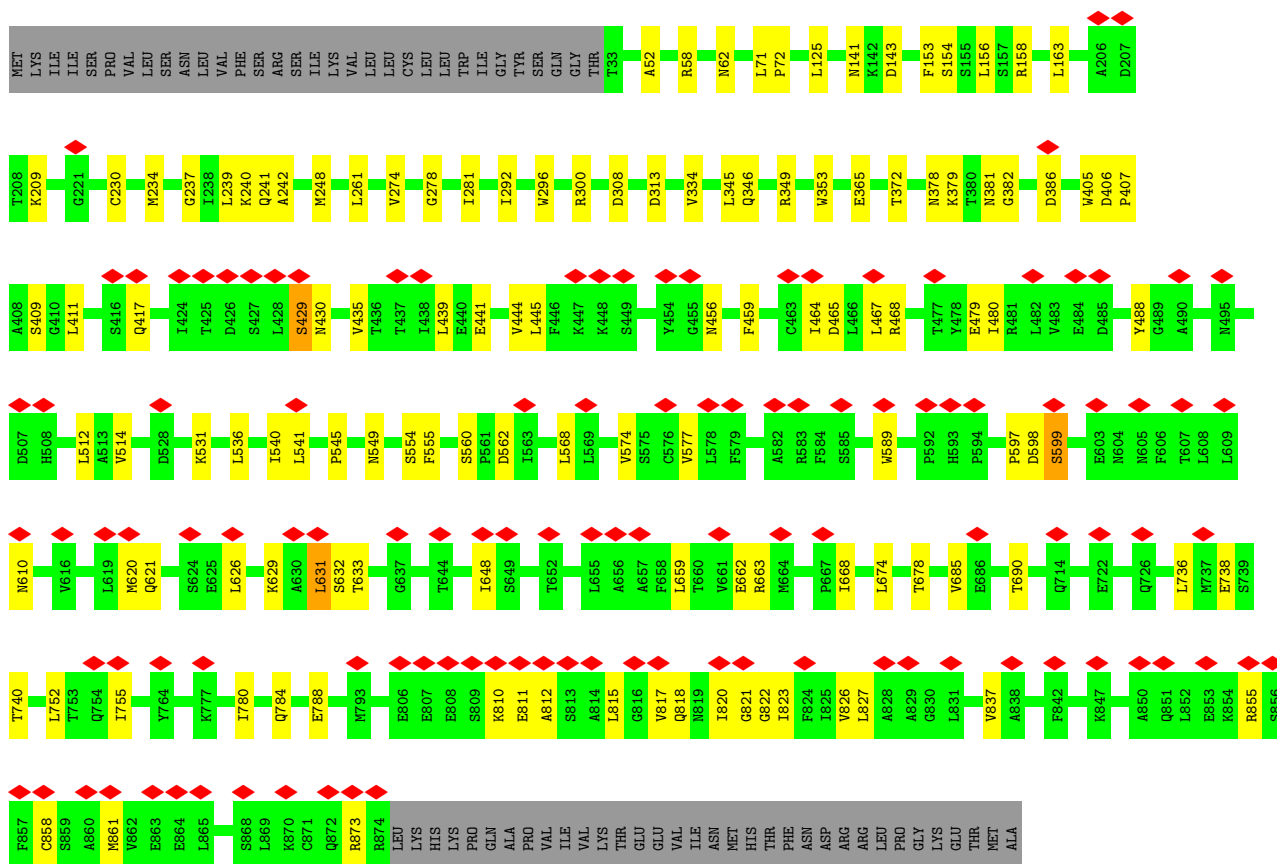
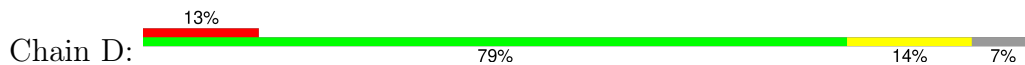


- Molecule 1: Glutamate receptor ionotropic, kainate 2

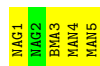




- Molecule 1: Glutamate receptor ionotropic, kainate 2



- Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I: 100%



- Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K: 100%



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

Chain F: 50% 50%



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

Chain J: 50% 50%



- Molecule 4: 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 H: 25% 75% 75%



- Molecule 4: 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 L: 25% 50% 75%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	115620	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	58.8	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	66.144	Depositor
Minimum map value	-40.431	Depositor
Average map value	0.037	Depositor
Map value standard deviation	1.295	Depositor
Recommended contour level	4.1	Depositor
Map size ( $\text{\AA}$ )	318.72, 318.72, 318.72	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	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: BMA, 2J9, NAG, KAI, POV, MAN

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	0.33	1/6833 (0.0%)	0.78	3/9248 (0.0%)
1	B	0.34	0/6833	0.81	10/9248 (0.1%)
1	C	0.33	1/6833 (0.0%)	0.78	3/9248 (0.0%)
1	D	0.34	0/6833	0.81	10/9248 (0.1%)
All	All	0.33	2/27332 (0.0%)	0.80	26/36992 (0.1%)

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	7
1	B	0	3
1	C	0	7
1	D	0	3
All	All	0	20

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	557	ASN	C-N	5.56	1.39	1.34
1	A	557	ASN	C-N	5.48	1.39	1.34

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	597	PRO	CA-C-N	7.89	136.62	121.54
1	D	597	PRO	C-N-CA	7.89	136.62	121.54
1	B	597	PRO	CA-C-N	7.87	136.56	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	597	PRO	C-N-CA	7.87	136.56	121.54
1	C	424	ILE	CA-C-N	5.56	132.16	121.54
1	C	424	ILE	C-N-CA	5.56	132.16	121.54
1	A	424	ILE	CA-C-N	5.56	132.16	121.54
1	A	424	ILE	C-N-CA	5.56	132.16	121.54
1	B	678	THR	N-CA-C	-5.33	107.79	114.56
1	D	678	THR	N-CA-C	-5.32	107.80	114.56
1	B	313	ASP	CA-C-N	5.24	125.92	119.99
1	B	313	ASP	C-N-CA	5.24	125.92	119.99
1	D	313	ASP	CA-C-N	5.24	125.92	119.99
1	D	313	ASP	C-N-CA	5.24	125.92	119.99
1	A	285	GLU	N-CA-C	-5.18	108.23	114.75
1	B	429	SER	CA-C-N	5.16	128.56	120.82
1	B	429	SER	C-N-CA	5.16	128.56	120.82
1	C	285	GLU	N-CA-C	-5.16	108.25	114.75
1	D	555	PHE	N-CA-C	-5.14	106.78	113.16
1	D	429	SER	CA-C-N	5.14	128.53	120.82
1	D	429	SER	C-N-CA	5.14	128.53	120.82
1	B	555	PHE	N-CA-C	-5.09	106.84	113.16
1	D	855	ARG	N-CA-C	5.07	116.50	110.97
1	D	817	VAL	N-CA-C	-5.06	106.98	112.80
1	B	855	ARG	N-CA-C	5.04	116.46	110.97
1	B	817	VAL	N-CA-C	-5.03	107.02	112.80

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	422	ALA	Peptide
1	A	425	THR	Peptide
1	A	431	ARG	Peptide
1	A	476	PHE	Peptide
1	A	807	GLU	Peptide
1	A	808	GLU	Peptide
1	A	820	ILE	Peptide
1	B	554	SER	Peptide
1	B	598	ASP	Peptide
1	B	599	SER	Peptide
1	C	422	ALA	Peptide
1	C	425	THR	Peptide
1	C	431	ARG	Peptide
1	C	476	PHE	Peptide

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Mol	Chain	Res	Type	Group
1	C	807	GLU	Peptide
1	C	808	GLU	Peptide
1	C	820	ILE	Peptide
1	D	554	SER	Peptide
1	D	598	ASP	Peptide
1	D	599	SER	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	6680	0	6659	67	0
1	B	6680	0	6658	70	0
1	C	6680	0	6659	67	0
1	D	6680	0	6659	74	0
2	E	61	0	52	0	0
2	G	61	0	52	0	0
2	I	61	0	52	0	0
2	K	61	0	52	0	0
3	F	28	0	25	1	0
3	J	28	0	25	1	0
4	H	50	0	43	0	0
4	L	50	0	43	0	0
5	A	15	0	13	1	0
5	B	15	0	13	3	0
5	C	15	0	13	1	0
5	D	15	0	13	3	0
6	A	312	0	492	3	0
6	B	104	0	164	1	0
6	C	208	0	328	6	0
6	D	208	0	328	5	0
7	A	84	0	78	0	0
7	B	56	0	52	0	0
7	C	84	0	78	1	0
7	D	56	0	52	0	0
8	A	16	0	11	2	0
8	B	32	0	22	2	0
8	D	16	0	11	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	28356	0	28647	268	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 (268) 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:488:TYR:HE2	5:B:1002:KAI:HG	1.36	0.89
1:D:488:TYR:HE2	5:D:1002:KAI:HG	1.40	0.84
1:B:488:TYR:CE2	5:B:1002:KAI:HG	2.15	0.81
1:D:488:TYR:CE2	5:D:1002:KAI:HG	2.19	0.76
1:C:685:VAL:HG11	5:C:1001:KAI:HD23	1.68	0.75
1:D:435:VAL:HG12	1:D:512:LEU:HB2	1.74	0.70
1:B:435:VAL:HG12	1:B:512:LEU:HB2	1.74	0.70
1:B:685:VAL:HG11	5:B:1002:KAI:HD23	1.73	0.68
1:D:685:VAL:HG11	5:D:1002:KAI:HD23	1.77	0.66
1:A:406:ASP:HB3	1:A:409:SER:HB2	1.79	0.65
1:C:435:VAL:HG12	1:C:512:LEU:HB2	1.79	0.64
1:C:406:ASP:HB3	1:C:409:SER:HB2	1.79	0.64
1:A:685:VAL:HG11	5:A:1001:KAI:HD23	1.80	0.64
1:A:123:ASN:ND2	1:A:143:ASP:OD1	2.31	0.64
1:A:467:LEU:HD13	1:A:514:VAL:HG21	1.80	0.64
1:A:435:VAL:HG12	1:A:512:LEU:HB2	1.79	0.64
1:C:123:ASN:ND2	1:C:143:ASP:OD1	2.31	0.63
1:C:467:LEU:HD13	1:C:514:VAL:HG21	1.80	0.63
1:D:536:LEU:HB3	1:D:740:THR:HG23	1.82	0.62
1:B:536:LEU:HB3	1:B:740:THR:HG23	1.82	0.62
1:C:210:ASP:HA	1:C:241:GLN:HE22	1.65	0.62
1:B:818:GLN:HG3	6:B:1004:POV:H12	1.83	0.60
1:C:33:THR:N	1:C:339:GLN:OE1	2.34	0.60
1:A:33:THR:N	1:A:339:GLN:OE1	2.34	0.60
1:A:210:ASP:HA	1:A:241:GLN:HE22	1.65	0.60
1:A:110:SER:HB3	1:A:133:ARG:HE	1.66	0.59
1:A:505:LEU:HD11	1:A:513:ALA:HB2	1.84	0.59
1:C:110:SER:HB3	1:C:133:ARG:HE	1.66	0.59
1:D:818:GLN:HG3	6:D:1005:POV:H12	1.83	0.59
1:B:237:GLY:O	1:B:241:GLN:NE2	2.36	0.58
1:B:668:ILE:HG13	1:B:755:ILE:HG21	1.85	0.58
1:C:505:LEU:HD11	1:C:513:ALA:HB2	1.85	0.58
1:D:237:GLY:O	1:D:241:GLN:NE2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:668:ILE:HG13	1:D:755:ILE:HG21	1.85	0.57
1:A:536:LEU:HD22	1:A:738:GLU:HB3	1.86	0.57
1:A:593:HIS:HB3	1:A:596:ASN:HB3	1.87	0.57
1:B:154:SER:O	1:B:158:ARG:NH2	2.38	0.57
1:B:248:MET:HE3	1:B:274:VAL:HG11	1.87	0.56
1:C:536:LEU:HD22	1:C:738:GLU:HB3	1.86	0.56
1:A:430:ASN:ND2	1:A:774:TYR:OH	2.38	0.56
1:C:430:ASN:ND2	1:C:774:TYR:OH	2.38	0.56
1:D:154:SER:O	1:D:158:ARG:NH2	2.38	0.56
1:A:761:SER:HB2	8:A:1014:2J9:H4	1.88	0.56
1:C:593:HIS:HB3	1:C:596:ASN:HB3	1.87	0.56
1:A:786:GLN:HG3	8:D:1001:2J9:H3	1.87	0.56
1:D:248:MET:HE3	1:D:274:VAL:HG11	1.87	0.56
1:B:631:LEU:HB2	1:C:609:LEU:HD11	1.87	0.55
1:B:365:GLU:HG3	1:B:379:LYS:HE3	1.87	0.55
1:C:616:VAL:HG11	6:C:1002:POV:H31E	1.88	0.55
1:A:622:GLN:HE22	1:D:621:GLN:HA	1.71	0.55
1:D:365:GLU:HG3	1:D:379:LYS:HE3	1.87	0.55
1:B:668:ILE:HG21	1:B:674:LEU:HD23	1.90	0.54
1:C:603:GLU:HG3	1:D:873:ARG:HH22	1.73	0.54
1:B:240:LYS:NZ	1:B:308:ASP:O	2.41	0.54
1:D:668:ILE:HG21	1:D:674:LEU:HD23	1.90	0.54
1:C:367:HIS:ND1	1:C:376:THR:OG1	2.40	0.53
1:D:240:LYS:NZ	1:D:308:ASP:O	2.41	0.53
1:A:204:LEU:HD23	1:A:214:LEU:HD13	1.91	0.53
8:B:1001:2J9:H4	1:C:761:SER:HB2	1.91	0.53
1:B:153:PHE:HA	1:B:156:LEU:HB2	1.91	0.52
1:B:784:GLN:NE2	1:B:788:GLU:OE2	2.42	0.52
1:D:784:GLN:NE2	1:D:788:GLU:OE2	2.42	0.52
1:B:239:LEU:HA	1:B:242:ALA:HB3	1.92	0.52
1:C:204:LEU:HD23	1:C:214:LEU:HD13	1.91	0.52
1:C:751:ASN:HB3	7:C:1011:NAG:H82	1.90	0.52
1:C:668:ILE:HG21	1:C:674:LEU:HD23	1.90	0.52
1:D:405:TRP:HD1	1:D:411:LEU:HD22	1.75	0.52
1:B:549:ASN:ND2	1:B:662:GLU:OE2	2.43	0.52
1:B:621:GLN:HE21	1:B:648:ILE:HD12	1.75	0.52
1:D:621:GLN:HE21	1:D:648:ILE:HD12	1.75	0.52
1:B:405:TRP:HD1	1:B:411:LEU:HD22	1.75	0.52
1:C:44:TYR:HB2	1:C:82:LYS:HB3	1.92	0.52
1:B:71:LEU:HD21	1:B:334:VAL:HG23	1.92	0.52
6:C:1003:POV:H31F	6:C:1005:POV:H214	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:58:ARG:O	1:D:62:ASN:ND2	2.43	0.52
1:A:668:ILE:HG21	1:A:674:LEU:HD23	1.90	0.52
1:B:58:ARG:O	1:B:62:ASN:ND2	2.43	0.52
1:C:463:CYS:HB3	1:C:514:VAL:HG12	1.91	0.52
1:C:528:ASP:HB3	1:C:775:ARG:HD2	1.92	0.52
1:A:463:CYS:HB3	1:A:514:VAL:HG12	1.91	0.51
1:C:546:ASN:O	1:C:663:ARG:NH1	2.43	0.51
1:D:153:PHE:HA	1:D:156:LEU:HB2	1.91	0.51
1:D:549:ASN:ND2	1:D:662:GLU:OE2	2.43	0.51
1:A:44:TYR:HB2	1:A:82:LYS:HB3	1.92	0.51
1:B:690:THR:OG1	1:B:738:GLU:OE2	2.29	0.51
1:C:378:ASN:O	1:C:381:ASN:N	2.44	0.51
1:B:417:GLN:NE2	3:F:1:NAG:O3	2.35	0.51
1:C:694:PHE:HB3	1:C:706:TRP:HB2	1.93	0.51
1:D:141:ASN:ND2	1:D:143:ASP:OD2	2.44	0.51
1:D:71:LEU:HD21	1:D:334:VAL:HG23	1.92	0.51
1:D:239:LEU:HA	1:D:242:ALA:HB3	1.92	0.51
1:D:465:ASP:OD1	1:D:468:ARG:NH1	2.44	0.51
1:B:465:ASP:OD1	1:B:468:ARG:NH1	2.44	0.51
1:A:546:ASN:O	1:A:663:ARG:NH1	2.43	0.51
1:B:141:ASN:ND2	1:B:143:ASP:OD2	2.44	0.51
1:B:378:ASN:HB3	1:B:381:ASN:HB2	1.93	0.51
1:B:406:ASP:HB3	1:B:409:SER:HB2	1.93	0.50
1:A:694:PHE:HB3	1:A:706:TRP:HB2	1.93	0.50
1:A:528:ASP:HB3	1:A:775:ARG:HD2	1.92	0.50
1:C:202:ARG:NH1	1:C:217:GLU:OE1	2.44	0.50
1:D:690:THR:OG1	1:D:738:GLU:OE2	2.29	0.50
1:B:378:ASN:O	1:B:382:GLY:N	2.43	0.50
1:D:429:SER:OG	1:D:430:ASN:N	2.42	0.50
1:D:346:GLN:OE1	1:D:349:ARG:NH1	2.45	0.50
1:D:378:ASN:HB3	1:D:381:ASN:HB2	1.93	0.50
1:A:202:ARG:NH1	1:A:217:GLU:OE1	2.44	0.50
1:B:346:GLN:OE1	1:B:349:ARG:NH1	2.45	0.50
1:D:541:LEU:HD21	1:D:752:LEU:HD23	1.94	0.50
1:D:560:SER:OG	1:D:562:ASP:OD1	2.28	0.50
1:A:176:TYR:HA	1:A:229:ASP:HB3	1.94	0.49
8:B:1009:2J9:H3	1:C:786:GLN:HG3	1.94	0.49
1:D:467:LEU:HD13	1:D:514:VAL:HG21	1.95	0.49
1:A:367:HIS:ND1	1:A:376:THR:OG1	2.40	0.49
1:A:547:GLY:HA2	1:A:663:ARG:HH12	1.77	0.49
1:D:823:ILE:O	1:D:827:LEU:N	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:ASN:O	1:A:381:ASN:N	2.44	0.49
1:C:176:TYR:HA	1:C:229:ASP:HB3	1.94	0.49
1:A:155:SER:HA	1:A:158:ARG:HD3	1.95	0.49
1:C:155:SER:HA	1:C:158:ARG:HD3	1.95	0.49
1:D:406:ASP:HB3	1:D:409:SER:HB2	1.93	0.48
1:D:456:ASN:HD21	1:D:480:ILE:H	1.61	0.48
1:B:467:LEU:HD13	1:B:514:VAL:HG21	1.95	0.48
1:B:574:VAL:HA	1:B:577:VAL:HG12	1.95	0.48
1:D:574:VAL:HA	1:D:577:VAL:HG12	1.95	0.48
1:C:547:GLY:HA2	1:C:663:ARG:HH12	1.77	0.48
1:B:541:LEU:HD21	1:B:752:LEU:HD23	1.94	0.48
1:C:820:ILE:O	1:C:822:GLY:N	2.46	0.48
1:A:820:ILE:O	1:A:822:GLY:N	2.46	0.48
1:A:98:GLN:HB3	1:A:103:VAL:HG11	1.96	0.48
1:C:661:VAL:HG13	1:C:662:GLU:H	1.79	0.48
1:B:796:GLU:OE2	1:B:800:ARG:NE	2.42	0.47
1:D:378:ASN:O	1:D:382:GLY:N	2.43	0.47
1:D:386:ASP:HA	1:D:407:PRO:HG2	1.95	0.47
1:D:417:GLN:NE2	3:J:1:NAG:O3	2.37	0.47
1:D:459:PHE:HB3	1:D:464:ILE:HG13	1.95	0.47
1:A:609:LEU:HD11	1:D:631:LEU:HB2	1.96	0.47
1:B:386:ASP:HA	1:B:407:PRO:HG2	1.95	0.47
1:C:98:GLN:HB3	1:C:103:VAL:HG11	1.96	0.47
1:A:661:VAL:HG13	1:A:662:GLU:H	1.79	0.47
1:D:823:ILE:HA	1:D:826:VAL:HG22	1.97	0.47
1:B:459:PHE:HB3	1:B:464:ILE:HG13	1.95	0.47
1:D:540:ILE:HG12	1:D:736:LEU:HG	1.97	0.47
1:A:530:SER:O	1:D:531:LYS:NZ	2.43	0.47
1:C:553:PHE:HB3	1:C:556:LEU:HD23	1.96	0.47
6:C:1005:POV:H27A	6:C:1005:POV:H24	1.57	0.47
1:B:439:LEU:HA	1:B:444:VAL:HB	1.97	0.47
1:B:540:ILE:HG12	1:B:736:LEU:HG	1.97	0.47
1:A:531:LYS:HE3	1:D:531:LYS:HA	1.97	0.47
1:B:456:ASN:HD21	1:B:480:ILE:H	1.61	0.47
1:A:831:LEU:HD11	1:D:574:VAL:HG22	1.97	0.47
1:A:169:TRP:HE3	1:A:172:VAL:HG12	1.81	0.46
1:B:627:MET:HB2	1:C:625:GLU:HB3	1.98	0.46
1:D:439:LEU:HA	1:D:444:VAL:HB	1.97	0.46
1:B:823:ILE:O	1:B:827:LEU:N	2.45	0.46
1:A:112:SER:O	1:A:116:ASN:ND2	2.49	0.46
1:B:823:ILE:HA	1:B:826:VAL:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:HIS:HD2	1:A:74:THR:HA	1.80	0.46
1:A:553:PHE:HB3	1:A:556:LEU:HD23	1.96	0.46
1:C:433:LEU:HD13	1:C:476:PHE:HB2	1.98	0.46
1:B:641:TRP:CD1	1:C:622:GLN:HG3	2.51	0.46
1:C:169:TRP:HE3	1:C:172:VAL:HG12	1.81	0.46
1:B:560:SER:OG	1:B:562:ASP:OD1	2.28	0.46
1:C:112:SER:O	1:C:116:ASN:ND2	2.49	0.46
1:D:629:LYS:O	1:D:633:THR:OG1	2.34	0.46
1:C:635:ILE:HD12	1:D:837:VAL:HG21	1.98	0.46
1:C:34:HIS:HD2	1:C:74:THR:HA	1.80	0.45
1:B:629:LYS:O	1:B:633:THR:OG1	2.34	0.45
1:C:820:ILE:HG13	1:C:821:GLY:H	1.81	0.45
1:B:281:ILE:HG12	1:B:372:THR:HB	1.99	0.45
1:D:281:ILE:HG12	1:D:372:THR:HB	1.99	0.45
1:A:820:ILE:HG13	1:A:821:GLY:H	1.81	0.45
6:C:1004:POV:H26	6:C:1004:POV:H29	1.65	0.45
1:C:436:THR:HG23	1:C:510:ALA:HB3	1.99	0.45
1:B:52:ALA:HA	1:B:300:ARG:HH22	1.82	0.45
1:A:40:GLY:HA3	1:A:80:THR:HA	1.98	0.45
1:A:389:LEU:HB2	1:A:405:TRP:HB3	1.99	0.45
1:C:591:ASN:HD22	1:C:592:PRO:HD2	1.82	0.45
1:D:858:CYS:HA	1:D:861:MET:HE2	1.99	0.45
1:B:641:TRP:CG	1:C:622:GLN:HG3	2.52	0.44
1:D:545:PRO:O	1:D:663:ARG:NH1	2.48	0.44
1:B:858:CYS:HA	1:B:861:MET:HE2	1.99	0.44
1:D:52:ALA:HA	1:D:300:ARG:HH22	1.82	0.44
1:A:125:LEU:HD12	1:A:345:LEU:HB3	1.99	0.44
1:A:433:LEU:HD13	1:A:476:PHE:HB2	1.98	0.44
1:A:436:THR:HG23	1:A:510:ALA:HB3	1.99	0.44
1:A:831:LEU:HD13	1:D:577:VAL:HG11	2.00	0.44
1:C:389:LEU:HB2	1:C:405:TRP:HB3	2.00	0.44
1:C:855:ARG:HB3	1:C:859:SER:HB3	1.99	0.44
6:C:1002:POV:H2	6:C:1003:POV:H22A	2.00	0.44
1:A:591:ASN:HD22	1:A:592:PRO:HD2	1.82	0.44
1:A:425:THR:O	1:A:427:SER:N	2.51	0.44
6:A:1012:POV:H14A	6:A:1012:POV:H11A	1.87	0.44
1:C:125:LEU:HD12	1:C:345:LEU:HB3	1.99	0.44
1:A:560:SER:OG	1:A:562:ASP:OD1	2.27	0.43
1:C:40:GLY:HA3	1:C:80:THR:HA	1.98	0.43
1:C:425:THR:O	1:C:427:SER:N	2.51	0.43
1:B:456:ASN:HD21	1:B:479:GLU:HA	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:456:ASN:HD21	1:D:479:GLU:HA	1.83	0.43
1:A:403:GLY:HA2	1:A:413:MET:HA	1.99	0.43
1:A:855:ARG:HB3	1:A:859:SER:HB3	1.99	0.43
1:C:560:SER:OG	1:C:562:ASP:OD1	2.27	0.43
6:A:1002:POV:H2	6:A:1003:POV:H22A	2.00	0.43
1:B:261:LEU:HD12	1:B:278:GLY:HA3	2.01	0.43
1:C:83:ILE:HG13	1:C:85:LEU:HD22	2.00	0.43
1:C:403:GLY:HA2	1:C:413:MET:HA	1.99	0.43
1:A:438:ILE:HG22	1:A:515:ALA:HB1	2.01	0.43
6:A:1005:POV:H27A	6:A:1005:POV:H24	1.59	0.43
1:B:238:ILE:O	1:B:242:ALA:N	2.48	0.43
1:C:438:ILE:HG22	1:C:515:ALA:HB1	2.01	0.43
1:D:659:LEU:HD21	1:D:815:LEU:HD11	2.01	0.43
1:D:261:LEU:HD12	1:D:278:GLY:HA3	2.01	0.43
1:C:829:ALA:HB1	6:C:1004:POV:H314	2.01	0.42
1:A:217:GLU:HA	1:A:220:ARG:HG2	2.00	0.42
1:B:659:LEU:HD21	1:B:815:LEU:HD11	2.01	0.42
1:C:153:PHE:HA	1:C:156:LEU:HB3	2.01	0.42
1:B:292:ILE:O	1:B:296:TRP:N	2.50	0.42
1:B:545:PRO:O	1:B:663:ARG:NH1	2.48	0.42
1:B:577:VAL:HG11	1:C:831:LEU:HD13	2.01	0.42
1:A:83:ILE:HG13	1:A:85:LEU:HD22	2.00	0.42
1:C:217:GLU:HA	1:C:220:ARG:HG2	2.00	0.42
1:C:405:TRP:HD1	1:C:411:LEU:HD23	1.83	0.42
1:A:89:PHE:HD1	1:B:121:ILE:HG12	1.85	0.42
1:B:444:VAL:HG13	1:B:464:ILE:HD11	2.02	0.42
1:D:568:LEU:HD11	6:D:1004:POV:H212	2.01	0.42
1:A:405:TRP:HD1	1:A:411:LEU:HD23	1.83	0.42
6:D:1003:POV:H34A	6:D:1004:POV:H24A	2.01	0.42
6:D:1004:POV:H14A	6:D:1004:POV:H11A	1.88	0.42
1:B:345:LEU:HD11	1:B:353:TRP:HD1	1.86	0.41
1:B:621:GLN:HA	1:C:622:GLN:HE22	1.85	0.41
8:A:1014:2J9:H1	8:A:1014:2J9:H7	1.88	0.41
1:D:345:LEU:HD11	1:D:353:TRP:HD1	1.86	0.41
1:A:153:PHE:HA	1:A:156:LEU:HB3	2.01	0.41
1:B:209:LYS:O	1:B:241:GLN:NE2	2.53	0.41
1:D:209:LYS:O	1:D:241:GLN:NE2	2.54	0.41
1:B:441:GLU:HG3	1:B:445:LEU:HD13	2.03	0.41
1:A:34:HIS:CD2	1:A:74:THR:HA	2.56	0.41
1:C:715:SER:O	1:C:727:ARG:NH1	2.42	0.41
1:D:620:MET:HE1	6:D:1003:POV:H315	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:531:LYS:HA	1:D:531:LYS:HZ2	1.86	0.41
1:A:867:MET:SD	1:D:589:TRP:NE1	2.93	0.41
1:C:536:LEU:HB3	1:C:537:GLY:H	1.75	0.41
1:C:591:ASN:ND2	1:C:601:VAL:O	2.54	0.41
1:D:444:VAL:HG13	1:D:464:ILE:HD11	2.02	0.41
1:D:810:LYS:O	1:D:812:ALA:N	2.54	0.41
1:A:632:SER:O	1:B:834:SER:OG	2.37	0.41
1:A:834:SER:OG	1:D:632:SER:O	2.38	0.41
1:B:33:THR:OG1	1:B:34:HIS:N	2.53	0.41
1:B:256:PHE:HB2	1:B:261:LEU:HD11	2.03	0.41
1:B:531:LYS:NZ	1:C:530:SER:O	2.50	0.41
1:D:610:ASN:HB3	1:D:626:LEU:HD21	2.03	0.41
1:A:591:ASN:ND2	1:A:601:VAL:O	2.54	0.40
1:B:659:LEU:HG	1:B:815:LEU:HD21	2.03	0.40
1:D:292:ILE:O	1:D:296:TRP:N	2.50	0.40
1:D:441:GLU:HG3	1:D:445:LEU:HD13	2.03	0.40
1:D:659:LEU:HG	1:D:815:LEU:HD21	2.03	0.40
1:A:670:SER:OG	1:A:671:ALA:N	2.54	0.40
1:C:33:THR:OG1	1:C:34:HIS:N	2.54	0.40
1:A:33:THR:OG1	1:A:34:HIS:N	2.54	0.40
1:A:536:LEU:HD21	1:A:764:TYR:CZ	2.57	0.40
1:B:810:LYS:O	1:B:812:ALA:N	2.54	0.40
1:D:820:ILE:O	1:D:822:GLY:N	2.54	0.40
1:C:34:HIS:CD2	1:C:74:THR:HA	2.56	0.40
1:D:125:LEU:HD12	1:D:345:LEU:HD23	2.03	0.40
1:D:163:LEU:HD12	1:D:411:LEU:HD21	2.04	0.40
1:D:230:CYS:HB3	1:D:234:MET:HB2	2.04	0.40
1:A:543:ARG:HA	1:A:752:LEU:HD23	2.03	0.40
1:B:456:ASN:ND2	1:B:480:ILE:H	2.20	0.40
1:B:610:ASN:HB3	1:B:626:LEU:HD21	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	841/908 (93%)	733 (87%)	103 (12%)	5 (1%)	22	55
1	B	841/908 (93%)	737 (88%)	99 (12%)	5 (1%)	22	55
1	C	841/908 (93%)	733 (87%)	103 (12%)	5 (1%)	22	55
1	D	841/908 (93%)	736 (88%)	100 (12%)	5 (1%)	22	55
All	All	3364/3632 (93%)	2939 (87%)	405 (12%)	20 (1%)	24	55

