



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 05:02 PM UTC

PDB ID : 7WYX / pdb_00007wyx
EMDB ID : EMD-32897
Title : Cryo-EM structure of Na⁺,K⁺-ATPase in the E2P state formed by ATP with
istaroxime
Authors : Kanai, R.; Cornelius, F.; Vilsen, B.; Toyoshima, C.
Deposited on : 2022-02-16
Resolution : 3.40 Å(reported)
Based on initial model : 7D91

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

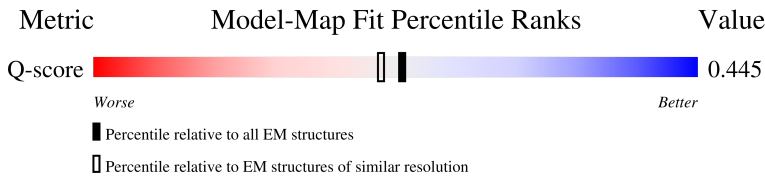
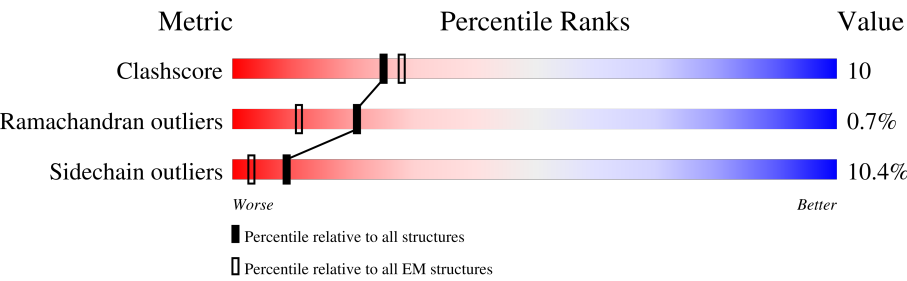
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14717 (2.90 - 3.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	1028	 21% 71% 23% . .
1	C	1028	 21% 71% 23% . .
2	B	305	 6% 60% 30% 6% .
2	D	305	 6% 59% 30% 7% .

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Mol	Chain	Length	Quality of chain
3	E	94	
3	G	94	
4	F	6	
4	K	6	
5	H	6	
5	L	6	
6	I	5	
6	M	5	
7	J	2	
7	N	2	

2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 22714 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 Sodium/potassium-transporting ATPase subunit alpha.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	993	Total	C	N	O	P	S	0	0
			7687	4890	1291	1459	1	46		
1	C	993	Total	C	N	O	P	S	0	0
			7687	4890	1291	1459	1	46		

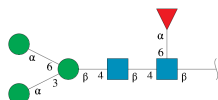
- Molecule 2 is a protein called Na⁺,K⁺-ATPase beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	294	Total	C	N	O	S	0	0
			2399	1551	394	443	11		
2	D	294	Total	C	N	O	S	0	0
			2399	1551	394	443	11		

- Molecule 3 is a protein called FXYD domain-containing ion transport regulator.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	40	Total	C	N	O	S	0	0
			311	203	51	55	2		
3	E	40	Total	C	N	O	S	0	0
			311	203	51	55	2		

- Molecule 4 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)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



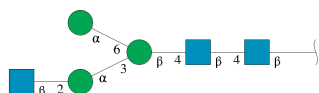
Mol	Chain	Residues	Atoms				AltConf	Trace
4	F	6	Total	C	N	O	0	0
			71	40	2	29		

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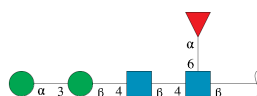
Mol	Chain	Residues	Atoms				AltConf	Trace
4	K	6	Total	C	N	O	0	0
			71	40	2	29		

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-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.



Mol	Chain	Residues	Atoms				AltConf	Trace
5	H	6	Total	C	N	O	0	0
			75	42	3	30		
5	L	6	Total	C	N	O	0	0
			75	42	3	30		

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
6	I	5	Total	C	N	O	0	0
			60	34	2	24		
6	M	5	Total	C	N	O	0	0
			60	34	2	24		

- Molecule 7 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
7	J	2	Total	C	N	O	0	0
			28	16	2	10		

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

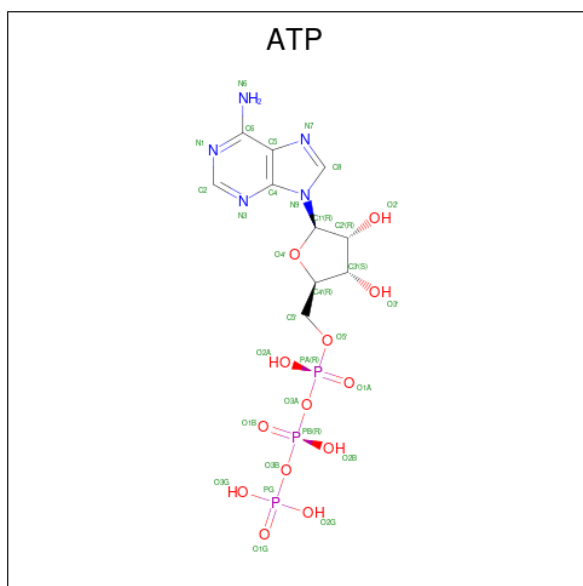
- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

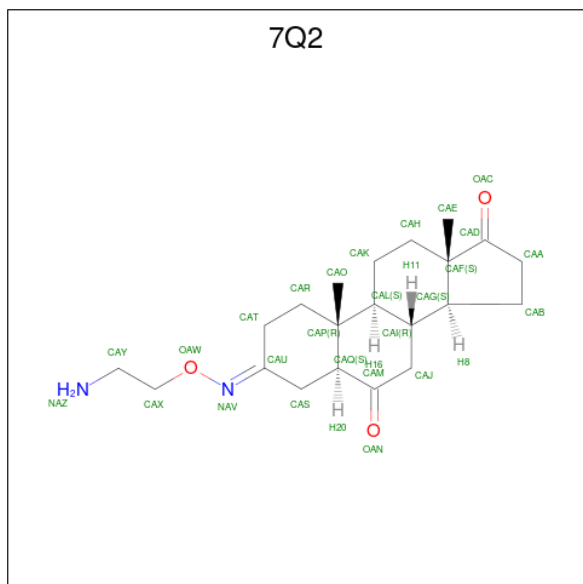
- Molecule 9 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
9	A	1	Total	Na	0
			1	1	
9	C	1	Total	Na	0
			1	1	

- Molecule 10 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).

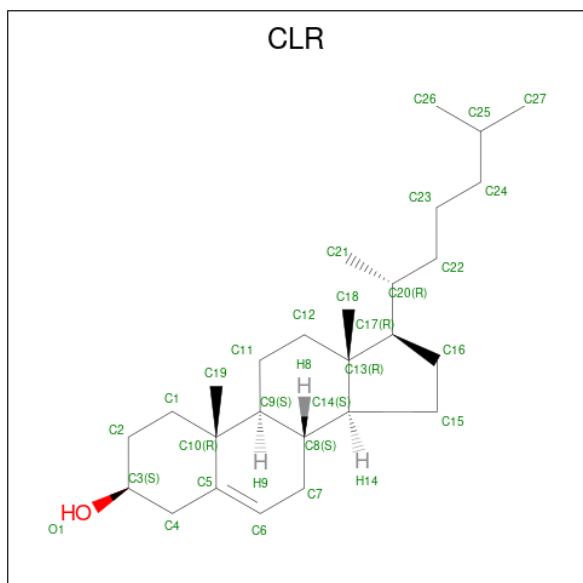


- Molecule 11 is (3E,5S,8R,9S,10R,13S,14S)-3-(2-azanylethoxyimino)-10,13-dimethyl-1,2,4,5,7,8,9,11,12,14,15,16-dodecahydrocyclopenta[a]phenanthrene-6,17-dione (CCD ID: 7Q2) (formula: $C_{21}H_{32}N_2O_3$) (labeled as "Ligand of Interest" by depositor).



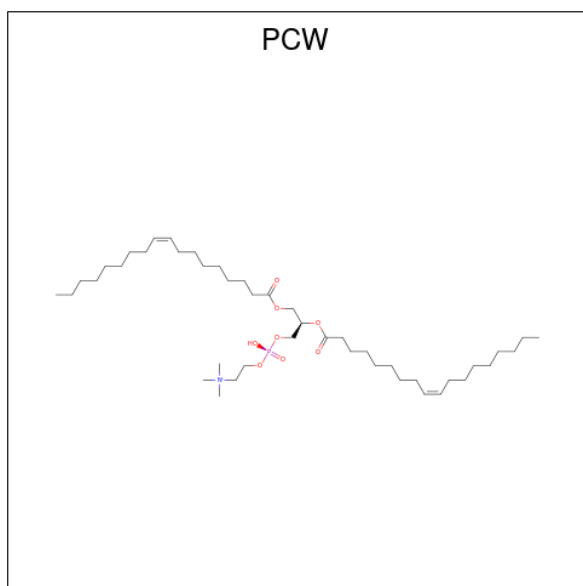
Mol	Chain	Residues	Atoms				AltConf
11	A	1	Total	C	N	O	0
			26	21	2	3	
11	C	1	Total	C	N	O	0
			26	21	2	3	

- Molecule 12 is CHOLESTEROL (CCD ID: CLR) (formula: $C_{27}H_{46}O$).



Mol	Chain	Residues	Atoms			AltConf
12	A	1	Total	C	O	0
			28	27	1	
12	B	1	Total	C	O	0
			28	27	1	
12	B	1	Total	C	O	0
			28	27	1	
12	G	1	Total	C	O	0
			28	27	1	
12	C	1	Total	C	O	0
			28	27	1	
12	D	1	Total	C	O	0
			28	27	1	
12	D	1	Total	C	O	0
			28	27	1	
12	E	1	Total	C	O	0
			28	27	1	

- Molecule 13 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PCW) (formula: $C_{44}H_{85}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
13	A	1	Total	C	N	O	P	0
			22	12	1	8	1	
13	A	1	Total	C	N	O	P	0
			22	12	1	8	1	
13	A	1	Total	C	N	O	P	0
			54	44	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
13	A	1	Total	C	N	O	P	0
			54	44	1	8	1	
13	A	1	Total	C	N	O	P	0
			54	44	1	8	1	
13	A	1	Total	C	N	O	P	0
			54	44	1	8	1	
13	A	1	Total	C	N	O	P	0
			54	44	1	8	1	
13	A	1	Total	C	N	O	P	0
			22	12	1	8	1	
13	A	1	Total	C	N	O	P	0
			54	44	1	8	1	
13	G	1	Total	C	N	O	P	0
			54	44	1	8	1	
13	G	1	Total	C	N	O	P	0
			54	44	1	8	1	
13	G	1	Total	C	N	O	P	0
			54	44	1	8	1	
13	C	1	Total	C	N	O	P	0
			22	12	1	8	1	
13	C	1	Total	C	N	O	P	0
			22	12	1	8	1	
13	C	1	Total	C	N	O	P	0
			54	44	1	8	1	
13	C	1	Total	C	N	O	P	0
			54	44	1	8	1	
13	C	1	Total	C	N	O	P	0
			54	44	1	8	1	
13	C	1	Total	C	N	O	P	0
			54	44	1	8	1	
13	C	1	Total	C	N	O	P	0
			22	12	1	8	1	
13	C	1	Total	C	N	O	P	0
			54	44	1	8	1	
13	E	1	Total	C	N	O	P	0
			54	44	1	8	1	
13	E	1	Total	C	N	O	P	0
			54	44	1	8	1	
13	E	1	Total	C	N	O	P	0
			54	44	1	8	1	

- Molecule 14 is water.

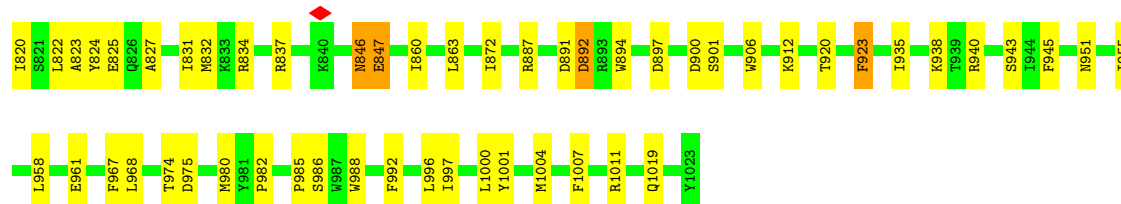
Mol	Chain	Residues	Atoms		AltConf
14	A	3	Total 3	O 3	0
14	C	3	Total 3	O 3	0

3 Residue-property plots

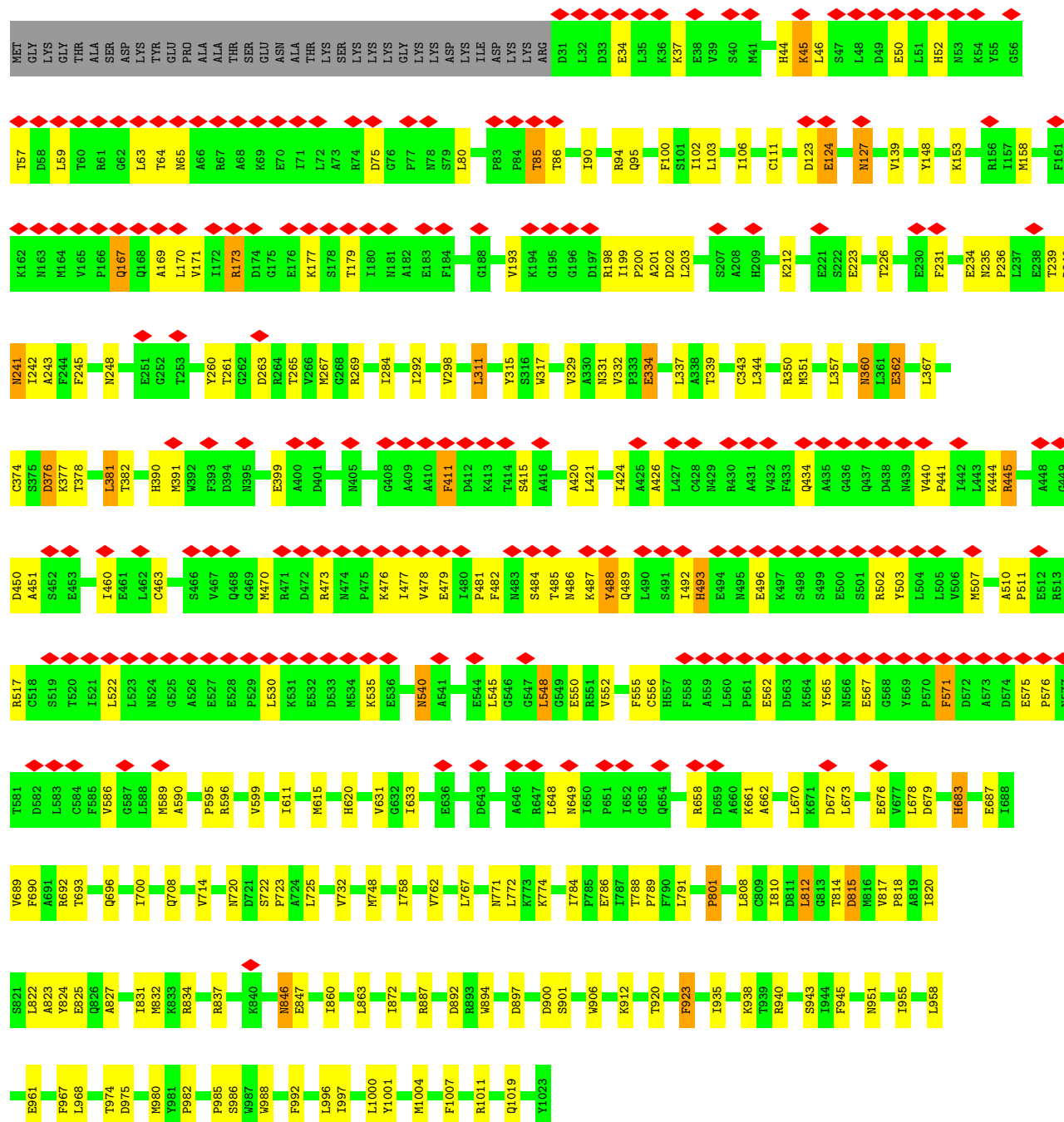
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

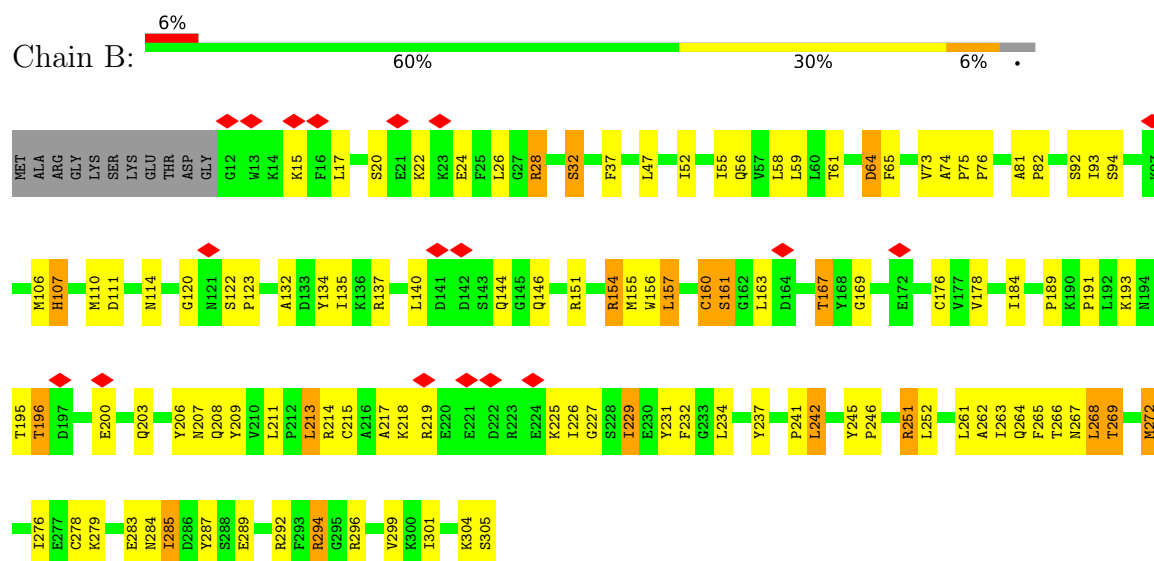




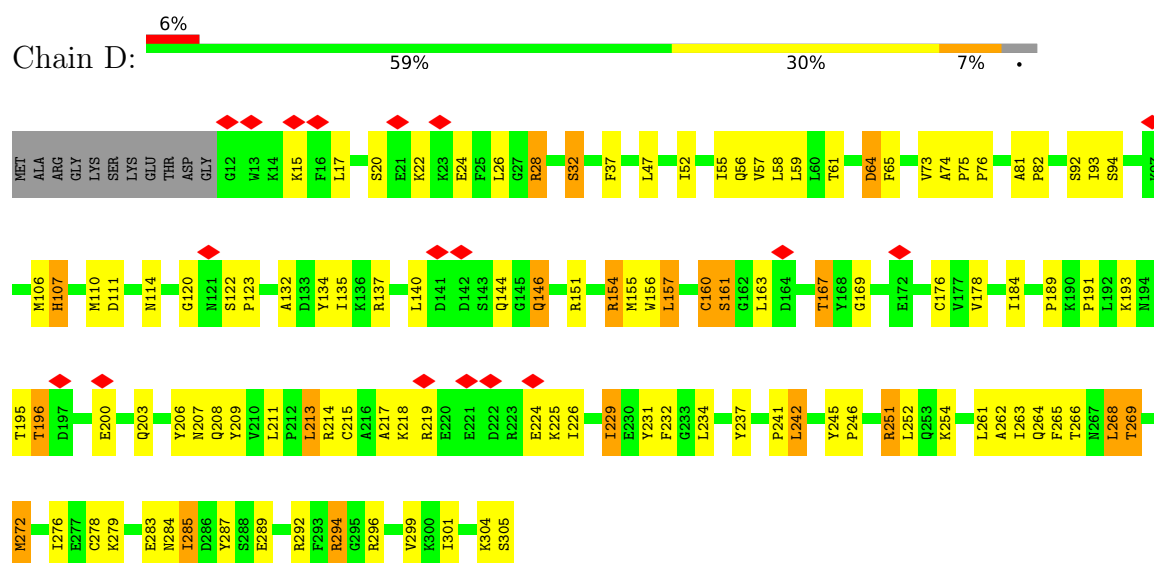
• Molecule 1: Sodium/potassium-transporting ATPase subunit alpha



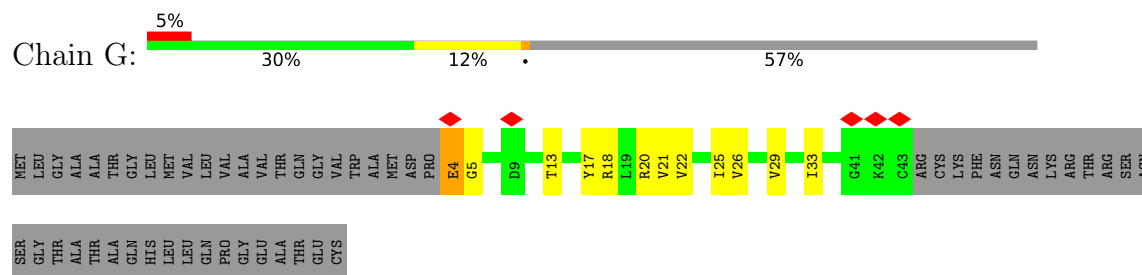
- Molecule 2: Na⁺,K⁺-ATPase beta subunit



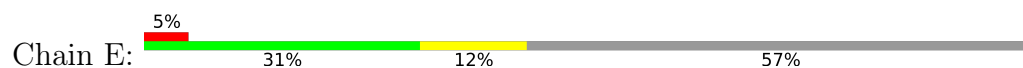
- Molecule 2: Na⁺,K⁺-ATPase beta subunit

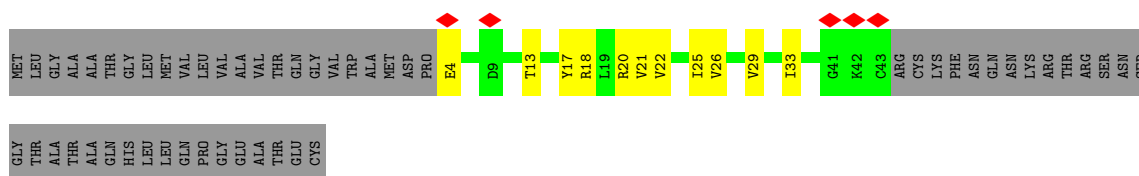


- Molecule 3: FXYP domain-containing ion transport regulator

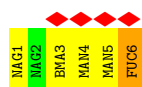


- Molecule 3: FXYP domain-containing ion transport regulator

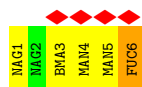




- Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



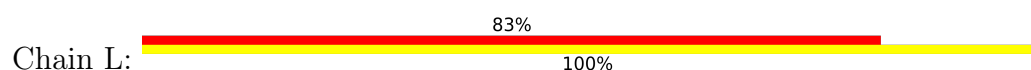
- Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



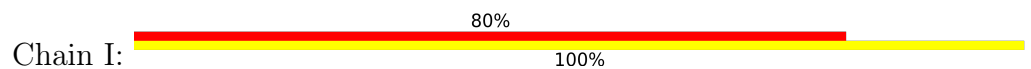
- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-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

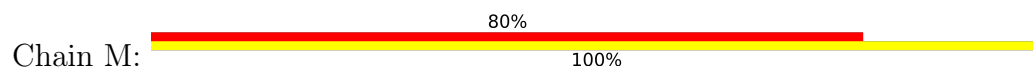


- Molecule 6: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose





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



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	137433	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.095	Depositor
Minimum map value	-0.046	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.019	Depositor
Map size ($\text{\AA}$)	258.24, 258.24, 258.24	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.076, 1.076, 1.076	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 7Q2, ATP, NA, NAG, MG, PHD, MAN, CLR, BMA, FUC, PCW

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	0.20	0/7824	0.62	0/10613
1	C	0.20	0/7824	0.62	0/10613
2	B	0.20	0/2462	0.71	0/3317
2	D	0.20	0/2462	0.71	0/3317
3	E	0.16	0/315	0.45	0/427
3	G	0.16	0/315	0.45	0/427
All	All	0.20	0/21202	0.64	0/28714

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	7687	0	7703	153	0
1	C	7687	0	7703	149	0
2	B	2399	0	2354	61	0
2	D	2399	0	2354	62	0
3	E	311	0	323	6	0
3	G	311	0	323	7	0
4	F	71	0	61	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	K	71	0	61	1	0
5	H	75	0	64	0	0
5	L	75	0	64	0	0
6	I	60	0	52	0	0
6	M	60	0	52	0	0
7	J	28	0	25	0	0
7	N	28	0	25	0	0
8	A	1	0	0	0	0
8	C	1	0	0	0	0
9	A	1	0	0	0	0
9	C	1	0	0	0	0
10	A	31	0	12	1	0
10	C	31	0	12	1	0
11	A	26	0	0	0	0
11	C	26	0	0	0	0
12	A	28	0	46	3	0
12	B	56	0	92	2	0
12	C	28	0	46	0	0
12	D	56	0	92	1	0
12	E	28	0	46	7	0
12	G	28	0	46	7	0
13	A	390	0	558	29	0
13	C	390	0	558	30	0
13	E	162	0	252	21	0
13	G	162	0	252	21	0
14	A	3	0	0	0	0
14	C	3	0	0	0	0
All	All	22714	0	23176	480	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 10.

