



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 01:08 AM UTC

PDB ID : 7OCA / pdb_00007oca
EMDB ID : EMD-12802
Title : Resting state full-length GluA1/A2 heterotrimer in complex with TARP
gamma 8 and CNIH2
Authors : Zhang, D.; Watson, J.F.; Matthews, P.M.; Cais, O.; Greger, I.H.
Deposited on : 2021-04-26
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

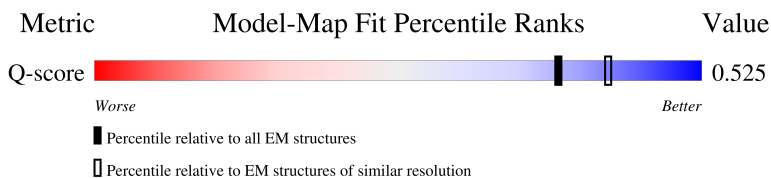
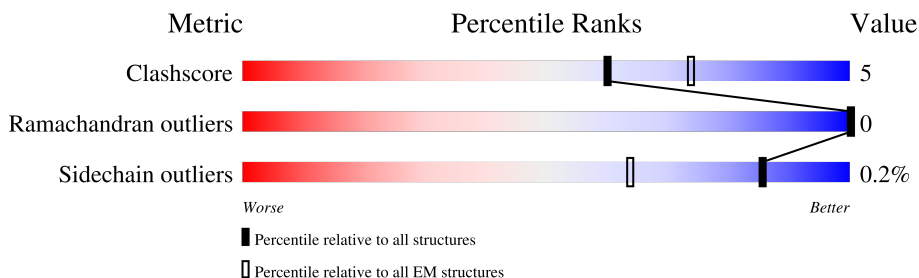
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.40 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	915	 5% 75% 10% 15%
1	C	915	 5% 76% 9% 15%
2	B	860	 1% 81% 10% 9%
2	D	860	 1% 81% 10% 9%

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Mol	Chain	Length	Quality of chain
3	E	188	<p>24% 74% 10% 16%</p>
3	G	188	<p>25% 76% 9% 16%</p>
4	I	423	<p>42% 56%</p>
4	J	423	<p>42% 56%</p>
5	F	3	<p>67% 33%</p>
5	M	3	<p>67% 33%</p>
6	H	2	<p>50% 100%</p>
6	K	2	<p>100%</p>
6	L	2	<p>100%</p>
6	N	2	<p>50% 100%</p>

2 Entry composition i

There are 10 unique types of molecules in this entry. The entry contains 29294 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Glutamate receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	775	Total	C	N	O	S	0	0
			5637	3660	939	1012	26		
1	C	775	Total	C	N	O	S	0	0
			5637	3660	939	1012	26		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	ASP	-	insertion	UNP P19490
A	-5	TYR	-	insertion	UNP P19490
A	-4	LYS	-	insertion	UNP P19490
A	-3	ASP	-	insertion	UNP P19490
A	-2	ASP	-	insertion	UNP P19490
A	-1	ASP	-	insertion	UNP P19490
A	0	ASP	-	insertion	UNP P19490
A	1	LYS	-	insertion	UNP P19490
C	-6	ASP	-	insertion	UNP P19490
C	-5	TYR	-	insertion	UNP P19490
C	-4	LYS	-	insertion	UNP P19490
C	-3	ASP	-	insertion	UNP P19490
C	-2	ASP	-	insertion	UNP P19490
C	-1	ASP	-	insertion	UNP P19490
C	0	ASP	-	insertion	UNP P19490
C	1	LYS	-	insertion	UNP P19490

- Molecule 2 is a protein called Glutamate receptor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	783	Total	C	N	O	S	0	0
			5815	3759	969	1060	27		
2	D	783	Total	C	N	O	S	0	0
			5815	3759	969	1060	27		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	586	ARG	GLN	conflict	UNP P19491
D	586	ARG	GLN	conflict	UNP P19491

- Molecule 3 is a protein called Protein cornichon homolog 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	158	Total	C	N	O	S	0	0
			1248	841	193	201	13		
3	E	158	Total	C	N	O	S	0	0
			1248	841	193	201	13		

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	161	GLU	-	expression tag	UNP Q5BJU5
G	162	ASN	-	expression tag	UNP Q5BJU5
G	163	LEU	-	expression tag	UNP Q5BJU5
G	164	TYR	-	expression tag	UNP Q5BJU5
G	165	PHE	-	expression tag	UNP Q5BJU5
G	166	GLN	-	expression tag	UNP Q5BJU5
G	167	SER	-	expression tag	UNP Q5BJU5
G	168	GLY	-	expression tag	UNP Q5BJU5
G	169	GLY	-	expression tag	UNP Q5BJU5
G	170	SER	-	expression tag	UNP Q5BJU5
G	171	THR	-	expression tag	UNP Q5BJU5
G	172	GLU	-	expression tag	UNP Q5BJU5
G	173	THR	-	expression tag	UNP Q5BJU5
G	174	SER	-	expression tag	UNP Q5BJU5
G	175	GLN	-	expression tag	UNP Q5BJU5
G	176	VAL	-	expression tag	UNP Q5BJU5
G	177	ALA	-	expression tag	UNP Q5BJU5
G	178	PRO	-	expression tag	UNP Q5BJU5
G	179	ALA	-	expression tag	UNP Q5BJU5
G	180	TYR	-	expression tag	UNP Q5BJU5
G	181	PRO	-	expression tag	UNP Q5BJU5
G	182	TYR	-	expression tag	UNP Q5BJU5
G	183	ASP	-	expression tag	UNP Q5BJU5
G	184	VAL	-	expression tag	UNP Q5BJU5
G	185	PRO	-	expression tag	UNP Q5BJU5
G	186	ASP	-	expression tag	UNP Q5BJU5
G	187	TYR	-	expression tag	UNP Q5BJU5

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Chain	Residue	Modelled	Actual	Comment	Reference
G	188	ALA	-	expression tag	UNP Q5BJU5
E	161	GLU	-	expression tag	UNP Q5BJU5
E	162	ASN	-	expression tag	UNP Q5BJU5
E	163	LEU	-	expression tag	UNP Q5BJU5
E	164	TYR	-	expression tag	UNP Q5BJU5
E	165	PHE	-	expression tag	UNP Q5BJU5
E	166	GLN	-	expression tag	UNP Q5BJU5
E	167	SER	-	expression tag	UNP Q5BJU5
E	168	GLY	-	expression tag	UNP Q5BJU5
E	169	GLY	-	expression tag	UNP Q5BJU5
E	170	SER	-	expression tag	UNP Q5BJU5
E	171	THR	-	expression tag	UNP Q5BJU5
E	172	GLU	-	expression tag	UNP Q5BJU5
E	173	THR	-	expression tag	UNP Q5BJU5
E	174	SER	-	expression tag	UNP Q5BJU5
E	175	GLN	-	expression tag	UNP Q5BJU5
E	176	VAL	-	expression tag	UNP Q5BJU5
E	177	ALA	-	expression tag	UNP Q5BJU5
E	178	PRO	-	expression tag	UNP Q5BJU5
E	179	ALA	-	expression tag	UNP Q5BJU5
E	180	TYR	-	expression tag	UNP Q5BJU5
E	181	PRO	-	expression tag	UNP Q5BJU5
E	182	TYR	-	expression tag	UNP Q5BJU5
E	183	ASP	-	expression tag	UNP Q5BJU5
E	184	VAL	-	expression tag	UNP Q5BJU5
E	185	PRO	-	expression tag	UNP Q5BJU5
E	186	ASP	-	expression tag	UNP Q5BJU5
E	187	TYR	-	expression tag	UNP Q5BJU5
E	188	ALA	-	expression tag	UNP Q5BJU5

- Molecule 4 is a protein called Voltage-dependent calcium channel gamma-8 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	I	185	1284	843	212	222	7	0	0
4	J	185	1284	843	212	222	7	0	0

There are 14 discrepancies between the modelled and reference sequences:

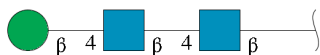
Chain	Residue	Modelled	Actual	Comment	Reference
I	1	GLY	-	expression tag	UNP Q8VHW5