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	426	ASP
1	B	811	GLU
1	C	426	ASP
1	D	811	GLU
1	A	423	ASN
1	B	599	SER
1	C	423	ASN
1	D	599	SER
1	A	808	GLU
1	B	631	LEU
1	C	808	GLU
1	D	631	LEU
1	B	821	GLY
1	D	821	GLY
1	A	379	LYS
1	C	379	LYS
1	A	821	GLY
1	B	72	PRO
1	C	821	GLY
1	D	72	PRO

### 5.3.2 Protein sidechains ⓘ

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	734/794 (92%)	731 (100%)	3 (0%)	89	94
1	B	734/794 (92%)	733 (100%)	1 (0%)	92	97
1	C	734/794 (92%)	731 (100%)	3 (0%)	89	94
1	D	734/794 (92%)	733 (100%)	1 (0%)	92	97
All	All	2936/3176 (92%)	2928 (100%)	8 (0%)	91	96

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

Mol	Chain	Res	Type
1	A	471[A]	SER
1	A	471[B]	SER
1	A	626	LEU
1	B	780	ILE
1	C	471[A]	SER
1	C	471[B]	SER
1	C	626	LEU
1	D	780	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	HIS
1	A	81	GLN
1	A	98	GLN
1	A	116	ASN
1	A	123	ASN
1	A	129	HIS
1	A	136	HIS
1	A	141	ASN
1	A	348	ASN
1	A	417	GLN
1	A	495	ASN
1	A	591	ASN
1	A	604	ASN
1	A	622	GLN
1	A	749	ASN
1	A	819	ASN
1	B	84	ASN
1	B	123	ASN
1	B	141	ASN

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Mol	Chain	Res	Type
1	B	241	GLN
1	B	348	ASN
1	B	456	ASN
1	B	557	ASN
1	B	604	ASN
1	B	610	ASN
1	B	621	GLN
1	B	721	ASN
1	B	802	ASN
1	C	34	HIS
1	C	81	GLN
1	C	98	GLN
1	C	116	ASN
1	C	123	ASN
1	C	129	HIS
1	C	141	ASN
1	C	339	GLN
1	C	348	ASN
1	C	417	GLN
1	C	495	ASN
1	C	591	ASN
1	C	596	ASN
1	C	604	ASN
1	C	622	GLN
1	C	749	ASN
1	C	819	ASN
1	D	84	ASN
1	D	123	ASN
1	D	137	GLN
1	D	141	ASN
1	D	241	GLN
1	D	348	ASN
1	D	456	ASN
1	D	557	ASN
1	D	604	ASN
1	D	610	ASN
1	D	621	GLN
1	D	622	GLN
1	D	721	ASN
1	D	802	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 ⓘ

32 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	1,2	14,14,15	0.52	0	17,19,21	0.86	1 (5%)
2	NAG	E	2	2	14,14,15	0.28	0	17,19,21	0.62	0
2	BMA	E	3	2	11,11,12	0.81	0	15,15,17	1.04	1 (6%)
2	MAN	E	4	2	11,11,12	0.92	0	15,15,17	0.87	1 (6%)
2	MAN	E	5	2	11,11,12	1.38	3 (27%)	15,15,17	1.77	4 (26%)
3	NAG	F	1	1,3	14,14,15	0.56	0	17,19,21	0.63	0
3	NAG	F	2	3	14,14,15	0.30	0	17,19,21	0.37	0
2	NAG	G	1	1,2	14,14,15	0.29	0	17,19,21	1.17	2 (11%)
2	NAG	G	2	2	14,14,15	1.22	1 (7%)	17,19,21	1.83	2 (11%)
2	BMA	G	3	2	11,11,12	1.41	2 (18%)	15,15,17	2.11	3 (20%)
2	MAN	G	4	2	11,11,12	1.01	0	15,15,17	1.10	2 (13%)
2	MAN	G	5	2	11,11,12	1.15	2 (18%)	15,15,17	1.14	1 (6%)
4	NAG	H	1	1,4	14,14,15	0.21	0	17,19,21	0.40	0
4	NAG	H	2	4	14,14,15	0.29	0	17,19,21	0.86	1 (5%)
4	BMA	H	3	4	11,11,12	2.16	3 (27%)	15,15,17	1.96	4 (26%)
4	BMA	H	4	4	11,11,12	1.32	2 (18%)	15,15,17	1.54	2 (13%)
2	NAG	I	1	1,2	14,14,15	0.48	0	17,19,21	0.74	1 (5%)
2	NAG	I	2	2	14,14,15	0.32	0	17,19,21	0.68	1 (5%)
2	BMA	I	3	2	11,11,12	1.29	2 (18%)	15,15,17	1.76	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	MAN	I	4	2	11,11,12	1.46	2 (18%)	15,15,17	1.76	6 (40%)
2	MAN	I	5	2	11,11,12	0.90	0	15,15,17	0.92	1 (6%)
3	NAG	J	1	1,3	14,14,15	0.54	0	17,19,21	0.61	0
3	NAG	J	2	3	14,14,15	0.33	0	17,19,21	0.36	0
2	NAG	K	1	1,2	14,14,15	0.68	1 (7%)	17,19,21	0.89	1 (5%)
2	NAG	K	2	2	14,14,15	1.14	1 (7%)	17,19,21	1.89	2 (11%)
2	BMA	K	3	2	11,11,12	1.40	2 (18%)	15,15,17	2.16	3 (20%)
2	MAN	K	4	2	11,11,12	0.94	0	15,15,17	1.15	2 (13%)
2	MAN	K	5	2	11,11,12	1.17	2 (18%)	15,15,17	1.14	1 (6%)
4	NAG	L	1	1,4	14,14,15	0.22	0	17,19,21	0.39	0
4	NAG	L	2	4	14,14,15	0.31	0	17,19,21	0.85	1 (5%)
4	BMA	L	3	4	11,11,12	2.13	3 (27%)	15,15,17	1.97	4 (26%)
4	BMA	L	4	4	11,11,12	1.16	1 (9%)	15,15,17	1.44	2 (13%)

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	1,2	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	BMA	E	3	2	-	2/2/19/22	0/1/1/1
2	MAN	E	4	2	-	2/2/19/22	0/1/1/1
2	MAN	E	5	2	-	0/2/19/22	0/1/1/1
3	NAG	F	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
2	NAG	G	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	G	2	2	-	4/6/23/26	0/1/1/1
2	BMA	G	3	2	-	2/2/19/22	0/1/1/1
2	MAN	G	4	2	-	0/2/19/22	0/1/1/1
2	MAN	G	5	2	-	0/2/19/22	1/1/1/1
4	NAG	H	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	H	2	4	-	0/6/23/26	0/1/1/1
4	BMA	H	3	4	-	0/2/19/22	0/1/1/1
4	BMA	H	4	4	-	0/2/19/22	0/1/1/1
2	NAG	I	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	I	2	2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BMA	I	3	2	-	0/2/19/22	0/1/1/1
2	MAN	I	4	2	-	2/2/19/22	0/1/1/1
2	MAN	I	5	2	-	1/2/19/22	0/1/1/1
3	NAG	J	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	J	2	3	-	2/6/23/26	0/1/1/1
2	NAG	K	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	K	2	2	-	4/6/23/26	0/1/1/1
2	BMA	K	3	2	-	2/2/19/22	0/1/1/1
2	MAN	K	4	2	-	0/2/19/22	0/1/1/1
2	MAN	K	5	2	-	0/2/19/22	1/1/1/1
4	NAG	L	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	L	2	4	-	0/6/23/26	0/1/1/1
4	BMA	L	3	4	-	0/2/19/22	0/1/1/1
4	BMA	L	4	4	-	2/2/19/22	0/1/1/1

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	3	BMA	C1-C2	4.40	1.62	1.52
2	G	2	NAG	O5-C1	4.38	1.51	1.43
4	L	3	BMA	C1-C2	4.30	1.62	1.52
2	K	2	NAG	O5-C1	3.99	1.50	1.43
4	L	3	BMA	C2-C3	3.70	1.58	1.52
4	H	3	BMA	C2-C3	3.67	1.58	1.52
2	I	4	MAN	C1-C2	3.44	1.60	1.52
2	K	3	BMA	C2-C3	3.34	1.57	1.52
2	G	3	BMA	C2-C3	3.29	1.57	1.52
4	H	3	BMA	O5-C1	3.10	1.48	1.43
4	L	3	BMA	O5-C1	3.02	1.48	1.43
2	I	4	MAN	C2-C3	2.83	1.56	1.52
2	G	3	BMA	O3-C3	2.77	1.49	1.43
2	E	5	MAN	C2-C3	2.73	1.56	1.52
2	K	3	BMA	O3-C3	2.71	1.49	1.43
2	I	3	BMA	O3-C3	2.39	1.48	1.43
4	H	4	BMA	C2-C3	2.26	1.55	1.52
4	H	4	BMA	C1-C2	2.23	1.57	1.52
2	E	5	MAN	O5-C5	2.21	1.47	1.43
2	I	3	BMA	O5-C5	2.20	1.47	1.43
2	K	5	MAN	C1-C2	2.18	1.57	1.52
2	G	5	MAN	C1-C2	2.16	1.57	1.52
4	L	4	BMA	C4-C3	2.12	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	1	NAG	C1-C2	2.11	1.55	1.52
2	K	5	MAN	O5-C5	2.09	1.47	1.43
2	E	5	MAN	C1-C2	2.07	1.57	1.52
2	G	5	MAN	O5-C5	2.05	1.47	1.43

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	2	NAG	C1-O5-C5	6.41	120.78	112.19
2	G	2	NAG	C1-O5-C5	6.17	120.46	112.19
2	K	3	BMA	O3-C3-C2	5.64	121.56	110.05
2	G	3	BMA	O3-C3-C2	5.52	121.33	110.05
2	E	5	MAN	C1-O5-C5	5.48	119.52	112.19
4	L	3	BMA	C1-O5-C5	5.34	119.34	112.19
4	H	3	BMA	C1-O5-C5	5.23	119.19	112.19
2	I	3	BMA	O3-C3-C2	4.71	119.66	110.05
4	H	4	BMA	C1-O5-C5	4.08	117.66	112.19
4	L	4	BMA	C1-O5-C5	3.99	117.54	112.19
2	K	3	BMA	C3-C4-C5	-3.82	103.30	110.23
2	G	3	BMA	C3-C4-C5	-3.82	103.31	110.23
2	I	3	BMA	C1-C2-C3	-3.77	104.15	109.64
2	K	3	BMA	C1-O5-C5	3.72	117.17	112.19
2	I	4	MAN	C1-O5-C5	3.45	116.81	112.19
2	G	3	BMA	C1-O5-C5	3.43	116.78	112.19
2	G	1	NAG	C2-N2-C7	3.33	127.37	122.90
2	I	4	MAN	C1-C2-C3	3.28	114.42	109.64
2	G	5	MAN	C1-O5-C5	3.27	116.57	112.19
2	K	5	MAN	C1-O5-C5	3.27	116.56	112.19
2	K	2	NAG	C2-N2-C7	3.25	127.25	122.90
2	G	2	NAG	C2-N2-C7	3.23	127.22	122.90
4	H	3	BMA	C1-C2-C3	3.10	114.15	109.64
4	L	3	BMA	C1-C2-C3	2.96	113.96	109.64
2	E	1	NAG	C1-O5-C5	2.90	116.07	112.19
2	I	1	NAG	C1-O5-C5	2.71	115.82	112.19
2	I	4	MAN	C2-C3-C4	2.65	115.53	110.86
2	K	4	MAN	C1-O5-C5	2.58	115.65	112.19
4	H	4	BMA	C2-C3-C4	2.47	115.20	110.86
2	E	3	BMA	O3-C3-C2	2.26	114.67	110.05
2	G	1	NAG	C1-O5-C5	2.25	115.21	112.19
2	E	4	MAN	O2-C2-C3	-2.25	105.48	110.15
2	G	4	MAN	C1-O5-C5	2.24	115.19	112.19
2	K	1	NAG	C2-N2-C7	2.20	125.84	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	4	MAN	O2-C2-C3	-2.17	105.66	110.15
4	L	4	BMA	C2-C3-C4	2.15	114.64	110.86
2	K	4	MAN	O2-C2-C3	-2.15	105.71	110.15
2	G	4	MAN	O2-C2-C3	-2.13	105.75	110.15
2	I	5	MAN	O2-C2-C3	-2.09	105.81	110.15
2	I	2	NAG	C1-O5-C5	2.09	114.99	112.19
4	L	3	BMA	O3-C3-C4	2.08	115.29	110.38
2	I	4	MAN	O5-C5-C4	-2.07	105.78	110.83
4	H	2	NAG	C1-O5-C5	2.07	114.96	112.19
4	H	3	BMA	O3-C3-C4	2.06	115.24	110.38
2	E	5	MAN	C2-C3-C4	2.06	114.49	110.86
2	E	5	MAN	O2-C2-C3	-2.04	105.92	110.15
2	E	5	MAN	C1-C2-C3	2.04	112.61	109.64
4	L	3	BMA	O2-C2-C1	2.03	113.88	109.22
4	H	3	BMA	O2-C2-C1	2.03	113.88	109.22
4	L	2	NAG	C1-O5-C5	2.02	114.89	112.19
2	I	4	MAN	O5-C1-C2	2.01	115.58	110.79

There are no chirality outliers.

All (40) torsion outliers are listed below:

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

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

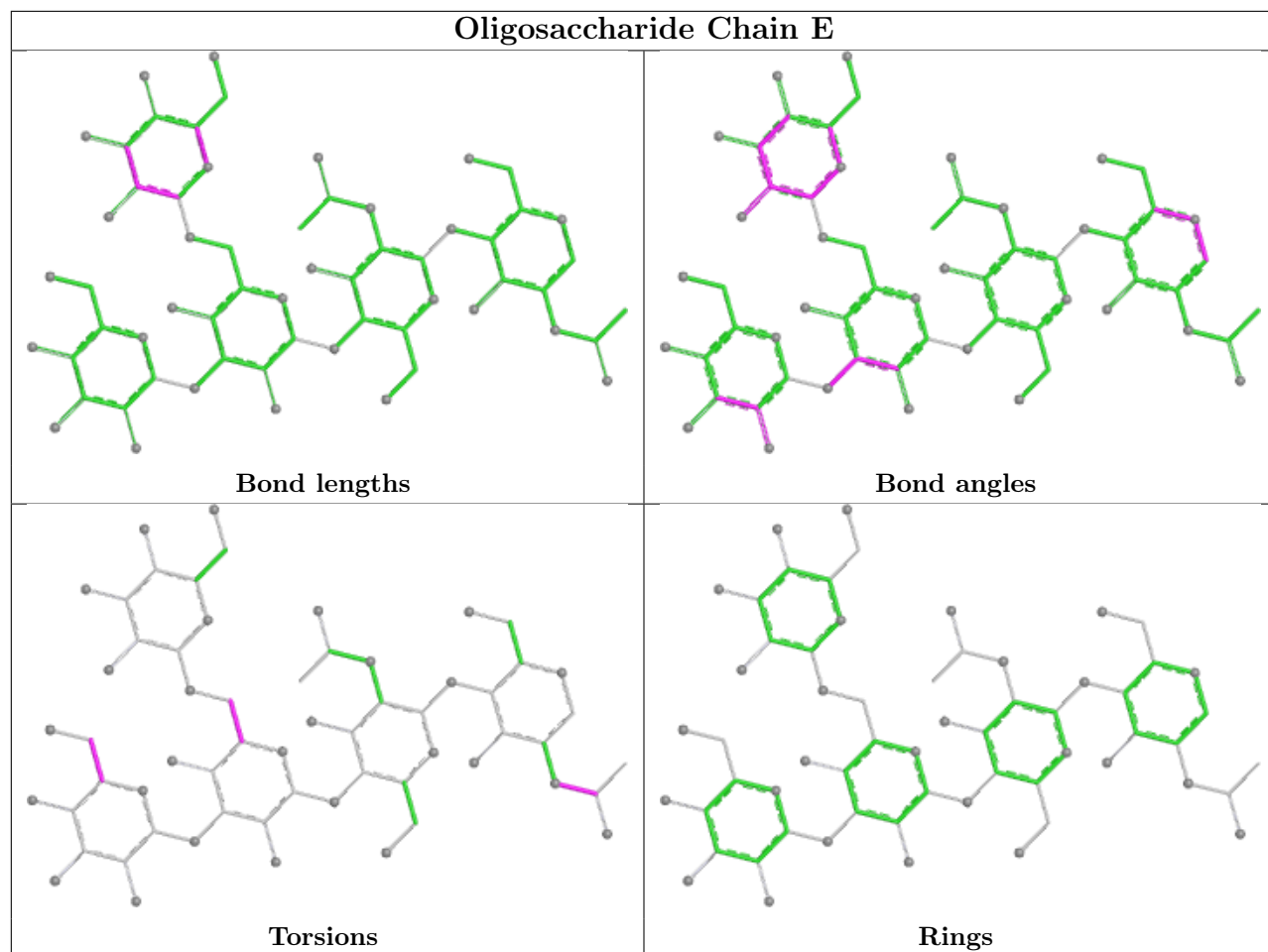
All (2) ring outliers are listed below:

