



## Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 06:59 PM EST

PDB ID : 7T4O  
EMDB ID : EMD-25683  
Title : CryoEM structure of *Methylococcus capsulatus* (Bath) pMMO treated with potassium cyanide in a native lipid nanodisc at 3.65 Angstrom resolution  
Authors : Koo, C.W.; Rosenzweig, A.C.  
Deposited on : 2021-12-10  
Resolution : 3.65 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>.

---

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

EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

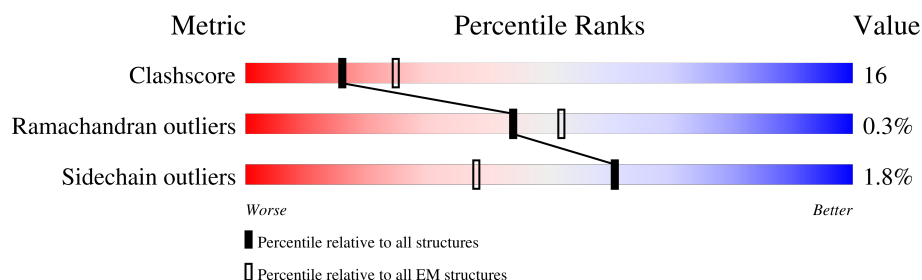
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.65 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	414	<div> <div>39%</div> <div> <div>71%</div> <div>21%</div> <div>8%</div> </div> </div>
1	E	414	<div> <div>40%</div> <div> <div>71%</div> <div>21%</div> <div>8%</div> </div> </div>
1	I	414	<div> <div>39%</div> <div> <div>71%</div> <div>20%</div> <div>8%</div> </div> </div>
2	C	260	<div> <div>45%</div> <div> <div>34%</div> <div>20%</div> <div>•</div> <div>43%</div> </div> </div>
2	G	260	<div> <div>46%</div> <div> <div>33%</div> <div>20%</div> <div>•</div> <div>43%</div> </div> </div>
2	K	260	<div> <div>45%</div> <div> <div>34%</div> <div>20%</div> <div>•</div> <div>43%</div> </div> </div>
3	B	247	<div> <div>34%</div> <div> <div>65%</div> <div>32%</div> <div>••</div> </div> </div>
3	F	247	<div> <div>34%</div> <div> <div>67%</div> <div>30%</div> <div>••</div> </div> </div>

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
3	J	247	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	D10	B	302	-	-	X	-
7	D10	F	302	-	-	X	-
7	D10	J	303	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 20036 atoms, of which 894 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 Particulate methane monooxygenase alpha subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	382	Total	C	N	O	S	0	0
			3017	1938	513	551	15		
1	E	382	Total	C	N	O	S	0	0
			3017	1938	513	551	15		
1	I	382	Total	C	N	O	S	0	0
			3017	1938	513	551	15		

- Molecule 2 is a protein called Ammonia monooxygenase/methane monooxygenase, subunit C family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	147	Total	C	N	O	S	0	0
			1200	815	186	196	3		
2	G	147	Total	C	N	O	S	0	0
			1200	815	186	196	3		
2	K	147	Total	C	N	O	S	0	0
			1200	815	186	196	3		

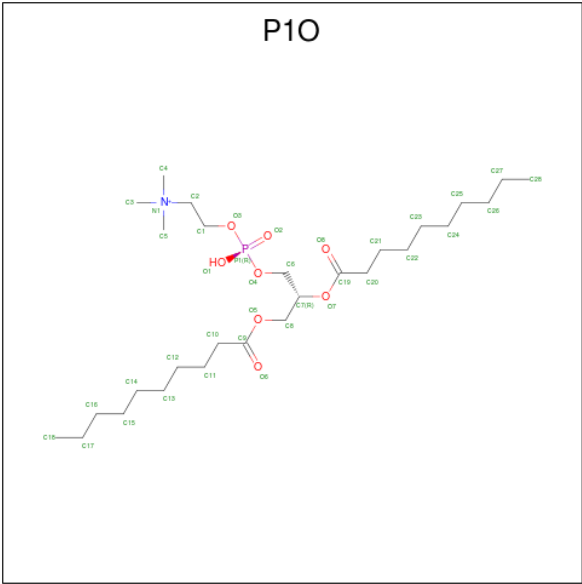
- Molecule 3 is a protein called Particulate methane monooxygenase beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	241	Total	C	N	O	S	0	0
			1976	1329	315	321	11		
3	F	241	Total	C	N	O	S	0	0
			1976	1329	315	321	11		
3	J	241	Total	C	N	O	S	0	0
			1976	1329	315	321	11		

- Molecule 4 is COPPER (II) ION (three-letter code: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	A	2	Total	Cu	0
			2	2	
4	E	2	Total	Cu	0
			2	2	
4	I	1	Total	Cu	0
			1	1	

- Molecule 5 is 1,2-DIDECANOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: P1O) (formula: C<sub>28</sub>H<sub>57</sub>NO<sub>8</sub>P) (labeled as "Ligand of Interest" by depositor).



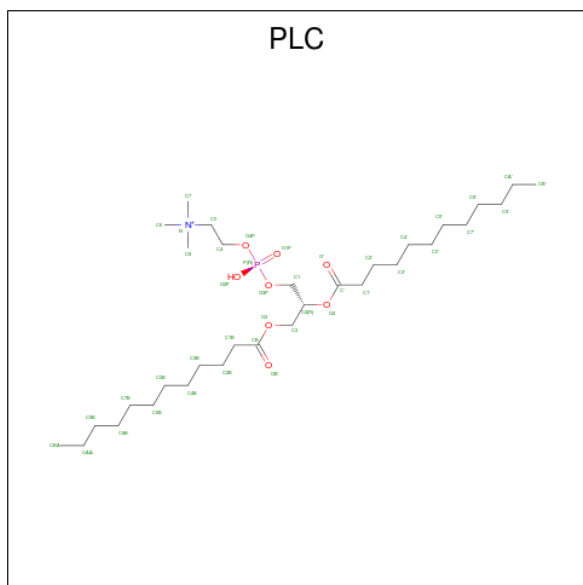
Mol	Chain	Residues	Atoms						AltConf
5	C	1	Total	C	H	N	O	P	0
			188	56	112	2	16	2	
5	C	1	Total	C	H	N	O	P	0
			188	56	112	2	16	2	
5	B	1	Total	C	H	N	O	P	0
			94	28	56	1	8	1	
5	G	1	Total	C	H	N	O	P	0
			188	56	112	2	16	2	
5	G	1	Total	C	H	N	O	P	0
			188	56	112	2	16	2	
5	K	1	Total	C	H	N	O	P	0
			188	56	112	2	16	2	
5	K	1	Total	C	H	N	O	P	0
			188	56	112	2	16	2	
5	F	1	Total	C	H	N	O	P	0
			94	28	56	1	8	1	

Continued on next page...

*Continued from previous page...*

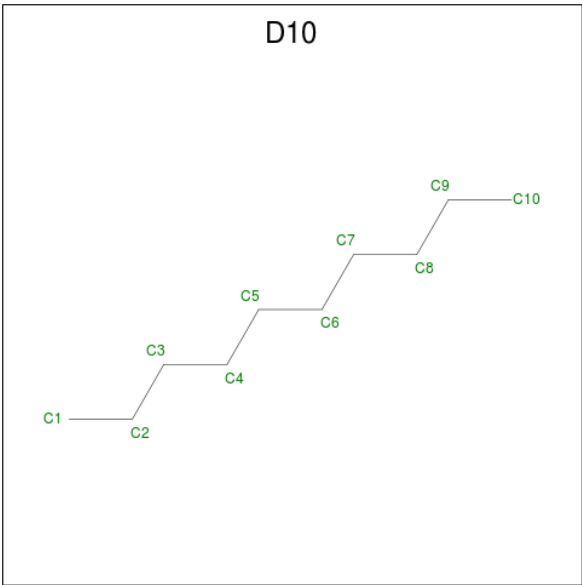
Mol	Chain	Residues	Atoms						AltConf
5	J	1	Total	C	H	N	O	P	0
			94	28	56	1	8	1	

- Molecule 6 is DIUNDECYL PHOSPHATIDYL CHOLINE (three-letter code: PLC) (formula:  $C_{32}H_{65}NO_8P$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
6	B	1	Total	C	H	N	O	P	0
			106	32	64	1	8	1	
6	F	1	Total	C	H	N	O	P	0
			106	32	64	1	8	1	
6	J	1	Total	C	H	N	O	P	0
			106	32	64	1	8	1	

- Molecule 7 is DECANE (three-letter code: D10) (formula:  $C_{10}H_{22}$ ) (labeled as "Ligand of Interest" by depositor).

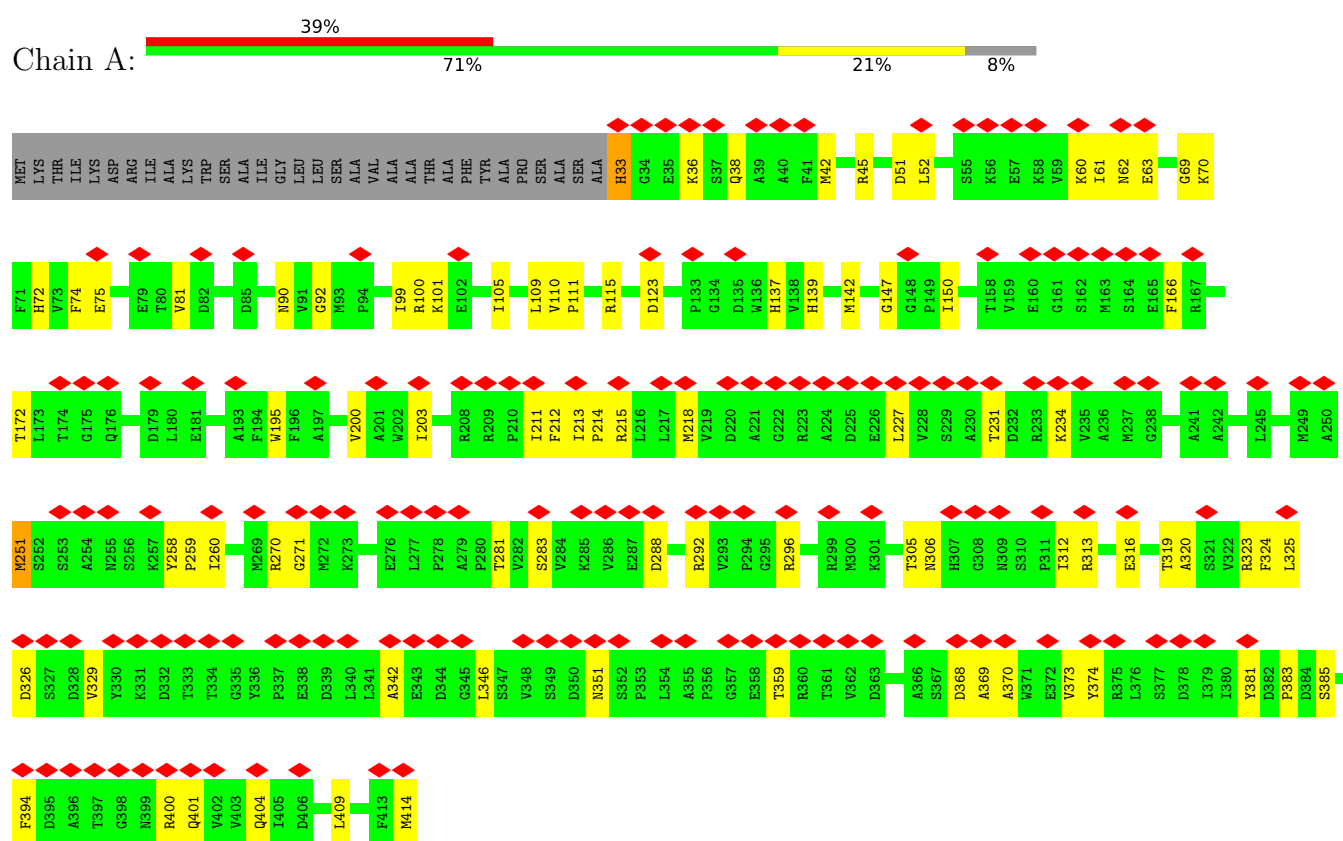


Mol	Chain	Residues	Atoms			AltConf
7	B	1	Total	C	H	0
			96	30	66	
7	B	1	Total	C	H	0
			96	30	66	
7	B	1	Total	C	H	0
			96	30	66	
7	F	1	Total	C	H	0
			96	30	66	
7	F	1	Total	C	H	0
			96	30	66	
7	F	1	Total	C	H	0
			96	30	66	
7	J	1	Total	C	H	0
			96	30	66	
7	J	1	Total	C	H	0
			96	30	66	
7	J	1	Total	C	H	0
			96	30	66	

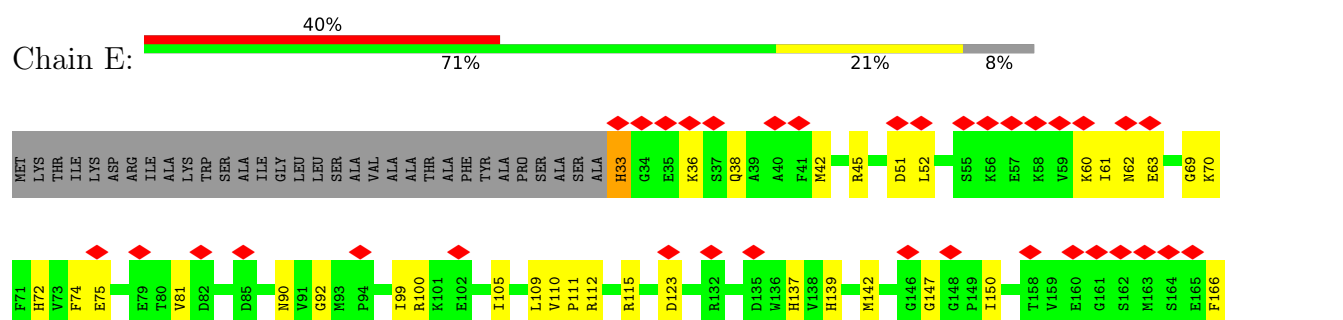
### 3 Residue-property plots

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.

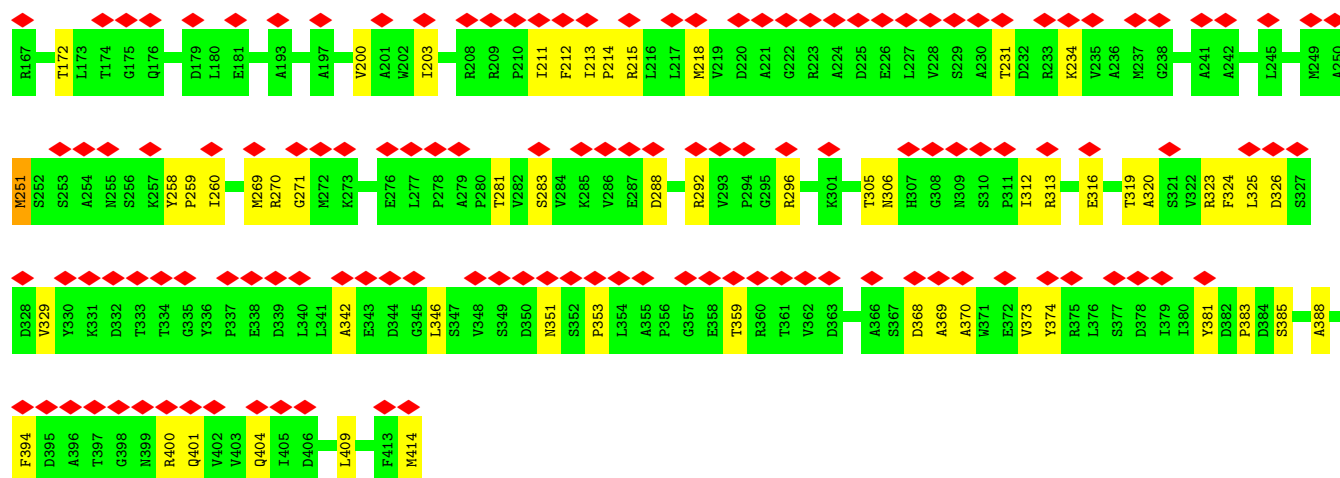
- Molecule 1: Particulate methane monooxygenase alpha subunit



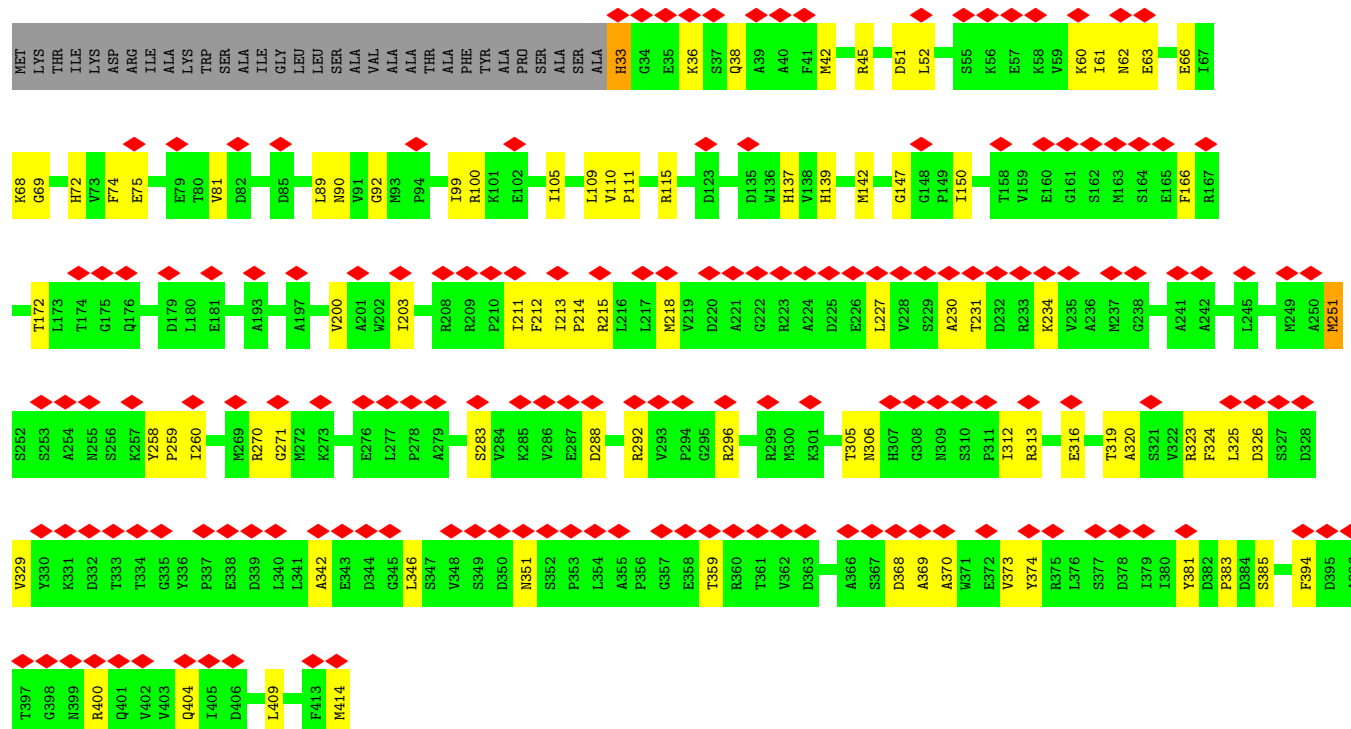
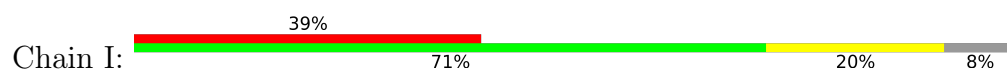
- Molecule 1: Particulate methane monooxygenase alpha subunit



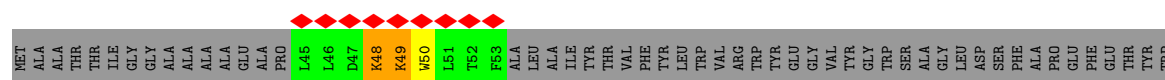
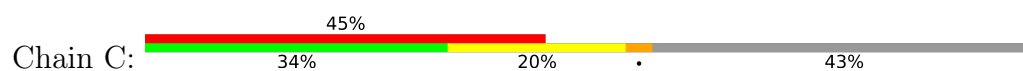


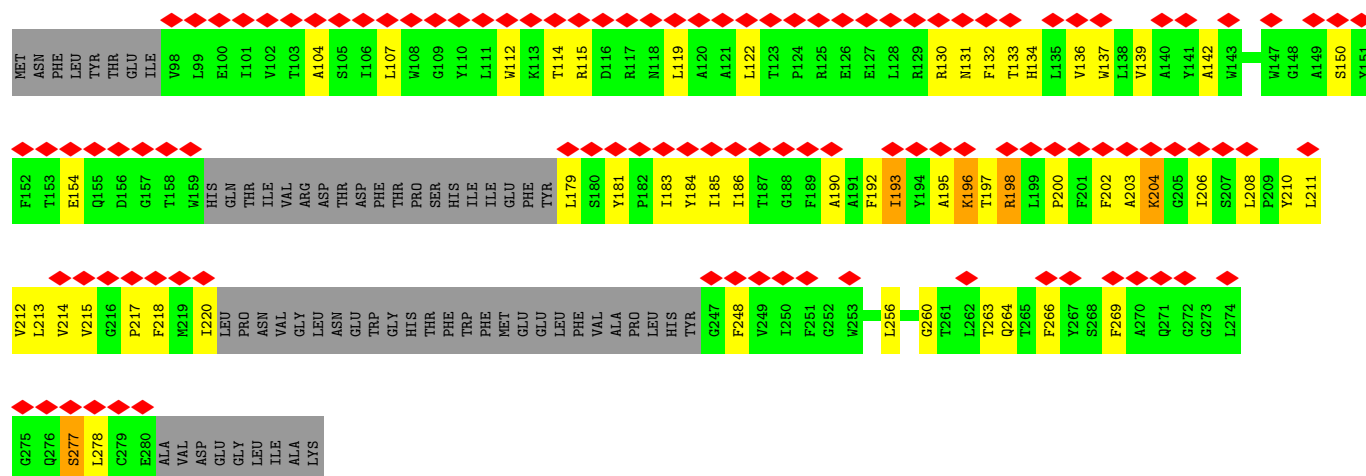


- Molecule 1: Particulate methane monooxygenase alpha subunit

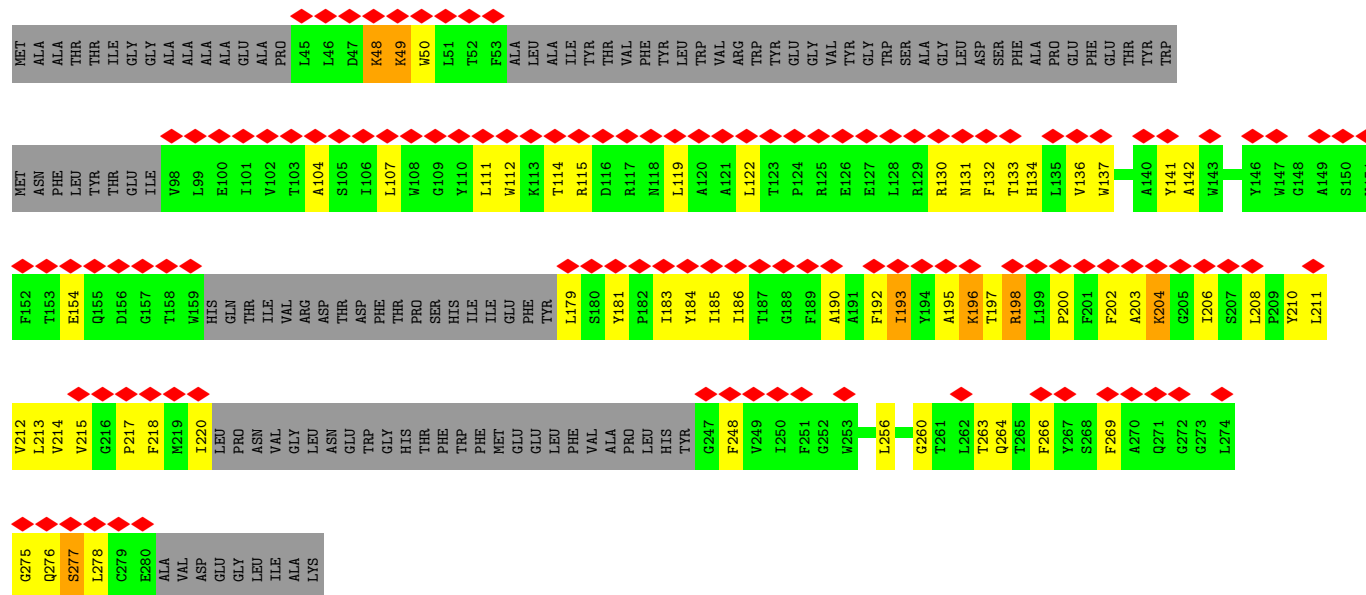
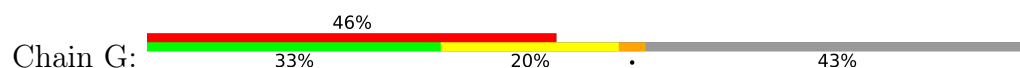