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Chain	Residue	Modelled	Actual	Comment	Reference
I	418	LEU	-	expression tag	UNP Q8VHW5
I	419	GLU	-	expression tag	UNP Q8VHW5
I	420	VAL	-	expression tag	UNP Q8VHW5
I	421	LEU	-	expression tag	UNP Q8VHW5
I	422	PHE	-	expression tag	UNP Q8VHW5
I	423	GLN	-	expression tag	UNP Q8VHW5
J	1	GLY	-	expression tag	UNP Q8VHW5
J	418	LEU	-	expression tag	UNP Q8VHW5
J	419	GLU	-	expression tag	UNP Q8VHW5
J	420	VAL	-	expression tag	UNP Q8VHW5
J	421	LEU	-	expression tag	UNP Q8VHW5
J	422	PHE	-	expression tag	UNP Q8VHW5
J	423	GLN	-	expression tag	UNP Q8VHW5

- Molecule 5 is an oligosaccharide called 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
			Total	C	N	O		
5	F	3	Total	C	N	O	0	0
			39	22	2	15		
5	M	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



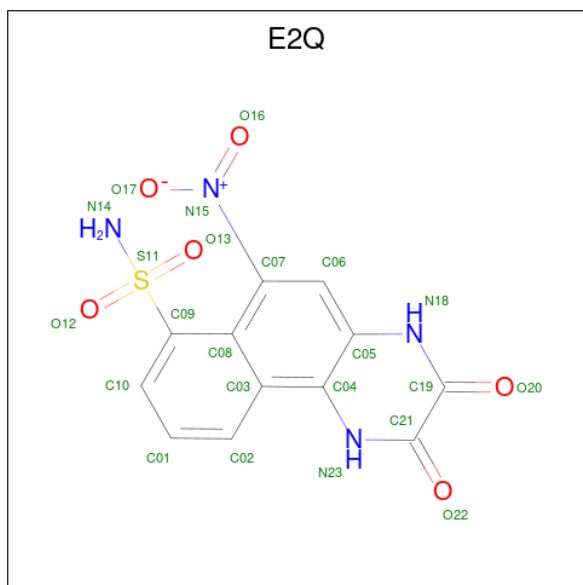
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	H	2	Total	C	N	O	0	0
			28	16	2	10		
6	K	2	Total	C	N	O	0	0
			28	16	2	10		
6	L	2	Total	C	N	O	0	0
			28	16	2	10		

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

- Molecule 7 is 6-nitro-2,3-bis(oxidanylidene)-1,4-dihydrobenzo[f]quinoxaline-7-sulfonamide (CCD ID: E2Q) (formula: C₁₂H₈N₄O₆S).



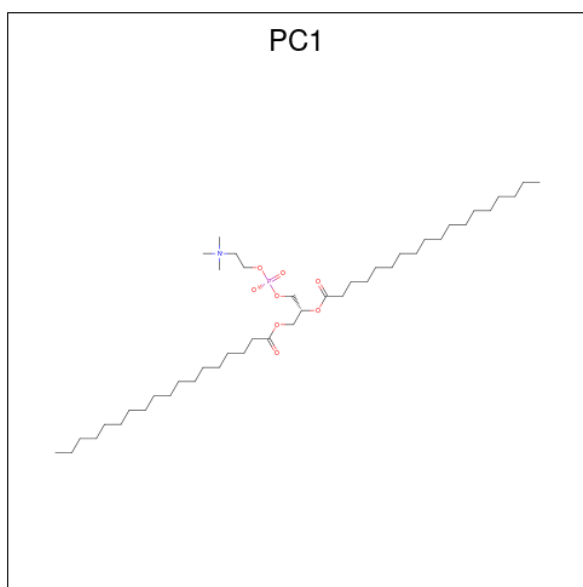
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
7	A	1	23	12	4	6	1	0
7	B	1	23	12	4	6	1	0
7	D	1	23	12	4	6	1	0
7	C	1	23	12	4	6	1	0

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 9 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms			AltConf
9	A	1	Total	C	O	0
			20	18	2	
9	A	1	Total	C	O	0
			18	16	2	
9	A	1	Total	C	O	0
			20	18	2	
9	A	1	Total	C	O	0
			18	16	2	
9	A	1	Total	C	O	0
			25	21	4	
9	A	1	Total	C	O	0
			18	16	2	
9	B	1	Total	C	O	0
			20	18	2	
9	B	1	Total	C	O	0
			16	14	2	
9	B	1	Total	C	O	0
			20	18	2	
9	B	1	Total	C	O	0
			20	18	2	
9	B	1	Total	C	O	0
			20	18	2	
9	B	1	Total	C	O	0
			18	16	2	
9	B	1	Total	C	O	0
			25	21	4	

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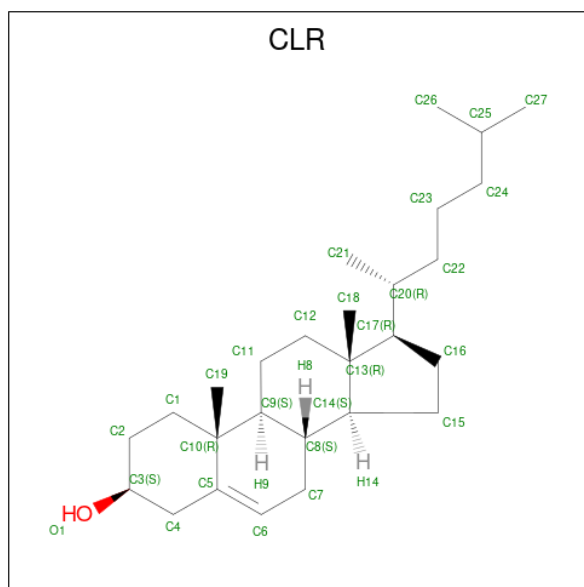
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
9	B	1	20	18	2	0
9	G	1	20	18	2	0
9	G	1	18	16	2	0
9	G	1	20	18	2	0
9	I	1	18	16	2	0
9	I	1	20	18	2	0
9	I	1	20	18	2	0
9	I	1	20	18	2	0
9	I	1	18	16	2	0
9	D	1	16	14	2	0
9	D	1	20	18	2	0
9	D	1	20	18	2	0
9	D	1	20	18	2	0
9	D	1	20	18	2	0
9	D	1	18	16	2	0
9	D	1	25	21	4	0
9	D	1	20	18	2	0
9	D	1	20	18	2	0
9	J	1	20	18	2	0
9	J	1	20	18	2	0
9	J	1	20	18	2	0

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Mol	Chain	Residues	Atoms			AltConf
9	J	1	Total	C	O	0
			18	16	2	
9	J	1	Total	C	O	0
			18	16	2	
9	C	1	Total	C	O	0
			18	16	2	
9	C	1	Total	C	O	0
			20	18	2	
9	C	1	Total	C	O	0
			18	16	2	
9	C	1	Total	C	O	0
			20	18	2	
9	C	1	Total	C	O	0
			18	16	2	
9	C	1	Total	C	O	0
			25	21	4	
9	E	1	Total	C	O	0
			18	16	2	
9	E	1	Total	C	O	0
			20	18	2	
9	E	1	Total	C	O	0
			20	18	2	

- Molecule 10 is CHOLESTEROL (CCD ID: CLR) (formula: $C_{27}H_{46}O$).