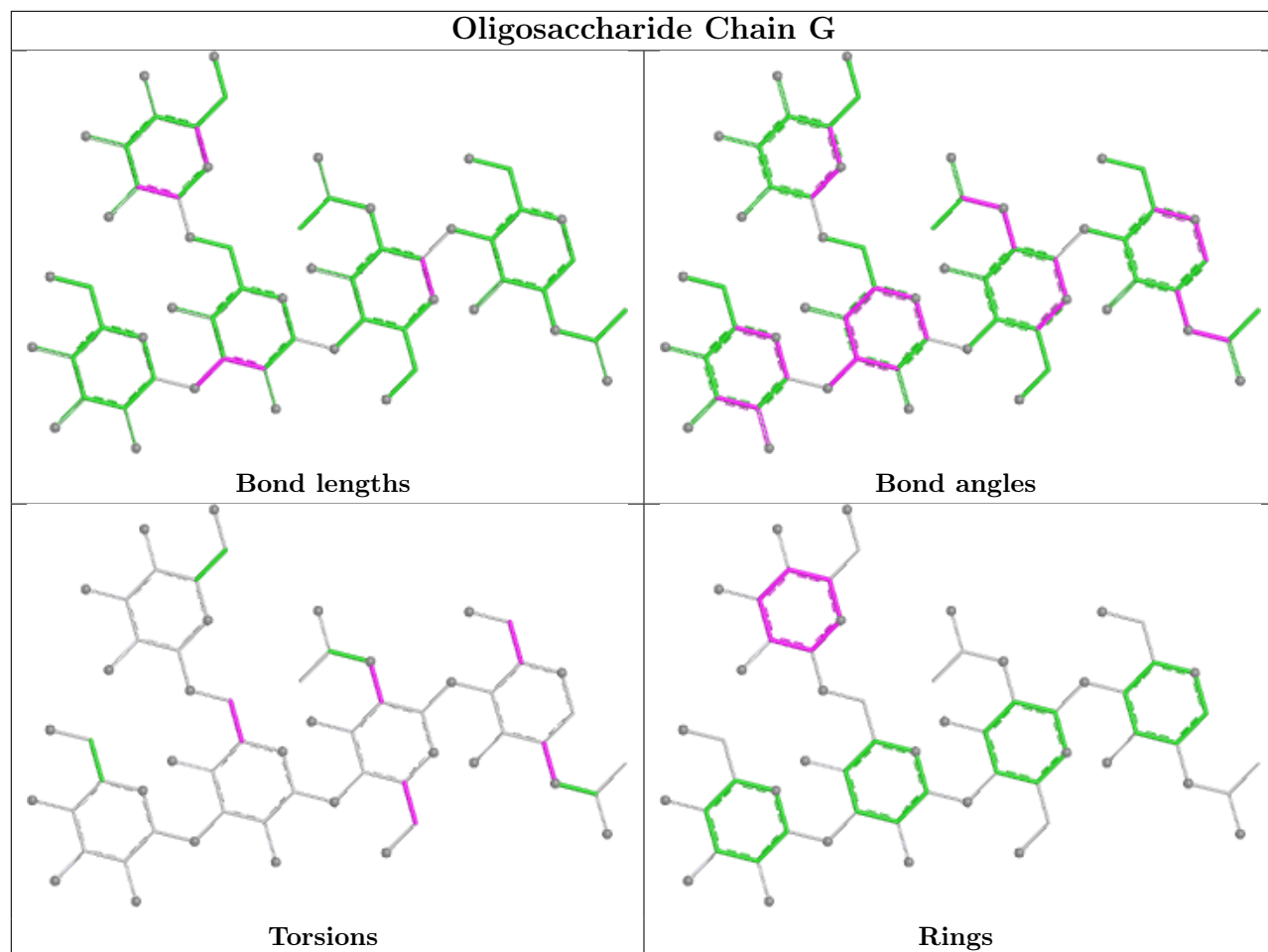
Mol	Chain	Res	Type	Atoms
2	K	5	MAN	C1-C2-C3-C4-C5-O5
2	G	5	MAN	C1-C2-C3-C4-C5-O5

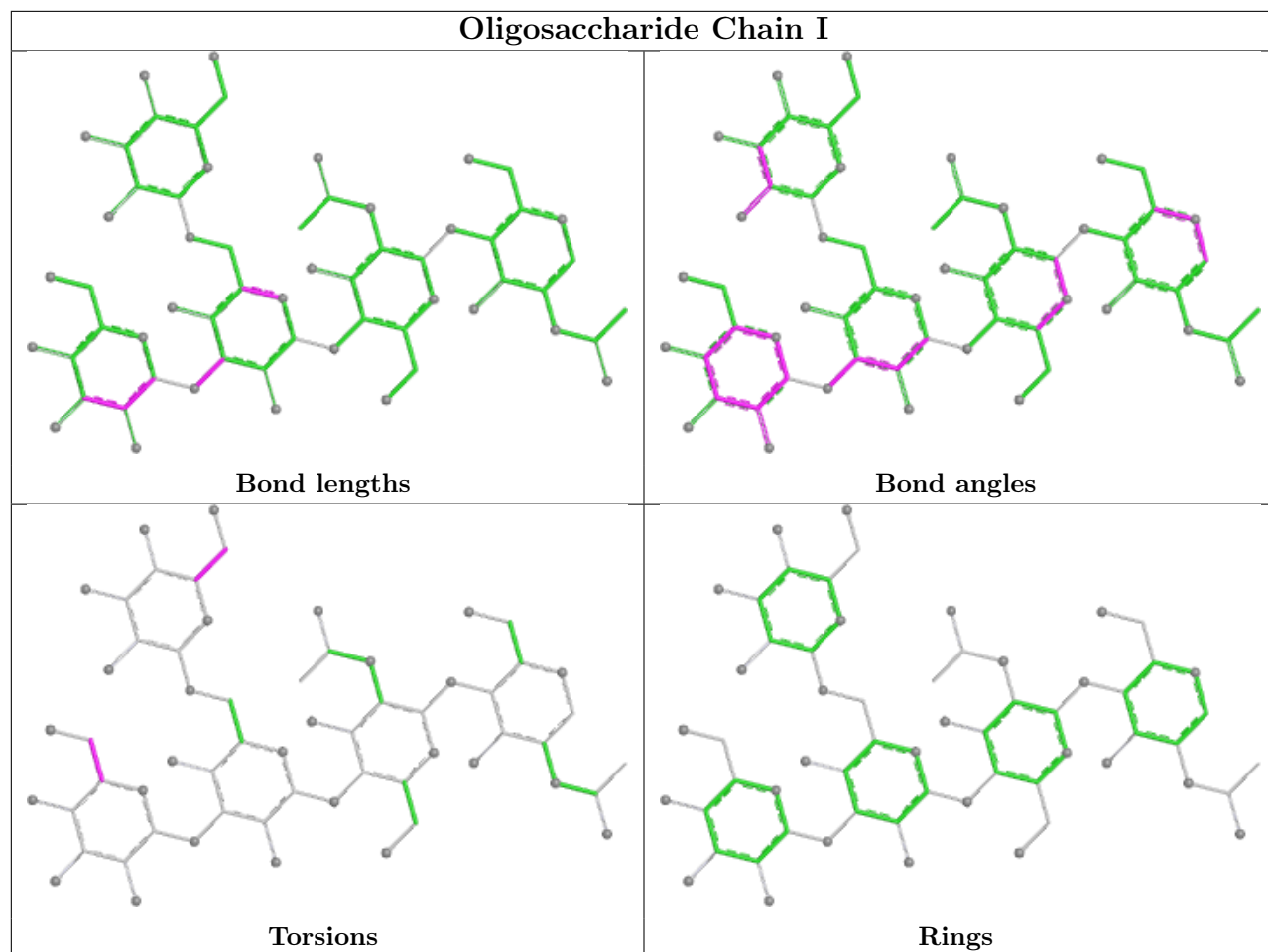
2 monomers are involved in 2 short contacts:

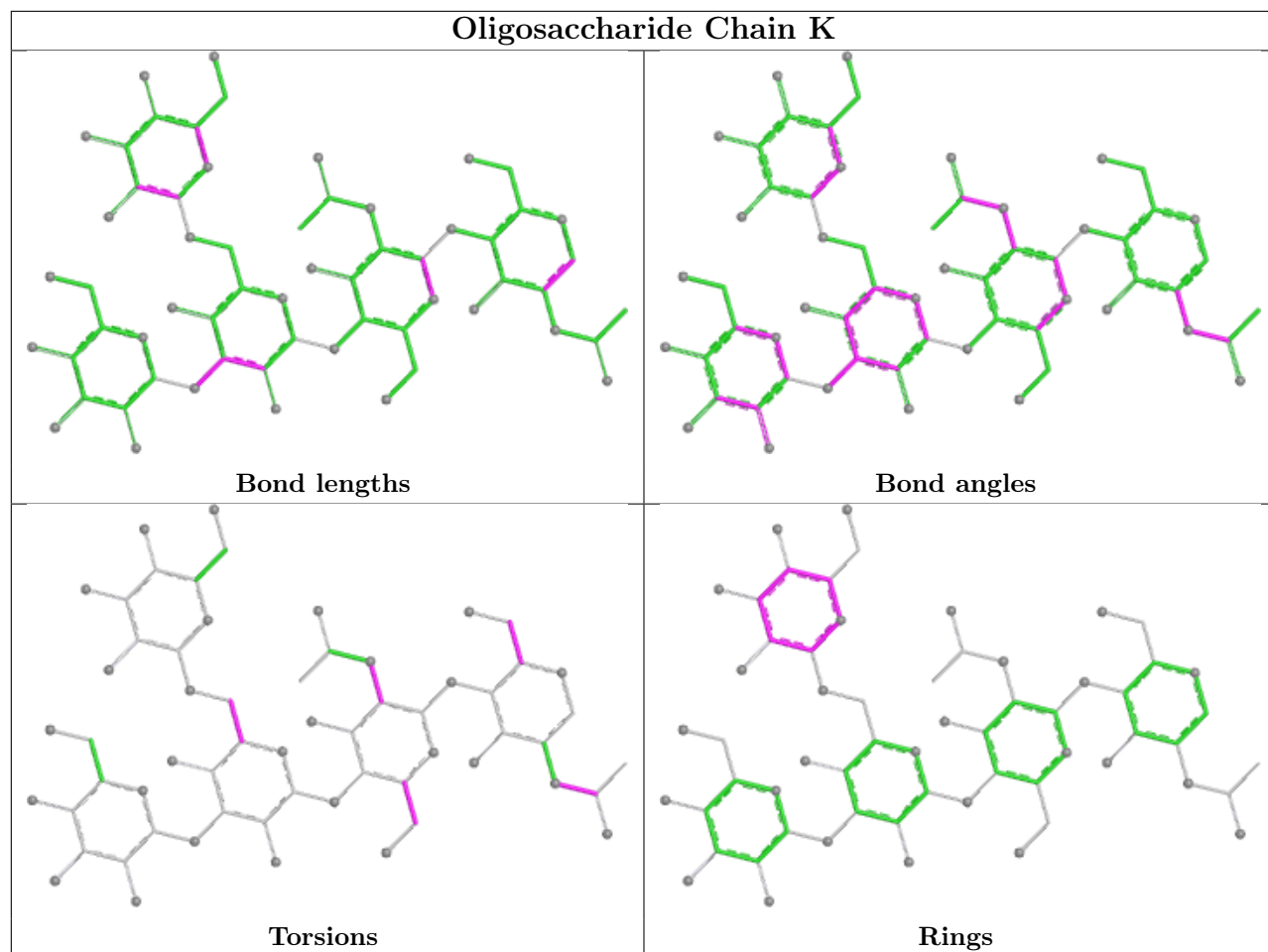
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	1	NAG	1	0
3	J	1	NAG	1	0

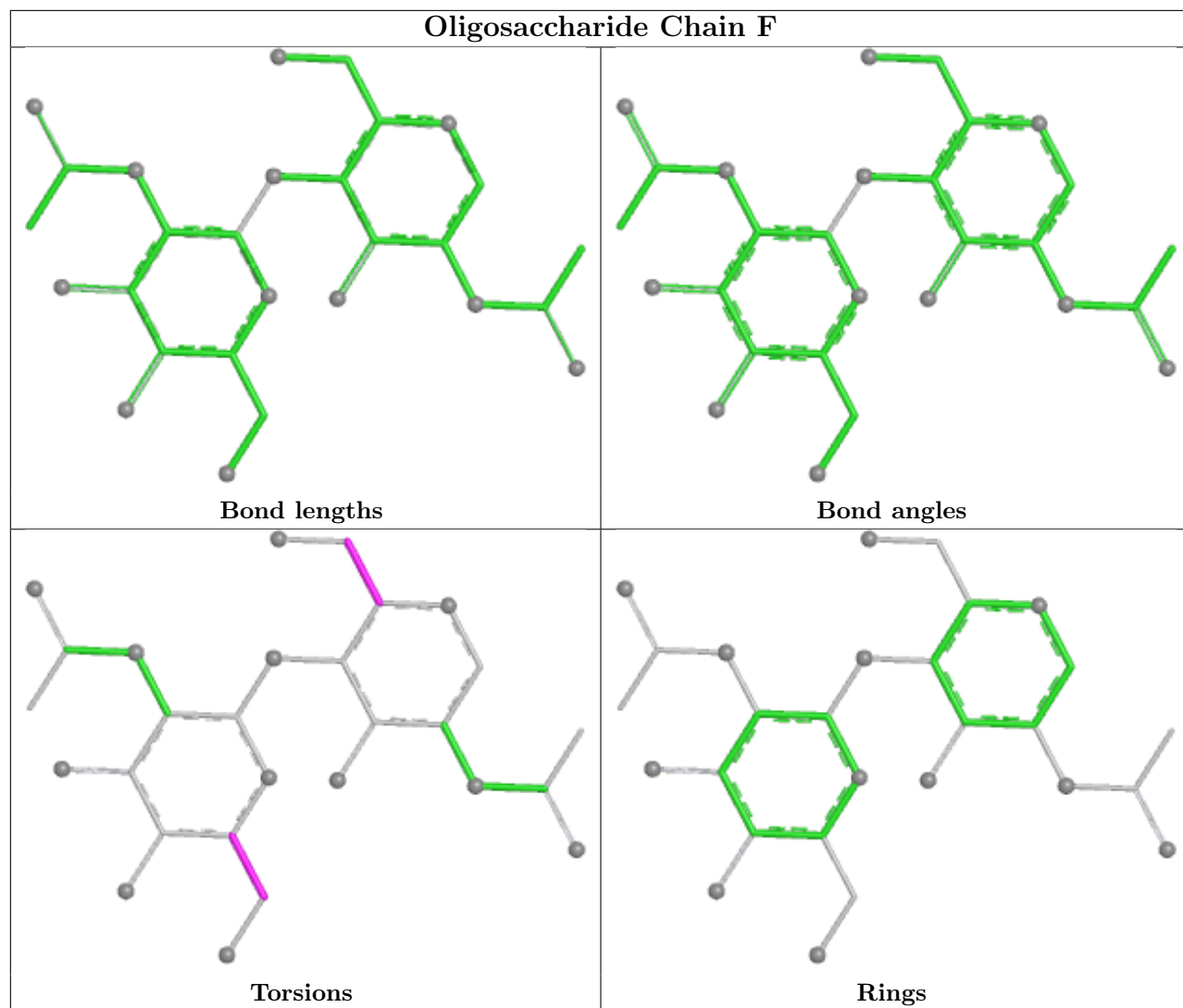
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