- Molecule 2: Ammonia monooxygenase/methane monooxygenase, subunit C family protein

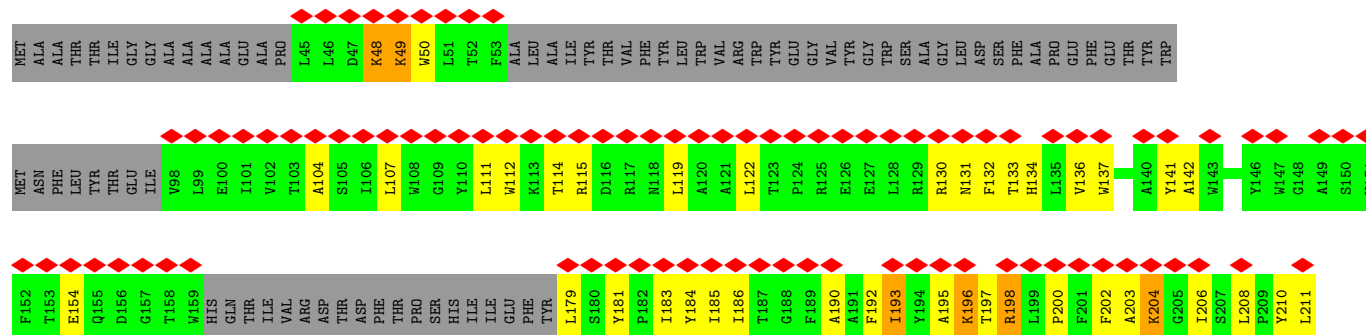


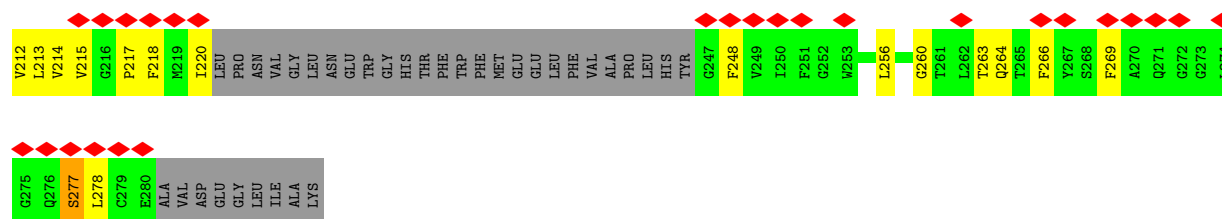


- Molecule 2: Ammonia monooxygenase/methane monooxygenase, subunit C family protein

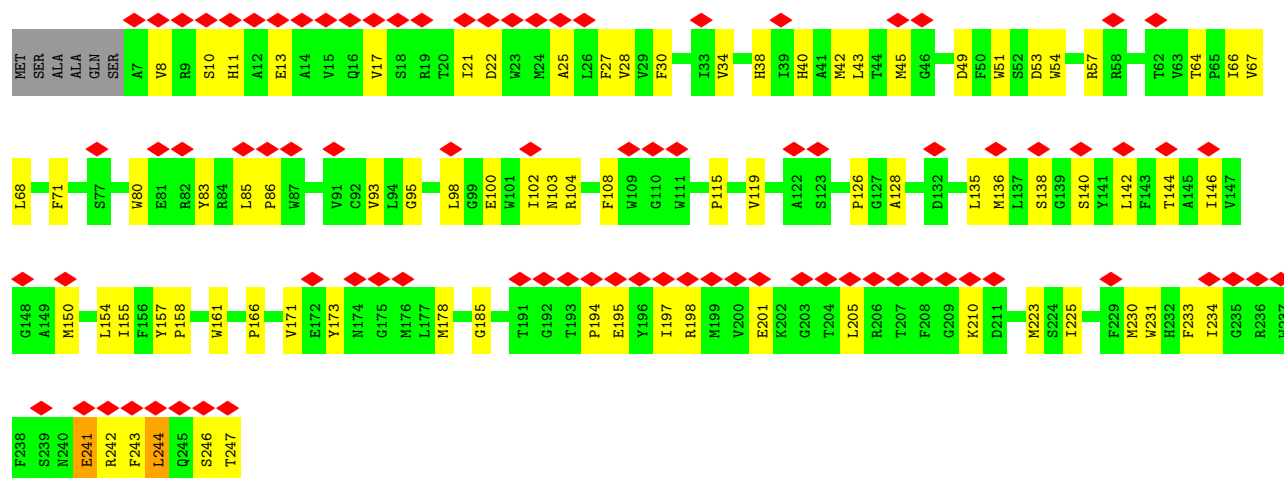


- Molecule 2: Ammonia monooxygenase/methane monooxygenase, subunit C family protein

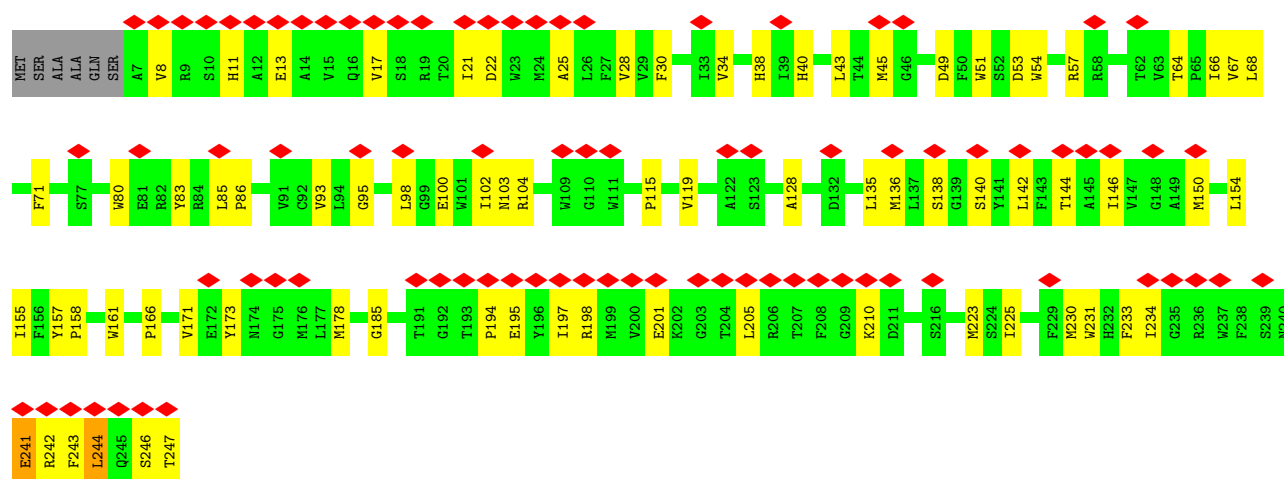




• Molecule 3: Particulate methane monooxygenase beta subunit

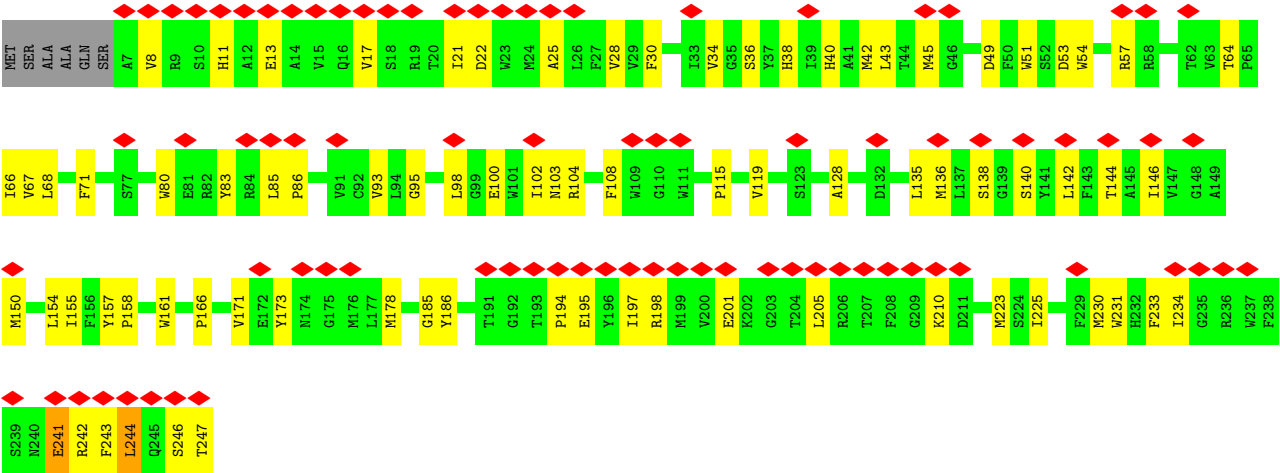


• Molecule 3: Particulate methane monooxygenase beta subunit



• Molecule 3: Particulate methane monooxygenase beta subunit





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	394208	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 ( $e^-/\text{\AA}^2$ )	1.2	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.046	Depositor
Minimum map value	-0.030	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0127	Depositor
Map size (Å)	153.29999, 153.29999, 153.29999	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.511, 0.511, 0.511	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CU, D10, P1O, PLC

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	0.28	0/3099	0.52	1/4215 (0.0%)
1	E	0.28	0/3099	0.52	1/4215 (0.0%)
1	I	0.28	0/3099	0.52	1/4215 (0.0%)
2	C	0.33	0/1239	0.50	0/1688
2	G	0.33	0/1239	0.50	0/1688
2	K	0.33	0/1239	0.50	0/1688
3	B	0.31	0/2052	0.50	0/2808
3	F	0.31	0/2052	0.50	0/2808
3	J	0.31	0/2052	0.50	0/2808
All	All	0.30	0/19170	0.51	3/26133 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	288	ASP	CB-CG-OD1	5.38	123.14	118.30
1	I	288	ASP	CB-CG-OD1	5.34	123.11	118.30
1	A	288	ASP	CB-CG-OD1	5.32	123.09	118.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3017	0	2980	63	0
1	E	3017	0	2980	62	0
1	I	3017	0	2980	63	0
2	C	1200	0	1201	80	0
2	G	1200	0	1201	80	0
2	K	1200	0	1201	81	0
3	B	1976	0	1936	93	0
3	F	1976	0	1936	86	0
3	J	1976	0	1936	91	0
4	A	2	0	0	0	0
4	E	2	0	0	0	0
4	I	1	0	0	0	0
5	B	38	56	56	4	0
5	C	76	112	112	34	0
5	F	38	56	56	4	0
5	G	76	112	112	34	0
5	J	38	56	56	5	0
5	K	76	112	112	35	0
6	B	42	64	64	5	0
6	F	42	64	64	5	0
6	J	42	64	64	5	0
7	B	30	66	66	10	0
7	F	30	66	66	11	0
7	J	30	66	66	10	0
All	All	19142	894	19245	618	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 16.

All (618) 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)
2:G:130:ARG:CD	5:G:301:P1O:H9	1.80	1.11
2:C:130:ARG:CD	5:C:301:P1O:H9	1.80	1.11
2:K:130:ARG:CD	5:K:301:P1O:H9	1.81	1.09
2:C:130:ARG:HD2	5:C:301:P1O:H9	1.40	1.04
2:K:130:ARG:HD2	5:K:301:P1O:H9	1.40	1.02
2:G:130:ARG:HD2	5:G:301:P1O:H9	1.40	1.01
2:C:112:TRP:CZ2	5:C:302:P1O:H6	2.00	0.96
2:G:137:TRP:HZ2	5:G:301:P1O:H19	1.31	0.96
2:K:112:TRP:CZ2	5:K:302:P1O:H6	2.00	0.96
2:K:137:TRP:HZ2	5:K:301:P1O:C10	1.79	0.95

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:112:TRP:CZ2	5:G:302:P1O:H6	2.00	0.95
2:K:137:TRP:HZ2	5:K:301:P1O:H19	1.31	0.95
2:C:137:TRP:HZ2	5:C:301:P1O:C10	1.79	0.95
2:C:137:TRP:HZ2	5:C:301:P1O:H19	1.31	0.94
2:G:137:TRP:HZ2	5:G:301:P1O:C10	1.79	0.94
2:G:130:ARG:HD3	5:G:301:P1O:H9	1.51	0.93
2:G:112:TRP:CH2	5:G:302:P1O:C1	2.53	0.92
2:K:112:TRP:CH2	5:K:302:P1O:C1	2.53	0.92
2:C:112:TRP:CH2	5:C:302:P1O:C1	2.53	0.91
2:C:130:ARG:HD3	5:C:301:P1O:H9	1.51	0.91
2:K:130:ARG:HD3	5:K:301:P1O:H9	1.52	0.91
2:G:112:TRP:HH2	5:G:302:P1O:C1	1.85	0.90
2:K:112:TRP:HH2	5:K:302:P1O:C1	1.85	0.89
2:C:112:TRP:HH2	5:C:302:P1O:C1	1.85	0.89
3:F:233:PHE:CG	7:F:302:D10:H51	2.08	0.89
3:J:233:PHE:CG	7:J:303:D10:H51	2.08	0.89
3:B:233:PHE:CG	7:B:302:D10:H51	2.08	0.87
2:G:137:TRP:CZ2	5:G:301:P1O:H19	2.11	0.85
2:C:137:TRP:CZ2	5:C:301:P1O:H19	2.11	0.85
2:K:137:TRP:CZ2	5:K:301:P1O:H19	2.11	0.84
2:K:112:TRP:HH2	5:K:302:P1O:H1	1.46	0.81
2:G:112:TRP:HH2	5:G:302:P1O:H1	1.46	0.80
2:K:196:LYS:HE3	2:K:206:ILE:HD13	1.64	0.79
2:C:130:ARG:HD3	5:C:301:P1O:C4	2.13	0.79
2:K:130:ARG:HD3	5:K:301:P1O:C4	2.13	0.79
2:C:112:TRP:HH2	5:C:302:P1O:H1	1.46	0.79
2:C:196:LYS:HE3	2:C:206:ILE:HD13	1.64	0.78
2:G:196:LYS:HE3	2:G:206:ILE:HD13	1.64	0.78
2:C:208:LEU:HD22	3:B:242:ARG:HD2	1.65	0.78
2:G:130:ARG:HD3	5:G:301:P1O:C4	2.13	0.78
2:G:208:LEU:HD22	3:F:242:ARG:HD2	1.65	0.77
2:K:208:LEU:CD2	3:J:242:ARG:HD2	2.15	0.77
2:K:208:LEU:HD22	3:J:242:ARG:HD2	1.67	0.77
2:C:208:LEU:CD2	3:B:242:ARG:HD2	2.16	0.76
2:C:112:TRP:CH2	5:C:302:P1O:H2	2.21	0.76
2:G:208:LEU:CD2	3:F:242:ARG:HD2	2.16	0.76
2:C:130:ARG:HD2	2:C:198:ARG:HG3	1.68	0.75
2:G:112:TRP:CH2	5:G:302:P1O:H2	2.21	0.75
2:G:130:ARG:HD2	2:G:198:ARG:HG3	1.68	0.75
2:K:130:ARG:HD2	2:K:198:ARG:HG3	1.68	0.75
1:A:51:ASP:OD1	1:A:400:ARG:NH2	2.21	0.74