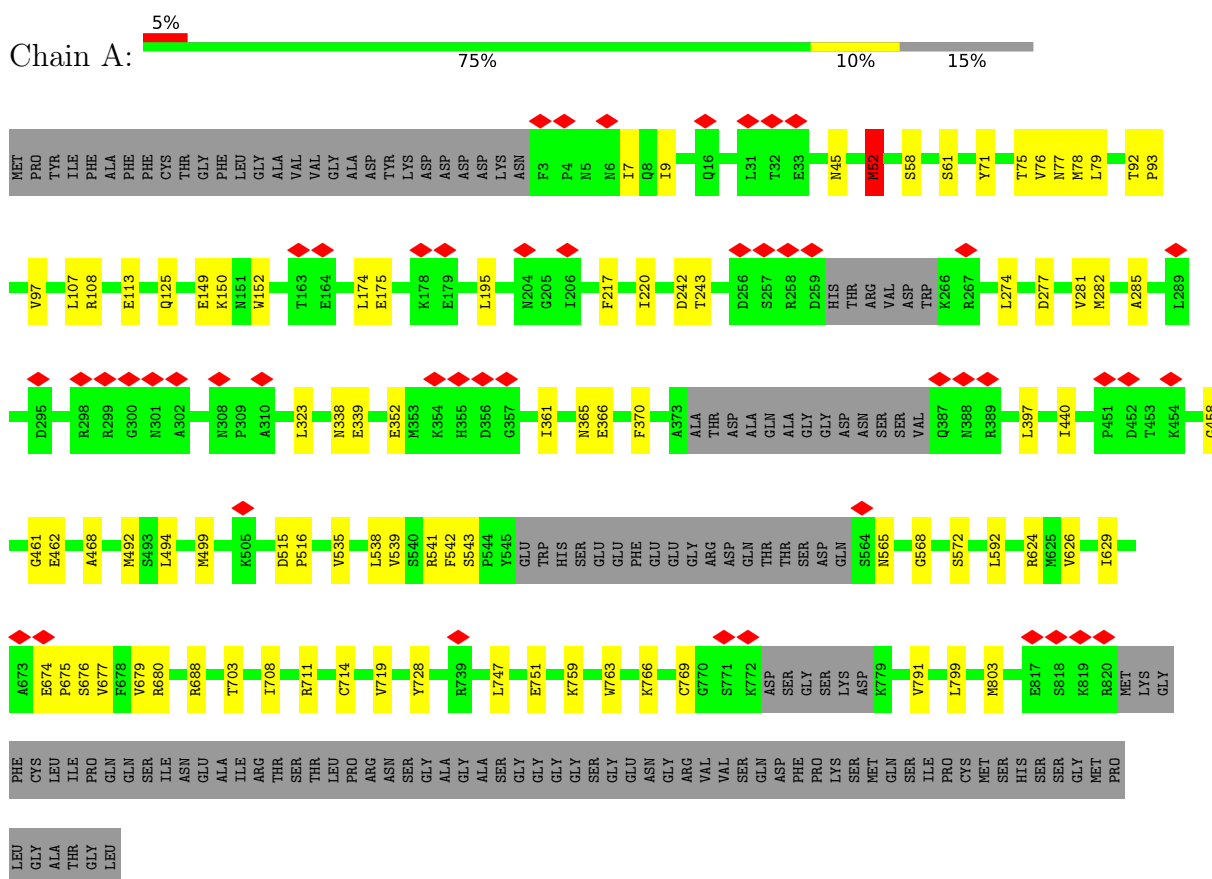


Mol	Chain	Residues	Atoms			AltConf
10	G	1	Total	C	O	0
			28	27	1	
10	E	1	Total	C	O	0
			28	27	1	

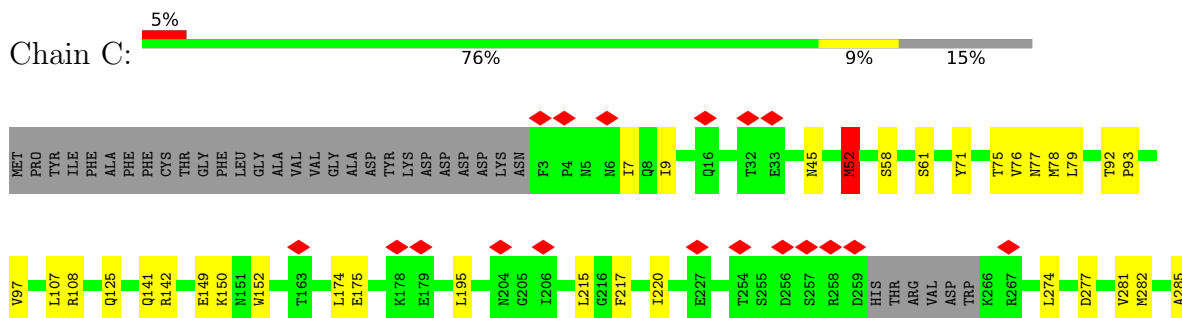
3 Residue-property plots

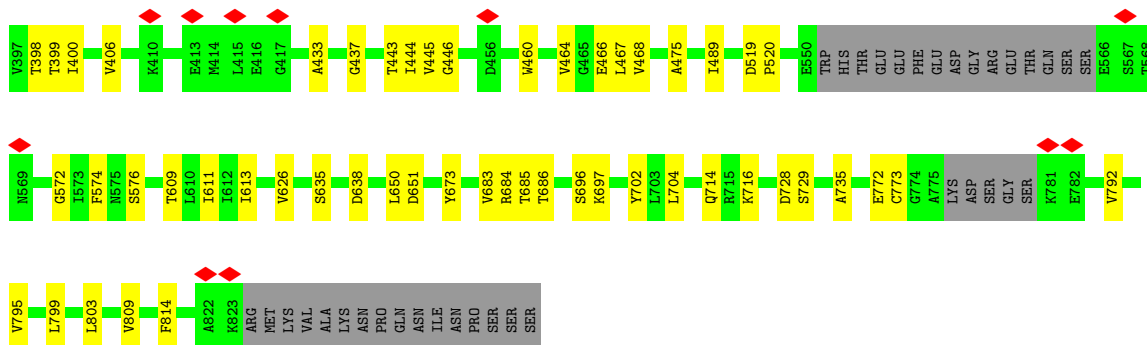
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Glutamate receptor 1

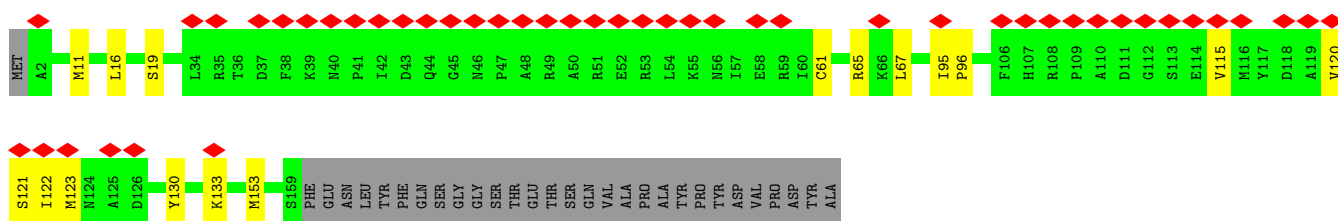
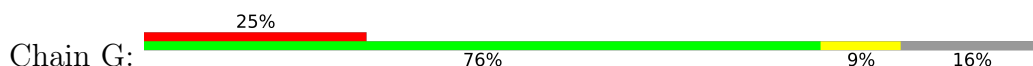


- Molecule 1: Glutamate receptor 1

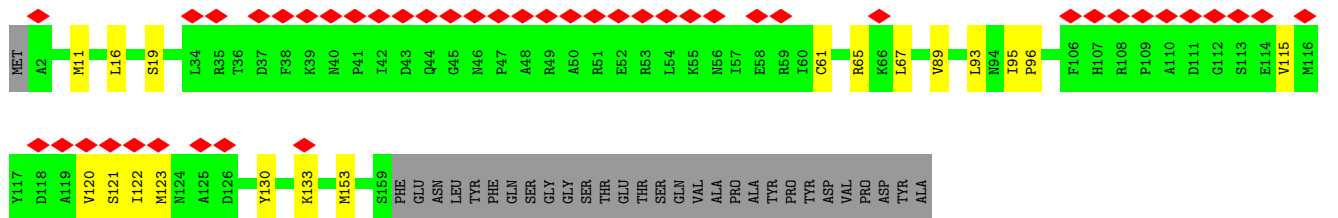
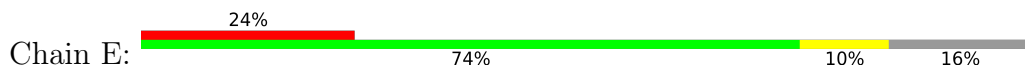




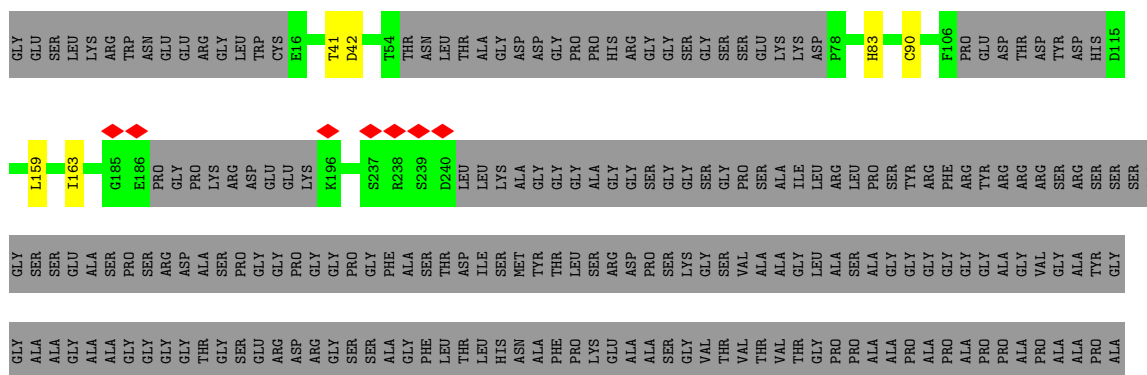
• Molecule 3: Protein cornichon homolog 2