All (480) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1000:LEU:HD21	13:C:1110:PCW:H39	1.55	0.87
1:A:1000:LEU:HD21	13:A:1110:PCW:H39	1.55	0.85
1:C:421:LEU:HG	1:C:589:MET:HE2	1.61	0.82
1:A:814:THR:HB	1:A:961:GLU:HG3	1.62	0.82
1:A:421:LEU:HG	1:A:589:MET:HE2	1.61	0.81
1:C:814:THR:HB	1:C:961:GLU:HG3	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:29:VAL:HG11	13:G:1303:PCW:H261	1.62	0.80
3:E:29:VAL:HG11	13:E:1303:PCW:H261	1.62	0.79
1:A:202:ASP:HB2	1:A:260:TYR:HB2	1.68	0.76
1:C:52:HIS:HE1	1:C:59:LEU:HD12	1.52	0.75
13:G:1304:PCW:H412	13:E:1304:PCW:H461	1.68	0.75
1:C:202:ASP:HB2	1:C:260:TYR:HB2	1.68	0.74
1:A:52:HIS:HE1	1:A:59:LEU:HD12	1.52	0.74
13:C:1109:PCW:H442	12:E:1301:CLR:H273	1.70	0.73
13:G:1304:PCW:H461	13:E:1304:PCW:H412	1.71	0.72
13:A:1109:PCW:H442	12:G:1301:CLR:H273	1.70	0.72
13:G:1304:PCW:H382	13:E:1304:PCW:H482	1.71	0.72
2:D:161:SER:HB3	2:D:163:LEU:HD12	1.72	0.72
2:B:74:ALA:HB3	2:B:75:PRO:HD3	1.72	0.72
1:C:241:ASN:H	1:C:241:ASN:HD22	1.38	0.71
2:B:176:CYS:SG	2:B:264:GLN:HG3	2.31	0.71
2:D:74:ALA:HB3	2:D:75:PRO:HD3	1.72	0.71
1:A:996:LEU:HD23	13:C:1110:PCW:H283	1.73	0.71
2:D:176:CYS:SG	2:D:264:GLN:HG3	2.31	0.71
2:B:161:SER:HB3	2:B:163:LEU:HD12	1.72	0.70
13:A:1110:PCW:H283	1:C:996:LEU:HD23	1.72	0.70
1:A:426:ALA:HB2	1:A:460:ILE:HG21	1.74	0.70
13:G:1304:PCW:H482	13:E:1304:PCW:H382	1.75	0.69
1:C:426:ALA:HB2	1:C:460:ILE:HG21	1.74	0.69
1:C:789:PRO:HB3	1:C:801:PRO:HB2	1.75	0.69
1:A:241:ASN:HD22	1:A:241:ASN:H	1.38	0.69
1:A:411:PHE:HZ	1:A:463:CYS:HG	1.40	0.69
3:G:26:VAL:HG11	12:G:1301:CLR:H71	1.75	0.69
1:A:789:PRO:HB3	1:A:801:PRO:HB2	1.75	0.69
1:C:982:PRO:HD3	3:E:20:ARG:HH21	1.58	0.69
1:C:411:PHE:HZ	1:C:463:CYS:HG	1.39	0.68
1:A:982:PRO:HD3	3:G:20:ARG:HH21	1.58	0.68
3:E:26:VAL:HG11	12:E:1301:CLR:H71	1.75	0.67
1:A:967:PHE:HZ	13:A:1112:PCW:H172	1.61	0.66
1:C:575:GLU:HB3	1:C:576:PRO:HD2	1.78	0.65
13:G:1304:PCW:H451	13:E:1304:PCW:H261	1.78	0.65
1:A:575:GLU:HB3	1:A:576:PRO:HD2	1.78	0.65
1:C:967:PHE:HZ	13:C:1112:PCW:H172	1.61	0.65
1:A:441:PRO:O	1:A:445:ARG:HG2	1.97	0.64
1:C:441:PRO:O	1:C:445:ARG:HG2	1.97	0.64
2:B:213:LEU:HD23	2:B:261:LEU:HD13	1.78	0.64
2:D:213:LEU:HD23	2:D:261:LEU:HD13	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:209:TYR:HA	2:B:242:LEU:HD22	1.80	0.63
1:C:103:LEU:HD22	1:C:292:ILE:HG23	1.79	0.63
2:D:209:TYR:HA	2:D:242:LEU:HD22	1.80	0.63
1:A:1001:TYR:HD1	13:A:1108:PCW:H40	1.64	0.63
1:A:103:LEU:HD22	1:A:292:ILE:HG23	1.79	0.62
1:A:46:LEU:HD22	1:A:50:GLU:HG2	1.82	0.62
1:A:503:TYR:CE2	1:A:567:GLU:HA	2.35	0.61
1:C:44:HIS:HB3	1:C:242:ILE:HD11	1.83	0.61
1:C:503:TYR:CE2	1:C:567:GLU:HA	2.35	0.61
1:A:239:THR:OG1	1:A:241:ASN:ND2	2.34	0.61
1:C:127:ASN:OD1	1:C:127:ASN:N	2.30	0.61
1:C:239:THR:OG1	1:C:241:ASN:ND2	2.34	0.61
1:C:1001:TYR:HD1	13:C:1108:PCW:H40	1.64	0.61
2:D:231:TYR:HD1	2:D:263:ILE:HG12	1.66	0.61
1:C:46:LEU:HD22	1:C:50:GLU:HG2	1.82	0.61
1:A:44:HIS:HB3	1:A:242:ILE:HD11	1.83	0.61
1:C:503:TYR:HE2	1:C:567:GLU:HA	1.66	0.61
1:A:503:TYR:HE2	1:A:567:GLU:HA	1.66	0.60
2:B:206:TYR:O	2:B:206:TYR:CD1	2.54	0.60
3:G:18:ARG:O	3:G:22:VAL:HG23	2.01	0.60
1:C:334:GLU:HG3	1:C:812:LEU:HD22	1.84	0.60
2:B:28:ARG:HD3	2:B:32:SER:HB3	1.82	0.60
2:B:231:TYR:HD1	2:B:263:ILE:HG12	1.66	0.60
2:D:206:TYR:O	2:D:206:TYR:CD1	2.54	0.60
3:E:18:ARG:O	3:E:22:VAL:HG23	2.01	0.59
2:D:28:ARG:HD3	2:D:32:SER:HB3	1.82	0.59
2:D:76:PRO:HG3	2:D:184:ILE:HD12	1.84	0.59
3:G:21:VAL:O	3:G:25:ILE:HG12	2.03	0.59
1:C:690:PHE:HB3	1:C:693:THR:HG21	1.85	0.59
12:G:1301:CLR:H241	13:E:1304:PCW:H462	1.83	0.59
13:E:1303:PCW:H262	13:E:1304:PCW:H20	1.85	0.59
1:A:265:THR:O	1:A:269:ARG:HG3	2.03	0.58
1:A:1000:LEU:CD2	13:A:1110:PCW:H39	2.30	0.58
13:G:1303:PCW:H262	13:G:1304:PCW:H20	1.85	0.58
1:A:992:PHE:HD2	13:A:1109:PCW:H271	1.69	0.58
1:A:171:VAL:HG11	1:A:173:ARG:HH11	1.69	0.58
2:B:217:ALA:HB2	2:B:226:ILE:HD12	1.84	0.58
2:D:217:ALA:HB2	2:D:226:ILE:HD12	1.84	0.58
12:G:1301:CLR:H263	13:E:1304:PCW:H441	1.85	0.58
13:G:1304:PCW:H261	13:E:1304:PCW:H451	1.85	0.58
2:B:64:ASP:N	2:B:64:ASP:OD1	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:76:PRO:HG3	2:B:184:ILE:HD12	1.84	0.58
3:E:21:VAL:O	3:E:25:ILE:HG12	2.03	0.58
1:A:334:GLU:HG3	1:A:812:LEU:HD22	1.84	0.58
1:A:690:PHE:HB3	1:A:693:THR:HG21	1.85	0.58
1:A:241:ASN:HD22	1:A:241:ASN:N	1.99	0.58
13:G:1304:PCW:H432	13:E:1304:PCW:H432	1.85	0.57
1:C:241:ASN:HD22	1:C:241:ASN:N	1.99	0.57
13:G:1304:PCW:H462	12:E:1301:CLR:H241	1.85	0.57
1:C:488:TYR:HD1	1:C:488:TYR:O	1.87	0.57
1:C:722:SER:HB2	1:C:723:PRO:HD3	1.87	0.57
1:C:992:PHE:CD2	13:C:1109:PCW:H271	2.39	0.57
2:D:64:ASP:N	2:D:64:ASP:OD1	2.36	0.57
1:C:193:VAL:HG11	1:C:199:ILE:HD13	1.86	0.57
1:C:265:THR:O	1:C:269:ARG:HG3	2.03	0.57
1:C:992:PHE:HD2	13:C:1109:PCW:H271	1.68	0.57
12:E:1301:CLR:H272	13:E:1304:PCW:H272	1.87	0.57
1:C:1000:LEU:CD2	13:C:1110:PCW:H39	2.31	0.57
1:A:153:LYS:NZ	13:A:1113:PCW:O2P	2.39	0.56
1:A:722:SER:HB2	1:A:723:PRO:HD3	1.87	0.56
1:C:171:VAL:HG11	1:C:173:ARG:HH11	1.69	0.56
1:C:80:LEU:HD11	1:C:267:MET:SD	2.46	0.56
1:A:488:TYR:HD1	1:A:488:TYR:O	1.87	0.56
1:A:992:PHE:CD2	13:A:1109:PCW:H271	2.40	0.56
1:C:153:LYS:NZ	13:C:1113:PCW:O2P	2.39	0.56
1:C:450:ASP:OD1	1:C:451:ALA:N	2.39	0.56
1:A:860:ILE:HG12	2:B:47:LEU:HD21	1.88	0.56
2:B:75:PRO:HB2	2:B:294:ARG:HD3	1.87	0.56
1:C:860:ILE:HG12	2:D:47:LEU:HD21	1.88	0.56
1:A:530:LEU:HD22	1:A:535:LYS:HE3	1.88	0.55
1:A:377:LYS:HA	1:A:381:LEU:HB2	1.88	0.55
2:D:75:PRO:HB2	2:D:294:ARG:HD3	1.87	0.55
1:A:441:PRO:HG2	1:A:444:LYS:HE3	1.88	0.55
1:A:80:LEU:HD11	1:A:267:MET:SD	2.46	0.55
1:A:193:VAL:HG11	1:A:199:ILE:HD13	1.86	0.55
12:G:1301:CLR:H272	13:G:1304:PCW:H272	1.87	0.55
1:C:486:ASN:HB3	1:C:488:TYR:CD1	2.42	0.55
1:C:771:ASN:ND2	1:C:823:ALA:O	2.40	0.55
13:A:1111:PCW:H241	13:A:1112:PCW:H441	1.88	0.55
1:C:377:LYS:HA	1:C:381:LEU:HB2	1.88	0.55
13:C:1111:PCW:H241	13:C:1112:PCW:H441	1.89	0.55
1:A:382:THR:HA	1:A:595:PRO:HA	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:771:ASN:ND2	1:A:823:ALA:O	2.40	0.55
1:C:382:THR:HA	1:C:595:PRO:HA	1.88	0.55
1:A:477:ILE:HG22	1:A:478:VAL:HG23	1.88	0.55
1:A:510:ALA:O	1:A:514:ILE:HG12	2.07	0.55
1:C:487:LYS:HE2	1:C:510:ALA:HB2	1.88	0.55
1:A:450:ASP:OD1	1:A:451:ALA:N	2.39	0.55
2:D:65:PHE:HE1	2:D:251:ARG:HH11	1.55	0.54
1:C:245:PHE:HD2	1:C:265:THR:HG21	1.73	0.54
1:A:486:ASN:HB3	1:A:488:TYR:CD1	2.42	0.54
1:C:339:THR:HA	1:C:820:ILE:HD11	1.90	0.54
1:C:441:PRO:HG2	1:C:444:LYS:HE3	1.88	0.54
1:A:245:PHE:HD2	1:A:265:THR:HG21	1.73	0.54
1:A:123:ASP:O	1:A:124:GLU:HG2	2.08	0.53
2:B:65:PHE:HE1	2:B:251:ARG:HH11	1.55	0.53
1:C:477:ILE:HG22	1:C:478:VAL:HG23	1.88	0.53
1:C:510:ALA:O	1:C:514:ILE:HG12	2.07	0.53
1:C:530:LEU:HD22	1:C:535:LYS:HE3	1.88	0.53
1:A:339:THR:HA	1:A:820:ILE:HD11	1.90	0.53
1:A:487:LYS:HE2	1:A:510:ALA:HB2	1.88	0.53
1:C:863:LEU:HD12	2:D:47:LEU:HD22	1.90	0.53
1:A:863:LEU:HD12	2:B:47:LEU:HD22	1.90	0.53
1:C:241:ASN:H	1:C:241:ASN:ND2	2.06	0.53
1:C:411:PHE:HZ	1:C:463:CYS:SG	2.32	0.53
1:C:123:ASP:O	1:C:124:GLU:HG2	2.08	0.53
3:G:17:TYR:O	3:G:21:VAL:HG23	2.08	0.53
2:D:92:SER:HA	2:D:304:LYS:O	2.09	0.53
2:B:279:LYS:HG3	2:B:296:ARG:HB3	1.91	0.52
3:E:17:TYR:O	3:E:21:VAL:HG23	2.08	0.52
2:B:92:SER:HA	2:B:304:LYS:O	2.10	0.52
13:G:1304:PCW:H441	12:E:1301:CLR:H263	1.91	0.52
2:D:58:LEU:O	2:D:61:THR:OG1	2.25	0.51
1:C:825:GLU:OE2	1:C:938:LYS:NZ	2.43	0.51
2:B:58:LEU:O	2:B:61:THR:OG1	2.26	0.51
2:D:191:PRO:HG3	2:D:208:GLN:O	2.11	0.51
2:D:279:LYS:HG3	2:D:296:ARG:HB3	1.92	0.51
1:A:411:PHE:HZ	1:A:463:CYS:SG	2.32	0.51
12:G:1301:CLR:H221	13:E:1304:PCW:H483	1.92	0.51
13:C:1108:PCW:H271	2:D:47:LEU:CD2	2.41	0.51
1:A:517:ARG:HG2	1:A:517:ARG:HH11	1.76	0.51
1:A:968:LEU:O	1:A:974:THR:HG21	2.11	0.51
1:A:212:LYS:HG2	1:A:226:THR:HG22	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:825:GLU:OE2	1:A:938:LYS:NZ	2.43	0.51
1:C:298:VAL:HG12	13:C:1114:PCW:H162	1.94	0.51
1:C:596:ARG:HB2	1:C:599:VAL:HG23	1.93	0.51
1:C:997:ILE:HG21	13:C:1108:PCW:H272	1.92	0.51
2:B:191:PRO:HG3	2:B:208:GLN:O	2.11	0.50
1:C:212:LYS:HG2	1:C:226:THR:HG22	1.93	0.50
1:A:997:ILE:HG21	13:A:1108:PCW:H272	1.92	0.50
1:C:762:VAL:HG13	1:C:832:MET:HE1	1.93	0.50
1:C:517:ARG:HG2	1:C:517:ARG:HH11	1.76	0.50
1:A:52:HIS:CE1	1:A:59:LEU:HD12	2.41	0.50
1:A:298:VAL:HG12	13:A:1114:PCW:H162	1.93	0.50
13:A:1108:PCW:H271	2:B:47:LEU:CD2	2.41	0.50
1:A:846:ASN:OD1	1:A:846:ASN:N	2.42	0.50
2:B:225:LYS:O	2:B:269:THR:OG1	2.30	0.50
1:A:565:TYR:HB3	1:A:571:PHE:HE2	1.77	0.50
1:C:565:TYR:HB3	1:C:571:PHE:HE2	1.77	0.50
1:C:897:ASP:OD1	1:C:897:ASP:N	2.45	0.50
1:A:920:THR:HG23	1:A:980:MET:HE2	1.93	0.50
1:C:424:ILE:HG21	1:C:555:PHE:HB3	1.94	0.50
1:C:515:LEU:HD11	1:C:535:LYS:HE2	1.94	0.50
13:C:1112:PCW:H19	13:E:1302:PCW:H40	1.94	0.50
1:C:968:LEU:O	1:C:974:THR:HG21	2.11	0.49
13:C:1114:PCW:H19	12:D:501:CLR:H151	1.93	0.49
1:A:241:ASN:H	1:A:241:ASN:ND2	2.06	0.49
1:A:391:MET:HE1	1:A:411:PHE:CD2	2.48	0.49
1:A:424:ILE:HG21	1:A:555:PHE:HB3	1.94	0.49
1:C:920:THR:HG23	1:C:980:MET:HE2	1.93	0.49
1:A:762:VAL:HG13	1:A:832:MET:HE1	1.93	0.49
13:A:1114:PCW:H19	12:B:501:CLR:H151	1.93	0.49
1:C:492:ILE:HD12	1:C:578:PHE:CE1	2.47	0.49
13:A:1112:PCW:H19	13:G:1302:PCW:H40	1.94	0.49
1:A:596:ARG:HB2	1:A:599:VAL:HG23	1.93	0.49
1:C:411:PHE:CD1	1:C:411:PHE:N	2.81	0.49
1:C:714:VAL:HG12	1:C:725:LEU:HD23	1.95	0.49
2:D:56:GLN:HE22	2:D:59:LEU:HD12	1.78	0.49
2:D:132:ALA:O	2:D:209:TYR:HB3	2.13	0.49
1:A:897:ASP:OD1	1:A:897:ASP:N	2.45	0.49
2:B:132:ALA:O	2:B:209:TYR:HB3	2.13	0.49
1:C:391:MET:HE1	1:C:411:PHE:CD2	2.48	0.49
1:C:52:HIS:CE1	1:C:59:LEU:HB2	2.48	0.49
1:A:492:ILE:HD12	1:A:578:PHE:CE1	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:424:ILE:HG22	1:C:555:PHE:HD2	1.78	0.48
1:C:167:GLN:HE22	1:C:198:ARG:NH2	2.11	0.48
1:C:846:ASN:OD1	1:C:846:ASN:N	2.42	0.48
1:A:52:HIS:CE1	1:A:59:LEU:HB2	2.48	0.48
1:A:411:PHE:N	1:A:411:PHE:CD1	2.81	0.48
1:A:714:VAL:HG12	1:A:725:LEU:HD23	1.95	0.48
1:C:615:MET:HB3	1:C:689:VAL:HG22	1.96	0.48
1:A:390:HIS:CD2	1:A:399:GLU:HG2	2.49	0.48
2:B:110:MET:HE1	2:B:157:LEU:HD13	1.96	0.48
2:D:81:ALA:HB3	2:D:82:PRO:HD3	1.96	0.48
2:D:163:LEU:HD23	4:K:6:FUC:H61	1.95	0.48
1:A:170:LEU:HD11	1:A:177:LYS:HB3	1.96	0.48
1:A:515:LEU:HD11	1:A:535:LYS:HE2	1.94	0.48
1:C:52:HIS:CE1	1:C:59:LEU:HD12	2.41	0.48
1:A:167:GLN:HE22	1:A:198:ARG:NH2	2.11	0.48
2:B:81:ALA:HB3	2:B:82:PRO:HD3	1.96	0.48
2:D:225:LYS:O	2:D:269:THR:OG1	2.30	0.48
1:A:102:ILE:O	1:A:106:ILE:HG23	2.14	0.48
1:A:615:MET:HB2	1:A:633:ILE:HD13	1.96	0.48
1:C:390:HIS:CD2	1:C:399:GLU:HG2	2.49	0.48
1:C:540:ASN:N	1:C:540:ASN:HD22	2.12	0.48
2:D:110:MET:HE1	2:D:157:LEU:HD13	1.96	0.48
1:A:424:ILE:HG22	1:A:555:PHE:HD2	1.78	0.48
1:C:170:LEU:HD11	1:C:177:LYS:HB3	1.96	0.48
1:C:615:MET:HB2	1:C:633:ILE:HD13	1.96	0.48
2:B:56:GLN:HE22	2:B:59:LEU:HD12	1.78	0.47
1:C:827:ALA:HB2	1:C:831:ILE:HD11	1.96	0.47
1:A:827:ALA:HB2	1:A:831:ILE:HD11	1.96	0.47
1:C:102:ILE:O	1:C:106:ILE:HG23	2.14	0.47
1:C:203:LEU:HB2	1:C:243:ALA:HB3	1.97	0.47
2:B:134:TYR:HE1	2:B:242:LEU:HG	1.80	0.47
13:G:1304:PCW:H471	13:E:1304:PCW:H241	1.96	0.47
13:A:1108:PCW:H72	13:A:1108:PCW:H41	1.69	0.47
2:D:134:TYR:HE1	2:D:242:LEU:HG	1.80	0.47
2:B:163:LEU:HD23	4:F:6:FUC:H61	1.96	0.47
13:G:1304:PCW:H483	12:E:1301:CLR:H221	1.95	0.47
1:A:203:LEU:HB2	1:A:243:ALA:HB3	1.97	0.47
13:A:1110:PCW:H282	13:C:1110:PCW:H282	1.97	0.47
1:A:111:CYS:SG	1:A:329:VAL:HG11	2.55	0.46
1:A:615:MET:HB3	1:A:689:VAL:HG22	1.96	0.46
1:A:900:ASP:OD2	1:A:906:TRP:NE1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:810:ILE:HG12	1:A:923:PHE:HD2	1.81	0.46
1:C:997:ILE:HG12	13:C:1108:PCW:H472	1.98	0.46
1:A:36:LYS:HZ1	1:A:272:THR:HB	1.81	0.46
2:B:229:ILE:H	2:B:229:ILE:HG13	1.56	0.46
1:C:482:PHE:CE1	1:C:487:LYS:HA	2.50	0.46
1:C:955:ILE:HA	1:C:958:LEU:HD12	1.98	0.46
1:A:540:ASN:N	1:A:540:ASN:HD22	2.12	0.46
13:G:1302:PCW:H382	13:G:1302:PCW:H411	1.80	0.46
1:A:482:PHE:CE1	1:A:487:LYS:HA	2.50	0.46
1:A:696:GLN:O	1:A:700:ILE:HG12	2.16	0.46
2:B:122:SER:HA	2:B:123:PRO:HA	1.57	0.46
1:C:517:ARG:HH11	1:C:517:ARG:CG	2.29	0.46
2:B:107:HIS:O	2:B:111:ASP:HB2	2.15	0.46
1:A:477:ILE:CD1	1:A:503:TYR:HE1	2.29	0.46
1:A:517:ARG:HH11	1:A:517:ARG:CG	2.29	0.46
1:C:810:ILE:HG12	1:C:923:PHE:HD2	1.80	0.46
1:C:900:ASP:OD2	1:C:906:TRP:NE1	2.48	0.46
2:D:120:GLY:O	2:D:151:ARG:NH2	2.49	0.46
2:D:215:CYS:SG	2:D:263:ILE:HD13	2.56	0.46
1:A:955:ILE:HA	1:A:958:LEU:HD12	1.98	0.45
1:C:376:PHD:OD2	1:C:378:THR:O	2.34	0.45
2:D:140:LEU:HD23	2:D:252:LEU:HD12	1.98	0.45
1:A:376:PHD:OD2	1:A:378:THR:O	2.34	0.45
1:A:679:ASP:O	1:A:683:HIS:HB2	2.16	0.45
2:D:15:LYS:C	2:D:17:LEU:H	2.25	0.45
1:A:997:ILE:HG12	13:A:1108:PCW:H472	1.98	0.45
2:B:65:PHE:HE1	2:B:251:ARG:NH1	2.14	0.45
1:C:696:GLN:O	1:C:700:ILE:HG12	2.16	0.45
1:A:127:ASN:OD1	1:A:127:ASN:N	2.30	0.45
2:D:107:HIS:O	2:D:111:ASP:HB2	2.15	0.45
2:D:229:ILE:HD12	2:D:229:ILE:O	2.16	0.45
2:B:120:GLY:O	2:B:151:ARG:NH2	2.49	0.45
2:B:215:CYS:SG	2:B:263:ILE:HD13	2.56	0.45
2:B:229:ILE:HD12	2:B:229:ILE:O	2.16	0.45
1:A:45:LYS:NZ	1:A:234:GLU:OE1	2.40	0.45
1:C:235:ASN:OD1	1:C:236:PRO:HD2	2.17	0.45
1:C:732:VAL:HG13	1:C:748:MET:HE3	1.97	0.45
1:A:421:LEU:HD13	1:A:586:VAL:HG12	1.99	0.45
1:C:477:ILE:CD1	1:C:503:TYR:HE1	2.29	0.45
1:C:648:LEU:O	1:C:649:ASN:HB2	2.16	0.45
1:C:679:ASP:O	1:C:683:HIS:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:THR:OG1	1:A:86:THR:N	2.49	0.45
1:A:420:ALA:O	1:A:424:ILE:HG13	2.16	0.45
2:B:140:LEU:HD23	2:B:252:LEU:HD12	1.98	0.45
1:C:52:HIS:CD2	1:C:57:THR:HG23	2.52	0.45
1:C:85:THR:OG1	1:C:86:THR:N	2.49	0.45
2:D:215:CYS:HA	2:D:278:CYS:HA	1.98	0.45
1:A:52:HIS:CD2	1:A:57:THR:HG23	2.52	0.45
1:A:810:ILE:O	1:A:815:ASP:HB2	2.17	0.45
1:C:111:CYS:SG	1:C:329:VAL:HG11	2.55	0.45
1:A:235:ASN:OD1	1:A:236:PRO:HD2	2.17	0.45
1:A:648:LEU:O	1:A:649:ASN:HB2	2.17	0.45
1:A:732:VAL:HG13	1:A:748:MET:HE3	1.97	0.45
1:A:1004:MET:SD	13:A:1108:PCW:H422	2.57	0.45
2:B:15:LYS:C	2:B:17:LEU:H	2.25	0.45
2:B:225:LYS:HD2	2:B:272:MET:SD	2.57	0.44
2:B:265:PHE:HB3	2:B:268:LEU:HD12	1.99	0.44
1:C:420:ALA:O	1:C:424:ILE:HG13	2.16	0.44
1:C:1004:MET:SD	13:C:1108:PCW:H422	2.57	0.44
2:D:122:SER:HA	2:D:123:PRO:HA	1.57	0.44
1:A:594:PRO:HA	1:A:595:PRO:HD3	1.85	0.44
1:A:1004:MET:HE3	2:D:57:VAL:HG22	1.99	0.44
13:A:1108:PCW:H271	2:B:47:LEU:HD23	1.99	0.44
1:C:284:ILE:HG21	1:C:362:GLU:HB3	1.99	0.44
1:C:511:PRO:O	1:C:515:LEU:HB2	2.18	0.44
2:D:65:PHE:HE1	2:D:251:ARG:NH1	2.14	0.44
2:D:225:LYS:HD2	2:D:272:MET:SD	2.57	0.44
2:D:265:PHE:CZ	2:D:276:ILE:HD12	2.52	0.44
2:B:215:CYS:HA	2:B:278:CYS:HA	1.98	0.44
1:A:100:PHE:HB3	1:A:337:LEU:HD13	1.99	0.44
2:B:265:PHE:CZ	2:B:276:ILE:HD12	2.52	0.44
1:A:476:LYS:HD3	1:A:479:GLU:HB3	1.99	0.44
1:A:774:LYS:HE2	1:A:940:ARG:HG3	1.99	0.44
1:C:45:LYS:NZ	1:C:234:GLU:OE1	2.40	0.44
1:C:476:LYS:HD3	1:C:479:GLU:HB3	1.99	0.44
2:D:114:ASN:OD1	2:D:154:ARG:NH1	2.51	0.44
1:A:311:LEU:HD11	1:A:317:TRP:CZ3	2.53	0.44
1:A:545:LEU:HB2	1:A:552:VAL:HG21	2.00	0.44
1:A:672:ASP:O	1:A:673:LEU:HD23	2.18	0.44
1:C:339:THR:HG23	1:C:820:ILE:HD13	2.00	0.44
1:A:945:PHE:HD1	13:A:1109:PCW:H121	1.83	0.44
3:G:4:GLU:HB2	3:G:5:GLY:H	1.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:810:ILE:O	1:C:815:ASP:HB2	2.17	0.44
2:B:114:ASN:OD1	2:B:154:ARG:NH1	2.51	0.44
1:C:374:CYS:HB2	1:C:714:VAL:HG22	2.00	0.44
1:C:421:LEU:HD13	1:C:586:VAL:HG12	1.99	0.44
13:E:1303:PCW:H283	13:E:1304:PCW:H222	2.00	0.44
1:A:817:VAL:HB	1:A:818:PRO:HD3	2.00	0.44
1:C:774:LYS:HE2	1:C:940:ARG:HG3	1.99	0.44
1:A:339:THR:HG23	1:A:820:ILE:HD13	2.00	0.43
2:B:81:ALA:HB2	2:B:178:VAL:HB	1.99	0.43
1:C:90:ILE:O	1:C:94:ARG:HG2	2.18	0.43
1:C:548:LEU:HB3	1:C:550:GLU:HG3	2.00	0.43
1:C:817:VAL:HB	1:C:818:PRO:HD3	2.00	0.43
1:A:95:GLN:HG3	1:A:148:TYR:HB2	2.00	0.43
1:A:284:ILE:HG21	1:A:362:GLU:HB3	2.00	0.43
1:A:507:MET:HG2	1:A:556:CYS:SG	2.59	0.43
13:G:1303:PCW:H283	13:G:1304:PCW:H222	2.00	0.43
1:A:139:VAL:HG21	1:A:812:LEU:HD21	2.00	0.43
2:D:81:ALA:HB2	2:D:178:VAL:HB	1.99	0.43
2:D:234:LEU:HG	2:D:241:PRO:HG3	2.01	0.43
1:C:808:LEU:HD23	1:C:808:LEU:HA	1.84	0.43
2:D:265:PHE:HB3	2:D:268:LEU:HD12	1.99	0.43
1:A:631:VAL:HG23	1:A:633:ILE:HG13	2.01	0.43
2:B:299:VAL:HG12	2:B:301:ILE:HG13	2.00	0.43
1:C:100:PHE:HB3	1:C:337:LEU:HD13	1.99	0.43
1:C:545:LEU:HB2	1:C:552:VAL:HG21	2.00	0.43
1:C:732:VAL:HG11	1:C:758:ILE:HD11	2.01	0.43
13:C:1108:PCW:H271	2:D:47:LEU:HD23	1.99	0.43
2:D:232:PHE:HB2	2:D:262:ALA:HB3	2.01	0.43
1:A:374:CYS:HB2	1:A:714:VAL:HG22	2.00	0.43
2:B:167:THR:HG22	2:B:169:GLY:H	1.84	0.43
1:C:912:LYS:HD3	1:C:912:LYS:HA	1.87	0.43
13:E:1303:PCW:H262	13:E:1304:PCW:C20	2.48	0.43
1:C:486:ASN:HB3	1:C:488:TYR:CE1	2.54	0.43
1:C:945:PHE:HD1	13:C:1109:PCW:H121	1.83	0.43
13:E:1302:PCW:H411	13:E:1302:PCW:H382	1.80	0.43
1:A:201:ALA:HB1	1:A:260:TYR:O	2.19	0.43
1:A:511:PRO:O	1:A:515:LEU:HB2	2.17	0.43
1:C:311:LEU:HD11	1:C:317:TRP:CZ3	2.53	0.43
1:C:507:MET:HG2	1:C:556:CYS:SG	2.59	0.43
1:A:996:LEU:CD2	13:C:1110:PCW:H283	2.47	0.43
12:A:1105:CLR:H161	12:A:1105:CLR:H222	1.97	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A:1110:PCW:H283	1:C:996:LEU:CD2	2.43	0.43
13:A:1111:PCW:H221	13:A:1111:PCW:H471	2.01	0.43
13:G:1303:PCW:H262	13:G:1304:PCW:C20	2.48	0.43
1:C:139:VAL:HG21	1:C:812:LEU:HD21	2.00	0.43
1:A:997:ILE:HG21	13:A:1108:PCW:C27	2.49	0.42
2:B:206:TYR:O	2:B:206:TYR:HD1	2.02	0.42
2:B:232:PHE:HB2	2:B:262:ALA:HB3	2.01	0.42
1:C:672:ASP:O	1:C:673:LEU:HD23	2.18	0.42
13:C:1111:PCW:H221	13:C:1111:PCW:H471	2.01	0.42
2:D:299:VAL:HG12	2:D:301:ILE:HG13	2.00	0.42
1:A:732:VAL:HG11	1:A:758:ILE:HD11	2.01	0.42
1:A:90:ILE:O	1:A:94:ARG:HG2	2.18	0.42
2:D:52:ILE:O	2:D:55:ILE:HG22	2.20	0.42
2:D:206:TYR:O	2:D:206:TYR:HD1	2.02	0.42
13:A:1108:PCW:C40	13:A:1108:PCW:H20	2.50	0.42
1:C:476:LYS:HE2	1:C:493:HIS:CE1	2.55	0.42
1:C:720:ASN:OD1	1:C:720:ASN:N	2.53	0.42
2:D:207:ASN:ND2	2:D:237:TYR:CZ	2.88	0.42
2:D:224:GLU:H	2:D:224:GLU:HG3	1.46	0.42
1:A:486:ASN:HB3	1:A:488:TYR:CE1	2.54	0.42
1:A:548:LEU:HB3	1:A:550:GLU:HG3	2.00	0.42
1:C:95:GLN:HG3	1:C:148:TYR:HB2	2.00	0.42
1:C:169:ALA:O	1:C:179:THR:HA	2.20	0.42
1:C:502:ARG:HG2	1:C:562:GLU:HB3	2.02	0.42
1:C:676:GLU:OE1	1:C:676:GLU:N	2.46	0.42
12:A:1105:CLR:H273	13:C:1110:PCW:H281	2.02	0.42
1:A:847:GLU:H	1:A:847:GLU:HG3	1.49	0.42
2:B:207:ASN:ND2	2:B:237:TYR:CZ	2.88	0.42
2:B:234:LEU:HG	2:B:241:PRO:HG3	2.01	0.42
13:C:1108:PCW:C40	13:C:1108:PCW:H20	2.50	0.42
1:A:169:ALA:O	1:A:179:THR:HA	2.20	0.42
1:A:502:ARG:HG2	1:A:562:GLU:HB3	2.02	0.42
13:G:1304:PCW:C41	13:E:1304:PCW:H461	2.45	0.42
1:A:997:ILE:HG21	13:A:1108:PCW:C26	2.50	0.42
2:B:189:PRO:HG2	2:B:245:TYR:CD2	2.55	0.42
13:G:1304:PCW:H451	13:E:1304:PCW:C26	2.47	0.42
1:A:476:LYS:HE2	1:A:493:HIS:CE1	2.55	0.41
1:C:791:LEU:HB3	13:C:1114:PCW:H282	2.02	0.41
2:D:160:CYS:SG	2:D:262:ALA:HB1	2.60	0.41
2:D:167:THR:HG22	2:D:169:GLY:H	1.84	0.41
2:D:265:PHE:HB3	2:D:268:LEU:CD1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:662:ALA:HB2	1:A:687:GLU:HB2	2.02	0.41
2:B:52:ILE:O	2:B:55:ILE:HG22	2.20	0.41
2:B:245:TYR:HB3	2:B:246:PRO:HA	2.02	0.41
1:C:201:ALA:HB1	1:C:260:TYR:O	2.19	0.41
1:A:482:PHE:HD2	1:A:489:GLN:HB2	1.85	0.41
1:A:548:LEU:HD12	1:A:548:LEU:HA	1.89	0.41
1:A:997:ILE:HG21	13:A:1108:PCW:H261	2.02	0.41
12:A:1105:CLR:H273	13:C:1110:PCW:C27	2.51	0.41
13:A:1112:PCW:H381	13:A:1112:PCW:H411	1.87	0.41
1:C:552:VAL:HA	1:C:590:ALA:HA	2.03	0.41
1:C:631:VAL:HG23	1:C:633:ILE:HG13	2.01	0.41
10:C:1103:ATP:H5'1	10:C:1103:ATP:O1B	2.20	0.41
2:D:193:LYS:HA	2:D:206:TYR:OH	2.21	0.41
1:A:791:LEU:HB3	13:A:1114:PCW:H282	2.02	0.41
1:A:992:PHE:HZ	12:G:1301:CLR:H20	1.85	0.41
2:B:265:PHE:HB3	2:B:268:LEU:CD1	2.50	0.41
1:C:473:ARG:HD3	1:C:496:GLU:OE1	2.21	0.41
1:C:611:ILE:HD11	1:C:762:VAL:HG21	2.03	0.41
1:A:488:TYR:CD1	1:A:488:TYR:C	2.99	0.41
13:G:1304:PCW:H241	13:E:1304:PCW:H471	2.02	0.41
2:D:189:PRO:HG2	2:D:245:TYR:CD2	2.55	0.41
10:A:1103:ATP:H5'1	10:A:1103:ATP:O1B	2.20	0.41
1:C:997:ILE:HG21	13:C:1108:PCW:C27	2.49	0.41
2:D:93:ILE:HB	2:D:305:SER:OG	2.20	0.41
2:D:106:MET:O	2:D:110:MET:HG2	2.21	0.41
1:A:552:VAL:HA	1:A:590:ALA:HA	2.02	0.41
2:B:106:MET:O	2:B:110:MET:HG2	2.21	0.41
1:C:488:TYR:CD1	1:C:488:TYR:C	2.99	0.41
1:C:997:ILE:HG21	13:C:1108:PCW:C26	2.50	0.41
2:B:93:ILE:HB	2:B:305:SER:OG	2.20	0.41
2:B:193:LYS:HA	2:B:206:TYR:OH	2.21	0.41
1:C:658:ARG:HA	1:C:658:ARG:HD3	1.90	0.41
13:C:1108:PCW:H72	13:C:1108:PCW:H41	1.69	0.41
1:A:473:ARG:HD3	1:A:496:GLU:OE1	2.21	0.41
1:A:602:ALA:HB3	1:A:755:PHE:HD2	1.86	0.41
1:A:720:ASN:N	1:A:720:ASN:OD1	2.53	0.41
1:A:808:LEU:HD23	1:A:808:LEU:HA	1.84	0.41
1:A:812:LEU:HD13	1:A:812:LEU:HA	1.92	0.41
1:A:912:LYS:HD3	1:A:912:LYS:HA	1.87	0.41
2:B:160:CYS:SG	2:B:262:ALA:HB1	2.60	0.41
2:B:195:THR:HG22	2:B:196:THR:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:B:502:CLR:H161	12:B:502:CLR:H222	1.96	0.41
2:D:22:LYS:HB2	2:D:24:GLU:HG3	2.03	0.41
2:D:195:THR:HG22	2:D:196:THR:N	2.36	0.41
2:B:22:LYS:HB2	2:B:24:GLU:HG3	2.03	0.40
1:A:611:ILE:HD11	1:A:762:VAL:HG21	2.03	0.40
1:C:360:ASN:HD22	1:C:360:ASN:HA	1.47	0.40
1:A:575:GLU:HB3	1:A:576:PRO:CD	2.50	0.40
1:C:696:GLN:OE1	1:C:696:GLN:N	2.47	0.40
2:D:283:GLU:C	2:D:285:ILE:H	2.30	0.40
1:A:540:ASN:HD22	1:A:540:ASN:H	1.70	0.40
1:A:891:ASP:O	1:A:892:ASP:C	2.64	0.40
2:B:227:GLY:HA3	2:B:267:ASN:HB3	2.04	0.40
1:C:482:PHE:HD2	1:C:489:GLN:HB2	1.85	0.40
1:C:772:LEU:HD23	1:C:772:LEU:HA	1.97	0.40
1:C:784:ILE:C	1:C:786:GLU:H	2.30	0.40
1:C:992:PHE:HZ	12:E:1301:CLR:H20	1.85	0.40
1:C:997:ILE:HG21	13:C:1108:PCW:H261	2.02	0.40
2:D:146:GLN:NE2	2:D:254:LYS:HG2	2.36	0.40
2:D:245:TYR:HB3	2:D:246:PRO:HA	2.02	0.40
1:A:824:TYR:HB2	1:A:951:ASN:HD21	1.86	0.40
2:B:283:GLU:C	2:B:285:ILE:H	2.30	0.40
1:C:662:ALA:HB2	1:C:687:GLU:HB2	2.02	0.40
1:C:824:TYR:HB2	1:C:951:ASN:HD21	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	990/1028 (96%)	911 (92%)	71 (7%)	8 (1%)	16 44
1	C	990/1028 (96%)	911 (92%)	71 (7%)	8 (1%)	16 44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	292/305 (96%)	256 (88%)	35 (12%)	1 (0%)	36	65
2	D	292/305 (96%)	256 (88%)	35 (12%)	1 (0%)	36	65
3	E	38/94 (40%)	33 (87%)	5 (13%)	0	100	100
3	G	38/94 (40%)	33 (87%)	5 (13%)	0	100	100
All	All	2640/2854 (92%)	2400 (91%)	222 (8%)	18 (1%)	20	47

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	85	THR
1	C	85	THR
1	A	315	TYR
1	C	315	TYR
1	A	481	PRO
1	A	988	TRP
1	C	481	PRO
1	C	988	TRP
1	A	200	PRO
1	A	985	PRO
2	B	155	MET
1	C	200	PRO
1	C	985	PRO
2	D	155	MET
1	A	124	GLU
1	C	124	GLU
1	A	801	PRO
1	C	801	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	840/868 (97%)	765 (91%)	75 (9%)	9	31
1	C	840/868 (97%)	765 (91%)	75 (9%)	9	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	258/266 (97%)	218 (84%)	40 (16%)	2	10
2	D	258/266 (97%)	218 (84%)	40 (16%)	2	10
3	E	33/75 (44%)	30 (91%)	3 (9%)	9	30
3	G	33/75 (44%)	30 (91%)	3 (9%)	9	30
All	All	2262/2418 (94%)	2026 (90%)	236 (10%)	9	24

All (236) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	GLU
1	A	37	LYS
1	A	45	LYS
1	A	63	LEU
1	A	64	THR
1	A	65	ASN
1	A	75	ASP
1	A	127	ASN
1	A	158	MET
1	A	167	GLN
1	A	173	ARG
1	A	223	GLU
1	A	231	PHE
1	A	240	ARG
1	A	241	ASN
1	A	248	ASN
1	A	261	THR
1	A	263	ASP
1	A	311	LEU
1	A	331	ASN
1	A	332	VAL
1	A	334	GLU
1	A	343	CYS
1	A	344	LEU
1	A	350	ARG
1	A	351	MET
1	A	357	LEU
1	A	360	ASN
1	A	362	GLU
1	A	367	LEU
1	A	381	LEU
1	A	411	PHE

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Mol	Chain	Res	Type
1	A	415	SER
1	A	434	GLN
1	A	440	VAL
1	A	445	ARG
1	A	470	MET
1	A	484	SER
1	A	485	THR
1	A	488	TYR
1	A	493	HIS
1	A	515	LEU
1	A	522	LEU
1	A	540	ASN
1	A	548	LEU
1	A	571	PHE
1	A	620	HIS
1	A	661	LYS
1	A	670	LEU
1	A	678	LEU
1	A	683	HIS
1	A	692	ARG
1	A	708	GLN
1	A	767	LEU
1	A	788	THR
1	A	812	LEU
1	A	815	ASP
1	A	822	LEU
1	A	834	ARG
1	A	837	ARG
1	A	846	ASN
1	A	847	GLU
1	A	872	ILE
1	A	887	ARG
1	A	892	ASP
1	A	894	TRP
1	A	901	SER
1	A	923	PHE
1	A	935	ILE
1	A	943	SER
1	A	975	ASP
1	A	986	SER
1	A	1007	PHE
1	A	1011	ARG

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Mol	Chain	Res	Type
1	A	1019	GLN
2	B	20	SER
2	B	26	LEU
2	B	28	ARG
2	B	32	SER
2	B	37	PHE
2	B	64	ASP
2	B	73	VAL
2	B	94	SER
2	B	107	HIS
2	B	135	ILE
2	B	137	ARG
2	B	144	GLN
2	B	146	GLN
2	B	154	ARG
2	B	156	TRP
2	B	157	LEU
2	B	160	CYS
2	B	161	SER
2	B	167	THR
2	B	196	THR
2	B	200	GLU
2	B	203	GLN
2	B	211	LEU
2	B	213	LEU
2	B	214	ARG
2	B	218	LYS
2	B	219	ARG
2	B	229	ILE
2	B	242	LEU
2	B	251	ARG
2	B	266	THR
2	B	268	LEU
2	B	269	THR
2	B	272	MET
2	B	284	ASN
2	B	285	ILE
2	B	287	TYR
2	B	289	GLU
2	B	292	ARG
2	B	294	ARG
3	G	4	GLU

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Mol	Chain	Res	Type
3	G	13	THR
3	G	33	ILE
1	C	34	GLU
1	C	37	LYS
1	C	45	LYS
1	C	63	LEU
1	C	64	THR
1	C	65	ASN
1	C	75	ASP
1	C	127	ASN
1	C	158	MET
1	C	167	GLN
1	C	173	ARG
1	C	223	GLU
1	C	231	PHE
1	C	240	ARG
1	C	241	ASN
1	C	248	ASN
1	C	261	THR
1	C	263	ASP
1	C	311	LEU
1	C	331	ASN
1	C	332	VAL
1	C	334	GLU
1	C	343	CYS
1	C	344	LEU
1	C	350	ARG
1	C	351	MET
1	C	357	LEU
1	C	360	ASN
1	C	362	GLU
1	C	367	LEU
1	C	381	LEU
1	C	411	PHE
1	C	415	SER
1	C	434	GLN
1	C	440	VAL
1	C	445	ARG
1	C	470	MET
1	C	484	SER
1	C	485	THR
1	C	488	TYR

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Mol	Chain	Res	Type
1	C	493	HIS
1	C	515	LEU
1	C	522	LEU
1	C	540	ASN
1	C	548	LEU
1	C	571	PHE
1	C	620	HIS
1	C	661	LYS
1	C	670	LEU
1	C	678	LEU
1	C	683	HIS
1	C	692	ARG
1	C	708	GLN
1	C	767	LEU
1	C	788	THR
1	C	812	LEU
1	C	815	ASP
1	C	822	LEU
1	C	834	ARG
1	C	837	ARG
1	C	846	ASN
1	C	847	GLU
1	C	872	ILE
1	C	887	ARG
1	C	892	ASP
1	C	894	TRP
1	C	901	SER
1	C	923	PHE
1	C	935	ILE
1	C	943	SER
1	C	975	ASP
1	C	986	SER
1	C	1007	PHE
1	C	1011	ARG
1	C	1019	GLN
2	D	20	SER
2	D	26	LEU
2	D	28	ARG
2	D	32	SER
2	D	37	PHE
2	D	64	ASP
2	D	73	VAL

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Mol	Chain	Res	Type
2	D	94	SER
2	D	107	HIS
2	D	135	ILE
2	D	137	ARG
2	D	144	GLN
2	D	146	GLN
2	D	154	ARG
2	D	156	TRP
2	D	157	LEU
2	D	160	CYS
2	D	161	SER
2	D	167	THR
2	D	196	THR
2	D	200	GLU
2	D	203	GLN
2	D	211	LEU
2	D	213	LEU
2	D	214	ARG
2	D	218	LYS
2	D	219	ARG
2	D	229	ILE
2	D	242	LEU
2	D	251	ARG
2	D	266	THR
2	D	268	LEU
2	D	269	THR
2	D	272	MET
2	D	284	ASN
2	D	285	ILE
2	D	287	TYR
2	D	289	GLU
2	D	292	ARG
2	D	294	ARG
3	E	4	GLU
3	E	13	THR
3	E	33	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	HIS
1	A	241	ASN

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Mol	Chain	Res	Type
1	A	360	ASN
1	A	434	GLN
1	A	474	ASN
1	A	539	GLN
1	A	540	ASN
1	A	904	GLN
2	B	56	GLN
2	B	80	HIS
2	B	203	GLN
1	C	52	HIS
1	C	241	ASN
1	C	360	ASN
1	C	434	GLN
1	C	474	ASN
1	C	540	ASN
1	C	649	ASN
1	C	904	GLN
2	D	56	GLN
2	D	80	HIS
2	D	203	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	PHD	A	376	1,8	9,11,12	1.82	1 (11%)	9,15,17	1.28	1 (11%)
1	PHD	C	376	1,8	9,11,12	1.83	1 (11%)	9,15,17	1.28	1 (11%)

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
1	PHD	A	376	1,8	-	2/8/11/13	-
1	PHD	C	376	1,8	-	2/8/11/13	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	376	PHD	P-OD1	-4.66	1.51	1.59
1	A	376	PHD	P-OD1	-4.61	1.51	1.59

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	376	PHD	OD1-CG-CB	2.54	116.91	110.95
1	A	376	PHD	OD1-CG-CB	2.54	116.91	110.95

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	376	PHD	CA-CB-CG-OD1
1	C	376	PHD	CA-CB-CG-OD1
1	A	376	PHD	CA-CB-CG-OD2
1	C	376	PHD	CA-CB-CG-OD2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	376	PHD	1	0
1	C	376	PHD	1	0