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:215:VAL:HG21	3:F:142:LEU:HD21	1.69	0.74
2:K:112:TRP:CH2	5:K:302:P1O:H2	2.21	0.74
1:E:51:ASP:OD1	1:E:400:ARG:NH2	2.21	0.74
1:I:51:ASP:OD1	1:I:400:ARG:NH2	2.20	0.73
2:G:215:VAL:HG21	3:J:142:LEU:HD21	1.70	0.73
2:G:217:PRO:HA	2:G:220:ILE:HD12	1.71	0.73
2:G:197:THR:HG22	2:G:198:ARG:HD3	1.71	0.73
2:C:112:TRP:CZ2	5:C:302:P1O:C3	2.72	0.73
2:C:217:PRO:HA	2:C:220:ILE:HD12	1.71	0.73
2:C:197:THR:HG22	2:C:198:ARG:HD3	1.71	0.73
2:K:197:THR:HG22	2:K:198:ARG:HD3	1.71	0.73
2:K:217:PRO:HA	2:K:220:ILE:HD12	1.71	0.72
3:B:142:LEU:HD21	2:K:215:VAL:HG21	1.72	0.72
1:I:115:ARG:HD2	1:I:270:ARG:HG3	1.71	0.72
2:K:112:TRP:CZ2	5:K:302:P1O:C3	2.72	0.72
2:G:112:TRP:CZ2	5:G:302:P1O:C3	2.72	0.72
3:J:150:MET:HG3	3:J:225:ILE:HD11	1.72	0.72
1:A:115:ARG:HD2	1:A:270:ARG:HG3	1.72	0.71
1:E:90:ASN:HA	1:E:100:ARG:HH12	1.55	0.71
3:B:150:MET:HG3	3:B:225:ILE:HD11	1.72	0.71
3:F:150:MET:HG3	3:F:225:ILE:HD11	1.72	0.71
1:E:72:HIS:HE1	1:E:404:GLN:HE22	1.39	0.71
1:E:115:ARG:HD2	1:E:270:ARG:HG3	1.71	0.71
1:I:72:HIS:HE1	1:I:404:GLN:HE22	1.39	0.71
1:I:90:ASN:HA	1:I:100:ARG:HH12	1.55	0.70
1:A:72:HIS:HE1	1:A:404:GLN:HE22	1.39	0.70
2:C:248:PHE:HB2	3:B:43:LEU:HD12	1.74	0.70
5:C:302:P1O:H29	3:F:146:ILE:HD12	1.74	0.69
2:G:130:ARG:CD	5:G:301:P1O:C4	2.66	0.69
3:J:205:LEU:HG	1:E:42:MET:HG2	1.75	0.68
1:A:90:ASN:HA	1:A:100:ARG:HH12	1.55	0.68
3:F:53:ASP:HB2	3:F:198:ARG:HH21	1.57	0.68
3:B:53:ASP:HB2	3:B:198:ARG:HH21	1.57	0.68
3:J:233:PHE:CD2	7:J:303:D10:H51	2.29	0.68
3:F:233:PHE:CD2	7:F:302:D10:H51	2.29	0.67
2:G:248:PHE:HB2	3:F:43:LEU:HD12	1.76	0.67
3:J:53:ASP:HB2	3:J:198:ARG:HH21	1.57	0.67
3:B:233:PHE:CD2	7:B:302:D10:H51	2.29	0.67
2:C:130:ARG:CD	5:C:301:P1O:C4	2.66	0.67
2:K:112:TRP:CH2	5:K:302:P1O:C2	2.79	0.65
2:C:112:TRP:CH2	5:C:302:P1O:C2	2.79	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:100:GLU:OE2	3:J:104:ARG:NH1	2.29	0.65
2:G:112:TRP:CH2	5:G:302:P1O:C2	2.79	0.65
2:K:137:TRP:CZ2	5:K:301:P1O:C10	2.71	0.65
2:C:181:TYR:HA	2:C:184:TYR:CE1	2.32	0.65
2:G:181:TYR:HA	2:G:184:TYR:CE1	2.32	0.65
1:E:326:ASP:OD2	1:E:351:ASN:ND2	2.30	0.65
1:I:326:ASP:OD2	1:I:351:ASN:ND2	2.30	0.65
2:K:130:ARG:CD	5:K:301:P1O:C4	2.66	0.64
3:F:100:GLU:OE2	3:F:104:ARG:NH1	2.29	0.64
1:A:326:ASP:OD2	1:A:351:ASN:ND2	2.30	0.64
3:B:100:GLU:OE2	3:B:104:ARG:NH1	2.29	0.64
1:E:324:PHE:HA	1:E:342:ALA:HB3	1.79	0.64
2:C:112:TRP:CH2	5:C:302:P1O:C3	2.81	0.64
2:K:248:PHE:HB2	3:J:43:LEU:HD12	1.80	0.64
1:A:52:LEU:HD23	1:A:69:GLY:HA3	1.80	0.64
2:G:112:TRP:CH2	5:G:302:P1O:C3	2.81	0.64
2:G:206:ILE:HB	3:F:244:LEU:CD2	2.28	0.64
3:J:244:LEU:HA	5:J:301:P1O:H3	1.80	0.64
2:K:112:TRP:CH2	5:K:302:P1O:C3	2.81	0.64
2:K:181:TYR:HA	2:K:184:TYR:CE1	2.32	0.64
1:I:52:LEU:HD23	1:I:69:GLY:HA3	1.80	0.64
2:G:154:GLU:HB3	3:F:103:ASN:ND2	2.13	0.63
1:A:324:PHE:HA	1:A:342:ALA:HB3	1.79	0.63
1:E:52:LEU:HD23	1:E:69:GLY:HA3	1.80	0.63
1:I:324:PHE:HA	1:I:342:ALA:HB3	1.79	0.63
5:G:302:P1O:H29	3:J:146:ILE:HD12	1.79	0.63
1:A:42:MET:HG2	3:F:205:LEU:HG	1.80	0.63
3:B:146:ILE:HD12	5:K:302:P1O:H29	1.81	0.63
2:C:206:ILE:HB	3:B:244:LEU:CD2	2.29	0.63
2:K:212:VAL:HG22	5:J:301:P1O:H50	1.81	0.63
5:C:302:P1O:O8	5:C:302:P1O:H7	1.99	0.62
5:G:301:P1O:H24	5:G:301:P1O:H18	1.82	0.62
5:K:302:P1O:O8	5:K:302:P1O:H7	1.99	0.62
2:C:154:GLU:HB3	3:B:103:ASN:ND2	2.14	0.62
2:C:212:VAL:HG22	5:B:305:P1O:H50	1.81	0.62
1:A:316:GLU:OE2	1:A:323:ARG:NH2	2.30	0.62
5:C:301:P1O:H18	5:C:301:P1O:H24	1.82	0.62
5:G:302:P1O:H7	5:G:302:P1O:O8	1.99	0.62
2:K:154:GLU:HB3	3:J:103:ASN:ND2	2.15	0.62
3:F:244:LEU:HA	5:F:305:P1O:H3	1.81	0.62
2:C:137:TRP:CZ2	5:C:301:P1O:C10	2.71	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:212:VAL:HG22	5:F:305:P1O:H50	1.83	0.61
3:B:205:LEU:HG	1:I:42:MET:HG2	1.80	0.61
1:A:105:ILE:HG12	1:A:110:VAL:HG21	1.83	0.61
3:B:244:LEU:HA	5:B:305:P1O:H3	1.82	0.61
2:G:137:TRP:CZ2	5:G:301:P1O:C10	2.71	0.61
5:K:301:P1O:H18	5:K:301:P1O:H24	1.82	0.61
3:J:34:VAL:O	3:J:38:HIS:HB2	2.01	0.61
3:B:230:MET:HG2	3:B:234:ILE:HD11	1.83	0.61
3:F:57:ARG:NE	3:F:201:GLU:OE1	2.33	0.61
1:A:109:LEU:HG	1:A:111:PRO:HD3	1.83	0.61
1:A:259:PRO:HG2	1:A:260:ILE:HD12	1.82	0.61
5:C:302:P1O:H29	3:F:146:ILE:CD1	2.31	0.61
3:B:233:PHE:CD2	7:B:302:D10:C7	2.84	0.61
1:I:259:PRO:HG2	1:I:260:ILE:HD12	1.82	0.61
2:C:112:TRP:CH2	5:C:302:P1O:H4	2.36	0.61
2:K:132:PHE:HZ	3:J:17:VAL:HG13	1.65	0.61
3:J:230:MET:HG2	3:J:234:ILE:HD11	1.83	0.61
3:J:233:PHE:CD2	7:J:303:D10:C7	2.84	0.61
2:C:48:LYS:HG3	2:C:50:TRP:HD1	1.66	0.60
2:G:48:LYS:HG3	2:G:50:TRP:HD1	1.66	0.60
3:F:233:PHE:CD2	7:F:302:D10:C7	2.84	0.60
2:K:48:LYS:HG3	2:K:50:TRP:HD1	1.66	0.60
3:B:34:VAL:O	3:B:38:HIS:HB2	2.01	0.60
3:F:230:MET:HG2	3:F:234:ILE:HD11	1.83	0.60
1:E:259:PRO:HG2	1:E:260:ILE:HD12	1.82	0.60
2:K:112:TRP:CH2	5:K:302:P1O:H4	2.36	0.60
3:F:34:VAL:O	3:F:38:HIS:HB2	2.01	0.60
1:I:109:LEU:HG	1:I:111:PRO:HD3	1.83	0.60
5:C:302:P1O:H34	3:F:146:ILE:HG21	1.84	0.60
2:G:112:TRP:CZ2	5:G:302:P1O:H4	2.37	0.60
5:C:301:P1O:O2	5:C:301:P1O:H4	2.02	0.60
2:K:112:TRP:CZ2	5:K:302:P1O:H4	2.37	0.60
5:G:301:P1O:H4	5:G:301:P1O:O2	2.02	0.59
2:C:132:PHE:HZ	3:B:17:VAL:HG13	1.68	0.59
2:G:112:TRP:CH2	5:G:302:P1O:H4	2.36	0.59
3:B:57:ARG:NE	3:B:201:GLU:OE1	2.33	0.59
3:J:21:ILE:HG21	1:I:213:ILE:HD11	1.84	0.59
2:C:112:TRP:CZ2	5:C:302:P1O:H4	2.37	0.59
3:F:242:ARG:HD3	5:F:305:P1O:C5	2.33	0.59
1:I:105:ILE:HG12	1:I:110:VAL:HG21	1.83	0.59
2:G:112:TRP:CH2	5:G:302:P1O:H7	2.37	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:301:P1O:O2	5:K:301:P1O:H4	2.02	0.59
3:J:57:ARG:NE	3:J:201:GLU:OE1	2.33	0.59
1:E:105:ILE:HG12	1:E:110:VAL:HG21	1.83	0.59
2:C:112:TRP:CH2	5:C:302:P1O:H7	2.37	0.59
1:E:109:LEU:HG	1:E:111:PRO:HD3	1.83	0.59
2:K:112:TRP:CH2	5:K:302:P1O:H7	2.37	0.59
2:K:278:LEU:HD22	1:I:214:PRO:HB3	1.83	0.59
2:C:179:LEU:O	2:C:183:ILE:HG12	2.03	0.58
1:I:316:GLU:OE2	1:I:323:ARG:NH2	2.30	0.58
2:G:132:PHE:HZ	3:F:17:VAL:HG13	1.67	0.58
2:G:206:ILE:HB	3:F:244:LEU:HD22	1.85	0.58
2:G:179:LEU:O	2:G:183:ILE:HG12	2.03	0.58
5:C:301:P1O:O2	5:C:301:P1O:H6	2.04	0.58
5:G:301:P1O:O2	5:G:301:P1O:H6	2.04	0.58
2:C:206:ILE:HB	3:B:244:LEU:HD22	1.85	0.57
2:K:179:LEU:O	2:K:183:ILE:HG12	2.03	0.57
5:K:301:P1O:O2	5:K:301:P1O:H6	2.04	0.57
3:F:233:PHE:CD2	7:F:302:D10:H71	2.39	0.57
2:K:206:ILE:HB	3:J:244:LEU:CD2	2.35	0.57
3:F:30:PHE:O	3:F:34:VAL:HG23	2.04	0.57
3:F:21:ILE:HG21	1:E:213:ILE:HD11	1.87	0.57
3:B:242:ARG:HD3	5:B:305:P1O:C5	2.35	0.57
3:J:233:PHE:CD2	7:J:303:D10:H71	2.39	0.57
3:B:30:PHE:O	3:B:34:VAL:HG23	2.04	0.57
3:B:233:PHE:CD2	7:B:302:D10:H71	2.39	0.56
3:J:30:PHE:O	3:J:34:VAL:HG23	2.04	0.56
1:E:270:ARG:HG2	1:E:271:GLY:H	1.70	0.56
1:A:214:PRO:HB3	2:C:278:LEU:HD22	1.87	0.56
1:E:316:GLU:OE2	1:E:323:ARG:NH2	2.30	0.56
3:F:242:ARG:HD3	5:F:305:P1O:H11	1.86	0.56
2:G:278:LEU:HD22	1:E:214:PRO:HB3	1.87	0.56
3:J:51:TRP:HB2	3:J:54:TRP:HB2	1.87	0.56
1:A:381:TYR:HB2	3:F:210:LYS:HE3	1.87	0.56
2:C:131:ASN:HD21	2:C:269:PHE:HD1	1.53	0.56
2:G:131:ASN:HD21	2:G:269:PHE:HD1	1.53	0.56
5:G:302:P1O:H29	3:J:146:ILE:CD1	2.36	0.56
1:I:270:ARG:HG2	1:I:271:GLY:H	1.70	0.56
3:B:51:TRP:HB2	3:B:54:TRP:HB2	1.87	0.55
3:F:40:HIS:NE2	3:F:67:VAL:O	2.35	0.55
3:F:51:TRP:HB2	3:F:54:TRP:HB2	1.87	0.55
3:F:194:PRO:HD2	3:F:197:ILE:HD12	1.88	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:ARG:HD2	1:A:369:ALA:HA	1.89	0.55
3:B:83:TYR:HB2	3:B:85:LEU:HD13	1.89	0.55
1:E:296:ARG:HD2	1:E:369:ALA:HA	1.88	0.55
2:K:131:ASN:HD21	2:K:269:PHE:HD1	1.53	0.55
3:B:146:ILE:CD1	5:K:302:P1O:H29	2.36	0.55
2:G:131:ASN:ND2	2:G:269:PHE:HD1	2.05	0.55
2:K:104:ALA:HB2	2:K:186:ILE:HG12	1.89	0.55
2:G:192:PHE:HZ	2:G:206:ILE:HG23	1.72	0.55
1:A:270:ARG:HG2	1:A:271:GLY:H	1.70	0.55
2:K:192:PHE:HZ	2:K:206:ILE:HG23	1.72	0.55
1:E:385:SER:OG	1:E:409:LEU:O	2.22	0.55
1:A:213:ILE:HD11	3:B:21:ILE:HG21	1.89	0.54
2:C:131:ASN:ND2	2:C:269:PHE:HD1	2.05	0.54
3:B:194:PRO:HD2	3:B:197:ILE:HD12	1.88	0.54
3:B:242:ARG:HD3	5:B:305:P1O:H11	1.89	0.54
2:G:112:TRP:CE2	5:G:302:P1O:H6	2.40	0.54
2:K:131:ASN:ND2	2:K:269:PHE:HD1	2.05	0.54
2:K:208:LEU:HD23	3:J:242:ARG:HD2	1.89	0.54
1:A:385:SER:OG	1:A:409:LEU:O	2.22	0.54
2:C:192:PHE:HZ	2:C:206:ILE:HG23	1.72	0.54
3:B:40:HIS:NE2	3:B:67:VAL:O	2.35	0.54
3:F:83:TYR:HB2	3:F:85:LEU:HD13	1.89	0.54
3:J:83:TYR:HB2	3:J:85:LEU:HD13	1.89	0.54
2:G:104:ALA:HB2	2:G:186:ILE:HG12	1.89	0.54
2:K:142:ALA:HB2	3:J:28:VAL:HG23	1.89	0.54
3:J:194:PRO:HD2	3:J:197:ILE:HD12	1.88	0.54
1:I:296:ARG:HD2	1:I:369:ALA:HA	1.89	0.54
3:J:242:ARG:HD3	5:J:301:P1O:H11	1.90	0.54
3:J:210:LYS:HE3	1:E:381:TYR:HB2	1.89	0.54
3:J:231:TRP:HA	3:J:234:ILE:HD12	1.90	0.54
2:K:112:TRP:CE2	5:K:302:P1O:H6	2.40	0.54
2:C:104:ALA:HB2	2:C:186:ILE:HG12	1.89	0.54
2:G:142:ALA:HB2	3:F:28:VAL:HG23	1.88	0.53
3:F:230:MET:HG3	7:F:303:D10:H101	1.90	0.53
2:K:115:ARG:HA	2:K:197:THR:HG21	1.90	0.53
3:J:40:HIS:NE2	3:J:67:VAL:O	2.35	0.53
3:B:230:MET:HG3	7:B:303:D10:H101	1.89	0.53
3:J:230:MET:HG3	7:J:304:D10:H101	1.90	0.53
3:B:205:LEU:HD22	1:I:38:GLN:OE1	2.09	0.53
3:B:210:LYS:HE3	1:I:381:TYR:HB2	1.91	0.53
2:C:112:TRP:CE2	5:C:302:P1O:H6	2.40	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:266:PHE:CE1	1:E:212:PHE:HB3	2.44	0.53
3:F:231:TRP:HA	3:F:234:ILE:HD12	1.90	0.53
3:J:233:PHE:CD1	7:J:303:D10:H51	2.44	0.53
3:F:233:PHE:CD1	7:F:302:D10:H51	2.44	0.53
2:C:115:ARG:HA	2:C:197:THR:HG21	1.90	0.52
3:B:93:VAL:HG21	3:B:128:ALA:HB2	1.91	0.52
1:I:214:PRO:O	1:I:218:MET:HG2	2.09	0.52
1:I:368:ASP:OD2	1:I:369:ALA:N	2.42	0.52
1:A:214:PRO:O	1:A:218:MET:HG2	2.09	0.52
3:B:146:ILE:HG21	5:K:302:P1O:H34	1.91	0.52
2:G:115:ARG:HA	2:G:197:THR:HG21	1.90	0.52
2:K:112:TRP:HB2	2:K:193:ILE:HG21	1.92	0.52
2:G:208:LEU:HD23	3:F:242:ARG:HD2	1.92	0.52
2:K:211:LEU:HD22	3:J:247:THR:HG22	1.90	0.52
1:E:60:LYS:NZ	1:E:63:GLU:OE2	2.42	0.52
3:B:231:TRP:HA	3:B:234:ILE:HD12	1.90	0.52
3:J:93:VAL:HG21	3:J:128:ALA:HB2	1.91	0.52
1:A:368:ASP:OD2	1:A:369:ALA:N	2.42	0.52
2:C:112:TRP:HB2	2:C:193:ILE:HG21	1.92	0.52
2:G:112:TRP:HB2	2:G:193:ILE:HG21	1.92	0.52
1:E:214:PRO:O	1:E:218:MET:HG2	2.09	0.52
1:E:316:GLU:HG2	1:E:325:LEU:HG	1.92	0.52
2:C:142:ALA:HB2	3:B:28:VAL:HG23	1.90	0.52
2:G:192:PHE:CD1	2:G:214:VAL:HG11	2.45	0.52
1:E:368:ASP:OD2	1:E:369:ALA:N	2.42	0.52
3:F:93:VAL:HG21	3:F:128:ALA:HB2	1.91	0.52
1:A:60:LYS:NZ	1:A:63:GLU:OE2	2.42	0.52
2:C:192:PHE:CD1	2:C:214:VAL:HG11	2.45	0.52
3:J:210:LYS:HA	1:E:381:TYR:CE2	2.45	0.52
3:J:242:ARG:HD3	5:J:301:P1O:C5	2.39	0.52
1:I:60:LYS:NZ	1:I:63:GLU:OE2	2.42	0.52
1:A:381:TYR:CE2	3:F:210:LYS:HA	2.45	0.52
1:A:306:ASN:ND2	1:A:312:ILE:HG12	2.25	0.51
5:G:302:P1O:H34	3:J:146:ILE:HG21	1.91	0.51
2:K:192:PHE:CD1	2:K:214:VAL:HG11	2.45	0.51
3:F:230:MET:O	3:F:234:ILE:HG13	2.10	0.51
1:I:306:ASN:ND2	1:I:312:ILE:HG12	2.25	0.51
3:B:230:MET:O	3:B:234:ILE:HG13	2.10	0.51
3:B:233:PHE:CD1	7:B:302:D10:H51	2.44	0.51
2:C:211:LEU:HD22	3:B:247:THR:HG22	1.92	0.51
2:G:211:LEU:HD22	3:F:247:THR:HG22	1.91	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:154:LEU:HD13	6:J:302:PLC:C9'	2.41	0.51
1:A:212:PHE:HB3	2:C:266:PHE:CE1	2.45	0.51
3:J:171:VAL:HG22	1:I:172:THR:HA	1.93	0.51
1:A:316:GLU:HG2	1:A:325:LEU:HG	1.92	0.51
5:C:302:P1O:H12	5:C:302:P1O:H16	1.93	0.51
1:E:306:ASN:ND2	1:E:312:ILE:HG12	2.25	0.51
1:A:283:SER:HB3	1:A:305:THR:HB	1.93	0.51
1:E:283:SER:HB3	1:E:305:THR:HB	1.93	0.51
3:B:154:LEU:HD13	6:B:301:PLC:C9'	2.41	0.51
1:I:316:GLU:HG2	1:I:325:LEU:HG	1.92	0.51
2:K:266:PHE:CE1	1:I:212:PHE:HB3	2.46	0.50
1:I:305:THR:HA	1:I:359:THR:HG22	1.92	0.50
3:B:86:PRO:HB3	3:B:136:MET:HB2	1.94	0.50
1:I:283:SER:HB3	1:I:305:THR:HB	1.93	0.50
1:A:305:THR:HA	1:A:359:THR:HG22	1.92	0.50
3:J:230:MET:O	3:J:234:ILE:HG13	2.10	0.50
1:E:305:THR:HA	1:E:359:THR:HG22	1.93	0.50
3:F:154:LEU:HD13	6:F:301:PLC:C9'	2.41	0.50
1:A:373:VAL:HG12	1:A:374:TYR:HD2	1.77	0.50
5:K:302:P1O:H16	5:K:302:P1O:H12	1.93	0.50
3:F:86:PRO:HB3	3:F:136:MET:HB2	1.94	0.50
5:G:302:P1O:H16	5:G:302:P1O:H12	1.93	0.50
1:I:373:VAL:HG12	1:I:374:TYR:HD2	1.77	0.50
2:C:190:ALA:HA	2:C:193:ILE:HD12	1.94	0.49
3:B:155:ILE:HA	3:B:158:PRO:HG2	1.94	0.49
1:E:373:VAL:HG12	1:E:374:TYR:HD2	1.77	0.49
3:J:86:PRO:HB3	3:J:136:MET:HB2	1.94	0.49
1:I:92:GLY:N	1:I:139:HIS:O	2.38	0.49
3:B:45:MET:SD	3:B:49:ASP:HB2	2.53	0.49
3:J:45:MET:SD	3:J:49:ASP:HB2	2.53	0.49
1:E:33:HIS:CE1	1:E:137:HIS:ND1	2.81	0.49
1:A:92:GLY:N	1:A:139:HIS:O	2.38	0.49
2:C:208:LEU:HD23	3:B:242:ARG:HD2	1.92	0.49
1:I:33:HIS:CE1	1:I:137:HIS:ND1	2.81	0.49
3:J:155:ILE:HA	3:J:158:PRO:HG2	1.94	0.49
2:K:190:ALA:HA	2:K:193:ILE:HD12	1.95	0.49
1:A:33:HIS:CE1	1:A:137:HIS:ND1	2.81	0.48
3:F:98:LEU:O	3:F:102:ILE:HG12	2.13	0.48
2:G:190:ALA:HA	2:G:193:ILE:HD12	1.95	0.48
1:A:370:ALA:HA	1:A:373:VAL:HB	1.96	0.48
3:B:154:LEU:HD22	6:B:301:PLC:H6'2	1.95	0.48

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:130:ARG:O	2:K:133:THR:OG1	2.27	0.48
2:K:206:ILE:HB	3:J:244:LEU:HD22	1.93	0.48
3:F:155:ILE:HA	3:F:158:PRO:HG2	1.94	0.48
1:I:370:ALA:HA	1:I:373:VAL:HB	1.95	0.48
3:B:210:LYS:HA	1:I:381:TYR:CE2	2.48	0.48
3:F:45:MET:SD	3:F:49:ASP:HB2	2.53	0.48
3:J:98:LEU:O	3:J:102:ILE:HG12	2.13	0.48
1:A:172:THR:HA	3:B:171:VAL:HG22	1.94	0.48
3:J:205:LEU:HD22	1:E:38:GLN:OE1	2.13	0.48
1:I:81:VAL:HG13	1:I:147:GLY:HA3	1.96	0.48
1:I:385:SER:OG	1:I:409:LEU:O	2.22	0.48
2:C:203:ALA:O	2:C:204:LYS:HG3	2.13	0.48
2:G:203:ALA:O	2:G:204:LYS:HG3	2.13	0.48
1:E:81:VAL:HG13	1:E:147:GLY:HA3	1.96	0.48
3:B:98:LEU:O	3:B:102:ILE:HG12	2.13	0.48
2:G:130:ARG:O	2:G:133:THR:OG1	2.27	0.48
2:K:203:ALA:O	2:K:204:LYS:HG3	2.13	0.48
2:C:192:PHE:HA	2:C:210:TYR:HE1	1.78	0.47
2:K:192:PHE:HA	2:K:210:TYR:HE1	1.79	0.47
1:E:370:ALA:HA	1:E:373:VAL:HB	1.96	0.47
2:C:264:GLN:HG3	3:B:241:GLU:HG2	1.96	0.47
2:K:136:VAL:HG12	5:K:301:P1O:O8	2.14	0.47
3:F:154:LEU:HD22	6:F:301:PLC:H6'2	1.95	0.47
2:K:112:TRP:CH2	5:K:302:P1O:H1	2.33	0.47
3:F:161:TRP:CD1	1:E:251:MET:HG2	2.49	0.47
1:A:38:GLN:OE1	3:F:205:LEU:HD22	2.14	0.47
3:J:154:LEU:HD22	6:J:302:PLC:H6'2	1.95	0.47
2:C:196:LYS:HD2	2:C:196:LYS:HA	1.62	0.47
2:C:136:VAL:HG12	5:C:301:P1O:O8	2.14	0.47
2:C:154:GLU:HB3	3:B:103:ASN:HD22	1.79	0.47
2:G:136:VAL:HG12	5:G:301:P1O:O8	2.14	0.47
2:G:264:GLN:HG3	3:F:241:GLU:HG2	1.96	0.47
2:K:211:LEU:CD2	3:J:247:THR:HG22	2.45	0.47
3:F:171:VAL:HG22	1:E:172:THR:HA	1.95	0.47
2:G:192:PHE:HA	2:G:210:TYR:HE1	1.79	0.47
3:J:54:TRP:CZ2	3:J:198:ARG:HA	2.50	0.47
2:C:256:LEU:HD21	3:B:71:PHE:CD2	2.50	0.47
3:F:54:TRP:CZ2	3:F:198:ARG:HA	2.50	0.47
3:J:210:LYS:HA	1:E:381:TYR:CZ	2.50	0.47
1:A:81:VAL:HG13	1:A:147:GLY:HA3	1.96	0.46
3:B:54:TRP:CZ2	3:B:198:ARG:HA	2.50	0.46