• Molecule 3: Protein cornichon homolog 2



• Molecule 4: Voltage-dependent calcium channel gamma-8 subunit



Chain K:  100%

MAG1
MAG2

- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:  100%

MAG1
MAG2

- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  50%  100%

MAG1
MAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	218320	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.195	Depositor
Minimum map value	-0.118	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.02	Depositor
Map size (\AA)	342.40002, 342.40002, 342.40002	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.07, 1.07, 1.07	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: PC1, E2Q, CLR, NAG, BMA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.28	0/5766	0.37	1/7872 (0.0%)
1	C	0.29	0/5766	0.37	1/7872 (0.0%)
2	B	0.37	0/5945	0.36	0/8088
2	D	0.37	0/5945	0.36	0/8088
3	E	0.15	0/1289	0.29	0/1760
3	G	0.15	0/1289	0.29	0/1760
4	I	0.25	0/1305	0.32	0/1782
4	J	0.25	0/1305	0.32	0/1782
All	All	0.31	0/28610	0.35	2/39004 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	52	MET	CB-CG-SD	10.13	143.10	112.70
1	A	52	MET	CB-CG-SD	10.12	143.05	112.70

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	5637	0	5182	61	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	5637	0	5182	61	0
2	B	5815	0	5490	52	0
2	D	5815	0	5490	54	0
3	E	1248	0	1186	13	0
3	G	1248	0	1186	12	0
4	I	1284	0	1219	3	0
4	J	1284	0	1219	5	0
5	F	39	0	34	1	0
5	M	39	0	34	1	0
6	H	28	0	25	0	0
6	K	28	0	25	0	0
6	L	28	0	25	0	0
6	N	28	0	25	0	0
7	A	23	0	0	0	0
7	B	23	0	0	1	0
7	C	23	0	0	0	0
7	D	23	0	0	1	0
8	A	28	0	26	0	0
8	B	14	0	13	1	0
8	C	28	0	26	0	0
8	D	14	0	13	1	0
9	A	119	0	194	0	0
9	B	179	0	302	1	0
9	C	119	0	194	0	0
9	D	179	0	302	1	0
9	E	58	0	98	0	0
9	G	58	0	98	0	0
9	I	96	0	161	0	0
9	J	96	0	161	1	0
10	E	28	0	46	3	0
10	G	28	0	46	3	0
All	All	29294	0	28002	259	0

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

The worst 5 of 259 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:716:LYS:N	2:B:772:GLU:OE2	2.10	0.84
2:D:716:LYS:N	2:D:772:GLU:OE2	2.10	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:624:ARG:NH2	2:B:626:VAL:O	2.12	0.83
2:B:728:ASP:OD2	2:B:729:SER:N	2.14	0.81
2:D:626:VAL:O	1:C:624:ARG:NH2	2.13	0.81

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	765/915 (84%)	741 (97%)	24 (3%)	0	100	100
1	C	765/915 (84%)	741 (97%)	24 (3%)	0	100	100
2	B	775/860 (90%)	743 (96%)	32 (4%)	0	100	100
2	D	775/860 (90%)	743 (96%)	32 (4%)	0	100	100
3	E	156/188 (83%)	153 (98%)	3 (2%)	0	100	100
3	G	156/188 (83%)	153 (98%)	3 (2%)	0	100	100
4	I	177/423 (42%)	170 (96%)	7 (4%)	0	100	100
4	J	177/423 (42%)	170 (96%)	7 (4%)	0	100	100
All	All	3746/4772 (78%)	3614 (96%)	132 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	517/778 (66%)	516 (100%)	1 (0%)	87	85
1	C	517/778 (66%)	516 (100%)	1 (0%)	87	85
2	B	563/737 (76%)	562 (100%)	1 (0%)	87	85
2	D	563/737 (76%)	562 (100%)	1 (0%)	87	85
3	E	123/166 (74%)	123 (100%)	0	100	100
3	G	123/166 (74%)	123 (100%)	0	100	100
4	I	114/309 (37%)	114 (100%)	0	100	100
4	J	114/309 (37%)	114 (100%)	0	100	100
All	All	2634/3980 (66%)	2630 (100%)	4 (0%)	85	85

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	MET
2	B	106	GLN
2	D	106	GLN
1	C	52	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	714	GLN
1	C	101	ASN
1	C	710	GLN
1	C	324	GLN
2	B	714	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates i

14 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
5	NAG	F	1	5,1	14,14,15	0.75	1 (7%)	17,19,21	1.54	1 (5%)
5	NAG	F	2	5	14,14,15	0.26	0	17,19,21	0.40	0
5	BMA	F	3	5	11,11,12	0.60	0	15,15,17	0.70	0
6	NAG	H	1	6,1	14,14,15	0.20	0	17,19,21	0.42	0
6	NAG	H	2	6	14,14,15	0.25	0	17,19,21	0.43	0
6	NAG	K	1	6,2	14,14,15	0.43	0	17,19,21	0.65	0
6	NAG	K	2	6	14,14,15	0.46	0	17,19,21	0.61	0
6	NAG	L	1	6,2	14,14,15	0.42	0	17,19,21	0.65	0
6	NAG	L	2	6	14,14,15	0.46	0	17,19,21	0.60	0
5	NAG	M	1	5,1	14,14,15	0.77	1 (7%)	17,19,21	1.53	1 (5%)
5	NAG	M	2	5	14,14,15	0.26	0	17,19,21	0.41	0
5	BMA	M	3	5	11,11,12	0.58	0	15,15,17	0.69	0
6	NAG	N	1	6,1	14,14,15	0.20	0	17,19,21	0.43	0
6	NAG	N	2	6	14,14,15	0.25	0	17,19,21	0.43	0

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

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

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	1	NAG	O5-C1	2.71	1.48	1.43
5	F	1	NAG	O5-C1	2.63	1.48	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	1	NAG	C1-O5-C5	6.01	120.24	112.19
5	M	1	NAG	C1-O5-C5	5.99	120.21	112.19