5.5 Carbohydrates

38 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	$\# Z > 2$
4	NAG	F	1	4,2	14,14,15	1.12	1 (7%)	17,19,21	1.25	1 (5%)
4	NAG	F	2	4	14,14,15	0.21	0	17,19,21	0.58	0
4	BMA	F	3	4	11,11,12	0.77	0	15,15,17	1.19	2 (13%)
4	MAN	F	4	4	11,11,12	0.73	0	15,15,17	0.96	2 (13%)
4	MAN	F	5	4	11,11,12	0.69	0	15,15,17	0.91	2 (13%)
4	FUC	F	6	4	10,10,11	1.03	1 (10%)	14,14,16	0.66	0
5	NAG	H	1	5,2	14,14,15	0.63	1 (7%)	17,19,21	1.16	2 (11%)
5	NAG	H	2	5	14,14,15	0.33	0	17,19,21	1.61	2 (11%)
5	BMA	H	3	5	11,11,12	1.22	1 (9%)	15,15,17	0.96	1 (6%)
5	MAN	H	4	5	11,11,12	1.41	3 (27%)	15,15,17	1.27	2 (13%)
5	NAG	H	5	5	14,14,15	0.69	0	17,19,21	0.83	1 (5%)
5	MAN	H	6	5	11,11,12	0.71	0	15,15,17	0.91	2 (13%)
6	NAG	I	1	6,2	14,14,15	0.79	1 (7%)	17,19,21	1.57	1 (5%)
6	NAG	I	2	6	14,14,15	0.20	0	17,19,21	0.62	1 (5%)
6	BMA	I	3	6	11,11,12	0.58	0	15,15,17	1.17	1 (6%)
6	MAN	I	4	6	11,11,12	0.65	0	15,15,17	0.94	2 (13%)
6	FUC	I	5	6	10,10,11	0.99	1 (10%)	14,14,16	0.66	0
7	NAG	J	1	7,2	14,14,15	0.49	0	17,19,21	0.63	0
7	NAG	J	2	7	14,14,15	0.19	0	17,19,21	0.40	0
4	NAG	K	1	4,2	14,14,15	1.12	1 (7%)	17,19,21	1.25	1 (5%)
4	NAG	K	2	4	14,14,15	0.21	0	17,19,21	0.59	0
4	BMA	K	3	4	11,11,12	0.79	0	15,15,17	1.18	2 (13%)
4	MAN	K	4	4	11,11,12	0.73	0	15,15,17	0.97	2 (13%)
4	MAN	K	5	4	11,11,12	0.69	0	15,15,17	0.91	2 (13%)
4	FUC	K	6	4	10,10,11	1.03	1 (10%)	14,14,16	0.66	0
5	NAG	L	1	5,2	14,14,15	0.62	1 (7%)	17,19,21	1.16	2 (11%)
5	NAG	L	2	5	14,14,15	0.33	0	17,19,21	1.61	2 (11%)
5	BMA	L	3	5	11,11,12	1.22	1 (9%)	15,15,17	0.96	1 (6%)
5	MAN	L	4	5	11,11,12	1.41	2 (18%)	15,15,17	1.27	2 (13%)
5	NAG	L	5	5	14,14,15	0.70	0	17,19,21	0.83	1 (5%)
5	MAN	L	6	5	11,11,12	0.71	0	15,15,17	0.92	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	M	1	6,2	14,14,15	0.79	1 (7%)	17,19,21	1.57	1 (5%)
6	NAG	M	2	6	14,14,15	0.20	0	17,19,21	0.63	1 (5%)
6	BMA	M	3	6	11,11,12	0.58	0	15,15,17	1.17	1 (6%)
6	MAN	M	4	6	11,11,12	0.65	0	15,15,17	0.94	2 (13%)
6	FUC	M	5	6	10,10,11	0.99	1 (10%)	14,14,16	0.65	0
7	NAG	N	1	7,2	14,14,15	0.49	0	17,19,21	0.63	0
7	NAG	N	2	7	14,14,15	0.19	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
4	NAG	F	1	4,2	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1
4	BMA	F	3	4	-	1/2/19/22	0/1/1/1
4	MAN	F	4	4	-	0/2/19/22	0/1/1/1
4	MAN	F	5	4	-	0/2/19/22	0/1/1/1
4	FUC	F	6	4	-	-	0/1/1/1
5	NAG	H	1	5,2	-	0/6/23/26	0/1/1/1
5	NAG	H	2	5	-	3/6/23/26	0/1/1/1
5	BMA	H	3	5	-	2/2/19/22	0/1/1/1
5	MAN	H	4	5	-	0/2/19/22	0/1/1/1
5	NAG	H	5	5	-	4/6/23/26	0/1/1/1
5	MAN	H	6	5	-	2/2/19/22	0/1/1/1
6	NAG	I	1	6,2	-	0/6/23/26	0/1/1/1
6	NAG	I	2	6	-	0/6/23/26	0/1/1/1
6	BMA	I	3	6	-	1/2/19/22	0/1/1/1
6	MAN	I	4	6	-	0/2/19/22	0/1/1/1
6	FUC	I	5	6	-	-	0/1/1/1
7	NAG	J	1	7,2	-	0/6/23/26	0/1/1/1
7	NAG	J	2	7	-	1/6/23/26	0/1/1/1
4	NAG	K	1	4,2	-	0/6/23/26	0/1/1/1
4	NAG	K	2	4	-	0/6/23/26	0/1/1/1
4	BMA	K	3	4	-	1/2/19/22	0/1/1/1
4	MAN	K	4	4	-	0/2/19/22	0/1/1/1
4	MAN	K	5	4	-	0/2/19/22	0/1/1/1
4	FUC	K	6	4	-	-	0/1/1/1
5	NAG	L	1	5,2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	L	2	5	-	3/6/23/26	0/1/1/1
5	BMA	L	3	5	-	2/2/19/22	0/1/1/1
5	MAN	L	4	5	-	0/2/19/22	0/1/1/1
5	NAG	L	5	5	-	4/6/23/26	0/1/1/1
5	MAN	L	6	5	-	2/2/19/22	0/1/1/1
6	NAG	M	1	6,2	-	0/6/23/26	0/1/1/1
6	NAG	M	2	6	-	0/6/23/26	0/1/1/1
6	BMA	M	3	6	-	1/2/19/22	0/1/1/1
6	MAN	M	4	6	-	0/2/19/22	0/1/1/1
6	FUC	M	5	6	-	-	0/1/1/1
7	NAG	N	1	7,2	-	0/6/23/26	0/1/1/1
7	NAG	N	2	7	-	1/6/23/26	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	1	NAG	O5-C1	3.64	1.49	1.43
4	K	1	NAG	O5-C1	3.64	1.49	1.43
5	H	4	MAN	O2-C2	3.06	1.49	1.43
5	L	4	MAN	O2-C2	3.05	1.49	1.43
4	K	6	FUC	O5-C1	-2.73	1.39	1.43
4	F	6	FUC	O5-C1	-2.70	1.39	1.43
6	I	5	FUC	O5-C1	-2.33	1.39	1.43
6	M	5	FUC	O5-C1	-2.32	1.39	1.43
6	M	1	NAG	O5-C1	2.32	1.47	1.43
6	I	1	NAG	O5-C1	2.29	1.47	1.43
5	H	3	BMA	C2-C3	2.17	1.55	1.52
5	L	3	BMA	C2-C3	2.16	1.55	1.52
5	L	4	MAN	C1-C2	2.15	1.57	1.52
5	H	1	NAG	C1-C2	2.14	1.55	1.52
5	L	1	NAG	C1-C2	2.11	1.55	1.52
5	H	4	MAN	C1-C2	2.10	1.57	1.52
5	H	4	MAN	C2-C3	2.03	1.55	1.52

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	1	NAG	C1-O5-C5	5.98	120.20	112.19
6	I	1	NAG	C1-O5-C5	5.96	120.18	112.19
4	F	1	NAG	C1-O5-C5	4.72	118.51	112.19
4	K	1	NAG	C1-O5-C5	4.70	118.49	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	2	NAG	C1-O5-C5	4.70	118.49	112.19
5	H	2	NAG	C1-O5-C5	4.69	118.47	112.19
5	L	2	NAG	C2-N2-C7	4.06	128.34	122.90
5	H	2	NAG	C2-N2-C7	4.05	128.32	122.90
5	L	4	MAN	O2-C2-C1	3.72	117.74	109.22
5	H	4	MAN	O2-C2-C1	3.71	117.73	109.22
5	H	5	NAG	C1-O5-C5	3.19	116.46	112.19
5	L	5	NAG	C1-O5-C5	3.19	116.46	112.19
5	H	1	NAG	O4-C4-C5	3.09	116.92	109.32
5	L	1	NAG	O4-C4-C5	3.07	116.90	109.32
5	L	3	BMA	O3-C3-C2	3.02	116.22	110.05
5	H	3	BMA	O3-C3-C2	3.00	116.17	110.05
5	H	1	NAG	C1-O5-C5	2.83	115.97	112.19
5	L	1	NAG	C1-O5-C5	2.82	115.96	112.19
5	L	4	MAN	C1-O5-C5	2.73	115.84	112.19
5	H	4	MAN	C1-O5-C5	2.72	115.84	112.19
6	I	3	BMA	C3-C4-C5	-2.29	106.08	110.23
6	M	3	BMA	C3-C4-C5	-2.29	106.08	110.23
4	K	5	MAN	O2-C2-C3	-2.26	105.48	110.15
4	F	5	MAN	O2-C2-C3	-2.25	105.49	110.15
4	K	4	MAN	C1-O5-C5	2.22	115.16	112.19
5	L	6	MAN	C1-O5-C5	2.21	115.15	112.19
4	F	4	MAN	C1-O5-C5	2.21	115.14	112.19
5	H	6	MAN	C1-O5-C5	2.20	115.13	112.19
6	I	4	MAN	C1-O5-C5	2.19	115.12	112.19
4	K	4	MAN	O2-C2-C3	-2.18	105.63	110.15
6	M	2	NAG	C1-O5-C5	2.18	115.11	112.19
4	F	3	BMA	C3-C4-C5	-2.18	106.28	110.23
4	F	4	MAN	O2-C2-C3	-2.18	105.64	110.15
5	H	6	MAN	O2-C2-C3	-2.17	105.67	110.15
6	M	4	MAN	C1-O5-C5	2.16	115.08	112.19
6	I	2	NAG	C1-O5-C5	2.15	115.06	112.19
5	L	6	MAN	O2-C2-C3	-2.14	105.71	110.15
4	K	3	BMA	C3-C4-C5	-2.14	106.35	110.23
6	M	4	MAN	O2-C2-C3	-2.11	105.79	110.15
6	I	4	MAN	O2-C2-C3	-2.09	105.81	110.15
4	F	3	BMA	O5-C5-C6	2.05	111.65	107.66
4	K	3	BMA	O5-C5-C6	2.02	111.60	107.66
4	F	5	MAN	C1-O5-C5	2.01	114.88	112.19
4	K	5	MAN	C1-O5-C5	2.00	114.87	112.19

There are no chirality outliers.

All (28) torsion outliers are listed below:

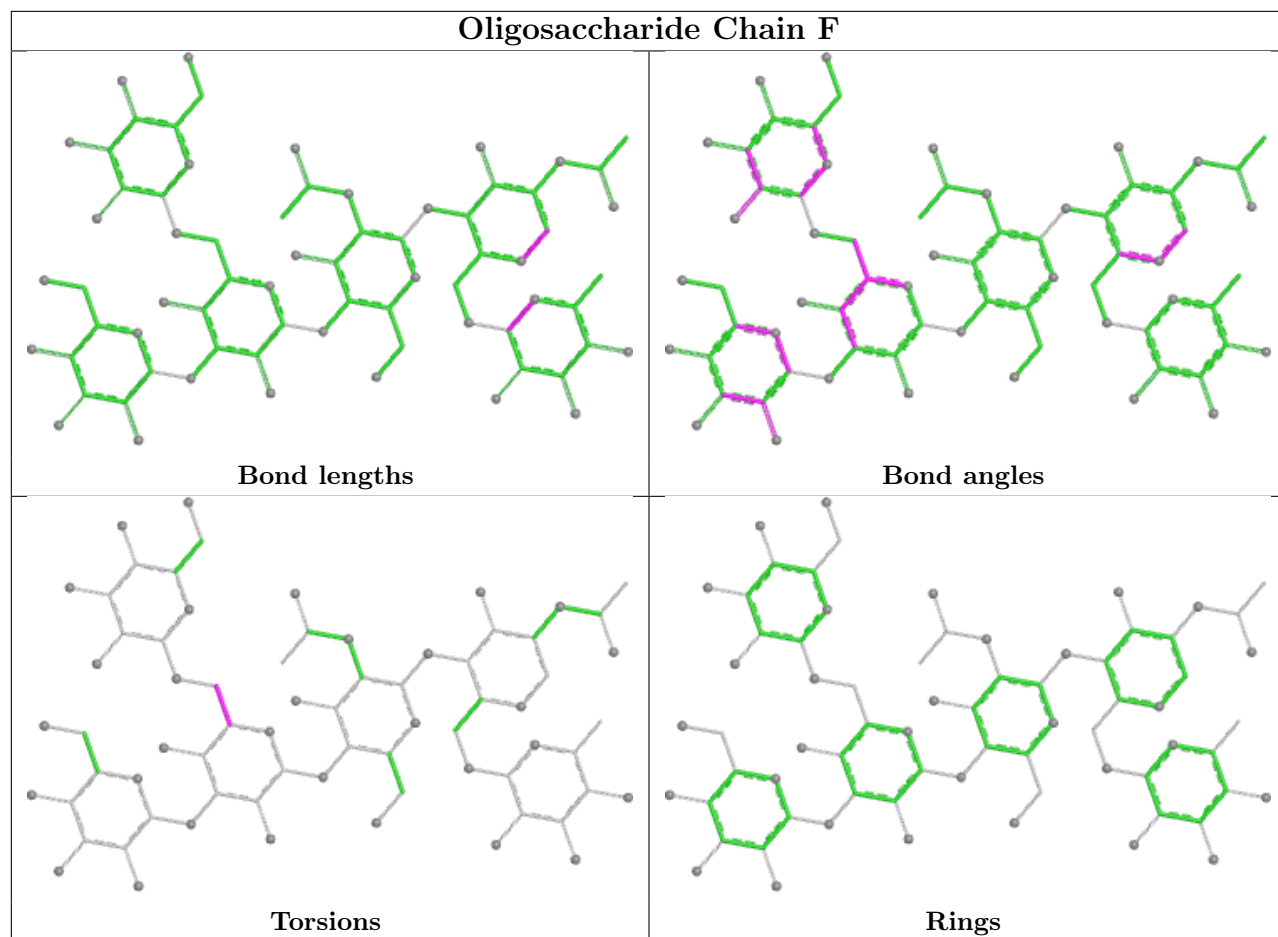
Mol	Chain	Res	Type	Atoms
5	H	2	NAG	C3-C2-N2-C7
5	L	2	NAG	C3-C2-N2-C7
5	H	5	NAG	O5-C5-C6-O6
5	H	6	MAN	O5-C5-C6-O6
5	L	5	NAG	O5-C5-C6-O6
5	L	6	MAN	O5-C5-C6-O6
5	H	2	NAG	O5-C5-C6-O6
5	L	2	NAG	O5-C5-C6-O6
5	H	6	MAN	C4-C5-C6-O6
5	L	6	MAN	C4-C5-C6-O6
5	H	3	BMA	O5-C5-C6-O6
5	L	3	BMA	O5-C5-C6-O6
5	H	2	NAG	C4-C5-C6-O6
5	L	2	NAG	C4-C5-C6-O6
5	H	5	NAG	C4-C5-C6-O6
5	L	5	NAG	C4-C5-C6-O6
5	H	3	BMA	C4-C5-C6-O6
5	L	3	BMA	C4-C5-C6-O6
5	H	5	NAG	C8-C7-N2-C2
5	H	5	NAG	O7-C7-N2-C2
5	L	5	NAG	C8-C7-N2-C2
5	L	5	NAG	O7-C7-N2-C2
6	I	3	BMA	O5-C5-C6-O6
6	M	3	BMA	O5-C5-C6-O6
4	K	3	BMA	O5-C5-C6-O6
4	F	3	BMA	O5-C5-C6-O6
7	J	2	NAG	C1-C2-N2-C7
7	N	2	NAG	C1-C2-N2-C7

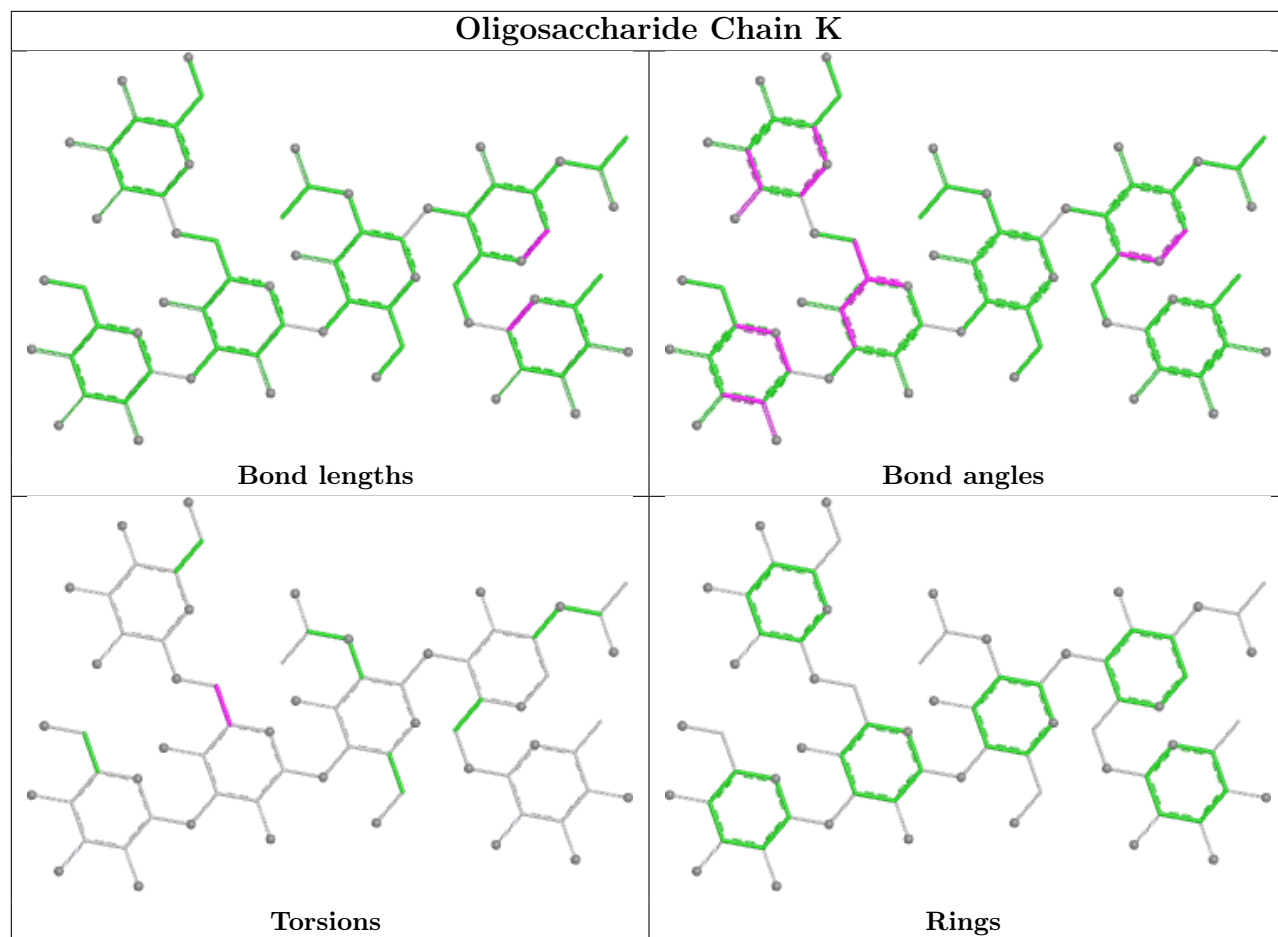
There are no ring outliers.

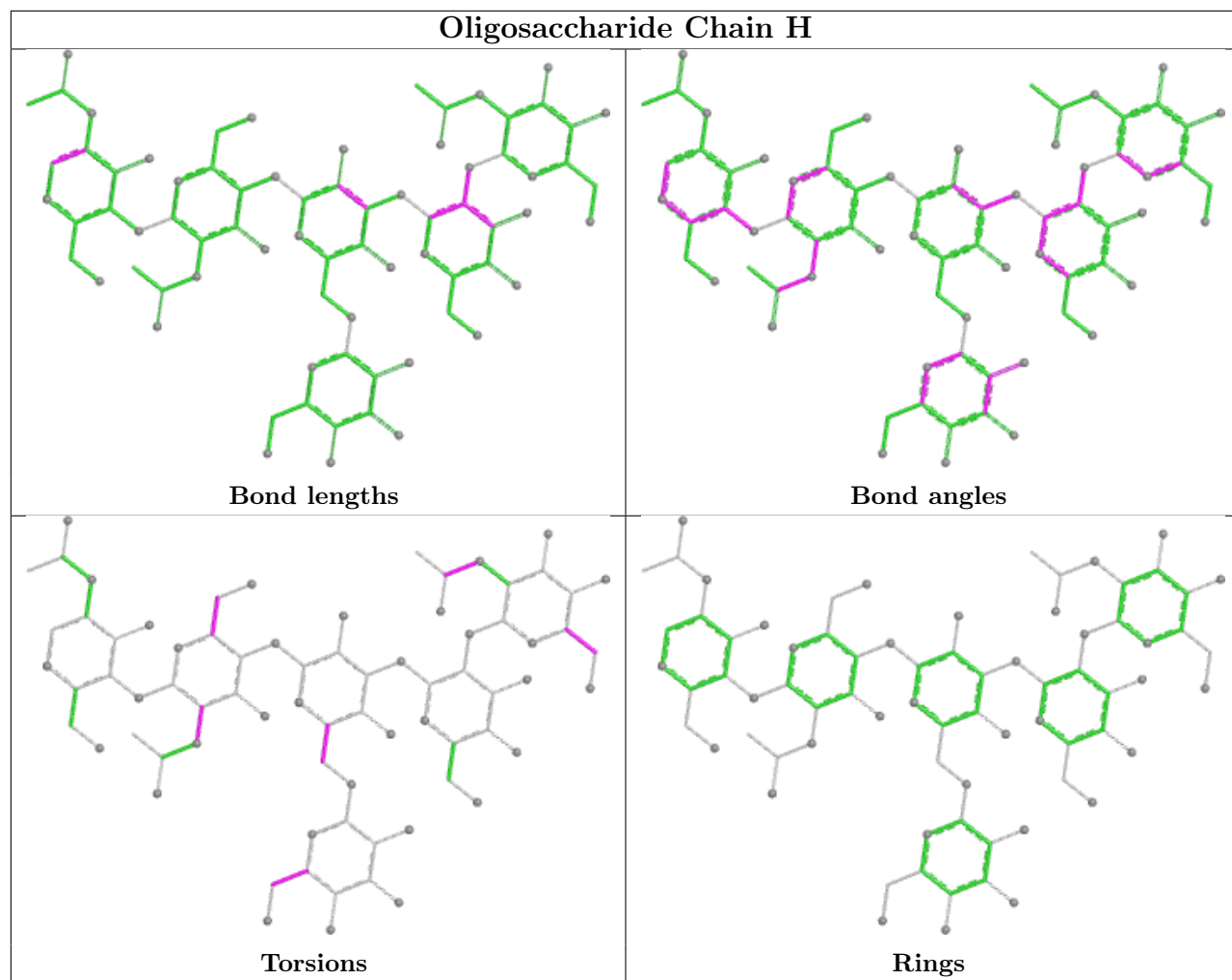
2 monomers are involved in 2 short contacts:

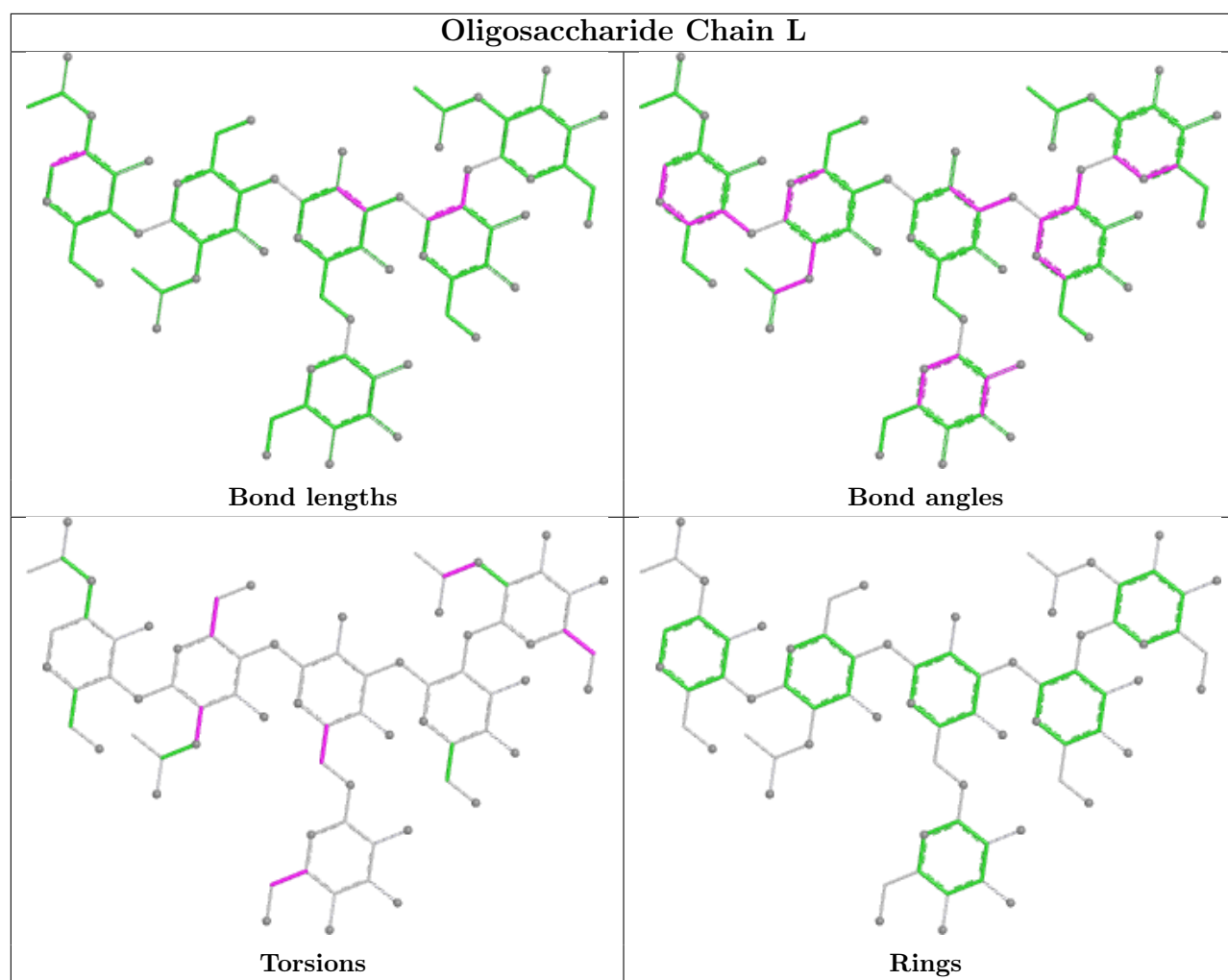
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	6	FUC	1	0
4	K	6	FUC	1	0

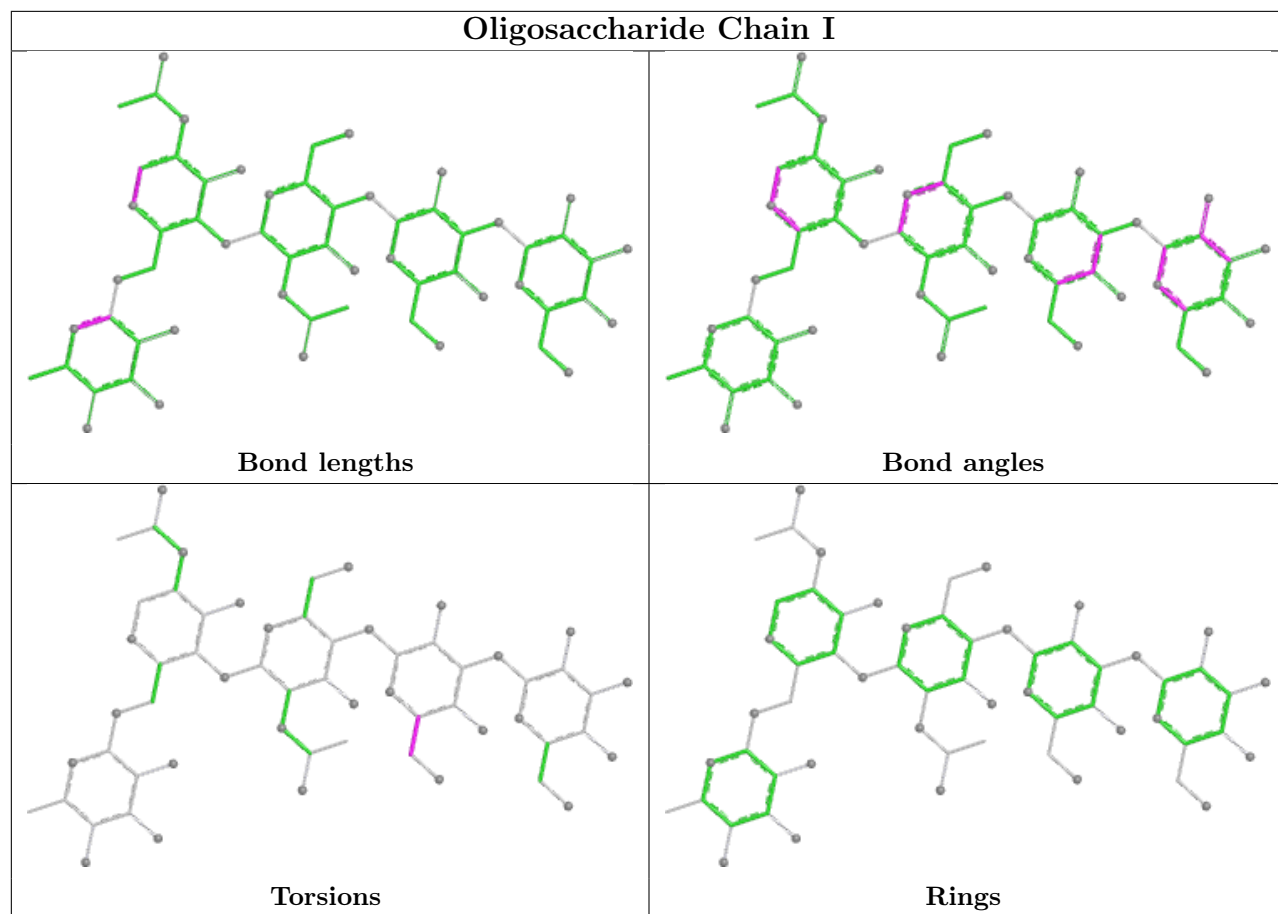
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