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:66:GLU:OE2	1:I:68:LYS:NZ	2.38	0.46
3:B:233:PHE:CD2	7:B:302:D10:H72	2.51	0.46
3:J:25:ALA:HA	3:J:28:VAL:HG12	1.97	0.46
2:C:130:ARG:O	2:C:133:THR:OG1	2.27	0.46
2:C:154:GLU:HB2	3:B:42:MET:HE3	1.97	0.46
2:K:181:TYR:HD1	2:K:184:TYR:HE1	1.63	0.46
3:J:166:PRO:HG3	1:I:258:TYR:CE2	2.51	0.46
1:A:99:ILE:HD13	1:A:166:PHE:HZ	1.81	0.46
2:C:193:ILE:H	2:C:193:ILE:HG13	1.55	0.46
3:F:233:PHE:CD2	7:F:302:D10:H72	2.50	0.46
2:G:200:PRO:C	2:G:202:PHE:H	2.19	0.46
1:E:99:ILE:HD13	1:E:166:PHE:HZ	1.81	0.46
3:F:166:PRO:HG3	1:E:258:TYR:CE2	2.51	0.46
1:I:61:ILE:HG22	1:I:62:ASN:OD1	2.16	0.46
1:A:251:MET:HG2	3:B:161:TRP:CD1	2.51	0.46
2:G:134:HIS:CD2	2:G:195:ALA:HB2	2.51	0.46
1:I:99:ILE:HD13	1:I:166:PHE:HZ	1.81	0.46
2:K:137:TRP:HZ2	5:K:301:P1O:H20	1.73	0.46
3:F:25:ALA:HA	3:F:28:VAL:HG12	1.98	0.46
2:C:134:HIS:CD2	2:C:195:ALA:HB2	2.51	0.45
2:C:213:LEU:O	2:C:217:PRO:HD2	2.16	0.45
3:B:34:VAL:HG22	3:B:95:GLY:HA3	1.99	0.45
2:G:256:LEU:HD21	3:F:71:PHE:CD2	2.51	0.45
1:A:75:GLU:O	1:E:270:ARG:HD2	2.17	0.45
2:K:134:HIS:CD2	2:K:195:ALA:HB2	2.51	0.45
3:F:8:VAL:HG22	3:F:13:GLU:OE2	2.17	0.45
2:G:213:LEU:O	2:G:217:PRO:HD2	2.16	0.45
2:K:200:PRO:C	2:K:202:PHE:H	2.19	0.45
3:F:173:TYR:HB3	3:F:178:MET:HG3	1.98	0.45
1:E:61:ILE:HG22	1:E:62:ASN:OD1	2.17	0.45
2:C:137:TRP:HZ2	5:C:301:P1O:H20	1.74	0.45
3:B:25:ALA:HA	3:B:28:VAL:HG12	1.98	0.45
2:G:193:ILE:H	2:G:193:ILE:HG13	1.55	0.45
2:G:275:GLY:HA3	2:G:276:GLN:HA	1.80	0.45
2:K:213:LEU:O	2:K:217:PRO:HD2	2.16	0.45
1:E:281:THR:OG1	1:E:401:GLN:NE2	2.37	0.45
1:A:313:ARG:N	1:A:394:PHE:O	2.45	0.45
1:E:92:GLY:N	1:E:139:HIS:O	2.38	0.45
1:A:258:TYR:CE2	3:B:166:PRO:HG3	2.51	0.45
3:F:34:VAL:HG22	3:F:95:GLY:HA3	1.99	0.45
3:J:161:TRP:CD1	1:I:251:MET:HG2	2.51	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:ILE:HG22	1:A:62:ASN:OD1	2.16	0.45
1:A:211:ILE:O	1:A:215:ARG:HD3	2.17	0.45
3:B:8:VAL:HG22	3:B:13:GLU:OE2	2.17	0.45
3:B:138:SER:O	3:B:138:SER:OG	2.35	0.45
1:A:270:ARG:HD2	1:I:75:GLU:O	2.17	0.45
3:J:51:TRP:CD1	3:J:54:TRP:CD1	3.05	0.45
3:J:201:GLU:HG2	1:E:383:PRO:HG3	1.99	0.45
1:E:313:ARG:N	1:E:394:PHE:O	2.45	0.45
2:C:200:PRO:C	2:C:202:PHE:H	2.19	0.44
2:G:181:TYR:HD1	2:G:184:TYR:HE1	1.63	0.44
3:J:34:VAL:HG22	3:J:95:GLY:HA3	1.99	0.44
3:J:135:LEU:HA	3:J:144:THR:OG1	2.18	0.44
2:C:48:LYS:HG3	2:C:50:TRP:CD1	2.49	0.44
2:C:181:TYR:HD1	2:C:184:TYR:HE1	1.63	0.44
3:B:51:TRP:CD1	3:B:54:TRP:CD1	3.05	0.44
3:J:66:ILE:HG12	3:J:223:MET:HB3	1.99	0.44
1:E:211:ILE:O	1:E:215:ARG:HD3	2.17	0.44
2:G:48:LYS:HG3	2:G:50:TRP:CD1	2.49	0.44
2:G:112:TRP:CZ3	5:G:302:P1O:H2	2.53	0.44
2:K:154:GLU:HB3	3:J:103:ASN:HD22	1.81	0.44
3:F:66:ILE:HG12	3:F:223:MET:HB3	1.99	0.44
3:J:233:PHE:CD2	7:J:303:D10:H72	2.50	0.44
1:E:72:HIS:CE1	1:E:404:GLN:HE22	2.27	0.44
1:I:45:ARG:NH1	1:I:74:PHE:HE2	2.16	0.44
2:K:211:LEU:HD11	5:K:302:P1O:C11	2.48	0.44
1:I:211:ILE:O	1:I:215:ARG:HD3	2.17	0.44
3:B:10:SER:N	3:B:13:GLU:OE2	2.41	0.44
3:B:66:ILE:HG12	3:B:223:MET:HB3	1.99	0.44
3:F:157:TYR:HD1	6:F:301:PLC:H1'2	1.83	0.44
3:J:173:TYR:HB3	3:J:178:MET:HG3	1.98	0.44
1:E:45:ARG:NH1	1:E:74:PHE:HE2	2.16	0.44
3:B:135:LEU:HA	3:B:144:THR:OG1	2.18	0.44
3:B:157:TYR:HD1	6:B:301:PLC:H1'2	1.83	0.44
3:B:210:LYS:HA	1:I:381:TYR:CZ	2.53	0.44
3:F:135:LEU:HA	3:F:144:THR:OG1	2.18	0.44
3:J:157:TYR:HD1	6:J:302:PLC:H1'2	1.83	0.44
1:I:313:ARG:HH12	1:I:329:VAL:HA	1.82	0.44
2:K:264:GLN:HG3	3:J:241:GLU:HG2	1.99	0.44
3:F:51:TRP:CD1	3:F:54:TRP:CD1	3.05	0.44
1:I:72:HIS:CE1	1:I:404:GLN:HE22	2.27	0.44
2:C:150:SER:OG	3:B:38:HIS:ND1	2.42	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:256:LEU:HD21	3:J:71:PHE:CD2	2.52	0.44
3:F:138:SER:O	3:F:138:SER:OG	2.35	0.44
3:J:8:VAL:HG22	3:J:13:GLU:OE2	2.17	0.44
1:A:381:TYR:CZ	3:F:210:LYS:HA	2.52	0.44
2:G:211:LEU:CD2	3:F:247:THR:HG22	2.47	0.44
2:K:112:TRP:CZ3	5:K:302:P1O:H2	2.53	0.44
3:B:64:THR:O	3:B:68:LEU:HB2	2.18	0.43
3:F:51:TRP:HD1	3:F:54:TRP:CD1	2.36	0.43
1:E:313:ARG:HH12	1:E:329:VAL:HA	1.83	0.43
1:A:45:ARG:NH1	1:A:74:PHE:HE2	2.16	0.43
2:G:154:GLU:HB3	3:F:103:ASN:HD22	1.79	0.43
3:J:64:THR:O	3:J:68:LEU:HB2	2.18	0.43
3:B:138:SER:O	3:B:140:SER:N	2.52	0.43
3:F:138:SER:O	3:F:140:SER:N	2.52	0.43
3:J:138:SER:O	3:J:140:SER:N	2.52	0.43
3:B:80:TRP:CZ3	3:B:136:MET:HG3	2.54	0.43
3:B:173:TYR:HB3	3:B:178:MET:HG3	1.98	0.43
3:F:80:TRP:CZ3	3:F:136:MET:HG3	2.54	0.43
1:E:75:GLU:O	1:I:270:ARG:HD2	2.17	0.43
1:I:292:ARG:NH1	1:I:414:MET:O	2.49	0.43
1:A:319:THR:HG23	1:A:320:ALA:H	1.84	0.43
3:B:154:LEU:HD13	6:B:301:PLC:H9'1	2.01	0.43
3:B:234:ILE:HG12	7:B:303:D10:H91	2.01	0.43
2:G:211:LEU:HD11	5:G:302:P1O:C11	2.48	0.43
3:F:154:LEU:HD13	6:F:301:PLC:H9'1	2.01	0.43
1:E:319:THR:HG23	1:E:320:ALA:H	1.84	0.43
1:I:313:ARG:N	1:I:394:PHE:O	2.45	0.43
1:A:313:ARG:HH12	1:A:329:VAL:HA	1.83	0.43
3:J:234:ILE:HG12	7:J:304:D10:H91	2.01	0.43
2:C:211:LEU:HD11	5:C:302:P1O:C11	2.48	0.43
3:F:233:PHE:CD2	7:F:302:D10:C5	3.01	0.43
3:J:154:LEU:HD13	6:J:302:PLC:H9'1	2.01	0.43
3:J:51:TRP:HD1	3:J:54:TRP:CD1	2.36	0.43
2:C:112:TRP:CZ3	5:C:302:P1O:H2	2.53	0.43
3:B:195:GLU:HG2	3:B:198:ARG:HD2	2.01	0.43
1:E:200:VAL:HA	1:E:203:ILE:HG22	2.01	0.42
2:C:49:LYS:HA	2:C:49:LYS:CE	2.50	0.42
3:B:51:TRP:HD1	3:B:54:TRP:CD1	2.36	0.42
3:F:64:THR:O	3:F:68:LEU:HB2	2.18	0.42
2:C:211:LEU:CD2	3:B:247:THR:HG22	2.49	0.42
3:F:195:GLU:HG2	3:F:198:ARG:HD2	2.01	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:80:TRP:CZ3	3:J:136:MET:HG3	2.54	0.42
1:E:326:ASP:HB2	1:E:346:LEU:HD23	2.02	0.42
1:I:319:THR:HG23	1:I:320:ALA:H	1.84	0.42
3:F:53:ASP:OD2	3:F:185:GLY:HA3	2.20	0.42
2:K:48:LYS:HG3	2:K:50:TRP:CD1	2.49	0.42
3:J:195:GLU:HG2	3:J:198:ARG:HD2	2.01	0.42
2:K:48:LYS:HE3	2:K:48:LYS:HB3	1.77	0.42
2:C:277:SER:HA	3:B:11:HIS:CD2	2.55	0.42
2:G:49:LYS:HA	2:G:49:LYS:CE	2.50	0.42
3:F:22:ASP:HB3	1:E:211:ILE:HD12	2.01	0.42
1:A:292:ARG:HH12	1:A:414:MET:C	2.23	0.42
3:B:53:ASP:O	3:B:198:ARG:NH2	2.52	0.42
2:K:132:PHE:CZ	3:J:17:VAL:HG13	2.52	0.42
3:F:234:ILE:HG12	7:F:303:D10:H91	2.01	0.42
1:I:200:VAL:HA	1:I:203:ILE:HG22	2.01	0.42
1:A:142:MET:HB3	1:A:150:ILE:HB	2.02	0.42
1:A:326:ASP:HB2	1:A:346:LEU:HD23	2.02	0.42
3:B:233:PHE:CD2	7:B:302:D10:C5	3.01	0.42
2:K:192:PHE:HD1	2:K:214:VAL:HG11	1.84	0.42
1:E:142:MET:HB3	1:E:150:ILE:HB	2.02	0.42
1:A:200:VAL:HA	1:A:203:ILE:HG22	2.01	0.41
2:C:139:VAL:HG13	3:B:27:PHE:CE2	2.55	0.41
3:B:115:PRO:O	3:B:119:VAL:HG22	2.20	0.41
3:F:53:ASP:O	3:F:198:ARG:NH2	2.52	0.41
3:F:210:LYS:O	6:F:301:PLC:O1P	2.38	0.41
3:J:22:ASP:HB3	1:I:211:ILE:HD12	2.02	0.41
1:I:326:ASP:HB2	1:I:346:LEU:HD23	2.02	0.41
2:C:192:PHE:HD1	2:C:214:VAL:HG11	1.84	0.41
2:G:192:PHE:HD1	2:G:214:VAL:HG11	1.84	0.41
1:I:45:ARG:HB2	1:I:74:PHE:CD2	2.55	0.41
3:J:186:TYR:CE1	1:I:100:ARG:HD2	2.54	0.41
1:E:142:MET:O	1:E:150:ILE:N	2.48	0.41
1:E:231:THR:OG1	1:E:234:LYS:HB3	2.21	0.41
1:I:142:MET:HB3	1:I:150:ILE:HB	2.02	0.41
1:I:230:ALA:HA	1:I:231:THR:HA	1.79	0.41
1:A:142:MET:O	1:A:150:ILE:N	2.48	0.41
3:F:83:TYR:CB	3:F:85:LEU:HD13	2.51	0.41
3:J:36:SER:HG	3:J:71:PHE:HE2	1.66	0.41
1:A:195:TRP:CH2	3:B:126:PRO:HG3	2.56	0.41
2:C:260:GLY:HA2	2:C:263:THR:HG22	2.02	0.41
3:B:201:GLU:HG2	1:I:383:PRO:HG3	2.01	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:111:LEU:HD21	5:G:301:P1O:O6	2.21	0.41
2:K:49:LYS:CE	2:K:49:LYS:HA	2.50	0.41
3:F:115:PRO:O	3:F:119:VAL:HG22	2.20	0.41
3:J:83:TYR:CB	3:J:85:LEU:HD13	2.50	0.41
1:E:45:ARG:HB2	1:E:74:PHE:CD2	2.55	0.41
1:A:45:ARG:HB2	1:A:74:PHE:CD2	2.55	0.41
3:B:53:ASP:OD2	3:B:185:GLY:HA3	2.20	0.41
2:K:119:LEU:O	2:K:122:LEU:HD13	2.21	0.41
3:F:230:MET:HA	7:F:302:D10:H91	2.03	0.41
3:J:138:SER:O	3:J:138:SER:OG	2.35	0.41
1:E:313:ARG:HH11	1:E:329:VAL:HG22	1.86	0.41
1:I:313:ARG:HH11	1:I:329:VAL:HG22	1.86	0.41
2:G:107:LEU:HD11	2:G:137:TRP:HH2	1.86	0.41
2:G:114:THR:HG22	2:G:114:THR:O	2.21	0.41
2:K:111:LEU:HD21	5:K:301:P1O:O6	2.20	0.41
3:J:53:ASP:O	3:J:198:ARG:NH2	2.52	0.41
3:J:115:PRO:O	3:J:119:VAL:HG22	2.20	0.41
1:E:112:ARG:HG3	1:E:269:MET:HG3	2.03	0.41
1:E:292:ARG:NH1	1:E:414:MET:O	2.49	0.41
1:I:231:THR:OG1	1:I:234:LYS:HB3	2.21	0.41
1:A:215:ARG:CZ	1:A:227:LEU:HB3	2.51	0.41
1:A:281:THR:OG1	1:A:401:GLN:NE2	2.37	0.41
2:C:107:LEU:HD11	2:C:137:TRP:HH2	1.86	0.41
2:C:119:LEU:O	2:C:122:LEU:HD13	2.21	0.41
3:B:45:MET:HB2	3:B:67:VAL:HG21	2.03	0.41
3:B:210:LYS:O	6:B:301:PLC:O1P	2.38	0.41
2:K:154:GLU:HB2	3:J:42:MET:HE3	2.02	0.41
2:K:277:SER:HA	3:J:11:HIS:CD2	2.56	0.41
3:J:53:ASP:OD2	3:J:185:GLY:HA3	2.20	0.41
1:I:215:ARG:CZ	1:I:227:LEU:HB3	2.51	0.41
1:I:292:ARG:HH12	1:I:414:MET:C	2.23	0.41
1:A:231:THR:OG1	1:A:234:LYS:HB3	2.21	0.41
1:A:292:ARG:NH1	1:A:414:MET:O	2.49	0.41
2:C:114:THR:HG22	2:C:114:THR:O	2.21	0.41
3:B:104:ARG:HA	3:B:108:PHE:HB2	2.02	0.41
3:B:233:PHE:CE2	7:B:302:D10:H72	2.56	0.41
2:G:141:TYR:CE2	2:G:213:LEU:HD21	2.56	0.41
2:G:185:ILE:HG12	2:G:218:PHE:HA	2.03	0.41
2:G:196:LYS:HA	2:G:196:LYS:HD2	1.62	0.41
3:J:210:LYS:O	6:J:302:PLC:O1P	2.38	0.41
5:C:301:P1O:H7	5:C:301:P1O:H1	1.85	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:45:MET:HB2	3:J:67:VAL:HG21	2.03	0.41
3:J:100:GLU:O	3:J:104:ARG:HG2	2.21	0.41
3:J:233:PHE:CE2	7:J:303:D10:H72	2.56	0.41
1:A:383:PRO:HG3	3:F:201:GLU:HG2	2.03	0.40
2:K:193:ILE:H	2:K:193:ILE:HG13	1.55	0.40
1:E:45:ARG:HB3	1:E:388:ALA:HB3	2.03	0.40
1:E:70:LYS:HA	1:E:123:ASP:HA	2.03	0.40
1:I:72:HIS:HE1	1:I:404:GLN:NE2	2.14	0.40
1:A:101:LYS:HD2	1:A:101:LYS:HA	1.90	0.40
1:A:211:ILE:HD12	3:B:22:ASP:HB3	2.03	0.40
2:C:185:ILE:HG12	2:C:218:PHE:HA	2.03	0.40
3:B:100:GLU:O	3:B:104:ARG:HG2	2.21	0.40
2:G:119:LEU:O	2:G:122:LEU:HD13	2.21	0.40
2:K:260:GLY:HA2	2:K:263:THR:HG22	2.02	0.40
3:F:233:PHE:CE2	7:F:302:D10:H72	2.56	0.40
1:I:89:LEU:HD22	1:I:105:ILE:HD11	2.03	0.40
1:A:70:LYS:HA	1:A:123:ASP:HA	2.04	0.40
2:C:49:LYS:HA	2:C:49:LYS:NZ	2.37	0.40
2:G:49:LYS:HA	2:G:49:LYS:NZ	2.37	0.40
2:K:107:LEU:HD11	2:K:137:TRP:HH2	1.86	0.40
2:K:185:ILE:HG12	2:K:218:PHE:HA	2.03	0.40
3:J:104:ARG:HA	3:J:108:PHE:HB2	2.02	0.40
1:A:313:ARG:HH11	1:A:329:VAL:HG22	1.86	0.40
3:B:53:ASP:OD1	3:B:54:TRP:N	2.54	0.40
3:B:142:LEU:HD13	5:J:301:P1O:H42	2.04	0.40
2:G:260:GLY:HA2	2:G:263:THR:HG22	2.02	0.40
2:K:141:TYR:CE2	2:K:213:LEU:HD21	2.56	0.40
3:J:233:PHE:CD2	7:J:303:D10:C5	3.01	0.40
1:A:72:HIS:HE1	1:A:404:GLN:NE2	2.14	0.40
2:G:112:TRP:CH2	5:G:302:P1O:H1	2.33	0.40
2:G:277:SER:HA	3:F:11:HIS:CD2	2.56	0.40
2:K:114:THR:HG22	2:K:114:THR:O	2.21	0.40
3:F:45:MET:HB2	3:F:67:VAL:HG21	2.03	0.40
1:E:313:ARG:HD3	1:E:353:PRO:HG3	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	380/414 (92%)	361 (95%)	19 (5%)	0	100	100
1	E	380/414 (92%)	360 (95%)	20 (5%)	0	100	100
1	I	380/414 (92%)	361 (95%)	19 (5%)	0	100	100
2	C	139/260 (54%)	133 (96%)	5 (4%)	1 (1%)	22	59
2	G	139/260 (54%)	133 (96%)	5 (4%)	1 (1%)	22	59
2	K	139/260 (54%)	132 (95%)	6 (4%)	1 (1%)	22	59
3	B	239/247 (97%)	222 (93%)	16 (7%)	1 (0%)	34	69
3	F	239/247 (97%)	222 (93%)	16 (7%)	1 (0%)	34	69
3	J	239/247 (97%)	222 (93%)	16 (7%)	1 (0%)	34	69
All	All	2274/2763 (82%)	2146 (94%)	122 (5%)	6 (0%)	44	74

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	277	SER
3	B	246	SER
2	G	277	SER
2	K	277	SER
3	F	246	SER
3	J	246	SER

### 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	323/345 (94%)	320 (99%)	3 (1%)	78	88
1	E	323/345 (94%)	320 (99%)	3 (1%)	78	88
1	I	323/345 (94%)	320 (99%)	3 (1%)	78	88
2	C	121/212 (57%)	115 (95%)	6 (5%)	24	55
2	G	121/212 (57%)	115 (95%)	6 (5%)	24	55
2	K	121/212 (57%)	115 (95%)	6 (5%)	24	55
3	B	206/210 (98%)	203 (98%)	3 (2%)	65	81
3	F	206/210 (98%)	203 (98%)	3 (2%)	65	81
3	J	206/210 (98%)	203 (98%)	3 (2%)	65	81
All	All	1950/2301 (85%)	1914 (98%)	36 (2%)	61	77

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	HIS
1	A	36	LYS
1	A	251	MET
2	C	48	LYS
2	C	49	LYS
2	C	193	ILE
2	C	196	LYS
2	C	198	ARG
2	C	204	LYS
3	B	241	GLU
3	B	243	PHE
3	B	244	LEU
2	G	48	LYS
2	G	49	LYS
2	G	193	ILE
2	G	196	LYS
2	G	198	ARG
2	G	204	LYS
2	K	48	LYS
2	K	49	LYS
2	K	193	ILE
2	K	196	LYS
2	K	198	ARG
2	K	204	LYS
3	F	241	GLU
3	F	243	PHE

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
3	F	244	LEU
3	J	241	GLU
3	J	243	PHE
3	J	244	LEU
1	E	33	HIS
1	E	36	LYS
1	E	251	MET
1	I	33	HIS
1	I	36	LYS
1	I	251	MET

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

Mol	Chain	Res	Type
1	A	48	HIS
1	A	404	GLN
2	C	131	ASN
2	C	134	HIS
2	G	131	ASN
2	G	134	HIS
2	K	131	ASN
2	K	134	HIS
3	J	187	ASN
1	E	48	HIS
1	E	404	GLN
1	I	72	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

Of 26 ligands modelled in this entry, 5 are monoatomic - leaving 21 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	P1O	K	301	-	37,37,37	1.11	2 (5%)	43,45,45	1.11	3 (6%)
6	PLC	J	302	-	41,41,41	0.83	0	47,49,49	0.66	1 (2%)
5	P1O	G	301	-	37,37,37	1.10	2 (5%)	43,45,45	1.11	3 (6%)
5	P1O	B	305	-	37,37,37	0.83	0	43,45,45	0.70	1 (2%)
5	P1O	C	301	-	37,37,37	1.10	2 (5%)	43,45,45	1.11	3 (6%)
7	D10	F	303	-	9,9,9	0.21	0	8,8,8	0.55	0
7	D10	J	305	-	9,9,9	0.22	0	8,8,8	0.54	0
7	D10	J	304	-	9,9,9	0.22	0	8,8,8	0.56	0
7	D10	B	304	-	9,9,9	0.22	0	8,8,8	0.55	0
6	PLC	F	301	-	41,41,41	0.83	0	47,49,49	0.66	1 (2%)
5	P1O	J	301	-	37,37,37	0.83	0	43,45,45	0.70	1 (2%)
5	P1O	G	302	-	37,37,37	1.12	2 (5%)	43,45,45	1.11	3 (6%)
5	P1O	K	302	-	37,37,37	1.12	2 (5%)	43,45,45	1.12	3 (6%)
7	D10	F	302	-	9,9,9	0.21	0	8,8,8	0.56	0
7	D10	B	303	-	9,9,9	0.21	0	8,8,8	0.55	0
5	P1O	C	302	-	37,37,37	1.11	2 (5%)	43,45,45	1.12	3 (6%)
7	D10	F	304	-	9,9,9	0.22	0	8,8,8	0.55	0
7	D10	B	302	-	9,9,9	0.21	0	8,8,8	0.56	0
5	P1O	F	305	-	37,37,37	0.83	0	43,45,45	0.70	1 (2%)
6	PLC	B	301	-	41,41,41	0.83	0	47,49,49	0.66	1 (2%)
7	D10	J	303	-	9,9,9	0.21	0	8,8,8	0.56	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
5	P1O	K	301	-	-	19/41/41/41	-

*Continued on next page...*

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PLC	J	302	-	-	12/45/45/45	-
5	P1O	G	301	-	-	19/41/41/41	-
5	P1O	B	305	-	-	15/41/41/41	-
5	P1O	C	301	-	-	18/41/41/41	-
7	D10	F	303	-	-	2/7/7/7	-
7	D10	J	305	-	-	6/7/7/7	-
7	D10	J	304	-	-	2/7/7/7	-
7	D10	B	304	-	-	6/7/7/7	-
6	PLC	F	301	-	-	12/45/45/45	-
5	P1O	J	301	-	-	15/41/41/41	-
5	P1O	G	302	-	-	26/41/41/41	-
5	P1O	K	302	-	-	26/41/41/41	-
7	D10	F	302	-	-	0/7/7/7	-
7	D10	B	303	-	-	2/7/7/7	-
5	P1O	C	302	-	-	26/41/41/41	-
7	D10	F	304	-	-	6/7/7/7	-
7	D10	B	302	-	-	0/7/7/7	-
5	P1O	F	305	-	-	15/41/41/41	-
6	PLC	B	301	-	-	12/45/45/45	-
7	D10	J	303	-	-	0/7/7/7	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	K	301	P1O	O5-C9	4.28	1.45	1.33
5	C	301	P1O	O5-C9	4.28	1.45	1.33
5	K	302	P1O	O5-C9	4.25	1.45	1.33
5	G	301	P1O	O5-C9	4.25	1.45	1.33
5	G	302	P1O	O5-C9	4.24	1.45	1.33
5	C	302	P1O	O5-C9	4.23	1.45	1.33
5	G	302	P1O	O7-C19	4.16	1.46	1.34
5	K	302	P1O	O7-C19	4.14	1.46	1.34
5	C	302	P1O	O7-C19	4.12	1.45	1.34
5	K	301	P1O	O7-C19	4.08	1.45	1.34
5	G	301	P1O	O7-C19	4.05	1.45	1.34
5	C	301	P1O	O7-C19	4.02	1.45	1.34

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	302	P1O	O7-C19-C20	4.18	120.51	111.50
5	C	302	P1O	O7-C19-C20	4.18	120.50	111.50
5	G	301	P1O	O7-C19-C20	4.17	120.49	111.50
5	G	302	P1O	O7-C19-C20	4.16	120.47	111.50
5	C	301	P1O	O7-C19-C20	4.15	120.44	111.50
5	K	301	P1O	O7-C19-C20	4.15	120.44	111.50
5	C	301	P1O	O5-C9-C10	2.67	120.28	111.91
5	K	301	P1O	O5-C9-C10	2.67	120.28	111.91
5	G	301	P1O	O5-C9-C10	2.66	120.27	111.91
5	C	302	P1O	O5-C9-C10	2.62	120.12	111.91
5	K	302	P1O	O5-C9-C10	2.61	120.11	111.91
5	G	302	P1O	O5-C9-C10	2.59	120.05	111.91
5	F	305	P1O	O7-C19-C20	2.42	116.72	111.50
5	B	305	P1O	O7-C19-C20	2.40	116.68	111.50
5	J	301	P1O	O7-C19-C20	2.39	116.66	111.50
5	C	302	P1O	C7-O7-C19	-2.39	111.91	117.79
5	G	302	P1O	C7-O7-C19	-2.37	111.96	117.79
5	K	302	P1O	C7-O7-C19	-2.37	111.96	117.79
5	K	301	P1O	C7-O7-C19	-2.24	112.28	117.79
5	G	301	P1O	C7-O7-C19	-2.23	112.29	117.79
5	C	301	P1O	C7-O7-C19	-2.22	112.33	117.79
6	J	302	PLC	O2-C2-C1	2.20	116.37	108.40
6	F	301	PLC	O2-C2-C1	2.18	116.28	108.40
6	B	301	PLC	O2-C2-C1	2.17	116.27	108.40

There are no chirality outliers.