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

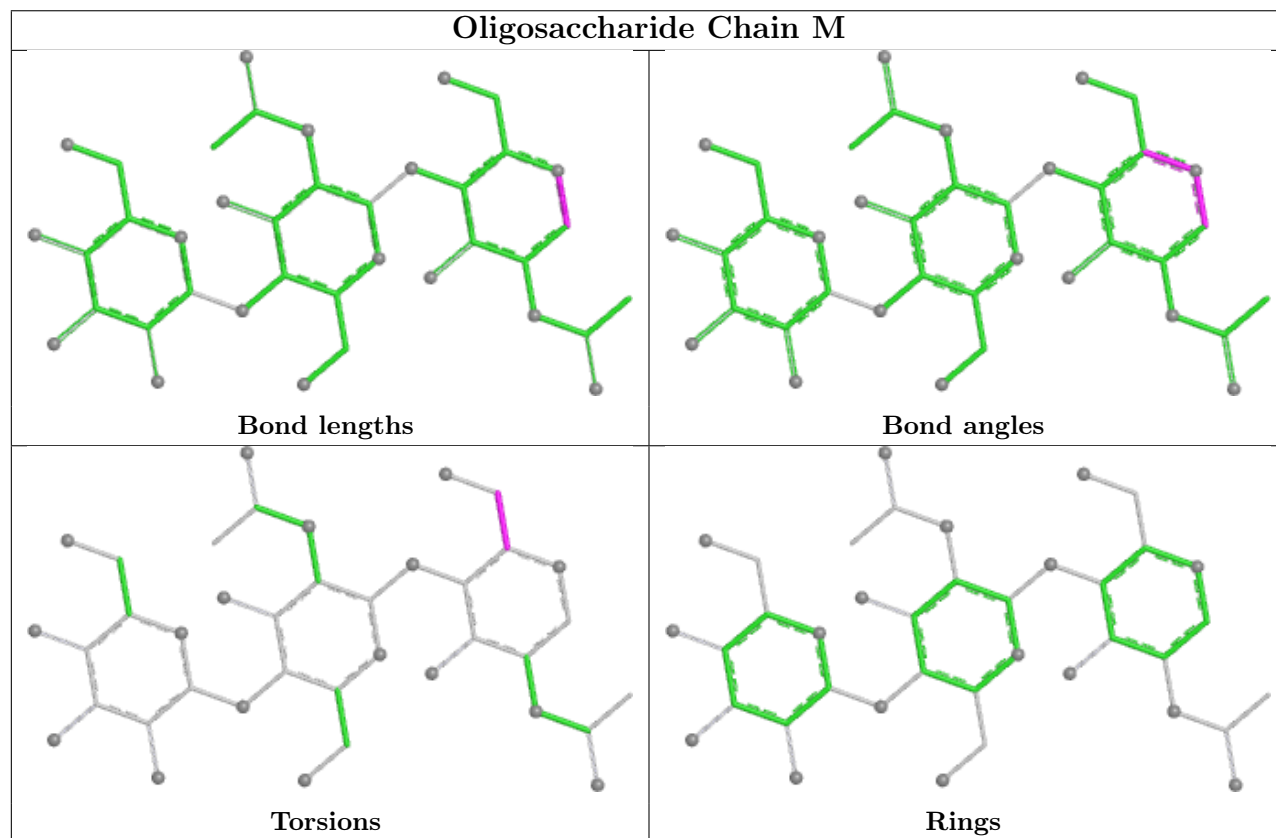
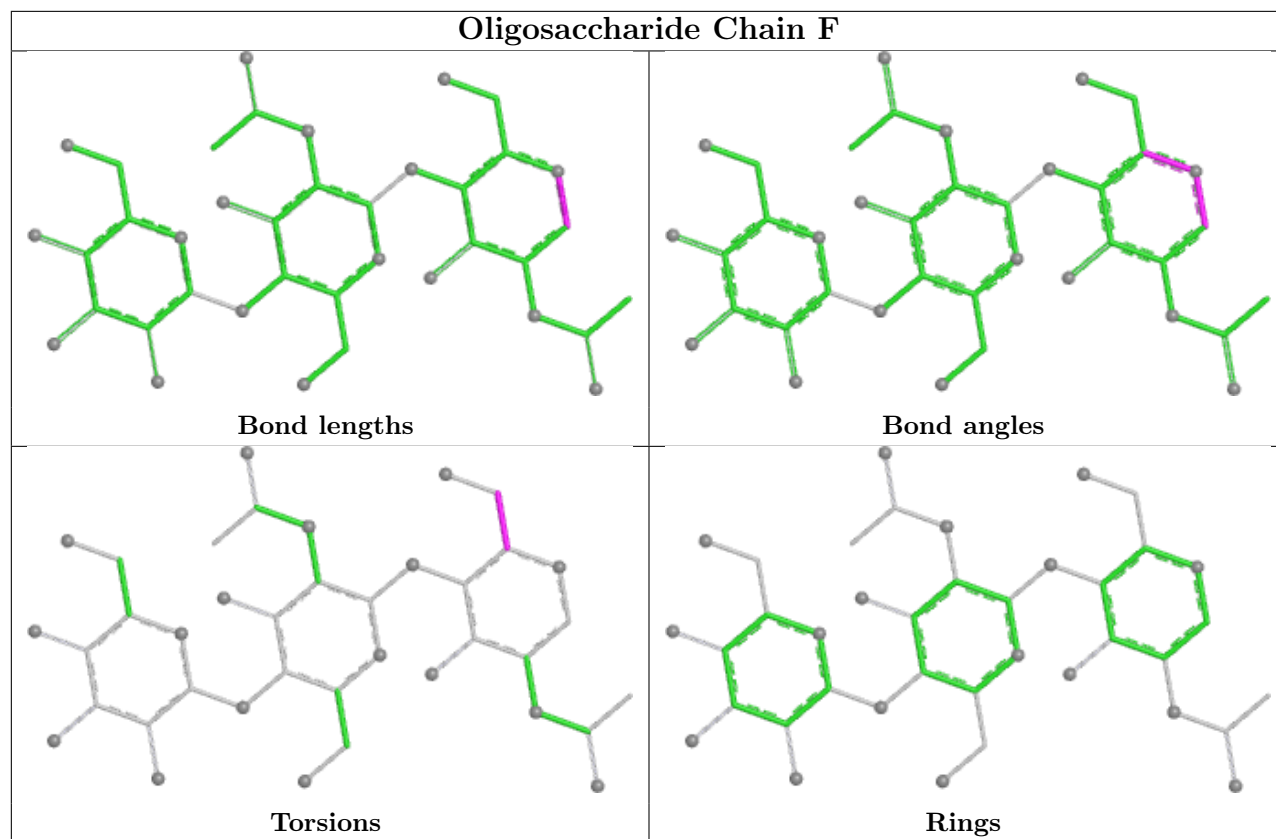
Mol	Chain	Res	Type	Atoms
6	K	2	NAG	C1-C2-N2-C7
6	L	2	NAG	C1-C2-N2-C7
6	H	1	NAG	O5-C5-C6-O6
6	N	1	NAG	O5-C5-C6-O6
6	K	2	NAG	C4-C5-C6-O6

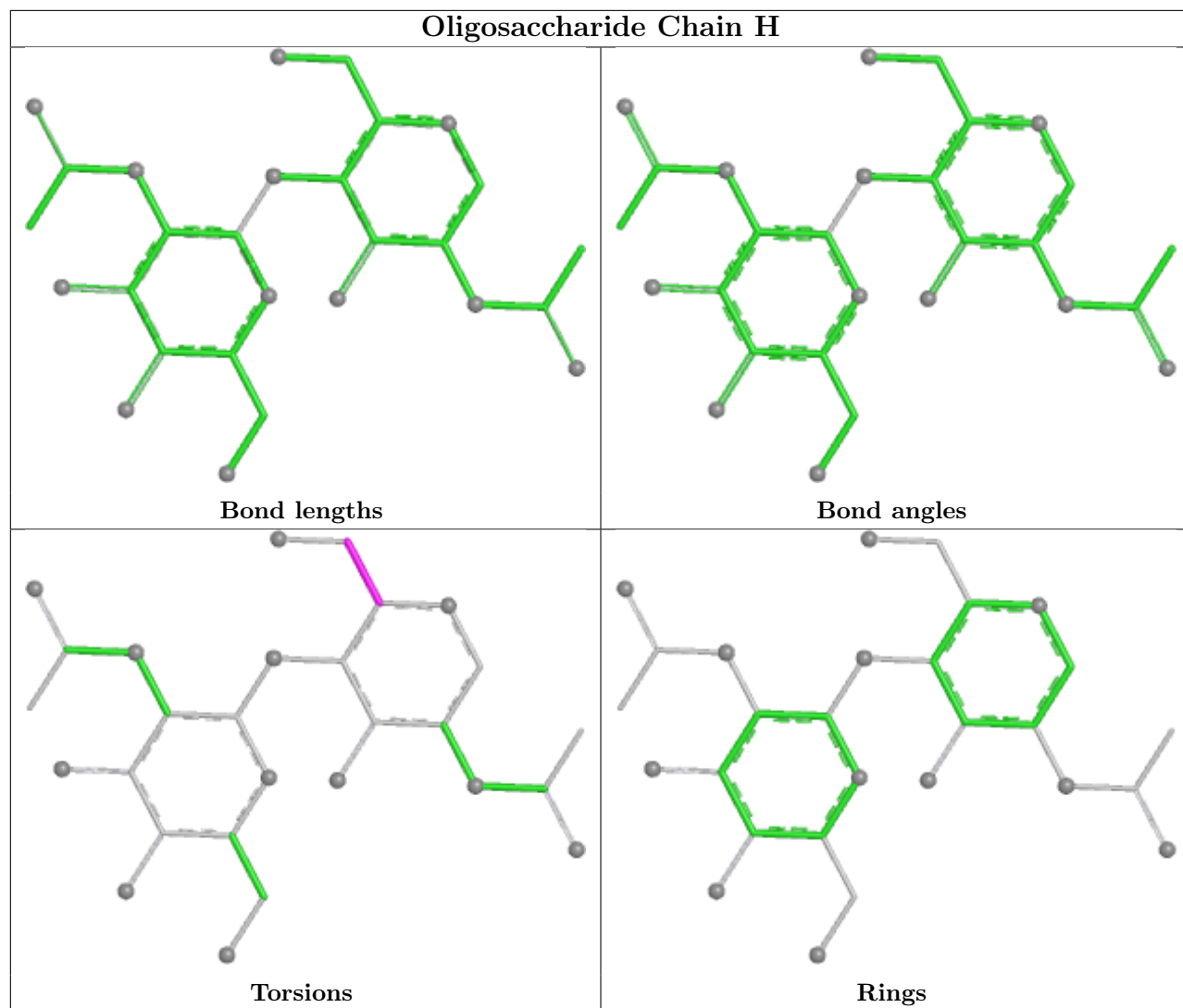
There are no ring outliers.