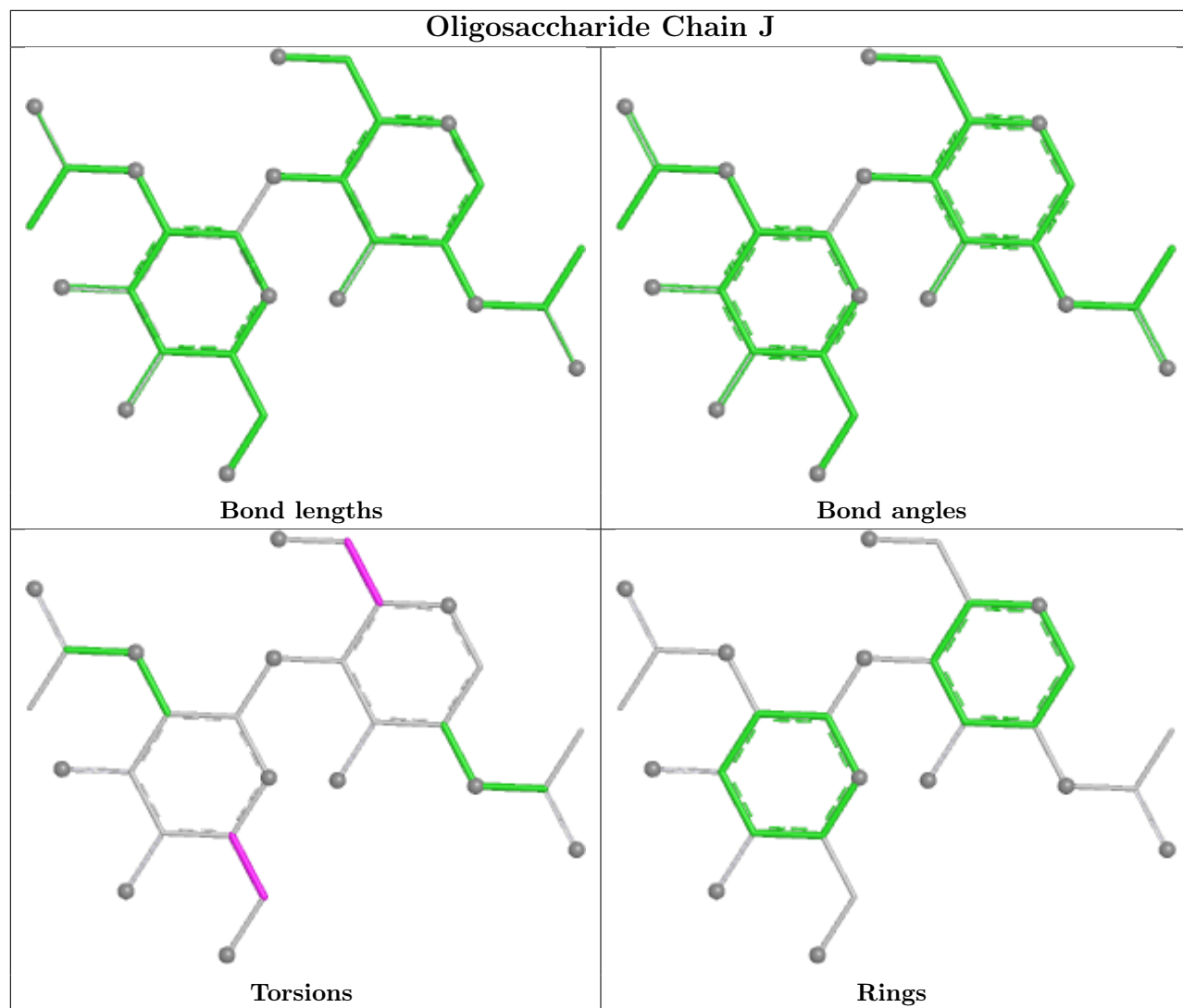




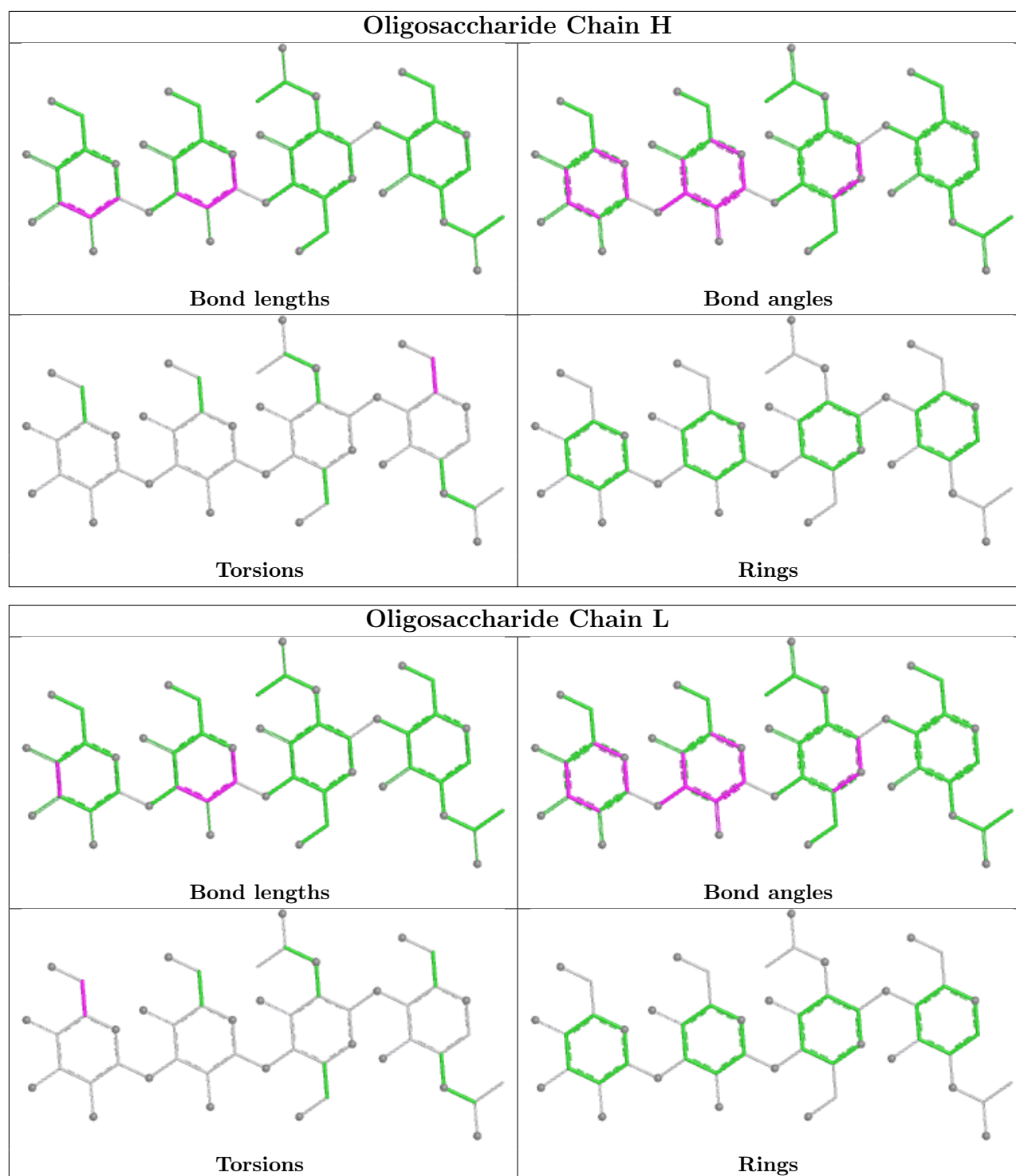












## 5.6 Ligand geometry [i](#)

44 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	NAG	D	1007	1	14,14,15	0.27	0	17,19,21	0.47	0
5	KAI	B	1002	-	13,15,15	1.12	1 (7%)	12,21,21	1.22	1 (8%)
6	POV	A	1003	-	51,51,51	1.09	3 (5%)	57,59,59	0.98	3 (5%)
7	NAG	C	1007	1	14,14,15	0.61	0	17,19,21	0.67	1 (5%)
6	POV	D	1004	-	51,51,51	1.08	3 (5%)	57,59,59	0.95	3 (5%)
7	NAG	A	1007	1	14,14,15	0.57	0	17,19,21	0.61	0
7	NAG	C	1009	1	14,14,15	0.42	0	17,19,21	0.98	1 (5%)
7	NAG	C	1010	1	14,14,15	0.31	0	17,19,21	0.49	0
6	POV	A	1005	-	51,51,51	1.09	3 (5%)	57,59,59	0.93	3 (5%)
6	POV	A	1004	-	51,51,51	1.09	2 (3%)	57,59,59	0.91	3 (5%)
7	NAG	B	1008	1	14,14,15	1.28	1 (7%)	17,19,21	1.65	1 (5%)
6	POV	A	1002	-	51,51,51	1.10	3 (5%)	57,59,59	0.93	3 (5%)
6	POV	B	1004	-	51,51,51	1.08	3 (5%)	57,59,59	0.99	3 (5%)
6	POV	A	1012	-	51,51,51	1.08	3 (5%)	57,59,59	0.96	3 (5%)
6	POV	C	1004	-	51,51,51	1.09	2 (3%)	57,59,59	0.91	3 (5%)
7	NAG	A	1008	1	14,14,15	1.32	1 (7%)	17,19,21	1.56	1 (5%)
6	POV	C	1003	-	51,51,51	1.09	3 (5%)	57,59,59	0.98	3 (5%)
6	POV	D	1003	-	51,51,51	1.06	3 (5%)	57,59,59	0.92	2 (3%)
6	POV	D	1005	-	51,51,51	1.08	3 (5%)	57,59,59	0.98	3 (5%)
7	NAG	A	1010	1	14,14,15	0.28	0	17,19,21	0.48	0
6	POV	A	1013	-	51,51,51	1.07	3 (5%)	57,59,59	0.90	3 (5%)
6	POV	C	1005	-	51,51,51	1.09	3 (5%)	57,59,59	0.93	3 (5%)
8	2J9	A	1014	-	17,18,18	0.62	0	24,28,28	3.93	2 (8%)
7	NAG	D	1010	1	14,14,15	1.29	1 (7%)	17,19,21	1.64	1 (5%)
7	NAG	A	1006	1	14,14,15	1.40	1 (7%)	17,19,21	1.29	1 (5%)
7	NAG	D	1008	1	14,14,15	0.35	0	17,19,21	0.35	0
7	NAG	C	1011	1	14,14,15	0.96	1 (7%)	17,19,21	2.37	3 (17%)
7	NAG	A	1009	1	14,14,15	0.42	0	17,19,21	0.97	1 (5%)
7	NAG	C	1008	1	14,14,15	1.33	1 (7%)	17,19,21	1.57	1 (5%)
5	KAI	A	1001	-	13,15,15	1.04	1 (7%)	12,21,21	1.00	0
7	NAG	B	1005	1	14,14,15	0.26	0	17,19,21	0.44	0
5	KAI	D	1002	-	13,15,15	1.11	1 (7%)	12,21,21	1.17	1 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	2J9	D	1001	-	17,18,18	0.67	0	24,28,28	4.65	2 (8%)
8	2J9	B	1009	-	17,18,18	0.66	0	24,28,28	4.67	2 (8%)
6	POV	B	1003	-	51,51,51	1.06	3 (5%)	57,59,59	0.92	2 (3%)
7	NAG	D	1009	1	14,14,15	0.34	0	17,19,21	0.39	0
7	NAG	B	1006	1	14,14,15	1.03	1 (7%)	17,19,21	2.37	3 (17%)
8	2J9	B	1001	-	17,18,18	0.61	0	24,28,28	3.73	2 (8%)
7	NAG	A	1011	1	14,14,15	0.48	0	17,19,21	0.57	0
7	NAG	C	1006	1	14,14,15	1.38	1 (7%)	17,19,21	1.31	1 (5%)
5	KAI	C	1001	-	13,15,15	1.06	1 (7%)	12,21,21	0.99	0
6	POV	D	1006	-	51,51,51	1.07	3 (5%)	57,59,59	0.91	3 (5%)
6	POV	C	1002	-	51,51,51	1.10	3 (5%)	57,59,59	0.92	3 (5%)
7	NAG	B	1007	1	14,14,15	0.36	0	17,19,21	0.39	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	D	1007	1	-	2/6/23/26	0/1/1/1
5	KAI	B	1002	-	-	2/12/25/25	0/1/1/1
6	POV	A	1003	-	-	29/55/55/55	-
7	NAG	C	1007	1	-	1/6/23/26	0/1/1/1
6	POV	D	1004	-	-	21/55/55/55	-
7	NAG	A	1007	1	-	2/6/23/26	0/1/1/1
7	NAG	C	1009	1	-	3/6/23/26	0/1/1/1
7	NAG	C	1010	1	-	4/6/23/26	0/1/1/1
6	POV	A	1005	-	-	28/55/55/55	-
6	POV	A	1004	-	-	28/55/55/55	-
7	NAG	B	1008	1	-	2/6/23/26	0/1/1/1
6	POV	A	1002	-	-	23/55/55/55	-
6	POV	B	1004	-	-	33/55/55/55	-
6	POV	A	1012	-	-	23/55/55/55	-
6	POV	C	1004	-	-	28/55/55/55	-
7	NAG	A	1008	1	-	2/6/23/26	0/1/1/1
6	POV	C	1003	-	-	28/55/55/55	-
6	POV	D	1003	-	-	31/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	POV	D	1005	-	-	31/55/55/55	-
7	NAG	A	1010	1	-	4/6/23/26	0/1/1/1
6	POV	A	1013	-	-	29/55/55/55	-
6	POV	C	1005	-	-	30/55/55/55	-
8	2J9	A	1014	-	-	3/4/22/22	0/3/3/3
7	NAG	D	1010	1	-	2/6/23/26	0/1/1/1
7	NAG	A	1006	1	-	2/6/23/26	0/1/1/1
7	NAG	D	1008	1	-	2/6/23/26	0/1/1/1
7	NAG	C	1011	1	-	6/6/23/26	0/1/1/1
7	NAG	A	1009	1	-	3/6/23/26	0/1/1/1
7	NAG	C	1008	1	-	2/6/23/26	0/1/1/1
5	KAI	A	1001	-	-	2/12/25/25	0/1/1/1
7	NAG	B	1005	1	-	2/6/23/26	0/1/1/1
5	KAI	D	1002	-	-	1/12/25/25	0/1/1/1
8	2J9	D	1001	-	-	2/4/22/22	0/3/3/3
8	2J9	B	1009	-	-	1/4/22/22	0/3/3/3
6	POV	B	1003	-	-	35/55/55/55	-
7	NAG	D	1009	1	-	2/6/23/26	0/1/1/1
7	NAG	B	1006	1	-	6/6/23/26	0/1/1/1
8	2J9	B	1001	-	-	3/4/22/22	0/3/3/3
7	NAG	A	1011	1	-	1/6/23/26	0/1/1/1
7	NAG	C	1006	1	-	3/6/23/26	0/1/1/1
5	KAI	C	1001	-	-	1/12/25/25	0/1/1/1
6	POV	D	1006	-	-	28/55/55/55	-
6	POV	C	1002	-	-	19/55/55/55	-
7	NAG	B	1007	1	-	2/6/23/26	0/1/1/1

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1006	NAG	O5-C1	4.89	1.51	1.43
7	C	1006	NAG	O5-C1	4.78	1.51	1.43
7	D	1010	NAG	O5-C1	4.72	1.51	1.43
7	B	1008	NAG	O5-C1	4.69	1.51	1.43
7	C	1008	NAG	O5-C1	4.60	1.51	1.43
7	A	1008	NAG	O5-C1	4.58	1.51	1.43
7	B	1006	NAG	C1-C2	3.30	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1004	POV	O21-C21	3.03	1.42	1.34
7	C	1011	NAG	C1-C2	3.02	1.56	1.52
6	C	1003	POV	O21-C21	3.01	1.42	1.34
6	A	1004	POV	O21-C21	3.00	1.42	1.34
6	A	1003	POV	O21-C21	2.99	1.42	1.34
6	D	1006	POV	O21-C21	2.97	1.42	1.34
6	A	1005	POV	O21-C21	2.95	1.42	1.34
6	A	1013	POV	O21-C21	2.94	1.42	1.34
6	C	1005	POV	O21-C21	2.91	1.42	1.34
6	B	1004	POV	O21-C21	2.89	1.42	1.34
6	D	1005	POV	O21-C21	2.86	1.42	1.34
6	A	1002	POV	O21-C21	2.84	1.42	1.34
6	D	1003	POV	O21-C21	2.82	1.42	1.34
6	A	1012	POV	O21-C21	2.81	1.42	1.34
6	C	1002	POV	O21-C21	2.80	1.42	1.34
6	B	1003	POV	O21-C21	2.80	1.42	1.34
6	A	1003	POV	O31-C31	2.80	1.41	1.33
6	C	1003	POV	O31-C31	2.80	1.41	1.33
6	D	1004	POV	O21-C21	2.79	1.42	1.34
6	D	1005	POV	O31-C31	2.76	1.41	1.33
6	A	1004	POV	O31-C31	2.76	1.41	1.33
6	C	1004	POV	O31-C31	2.75	1.41	1.33
6	B	1004	POV	O31-C31	2.75	1.41	1.33
6	A	1002	POV	O31-C31	2.74	1.41	1.33
6	C	1002	POV	O31-C31	2.73	1.41	1.33
6	A	1005	POV	O31-C31	2.67	1.41	1.33
6	B	1003	POV	O31-C31	2.66	1.41	1.33
6	C	1005	POV	O31-C31	2.66	1.41	1.33
6	D	1004	POV	O31-C31	2.65	1.41	1.33
6	A	1012	POV	O31-C31	2.65	1.41	1.33
6	D	1006	POV	O31-C31	2.65	1.41	1.33
6	D	1003	POV	O31-C31	2.64	1.41	1.33
6	A	1013	POV	O31-C31	2.63	1.41	1.33
6	C	1002	POV	O21-C2	-2.62	1.40	1.46
6	A	1002	POV	O21-C2	-2.58	1.40	1.46
6	D	1003	POV	O21-C2	-2.55	1.40	1.46
6	A	1012	POV	O21-C2	-2.53	1.40	1.46
6	D	1004	POV	O21-C2	-2.52	1.40	1.46
6	B	1003	POV	O21-C2	-2.52	1.40	1.46
6	A	1005	POV	O21-C2	-2.47	1.40	1.46
6	C	1005	POV	O21-C2	-2.46	1.40	1.46
6	D	1005	POV	O21-C2	-2.39	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1004	POV	O21-C2	-2.36	1.41	1.46
6	A	1003	POV	O21-C2	-2.33	1.41	1.46
6	C	1003	POV	O21-C2	-2.31	1.41	1.46
5	B	1002	KAI	OXT-C	-2.14	1.23	1.30
5	C	1001	KAI	OXT-C	-2.12	1.23	1.30
5	D	1002	KAI	OXT-C	-2.11	1.23	1.30
5	A	1001	KAI	OXT-C	-2.08	1.24	1.30
6	A	1013	POV	O21-C2	-2.05	1.41	1.46
6	D	1006	POV	O21-C2	-2.05	1.41	1.46

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	1009	2J9	CAI-NAO-CAL	22.32	123.37	110.17
8	D	1001	2J9	CAI-NAO-CAL	22.20	123.30	110.17
8	A	1014	2J9	CAI-NAO-CAL	18.65	121.20	110.17
8	B	1001	2J9	CAI-NAO-CAL	17.63	120.60	110.17
7	B	1006	NAG	C2-N2-C7	8.31	134.04	122.90
7	C	1011	NAG	C2-N2-C7	8.14	133.81	122.90
7	B	1008	NAG	C1-O5-C5	6.57	121.00	112.19
7	D	1010	NAG	C1-O5-C5	6.57	121.00	112.19
7	C	1008	NAG	C1-O5-C5	6.08	120.34	112.19
7	A	1008	NAG	C1-O5-C5	6.03	120.27	112.19
7	C	1006	NAG	C1-O5-C5	5.04	118.95	112.19
7	A	1006	NAG	C1-O5-C5	4.97	118.85	112.19
7	C	1011	NAG	C1-C2-N2	4.26	117.14	110.43
6	B	1004	POV	O21-C21-C22	4.24	120.66	111.48
6	A	1003	POV	O21-C21-C22	4.22	120.62	111.48
6	D	1005	POV	O21-C21-C22	4.20	120.56	111.48
6	C	1003	POV	O21-C21-C22	4.19	120.54	111.48
6	A	1002	POV	O21-C21-C22	4.17	120.50	111.48
6	C	1002	POV	O21-C21-C22	4.12	120.39	111.48
7	B	1006	NAG	C1-C2-N2	4.11	116.92	110.43
6	C	1005	POV	O21-C21-C22	3.93	119.99	111.48
6	D	1003	POV	O21-C21-C22	3.93	119.98	111.48
6	A	1005	POV	O21-C21-C22	3.90	119.91	111.48
6	B	1003	POV	O21-C21-C22	3.90	119.91	111.48
8	B	1001	2J9	CAK-CAF-CAM	3.86	119.23	116.92
6	A	1012	POV	O21-C21-C22	3.85	119.80	111.48
8	A	1014	2J9	CAK-CAF-CAM	3.83	119.21	116.92
6	D	1004	POV	O21-C21-C22	3.82	119.75	111.48
8	D	1001	2J9	CAK-CAF-CAM	3.79	119.19	116.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	1009	2J9	CAK-CAF-CAM	3.79	119.19	116.92
6	A	1004	POV	O21-C21-C22	3.64	119.36	111.48
6	C	1004	POV	O21-C21-C22	3.64	119.35	111.48
6	D	1006	POV	O21-C21-C22	3.56	119.18	111.48
6	A	1013	POV	O21-C21-C22	3.36	118.74	111.48
7	A	1009	NAG	C2-N2-C7	3.27	127.28	122.90
7	C	1009	NAG	C2-N2-C7	3.26	127.28	122.90
6	C	1005	POV	O31-C31-C32	2.72	120.12	111.83
6	A	1005	POV	O31-C31-C32	2.70	120.07	111.83
6	A	1002	POV	O31-C31-C32	2.67	119.97	111.83
6	C	1004	POV	O31-C31-C32	2.63	119.85	111.83
6	A	1004	POV	O31-C31-C32	2.63	119.84	111.83
6	A	1012	POV	C14-N-C12	2.61	120.28	109.91
6	C	1002	POV	O31-C31-C32	2.58	119.71	111.83
6	D	1004	POV	C14-N-C12	2.58	120.16	109.91
6	C	1003	POV	O31-C31-C32	2.58	119.69	111.83
6	A	1003	POV	O31-C31-C32	2.58	119.69	111.83
6	A	1003	POV	C14-N-C12	2.55	120.06	109.91
6	A	1012	POV	O31-C31-C32	2.54	119.57	111.83
6	D	1004	POV	O31-C31-C32	2.53	119.53	111.83
6	C	1003	POV	C14-N-C12	2.52	119.94	109.91
6	B	1004	POV	C14-N-C12	2.51	119.88	109.91
6	B	1004	POV	O31-C31-C32	2.51	119.48	111.83
6	D	1005	POV	O31-C31-C32	2.50	119.47	111.83
6	A	1013	POV	O31-C31-C32	2.50	119.46	111.83
6	D	1006	POV	O31-C31-C32	2.50	119.46	111.83
6	D	1005	POV	C14-N-C12	2.49	119.82	109.91
6	A	1004	POV	C14-N-C12	2.48	119.75	109.91
6	C	1004	POV	C14-N-C12	2.47	119.74	109.91
6	A	1005	POV	C14-N-C12	2.41	119.49	109.91
6	C	1005	POV	C14-N-C12	2.40	119.46	109.91
5	B	1002	KAI	O-C-CA	-2.35	114.07	121.86
6	B	1003	POV	O31-C31-C32	2.33	118.92	111.83
6	C	1002	POV	C14-N-C12	2.30	119.07	109.91
6	D	1003	POV	O31-C31-C32	2.30	118.86	111.83
6	A	1002	POV	C14-N-C12	2.29	119.00	109.91
6	A	1013	POV	C14-N-C12	2.27	118.92	109.91
6	D	1006	POV	C14-N-C12	2.24	118.81	109.91
7	C	1007	NAG	C1-O5-C5	2.22	115.16	112.19
7	B	1006	NAG	C8-C7-N2	2.22	119.79	116.12
5	D	1002	KAI	O-C-CA	-2.17	114.65	121.86
7	C	1011	NAG	C8-C7-N2	2.14	119.67	116.12



There are no chirality outliers.

All (512) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1002	POV	C1-O11-P-O12
6	A	1002	POV	C1-O11-P-O13
6	A	1002	POV	C11-O12-P-O11
6	A	1002	POV	C11-O12-P-O13
6	A	1002	POV	C11-O12-P-O14
6	A	1003	POV	O12-C11-C12-N
6	A	1003	POV	C22-C21-O21-C2
6	A	1003	POV	O22-C21-O21-C2
6	A	1004	POV	C11-O12-P-O11
6	A	1004	POV	C11-O12-P-O13
6	A	1004	POV	O12-C11-C12-N
6	A	1004	POV	O32-C31-O31-C3
6	A	1005	POV	C1-O11-P-O12
6	A	1005	POV	C1-O11-P-O13
6	A	1005	POV	O12-C11-C12-N
6	A	1012	POV	C11-O12-P-O14
6	A	1012	POV	O22-C21-O21-C2
6	A	1013	POV	C1-O11-P-O12
6	A	1013	POV	C11-O12-P-O11
6	A	1013	POV	O11-C1-C2-O21
6	A	1013	POV	O12-C11-C12-N
6	A	1013	POV	C22-C21-O21-C2
6	A	1013	POV	O32-C31-O31-C3
6	B	1003	POV	C1-O11-P-O12
6	B	1003	POV	C1-O11-P-O13
6	B	1003	POV	C1-O11-P-O14
6	B	1003	POV	C11-O12-P-O14
6	B	1003	POV	O21-C2-C3-O31
6	B	1003	POV	O22-C21-O21-C2
6	B	1004	POV	C1-O11-P-O12
6	B	1004	POV	C1-O11-P-O13
6	B	1004	POV	O12-C11-C12-N
6	B	1004	POV	C22-C21-O21-C2
6	B	1004	POV	O22-C21-O21-C2
6	C	1002	POV	C1-O11-P-O12
6	C	1002	POV	C11-O12-P-O11
6	C	1002	POV	C11-O12-P-O13
6	C	1002	POV	C11-O12-P-O14
6	C	1003	POV	O12-C11-C12-N
6	C	1003	POV	C22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
6	C	1003	POV	O22-C21-O21-C2
6	C	1004	POV	C11-O12-P-O11
6	C	1004	POV	C11-O12-P-O13
6	C	1004	POV	O12-C11-C12-N
6	C	1004	POV	O32-C31-O31-C3
6	C	1005	POV	C1-O11-P-O12
6	C	1005	POV	C1-O11-P-O13
6	C	1005	POV	O12-C11-C12-N
6	D	1003	POV	C1-O11-P-O12
6	D	1003	POV	C1-O11-P-O13
6	D	1003	POV	C1-O11-P-O14
6	D	1003	POV	C11-O12-P-O14
6	D	1003	POV	O21-C2-C3-O31
6	D	1003	POV	O22-C21-O21-C2
6	D	1004	POV	C11-O12-P-O14
6	D	1004	POV	O22-C21-O21-C2
6	D	1005	POV	O12-C11-C12-N
6	D	1005	POV	O22-C21-O21-C2
6	D	1006	POV	C1-O11-P-O12
6	D	1006	POV	C11-O12-P-O11
6	D	1006	POV	C11-O12-P-O13
6	D	1006	POV	O11-C1-C2-O21
6	D	1006	POV	O12-C11-C12-N
6	D	1006	POV	C22-C21-O21-C2
8	A	1014	2J9	CAG-CAN-NAO-CAI
8	B	1001	2J9	CAG-CAN-NAO-CAI
8	B	1009	2J9	CAH-CAN-NAO-CAI
8	D	1001	2J9	CAH-CAN-NAO-CAI
6	D	1005	POV	O32-C31-O31-C3
6	B	1004	POV	C32-C31-O31-C3
6	A	1005	POV	O32-C31-O31-C3
6	B	1004	POV	O32-C31-O31-C3
6	C	1005	POV	O32-C31-O31-C3
6	D	1006	POV	O32-C31-O31-C3
6	A	1004	POV	O22-C21-O21-C2
6	A	1013	POV	O22-C21-O21-C2
6	C	1004	POV	O22-C21-O21-C2
6	D	1006	POV	O22-C21-O21-C2
6	A	1004	POV	C32-C31-O31-C3
6	A	1005	POV	C32-C31-O31-C3
6	A	1013	POV	C32-C31-O31-C3
6	B	1003	POV	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
6	C	1004	POV	C32-C31-O31-C3
6	C	1005	POV	C32-C31-O31-C3
6	D	1005	POV	C32-C31-O31-C3
7	A	1010	NAG	O5-C5-C6-O6
6	A	1004	POV	C22-C21-O21-C2
6	A	1012	POV	C22-C21-O21-C2
6	B	1003	POV	C22-C21-O21-C2
6	C	1004	POV	C22-C21-O21-C2
6	D	1003	POV	C22-C21-O21-C2
6	D	1004	POV	C22-C21-O21-C2
6	D	1005	POV	C22-C21-O21-C2
7	C	1011	NAG	O5-C5-C6-O6
7	B	1005	NAG	C4-C5-C6-O6
6	D	1003	POV	C32-C31-O31-C3
6	D	1006	POV	C32-C31-O31-C3
6	B	1003	POV	O32-C31-O31-C3
7	D	1008	NAG	O5-C5-C6-O6
7	B	1007	NAG	C4-C5-C6-O6
7	D	1007	NAG	C4-C5-C6-O6
7	B	1005	NAG	O5-C5-C6-O6
7	C	1010	NAG	O5-C5-C6-O6
7	B	1006	NAG	O5-C5-C6-O6
7	A	1010	NAG	C4-C5-C6-O6
7	C	1010	NAG	C4-C5-C6-O6
7	C	1011	NAG	C4-C5-C6-O6
7	D	1008	NAG	C4-C5-C6-O6
7	D	1009	NAG	C4-C5-C6-O6
6	D	1003	POV	O32-C31-O31-C3
7	B	1007	NAG	O5-C5-C6-O6
7	B	1008	NAG	C4-C5-C6-O6
6	A	1012	POV	C24-C25-C26-C27
6	C	1005	POV	C24-C25-C26-C27
6	D	1004	POV	C24-C25-C26-C27
7	D	1007	NAG	O5-C5-C6-O6
6	A	1003	POV	C21-C22-C23-C24
7	D	1010	NAG	C4-C5-C6-O6
7	D	1009	NAG	O5-C5-C6-O6
6	B	1003	POV	C212-C213-C214-C215
6	A	1013	POV	C31-C32-C33-C34
6	C	1003	POV	C21-C22-C23-C24
6	C	1004	POV	C21-C22-C23-C24
7	B	1006	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	A	1005	POV	C24-C25-C26-C27
6	A	1004	POV	C21-C22-C23-C24
6	A	1012	POV	C21-C22-C23-C24
7	A	1006	NAG	C8-C7-N2-C2
7	A	1006	NAG	O7-C7-N2-C2
7	A	1008	NAG	C8-C7-N2-C2
7	A	1008	NAG	O7-C7-N2-C2
7	A	1010	NAG	C8-C7-N2-C2
7	A	1010	NAG	O7-C7-N2-C2
7	B	1006	NAG	C8-C7-N2-C2
7	B	1006	NAG	O7-C7-N2-C2
7	C	1006	NAG	C8-C7-N2-C2
7	C	1006	NAG	O7-C7-N2-C2
7	C	1008	NAG	C8-C7-N2-C2
7	C	1008	NAG	O7-C7-N2-C2
7	C	1010	NAG	C8-C7-N2-C2
7	C	1010	NAG	O7-C7-N2-C2
7	C	1011	NAG	C8-C7-N2-C2
7	C	1011	NAG	O7-C7-N2-C2
7	B	1008	NAG	O5-C5-C6-O6
7	D	1010	NAG	O5-C5-C6-O6
6	A	1003	POV	C31-C32-C33-C34
6	C	1003	POV	C31-C32-C33-C34
6	D	1004	POV	C21-C22-C23-C24
6	D	1006	POV	C31-C32-C33-C34
6	D	1003	POV	C212-C213-C214-C215
6	A	1004	POV	C31-C32-C33-C34
6	A	1004	POV	C23-C24-C25-C26
6	C	1004	POV	C23-C24-C25-C26
6	C	1004	POV	C31-C32-C33-C34
6	A	1013	POV	C3-C2-O21-C21
6	D	1006	POV	C3-C2-O21-C21
6	A	1005	POV	C39-C310-C311-C312
6	A	1005	POV	C25-C26-C27-C28
6	A	1002	POV	C22-C23-C24-C25
6	A	1002	POV	C24-C25-C26-C27
6	A	1003	POV	C36-C37-C38-C39
6	A	1012	POV	C34-C35-C36-C37
6	C	1002	POV	C22-C23-C24-C25
6	C	1003	POV	C32-C33-C34-C35
6	C	1005	POV	C25-C26-C27-C28
6	D	1004	POV	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
6	A	1003	POV	C32-C33-C34-C35
6	A	1004	POV	C311-C312-C313-C314
6	C	1003	POV	C36-C37-C38-C39
6	B	1004	POV	C213-C214-C215-C216
6	C	1005	POV	C35-C36-C37-C38
6	D	1005	POV	C213-C214-C215-C216
6	C	1005	POV	C39-C310-C311-C312
6	A	1004	POV	C22-C23-C24-C25
6	C	1004	POV	C311-C312-C313-C314
6	C	1004	POV	C22-C23-C24-C25
6	A	1002	POV	C25-C26-C27-C28
6	B	1004	POV	C24-C25-C26-C27
6	C	1002	POV	C24-C25-C26-C27
6	D	1005	POV	C24-C25-C26-C27
6	A	1004	POV	C211-C212-C213-C214
6	A	1005	POV	C34-C35-C36-C37
6	A	1005	POV	C35-C36-C37-C38
6	C	1004	POV	C211-C212-C213-C214
6	C	1002	POV	C25-C26-C27-C28
7	A	1007	NAG	C4-C5-C6-O6
6	C	1003	POV	C311-C312-C313-C314
6	A	1003	POV	C311-C312-C313-C314
6	A	1013	POV	C310-C311-C312-C313
6	D	1006	POV	C37-C38-C39-C310
6	B	1003	POV	C35-C36-C37-C38
6	A	1013	POV	C39-C310-C311-C312
6	D	1003	POV	C35-C36-C37-C38
6	A	1004	POV	C24-C25-C26-C27
6	A	1012	POV	C312-C313-C314-C315
6	A	1003	POV	C312-C313-C314-C315
6	A	1013	POV	C37-C38-C39-C310
6	C	1004	POV	C24-C25-C26-C27
6	C	1005	POV	C33-C34-C35-C36
6	D	1006	POV	C310-C311-C312-C313
6	B	1003	POV	C36-C37-C38-C39
6	D	1003	POV	C36-C37-C38-C39
6	C	1004	POV	C311-C310-C39-C38
6	A	1013	POV	C27-C28-C29-C210
6	B	1003	POV	C27-C28-C29-C210
6	A	1002	POV	C22-C21-O21-C2
6	C	1002	POV	C22-C21-O21-C2
6	C	1004	POV	C212-C213-C214-C215