All (239) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	301	P1O	C1-O3-P1-O1
5	C	301	P1O	C2-C1-O3-P1
5	C	301	P1O	O3-C1-C2-N1
5	C	301	P1O	O6-C9-O5-C8
5	C	301	P1O	C10-C9-O5-C8
5	C	301	P1O	O8-C19-O7-C7
5	C	302	P1O	C1-O3-P1-O1
5	C	302	P1O	C1-O3-P1-O2
5	C	302	P1O	C6-O4-P1-O1
5	C	302	P1O	C6-O4-P1-O2
5	B	305	P1O	C1-O3-P1-O1
5	B	305	P1O	C1-O3-P1-O2
5	B	305	P1O	C6-O4-P1-O1
5	B	305	P1O	C6-O4-P1-O2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
5	B	305	P1O	C20-C19-O7-C7
5	G	301	P1O	C1-O3-P1-O1
5	G	301	P1O	C2-C1-O3-P1
5	G	301	P1O	O3-C1-C2-N1
5	G	301	P1O	O6-C9-O5-C8
5	G	301	P1O	C10-C9-O5-C8
5	G	301	P1O	O8-C19-O7-C7
5	G	302	P1O	C1-O3-P1-O1
5	G	302	P1O	C1-O3-P1-O2
5	G	302	P1O	C6-O4-P1-O1
5	G	302	P1O	C6-O4-P1-O2
5	K	301	P1O	C1-O3-P1-O1
5	K	301	P1O	C2-C1-O3-P1
5	K	301	P1O	O3-C1-C2-N1
5	K	301	P1O	O6-C9-O5-C8
5	K	301	P1O	C10-C9-O5-C8
5	K	301	P1O	O8-C19-O7-C7
5	K	302	P1O	C1-O3-P1-O1
5	K	302	P1O	C1-O3-P1-O2
5	K	302	P1O	C6-O4-P1-O1
5	K	302	P1O	C6-O4-P1-O2
5	F	305	P1O	C1-O3-P1-O1
5	F	305	P1O	C1-O3-P1-O2
5	F	305	P1O	C6-O4-P1-O1
5	F	305	P1O	C6-O4-P1-O2
5	F	305	P1O	C20-C19-O7-C7
5	J	301	P1O	C1-O3-P1-O1
5	J	301	P1O	C1-O3-P1-O2
5	J	301	P1O	C6-O4-P1-O1
5	J	301	P1O	C6-O4-P1-O2
5	J	301	P1O	C20-C19-O7-C7
6	B	301	PLC	C1-C2-O2-C'
6	B	301	PLC	C1'-C'-O2-C2
6	B	301	PLC	C1-O3P-P-O2P
6	F	301	PLC	C1-C2-O2-C'
6	F	301	PLC	C1'-C'-O2-C2
6	F	301	PLC	C1-O3P-P-O2P
6	J	302	PLC	C1-C2-O2-C'
6	J	302	PLC	C1'-C'-O2-C2
6	J	302	PLC	C1-O3P-P-O2P
5	B	305	P1O	O8-C19-O7-C7
5	F	305	P1O	O8-C19-O7-C7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
5	J	301	P1O	O8-C19-O7-C7
6	B	301	PLC	O'-C'-O2-C2
6	F	301	PLC	O'-C'-O2-C2
6	J	302	PLC	O'-C'-O2-C2
5	C	301	P1O	C20-C19-O7-C7
5	G	301	P1O	C20-C19-O7-C7
5	K	301	P1O	C20-C19-O7-C7
6	B	301	PLC	OB-CB-O3-C3
6	F	301	PLC	OB-CB-O3-C3
6	J	302	PLC	OB-CB-O3-C3
6	B	301	PLC	C1B-CB-O3-C3
6	F	301	PLC	C1B-CB-O3-C3
6	J	302	PLC	C1B-CB-O3-C3
5	B	305	P1O	C10-C9-O5-C8
5	F	305	P1O	C10-C9-O5-C8
5	J	301	P1O	C10-C9-O5-C8
5	C	301	P1O	C9-C10-C11-C12
5	G	301	P1O	C9-C10-C11-C12
5	K	301	P1O	C9-C10-C11-C12
5	B	305	P1O	O6-C9-O5-C8
5	F	305	P1O	O6-C9-O5-C8
5	J	301	P1O	O6-C9-O5-C8
5	C	302	P1O	C10-C9-O5-C8
5	G	302	P1O	C10-C9-O5-C8
5	K	302	P1O	C10-C9-O5-C8
5	C	302	P1O	C7-C6-O4-P1
5	G	302	P1O	C7-C6-O4-P1
5	K	302	P1O	C7-C6-O4-P1
5	C	301	P1O	C1-O3-P1-O4
5	C	301	P1O	C6-O4-P1-O3
5	C	302	P1O	C1-O3-P1-O4
5	C	302	P1O	C6-O4-P1-O3
5	B	305	P1O	C1-O3-P1-O4
5	B	305	P1O	C6-O4-P1-O3
5	G	301	P1O	C1-O3-P1-O4
5	G	301	P1O	C6-O4-P1-O3
5	G	302	P1O	C1-O3-P1-O4
5	G	302	P1O	C6-O4-P1-O3
5	K	301	P1O	C1-O3-P1-O4
5	K	301	P1O	C6-O4-P1-O3
5	K	302	P1O	C1-O3-P1-O4
5	K	302	P1O	C6-O4-P1-O3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
5	F	305	P1O	C1-O3-P1-O4
5	F	305	P1O	C6-O4-P1-O3
5	J	301	P1O	C1-O3-P1-O4
5	J	301	P1O	C6-O4-P1-O3
5	C	301	P1O	C21-C22-C23-C24
5	C	302	P1O	C13-C14-C15-C16
5	G	301	P1O	C21-C22-C23-C24
5	G	302	P1O	C13-C14-C15-C16
5	K	301	P1O	C21-C22-C23-C24
5	K	302	P1O	C13-C14-C15-C16
5	C	302	P1O	O6-C9-O5-C8
5	G	302	P1O	O6-C9-O5-C8
5	K	302	P1O	O6-C9-O5-C8
5	G	302	P1O	C24-C25-C26-C27
5	K	302	P1O	C24-C25-C26-C27
7	B	304	D10	C5-C6-C7-C8
7	F	304	D10	C5-C6-C7-C8
7	J	305	D10	C5-C6-C7-C8
5	C	302	P1O	C24-C25-C26-C27
5	C	302	P1O	C21-C22-C23-C24
5	G	302	P1O	C21-C22-C23-C24
5	K	302	P1O	C21-C22-C23-C24
5	C	302	P1O	C12-C13-C14-C15
5	G	302	P1O	C12-C13-C14-C15
5	K	302	P1O	C12-C13-C14-C15
5	K	302	P1O	C20-C19-O7-C7
5	C	302	P1O	C10-C11-C12-C13
5	G	302	P1O	C10-C11-C12-C13
5	K	302	P1O	C10-C11-C12-C13
6	B	301	PLC	C5B-C6B-C7B-C8B
6	J	302	PLC	C5B-C6B-C7B-C8B
6	F	301	PLC	C5B-C6B-C7B-C8B
5	C	302	P1O	C20-C19-O7-C7
5	G	302	P1O	C20-C19-O7-C7
5	C	302	P1O	O8-C19-O7-C7
5	G	302	P1O	O8-C19-O7-C7
5	K	302	P1O	O8-C19-O7-C7
7	B	303	D10	C5-C6-C7-C8
7	B	304	D10	C4-C5-C6-C7
7	F	303	D10	C5-C6-C7-C8
7	F	304	D10	C4-C5-C6-C7
7	J	304	D10	C5-C6-C7-C8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
7	J	305	D10	C4-C5-C6-C7
6	B	301	PLC	C1-O3P-P-O4P
6	F	301	PLC	C1-O3P-P-O4P
6	J	302	PLC	C1-O3P-P-O4P
5	K	301	P1O	C22-C23-C24-C25
5	C	301	P1O	C22-C23-C24-C25
5	G	301	P1O	C22-C23-C24-C25
7	F	304	D10	C2-C3-C4-C5
7	J	305	D10	C2-C3-C4-C5
7	B	304	D10	C2-C3-C4-C5
5	B	305	P1O	C6-C7-O7-C19
5	F	305	P1O	C6-C7-O7-C19
5	J	301	P1O	C6-C7-O7-C19
7	J	305	D10	C6-C7-C8-C9
7	B	304	D10	C6-C7-C8-C9
7	F	304	D10	C6-C7-C8-C9
5	C	302	P1O	O4-C6-C7-C8
5	G	302	P1O	O4-C6-C7-C8
5	K	302	P1O	O4-C6-C7-C8
5	C	302	P1O	C19-C20-C21-C22
5	G	302	P1O	C19-C20-C21-C22
5	K	302	P1O	C19-C20-C21-C22
5	C	302	P1O	C15-C16-C17-C18
5	G	302	P1O	C15-C16-C17-C18
5	K	302	P1O	C15-C16-C17-C18
7	B	304	D10	C3-C4-C5-C6
7	F	304	D10	C3-C4-C5-C6
7	J	305	D10	C3-C4-C5-C6
5	C	302	P1O	C14-C15-C16-C17
5	C	302	P1O	C22-C23-C24-C25
5	G	302	P1O	C14-C15-C16-C17
5	K	302	P1O	C14-C15-C16-C17
5	G	301	P1O	C11-C12-C13-C14
5	G	302	P1O	C22-C23-C24-C25
5	K	302	P1O	C22-C23-C24-C25
5	C	301	P1O	C11-C12-C13-C14
5	K	301	P1O	C11-C12-C13-C14
5	C	302	P1O	O4-C6-C7-O7
5	G	302	P1O	O4-C6-C7-O7
5	K	302	P1O	O4-C6-C7-O7
5	C	302	P1O	O7-C7-C8-O5
5	G	302	P1O	O7-C7-C8-O5

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
5	K	302	P1O	O7-C7-C8-O5
6	F	301	PLC	C2B-C3B-C4B-C5B
5	C	301	P1O	C6-O4-P1-O2
5	G	301	P1O	C6-O4-P1-O2
5	K	301	P1O	C6-O4-P1-O2
6	J	302	PLC	C2B-C3B-C4B-C5B
6	B	301	PLC	C2B-C3B-C4B-C5B
6	B	301	PLC	O4P-C4-C5-N
6	F	301	PLC	O4P-C4-C5-N
6	J	302	PLC	O4P-C4-C5-N
5	G	301	P1O	C24-C25-C26-C27
5	C	301	P1O	C24-C25-C26-C27
5	K	301	P1O	C24-C25-C26-C27
5	C	302	P1O	C6-C7-C8-O5
5	G	302	P1O	C6-C7-C8-O5
5	K	302	P1O	C6-C7-C8-O5
7	B	304	D10	C7-C8-C9-C10
7	F	304	D10	C7-C8-C9-C10
7	J	305	D10	C7-C8-C9-C10
5	G	302	P1O	C23-C24-C25-C26
5	K	302	P1O	C23-C24-C25-C26
5	C	302	P1O	C23-C24-C25-C26
6	B	301	PLC	C4B-C5B-C6B-C7B
6	J	302	PLC	C4B-C5B-C6B-C7B
6	F	301	PLC	C4B-C5B-C6B-C7B
5	K	302	P1O	C9-C10-C11-C12
5	G	302	P1O	C9-C10-C11-C12
5	B	305	P1O	O7-C19-C20-C21
5	J	301	P1O	O7-C19-C20-C21
5	C	302	P1O	C9-C10-C11-C12
5	F	305	P1O	C11-C10-C9-O5
5	F	305	P1O	O7-C19-C20-C21
5	J	301	P1O	C11-C10-C9-O5
5	B	305	P1O	C11-C10-C9-O5
7	B	303	D10	C7-C8-C9-C10
7	F	303	D10	C7-C8-C9-C10
7	J	304	D10	C7-C8-C9-C10
5	B	305	P1O	O8-C19-C20-C21
5	F	305	P1O	O8-C19-C20-C21
5	J	301	P1O	O8-C19-C20-C21
5	G	301	P1O	C10-C11-C12-C13
5	C	301	P1O	C10-C11-C12-C13

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
5	K	301	P1O	C10-C11-C12-C13
5	C	301	P1O	C7-C6-O4-P1
5	G	301	P1O	C7-C6-O4-P1
5	K	301	P1O	C7-C6-O4-P1
5	F	305	P1O	C11-C10-C9-O6
5	J	301	P1O	C11-C10-C9-O6
6	B	301	PLC	C1-O3P-P-O1P
6	F	301	PLC	C1-O3P-P-O1P
6	J	302	PLC	C1-O3P-P-O1P
5	B	305	P1O	C11-C10-C9-O6
5	C	301	P1O	C11-C10-C9-O5
5	G	301	P1O	C11-C10-C9-O5
5	K	301	P1O	C11-C10-C9-O5
5	G	301	P1O	C11-C10-C9-O6
5	K	301	P1O	C11-C10-C9-O6

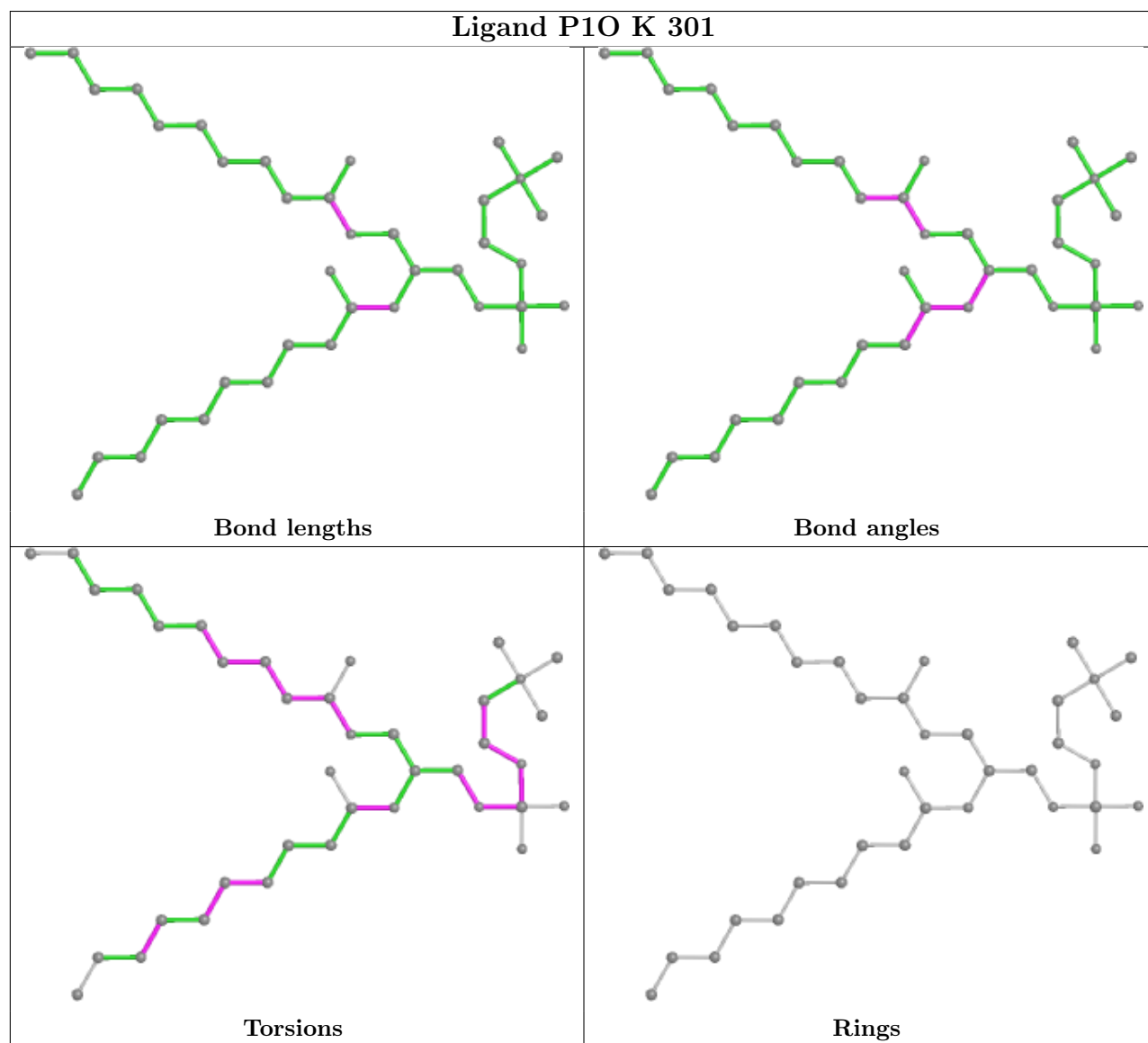
There are no ring outliers.

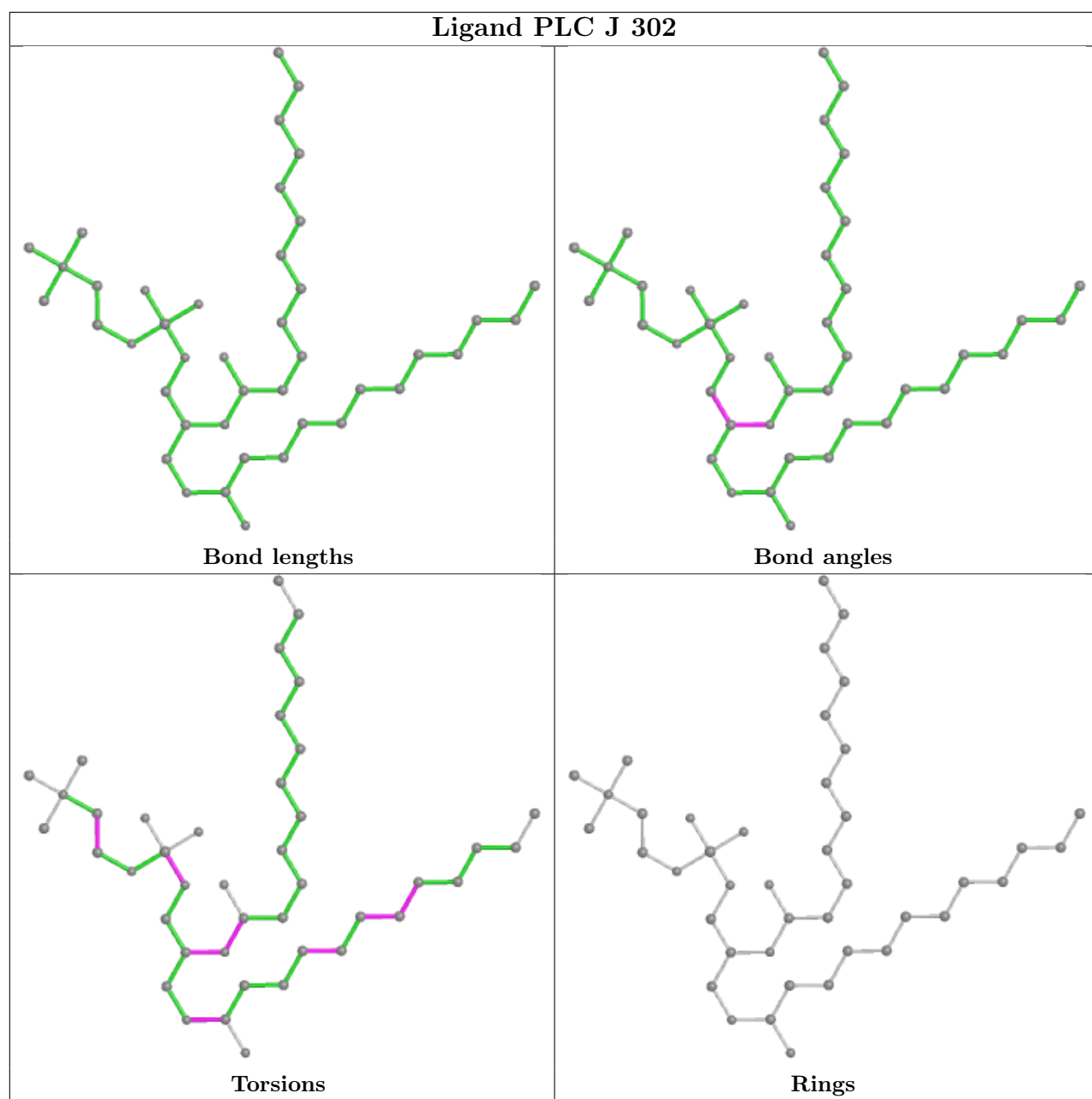
18 monomers are involved in 162 short contacts:

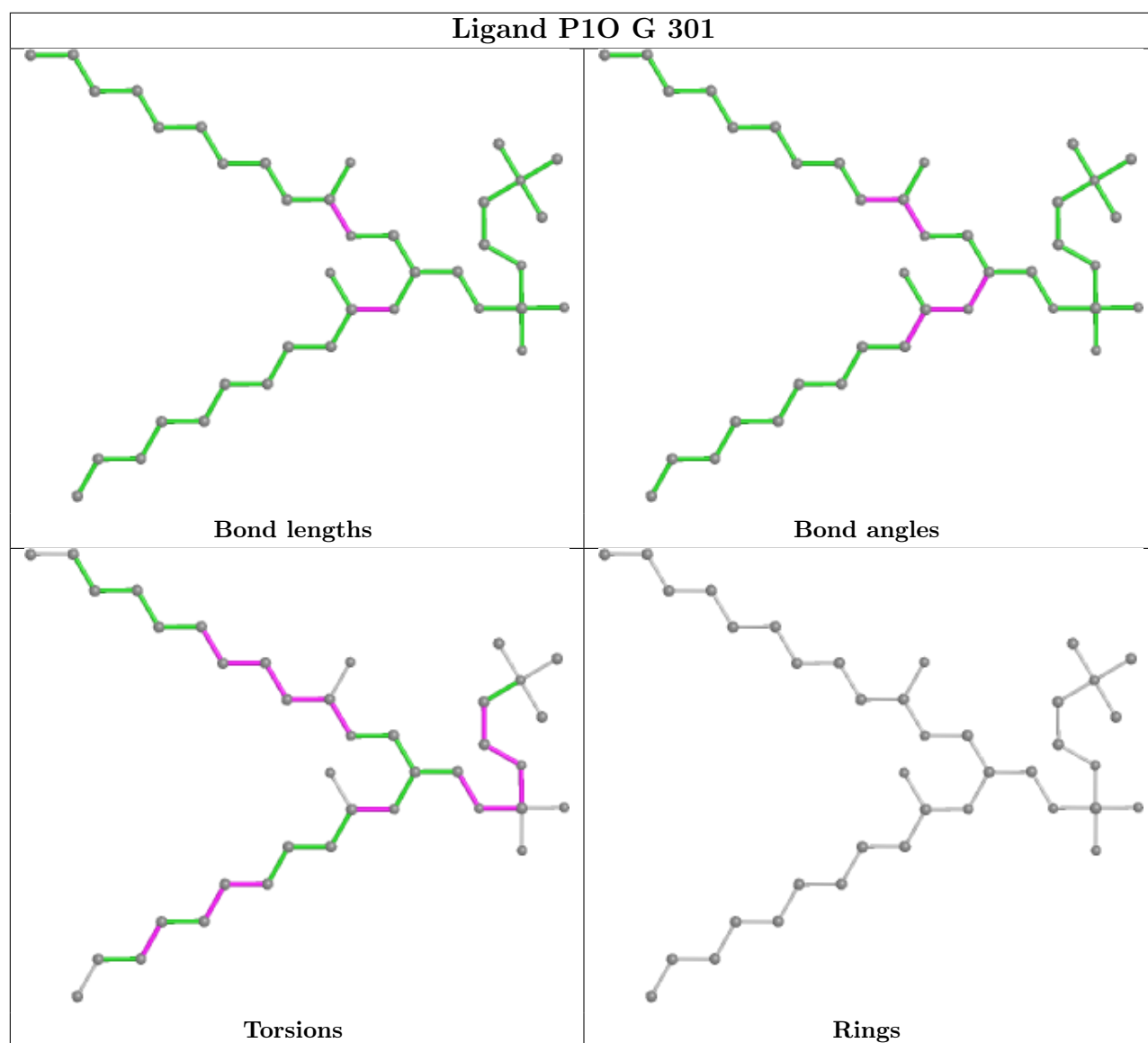
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	K	301	P1O	15	0
6	J	302	PLC	5	0
5	G	301	P1O	14	0
5	B	305	P1O	4	0
5	C	301	P1O	15	0
7	F	303	D10	2	0
7	J	304	D10	2	0
6	F	301	PLC	5	0
5	J	301	P1O	5	0
5	G	302	P1O	20	0
5	K	302	P1O	20	0
7	F	302	D10	9	0
7	B	303	D10	2	0
5	C	302	P1O	19	0
7	B	302	D10	8	0
5	F	305	P1O	4	0
6	B	301	PLC	5	0
7	J	303	D10	8	0

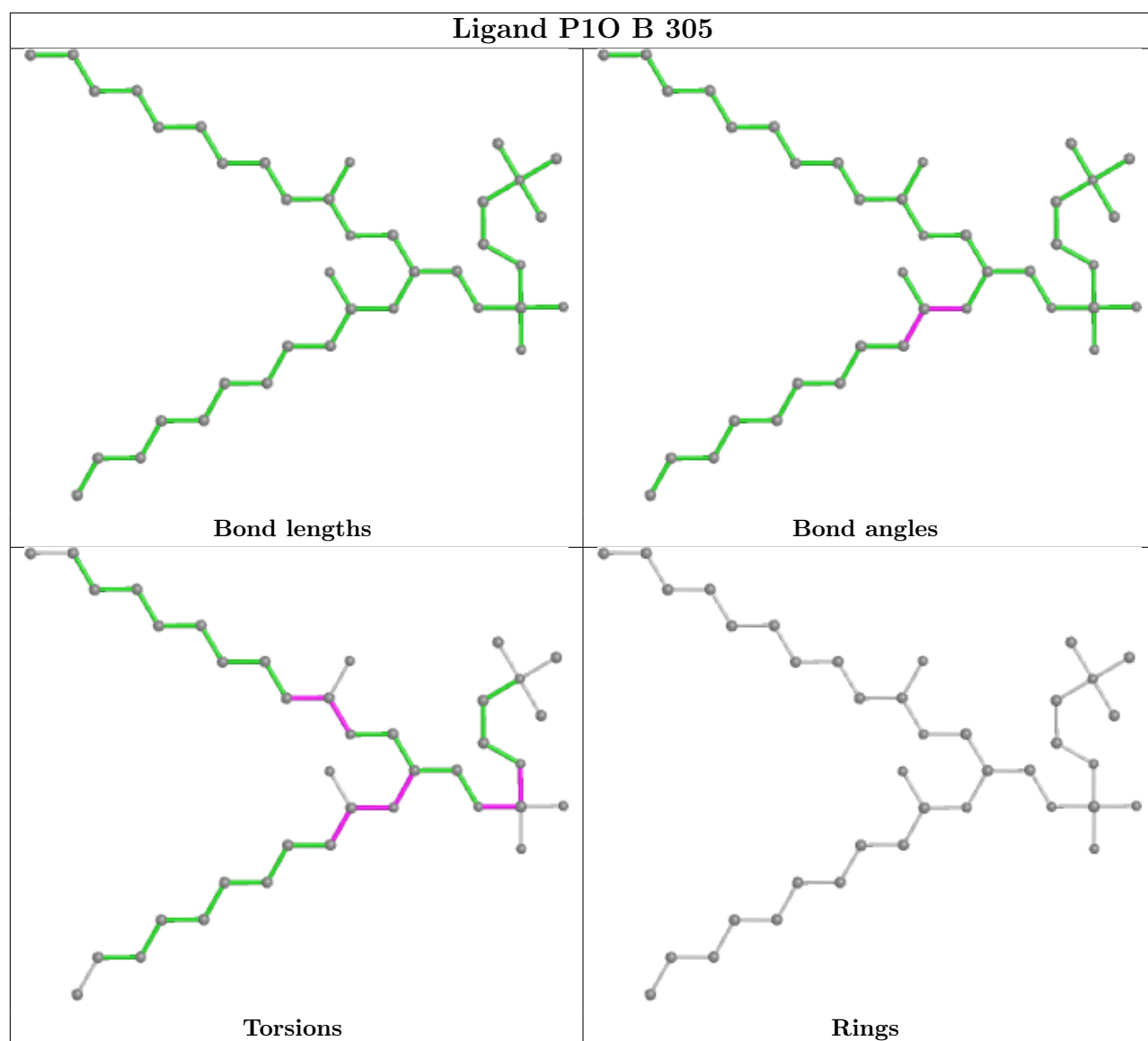
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