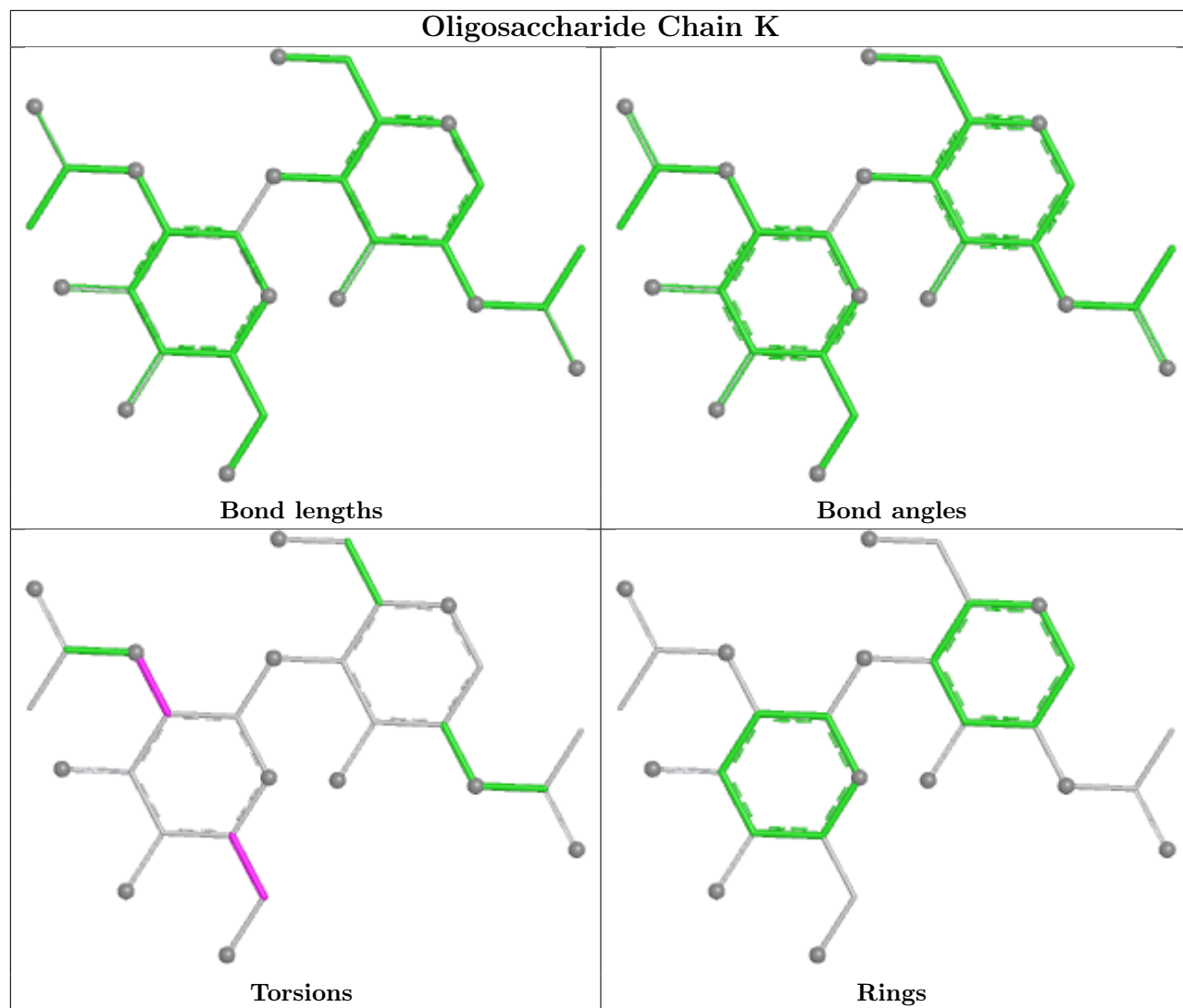
2 monomers are involved in 2 short contacts:

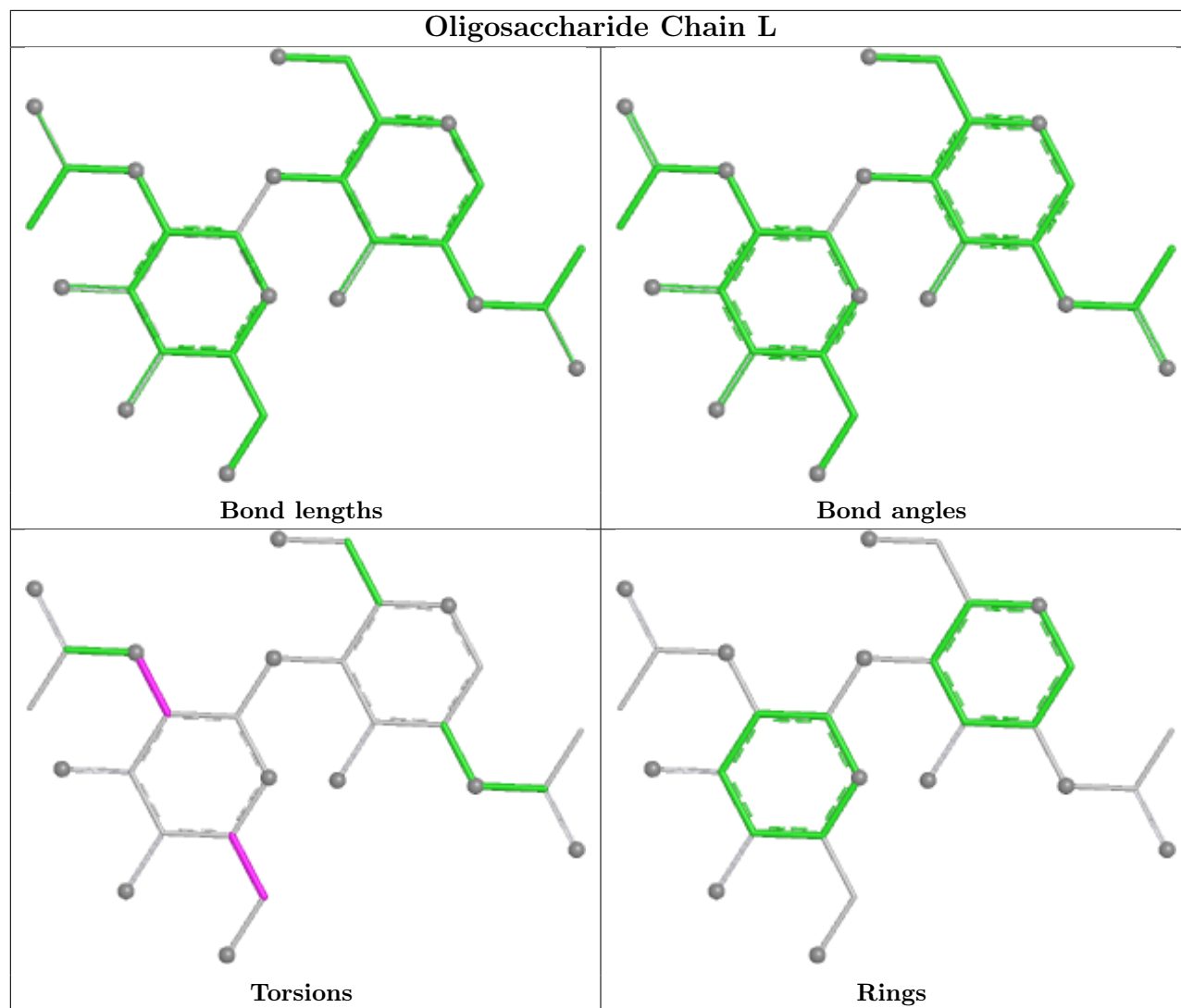
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	M	1	NAG	1	0
5	F	1	NAG	1	0