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Mol	Chain	Res	Type	Atoms
6	D	1006	POV	C39-C310-C311-C312
6	D	1003	POV	C313-C314-C315-C316
6	C	1005	POV	C34-C35-C36-C37
6	A	1004	POV	C212-C213-C214-C215
6	D	1005	POV	C22-C23-C24-C25
6	A	1003	POV	O11-C1-C2-O21
6	C	1003	POV	O11-C1-C2-O21
6	A	1004	POV	C311-C310-C39-C38
7	A	1009	NAG	O5-C5-C6-O6
7	C	1009	NAG	O5-C5-C6-O6
6	A	1005	POV	O21-C2-C3-O31
6	C	1005	POV	O21-C2-C3-O31
6	D	1005	POV	C210-C211-C212-C213
6	D	1003	POV	C22-C23-C24-C25
6	D	1005	POV	C311-C310-C39-C38
6	B	1004	POV	C311-C310-C39-C38
6	C	1003	POV	C22-C23-C24-C25
6	A	1013	POV	C33-C34-C35-C36
6	B	1004	POV	C312-C313-C314-C315
6	D	1003	POV	C27-C28-C29-C210
6	D	1006	POV	C27-C28-C29-C210
6	A	1003	POV	C22-C23-C24-C25
6	A	1013	POV	C22-C23-C24-C25
6	C	1002	POV	O22-C21-O21-C2
6	A	1002	POV	C39-C310-C311-C312
6	B	1004	POV	C22-C23-C24-C25
6	B	1004	POV	C210-C211-C212-C213
6	D	1003	POV	C210-C211-C212-C213
6	D	1004	POV	C210-C211-C212-C213
6	D	1006	POV	C311-C310-C39-C38
6	A	1003	POV	O11-C1-C2-C3
6	A	1013	POV	O11-C1-C2-C3
6	A	1002	POV	O22-C21-O21-C2
6	B	1004	POV	C36-C37-C38-C39
6	D	1006	POV	C33-C34-C35-C36
6	B	1004	POV	C35-C36-C37-C38
6	D	1005	POV	C35-C36-C37-C38
7	A	1007	NAG	O5-C5-C6-O6
6	B	1003	POV	C39-C310-C311-C312
6	C	1005	POV	C211-C212-C213-C214
6	C	1005	POV	C23-C24-C25-C26
6	D	1003	POV	C310-C311-C312-C313

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Mol	Chain	Res	Type	Atoms
6	D	1006	POV	C22-C23-C24-C25
6	A	1003	POV	C1-C2-C3-O31
6	A	1005	POV	C1-C2-C3-O31
6	C	1003	POV	C1-C2-C3-O31
6	B	1003	POV	C210-C211-C212-C213
6	D	1003	POV	C26-C27-C28-C29
6	A	1005	POV	C33-C34-C35-C36
6	D	1003	POV	C39-C310-C311-C312
6	D	1005	POV	C36-C37-C38-C39
7	C	1006	NAG	O5-C5-C6-O6
6	D	1003	POV	C25-C26-C27-C28
6	B	1003	POV	C33-C34-C35-C36
6	A	1002	POV	C310-C311-C312-C313
8	A	1014	2J9	CAH-CAN-NAO-CAL
8	B	1001	2J9	CAH-CAN-NAO-CAL
6	A	1003	POV	C35-C36-C37-C38
6	A	1004	POV	C3-C2-O21-C21
6	B	1004	POV	C3-C2-O21-C21
6	C	1004	POV	C3-C2-O21-C21
6	A	1003	POV	C311-C310-C39-C38
6	C	1003	POV	C35-C36-C37-C38
6	A	1004	POV	C26-C27-C28-C29
6	B	1003	POV	C26-C27-C28-C29
6	C	1004	POV	C26-C27-C28-C29
6	B	1003	POV	C22-C23-C24-C25
6	C	1002	POV	C39-C310-C311-C312
6	D	1005	POV	C211-C212-C213-C214
6	D	1005	POV	C312-C313-C314-C315
6	C	1003	POV	C312-C313-C314-C315
6	A	1013	POV	C311-C310-C39-C38
6	D	1003	POV	C33-C34-C35-C36
6	B	1004	POV	C33-C34-C35-C36
6	A	1013	POV	C211-C212-C213-C214
6	D	1005	POV	C33-C34-C35-C36
6	A	1005	POV	C311-C312-C313-C314
6	A	1003	POV	C313-C314-C315-C316
6	D	1004	POV	C215-C216-C217-C218
6	C	1002	POV	C23-C24-C25-C26
6	A	1012	POV	C215-C216-C217-C218
6	A	1005	POV	C213-C214-C215-C216
6	A	1004	POV	C37-C38-C39-C310
6	A	1012	POV	C211-C212-C213-C214

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Mol	Chain	Res	Type	Atoms
6	B	1003	POV	C29-C210-C211-C212
6	A	1002	POV	C23-C24-C25-C26
6	B	1003	POV	C25-C26-C27-C28
6	D	1006	POV	C211-C212-C213-C214
6	C	1005	POV	C311-C312-C313-C314
6	A	1012	POV	C213-C214-C215-C216
6	D	1003	POV	C312-C313-C314-C315
6	C	1003	POV	O11-C1-C2-C3
6	D	1006	POV	O11-C1-C2-C3
6	C	1004	POV	C37-C38-C39-C310
6	A	1005	POV	C23-C24-C25-C26
6	D	1005	POV	C23-C24-C25-C26
6	B	1004	POV	C211-C212-C213-C214
6	B	1004	POV	C23-C24-C25-C26
6	A	1013	POV	C21-C22-C23-C24
6	D	1004	POV	C311-C312-C313-C314
6	A	1012	POV	C1-C2-C3-O31
6	B	1003	POV	C1-C2-C3-O31
6	C	1005	POV	C1-C2-C3-O31
6	D	1003	POV	C1-C2-C3-O31
6	D	1004	POV	C1-C2-C3-O31
6	A	1005	POV	C36-C37-C38-C39
6	C	1003	POV	C313-C314-C315-C316
6	C	1002	POV	C310-C311-C312-C313
6	C	1003	POV	C311-C310-C39-C38
6	D	1004	POV	C211-C212-C213-C214
6	A	1003	POV	C24-C25-C26-C27
6	C	1003	POV	C24-C25-C26-C27
6	C	1005	POV	C21-C22-C23-C24
6	C	1005	POV	C31-C32-C33-C34
6	A	1002	POV	C36-C37-C38-C39
7	A	1009	NAG	C1-C2-N2-C7
7	C	1009	NAG	C1-C2-N2-C7
6	C	1002	POV	C36-C37-C38-C39
6	D	1003	POV	C29-C210-C211-C212
6	D	1004	POV	C213-C214-C215-C216
6	D	1005	POV	C311-C312-C313-C314
6	B	1004	POV	C26-C27-C28-C29
6	D	1003	POV	C2-C1-O11-P
6	B	1004	POV	C311-C312-C313-C314
8	A	1014	2J9	CAG-CAN-NAO-CAL
6	A	1013	POV	C311-C312-C313-C314

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Mol	Chain	Res	Type	Atoms
6	D	1006	POV	C311-C312-C313-C314
6	A	1003	POV	C3-C2-O21-C21
6	C	1003	POV	C3-C2-O21-C21
6	D	1005	POV	C3-C2-O21-C21
6	C	1003	POV	C34-C35-C36-C37
6	C	1005	POV	C311-C310-C39-C38
6	D	1006	POV	C21-C22-C23-C24
6	D	1004	POV	C312-C313-C314-C315
6	A	1005	POV	O21-C21-C22-C23
6	A	1003	POV	C34-C35-C36-C37
6	B	1003	POV	C12-C11-O12-P
6	D	1003	POV	C12-C11-O12-P
6	A	1013	POV	O21-C2-C3-O31
6	D	1005	POV	C26-C27-C28-C29
6	D	1006	POV	O21-C2-C3-O31
6	B	1003	POV	C213-C214-C215-C216
6	B	1003	POV	C2-C1-O11-P
6	A	1002	POV	O12-C11-C12-N
6	A	1012	POV	O12-C11-C12-N
6	C	1002	POV	O12-C11-C12-N
6	D	1004	POV	O12-C11-C12-N
6	B	1004	POV	C21-C22-C23-C24
8	B	1001	2J9	CAG-CAN-NAO-CAL
6	A	1012	POV	C210-C211-C212-C213
6	A	1005	POV	C212-C213-C214-C215
6	B	1004	POV	C39-C310-C311-C312
6	D	1005	POV	C39-C310-C311-C312
6	C	1003	POV	C27-C28-C29-C210
6	A	1005	POV	C31-C32-C33-C34
6	C	1005	POV	C36-C37-C38-C39
6	B	1003	POV	C311-C312-C313-C314
5	A	1001	KAI	CA-CB-CB1-CG1
5	C	1001	KAI	CA-CB-CB1-CG1
6	C	1002	POV	C27-C28-C29-C210
6	A	1003	POV	O21-C2-C3-O31
6	A	1012	POV	O21-C2-C3-O31
6	B	1004	POV	O21-C2-C3-O31
6	C	1003	POV	O21-C2-C3-O31
6	D	1005	POV	O21-C2-C3-O31
6	A	1013	POV	C1-C2-C3-O31
6	D	1006	POV	C1-C2-C3-O31
6	A	1013	POV	C214-C215-C216-C217

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Mol	Chain	Res	Type	Atoms
6	C	1003	POV	C29-C210-C211-C212
6	A	1002	POV	C1-O11-P-O14
6	A	1004	POV	C1-O11-P-O12
6	A	1004	POV	C1-O11-P-O13
6	A	1004	POV	C1-O11-P-O14
6	A	1004	POV	C11-O12-P-O14
6	A	1005	POV	C1-O11-P-O14
6	A	1012	POV	C11-O12-P-O11
6	A	1012	POV	C11-O12-P-O13
6	A	1013	POV	C11-O12-P-O14
6	B	1004	POV	C1-O11-P-O14
6	B	1004	POV	C11-O12-P-O14
6	C	1002	POV	C1-O11-P-O14
6	C	1004	POV	C1-O11-P-O12
6	C	1004	POV	C1-O11-P-O13
6	C	1004	POV	C1-O11-P-O14
6	C	1004	POV	C11-O12-P-O14
6	C	1005	POV	C1-O11-P-O14
6	D	1004	POV	C11-O12-P-O11
6	D	1004	POV	C11-O12-P-O13
6	D	1005	POV	C1-O11-P-O14
6	D	1005	POV	C11-O12-P-O14
6	D	1006	POV	C11-O12-P-O14
7	B	1006	NAG	C3-C2-N2-C7
6	A	1013	POV	C2-C1-O11-P
6	C	1005	POV	C2-C1-O11-P
6	D	1006	POV	C2-C1-O11-P
6	D	1005	POV	C313-C314-C315-C316
6	C	1003	POV	C39-C310-C311-C312
6	C	1005	POV	C212-C213-C214-C215
6	A	1005	POV	C21-C22-C23-C24
6	B	1004	POV	C313-C314-C315-C316
6	D	1004	POV	C32-C33-C34-C35
6	B	1004	POV	C214-C215-C216-C217
6	A	1005	POV	C211-C212-C213-C214
6	C	1002	POV	C311-C310-C39-C38
6	C	1005	POV	O21-C21-C22-C23
6	A	1012	POV	C32-C33-C34-C35
6	A	1005	POV	C2-C1-O11-P
6	A	1012	POV	C311-C312-C313-C314
6	B	1004	POV	C310-C311-C312-C313
6	D	1004	POV	O21-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
6	A	1005	POV	C311-C310-C39-C38
6	D	1006	POV	O21-C21-C22-C23
6	B	1003	POV	C310-C311-C312-C313
6	B	1004	POV	C1-C2-C3-O31
6	D	1005	POV	C1-C2-C3-O31
6	D	1005	POV	C21-C22-C23-C24
6	A	1013	POV	O21-C21-C22-C23
6	A	1004	POV	C27-C28-C29-C210
6	A	1012	POV	C27-C28-C29-C210
6	C	1004	POV	C27-C28-C29-C210
6	D	1004	POV	C27-C28-C29-C210
6	A	1003	POV	C39-C310-C311-C312
6	B	1003	POV	C313-C314-C315-C316
8	D	1001	2J9	CAG-CAN-NAO-CAI
6	A	1002	POV	O21-C2-C3-O31
6	C	1002	POV	O21-C2-C3-O31
6	A	1003	POV	C211-C212-C213-C214
6	A	1002	POV	C311-C312-C313-C314
6	C	1005	POV	C214-C215-C216-C217
6	A	1003	POV	C215-C216-C217-C218
6	B	1003	POV	C311-C310-C39-C38
6	D	1003	POV	C311-C310-C39-C38
6	A	1004	POV	C29-C210-C211-C212
6	C	1004	POV	C29-C210-C211-C212
6	C	1005	POV	C27-C28-C29-C210
6	D	1005	POV	C310-C311-C312-C313
6	B	1003	POV	C32-C33-C34-C35
7	B	1006	NAG	C1-C2-N2-C7
7	C	1007	NAG	C1-C2-N2-C7
7	C	1011	NAG	C1-C2-N2-C7
6	C	1003	POV	C2-C1-O11-P
6	C	1003	POV	C215-C216-C217-C218
6	A	1002	POV	C27-C28-C29-C210
6	A	1003	POV	C29-C210-C211-C212
6	D	1005	POV	C29-C210-C211-C212
6	D	1003	POV	O31-C31-C32-C33
7	A	1009	NAG	C3-C2-N2-C7
7	C	1009	NAG	C3-C2-N2-C7
7	C	1011	NAG	C3-C2-N2-C7
6	A	1002	POV	C212-C213-C214-C215
6	B	1004	POV	C27-C28-C29-C210
6	B	1003	POV	O31-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
6	B	1003	POV	C37-C38-C39-C310
6	B	1004	POV	C32-C33-C34-C35
6	B	1003	POV	C11-C12-N-C15
6	A	1002	POV	C21-C22-C23-C24
6	D	1005	POV	C32-C33-C34-C35
6	A	1003	POV	C2-C1-O11-P
6	A	1003	POV	C213-C214-C215-C216
6	A	1005	POV	C27-C28-C29-C210
6	A	1012	POV	C29-C210-C211-C212
6	C	1003	POV	C33-C34-C35-C36
6	A	1003	POV	C27-C28-C29-C210
6	B	1004	POV	C29-C210-C211-C212
6	D	1004	POV	C29-C210-C211-C212
6	D	1005	POV	C27-C28-C29-C210
6	D	1003	POV	C11-C12-N-C15
6	A	1003	POV	C33-C34-C35-C36
6	A	1004	POV	O21-C21-C22-C23
5	D	1002	KAI	OXT-C-CA-CB
6	D	1006	POV	C32-C33-C34-C35
6	C	1004	POV	O21-C21-C22-C23
6	A	1004	POV	C25-C26-C27-C28
6	A	1013	POV	C25-C26-C27-C28
6	C	1003	POV	C213-C214-C215-C216
6	A	1012	POV	O11-C1-C2-O21
6	D	1005	POV	C214-C215-C216-C217
5	A	1001	KAI	CG-CB-CB1-CG1
5	B	1002	KAI	O-C-CA-CB
5	B	1002	KAI	OXT-C-CA-CB
6	A	1002	POV	C311-C310-C39-C38
6	B	1003	POV	C34-C35-C36-C37
6	A	1005	POV	C214-C215-C216-C217
6	D	1003	POV	C32-C33-C34-C35
6	A	1012	POV	C25-C26-C27-C28
6	C	1002	POV	C21-C22-C23-C24
6	A	1002	POV	C29-C210-C211-C212
6	C	1004	POV	C25-C26-C27-C28
7	A	1011	NAG	O5-C5-C6-O6
6	A	1003	POV	C11-C12-N-C14
6	B	1003	POV	C11-C12-N-C14
6	D	1004	POV	O21-C21-C22-C23
6	A	1004	POV	O22-C21-C22-C23
6	A	1005	POV	O22-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
6	C	1005	POV	O22-C21-O21-C2
6	C	1004	POV	O22-C21-C22-C23
6	A	1012	POV	O21-C21-C22-C23
6	B	1003	POV	C11-C12-N-C13
6	A	1013	POV	C23-C24-C25-C26
6	D	1003	POV	C34-C35-C36-C37
6	C	1005	POV	C213-C214-C215-C216
6	C	1005	POV	C22-C23-C24-C25
6	C	1005	POV	C313-C314-C315-C316
6	C	1003	POV	C211-C212-C213-C214

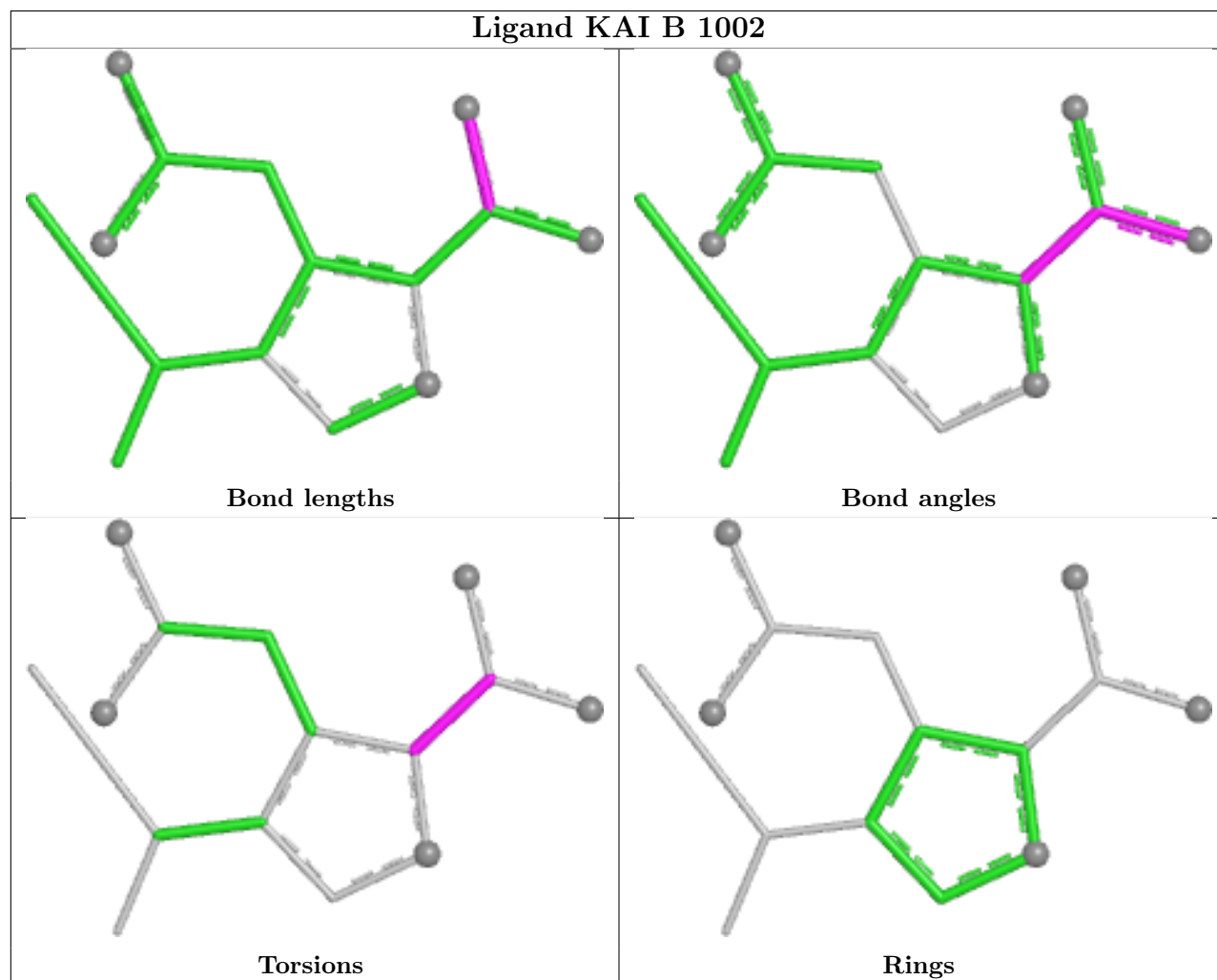
There are no ring outliers.

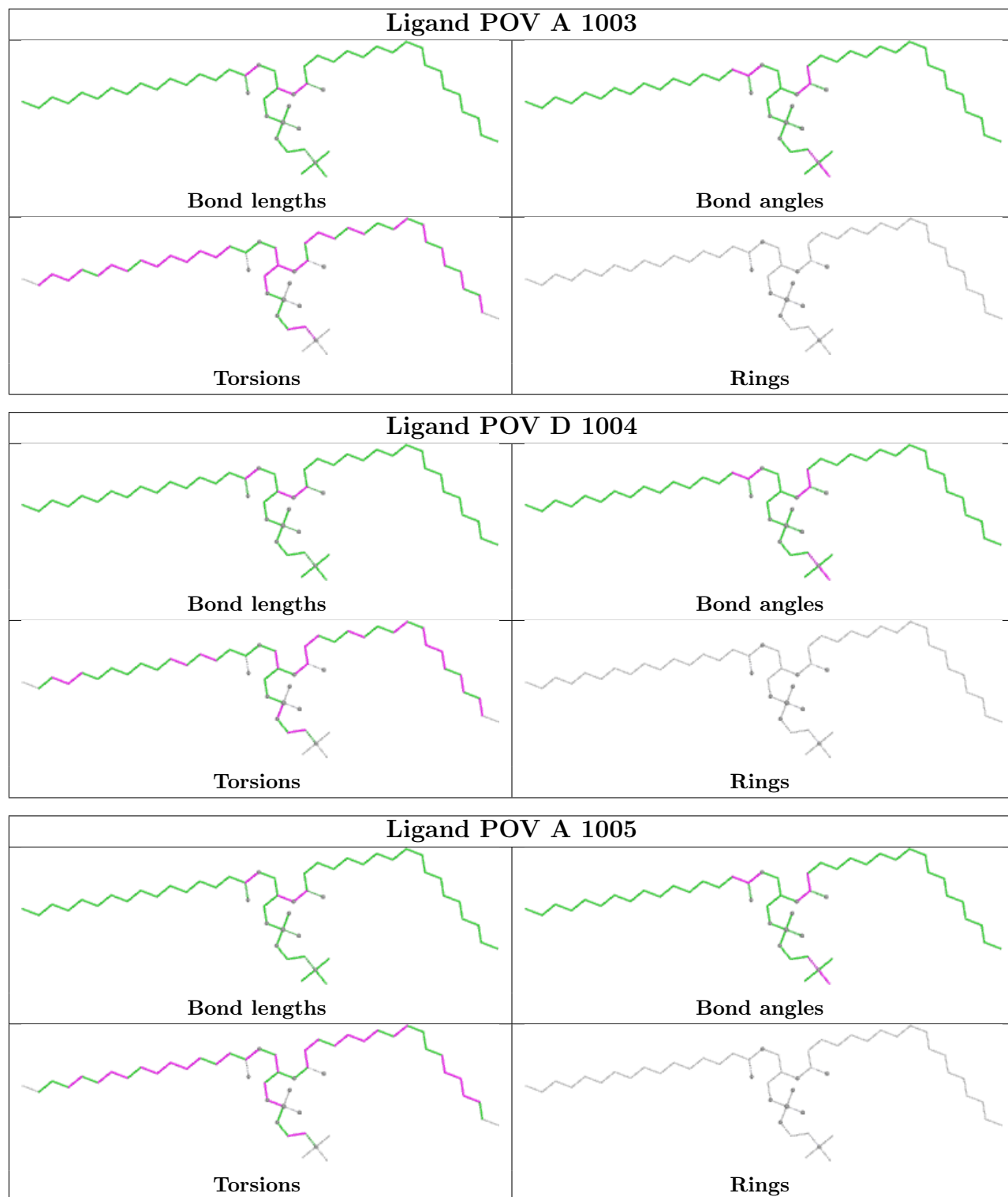
21 monomers are involved in 29 short contacts:

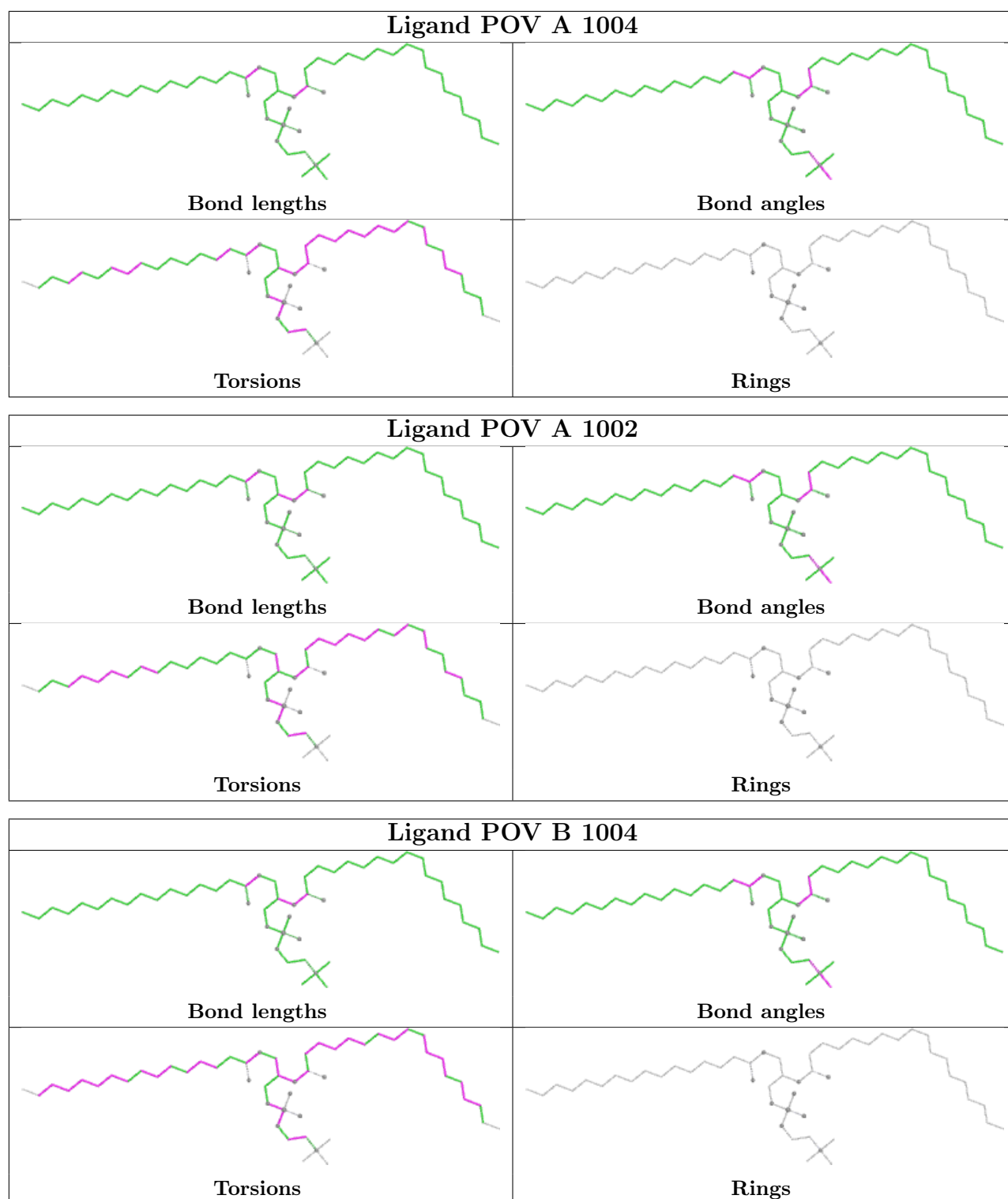
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1002	KAI	3	0
6	A	1003	POV	1	0
6	D	1004	POV	3	0
6	A	1005	POV	1	0
6	A	1002	POV	1	0
6	B	1004	POV	1	0
6	A	1012	POV	1	0
6	C	1004	POV	2	0
6	C	1003	POV	2	0
6	D	1003	POV	2	0
6	D	1005	POV	1	0
6	C	1005	POV	2	0
8	A	1014	2J9	2	0
7	C	1011	NAG	1	0
5	A	1001	KAI	1	0
5	D	1002	KAI	3	0
8	D	1001	2J9	1	0
8	B	1009	2J9	1	0
8	B	1001	2J9	1	0
5	C	1001	KAI	1	0
6	C	1002	POV	2	0

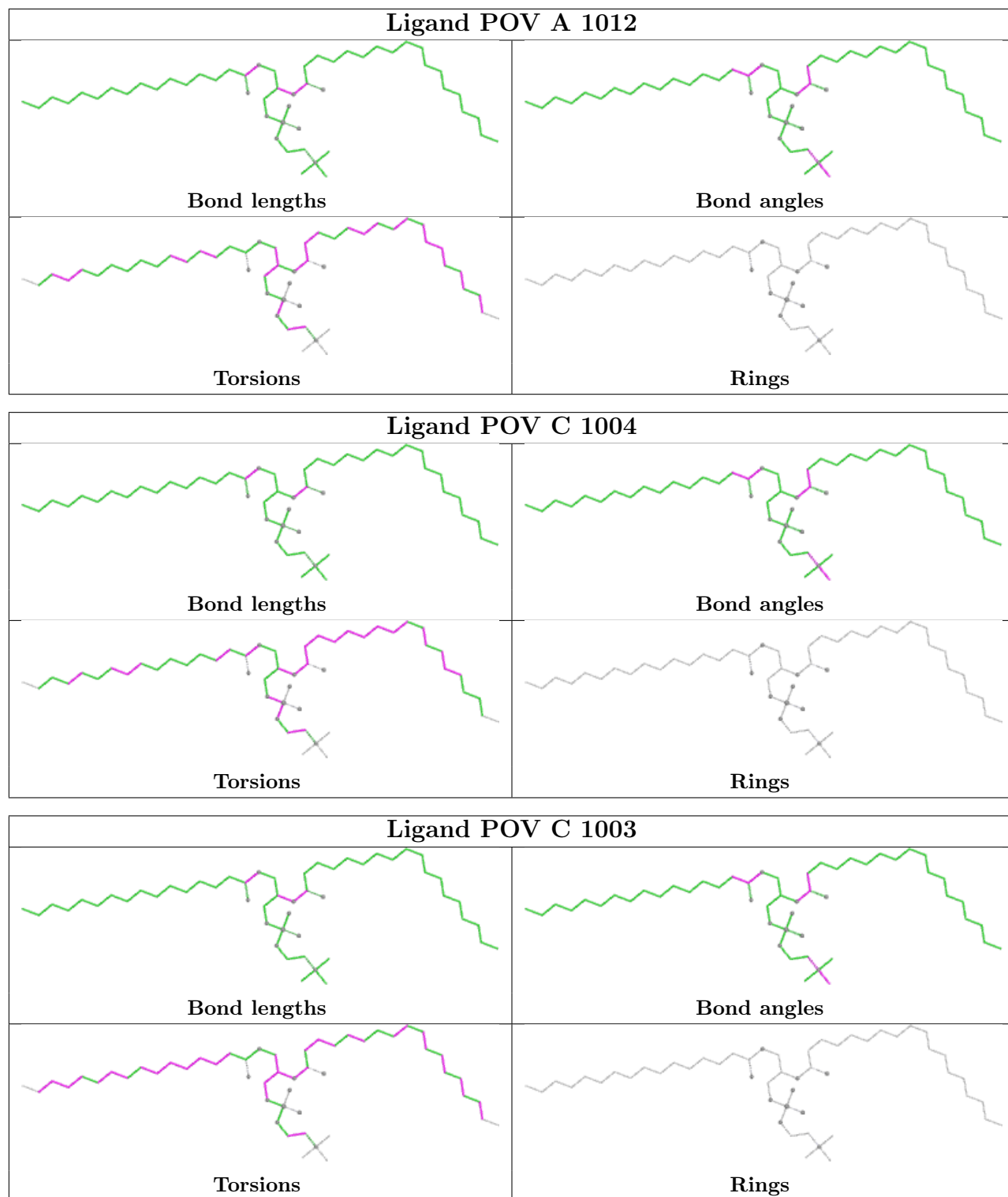
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

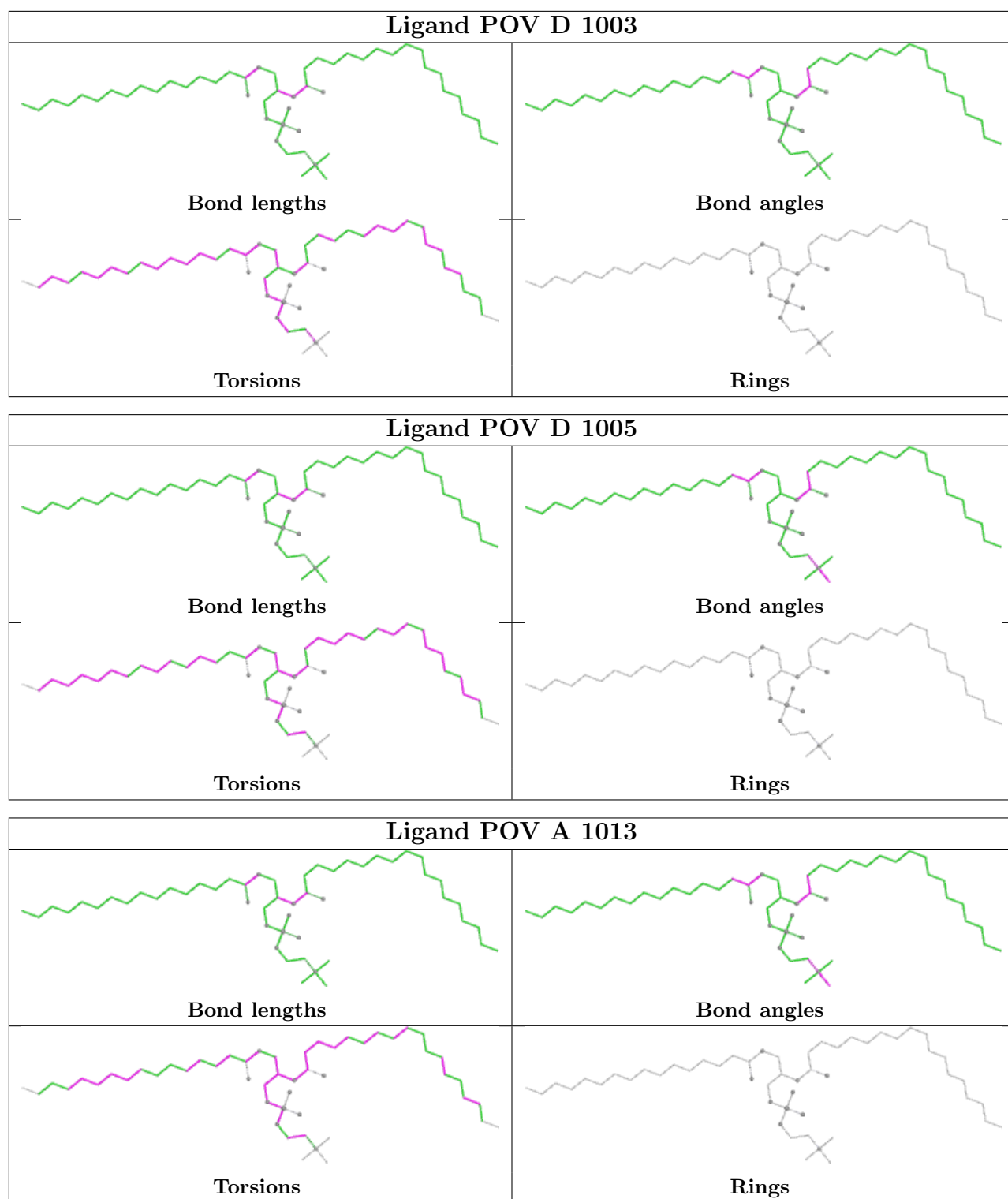


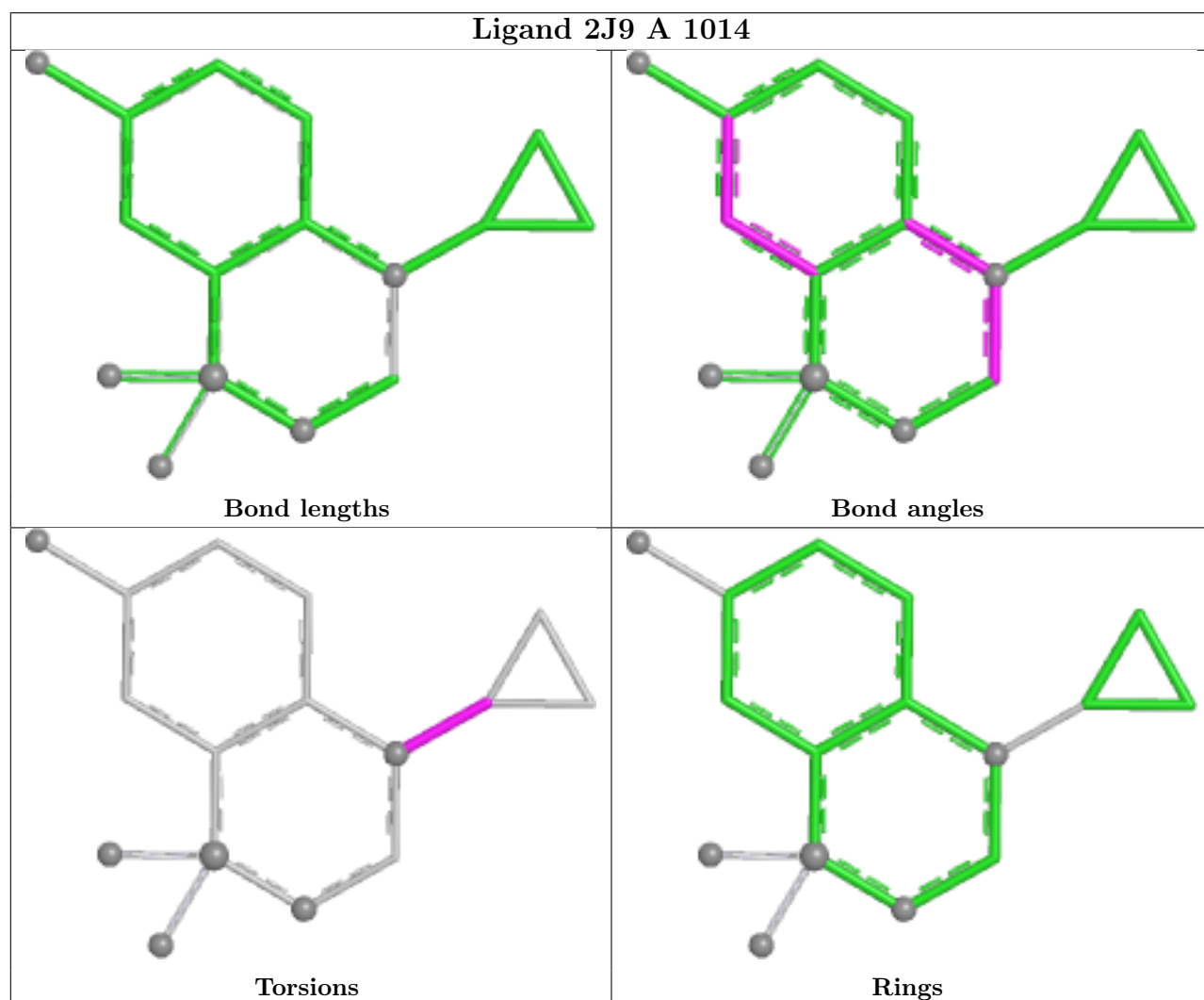
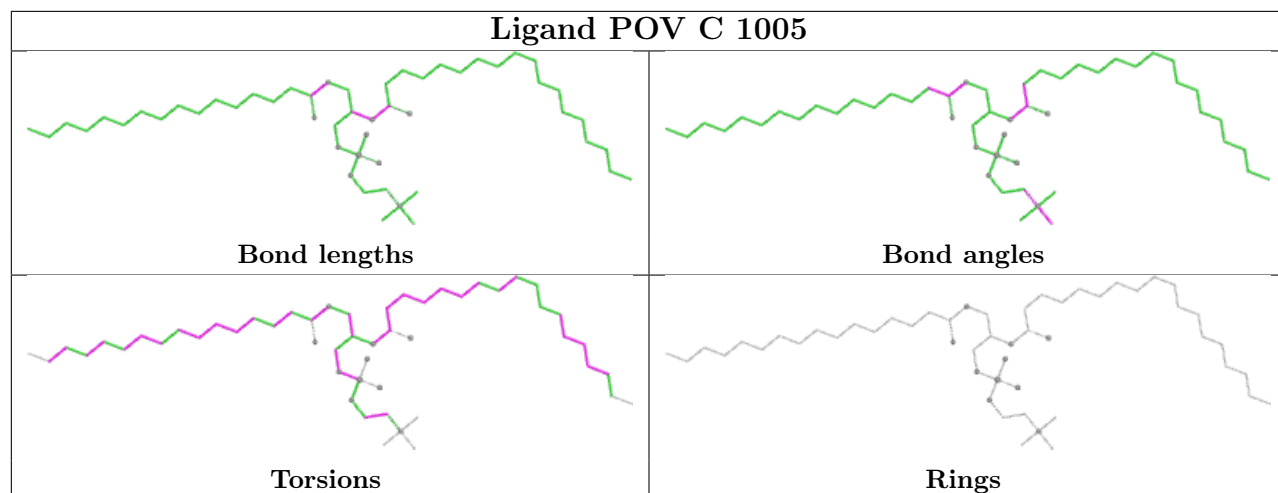