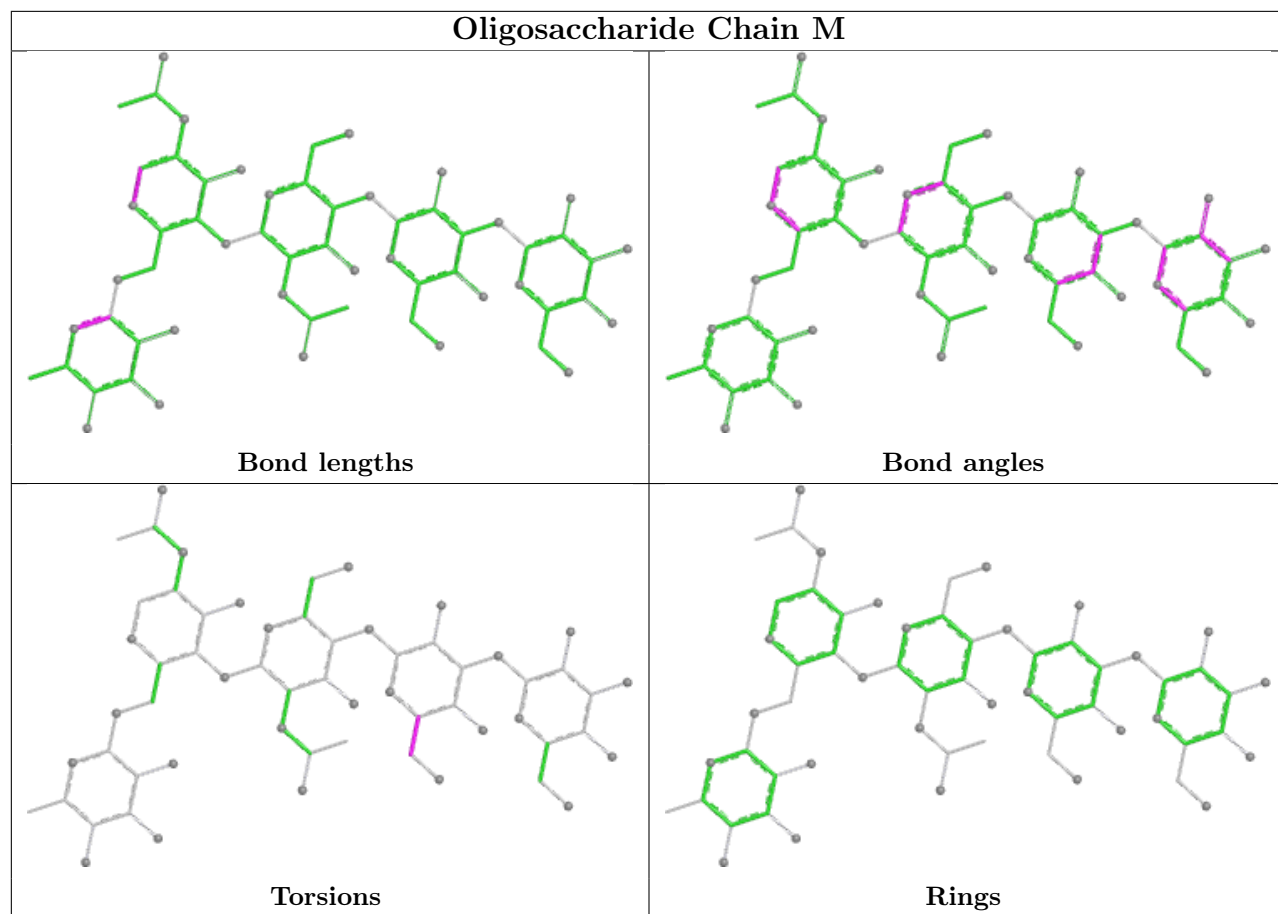


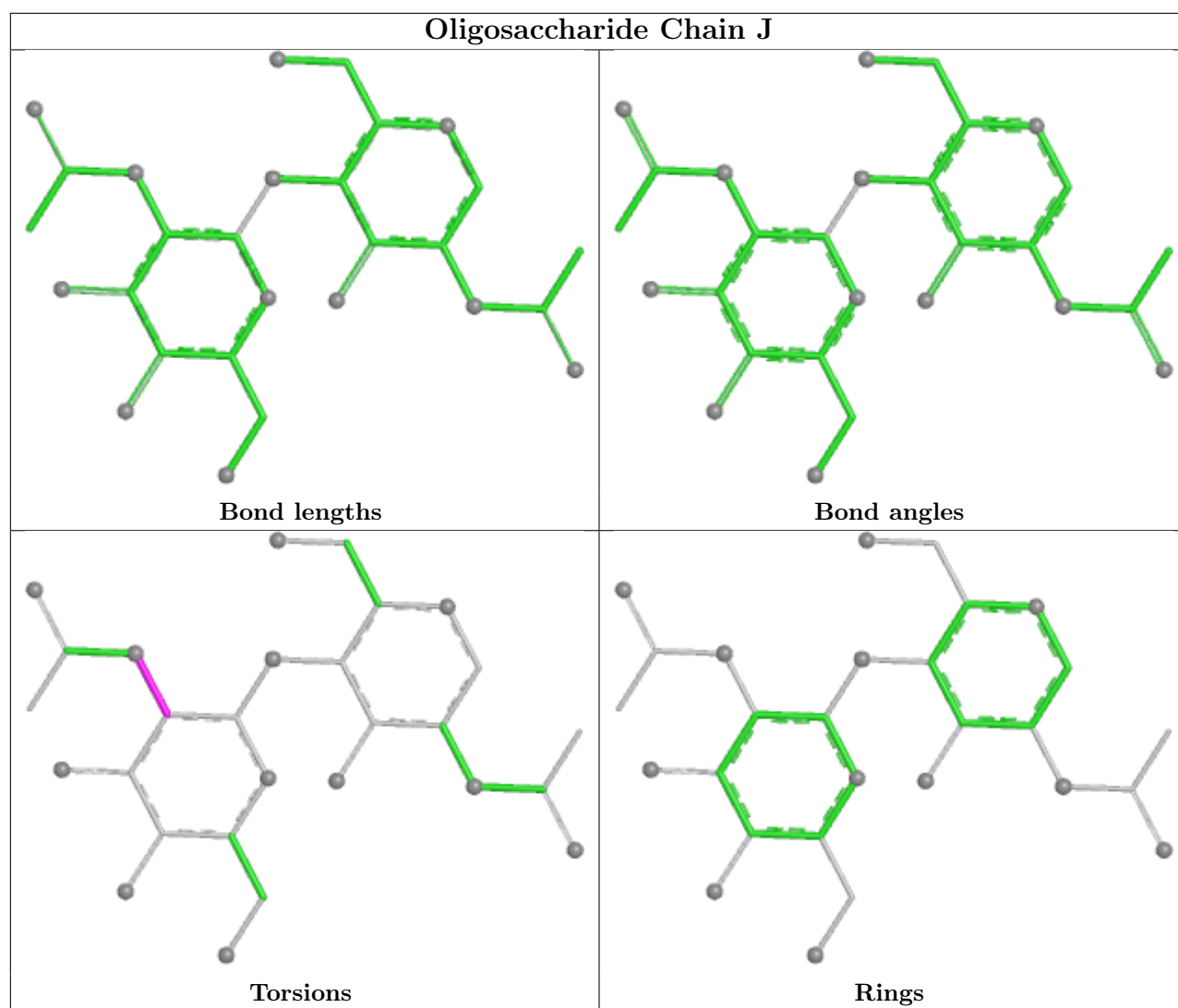


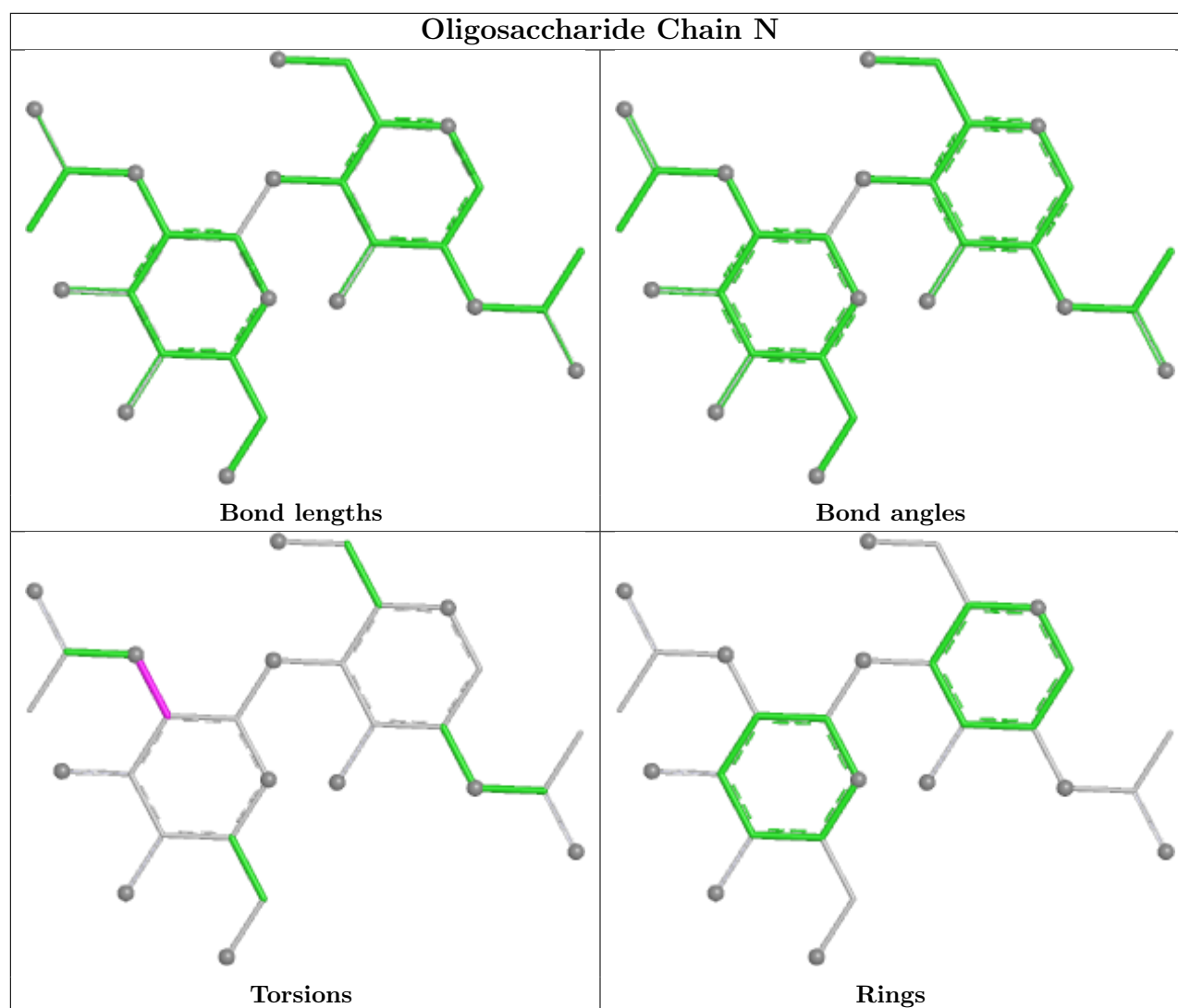












5.6 Ligand geometry [i](#)

Of 40 ligands modelled in this entry, 4 are monoatomic - leaving 36 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	$\# Z > 2$
13	PCW	C	1108	-	53,53,53	0.98	2 (3%)	59,61,61	0.74	0
12	CLR	A	1105	-	31,31,31	1.10	1 (3%)	48,48,48	1.39	8 (16%)
13	PCW	G	1302	-	53,53,53	1.00	2 (3%)	59,61,61	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	ATP	A	1103	-	32,33,33	0.31	0	48,52,52	0.30	0
13	PCW	C	1107	-	21,21,53	0.88	0	27,29,61	1.21	3 (11%)
12	CLR	B	501	-	31,31,31	1.12	1 (3%)	48,48,48	1.39	8 (16%)
13	PCW	E	1302	-	53,53,53	1.00	2 (3%)	59,61,61	0.75	0
11	7Q2	A	1104	-	29,29,29	3.72	15 (51%)	43,45,45	2.01	14 (32%)
13	PCW	C	1109	-	53,53,53	1.00	2 (3%)	59,61,61	0.77	0
13	PCW	A	1108	-	53,53,53	0.98	2 (3%)	59,61,61	0.75	0
13	PCW	C	1106	-	21,21,53	0.87	0	27,29,61	1.23	3 (11%)
13	PCW	C	1110	-	53,53,53	0.96	2 (3%)	59,61,61	0.81	0
13	PCW	A	1106	-	21,21,53	0.88	0	27,29,61	1.23	3 (11%)
13	PCW	G	1303	-	53,53,53	0.99	2 (3%)	59,61,61	0.79	0
13	PCW	E	1304	-	53,53,53	1.01	2 (3%)	59,61,61	0.69	0
13	PCW	C	1111	-	53,53,53	1.00	2 (3%)	59,61,61	0.71	0
12	CLR	G	1301	-	31,31,31	1.12	2 (6%)	48,48,48	1.39	8 (16%)
13	PCW	C	1113	-	21,21,53	0.88	0	27,29,61	1.34	3 (11%)
11	7Q2	C	1104	-	29,29,29	3.73	15 (51%)	43,45,45	2.02	14 (32%)
12	CLR	D	501	-	31,31,31	1.11	2 (6%)	48,48,48	1.39	8 (16%)
13	PCW	A	1107	-	21,21,53	0.88	0	27,29,61	1.20	3 (11%)
12	CLR	B	502	-	31,31,31	1.11	1 (3%)	48,48,48	1.39	8 (16%)
13	PCW	A	1111	-	53,53,53	1.00	2 (3%)	59,61,61	0.71	0
12	CLR	D	502	-	31,31,31	1.11	1 (3%)	48,48,48	1.39	8 (16%)
13	PCW	A	1109	-	53,53,53	1.00	2 (3%)	59,61,61	0.77	0
13	PCW	A	1110	-	53,53,53	0.96	2 (3%)	59,61,61	0.81	0
13	PCW	A	1113	-	21,21,53	0.87	0	27,29,61	1.34	3 (11%)
13	PCW	G	1304	-	53,53,53	1.01	2 (3%)	59,61,61	0.69	0
13	PCW	C	1112	-	53,53,53	1.00	2 (3%)	59,61,61	0.73	0
13	PCW	C	1114	-	53,53,53	1.01	2 (3%)	59,61,61	0.69	0
13	PCW	E	1303	-	53,53,53	0.99	2 (3%)	59,61,61	0.79	0
12	CLR	C	1105	-	31,31,31	1.11	1 (3%)	48,48,48	1.39	9 (18%)
12	CLR	E	1301	-	31,31,31	1.11	2 (6%)	48,48,48	1.39	8 (16%)
13	PCW	A	1114	-	53,53,53	1.01	2 (3%)	59,61,61	0.69	0
10	ATP	C	1103	-	32,33,33	0.31	0	48,52,52	0.30	0
13	PCW	A	1112	-	53,53,53	1.00	2 (3%)	59,61,61	0.73	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
13	PCW	C	1108	-	-	20/57/57/57	-
12	CLR	A	1105	-	-	2/10/68/68	0/4/4/4
13	PCW	G	1302	-	-	18/57/57/57	-
10	ATP	A	1103	-	-	3/22/38/38	0/3/3/3
13	PCW	C	1107	-	-	14/23/23/57	-
12	CLR	B	501	-	-	1/10/68/68	0/4/4/4
13	PCW	E	1302	-	-	18/57/57/57	-
11	7Q2	A	1104	-	-	2/5/66/66	0/4/4/4
13	PCW	C	1109	-	-	17/57/57/57	-
13	PCW	A	1108	-	-	20/57/57/57	-
13	PCW	C	1106	-	-	4/23/23/57	-
13	PCW	C	1110	-	-	13/57/57/57	-
13	PCW	A	1106	-	-	4/23/23/57	-
13	PCW	G	1303	-	-	22/57/57/57	-
13	PCW	E	1304	-	-	17/57/57/57	-
13	PCW	C	1111	-	-	21/57/57/57	-
12	CLR	G	1301	-	-	0/10/68/68	0/4/4/4
13	PCW	C	1113	-	-	8/23/23/57	-
11	7Q2	C	1104	-	-	2/5/66/66	0/4/4/4
12	CLR	D	501	-	-	1/10/68/68	0/4/4/4
13	PCW	A	1107	-	-	14/23/23/57	-
12	CLR	B	502	-	-	0/10/68/68	0/4/4/4
13	PCW	A	1111	-	-	21/57/57/57	-
12	CLR	D	502	-	-	0/10/68/68	0/4/4/4
13	PCW	A	1109	-	-	17/57/57/57	-
13	PCW	A	1110	-	-	13/57/57/57	-
13	PCW	A	1113	-	-	8/23/23/57	-
13	PCW	G	1304	-	-	17/57/57/57	-
13	PCW	C	1112	-	-	18/57/57/57	-
13	PCW	C	1114	-	-	21/57/57/57	-
13	PCW	E	1303	-	-	22/57/57/57	-
12	CLR	C	1105	-	-	2/10/68/68	0/4/4/4
12	CLR	E	1301	-	-	0/10/68/68	0/4/4/4
13	PCW	A	1114	-	-	21/57/57/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	ATP	C	1103	-	-	3/22/38/38	0/3/3/3
13	PCW	A	1112	-	-	18/57/57/57	-

All (77) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	1104	7Q2	CAF-CAD	-8.00	1.41	1.52
11	A	1104	7Q2	CAF-CAD	-7.98	1.41	1.52
11	C	1104	7Q2	CAS-CAU	-6.84	1.40	1.50
11	A	1104	7Q2	CAS-CAU	-6.79	1.40	1.50
11	C	1104	7Q2	CAT-CAU	-6.74	1.41	1.50
11	A	1104	7Q2	CAT-CAU	-6.70	1.41	1.50
11	C	1104	7Q2	CAU-NAV	6.35	1.33	1.28
11	A	1104	7Q2	CAU-NAV	6.33	1.33	1.28
11	A	1104	7Q2	CAF-CAG	-6.21	1.43	1.54
11	C	1104	7Q2	CAF-CAG	-6.17	1.43	1.54
11	C	1104	7Q2	CAB-CAG	-5.81	1.42	1.54
11	A	1104	7Q2	CAB-CAG	-5.79	1.42	1.54
11	C	1104	7Q2	CAQ-CAM	-5.17	1.42	1.51
11	A	1104	7Q2	CAQ-CAM	-5.11	1.43	1.51
11	C	1104	7Q2	CAP-CAL	-4.41	1.48	1.56
11	A	1104	7Q2	CAP-CAL	-4.40	1.48	1.56
11	C	1104	7Q2	CAJ-CAM	-4.16	1.43	1.50
11	A	1104	7Q2	CAJ-CAM	-4.16	1.43	1.50
13	G	1304	PCW	C40-C39	4.04	1.54	1.31
13	E	1304	PCW	C40-C39	4.04	1.54	1.31
11	A	1104	7Q2	CAI-CAG	-4.02	1.46	1.53
13	A	1109	PCW	C20-C19	3.98	1.54	1.31
11	C	1104	7Q2	CAI-CAG	-3.98	1.46	1.53
13	C	1114	PCW	C20-C19	3.98	1.54	1.31
13	C	1109	PCW	C20-C19	3.98	1.54	1.31
13	A	1114	PCW	C20-C19	3.97	1.54	1.31
13	E	1302	PCW	C40-C39	3.97	1.54	1.31
13	A	1112	PCW	C40-C39	3.96	1.54	1.31
13	A	1112	PCW	C20-C19	3.96	1.54	1.31
13	C	1112	PCW	C20-C19	3.96	1.54	1.31
13	A	1111	PCW	C20-C19	3.95	1.54	1.31
13	G	1302	PCW	C40-C39	3.95	1.54	1.31
13	C	1112	PCW	C40-C39	3.95	1.54	1.31
13	G	1303	PCW	C40-C39	3.95	1.54	1.31
13	E	1302	PCW	C20-C19	3.95	1.54	1.31
13	C	1111	PCW	C20-C19	3.95	1.54	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	G	1302	PCW	C20-C19	3.94	1.54	1.31
13	A	1111	PCW	C40-C39	3.94	1.54	1.31
13	E	1303	PCW	C40-C39	3.93	1.54	1.31
13	A	1114	PCW	C40-C39	3.93	1.54	1.31
13	C	1111	PCW	C40-C39	3.92	1.54	1.31
13	G	1304	PCW	C20-C19	3.92	1.54	1.31
13	E	1304	PCW	C20-C19	3.91	1.53	1.31
13	C	1114	PCW	C40-C39	3.91	1.53	1.31
13	A	1109	PCW	C40-C39	3.91	1.53	1.31
13	C	1109	PCW	C40-C39	3.90	1.53	1.31
13	A	1108	PCW	C20-C19	3.89	1.53	1.31
13	C	1108	PCW	C20-C19	3.88	1.53	1.31
13	C	1110	PCW	C20-C19	3.86	1.53	1.31
13	A	1110	PCW	C20-C19	3.85	1.53	1.31
13	C	1108	PCW	C40-C39	3.85	1.53	1.31
13	A	1108	PCW	C40-C39	3.84	1.53	1.31
13	G	1303	PCW	C20-C19	3.82	1.53	1.31
13	E	1303	PCW	C20-C19	3.82	1.53	1.31
13	A	1110	PCW	C40-C39	3.79	1.53	1.31
13	C	1110	PCW	C40-C39	3.78	1.53	1.31
11	A	1104	7Q2	CAH-CAF	-3.45	1.47	1.54
11	C	1104	7Q2	CAH-CAF	-3.45	1.47	1.54
12	G	1301	CLR	C16-C17	3.30	1.61	1.54
12	E	1301	CLR	C16-C17	3.29	1.61	1.54
12	A	1105	CLR	C16-C17	3.28	1.61	1.54
12	B	502	CLR	C16-C17	3.28	1.61	1.54
12	D	502	CLR	C16-C17	3.28	1.61	1.54
12	C	1105	CLR	C16-C17	3.26	1.61	1.54
12	B	501	CLR	C16-C17	3.26	1.61	1.54
12	D	501	CLR	C16-C17	3.25	1.61	1.54
11	A	1104	7Q2	CAP-CAQ	-3.11	1.51	1.56
11	C	1104	7Q2	CAP-CAQ	-3.08	1.51	1.56
11	C	1104	7Q2	CAK-CAL	2.71	1.58	1.53
11	A	1104	7Q2	CAK-CAL	2.68	1.58	1.53
11	C	1104	7Q2	OAW-NAV	2.41	1.46	1.42
11	A	1104	7Q2	OAW-NAV	2.40	1.46	1.42
11	A	1104	7Q2	CAH-CAK	2.23	1.57	1.53
11	C	1104	7Q2	CAH-CAK	2.21	1.57	1.53
12	E	1301	CLR	C16-C15	2.03	1.59	1.54
12	G	1301	CLR	C16-C15	2.01	1.59	1.54
12	D	501	CLR	C16-C15	2.00	1.59	1.54

All (111) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1104	7Q2	OAW-NAV-CAU	5.46	116.85	110.81
11	C	1104	7Q2	OAW-NAV-CAU	5.43	116.82	110.81
13	C	1113	PCW	C2-O2-C31	-4.70	109.55	117.85
13	A	1113	PCW	C2-O2-C31	-4.68	109.58	117.85
13	C	1107	PCW	C2-O2-C31	-4.51	109.89	117.85
13	A	1107	PCW	C2-O2-C31	-4.49	109.91	117.85
11	C	1104	7Q2	CAB-CAG-CAI	-4.08	112.60	119.10
11	A	1104	7Q2	CAB-CAG-CAI	-4.07	112.61	119.10
13	C	1106	PCW	C2-O2-C31	-3.98	110.82	117.85
13	A	1106	PCW	C2-O2-C31	-3.94	110.88	117.85
11	C	1104	7Q2	CAB-CAA-CAD	-3.57	102.25	105.70
11	A	1104	7Q2	CAB-CAA-CAD	-3.57	102.26	105.70
11	A	1104	7Q2	CAT-CAR-CAP	-3.55	109.01	113.44
11	C	1104	7Q2	CAT-CAR-CAP	-3.52	109.04	113.44
11	C	1104	7Q2	CAF-CAG-CAI	-3.36	109.60	113.13
11	A	1104	7Q2	CAF-CAG-CAI	-3.35	109.61	113.13
13	C	1113	PCW	C3-O3-C11	-3.29	108.97	117.08
13	A	1113	PCW	C3-O3-C11	-3.28	108.99	117.08
11	A	1104	7Q2	CAP-CAL-CAI	-3.27	109.11	112.43
11	C	1104	7Q2	CAP-CAL-CAI	-3.25	109.13	112.43
13	A	1106	PCW	C3-O3-C11	-3.01	109.65	117.08
13	C	1106	PCW	C3-O3-C11	-3.00	109.69	117.08
11	C	1104	7Q2	CAK-CAL-CAP	-2.96	110.58	113.91
11	A	1104	7Q2	CAK-CAL-CAP	-2.95	110.59	113.91
12	D	502	CLR	C22-C20-C17	-2.90	104.31	110.33
12	B	502	CLR	C22-C20-C17	-2.87	104.38	110.33
12	E	1301	CLR	C22-C20-C17	-2.81	104.50	110.33
12	D	501	CLR	C22-C20-C17	-2.81	104.51	110.33
12	G	1301	CLR	C22-C20-C17	-2.80	104.52	110.33
12	B	501	CLR	C22-C20-C17	-2.80	104.53	110.33
12	A	1105	CLR	C22-C20-C17	-2.77	104.58	110.33
12	C	1105	CLR	C22-C20-C17	-2.76	104.60	110.33
11	A	1104	7Q2	CAE-CAF-CAD	2.68	110.13	105.18
11	C	1104	7Q2	CAE-CAF-CAD	2.68	110.11	105.18
11	A	1104	7Q2	CAH-CAF-CAD	-2.65	112.96	116.71
11	C	1104	7Q2	CAH-CAF-CAD	-2.61	113.01	116.71
12	B	502	CLR	C7-C8-C14	-2.60	107.26	110.93
12	D	502	CLR	C7-C8-C14	-2.59	107.26	110.93
12	E	1301	CLR	C7-C8-C14	-2.56	107.31	110.93
12	G	1301	CLR	C7-C8-C14	-2.55	107.32	110.93
12	A	1105	CLR	C13-C17-C20	-2.54	115.57	119.50
12	D	501	CLR	C13-C17-C20	-2.54	115.58	119.50
12	C	1105	CLR	C13-C17-C20	-2.53	115.58	119.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	501	CLR	C13-C17-C20	-2.52	115.60	119.50
12	C	1105	CLR	C7-C8-C14	-2.52	107.37	110.93
12	A	1105	CLR	C7-C8-C14	-2.51	107.37	110.93
13	C	1107	PCW	C3-O3-C11	-2.49	110.93	117.08
13	A	1107	PCW	C3-O3-C11	-2.47	110.98	117.08
12	E	1301	CLR	C13-C17-C20	-2.47	115.69	119.50
12	G	1301	CLR	C13-C17-C20	-2.43	115.74	119.50
12	B	501	CLR	C7-C8-C14	-2.43	107.50	110.93
12	D	501	CLR	C7-C8-C14	-2.41	107.53	110.93
12	D	502	CLR	C13-C17-C20	-2.40	115.79	119.50
11	C	1104	7Q2	CAG-CAF-CAD	2.38	103.41	100.61
12	B	502	CLR	C13-C17-C20	-2.38	115.82	119.50
11	C	1104	7Q2	CAJ-CAM-CAQ	2.38	119.02	115.39
11	A	1104	7Q2	CAG-CAF-CAD	2.37	103.40	100.61
11	A	1104	7Q2	CAJ-CAM-CAQ	2.32	118.93	115.39
11	A	1104	7Q2	CAK-CAH-CAF	-2.27	107.95	112.78
11	C	1104	7Q2	CAK-CAH-CAF	-2.24	108.01	112.78
11	A	1104	7Q2	CAH-CAK-CAL	-2.23	109.34	113.14
11	C	1104	7Q2	CAH-CAK-CAL	-2.22	109.36	113.14
13	A	1107	PCW	O2-C31-C32	2.21	115.03	111.09
13	C	1107	PCW	O2-C31-C32	2.19	114.99	111.09
13	A	1113	PCW	O2-C31-C32	2.18	114.97	111.09
13	C	1113	PCW	O2-C31-C32	2.16	114.95	111.09
12	B	501	CLR	C24-C23-C22	-2.16	103.60	113.28
12	C	1105	CLR	C3-C4-C5	2.16	115.49	112.05
12	D	501	CLR	C24-C23-C22	-2.15	103.64	113.28
12	B	502	CLR	C24-C23-C22	-2.15	103.64	113.28
12	D	502	CLR	C24-C23-C22	-2.15	103.65	113.28
12	B	502	CLR	C3-C4-C5	2.15	115.48	112.05
12	G	1301	CLR	C24-C23-C22	-2.15	103.66	113.28
12	A	1105	CLR	C3-C4-C5	2.14	115.46	112.05
12	D	502	CLR	C3-C4-C5	2.14	115.46	112.05
12	E	1301	CLR	C3-C4-C5	2.14	115.46	112.05
12	E	1301	CLR	C24-C23-C22	-2.14	103.70	113.28
12	D	501	CLR	C3-C4-C5	2.13	115.45	112.05
12	G	1301	CLR	C3-C4-C5	2.13	115.44	112.05
12	C	1105	CLR	C19-C10-C9	-2.12	109.28	111.66
13	A	1106	PCW	O2-C31-C32	2.11	114.86	111.09
12	B	501	CLR	C3-C4-C5	2.11	115.41	112.05
12	C	1105	CLR	C24-C23-C22	-2.11	103.83	113.28
13	C	1106	PCW	O2-C31-C32	2.11	114.84	111.09
12	B	502	CLR	C19-C10-C9	-2.11	109.30	111.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	1105	CLR	C24-C23-C22	-2.10	103.86	113.28
12	E	1301	CLR	C19-C10-C9	-2.09	109.31	111.66
12	G	1301	CLR	C18-C13-C12	2.09	113.69	110.61
12	D	502	CLR	C19-C10-C9	-2.08	109.32	111.66
12	B	502	CLR	C18-C13-C12	2.07	113.66	110.61
12	E	1301	CLR	C18-C13-C12	2.07	113.66	110.61
12	D	501	CLR	C19-C10-C9	-2.07	109.34	111.66
12	B	502	CLR	C10-C5-C6	2.06	125.94	122.93
12	A	1105	CLR	C19-C10-C9	-2.06	109.35	111.66
12	D	502	CLR	C18-C13-C12	2.05	113.63	110.61
12	B	501	CLR	C18-C13-C12	2.05	113.62	110.61
11	C	1104	7Q2	CAE-CAF-CAG	-2.04	110.06	112.99
12	G	1301	CLR	C19-C10-C9	-2.04	109.37	111.66
12	A	1105	CLR	C10-C5-C6	2.04	125.91	122.93
12	C	1105	CLR	C10-C5-C6	2.04	125.91	122.93
12	D	501	CLR	C18-C13-C12	2.04	113.61	110.61
12	E	1301	CLR	C10-C5-C6	2.04	125.90	122.93
12	B	501	CLR	C19-C10-C9	-2.04	109.38	111.66
12	A	1105	CLR	C18-C13-C12	2.03	113.60	110.61
12	C	1105	CLR	C18-C13-C12	2.03	113.60	110.61
12	D	501	CLR	C11-C12-C13	-2.02	109.32	112.74
11	A	1104	7Q2	CAE-CAF-CAG	-2.02	110.09	112.99
12	D	502	CLR	C10-C5-C6	2.02	125.88	122.93
12	B	501	CLR	C11-C12-C13	-2.02	109.33	112.74
12	G	1301	CLR	C10-C5-C6	2.02	125.87	122.93
12	C	1105	CLR	C15-C14-C13	2.00	106.19	103.84

There are no chirality outliers.

All (402) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	1103	ATP	PB-O3A-PA-O5'
10	C	1103	ATP	PB-O3A-PA-O5'
11	A	1104	7Q2	OAW-CAX-CAY-NAZ
11	C	1104	7Q2	OAW-CAX-CAY-NAZ
13	A	1107	PCW	C1-O3P-P-O4P
13	A	1107	PCW	C4-O4P-P-O2P
13	A	1107	PCW	C4-O4P-P-O3P
13	A	1108	PCW	O4P-C4-C5-N
13	A	1108	PCW	C4-O4P-P-O1P
13	A	1108	PCW	C4-O4P-P-O3P
13	A	1109	PCW	O3P-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
13	A	1109	PCW	C1-O3P-P-O2P
13	A	1112	PCW	O2-C2-C3-O3
13	A	1113	PCW	C1-O3P-P-O2P
13	G	1302	PCW	O2-C2-C3-O3
13	G	1302	PCW	C1-O3P-P-O1P
13	G	1302	PCW	C1-O3P-P-O2P
13	G	1302	PCW	C1-O3P-P-O4P
13	G	1302	PCW	C4-O4P-P-O2P
13	G	1302	PCW	C4-O4P-P-O3P
13	G	1303	PCW	C4-O4P-P-O1P
13	G	1303	PCW	C4-O4P-P-O3P
13	C	1107	PCW	C1-O3P-P-O4P
13	C	1107	PCW	C4-O4P-P-O2P
13	C	1107	PCW	C4-O4P-P-O3P
13	C	1108	PCW	O4P-C4-C5-N
13	C	1108	PCW	C4-O4P-P-O1P
13	C	1108	PCW	C4-O4P-P-O3P
13	C	1109	PCW	O3P-C1-C2-O2
13	C	1109	PCW	C1-O3P-P-O2P
13	C	1112	PCW	O2-C2-C3-O3
13	C	1113	PCW	C1-O3P-P-O2P
13	E	1302	PCW	O2-C2-C3-O3
13	E	1302	PCW	C1-O3P-P-O1P
13	E	1302	PCW	C1-O3P-P-O2P
13	E	1302	PCW	C1-O3P-P-O4P
13	E	1302	PCW	C4-O4P-P-O2P
13	E	1302	PCW	C4-O4P-P-O3P
13	E	1303	PCW	C4-O4P-P-O1P
13	E	1303	PCW	C4-O4P-P-O3P
13	A	1107	PCW	C32-C31-O2-C2
13	C	1107	PCW	C32-C31-O2-C2
13	A	1107	PCW	C12-C11-O3-C3
13	C	1107	PCW	C12-C11-O3-C3
13	A	1111	PCW	C4-C5-N-C8
13	A	1112	PCW	C4-C5-N-C8
13	A	1114	PCW	C4-C5-N-C8
13	G	1302	PCW	C4-C5-N-C8
13	G	1303	PCW	C4-C5-N-C8
13	C	1111	PCW	C4-C5-N-C8
13	C	1112	PCW	C4-C5-N-C8
13	C	1114	PCW	C4-C5-N-C8
13	E	1302	PCW	C4-C5-N-C8

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Mol	Chain	Res	Type	Atoms
13	E	1303	PCW	C4-C5-N-C8
13	A	1107	PCW	O11-C11-O3-C3
13	C	1107	PCW	O11-C11-O3-C3
13	A	1107	PCW	O31-C31-O2-C2
13	C	1107	PCW	O31-C31-O2-C2
13	A	1108	PCW	C11-C12-C13-C14
13	A	1108	PCW	C31-C32-C33-C34
13	A	1110	PCW	C31-C32-C33-C34
13	A	1114	PCW	C11-C12-C13-C14
13	G	1303	PCW	C11-C12-C13-C14
13	C	1108	PCW	C11-C12-C13-C14
13	C	1108	PCW	C31-C32-C33-C34
13	C	1110	PCW	C31-C32-C33-C34
13	C	1114	PCW	C11-C12-C13-C14
13	E	1303	PCW	C11-C12-C13-C14
13	A	1112	PCW	C31-C32-C33-C34
13	C	1112	PCW	C31-C32-C33-C34
13	A	1111	PCW	C4-C5-N-C6
13	A	1111	PCW	C4-C5-N-C7
13	A	1112	PCW	C4-C5-N-C6
13	A	1112	PCW	C4-C5-N-C7
13	A	1114	PCW	C4-C5-N-C6
13	A	1114	PCW	C4-C5-N-C7
13	G	1302	PCW	C4-C5-N-C6
13	G	1302	PCW	C4-C5-N-C7
13	G	1303	PCW	C4-C5-N-C6
13	G	1303	PCW	C4-C5-N-C7
13	G	1304	PCW	C4-C5-N-C6
13	G	1304	PCW	C4-C5-N-C7
13	G	1304	PCW	C4-C5-N-C8
13	C	1111	PCW	C4-C5-N-C6
13	C	1111	PCW	C4-C5-N-C7
13	C	1112	PCW	C4-C5-N-C6
13	C	1112	PCW	C4-C5-N-C7
13	C	1114	PCW	C4-C5-N-C6
13	C	1114	PCW	C4-C5-N-C7
13	E	1302	PCW	C4-C5-N-C6
13	E	1302	PCW	C4-C5-N-C7
13	E	1303	PCW	C4-C5-N-C6
13	E	1303	PCW	C4-C5-N-C7
13	E	1304	PCW	C4-C5-N-C6
13	E	1304	PCW	C4-C5-N-C7

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Mol	Chain	Res	Type	Atoms
13	E	1304	PCW	C4-C5-N-C8
13	A	1110	PCW	C34-C35-C36-C37
13	C	1110	PCW	C34-C35-C36-C37
13	A	1111	PCW	C22-C23-C24-C25
13	G	1303	PCW	C13-C14-C15-C16
13	G	1304	PCW	C21-C22-C23-C24
13	C	1111	PCW	C22-C23-C24-C25
13	E	1303	PCW	C13-C14-C15-C16
13	E	1304	PCW	C21-C22-C23-C24
13	A	1111	PCW	C43-C44-C45-C46
13	G	1304	PCW	C34-C35-C36-C37
13	G	1304	PCW	C43-C44-C45-C46
13	C	1111	PCW	C43-C44-C45-C46
13	E	1304	PCW	C34-C35-C36-C37
13	E	1304	PCW	C43-C44-C45-C46
13	A	1112	PCW	C42-C43-C44-C45
13	C	1112	PCW	C42-C43-C44-C45
13	A	1109	PCW	C44-C45-C46-C47
13	C	1109	PCW	C44-C45-C46-C47
13	A	1108	PCW	C33-C34-C35-C36
13	C	1108	PCW	C33-C34-C35-C36
13	A	1109	PCW	C20-C21-C22-C23
13	C	1109	PCW	C20-C21-C22-C23
13	A	1110	PCW	C15-C16-C17-C18
13	C	1110	PCW	C15-C16-C17-C18
13	A	1111	PCW	C21-C22-C23-C24
13	C	1111	PCW	C21-C22-C23-C24
13	A	1111	PCW	C23-C24-C25-C26
13	C	1111	PCW	C23-C24-C25-C26
13	A	1112	PCW	C35-C36-C37-C38
13	C	1112	PCW	C35-C36-C37-C38
13	A	1111	PCW	C16-C17-C18-C19
13	A	1112	PCW	C40-C41-C42-C43
13	A	1114	PCW	C20-C21-C22-C23
13	C	1111	PCW	C16-C17-C18-C19
13	C	1112	PCW	C40-C41-C42-C43
13	G	1303	PCW	C34-C35-C36-C37
13	E	1303	PCW	C34-C35-C36-C37
13	A	1113	PCW	O3P-C1-C2-O2
13	C	1113	PCW	O3P-C1-C2-O2
13	A	1108	PCW	C16-C17-C18-C19
13	A	1108	PCW	C40-C41-C42-C43

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Mol	Chain	Res	Type	Atoms
13	C	1108	PCW	C16-C17-C18-C19
13	C	1108	PCW	C40-C41-C42-C43
13	C	1114	PCW	C20-C21-C22-C23
13	A	1112	PCW	C33-C34-C35-C36
13	G	1304	PCW	C33-C34-C35-C36
13	E	1304	PCW	C33-C34-C35-C36
13	C	1112	PCW	C33-C34-C35-C36
13	A	1110	PCW	C41-C42-C43-C44
13	C	1110	PCW	C41-C42-C43-C44
13	A	1110	PCW	C40-C41-C42-C43
13	G	1302	PCW	C40-C41-C42-C43
13	C	1110	PCW	C40-C41-C42-C43
13	E	1302	PCW	C40-C41-C42-C43
13	A	1109	PCW	O3P-C1-C2-C3
13	A	1111	PCW	O3P-C1-C2-C3
13	A	1112	PCW	O3P-C1-C2-C3
13	A	1114	PCW	O3P-C1-C2-C3
13	G	1304	PCW	O3P-C1-C2-C3
13	C	1109	PCW	O3P-C1-C2-C3
13	C	1111	PCW	O3P-C1-C2-C3
13	C	1112	PCW	O3P-C1-C2-C3
13	C	1114	PCW	O3P-C1-C2-C3
13	E	1304	PCW	O3P-C1-C2-C3
13	G	1304	PCW	C11-C12-C13-C14
13	E	1304	PCW	C11-C12-C13-C14
13	A	1107	PCW	C1-C2-C3-O3
13	A	1109	PCW	C1-C2-C3-O3
13	A	1112	PCW	C1-C2-C3-O3
13	C	1107	PCW	C1-C2-C3-O3
13	C	1109	PCW	C1-C2-C3-O3
13	C	1112	PCW	C1-C2-C3-O3
13	A	1112	PCW	C36-C37-C38-C39
13	C	1108	PCW	C20-C21-C22-C23
13	C	1112	PCW	C36-C37-C38-C39
13	G	1302	PCW	C43-C44-C45-C46
13	E	1302	PCW	C43-C44-C45-C46
13	A	1114	PCW	C31-C32-C33-C34
13	G	1303	PCW	C31-C32-C33-C34
13	E	1303	PCW	C31-C32-C33-C34
13	A	1108	PCW	C20-C21-C22-C23
13	A	1109	PCW	C40-C41-C42-C43
13	C	1109	PCW	C40-C41-C42-C43