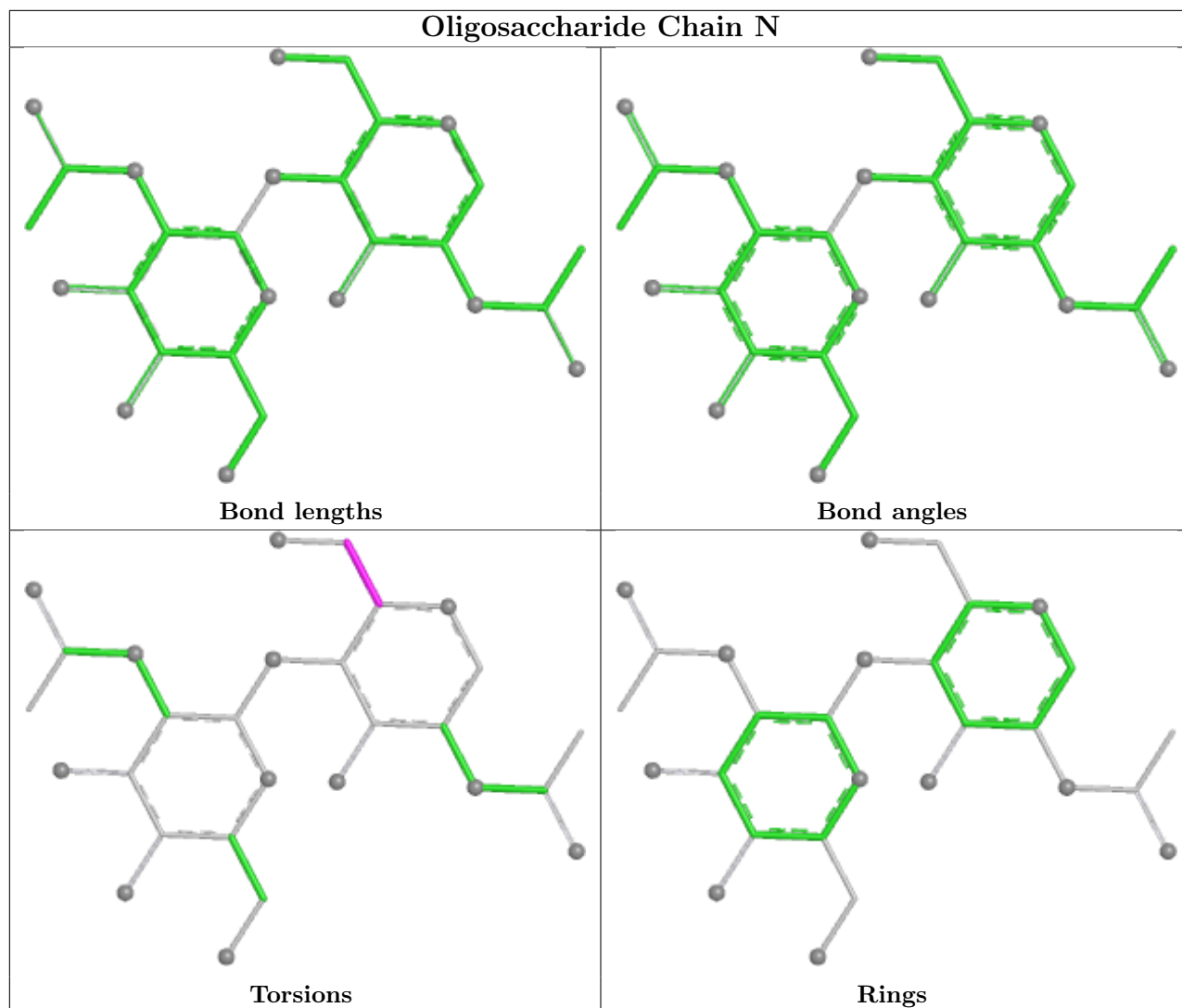
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