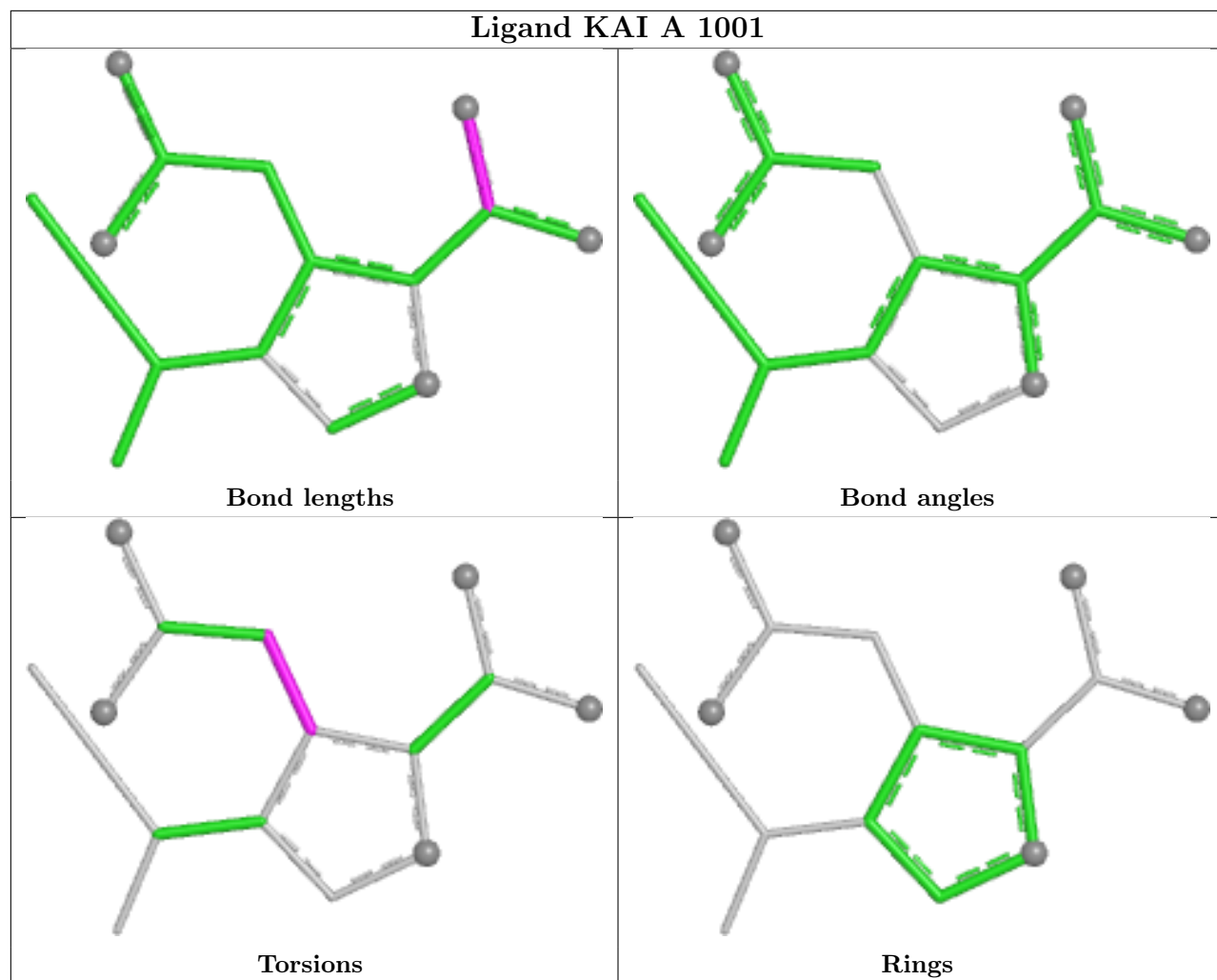


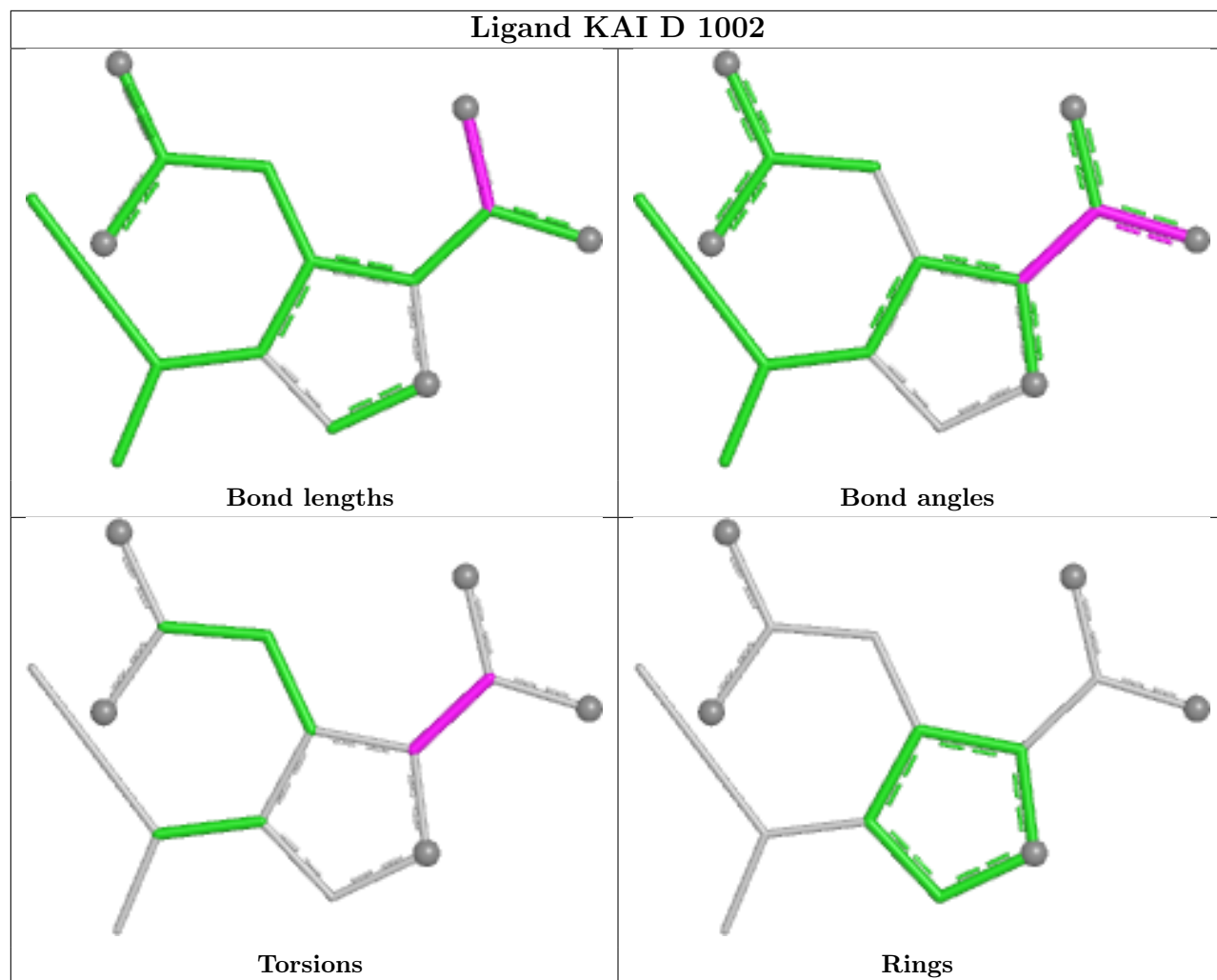




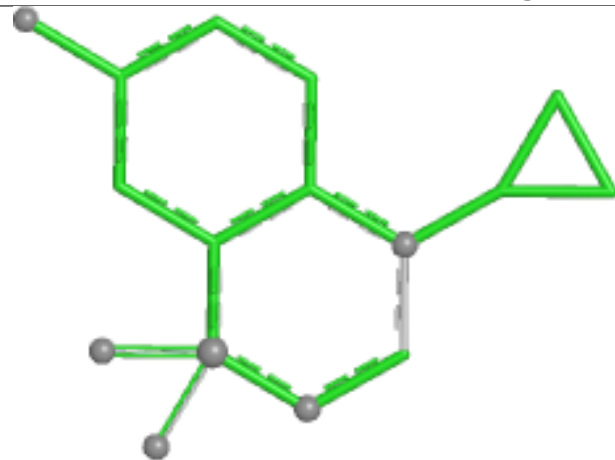




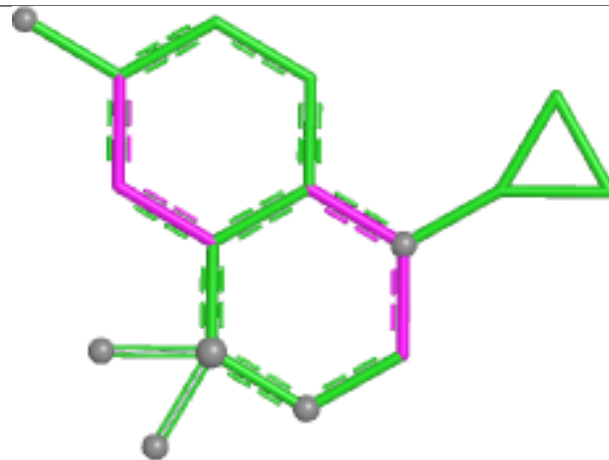




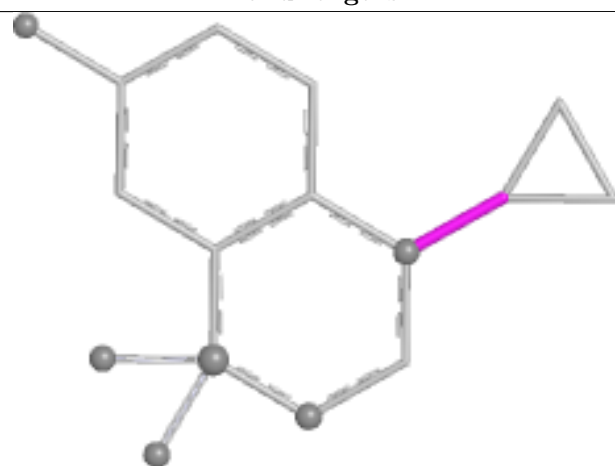
## Ligand 2J9 D 1001



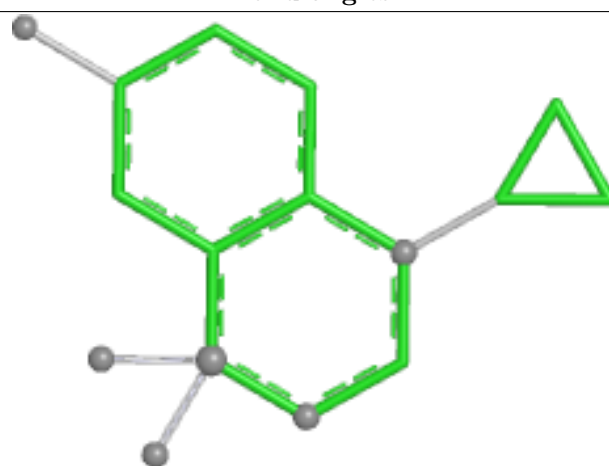
Bond lengths



Bond angles

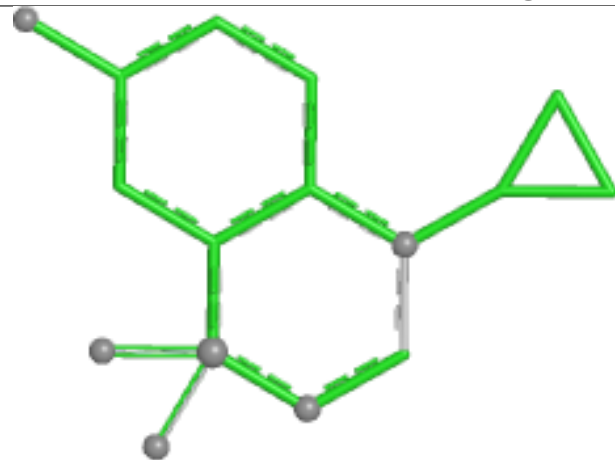


Torsions

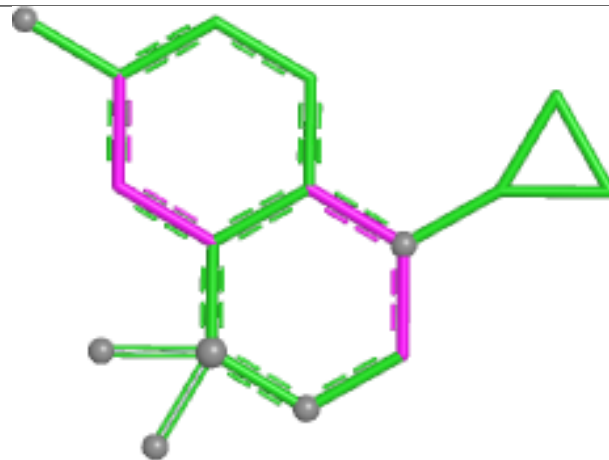


Rings

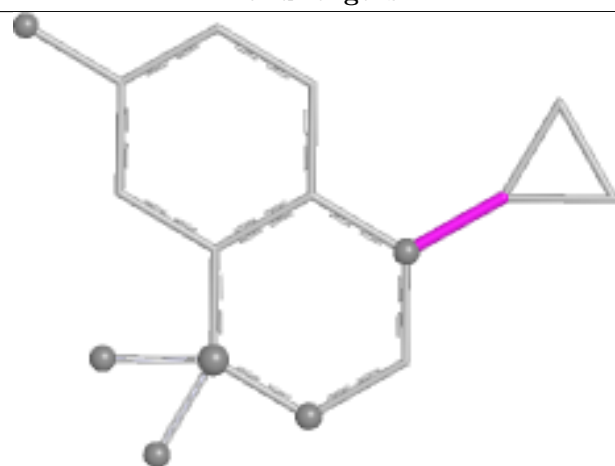
## Ligand 2J9 B 1009



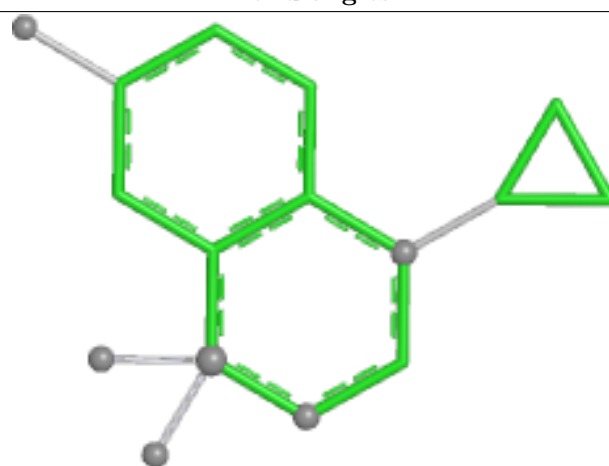
Bond lengths



Bond angles

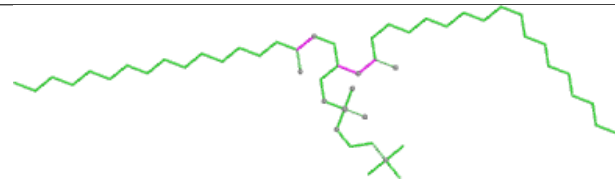


Torsions

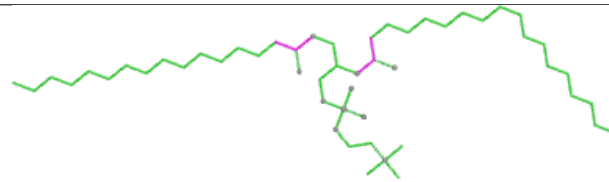


Rings

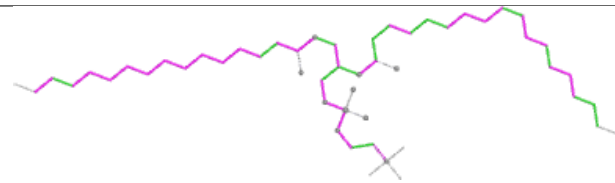
## Ligand POV B 1003



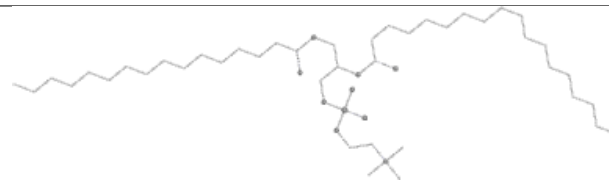
Bond lengths



Bond angles

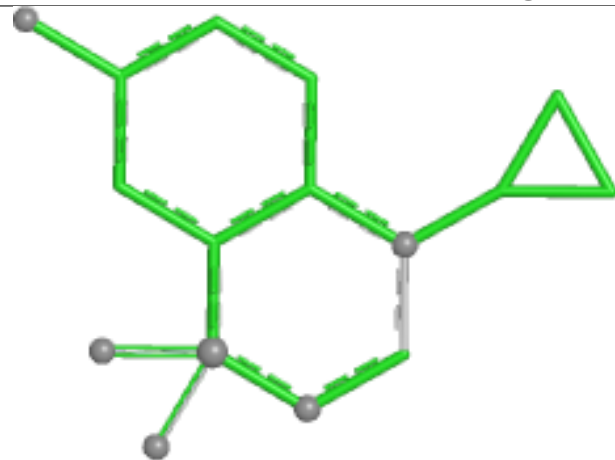


Torsions

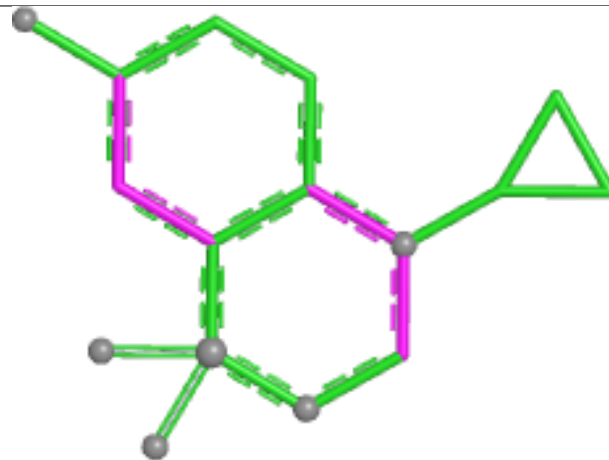


Rings

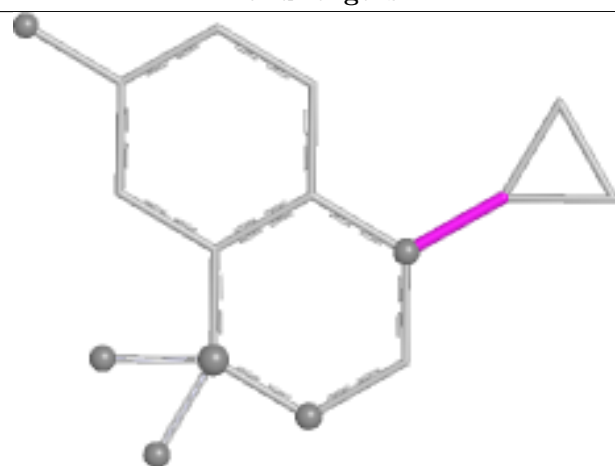
## Ligand 2J9 B 1001



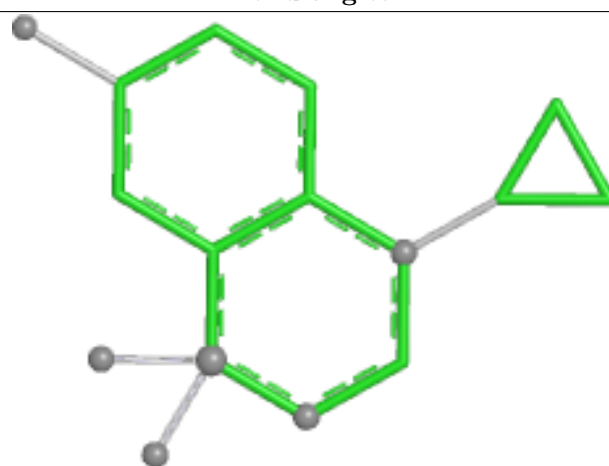
Bond lengths



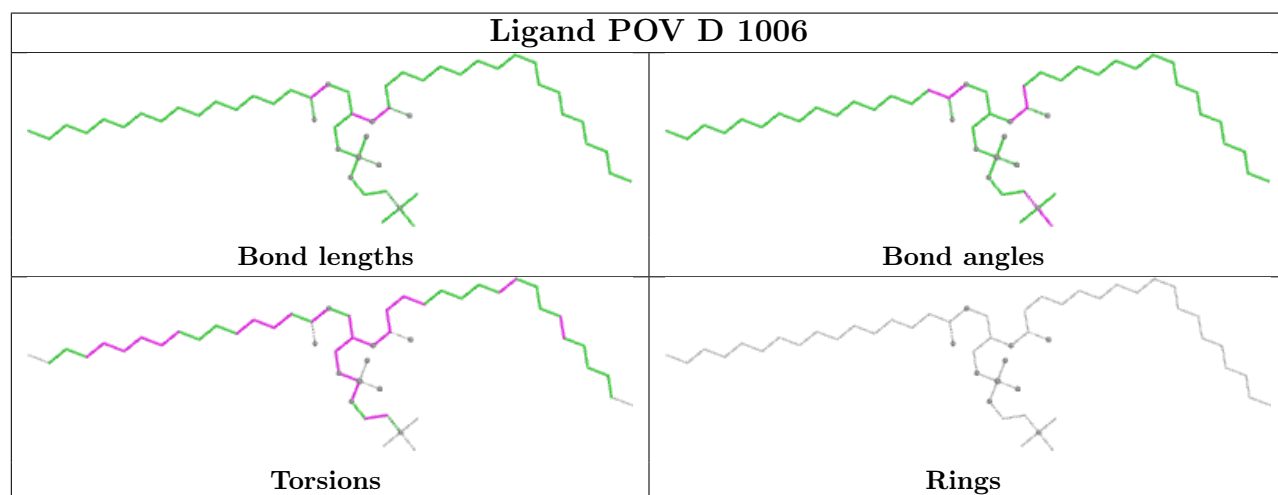
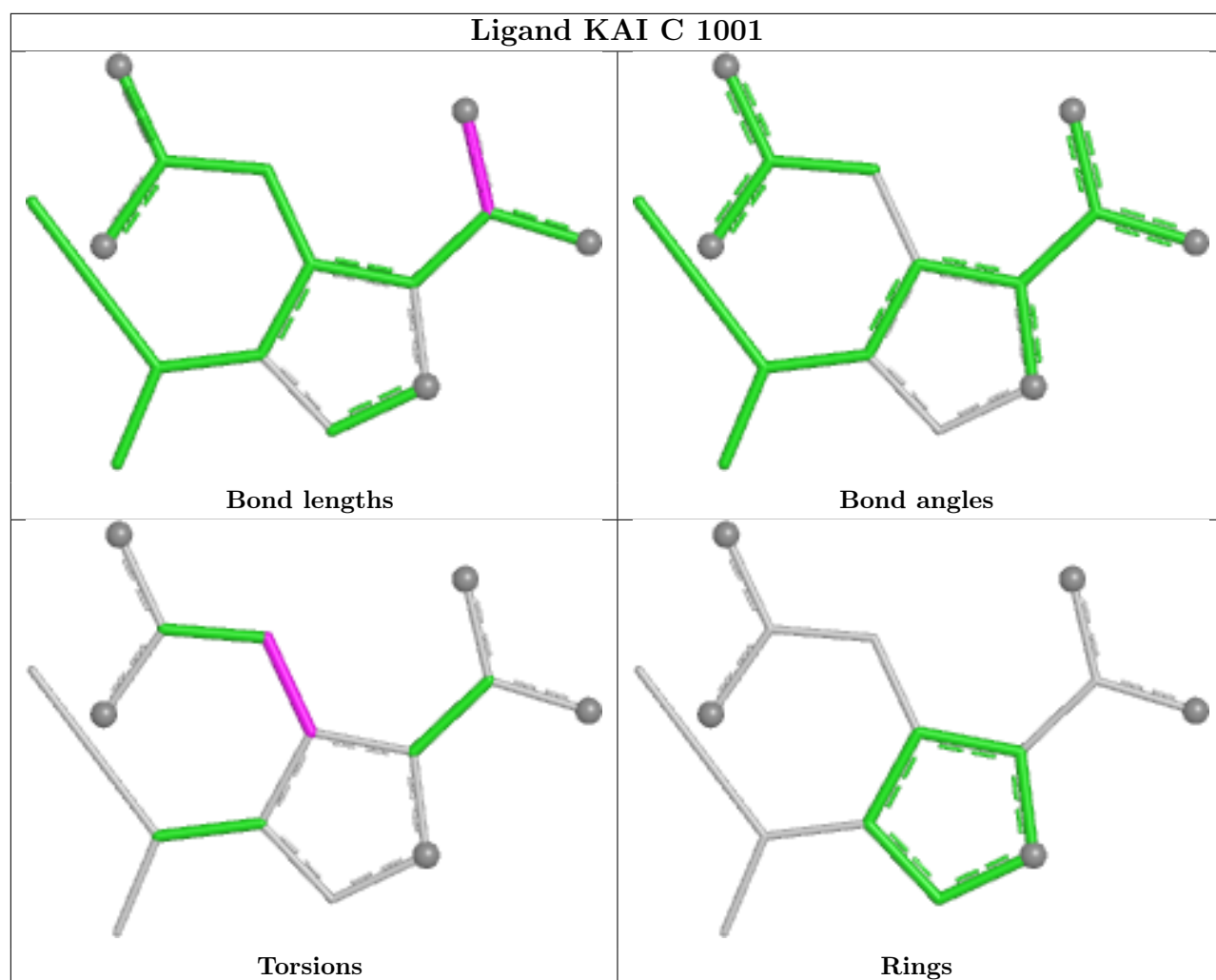
Bond angles



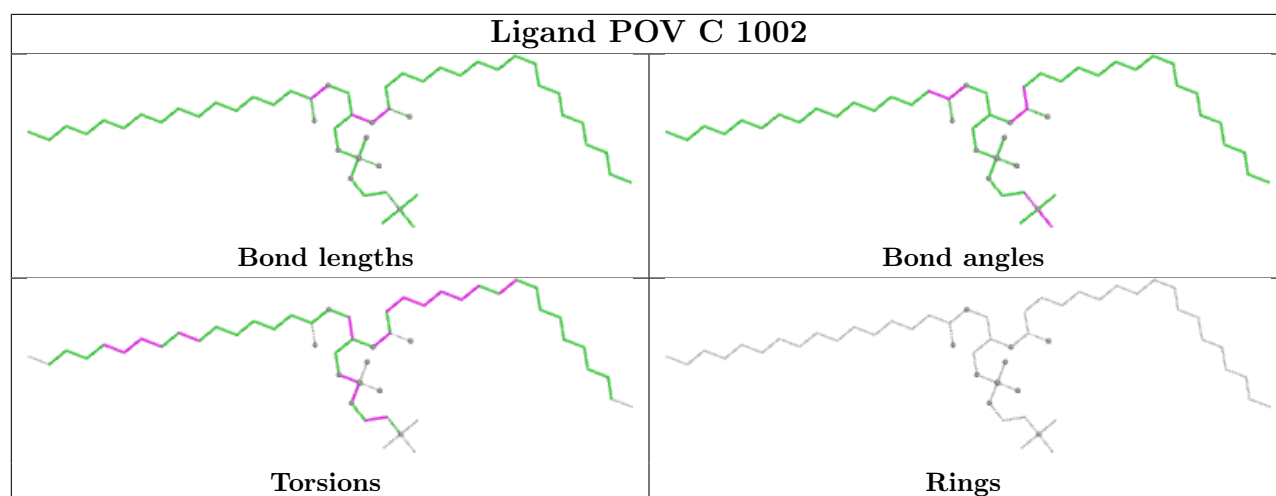
Torsions



Rings







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

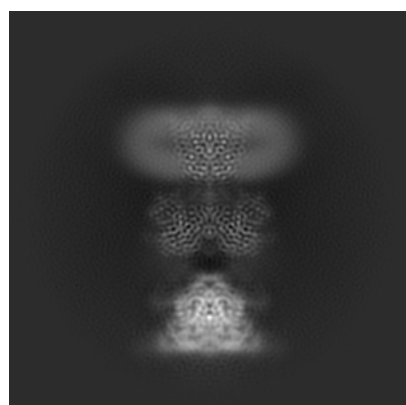
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-48903. These allow visual inspection of the internal detail of the map and identification of artifacts.

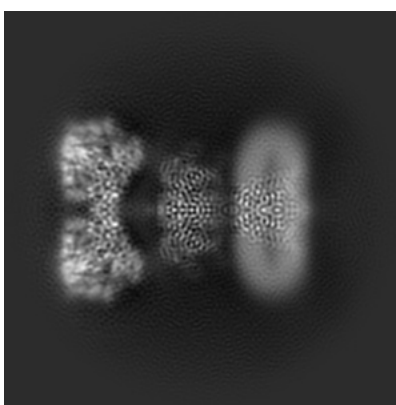
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

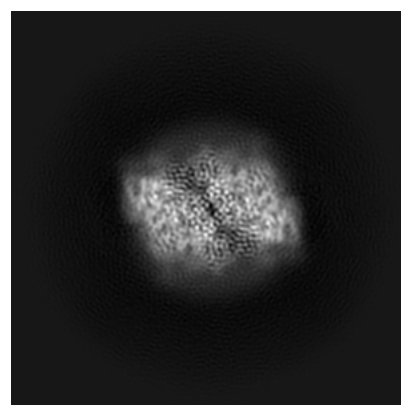
#### 6.1.1 Primary map



X



Y

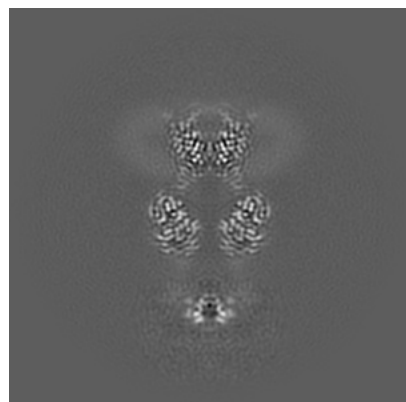


Z

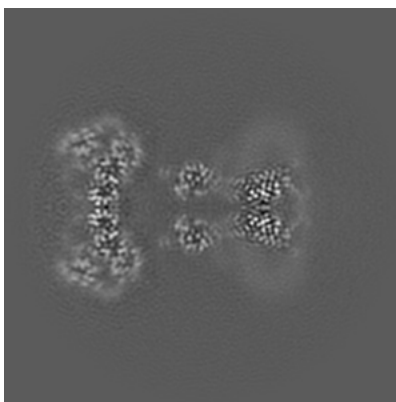
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

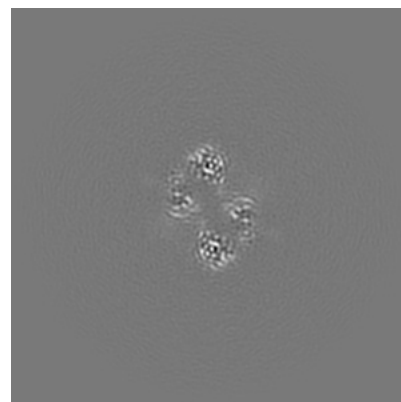
#### 6.2.1 Primary map



X Index: 192



Y Index: 192

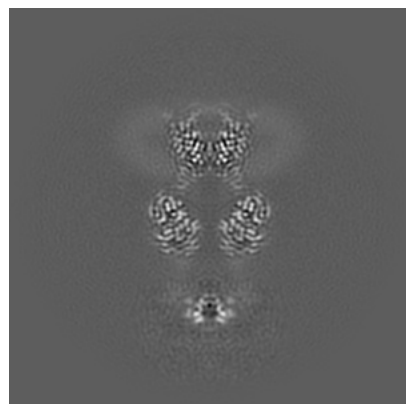


Z Index: 192

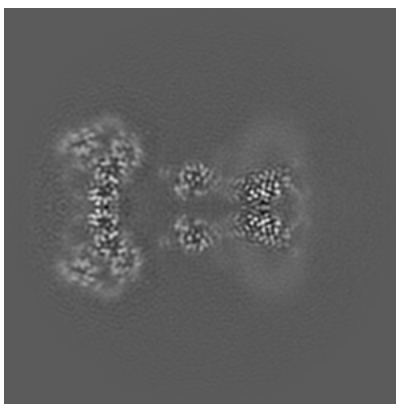
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