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Mol	Chain	Res	Type	Atoms
13	C	1114	PCW	C31-C32-C33-C34
13	A	1111	PCW	C32-C33-C34-C35
13	C	1111	PCW	C32-C33-C34-C35
13	A	1112	PCW	C14-C15-C16-C17
13	G	1302	PCW	C35-C36-C37-C38
13	C	1112	PCW	C14-C15-C16-C17
13	E	1302	PCW	C35-C36-C37-C38
13	G	1303	PCW	O2-C2-C3-O3
13	E	1303	PCW	O2-C2-C3-O3
13	G	1304	PCW	C16-C17-C18-C19
13	E	1304	PCW	C16-C17-C18-C19
13	A	1111	PCW	C14-C15-C16-C17
13	C	1111	PCW	C14-C15-C16-C17
13	A	1109	PCW	C14-C15-C16-C17
13	C	1109	PCW	C14-C15-C16-C17
13	A	1113	PCW	O3P-C1-C2-C3
13	C	1113	PCW	O3P-C1-C2-C3
11	A	1104	7Q2	CAY-CAX-OAW-NAV
11	C	1104	7Q2	CAY-CAX-OAW-NAV
13	A	1111	PCW	C1-C2-C3-O3
13	A	1113	PCW	C1-C2-C3-O3
13	A	1114	PCW	C1-C2-C3-O3
13	C	1111	PCW	C1-C2-C3-O3
13	C	1113	PCW	C1-C2-C3-O3
13	C	1114	PCW	C1-C2-C3-O3
13	G	1303	PCW	C23-C24-C25-C26
13	E	1303	PCW	C23-C24-C25-C26
13	A	1106	PCW	O3P-C1-C2-O2
13	A	1111	PCW	O3P-C1-C2-O2
13	A	1114	PCW	O3P-C1-C2-O2
13	C	1106	PCW	O3P-C1-C2-O2
13	C	1111	PCW	O3P-C1-C2-O2
13	C	1114	PCW	O3P-C1-C2-O2
13	G	1304	PCW	C31-C32-C33-C34
13	E	1304	PCW	C31-C32-C33-C34
13	A	1114	PCW	C25-C26-C27-C28
13	C	1114	PCW	C25-C26-C27-C28
13	A	1107	PCW	O2-C2-C3-O3
13	A	1108	PCW	O2-C2-C3-O3
13	A	1111	PCW	O2-C2-C3-O3
13	A	1113	PCW	O2-C2-C3-O3
13	C	1107	PCW	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
13	C	1108	PCW	O2-C2-C3-O3
13	C	1111	PCW	O2-C2-C3-O3
13	C	1113	PCW	O2-C2-C3-O3
13	A	1114	PCW	C45-C46-C47-C48
13	C	1114	PCW	C45-C46-C47-C48
13	A	1106	PCW	O3P-C1-C2-C3
13	C	1106	PCW	O3P-C1-C2-C3
13	A	1110	PCW	C43-C44-C45-C46
13	G	1303	PCW	C35-C36-C37-C38
13	C	1110	PCW	C43-C44-C45-C46
13	E	1303	PCW	C35-C36-C37-C38
13	G	1303	PCW	O3P-C1-C2-O2
13	E	1303	PCW	O3P-C1-C2-O2
13	G	1302	PCW	C1-C2-C3-O3
13	E	1302	PCW	C1-C2-C3-O3
13	A	1109	PCW	O2-C2-C3-O3
13	C	1109	PCW	O2-C2-C3-O3
13	A	1106	PCW	O4P-C4-C5-N
13	A	1107	PCW	O4P-C4-C5-N
13	A	1109	PCW	O4P-C4-C5-N
13	A	1110	PCW	O4P-C4-C5-N
13	A	1111	PCW	O4P-C4-C5-N
13	A	1112	PCW	O4P-C4-C5-N
13	A	1113	PCW	O4P-C4-C5-N
13	A	1114	PCW	O4P-C4-C5-N
13	G	1302	PCW	O4P-C4-C5-N
13	G	1303	PCW	O4P-C4-C5-N
13	G	1304	PCW	O4P-C4-C5-N
13	C	1106	PCW	O4P-C4-C5-N
13	C	1107	PCW	O4P-C4-C5-N
13	C	1109	PCW	O4P-C4-C5-N
13	C	1110	PCW	O4P-C4-C5-N
13	C	1111	PCW	O4P-C4-C5-N
13	C	1112	PCW	O4P-C4-C5-N
13	C	1113	PCW	O4P-C4-C5-N
13	C	1114	PCW	O4P-C4-C5-N
13	E	1302	PCW	O4P-C4-C5-N
13	E	1303	PCW	O4P-C4-C5-N
13	E	1304	PCW	O4P-C4-C5-N
13	C	1114	PCW	C15-C16-C17-C18
13	A	1114	PCW	C15-C16-C17-C18
13	A	1111	PCW	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
13	C	1111	PCW	C15-C16-C17-C18
13	G	1303	PCW	O3P-C1-C2-C3
13	E	1303	PCW	O3P-C1-C2-C3
13	A	1114	PCW	C39-C40-C41-C42
13	C	1114	PCW	C39-C40-C41-C42
13	A	1114	PCW	O2-C2-C3-O3
13	C	1114	PCW	O2-C2-C3-O3
13	A	1108	PCW	C1-C2-C3-O3
13	C	1108	PCW	C1-C2-C3-O3
13	A	1110	PCW	C32-C33-C34-C35
13	C	1110	PCW	C32-C33-C34-C35
13	A	1106	PCW	C4-O4P-P-O2P
13	A	1107	PCW	C1-O3P-P-O2P
13	A	1107	PCW	C4-O4P-P-O1P
13	A	1108	PCW	C1-O3P-P-O2P
13	A	1109	PCW	C4-O4P-P-O2P
13	A	1111	PCW	C4-O4P-P-O2P
13	A	1112	PCW	C4-O4P-P-O2P
13	A	1113	PCW	C1-O3P-P-O4P
13	A	1113	PCW	C4-O4P-P-O2P
13	A	1114	PCW	C4-O4P-P-O2P
13	C	1106	PCW	C4-O4P-P-O2P
13	C	1107	PCW	C1-O3P-P-O2P
13	C	1107	PCW	C4-O4P-P-O1P
13	C	1108	PCW	C1-O3P-P-O2P
13	C	1109	PCW	C4-O4P-P-O2P
13	C	1111	PCW	C4-O4P-P-O2P
13	C	1112	PCW	C4-O4P-P-O2P
13	C	1113	PCW	C1-O3P-P-O4P
13	C	1113	PCW	C4-O4P-P-O2P
13	C	1114	PCW	C4-O4P-P-O2P
13	A	1110	PCW	C14-C15-C16-C17
13	C	1110	PCW	C14-C15-C16-C17
13	E	1303	PCW	O2-C31-C32-C33
13	A	1109	PCW	C17-C18-C19-C20
13	A	1114	PCW	C19-C20-C21-C22
13	C	1109	PCW	C17-C18-C19-C20
13	C	1114	PCW	C19-C20-C21-C22
13	A	1107	PCW	O3P-C1-C2-O2
13	A	1112	PCW	O3P-C1-C2-O2
13	G	1304	PCW	O3P-C1-C2-O2
13	C	1107	PCW	O3P-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
13	C	1112	PCW	O3P-C1-C2-O2
13	E	1304	PCW	O3P-C1-C2-O2
13	G	1303	PCW	O2-C31-C32-C33
13	C	1108	PCW	C35-C36-C37-C38
13	A	1108	PCW	C35-C36-C37-C38
13	G	1304	PCW	C20-C21-C22-C23
13	E	1304	PCW	C20-C21-C22-C23
13	G	1303	PCW	C1-C2-C3-O3
13	E	1303	PCW	C1-C2-C3-O3
13	A	1111	PCW	C19-C20-C21-C22
13	G	1302	PCW	C17-C18-C19-C20
13	C	1111	PCW	C19-C20-C21-C22
13	E	1302	PCW	C17-C18-C19-C20
13	C	1111	PCW	C42-C43-C44-C45
10	A	1103	ATP	PG-O3B-PB-O3A
10	C	1103	ATP	PG-O3B-PB-O3A
13	A	1111	PCW	C42-C43-C44-C45
13	A	1111	PCW	C41-C42-C43-C44
13	C	1111	PCW	C41-C42-C43-C44
13	G	1302	PCW	C36-C37-C38-C39
13	E	1302	PCW	C36-C37-C38-C39
13	A	1114	PCW	C41-C42-C43-C44
13	C	1114	PCW	C41-C42-C43-C44
13	A	1107	PCW	O3P-C1-C2-C3
13	A	1108	PCW	O3P-C1-C2-C3
13	C	1107	PCW	O3P-C1-C2-C3
13	C	1108	PCW	O3P-C1-C2-C3
13	A	1110	PCW	O2-C2-C3-O3
13	C	1110	PCW	O2-C2-C3-O3
12	D	501	CLR	C23-C24-C25-C27
13	A	1114	PCW	C43-C44-C45-C46
13	C	1114	PCW	C43-C44-C45-C46
12	B	501	CLR	C23-C24-C25-C27
13	A	1110	PCW	C1-C2-C3-O3
13	C	1110	PCW	C1-C2-C3-O3
13	E	1303	PCW	C20-C21-C22-C23
13	A	1108	PCW	O3P-C1-C2-O2
13	C	1108	PCW	O3P-C1-C2-O2
13	G	1303	PCW	C20-C21-C22-C23
13	G	1303	PCW	C36-C37-C38-C39
13	E	1303	PCW	C36-C37-C38-C39
13	A	1110	PCW	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
13	G	1303	PCW	C17-C18-C19-C20
13	C	1110	PCW	C39-C40-C41-C42
13	E	1303	PCW	C17-C18-C19-C20
13	A	1108	PCW	C2-C1-O3P-P
13	C	1108	PCW	C2-C1-O3P-P
13	E	1302	PCW	C41-C42-C43-C44
13	G	1302	PCW	C41-C42-C43-C44
13	A	1109	PCW	C22-C23-C24-C25
13	C	1109	PCW	C22-C23-C24-C25
13	G	1303	PCW	C19-C20-C21-C22
13	G	1304	PCW	C19-C20-C21-C22
13	E	1303	PCW	C19-C20-C21-C22
13	E	1304	PCW	C19-C20-C21-C22
13	A	1108	PCW	C19-C20-C21-C22
13	C	1108	PCW	C19-C20-C21-C22
13	G	1304	PCW	C37-C38-C39-C40
13	E	1304	PCW	C37-C38-C39-C40
12	A	1105	CLR	C21-C20-C22-C23
12	C	1105	CLR	C21-C20-C22-C23
13	A	1109	PCW	C36-C37-C38-C39
13	C	1109	PCW	C36-C37-C38-C39
13	A	1112	PCW	C19-C20-C21-C22
13	C	1112	PCW	C19-C20-C21-C22
13	A	1114	PCW	O2-C31-C32-C33
13	C	1114	PCW	O2-C31-C32-C33
13	C	1109	PCW	O2-C31-C32-C33
13	A	1112	PCW	O2-C31-C32-C33
13	C	1112	PCW	O2-C31-C32-C33
13	A	1108	PCW	C37-C38-C39-C40
13	A	1109	PCW	C37-C38-C39-C40
13	A	1111	PCW	C37-C38-C39-C40
13	C	1108	PCW	C37-C38-C39-C40
13	C	1109	PCW	C37-C38-C39-C40
13	E	1303	PCW	C32-C33-C34-C35
13	G	1303	PCW	C32-C33-C34-C35
13	A	1109	PCW	O2-C31-C32-C33
10	A	1103	ATP	PG-O3B-PB-O1B
10	C	1103	ATP	PG-O3B-PB-O1B
13	A	1108	PCW	O2-C31-C32-C33
13	C	1108	PCW	O2-C31-C32-C33
13	C	1111	PCW	C37-C38-C39-C40
12	A	1105	CLR	C17-C20-C22-C23

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Mol	Chain	Res	Type	Atoms
12	C	1105	CLR	C17-C20-C22-C23
13	G	1304	PCW	C32-C33-C34-C35
13	A	1108	PCW	O31-C31-C32-C33
13	C	1108	PCW	O31-C31-C32-C33
13	E	1304	PCW	C32-C33-C34-C35
13	A	1109	PCW	O31-C31-C32-C33
13	C	1109	PCW	O31-C31-C32-C33
13	C	1114	PCW	O31-C31-C32-C33
13	A	1114	PCW	O31-C31-C32-C33
13	A	1110	PCW	O3P-C1-C2-C3
13	C	1110	PCW	O3P-C1-C2-C3
13	E	1302	PCW	O2-C31-C32-C33
13	G	1302	PCW	O2-C31-C32-C33

There are no ring outliers.

28 monomers are involved in 95 short contacts:

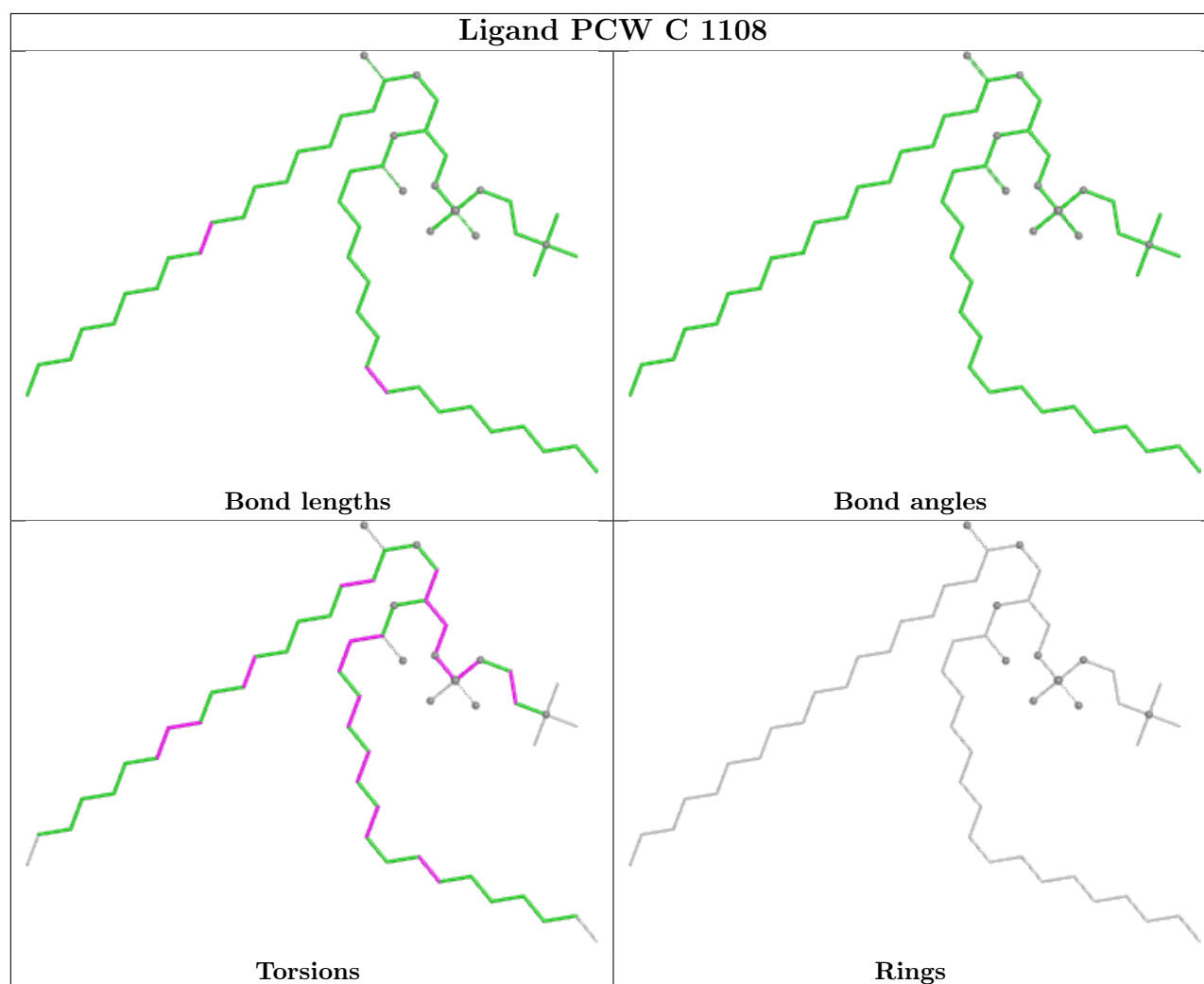
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	C	1108	PCW	11	0
12	A	1105	CLR	3	0
13	G	1302	PCW	2	0
10	A	1103	ATP	1	0
12	B	501	CLR	1	0
13	E	1302	PCW	2	0
13	C	1109	PCW	4	0
13	A	1108	PCW	11	0
13	C	1110	PCW	7	0
13	G	1303	PCW	4	0
13	E	1304	PCW	18	0
13	C	1111	PCW	2	0
12	G	1301	CLR	7	0
13	C	1113	PCW	1	0
12	D	501	CLR	1	0
12	B	502	CLR	1	0
13	A	1111	PCW	2	0
13	A	1109	PCW	4	0
13	A	1110	PCW	5	0
13	A	1113	PCW	1	0
13	G	1304	PCW	18	0
13	C	1112	PCW	3	0
13	C	1114	PCW	3	0
13	E	1303	PCW	4	0

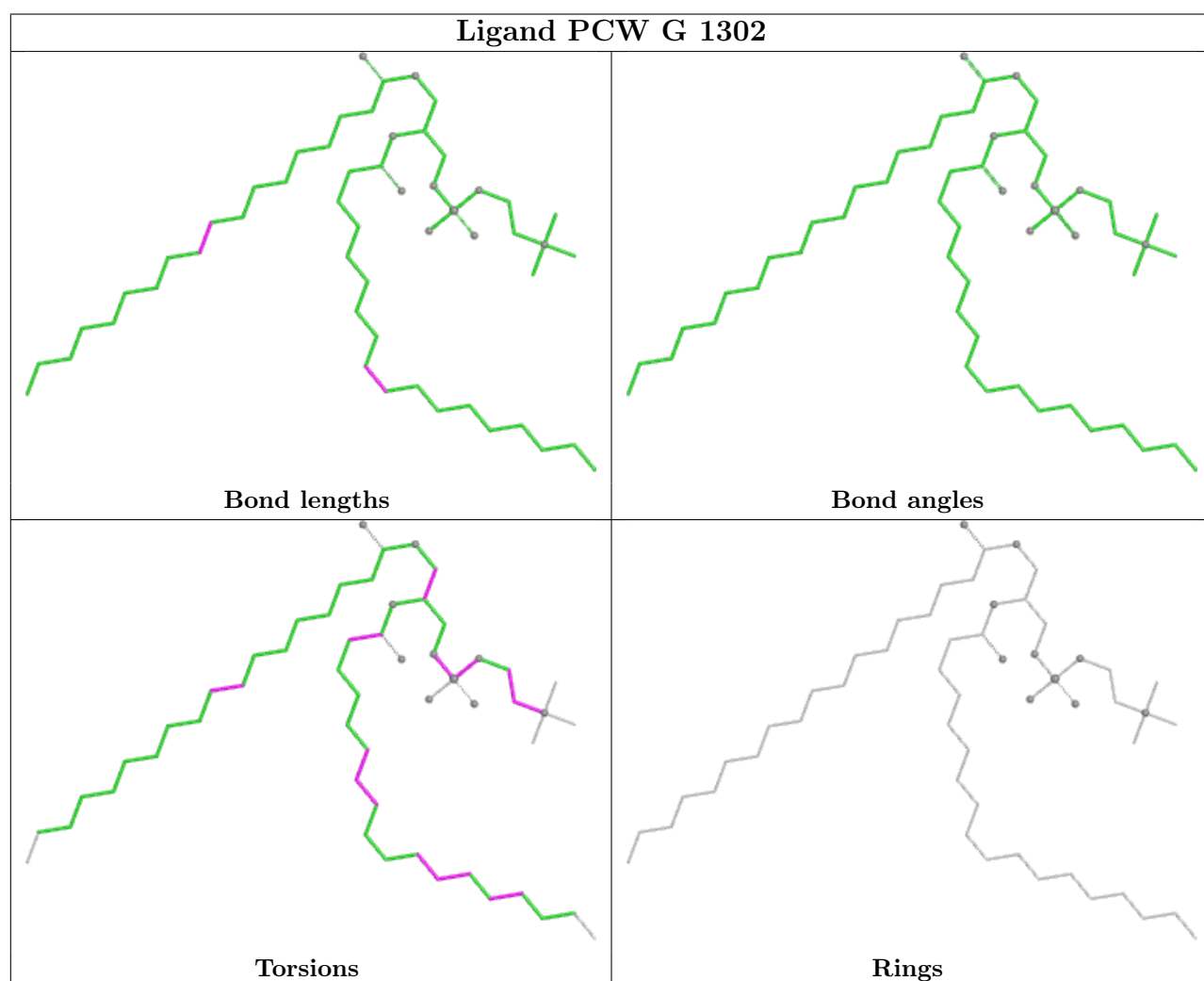
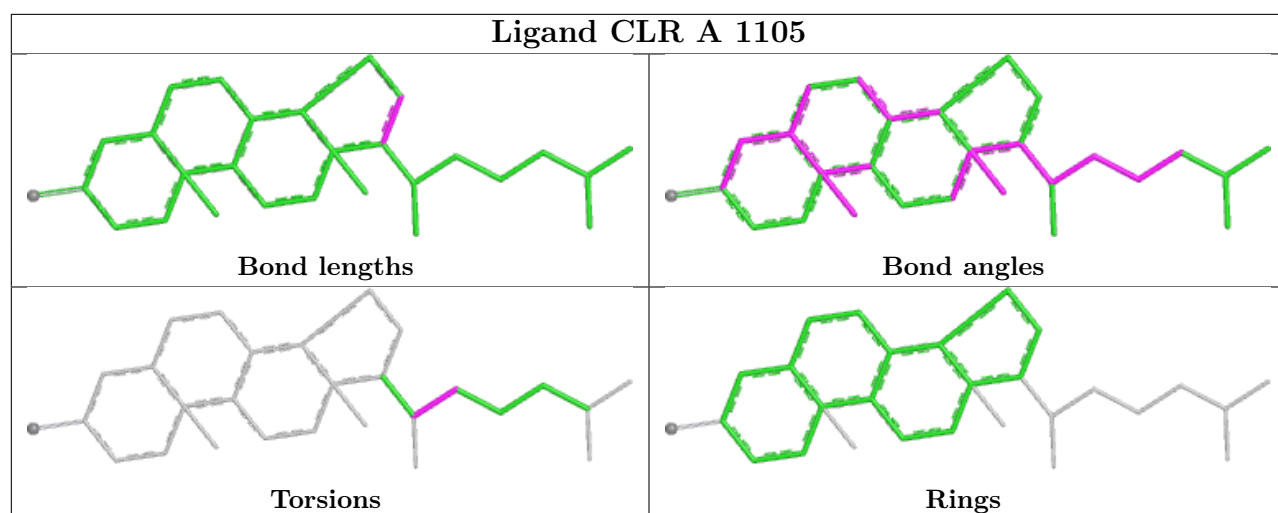
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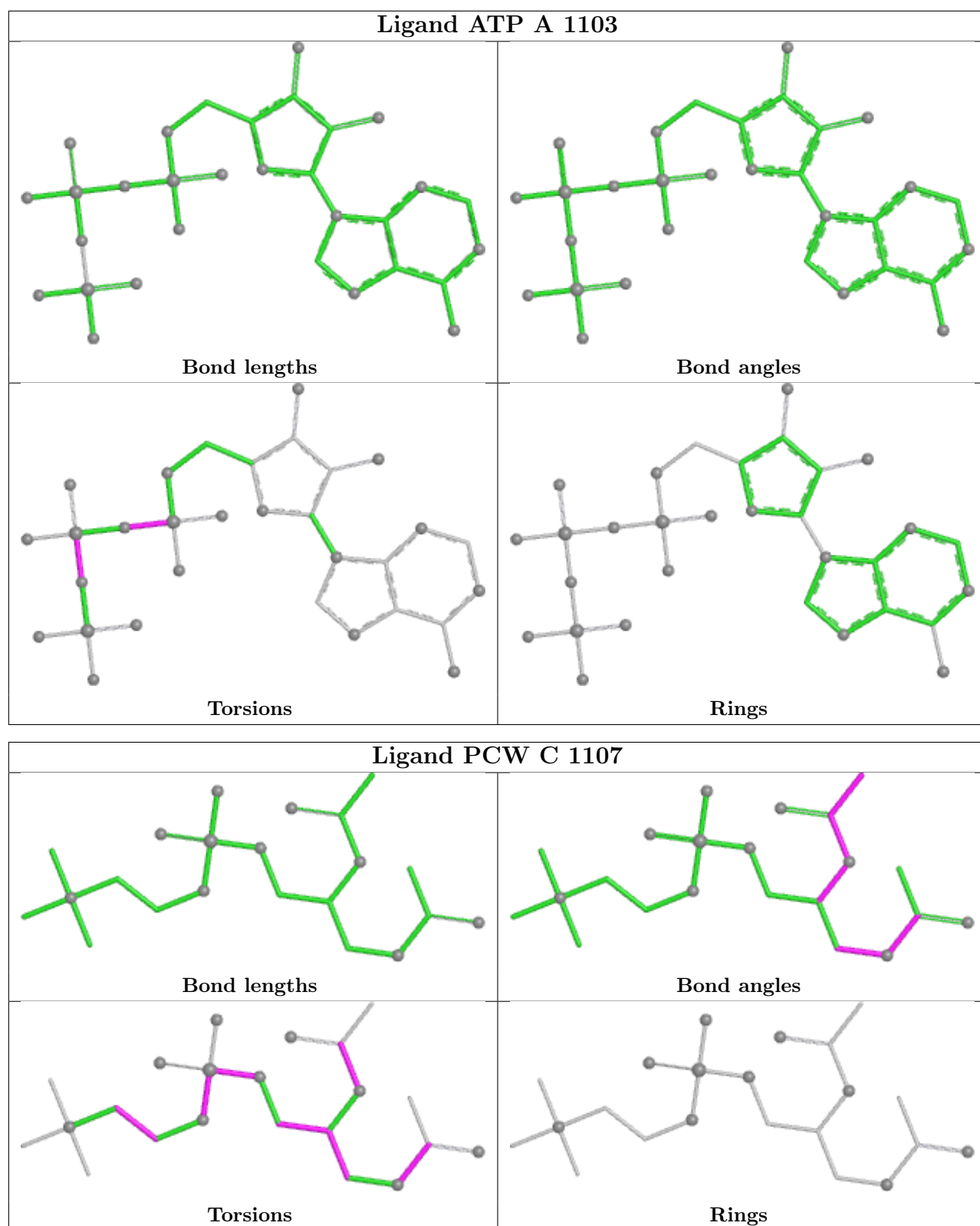
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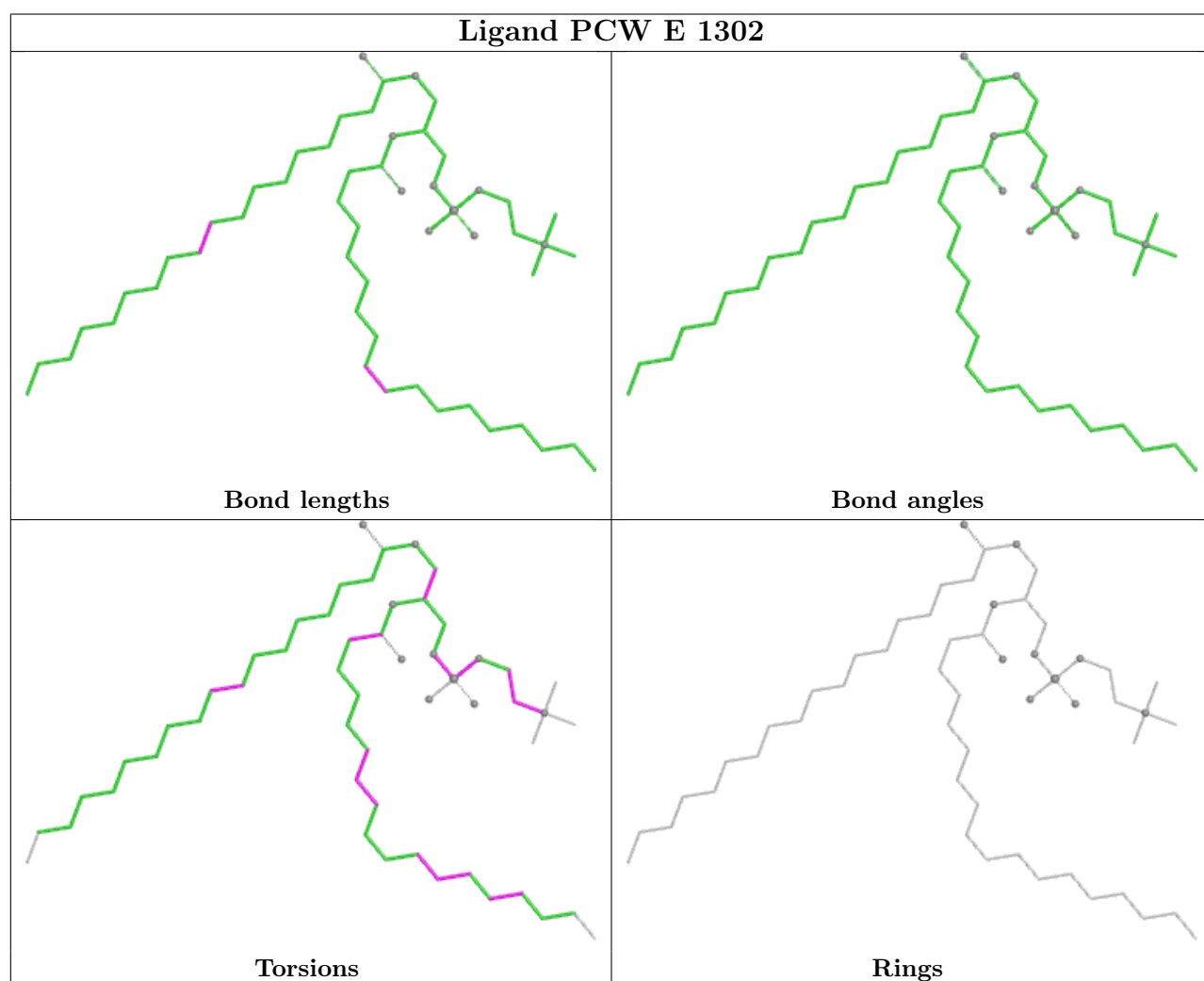
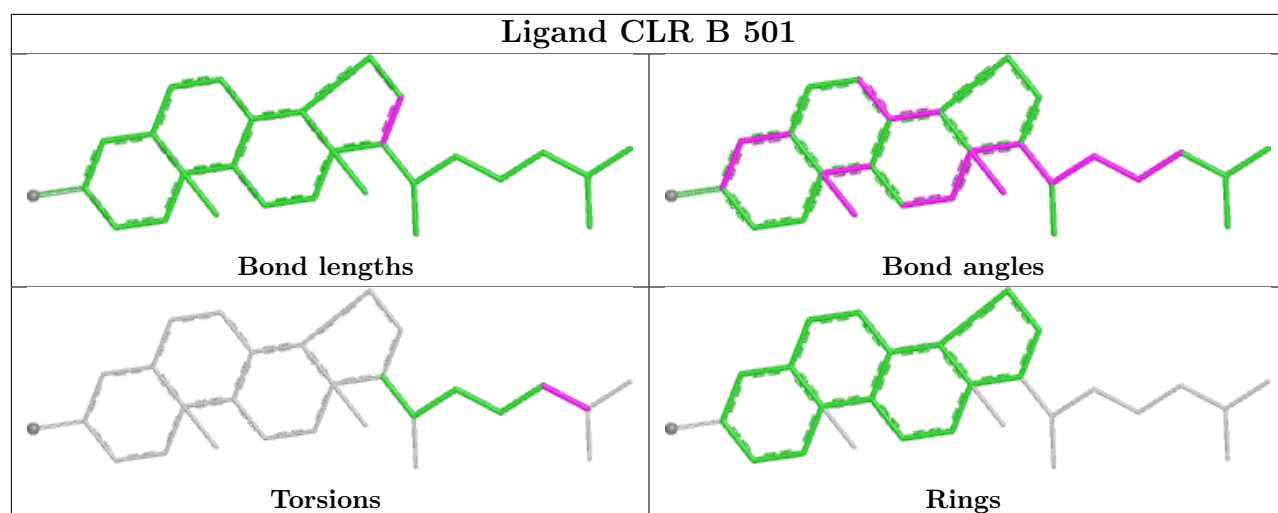
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	E	1301	CLR	7	0
13	A	1114	PCW	3	0
10	C	1103	ATP	1	0
13	A	1112	PCW	4	0

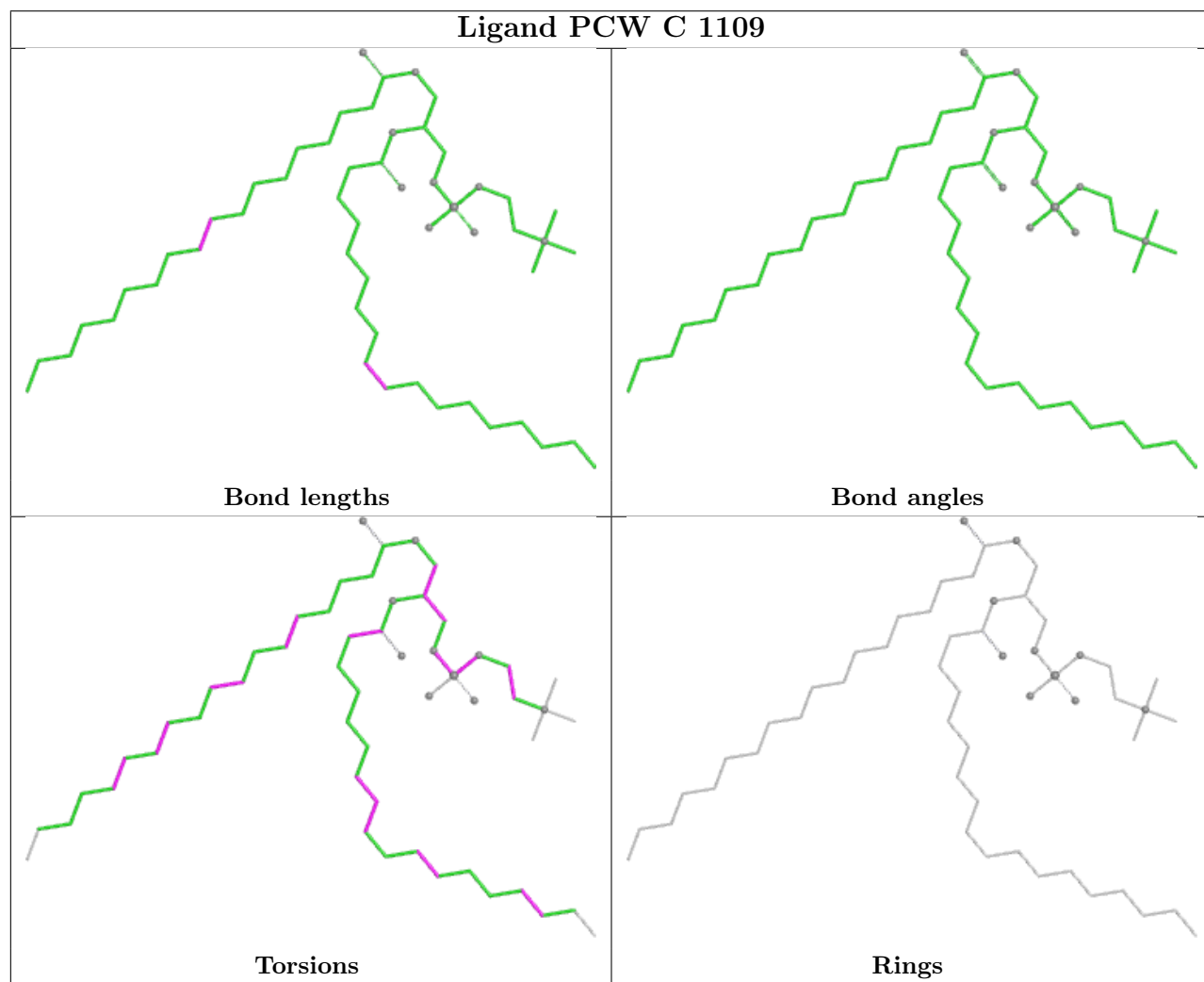
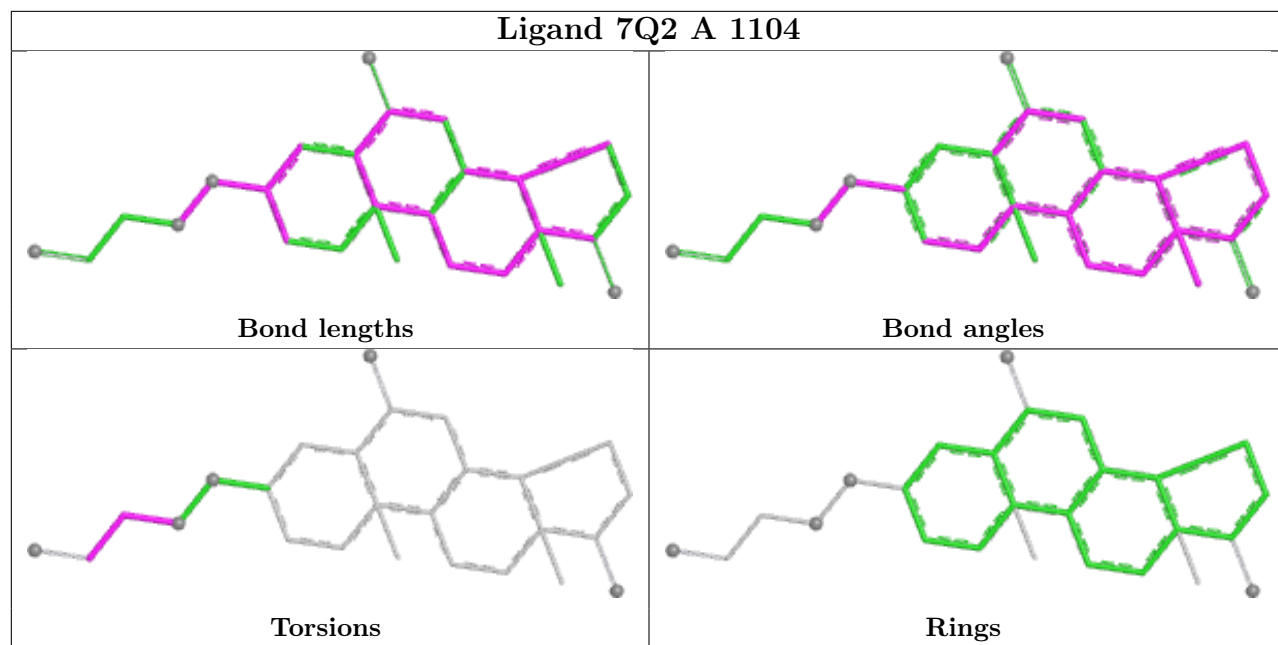
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