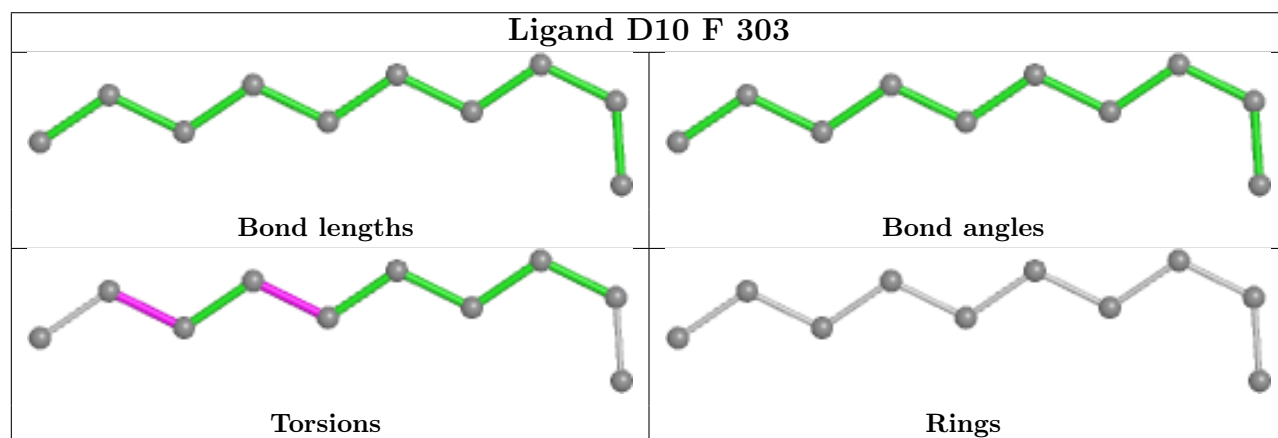
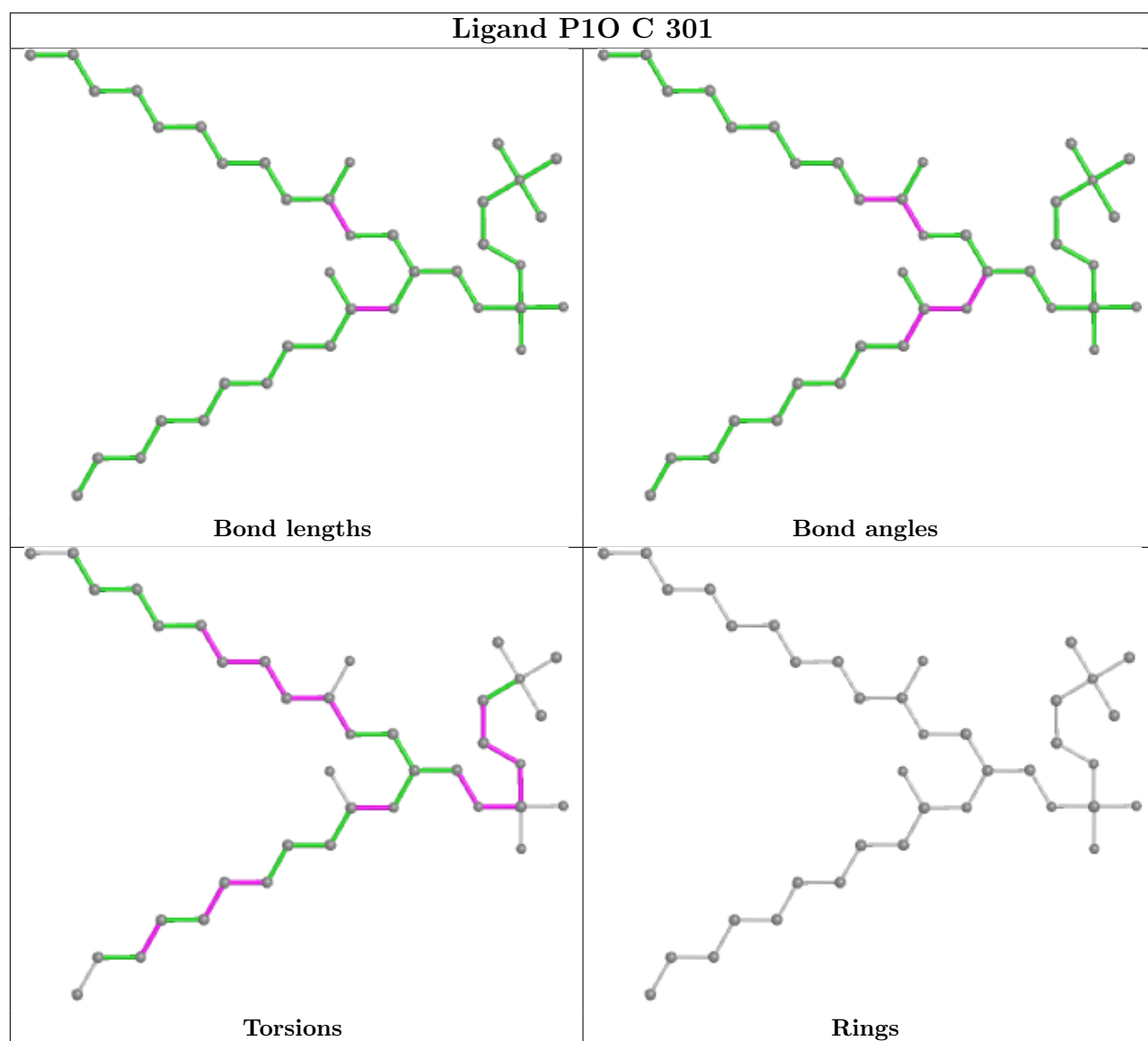
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.

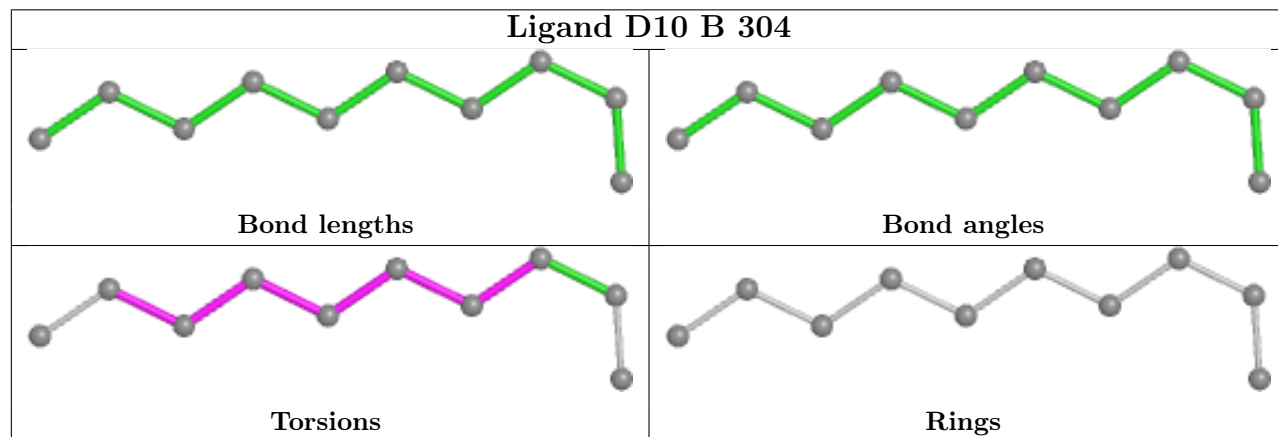
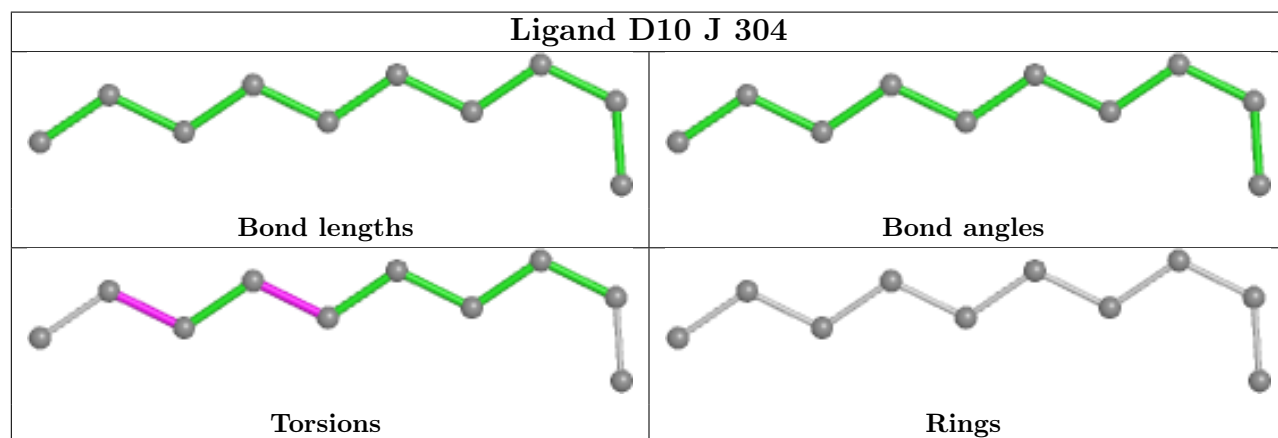
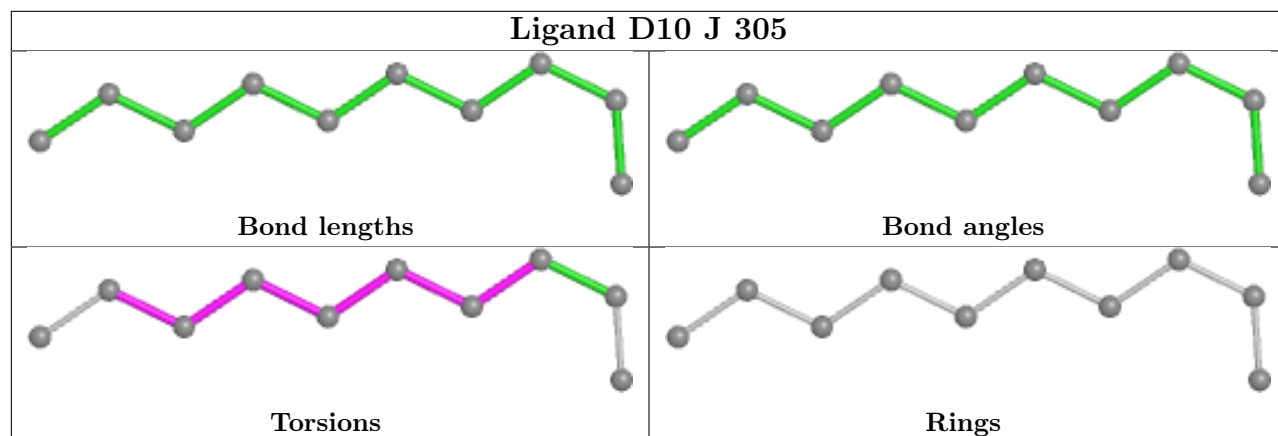




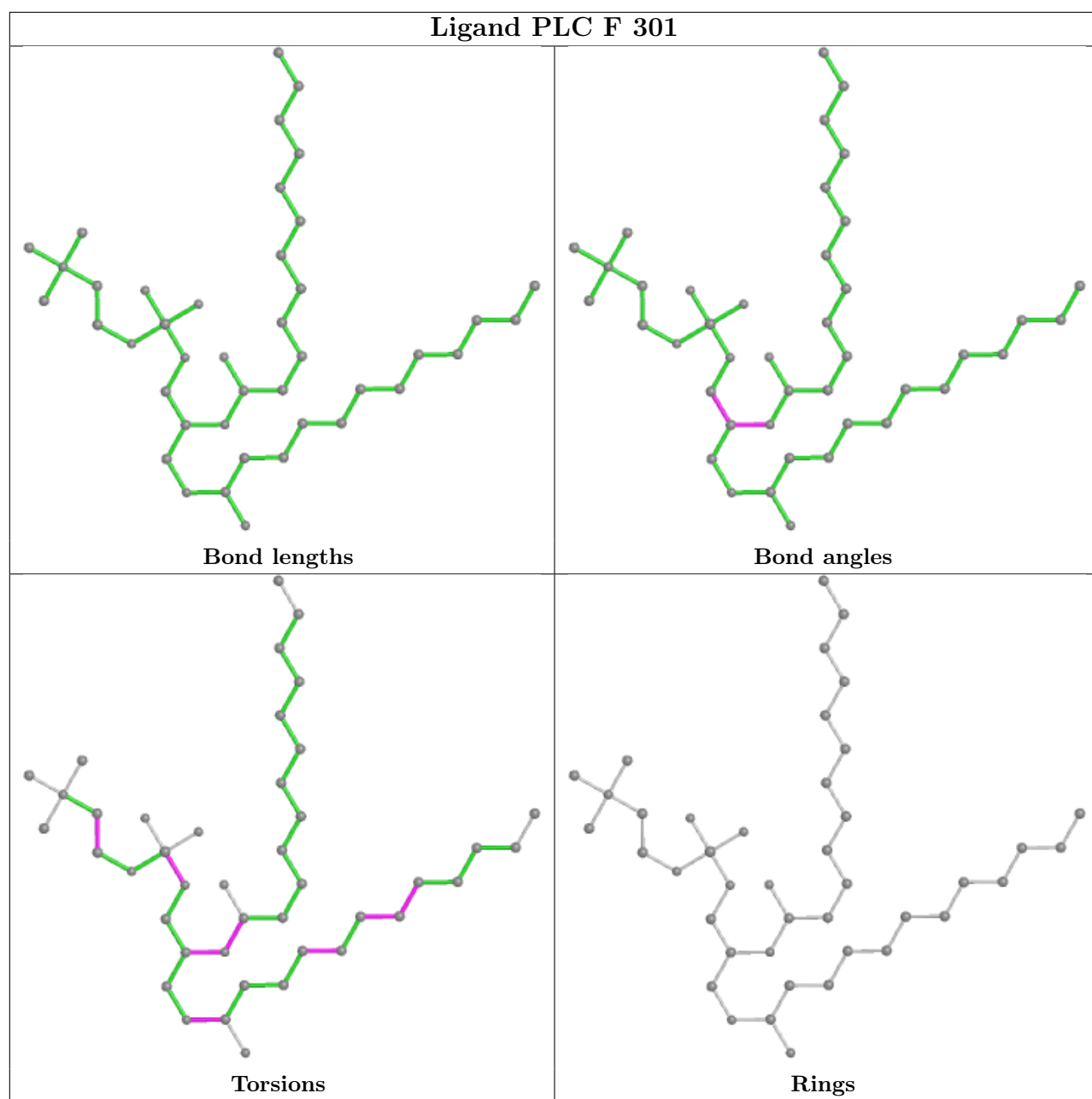


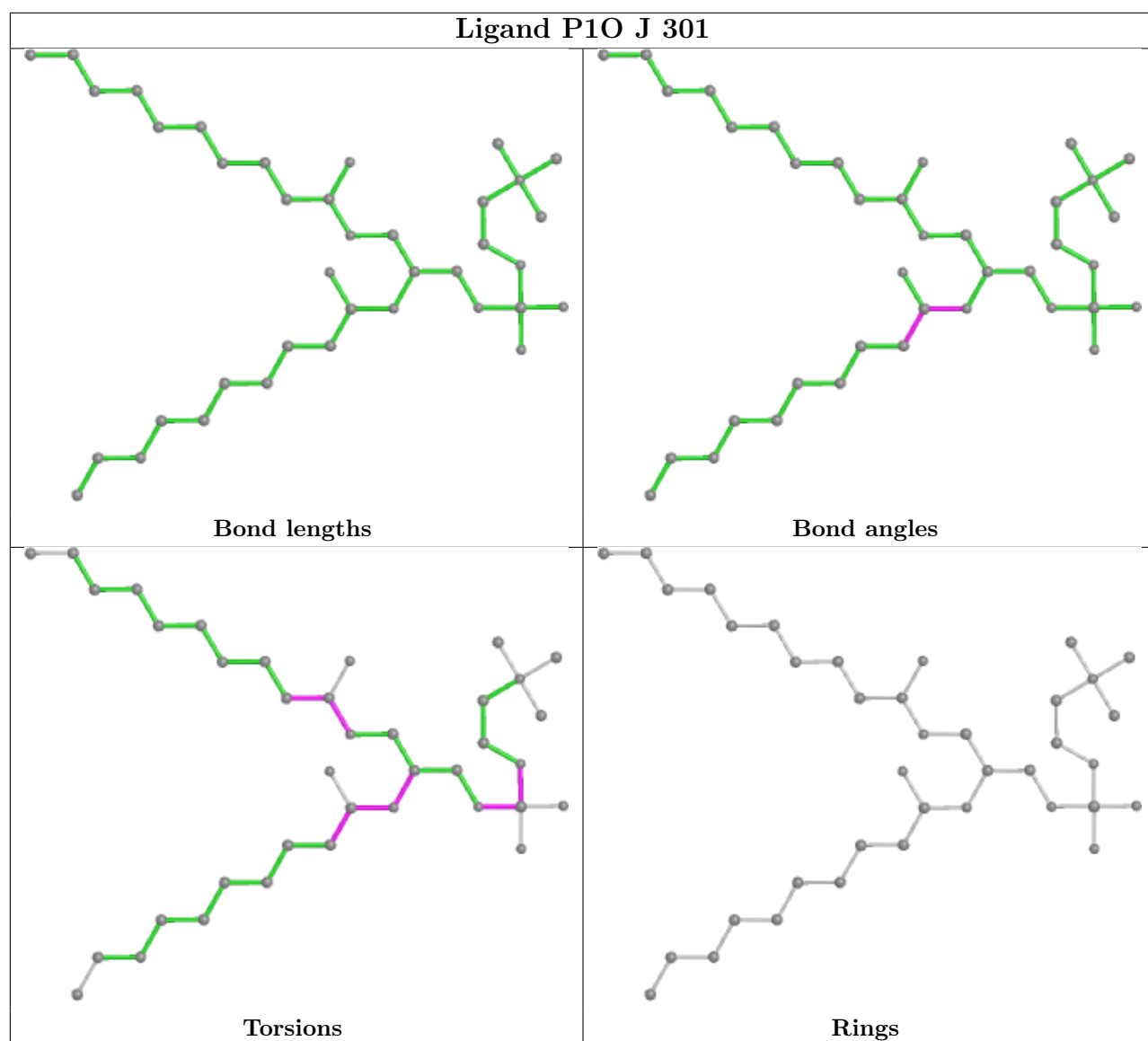


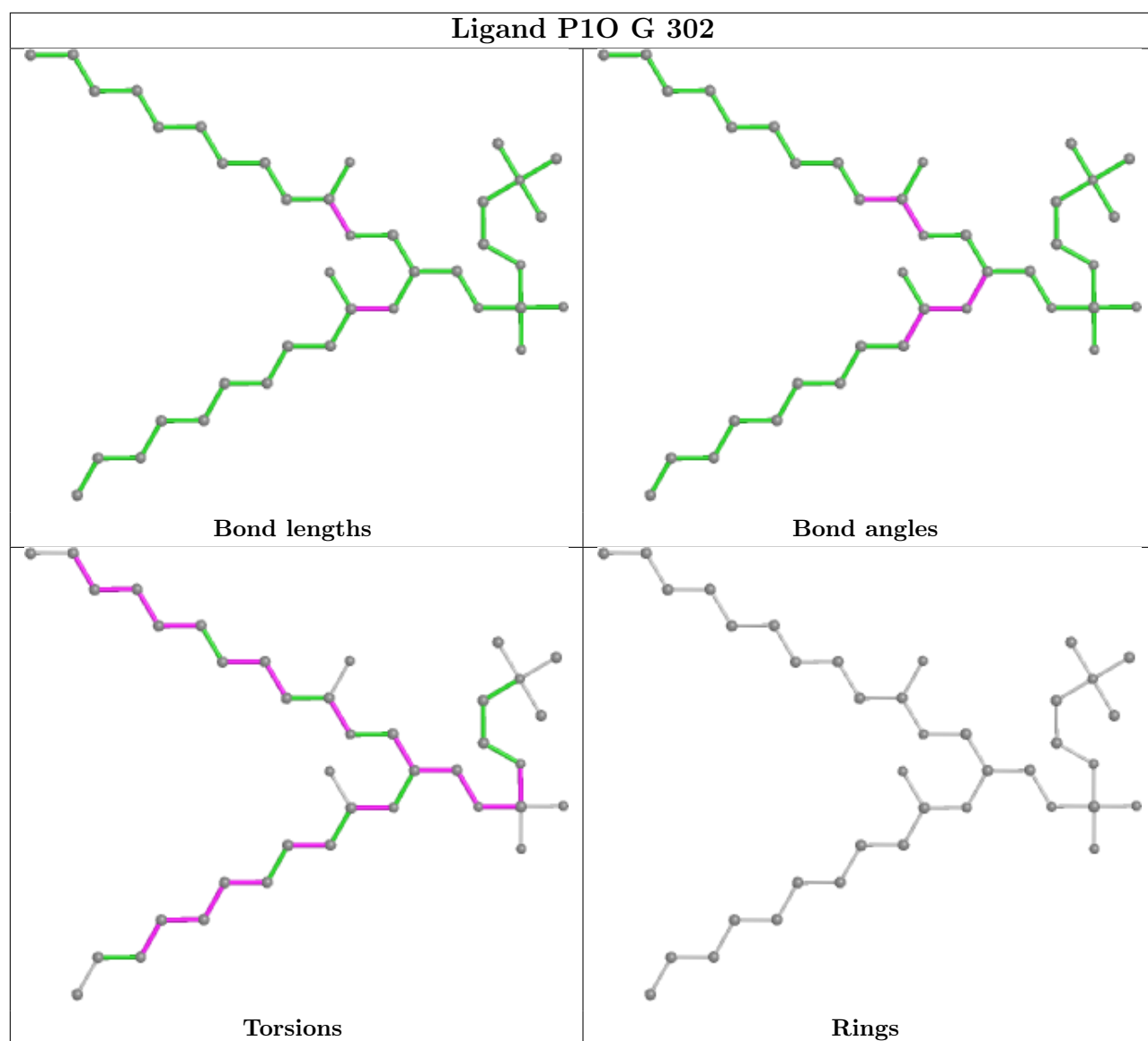


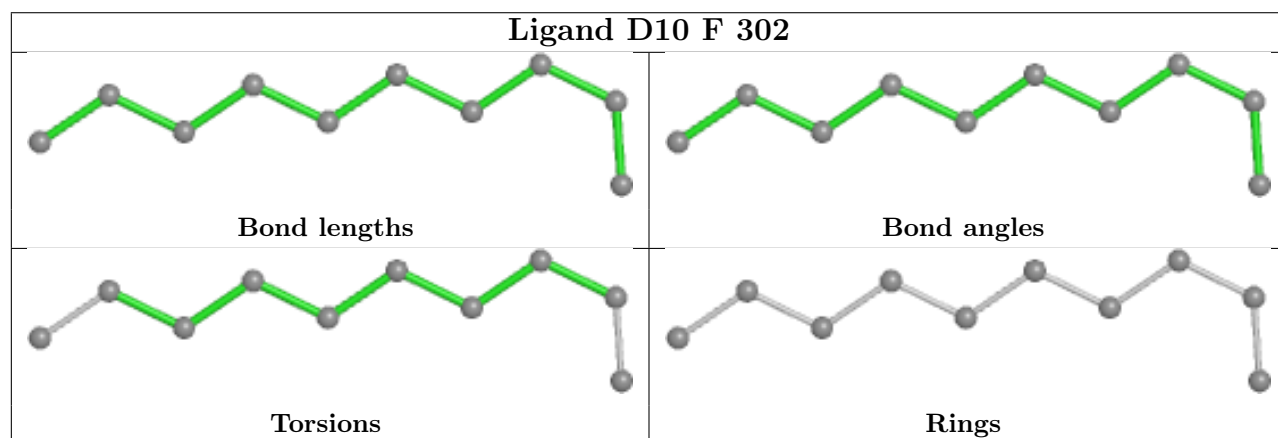
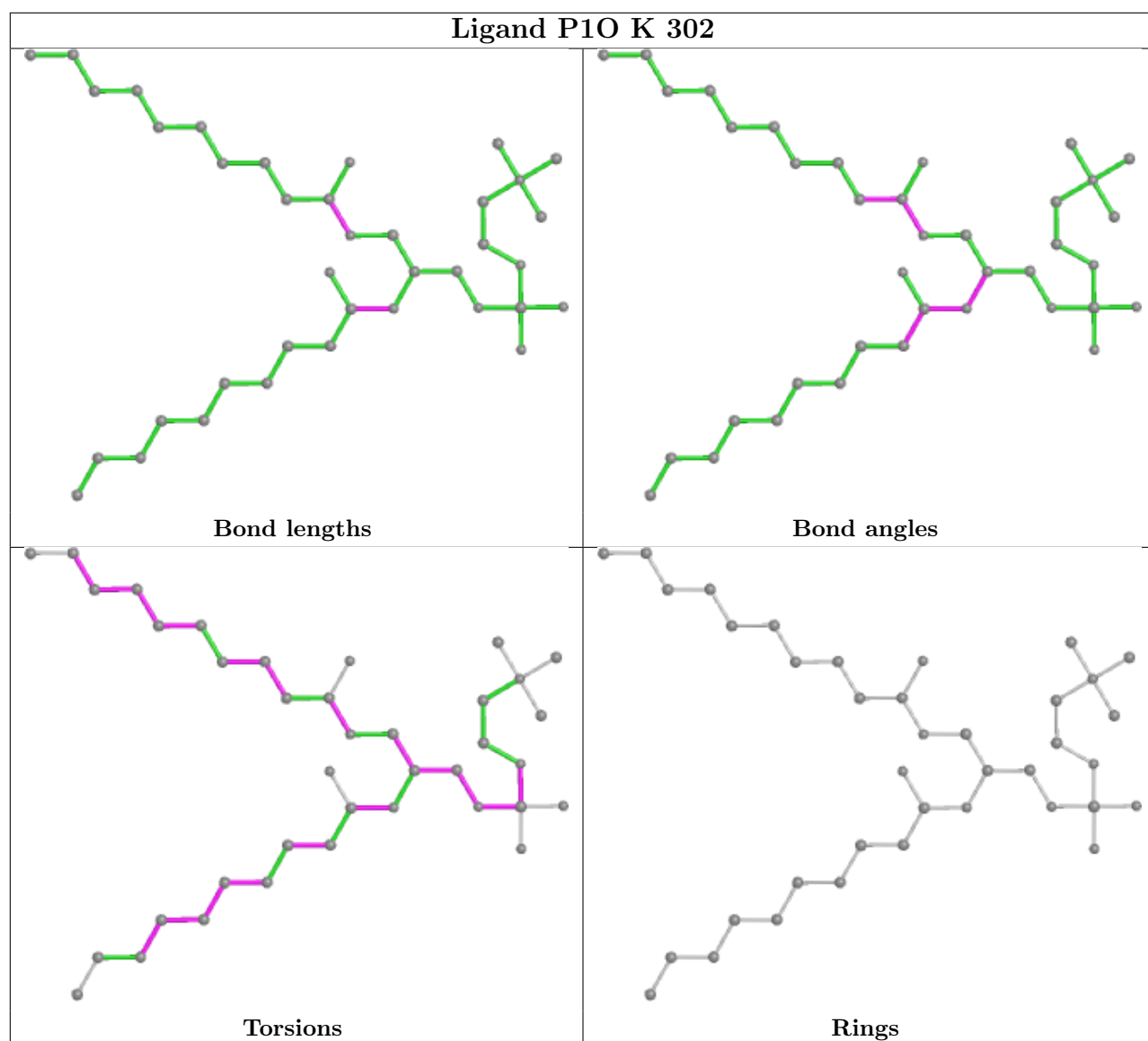