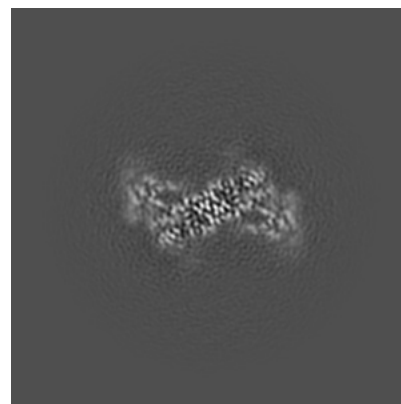
### 6.3.1 Primary map



X Index: 192



Y Index: 192

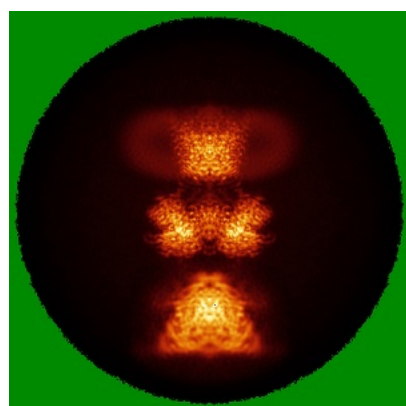


Z Index: 89

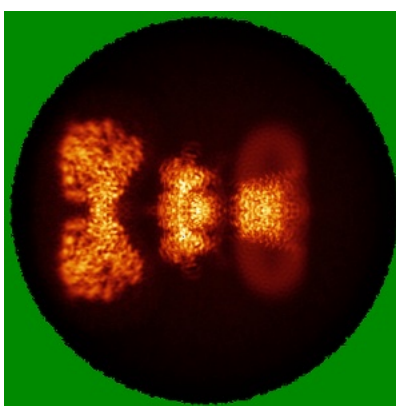
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

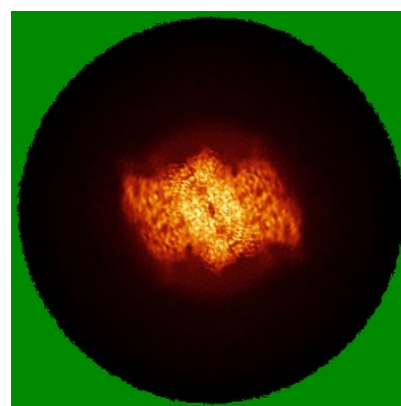
### 6.4.1 Primary map



X



Y

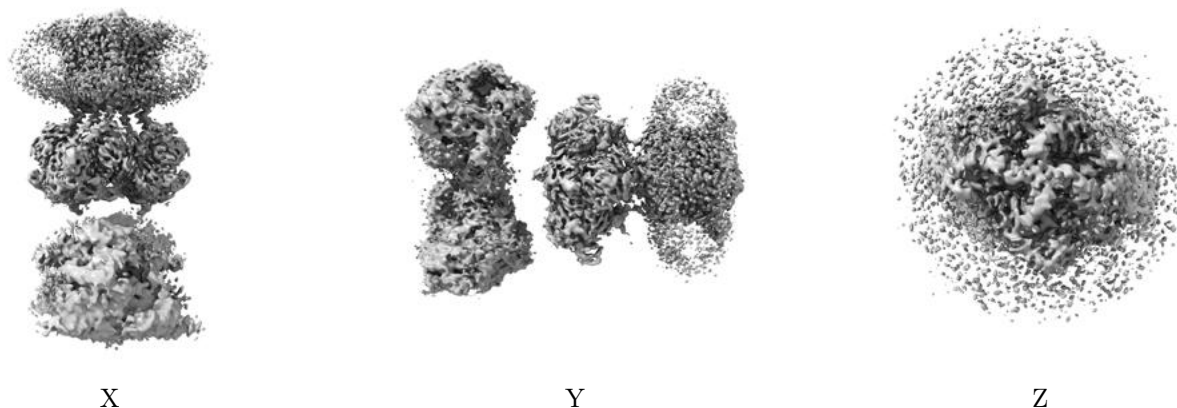


Z

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



The images above show the 3D surface view of the map at the recommended contour level 4.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

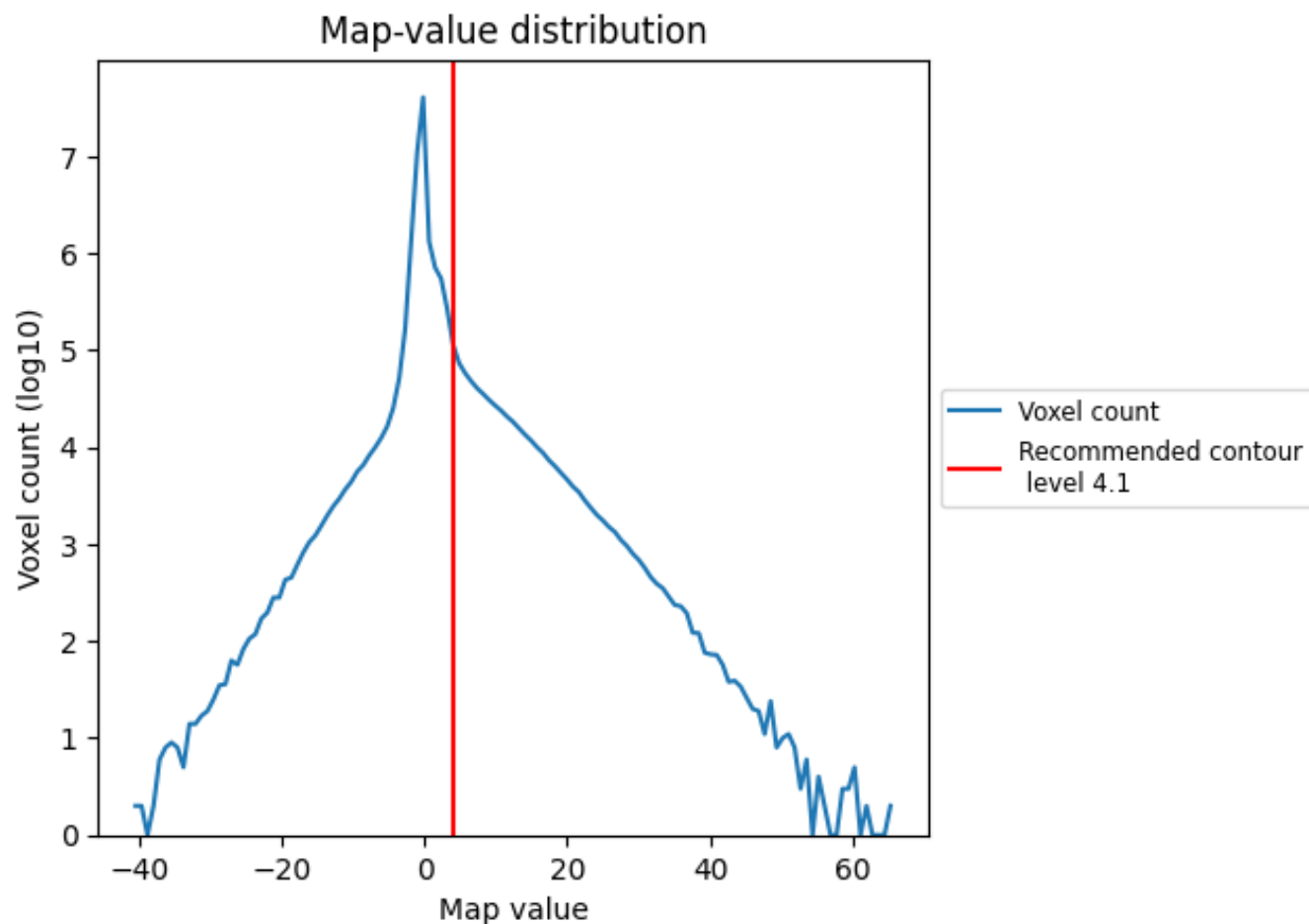
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

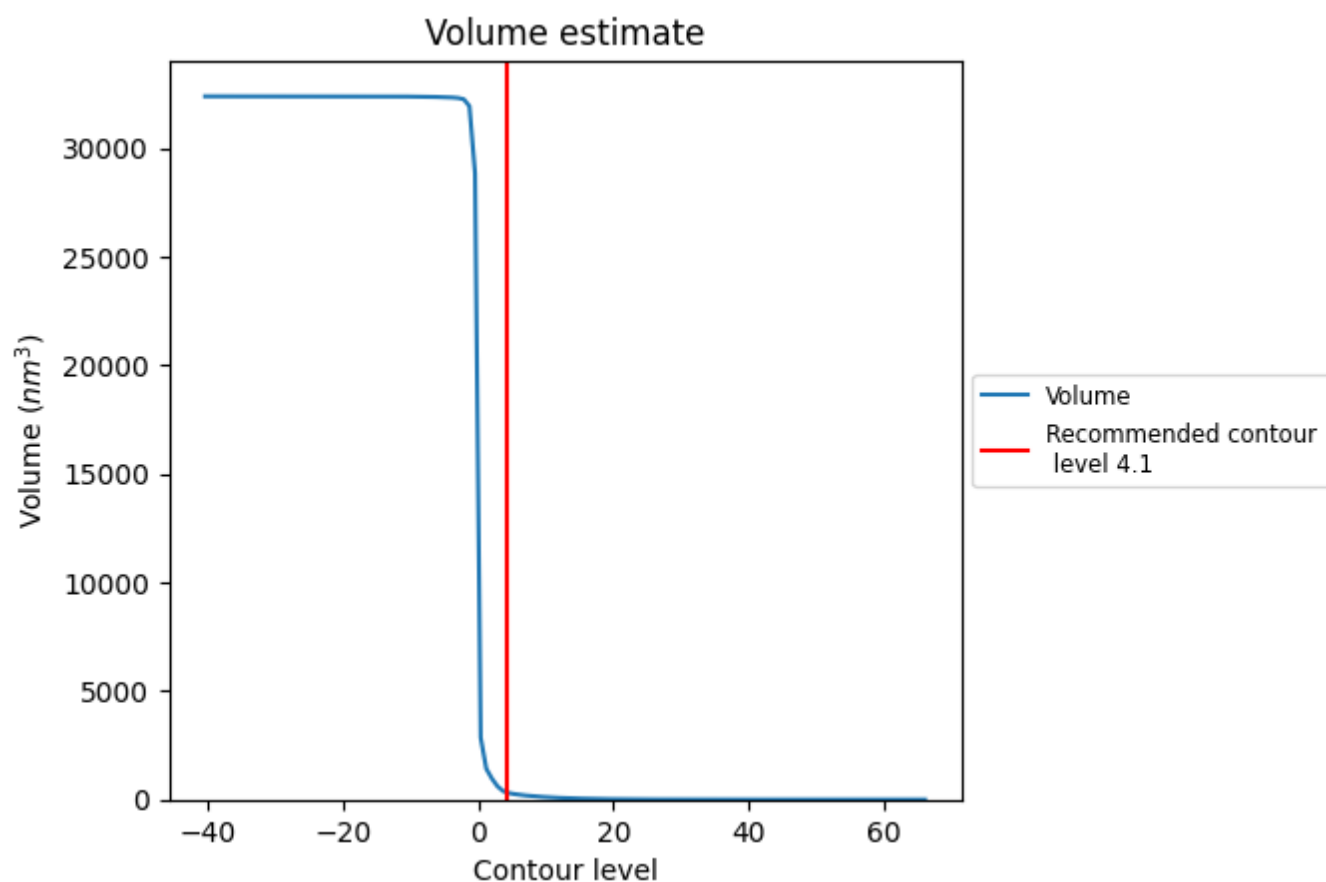
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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.

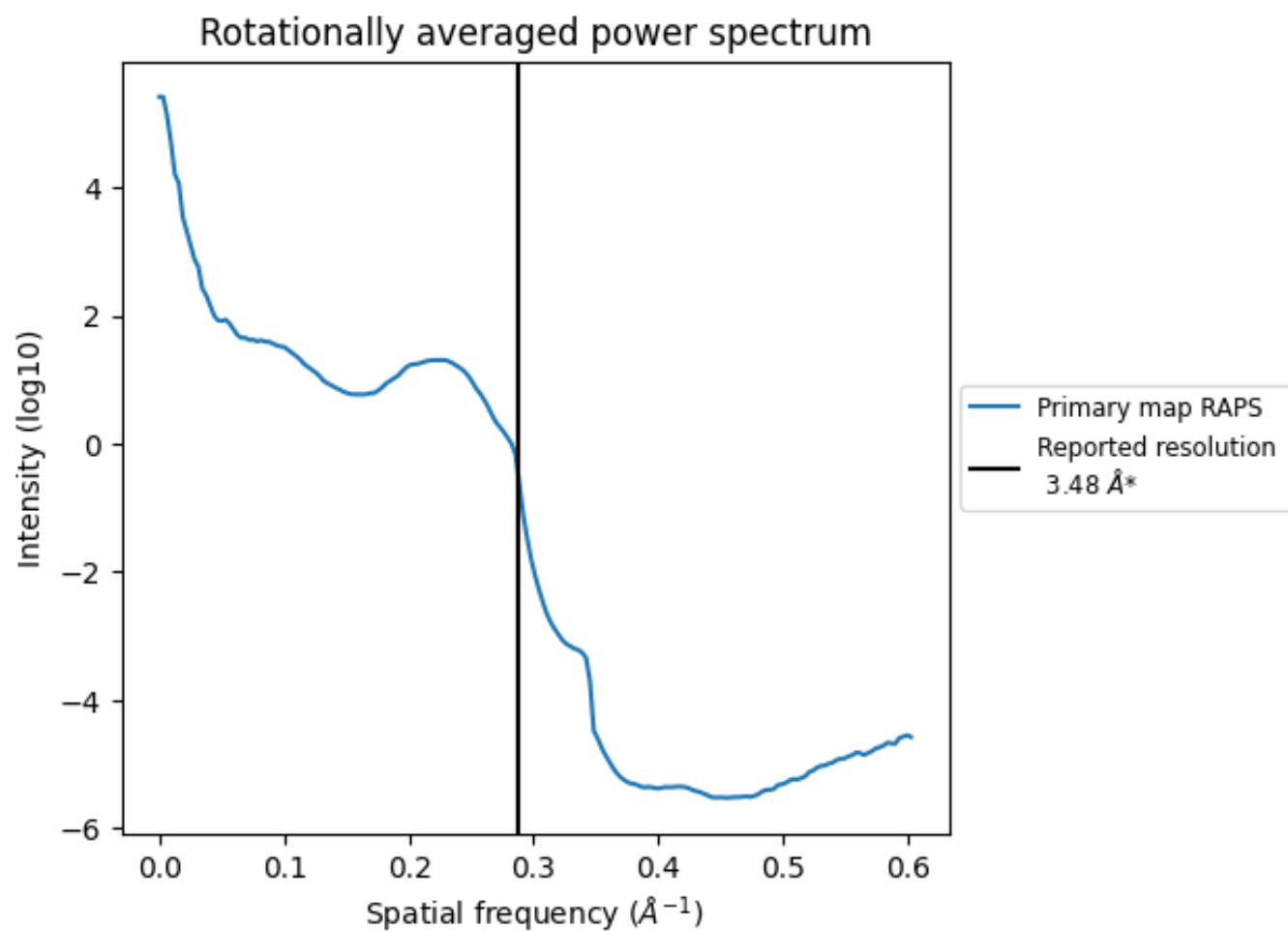
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 347 nm<sup>3</sup>; this corresponds to an approximate mass of 314 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 ⓘ



\*Reported resolution corresponds to spatial frequency of 0.287 Å<sup>-1</sup>

## 8 Fourier-Shell correlation ⓘ

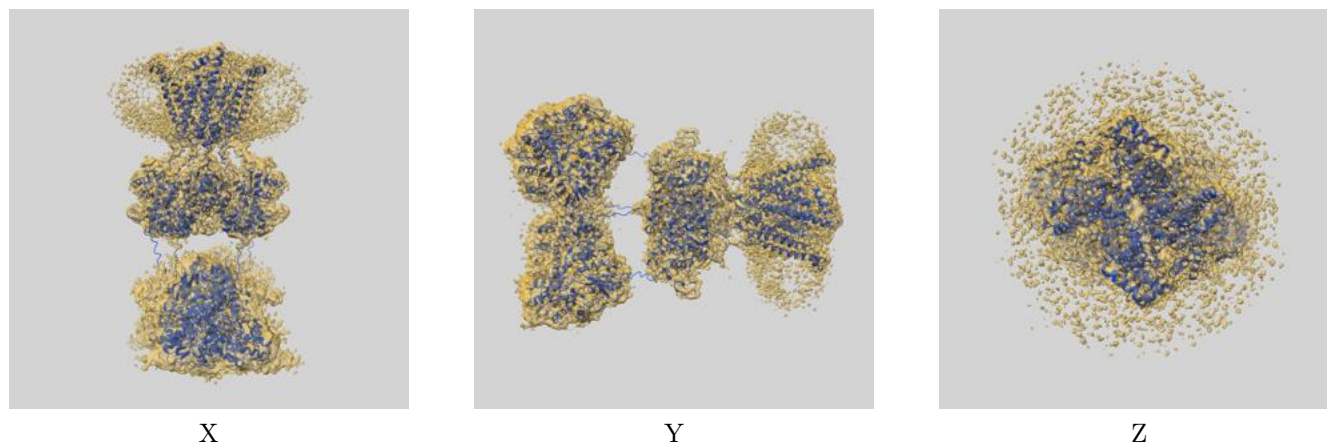
This section was not generated. No FSC curve or half-maps provided.



## 9 Map-model fit [i](#)

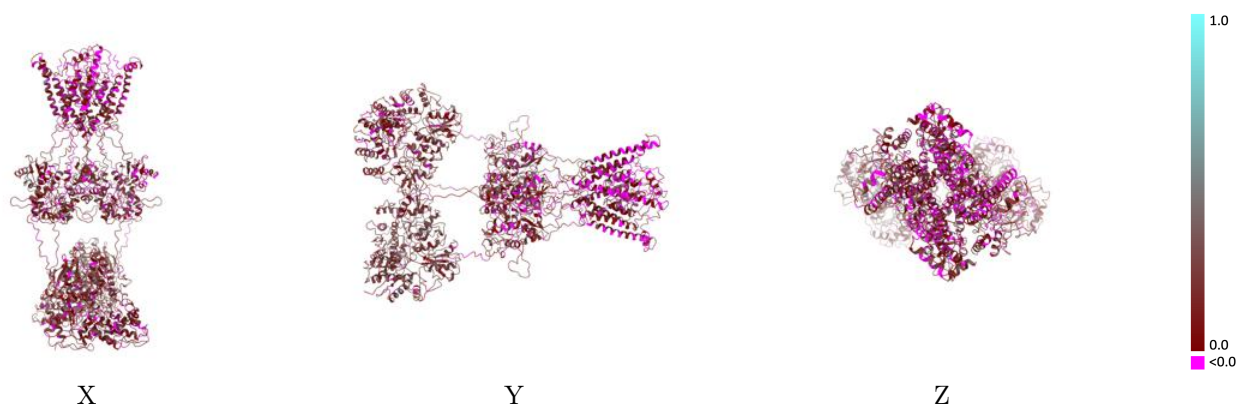
This section contains information regarding the fit between EMDB map EMD-48903 and PDB model 9N4R. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

### 9.1 Map-model overlay [i](#)



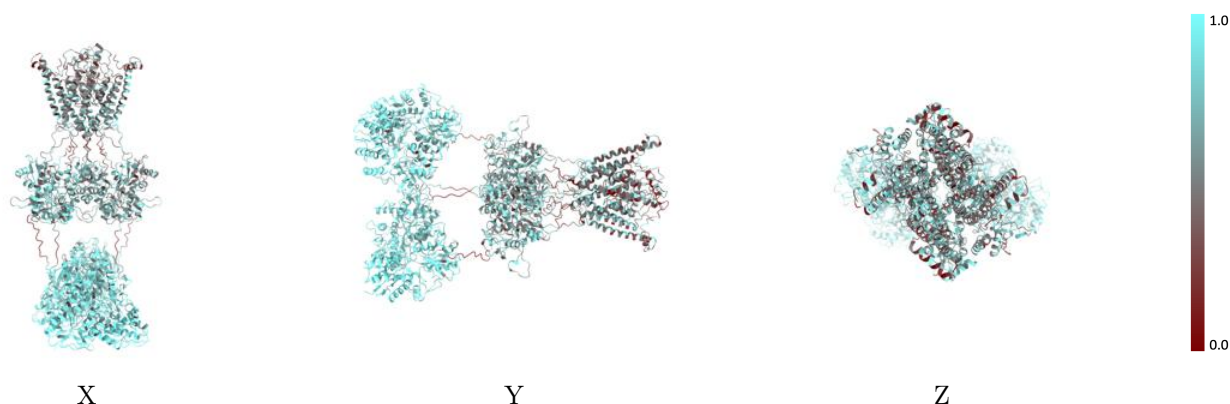
The images above show the 3D surface view of the map at the recommended contour level 4.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



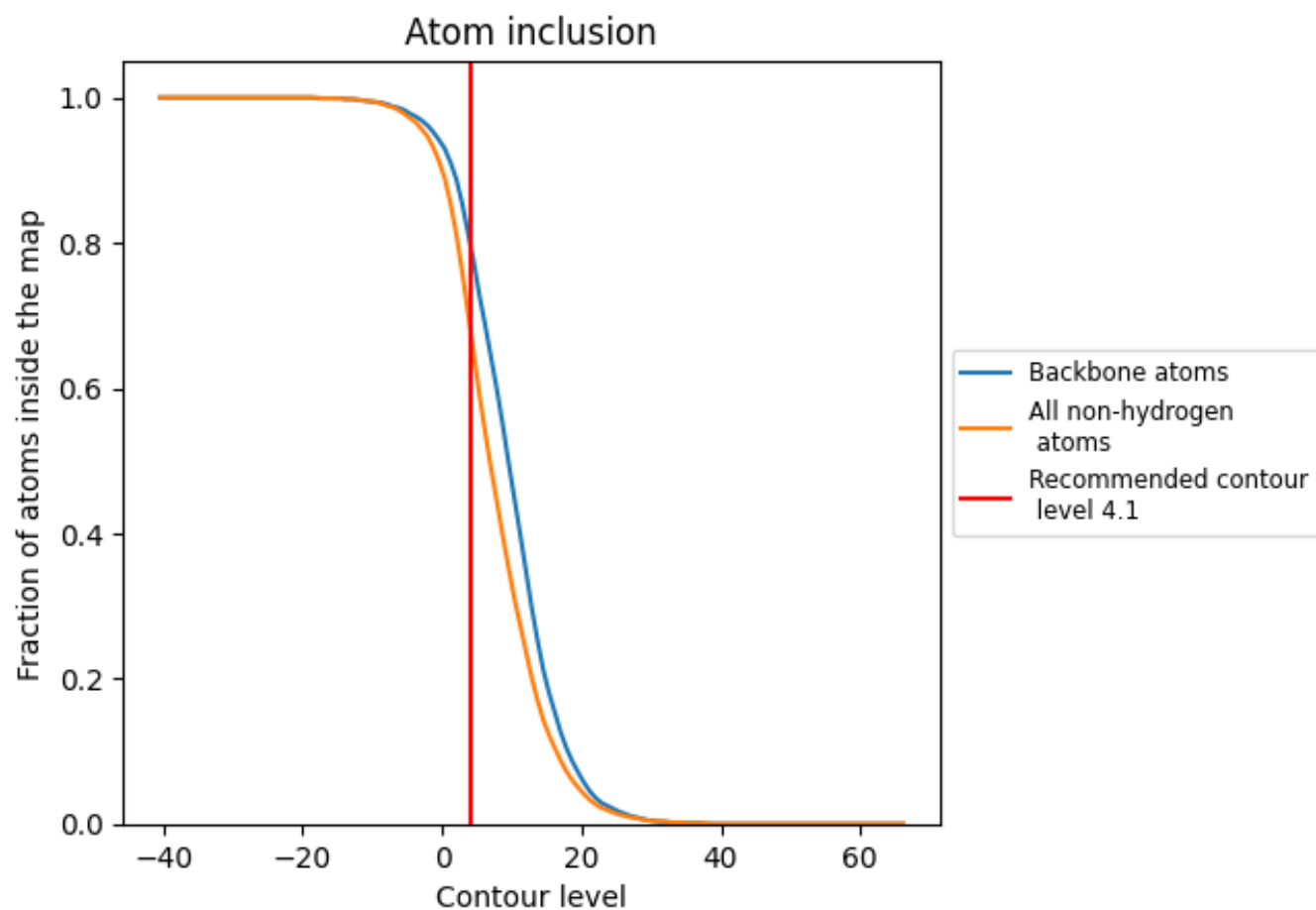
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (4.1).



























## 9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 68% 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 (4.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6770	 0.1630
A	 0.6540	 0.1400
B	 0.6640	 0.1440
C	 0.6930	 0.1880
D	 0.6960	 0.1770
E	 0.9180	 0.2070
F	 0.6790	 0.1950
G	 0.8030	 0.1440
H	 0.2400	 -0.0920
I	 0.8850	 0.3200
J	 0.7140	 0.2620
K	 0.9670	 0.2810
L	 0.4600	 0.1830