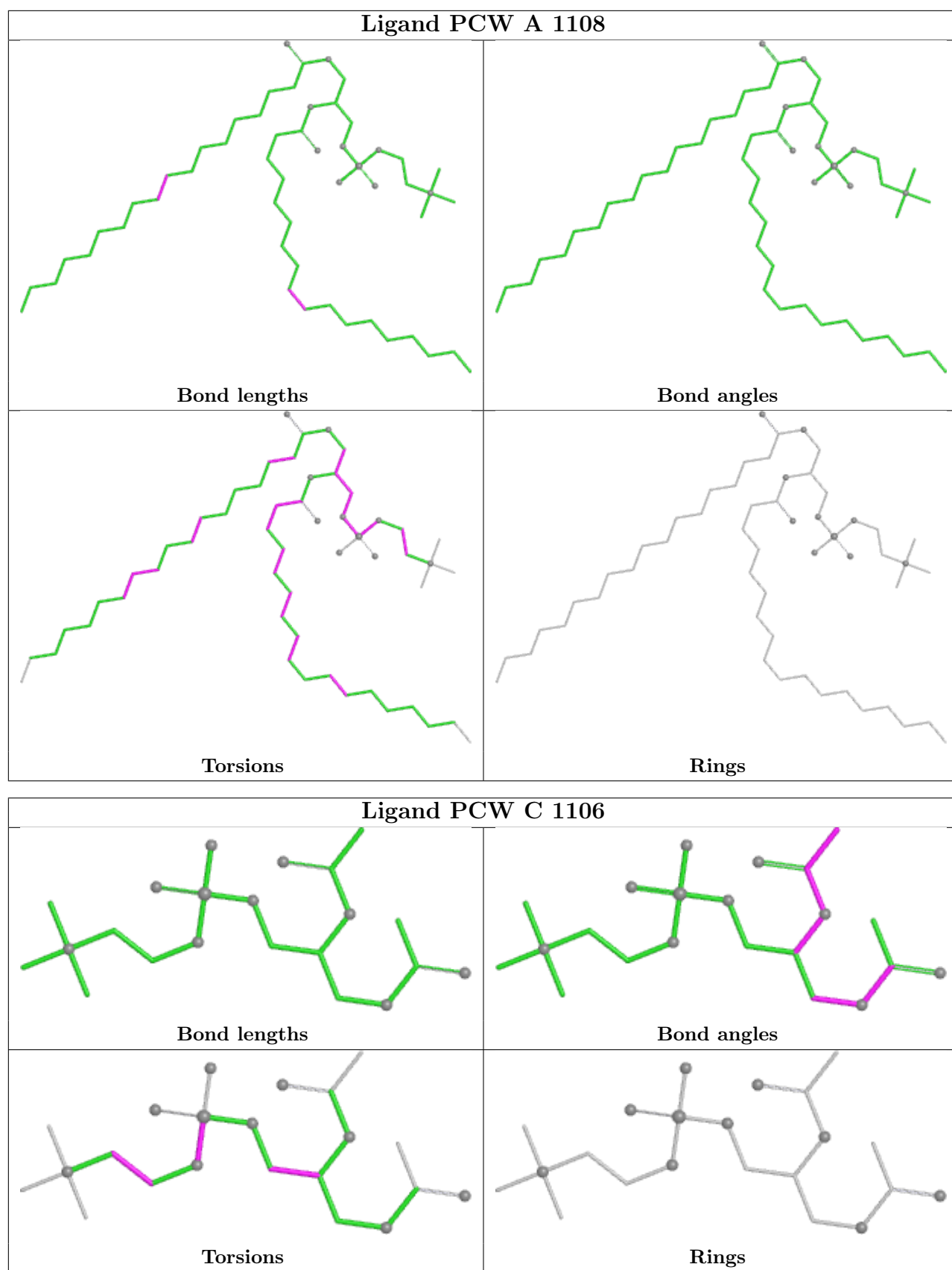


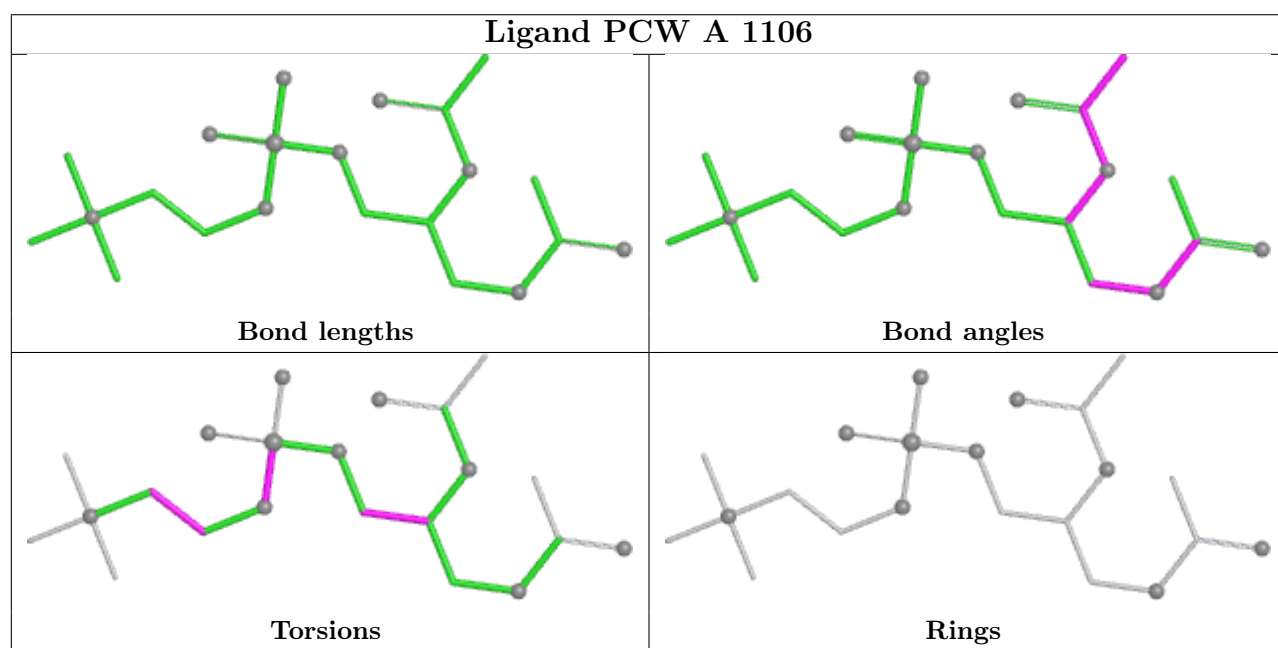
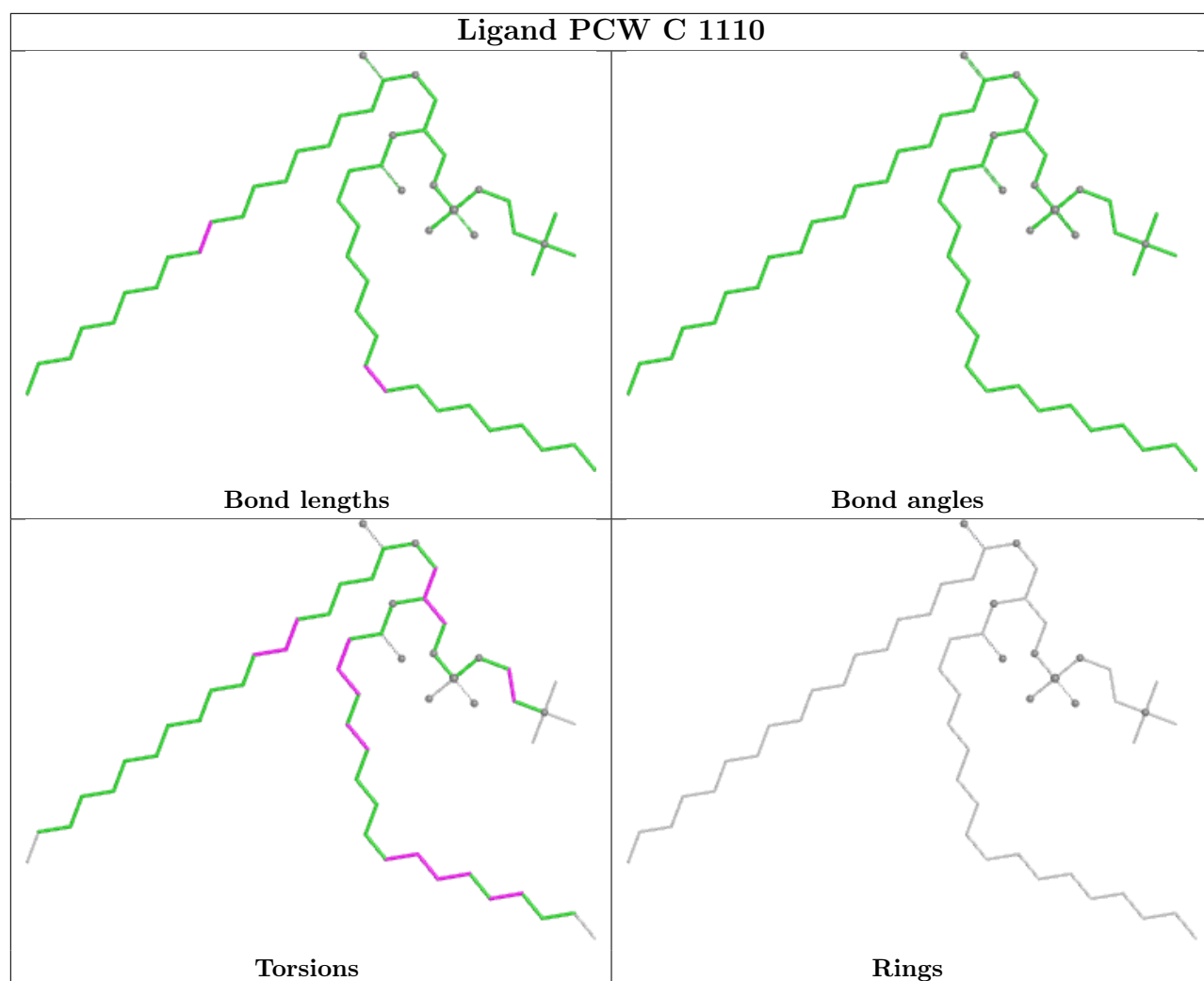


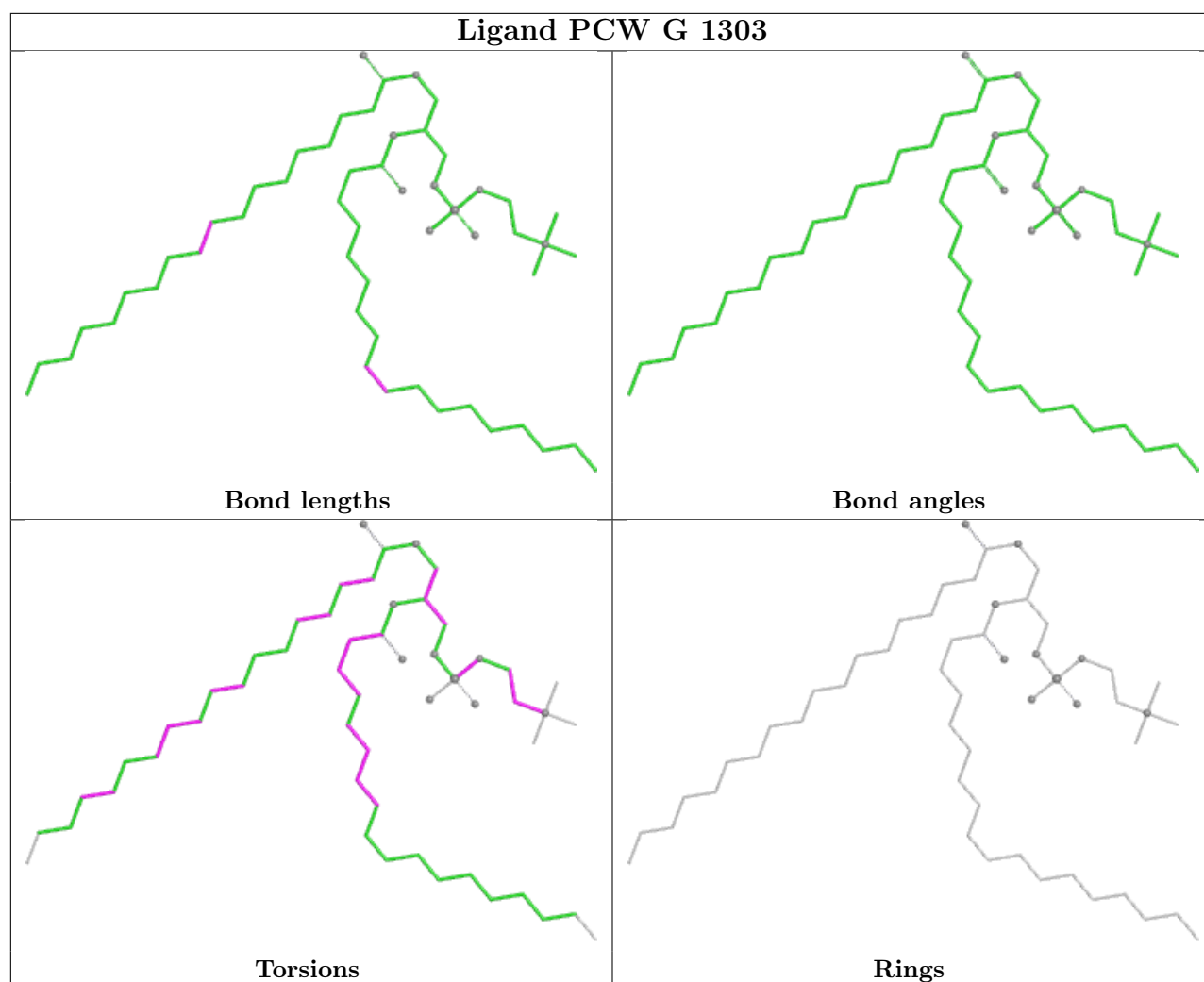


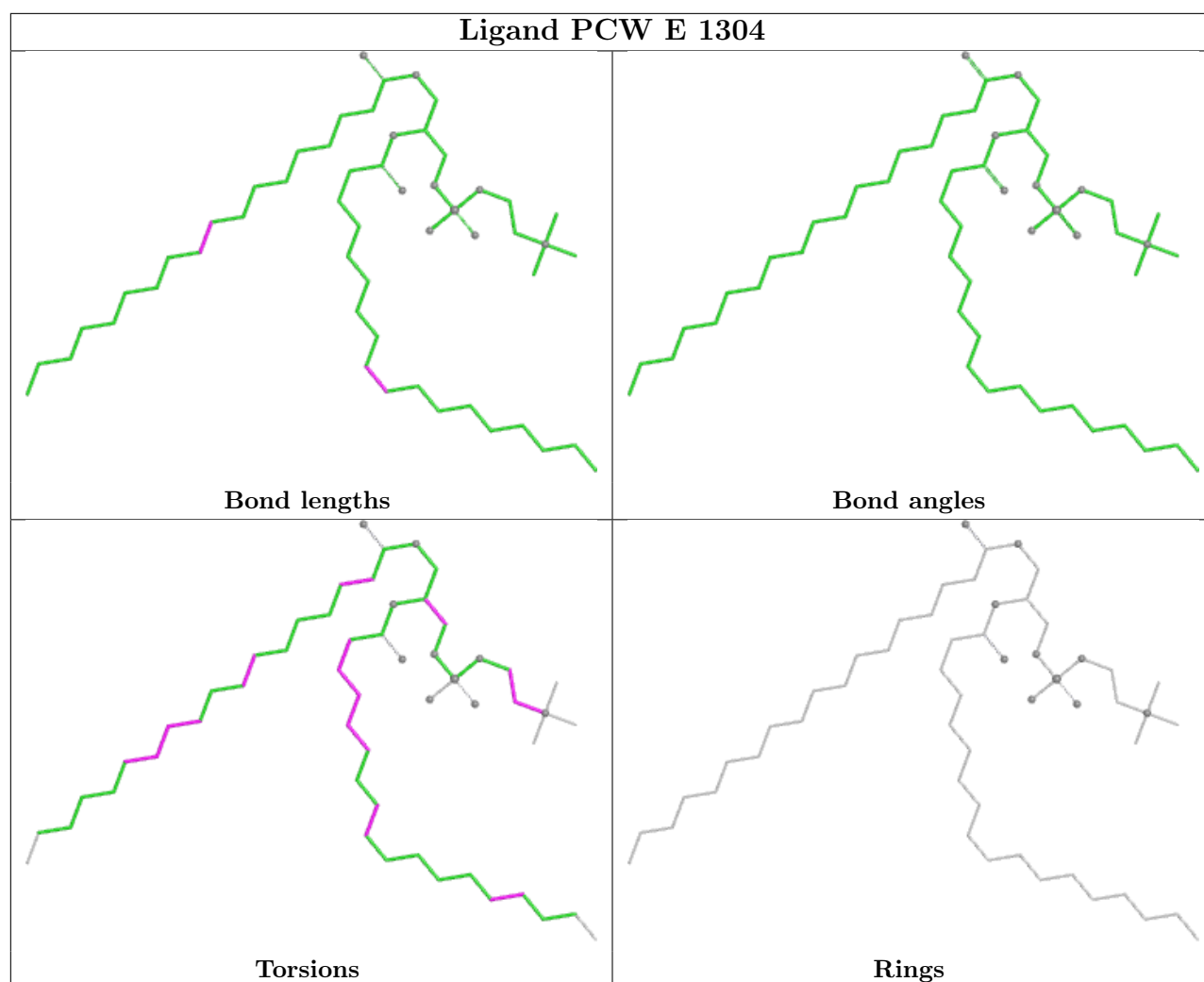


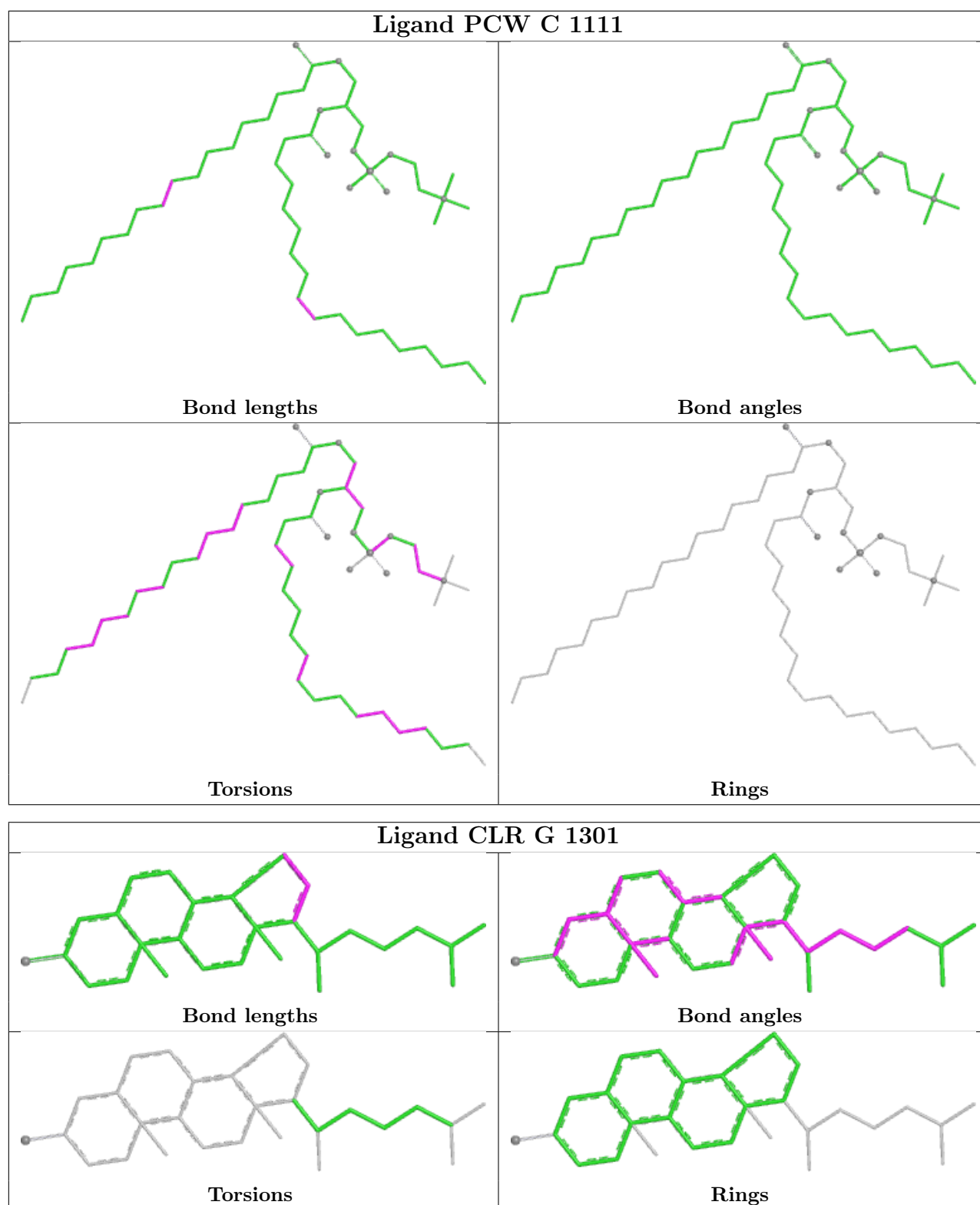




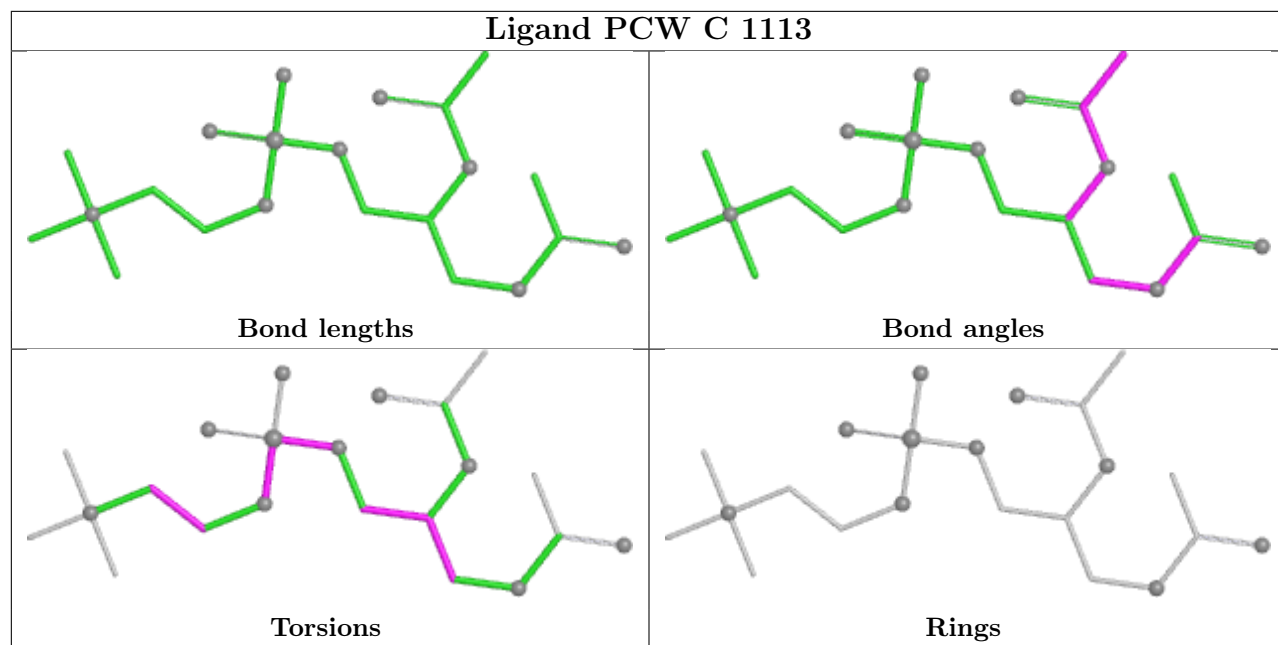




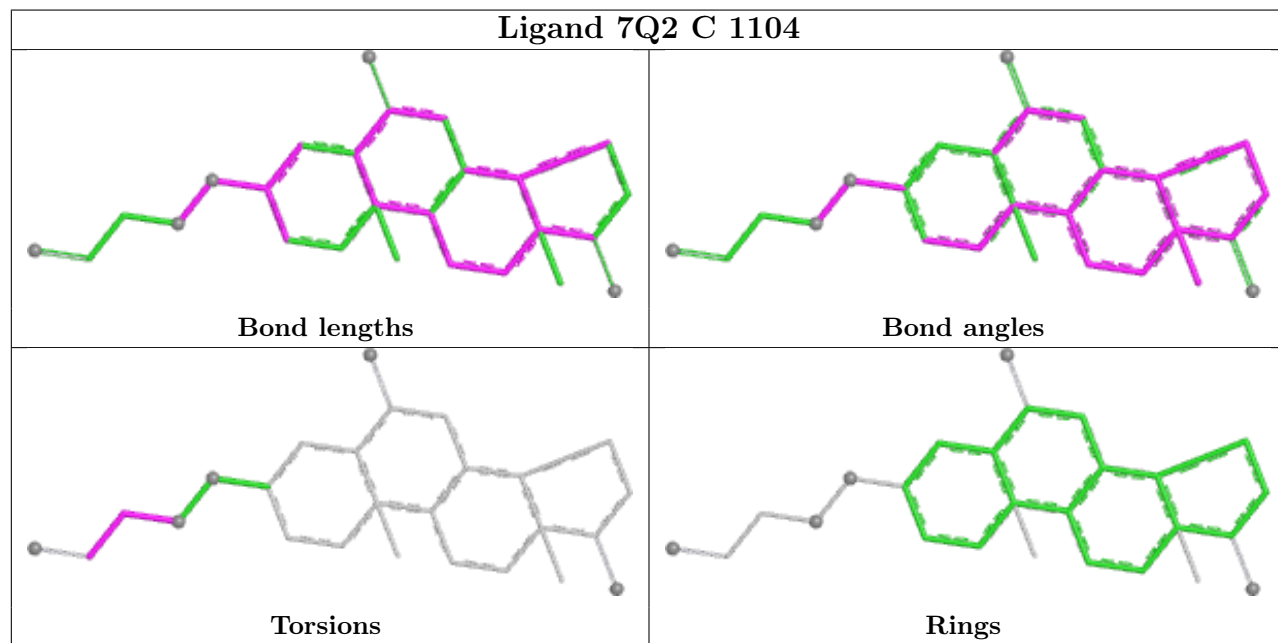


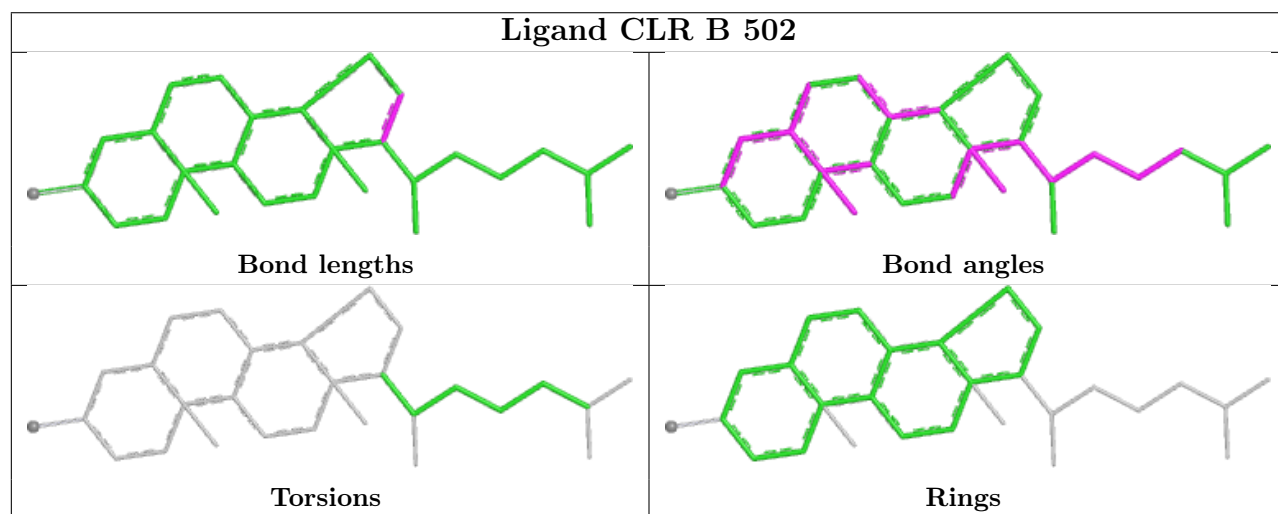
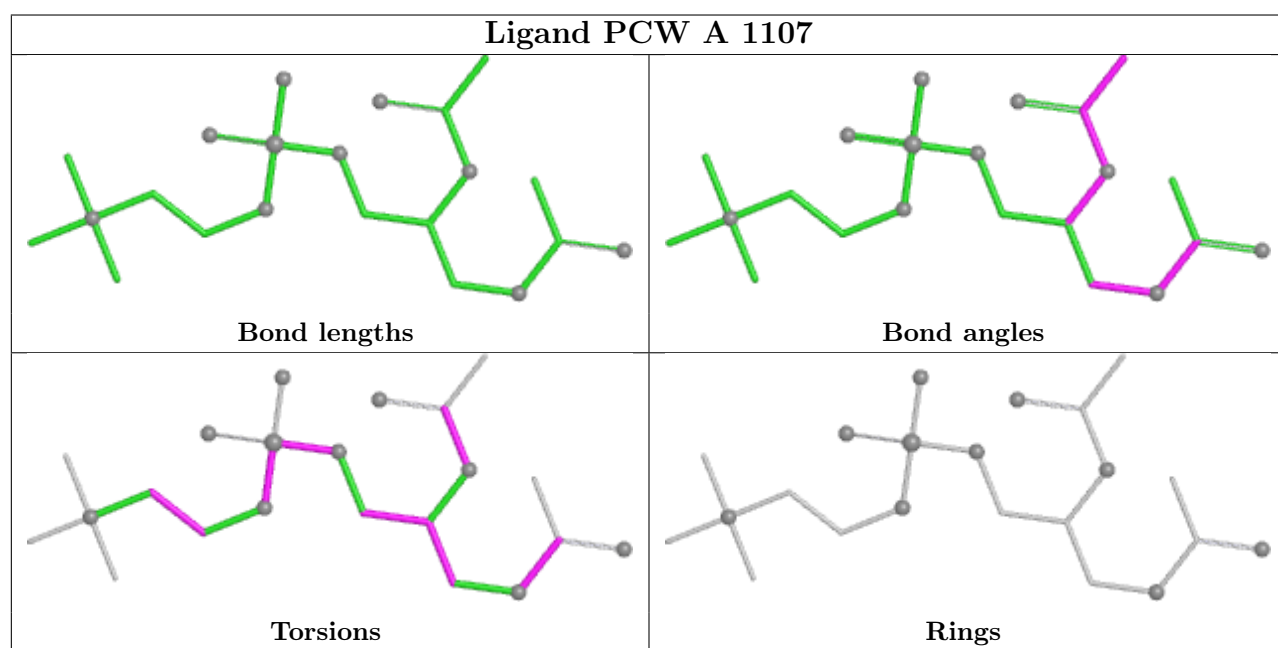
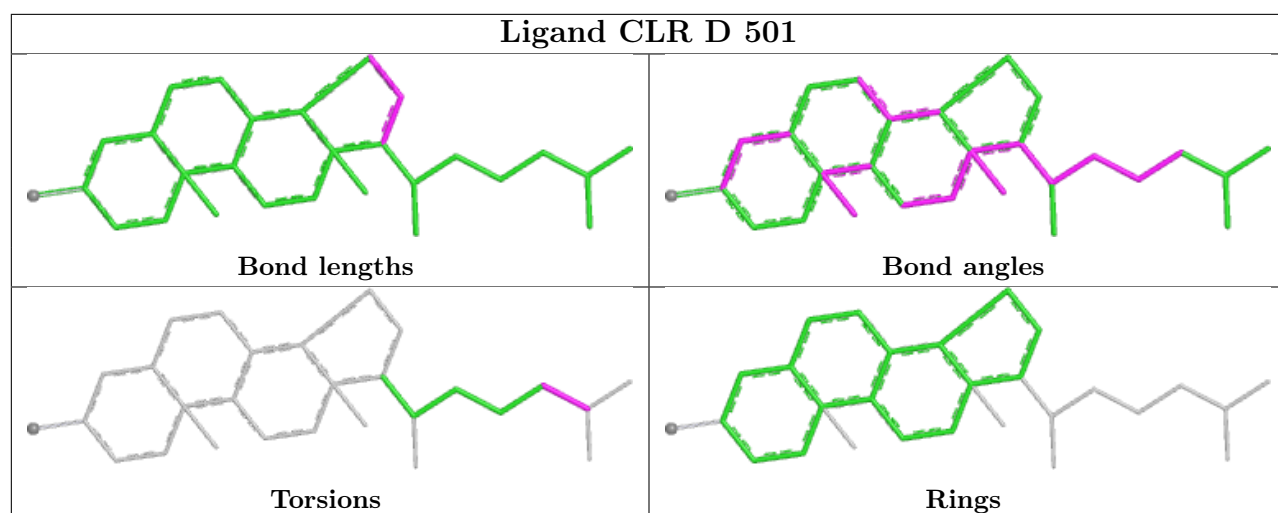


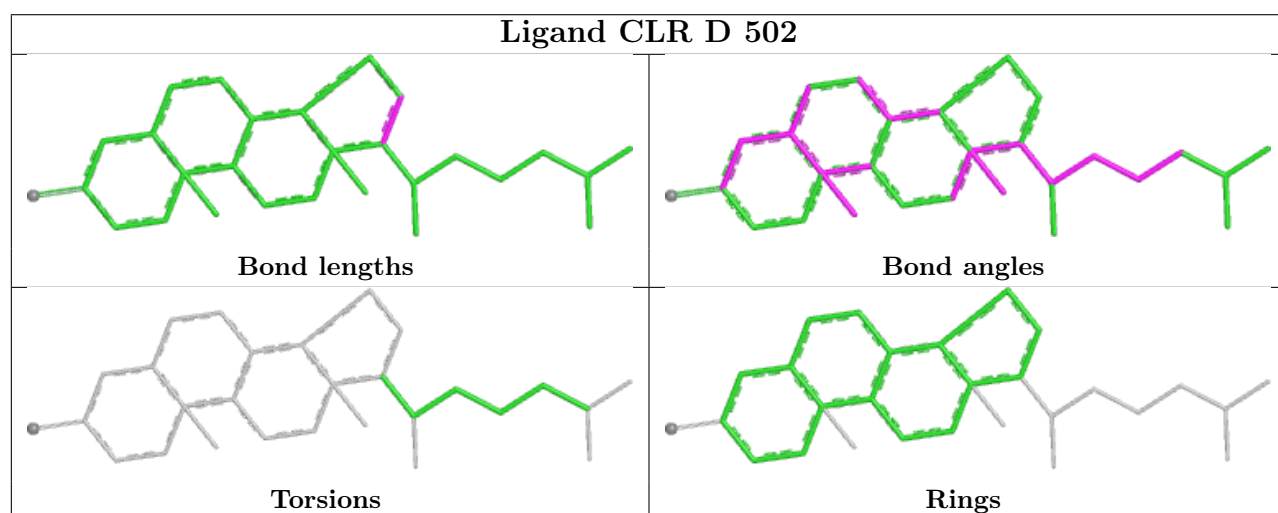
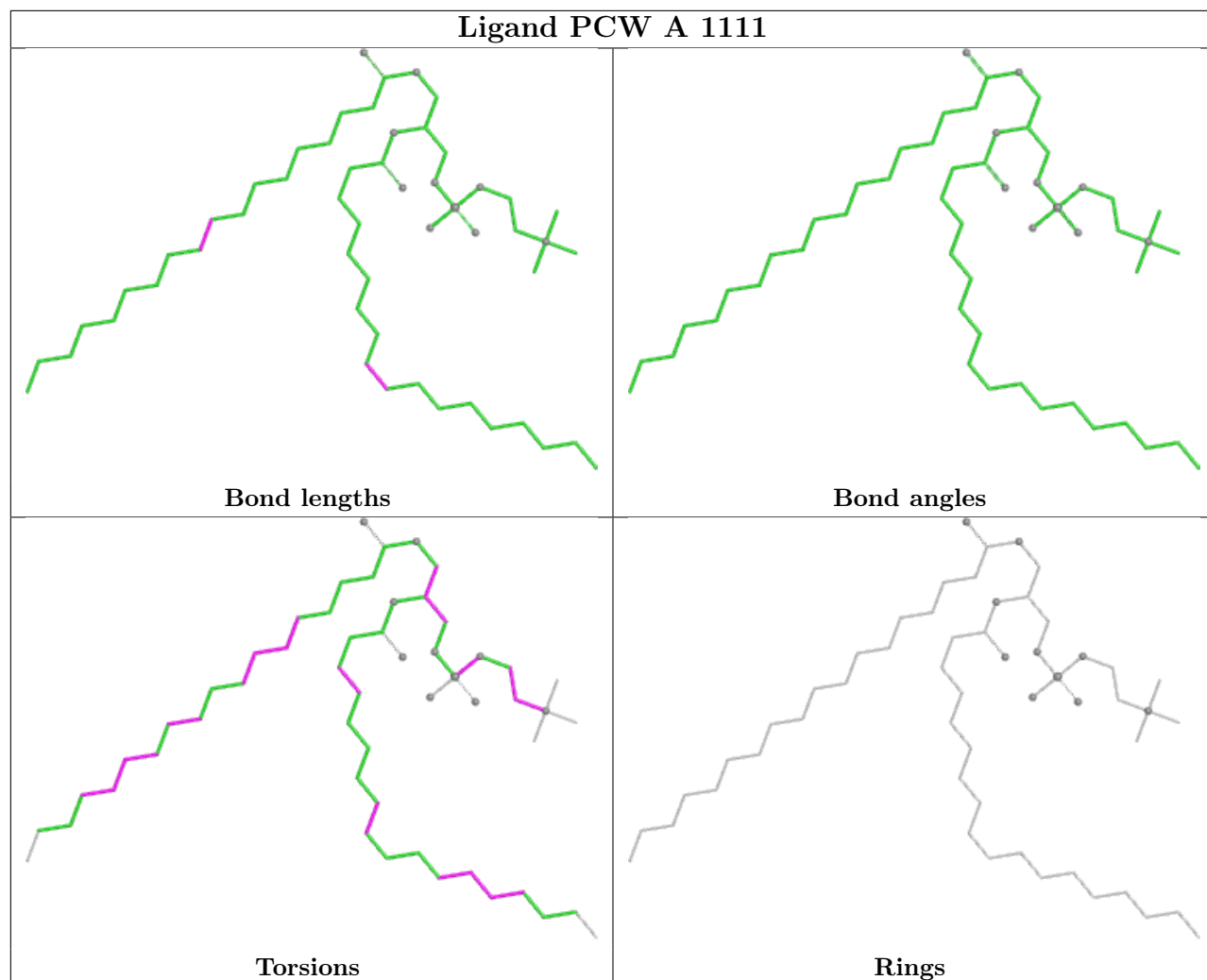
Ligand PCW C 1113