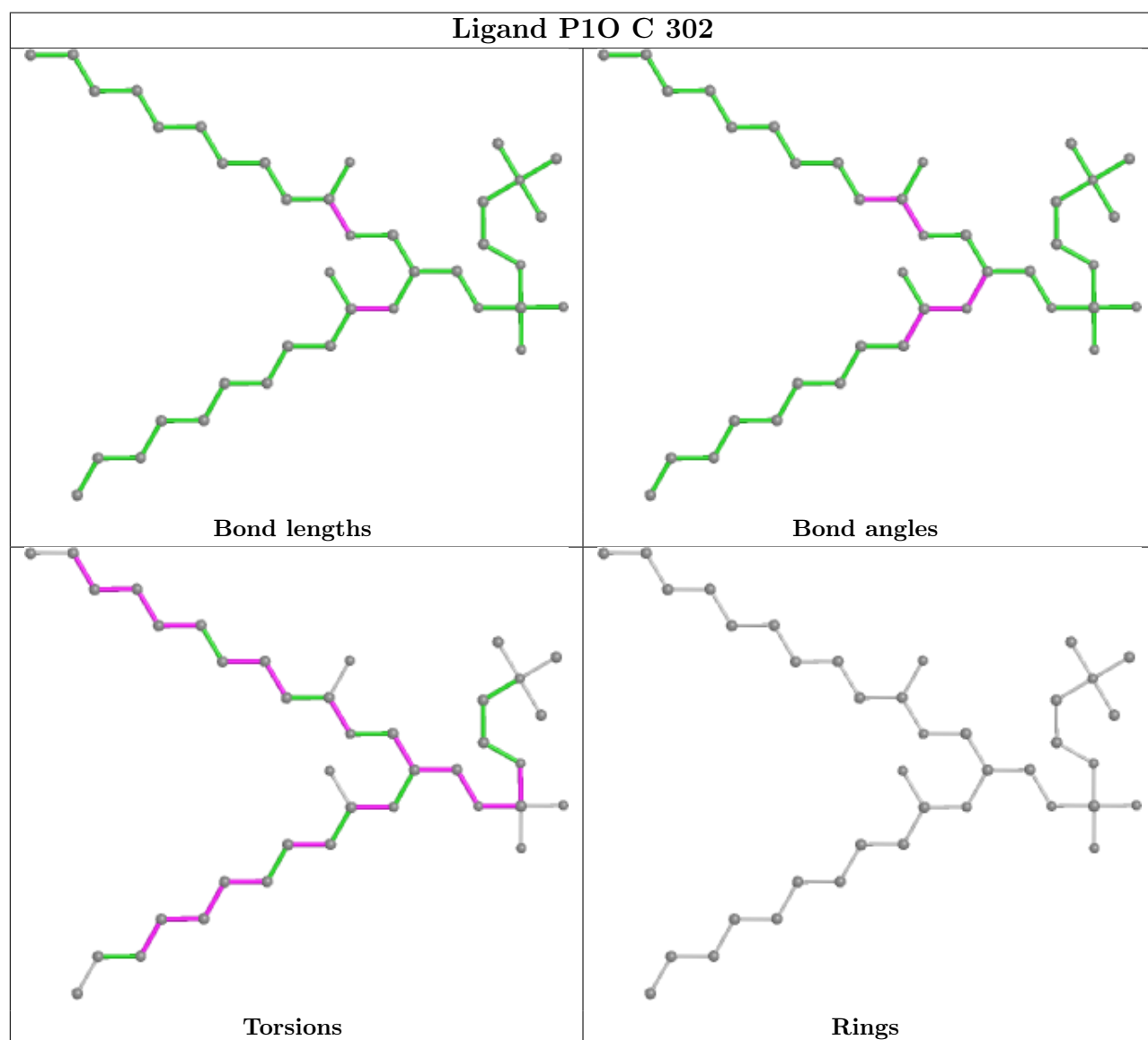
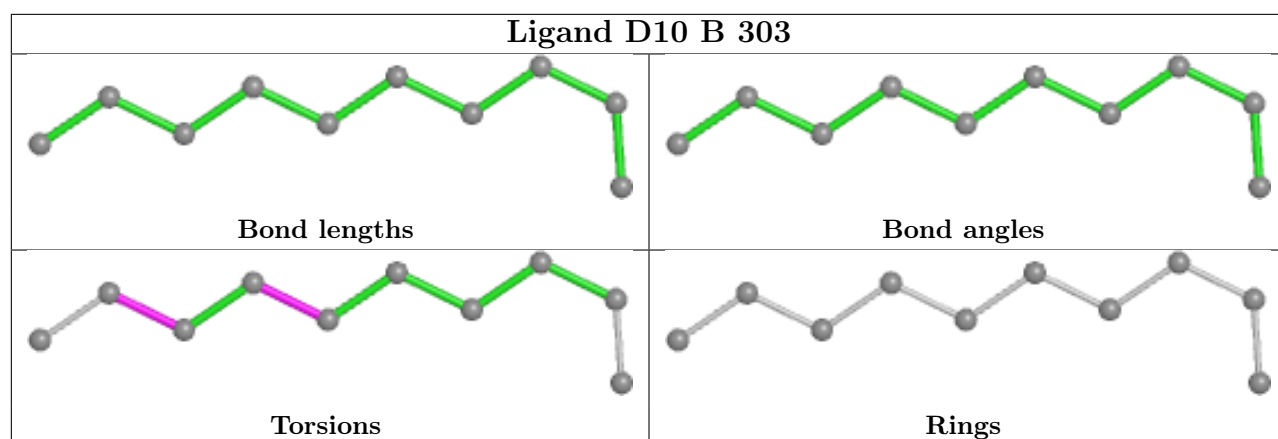


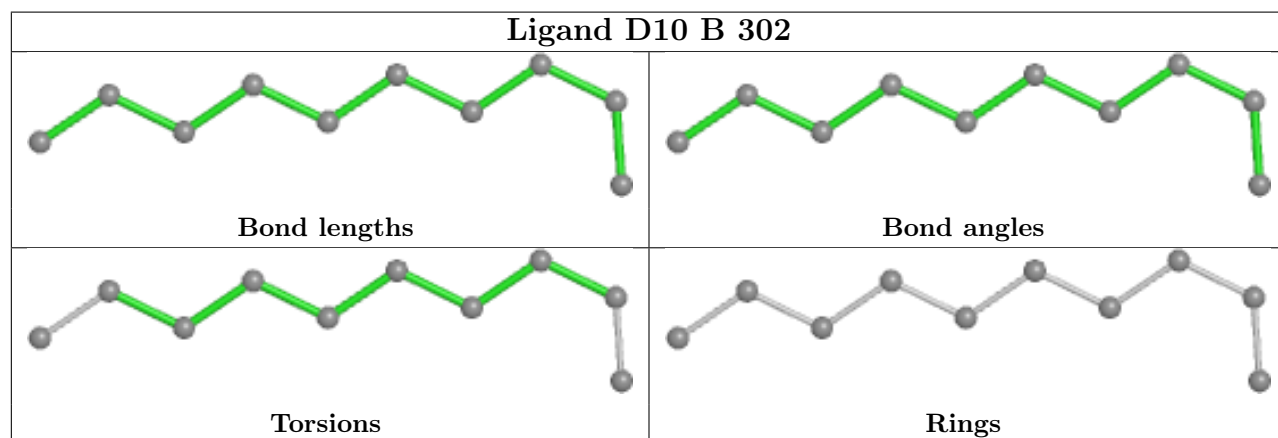
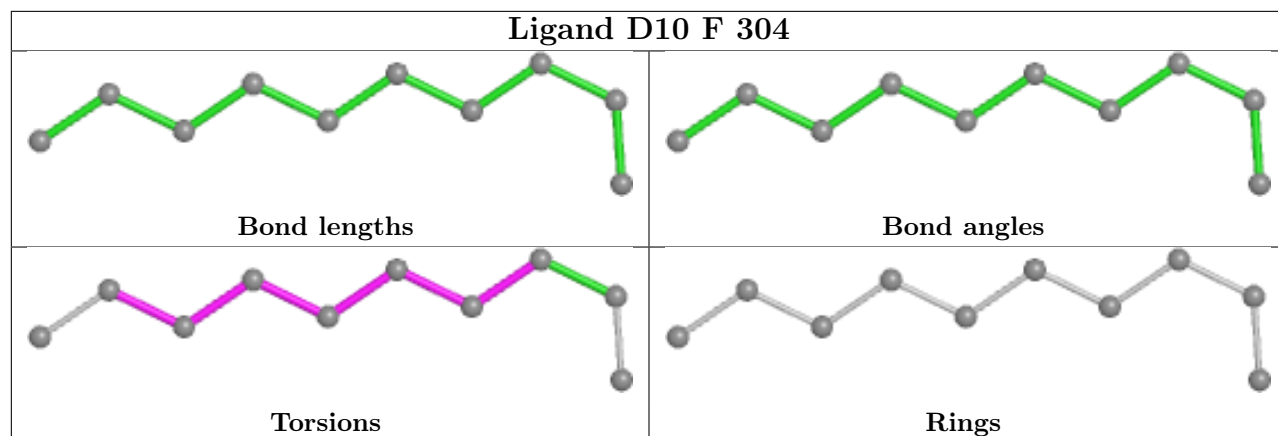


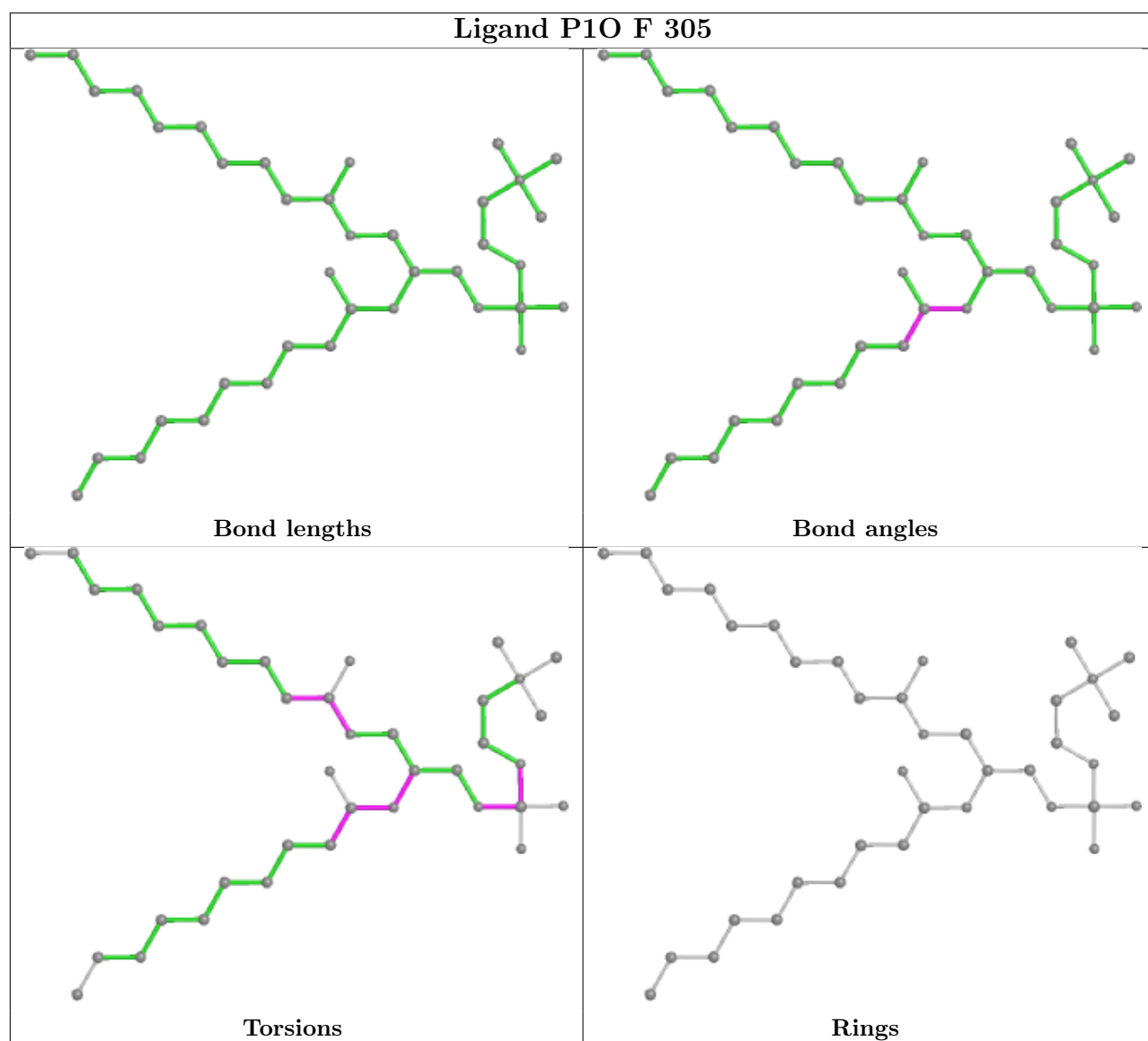


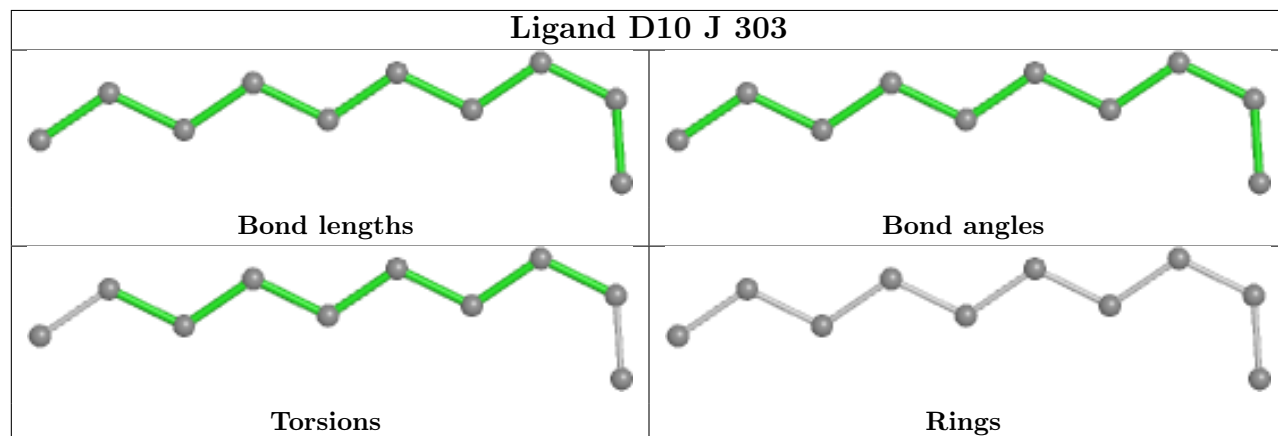
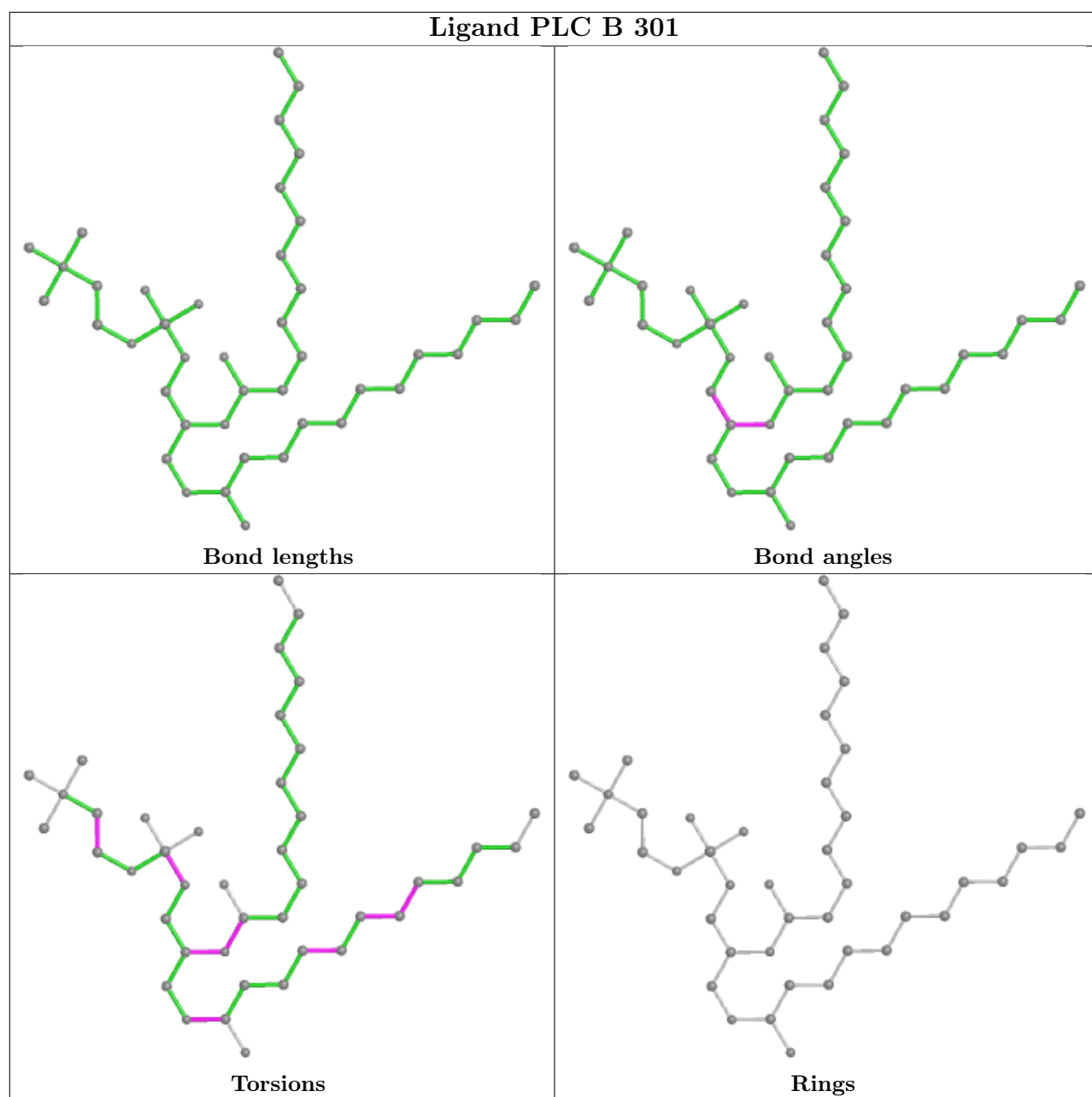














## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

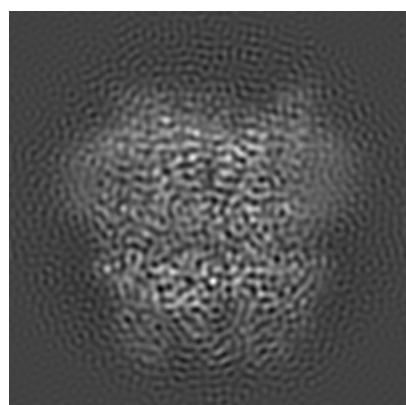
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25683. These allow visual inspection of the internal detail of the map and identification of artifacts.

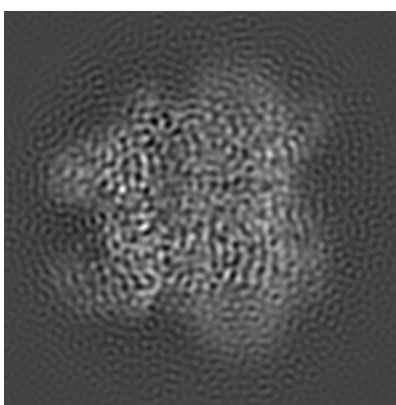
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

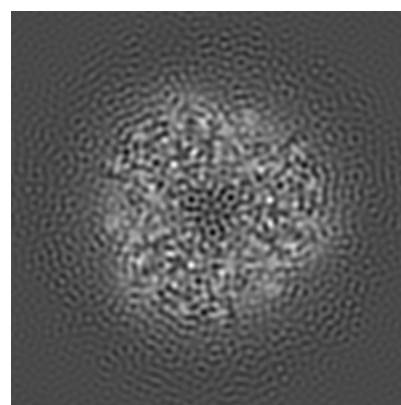
#### 6.1.1 Primary map



X



Y

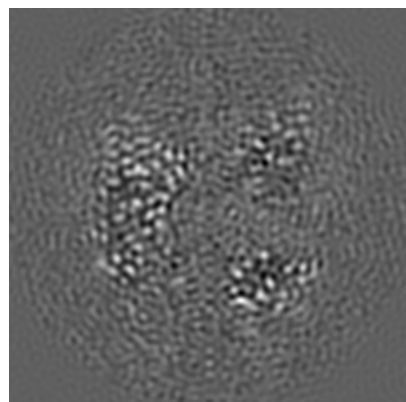


Z

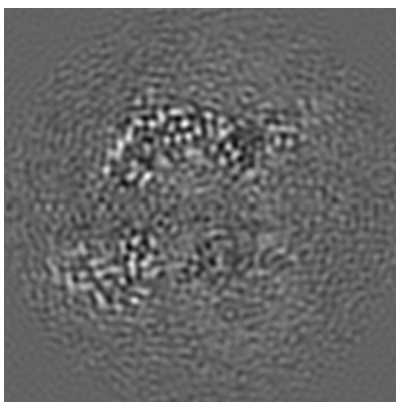
The images above show the map projected in three orthogonal directions.

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

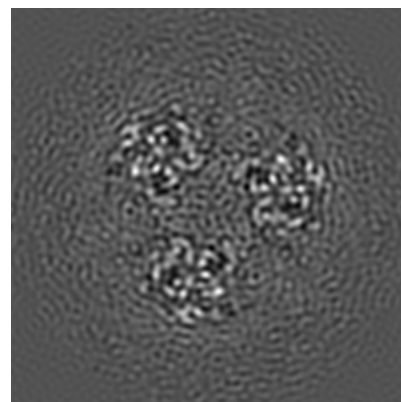
#### 6.2.1 Primary map



X Index: 150



Y Index: 150

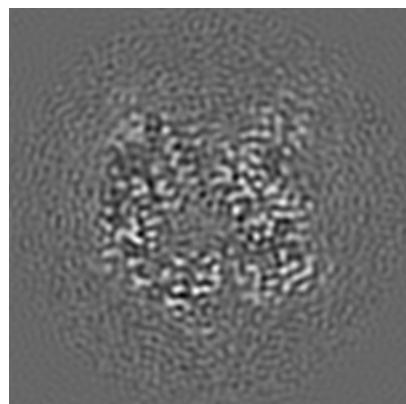


Z Index: 150

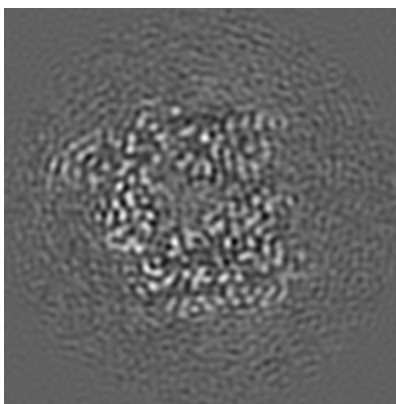
The images above show central slices of the map in three orthogonal directions.