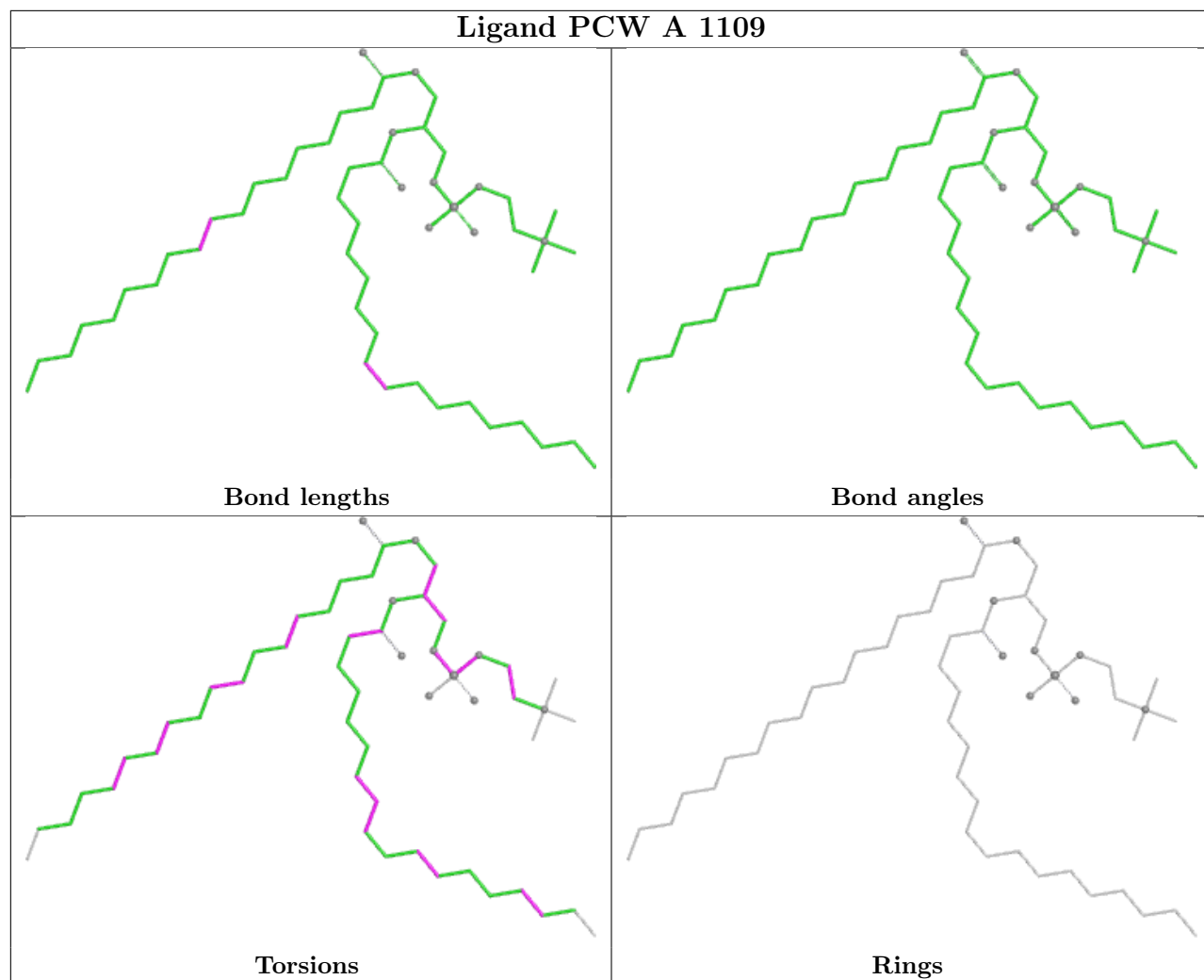


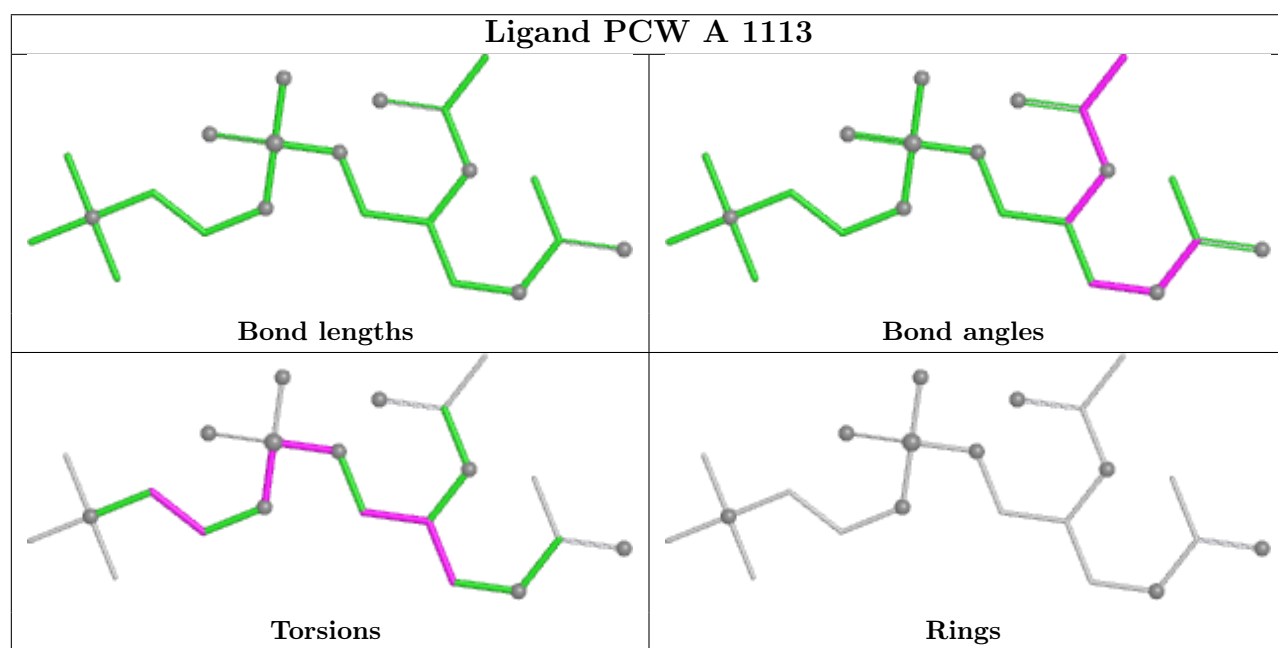
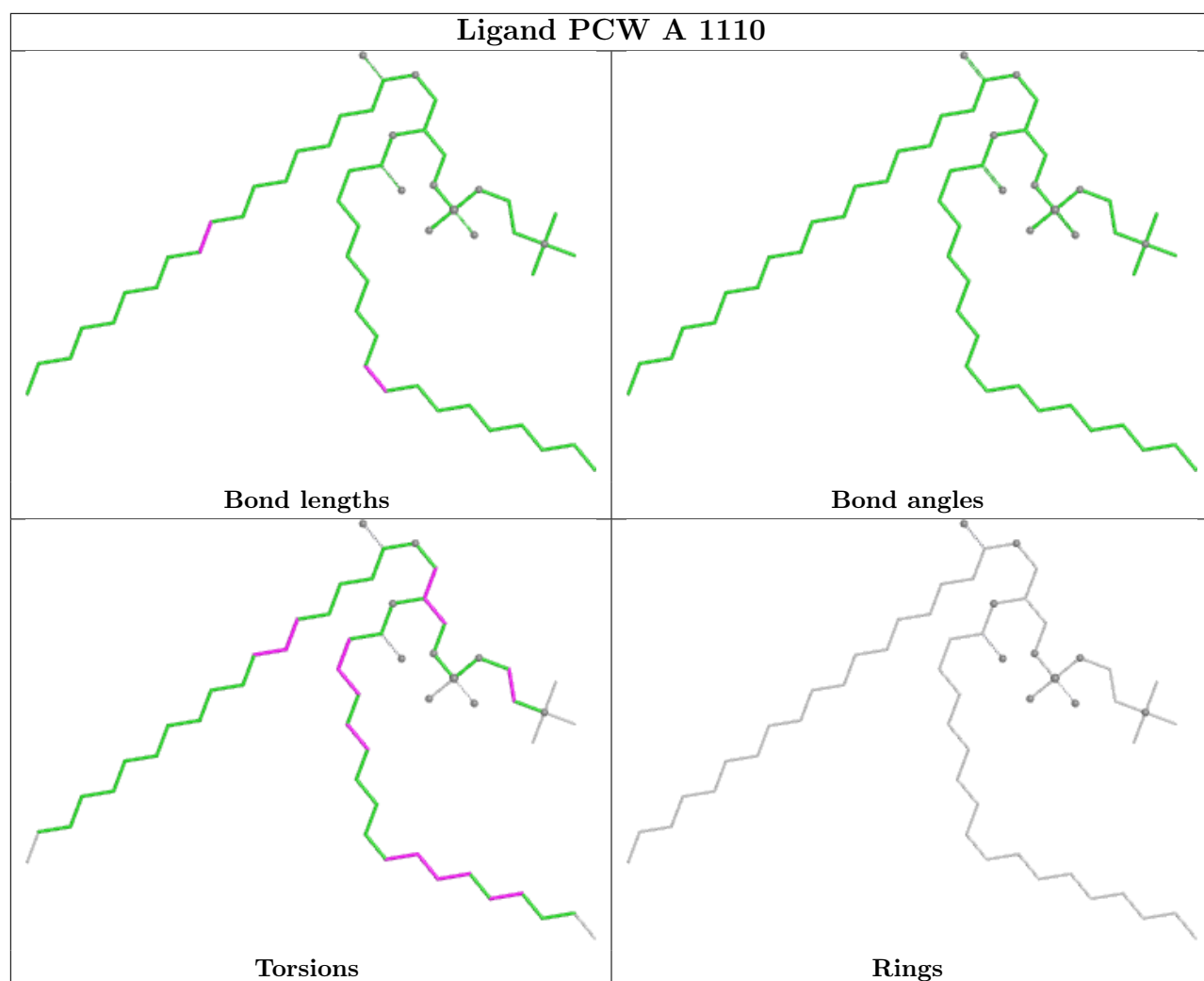
Ligand 7Q2 C 1104

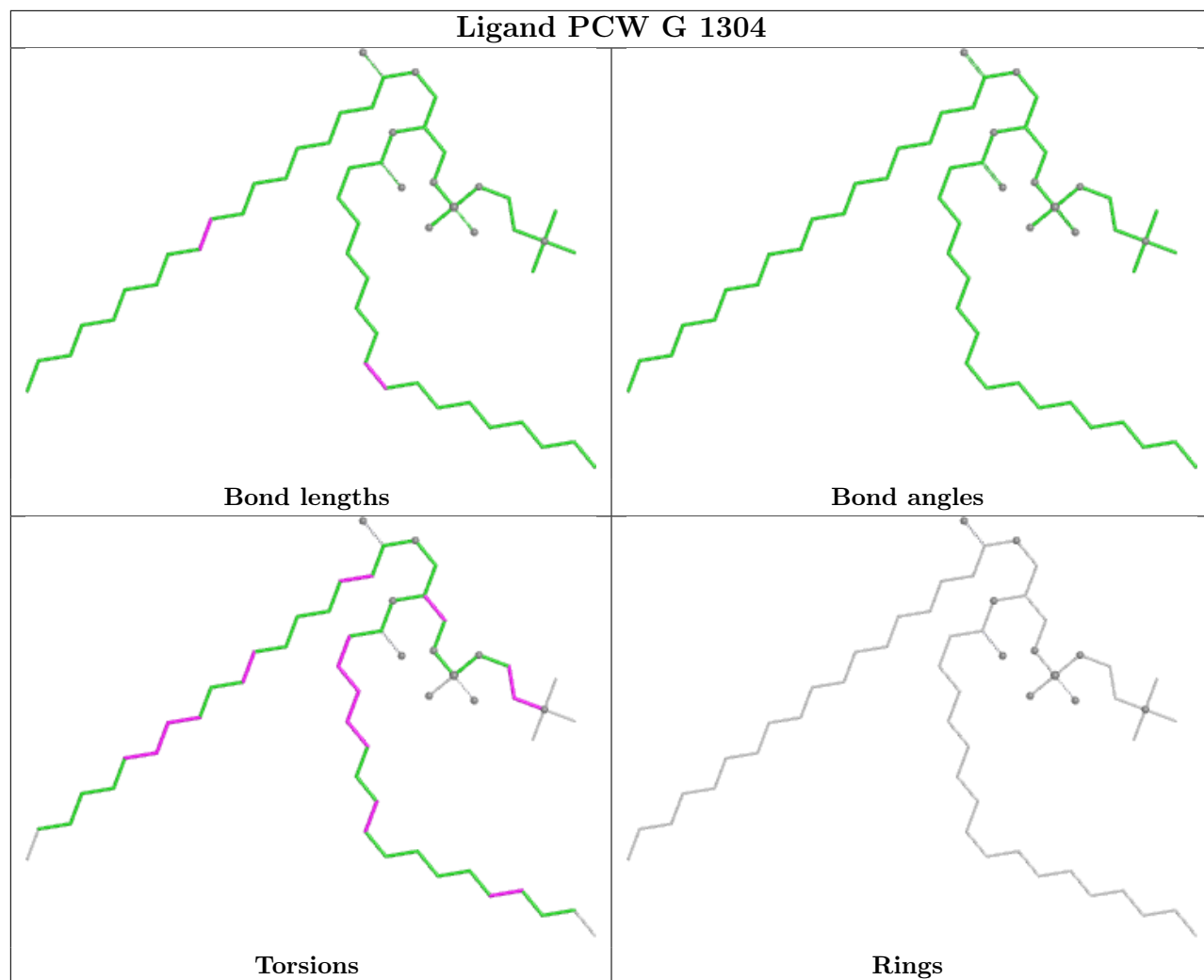


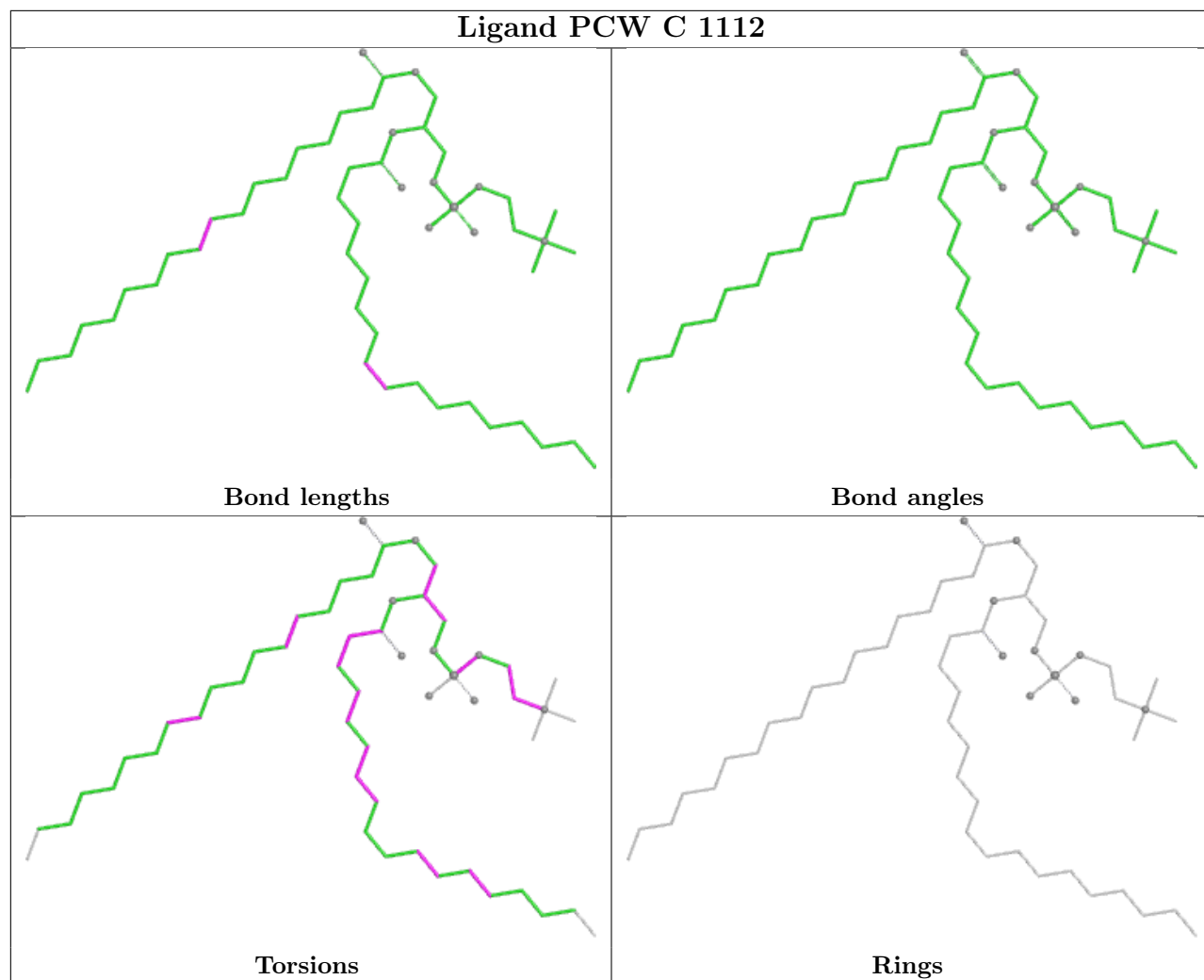


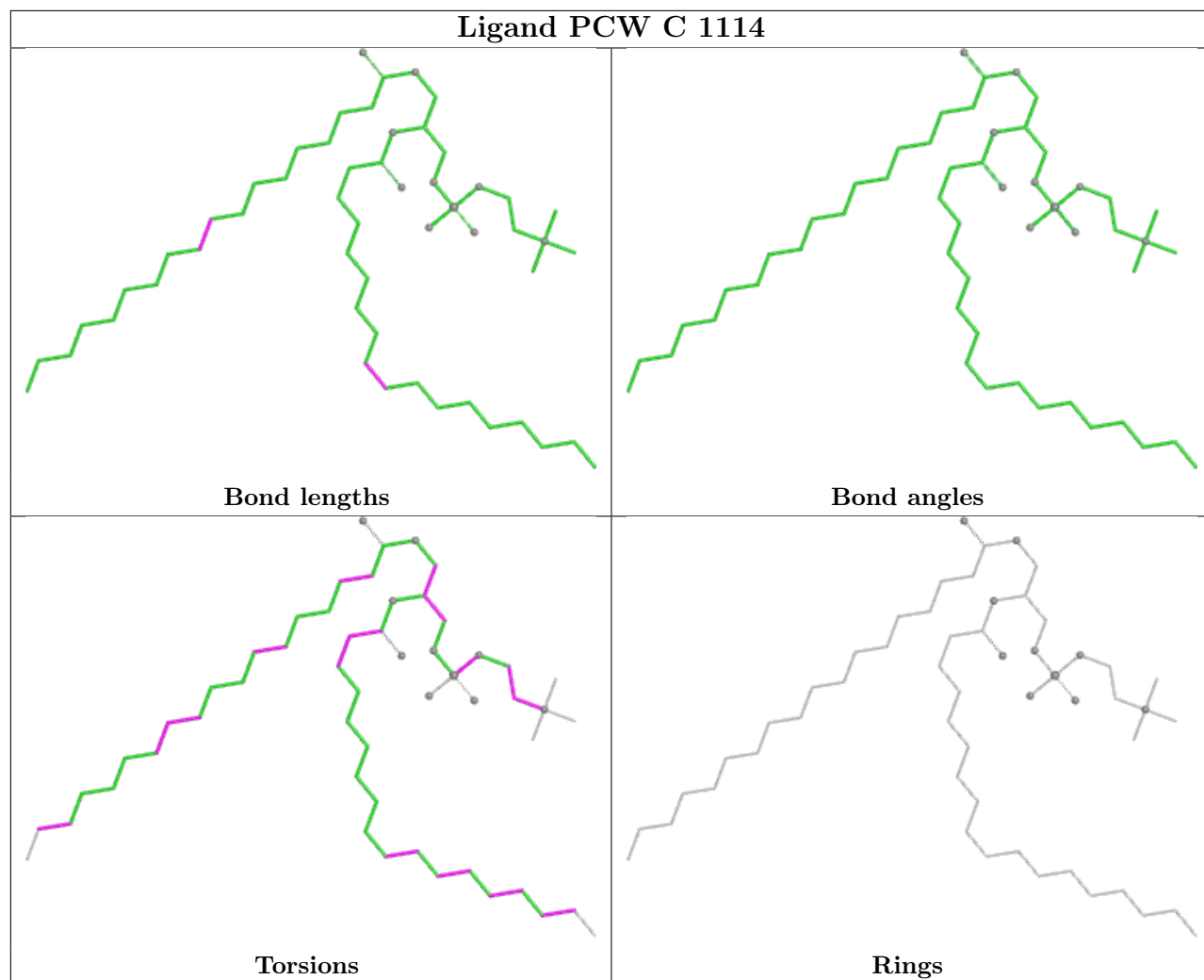




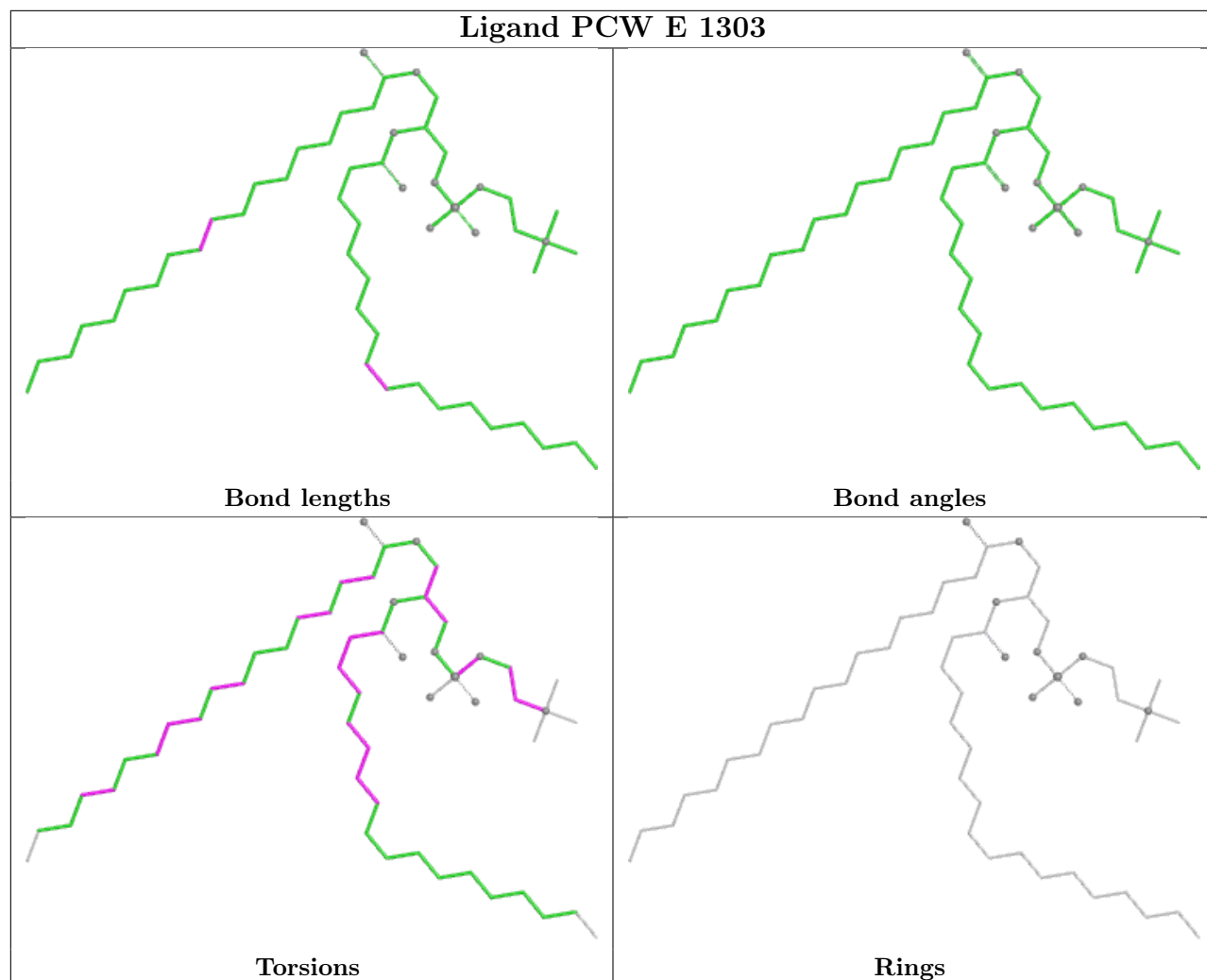




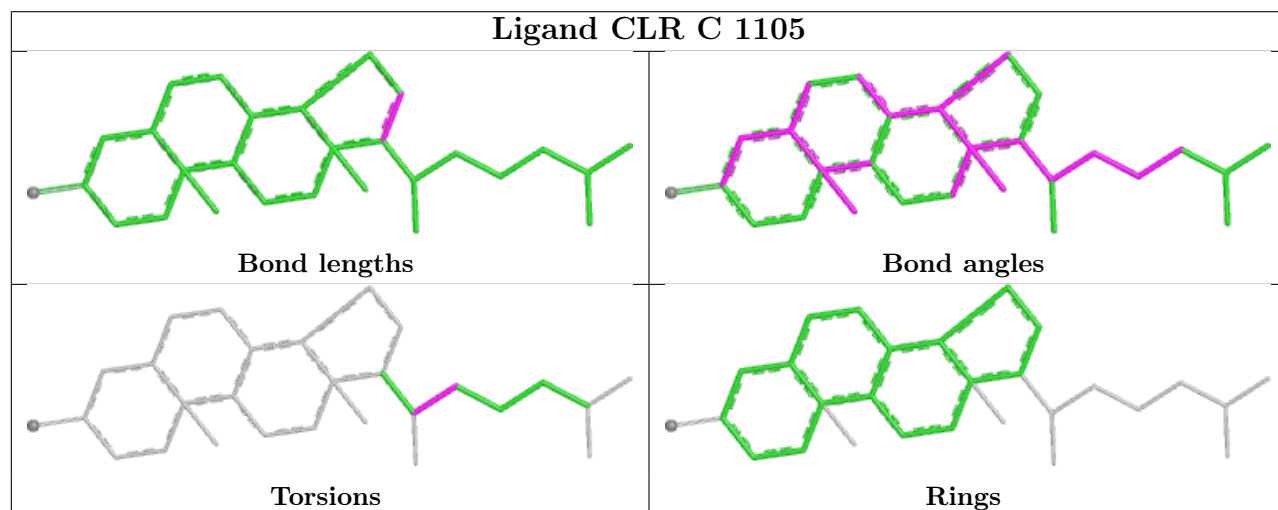


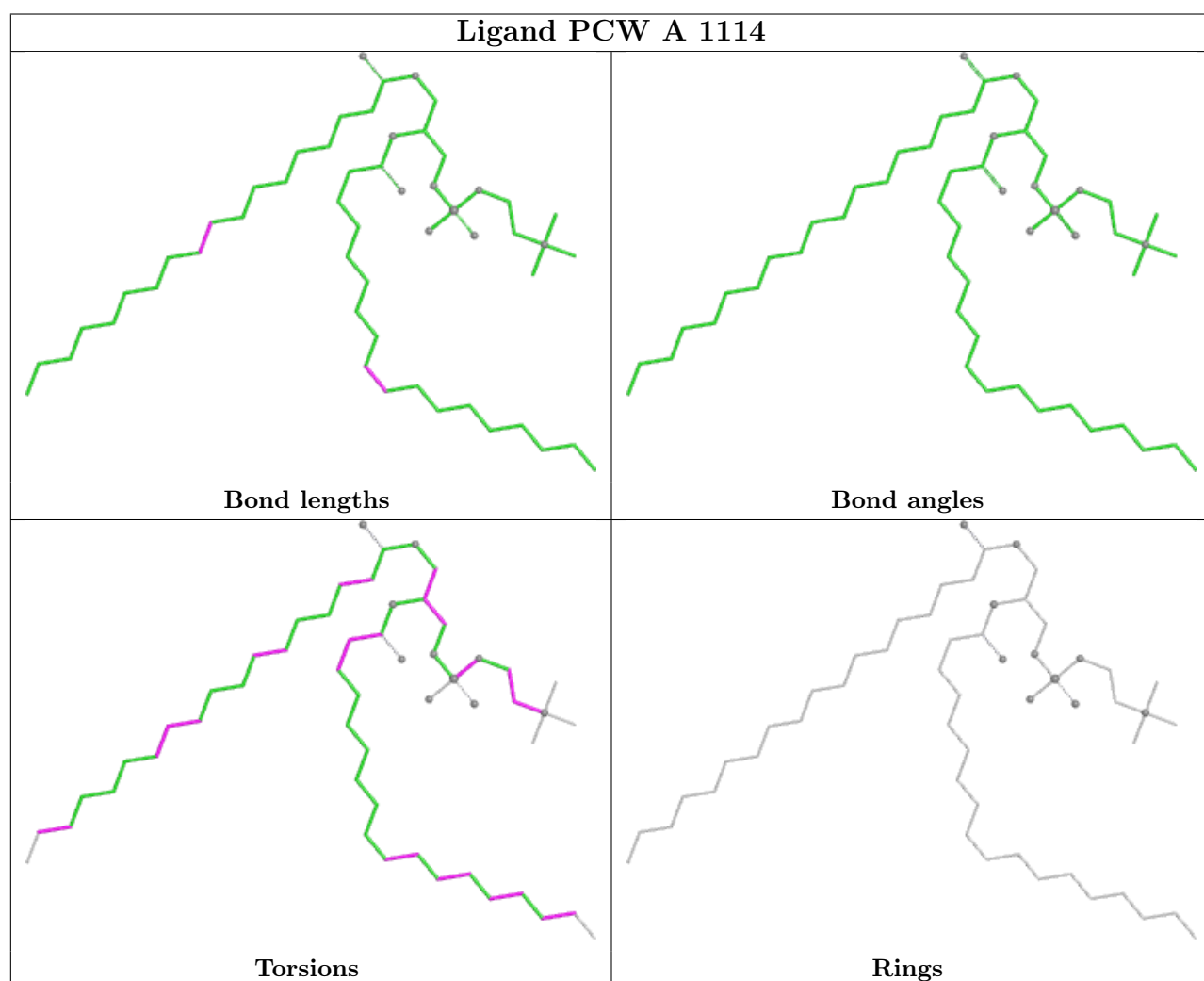
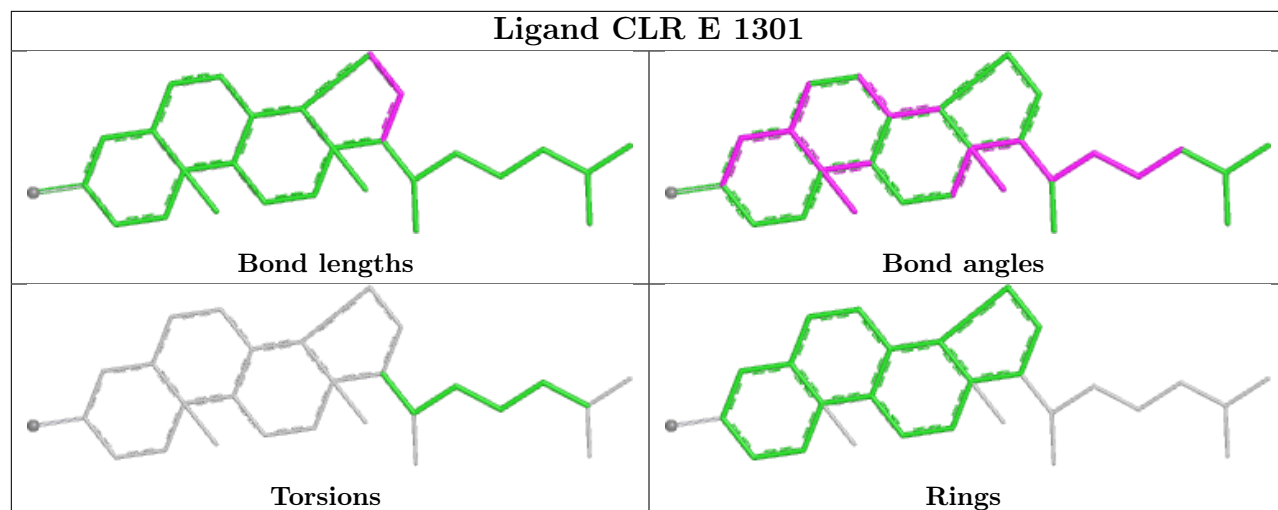


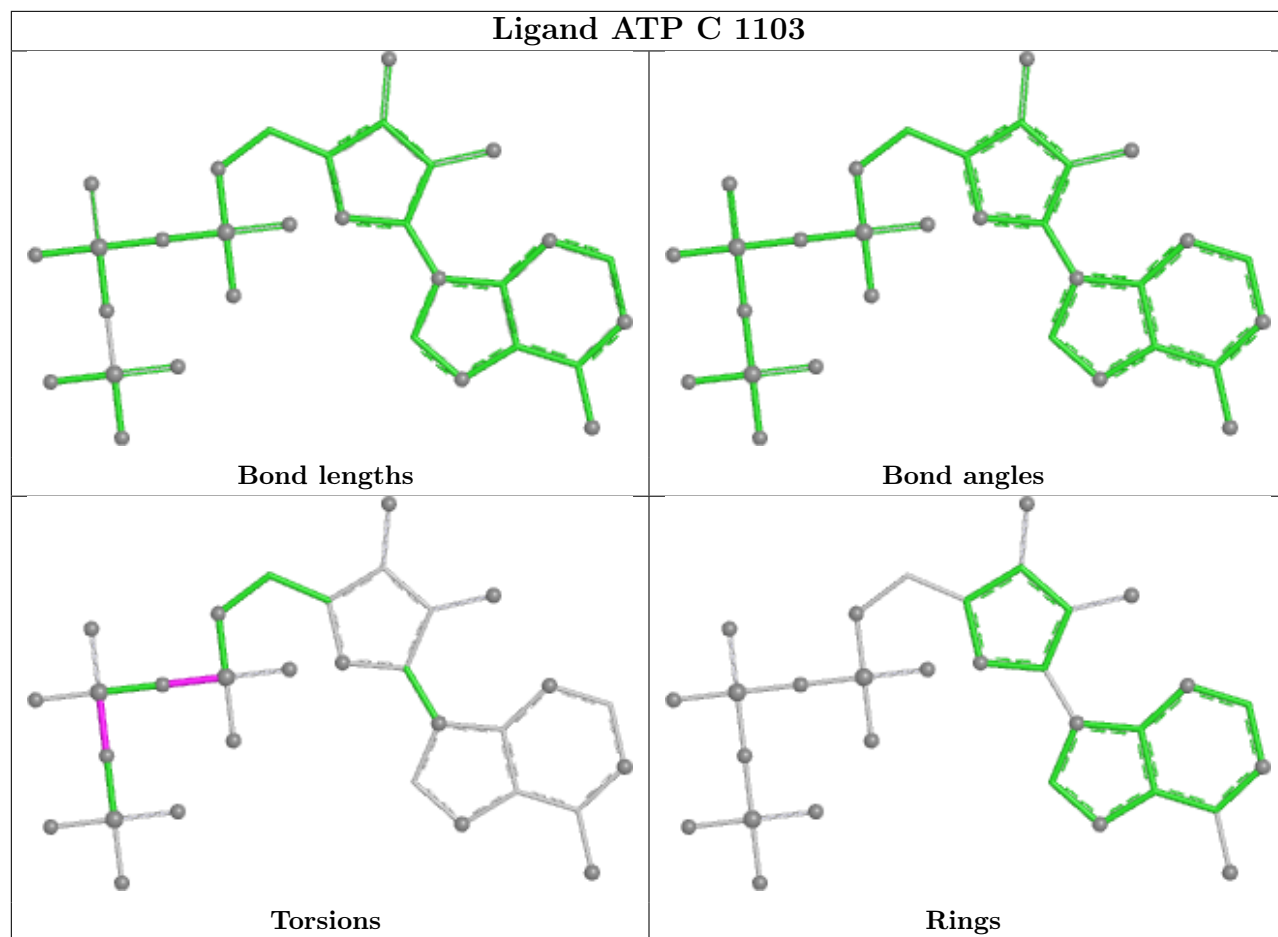
Ligand PCW E 1303

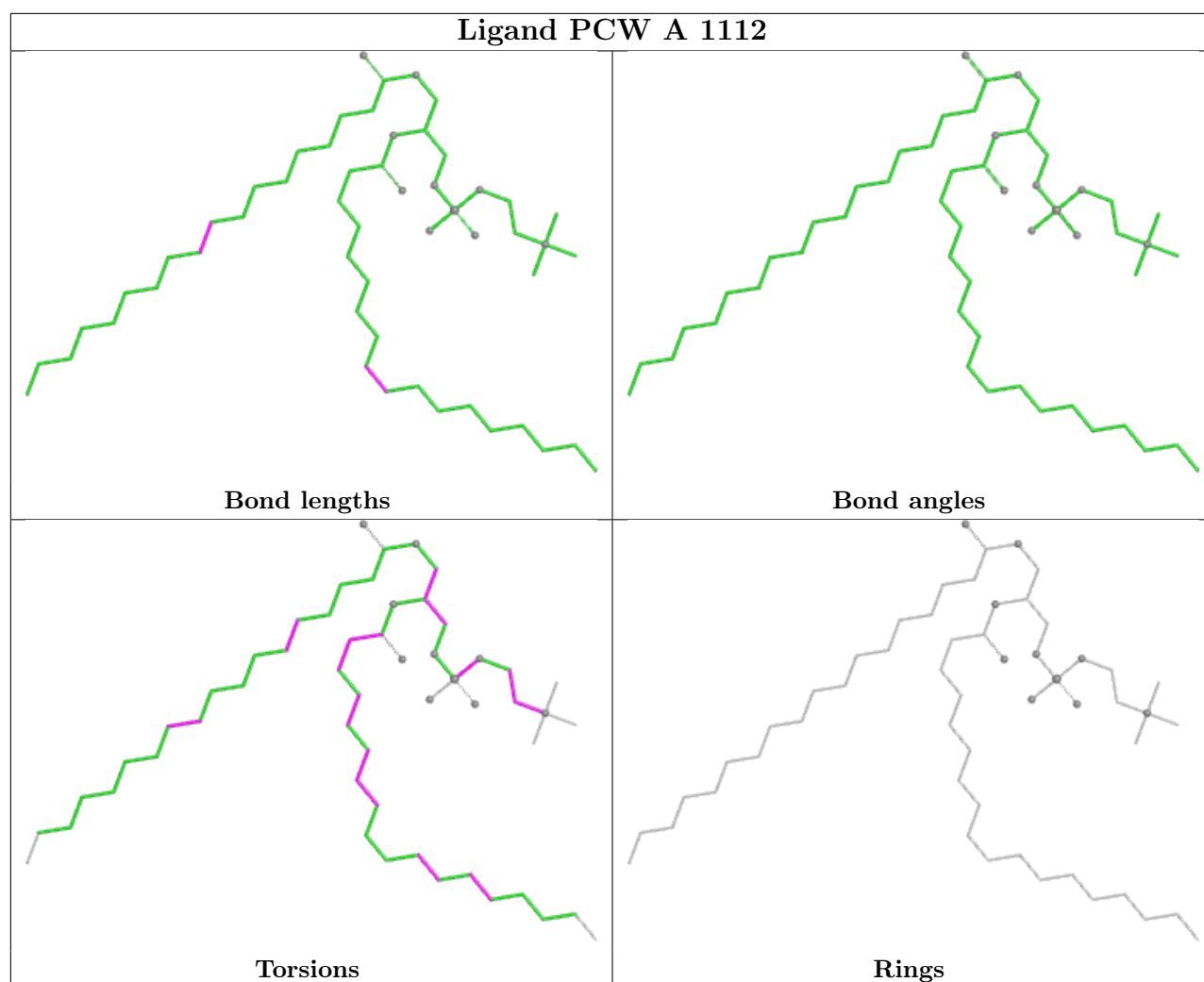


Ligand CLR C 1105









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.

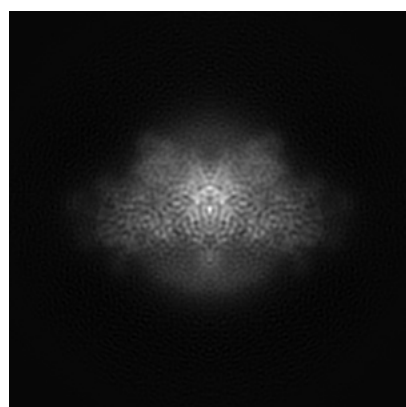
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32897. These allow visual inspection of the internal detail of the map and identification of artifacts.

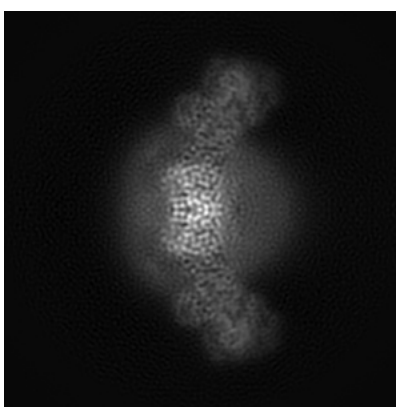
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

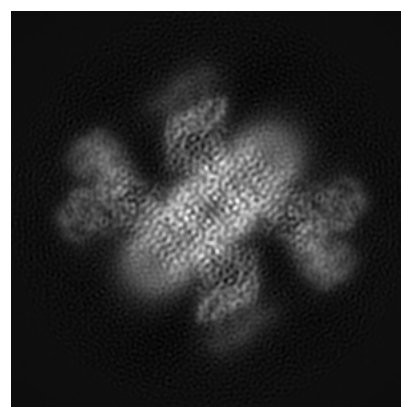
6.1.1 Primary map



X



Y

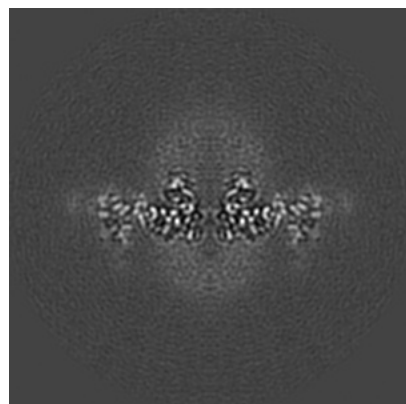


Z

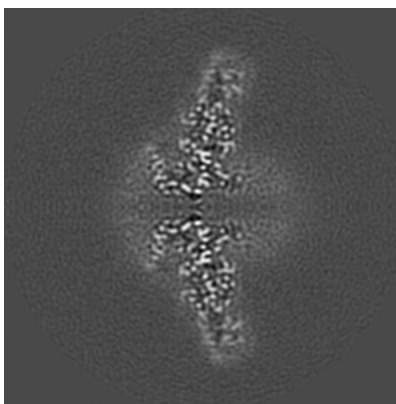
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

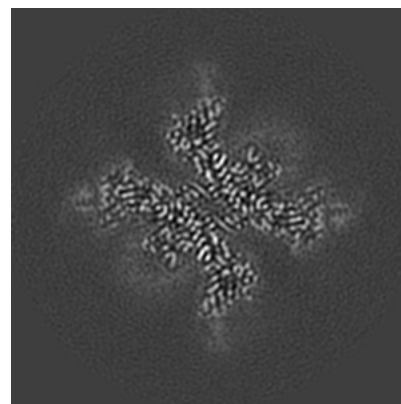
6.2.1 Primary map



X Index: 120



Y Index: 120

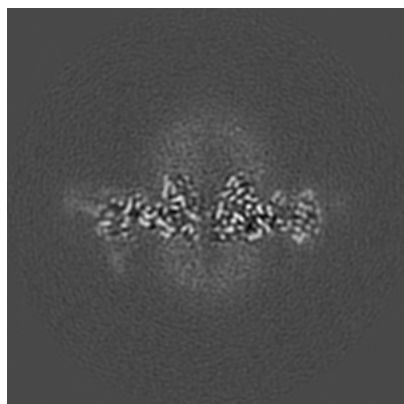


Z Index: 120

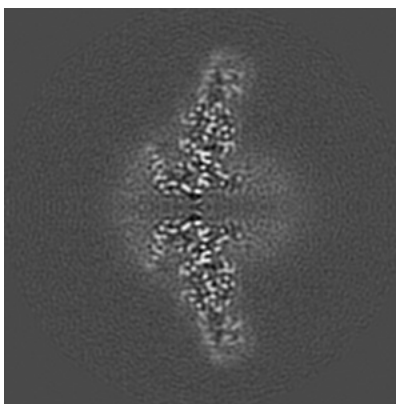
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

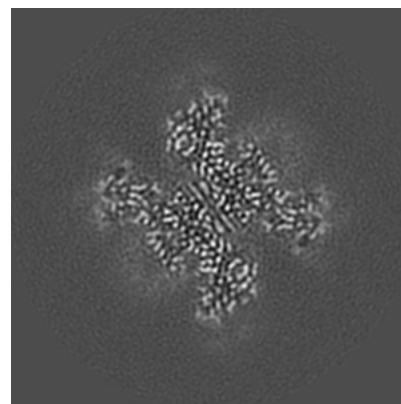
6.3.1 Primary map



X Index: 123



Y Index: 120

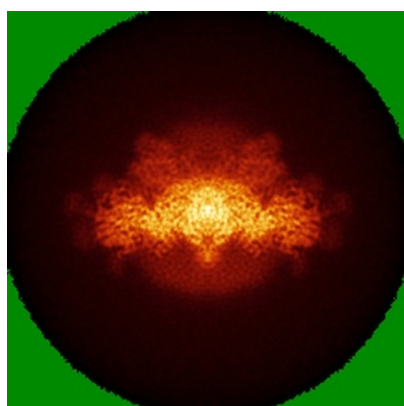


Z Index: 116

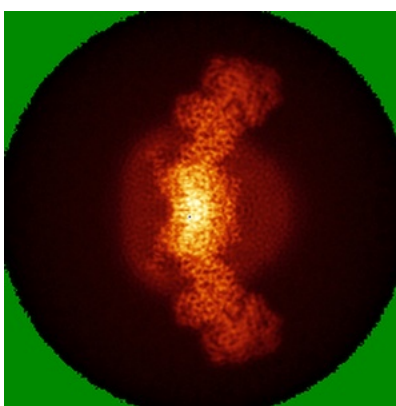
The images above show the largest variance slices of the map in three orthogonal directions.

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

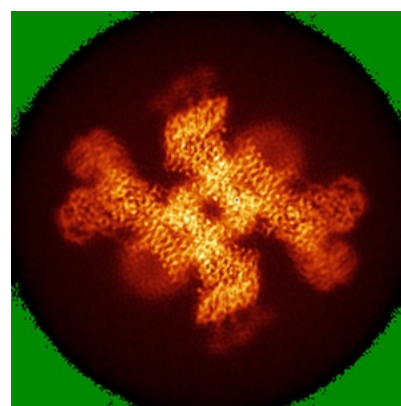
6.4.1 Primary map



X



Y

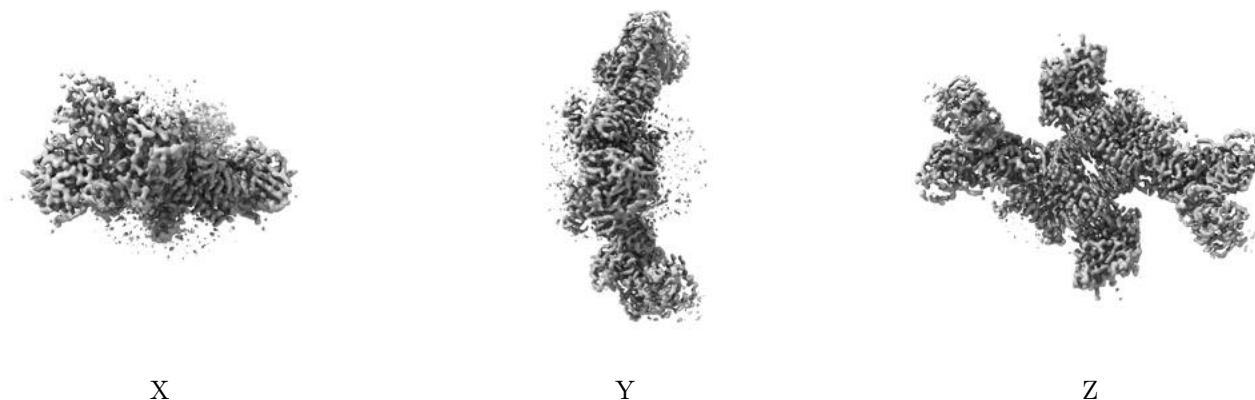


Z

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 0.019. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

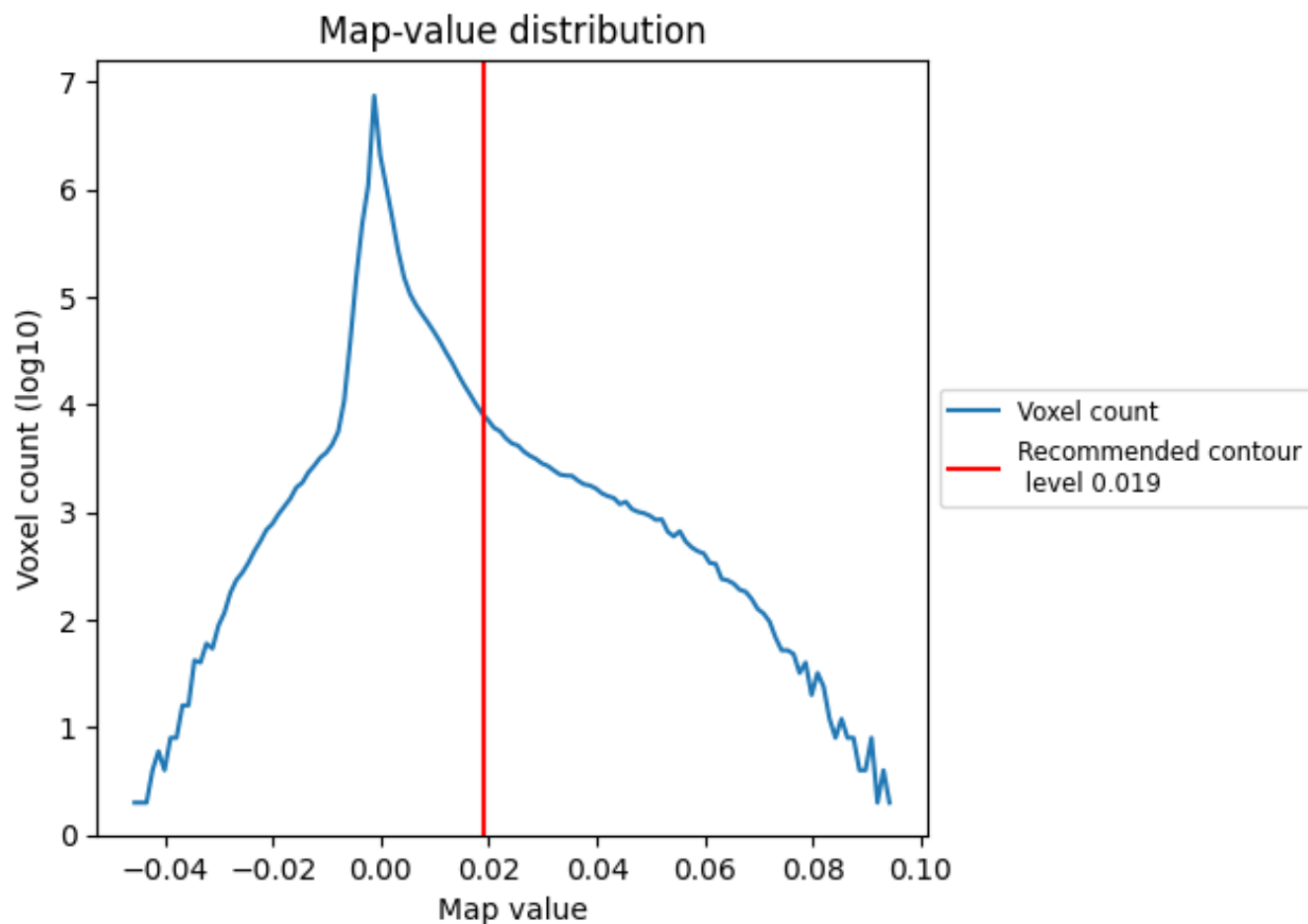
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

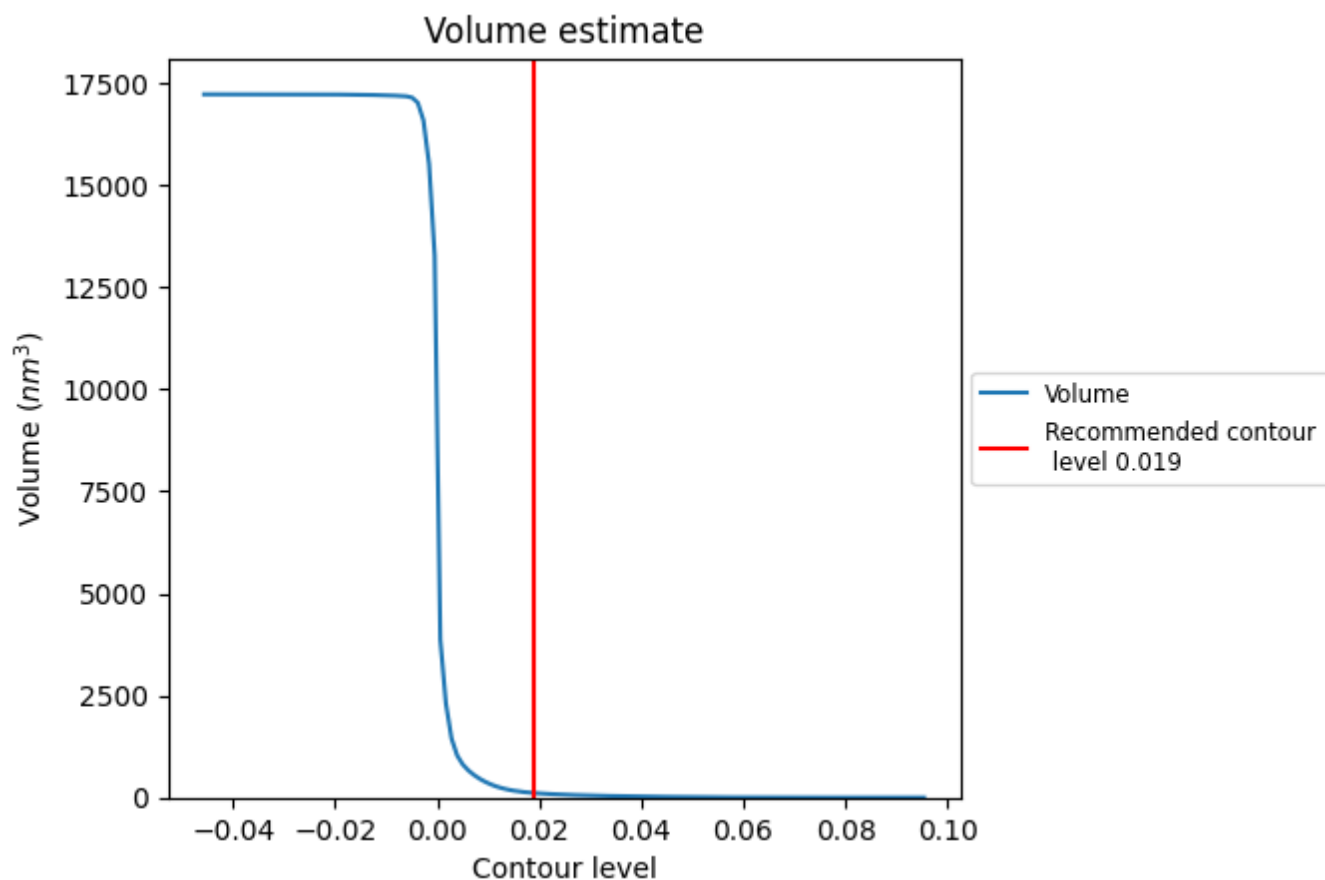
This section contains the results of statistical analysis of the map.

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.

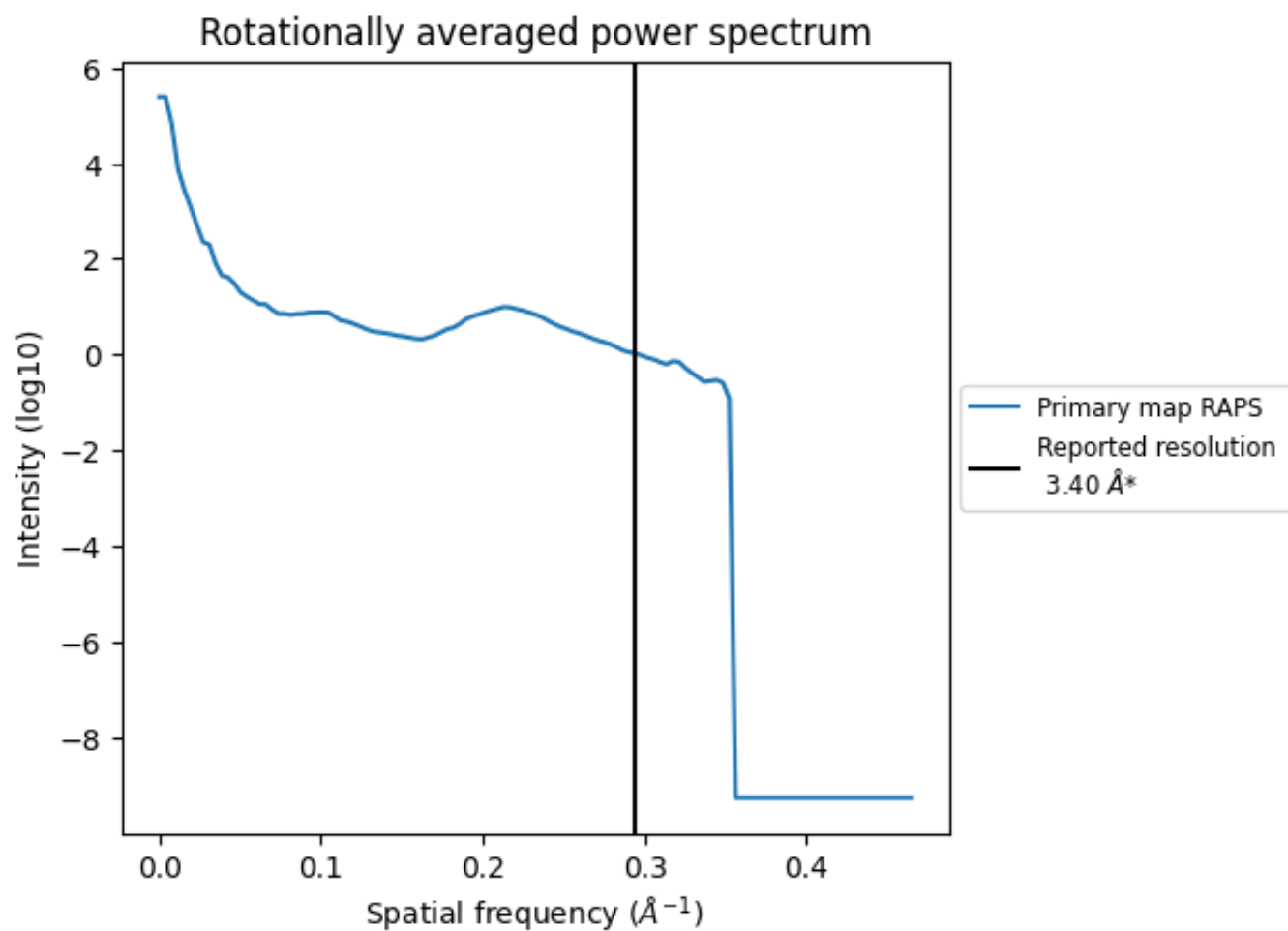
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 111 nm³; this corresponds to an approximate mass of 101 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 ⓘ

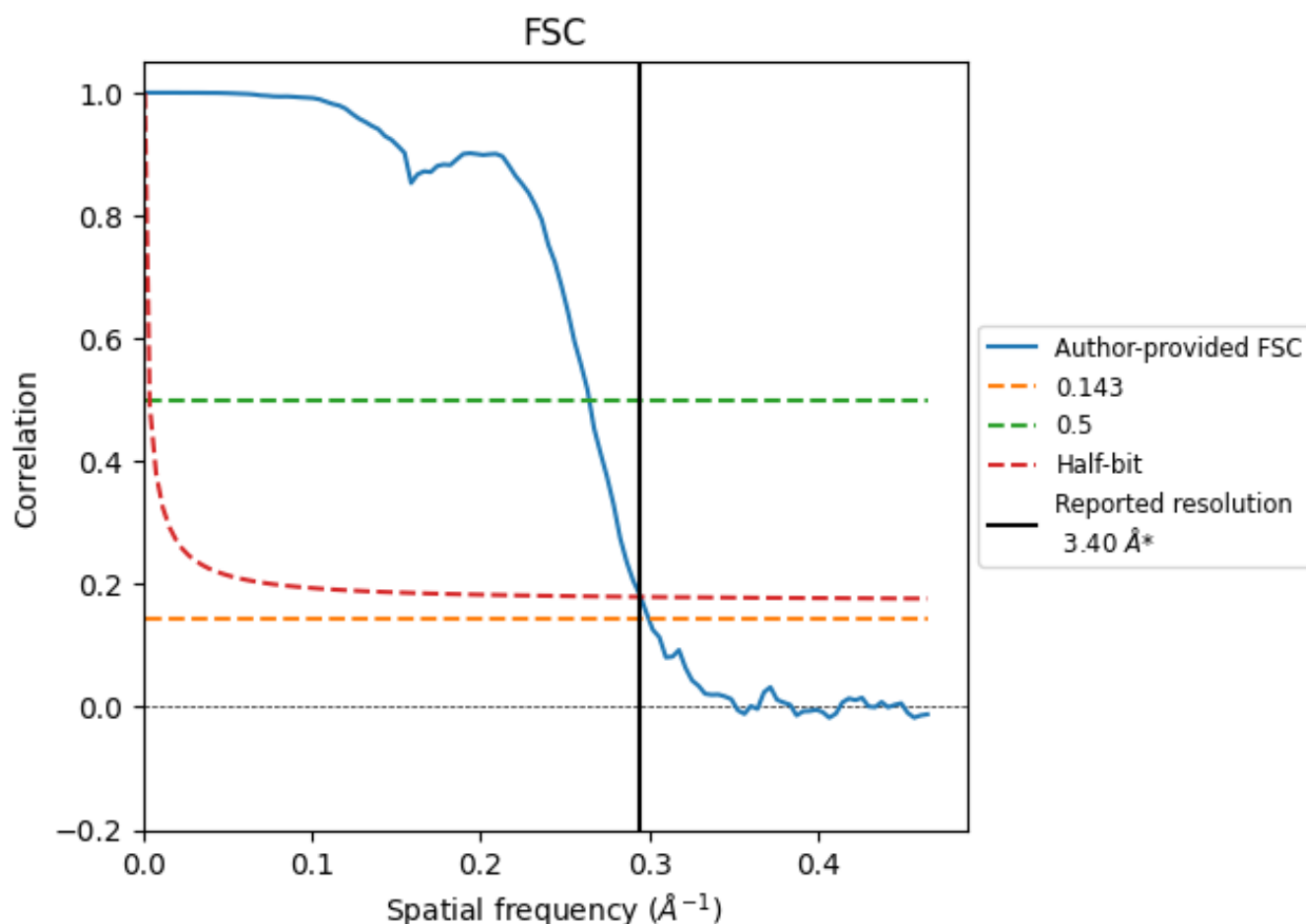


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 0.294 Å⁻¹

8.2 Resolution estimates [i](#)

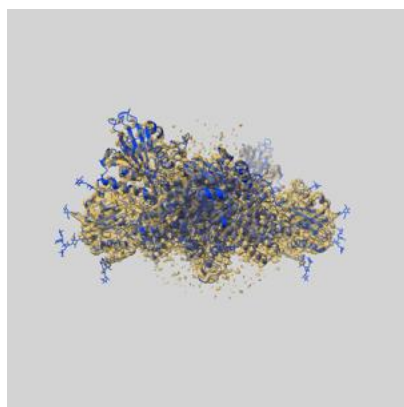
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.34	3.78	3.39
Unmasked-calculated*	-	-	-

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

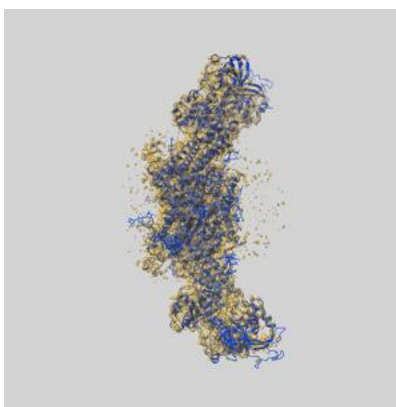
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-32897 and PDB model 7WYX. Per-residue inclusion information can be found in section [3](#) on page [11](#).

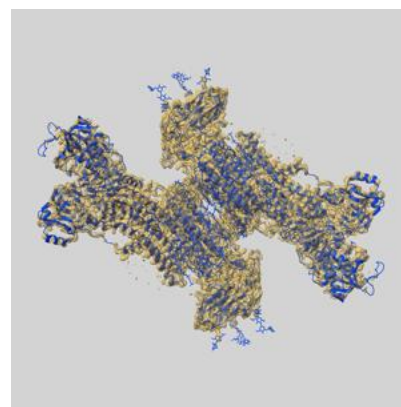
9.1 Map-model overlay [i](#)



X



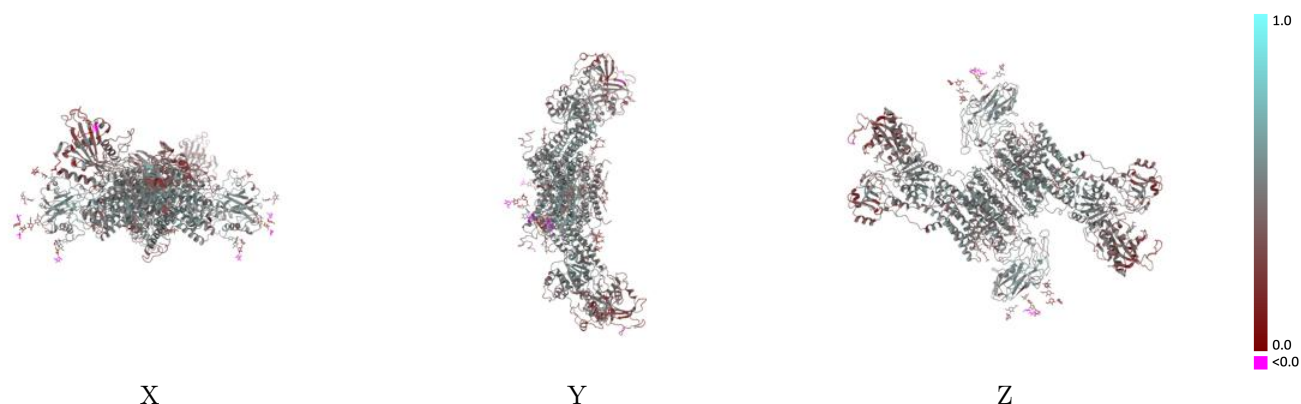
Y



Z

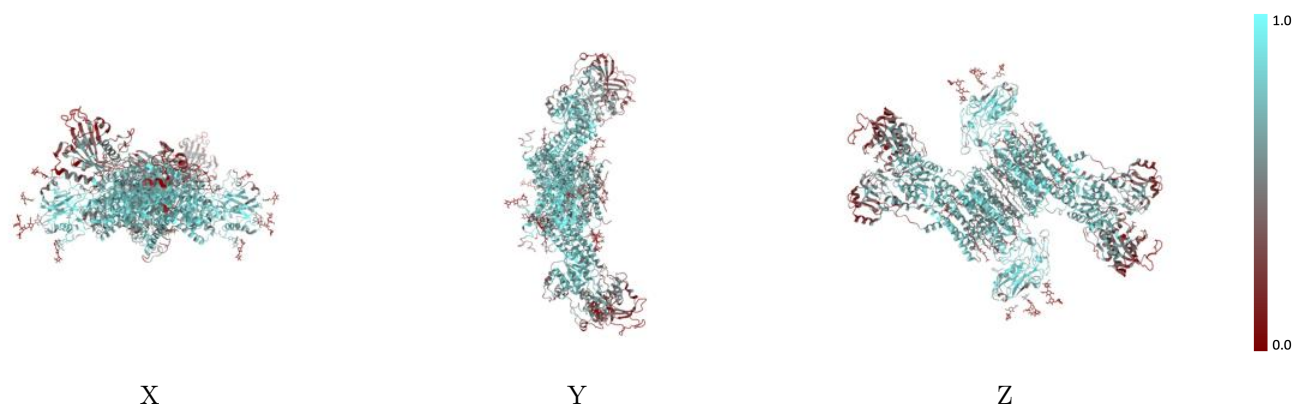
The images above show the 3D surface view of the map at the recommended contour level 0.019 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



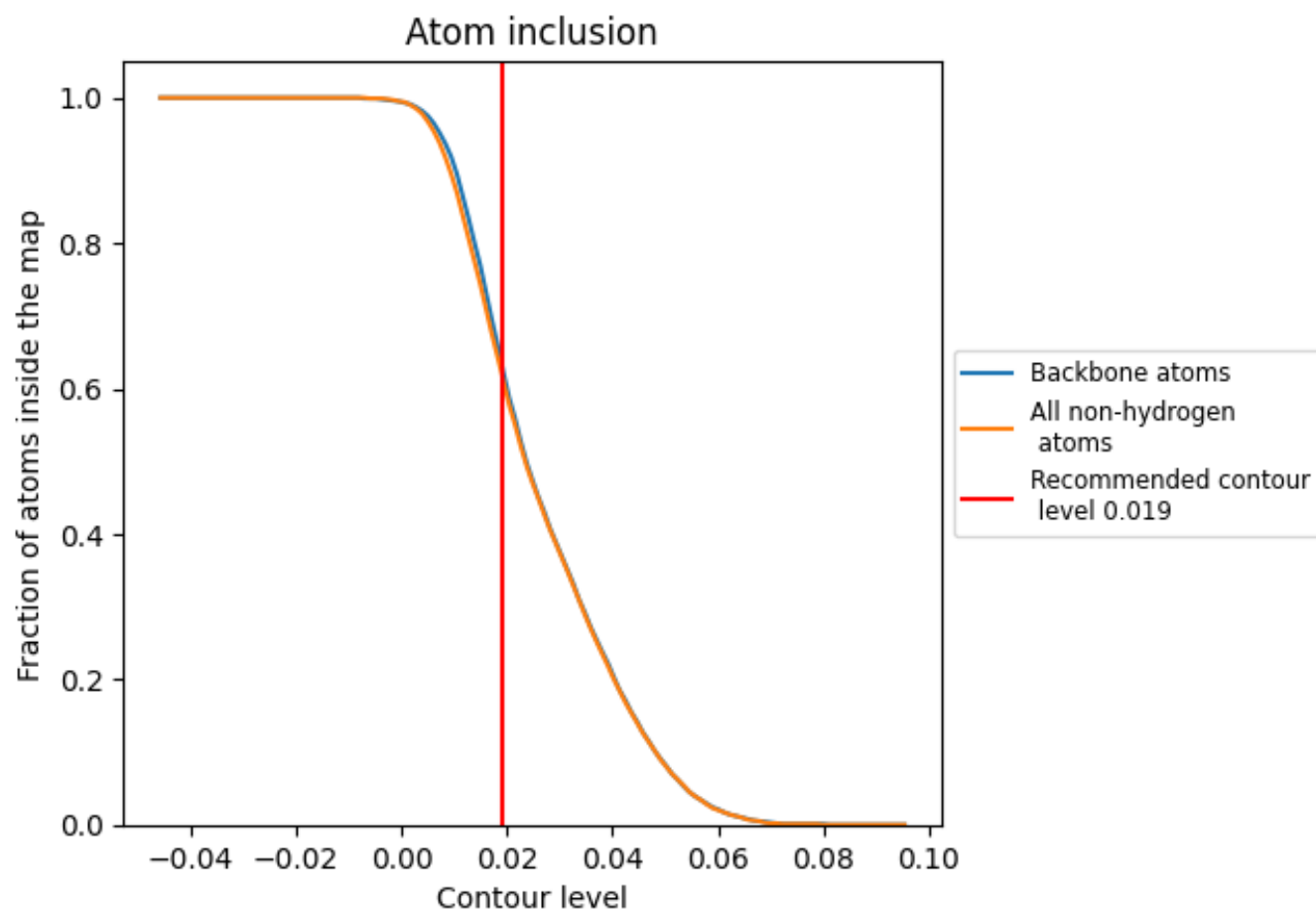
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.019).

9.4 Atom inclusion [i](#)



At the recommended contour level, 64% of all backbone atoms, 62% 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 (0.019) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6220	 0.4450
A	 0.6100	 0.4410
B	 0.7460	 0.4830
C	 0.6100	 0.4410
D	 0.7450	 0.4850
E	 0.5690	 0.4340
F	 0.3240	 0.2520
G	 0.5750	 0.4370
H	 0.0670	 0.0590
I	 0.1330	 0.2540
J	 0.1430	 0.3100
K	 0.3240	 0.2660
L	 0.0800	 0.0680
M	 0.1330	 0.2520
N	 0.1430	 0.3170