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

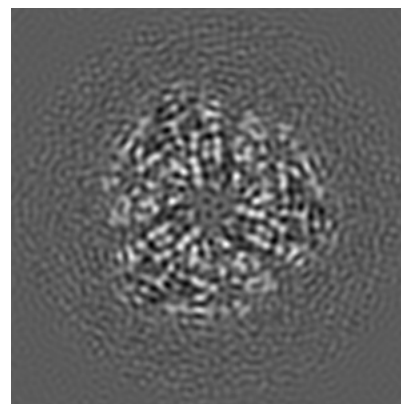
### 6.3.1 Primary map



X Index: 122



Y Index: 186



Z Index: 105

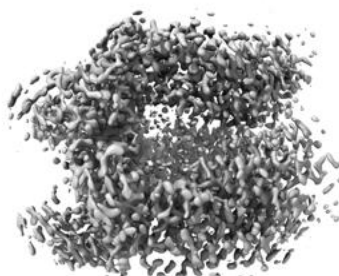
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0127. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

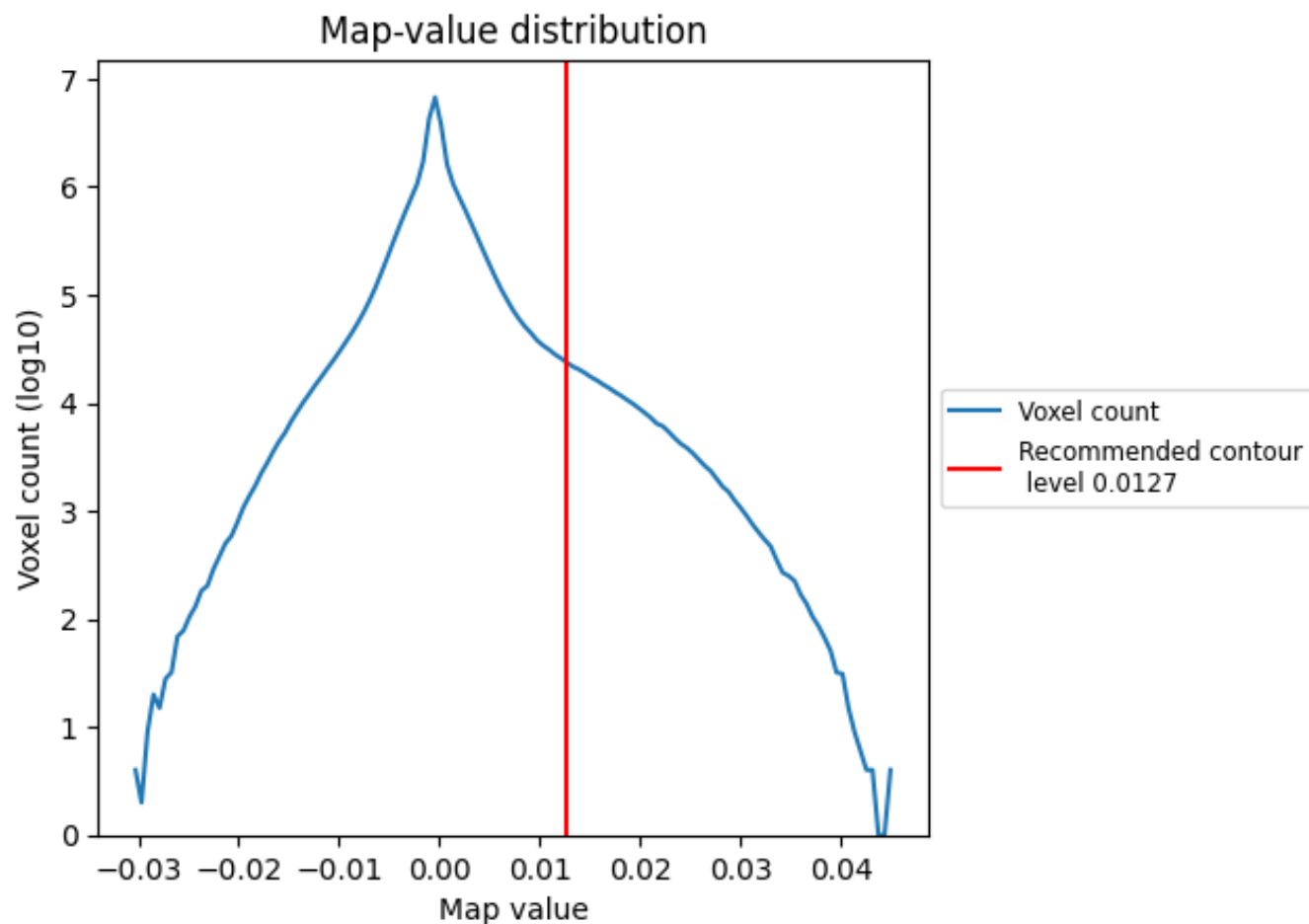
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

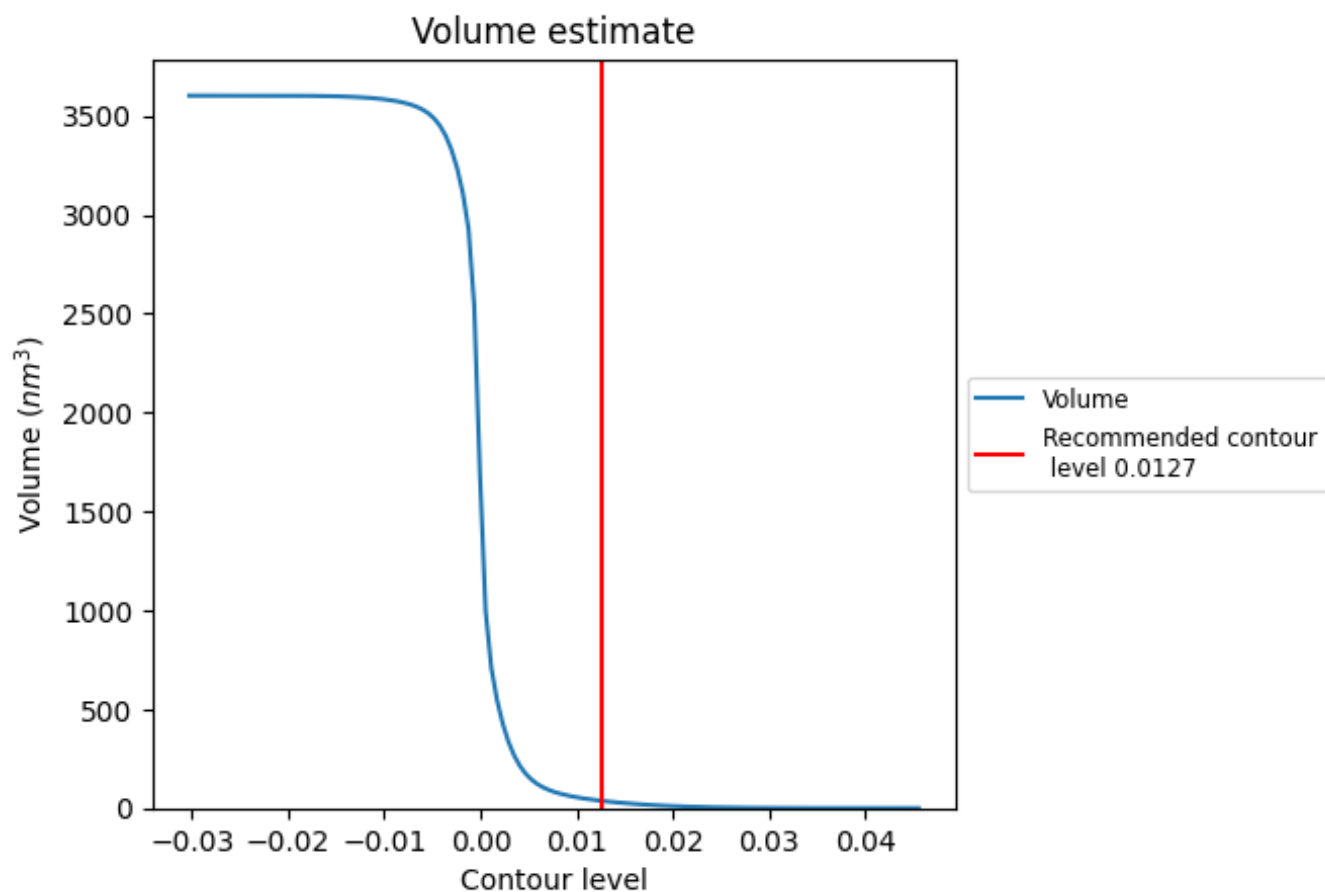
This section contains the results of statistical analysis of the map.

### 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.

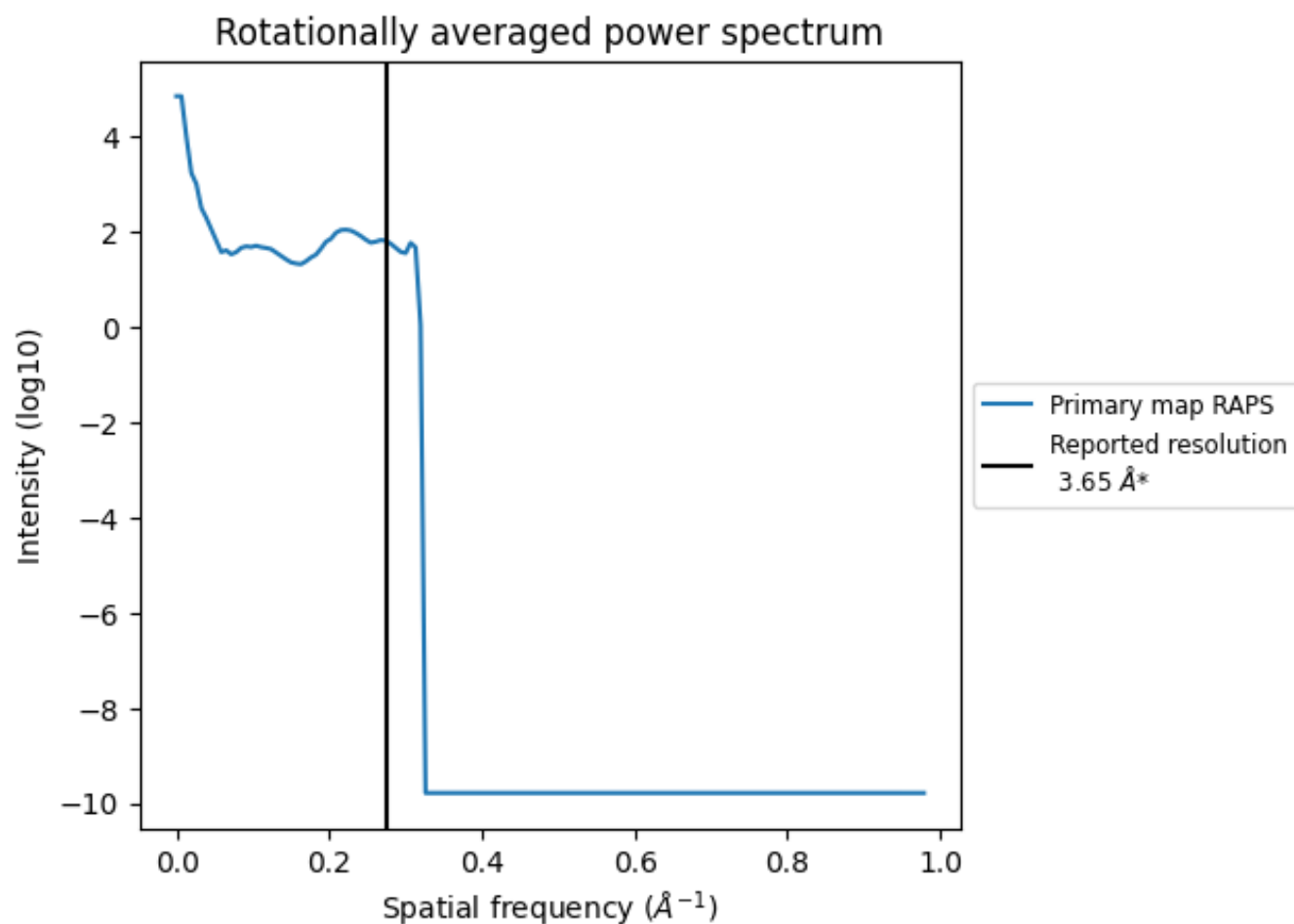
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 36 nm<sup>3</sup>; this corresponds to an approximate mass of 33 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 ⓘ

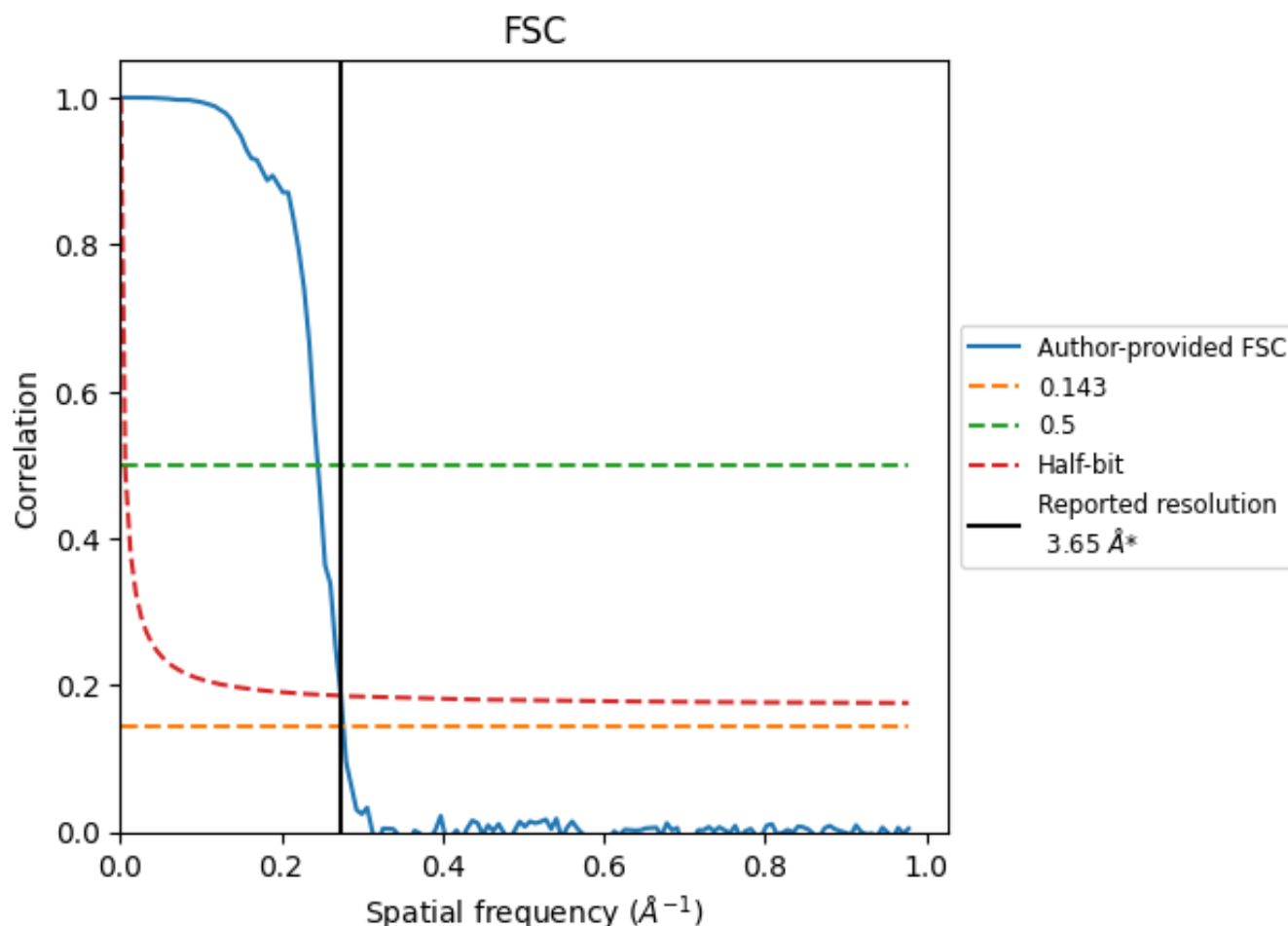


\*Reported resolution corresponds to spatial frequency of  $0.274 \text{ \AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

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 [i](#)



\*Reported resolution corresponds to spatial frequency of 0.274 Å<sup>-1</sup>



## 8.2 Resolution estimates [i](#)

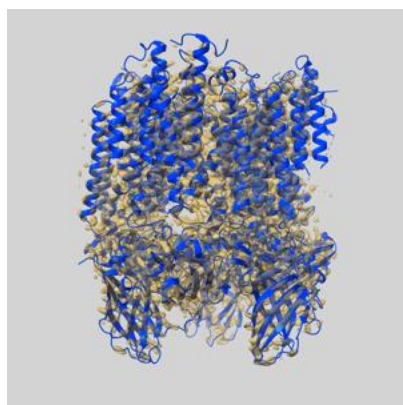
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.65	-	-
Author-provided FSC curve	3.61	4.08	3.65
Unmasked-calculated*	-	-	-

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

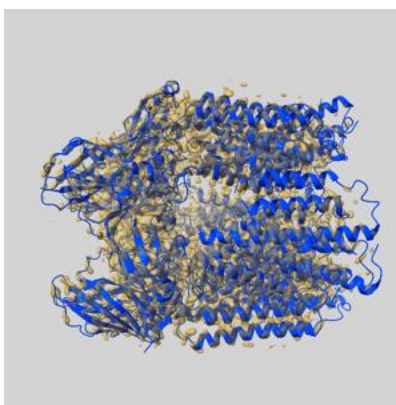
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-25683 and PDB model 7T4O. Per-residue inclusion information can be found in section [3](#) on page [8](#).

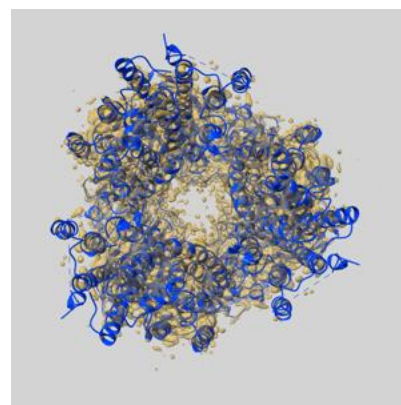
### 9.1 Map-model overlay [i](#)



X



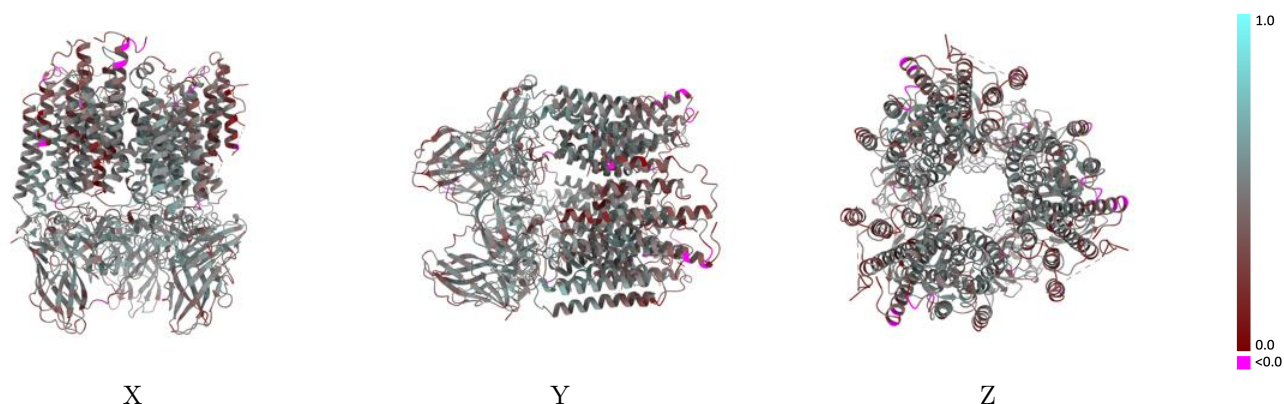
Y



Z

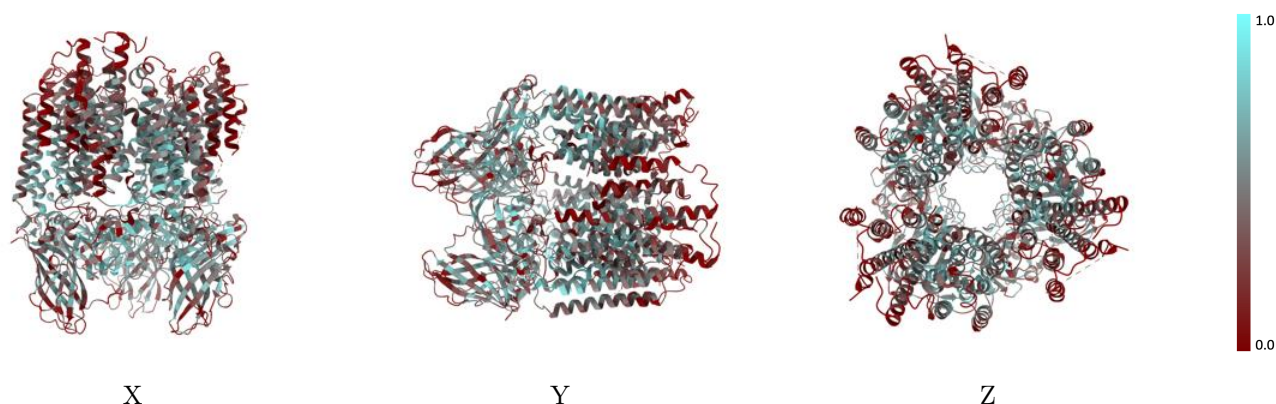
The images above show the 3D surface view of the map at the recommended contour level 0.0127 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



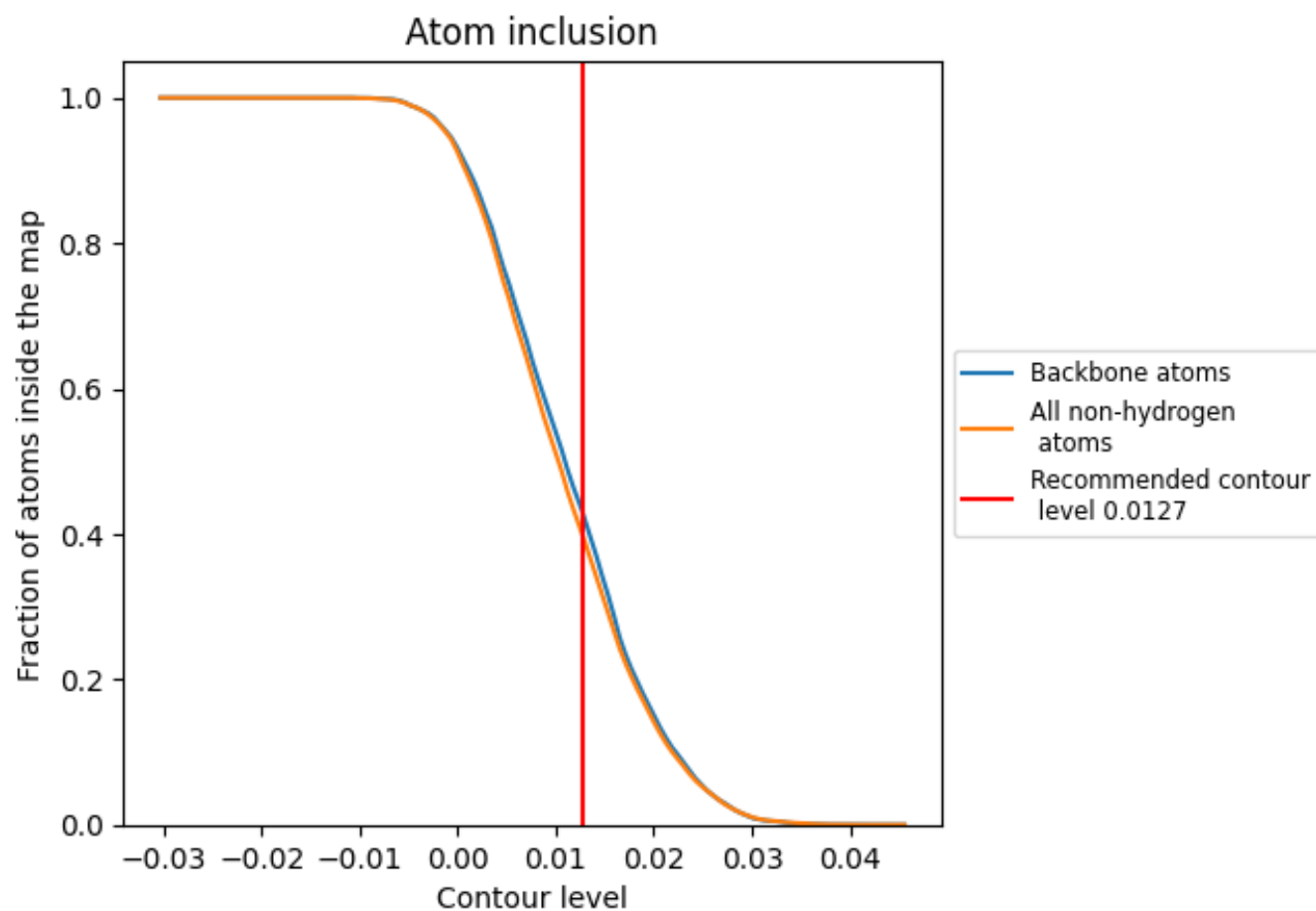
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0127).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 43% of all backbone atoms, 40% 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 (0.0127) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.4004	<div></div> 0.4280
A	<div></div> 0.4522	<div></div> 0.4620
B	<div></div> 0.4745	<div></div> 0.4530
C	<div></div> 0.1692	<div></div> 0.3130
E	<div></div> 0.4539	<div></div> 0.4600
F	<div></div> 0.4725	<div></div> 0.4530
G	<div></div> 0.1684	<div></div> 0.3100
I	<div></div> 0.4564	<div></div> 0.4600
J	<div></div> 0.4730	<div></div> 0.4530
K	<div></div> 0.1692	<div></div> 0.3120

1.0

0.0

<0.0