58 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	E2Q	A	901	-	25,25,25	1.77	6 (24%)	32,39,39	2.20	12 (37%)
8	NAG	D	902	2	14,14,15	0.42	0	17,19,21	0.48	0
8	NAG	A	902	1	14,14,15	0.53	0	17,19,21	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	PC1	B	2908	-	19,19,53	0.79	1 (5%)	19,19,61	0.96	0
9	PC1	D	904	-	19,19,53	0.79	1 (5%)	19,19,61	1.05	1 (5%)
9	PC1	E	3101	-	17,17,53	0.85	1 (5%)	17,17,61	1.03	0
9	PC1	G	3104	-	19,19,53	0.79	1 (5%)	19,19,61	1.07	0
9	PC1	C	2709	-	24,24,53	0.81	2 (8%)	25,25,61	1.04	1 (4%)
9	PC1	E	3102	-	19,19,53	0.79	1 (5%)	19,19,61	1.04	0
9	PC1	B	2904	-	15,15,53	0.85	1 (6%)	15,15,61	1.09	0
9	PC1	J	2501	-	19,19,53	0.79	1 (5%)	19,19,61	1.10	1 (5%)
9	PC1	D	905	-	19,19,53	0.79	1 (5%)	19,19,61	1.02	0
9	PC1	B	2907	-	19,19,53	0.77	1 (5%)	19,19,61	1.05	0
9	PC1	B	2909	-	17,17,53	0.83	1 (5%)	17,17,61	1.07	0
9	PC1	D	903	-	15,15,53	0.84	1 (6%)	15,15,61	1.09	0
9	PC1	I	3001	-	17,17,53	0.82	1 (5%)	17,17,61	1.11	0
9	PC1	J	2502	-	19,19,53	0.78	1 (5%)	19,19,61	1.02	0
9	PC1	J	2503	-	19,19,53	0.78	1 (5%)	19,19,61	1.07	0
9	PC1	I	3005	-	17,17,53	0.83	1 (5%)	17,17,61	1.07	0
9	PC1	B	2910	-	24,24,53	0.80	2 (8%)	25,25,61	1.05	1 (4%)
9	PC1	I	3002	-	19,19,53	0.78	1 (5%)	19,19,61	1.10	1 (5%)
10	CLR	E	3103	-	31,31,31	0.31	0	48,48,48	0.63	1 (2%)
9	PC1	C	2706	-	17,17,53	0.81	1 (5%)	17,17,61	1.10	0
9	PC1	I	3004	-	19,19,53	0.79	1 (5%)	19,19,61	1.06	0
9	PC1	A	906	-	19,19,53	0.77	1 (5%)	19,19,61	1.05	0
8	NAG	A	903	1	14,14,15	0.17	0	17,19,21	0.45	0
9	PC1	B	2901	-	19,19,53	0.78	1 (5%)	19,19,61	1.07	0
8	NAG	B	2903	2	14,14,15	0.41	0	17,19,21	0.50	0
9	PC1	G	3101	-	19,19,53	0.79	1 (5%)	19,19,61	1.04	0
9	PC1	D	907	-	19,19,53	0.79	1 (5%)	19,19,61	0.96	0
8	NAG	C	2703	1	14,14,15	0.55	0	17,19,21	0.40	0
9	PC1	D	908	-	17,17,53	0.83	1 (5%)	17,17,61	1.07	0
9	PC1	C	2701	-	17,17,53	0.83	1 (5%)	17,17,61	0.96	0
8	NAG	C	2704	1	14,14,15	0.18	0	17,19,21	0.46	0
7	E2Q	D	901	-	25,25,25	1.78	6 (24%)	32,39,39	2.17	11 (34%)
7	E2Q	C	2702	-	25,25,25	1.77	6 (24%)	32,39,39	2.20	12 (37%)
9	PC1	G	3102	-	17,17,53	0.84	1 (5%)	17,17,61	1.02	0
9	PC1	J	2505	-	17,17,53	0.82	1 (5%)	17,17,61	1.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	PC1	A	904	-	19,19,53	0.77	1 (5%)	19,19,61	1.03	0
9	PC1	J	2504	-	17,17,53	0.83	1 (5%)	17,17,61	1.08	0
9	PC1	D	910	-	19,19,53	0.78	1 (5%)	19,19,61	1.07	1 (5%)
9	PC1	A	907	-	17,17,53	0.82	1 (5%)	17,17,61	1.05	0
9	PC1	C	2708	-	17,17,53	0.82	1 (5%)	17,17,61	1.05	0
9	PC1	A	908	-	24,24,53	0.82	2 (8%)	25,25,61	1.04	1 (4%)
9	PC1	D	909	-	24,24,53	0.79	2 (8%)	25,25,61	1.05	1 (4%)
9	PC1	A	905	-	17,17,53	0.81	1 (5%)	17,17,61	1.10	0
9	PC1	I	3003	-	19,19,53	0.78	1 (5%)	19,19,61	1.02	0
9	PC1	D	906	-	19,19,53	0.77	1 (5%)	19,19,61	1.05	0
9	PC1	B	2906	-	19,19,53	0.80	1 (5%)	19,19,61	1.02	0
9	PC1	A	909	-	17,17,53	0.84	1 (5%)	17,17,61	0.97	0
9	PC1	D	911	-	19,19,53	0.77	1 (5%)	19,19,61	0.93	0
9	PC1	C	2707	-	19,19,53	0.78	1 (5%)	19,19,61	1.05	0
9	PC1	E	3104	-	19,19,53	0.79	1 (5%)	19,19,61	1.07	0
10	CLR	G	3103	-	31,31,31	0.31	0	48,48,48	0.63	1 (2%)
9	PC1	C	2705	-	19,19,53	0.77	1 (5%)	19,19,61	1.04	0
9	PC1	B	2911	-	19,19,53	0.77	1 (5%)	19,19,61	0.92	0
7	E2Q	B	2902	-	25,25,25	1.78	6 (24%)	32,39,39	2.18	11 (34%)
9	PC1	B	2905	-	19,19,53	0.78	1 (5%)	19,19,61	1.05	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	E2Q	A	901	-	-	3/8/10/10	0/3/3/3
8	NAG	D	902	2	-	3/6/23/26	0/1/1/1
8	NAG	A	902	1	-	2/6/23/26	0/1/1/1
9	PC1	B	2908	-	-	5/17/17/57	-
9	PC1	D	904	-	-	8/17/17/57	-
9	PC1	E	3101	-	-	2/15/15/57	-
9	PC1	G	3104	-	-	6/17/17/57	-
9	PC1	C	2709	-	-	12/24/24/57	-
9	PC1	E	3102	-	-	6/17/17/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	PC1	B	2904	-	-	5/13/13/57	-
9	PC1	J	2501	-	-	2/17/17/57	-
9	PC1	D	905	-	-	3/17/17/57	-
9	PC1	B	2907	-	-	4/17/17/57	-
9	PC1	B	2909	-	-	5/15/15/57	-
9	PC1	D	903	-	-	5/13/13/57	-
9	PC1	I	3001	-	-	5/15/15/57	-
9	PC1	J	2502	-	-	6/17/17/57	-
9	PC1	J	2503	-	-	4/17/17/57	-
9	PC1	I	3005	-	-	7/15/15/57	-
9	PC1	B	2910	-	-	10/24/24/57	-
9	PC1	I	3002	-	-	2/17/17/57	-
10	CLR	E	3103	-	-	4/10/68/68	0/4/4/4
9	PC1	C	2706	-	-	8/15/15/57	-
9	PC1	I	3004	-	-	4/17/17/57	-
9	PC1	A	906	-	-	5/17/17/57	-
8	NAG	A	903	1	-	2/6/23/26	0/1/1/1
9	PC1	B	2901	-	-	6/17/17/57	-
8	NAG	B	2903	2	-	3/6/23/26	0/1/1/1
9	PC1	G	3101	-	-	6/17/17/57	-
9	PC1	D	907	-	-	6/17/17/57	-
8	NAG	C	2703	1	-	2/6/23/26	0/1/1/1
9	PC1	D	908	-	-	5/15/15/57	-
9	PC1	C	2701	-	-	11/15/15/57	-
8	NAG	C	2704	1	-	2/6/23/26	0/1/1/1
7	E2Q	D	901	-	-	3/8/10/10	0/3/3/3
7	E2Q	C	2702	-	-	3/8/10/10	0/3/3/3
9	PC1	G	3102	-	-	2/15/15/57	-
9	PC1	J	2505	-	-	5/15/15/57	-
9	PC1	A	904	-	-	6/17/17/57	-
9	PC1	J	2504	-	-	7/15/15/57	-
9	PC1	D	910	-	-	6/17/17/57	-
9	PC1	A	907	-	-	3/15/15/57	-
9	PC1	C	2708	-	-	3/15/15/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	PC1	A	908	-	-	12/24/24/57	-
9	PC1	D	909	-	-	10/24/24/57	-
9	PC1	A	905	-	-	8/15/15/57	-
9	PC1	I	3003	-	-	6/17/17/57	-
9	PC1	D	906	-	-	4/17/17/57	-
9	PC1	B	2906	-	-	3/17/17/57	-
9	PC1	A	909	-	-	11/15/15/57	-
9	PC1	D	911	-	-	9/17/17/57	-
9	PC1	C	2707	-	-	5/17/17/57	-
9	PC1	E	3104	-	-	6/17/17/57	-
10	CLR	G	3103	-	-	4/10/68/68	0/4/4/4
9	PC1	C	2705	-	-	6/17/17/57	-
9	PC1	B	2911	-	-	9/17/17/57	-
7	E2Q	B	2902	-	-	3/8/10/10	0/3/3/3
9	PC1	B	2905	-	-	8/17/17/57	-

The worst 5 of 74 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	2702	E2Q	C09-S11	-5.79	1.69	1.77
7	D	901	E2Q	C09-S11	-5.74	1.69	1.77
7	A	901	E2Q	C09-S11	-5.73	1.69	1.77
7	B	2902	E2Q	C09-S11	-5.72	1.69	1.77
7	A	901	E2Q	C21-N23	3.21	1.40	1.35

The worst 5 of 57 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	901	E2Q	C09-C08-C03	5.44	119.76	116.78
7	C	2702	E2Q	C09-C08-C03	5.37	119.72	116.78
7	B	2902	E2Q	C09-C08-C03	5.37	119.72	116.78
7	D	901	E2Q	C09-C08-C03	5.34	119.71	116.78
7	C	2702	E2Q	O22-C21-C19	3.79	122.98	119.62

There are no chirality outliers.

5 of 311 torsion outliers are listed below:

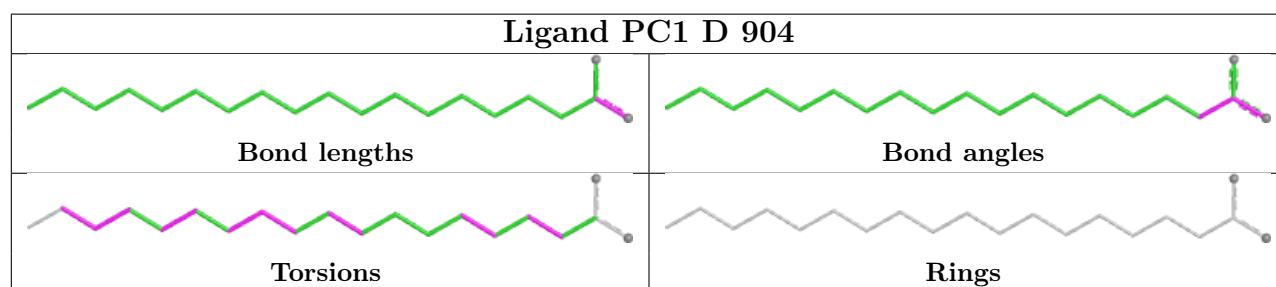
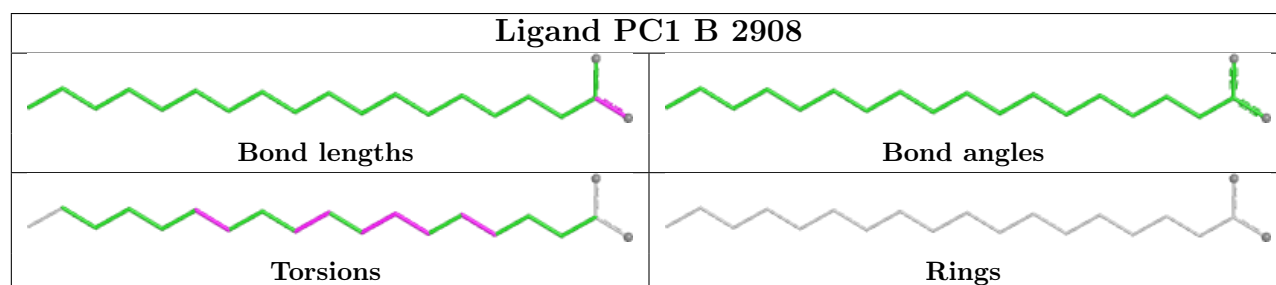
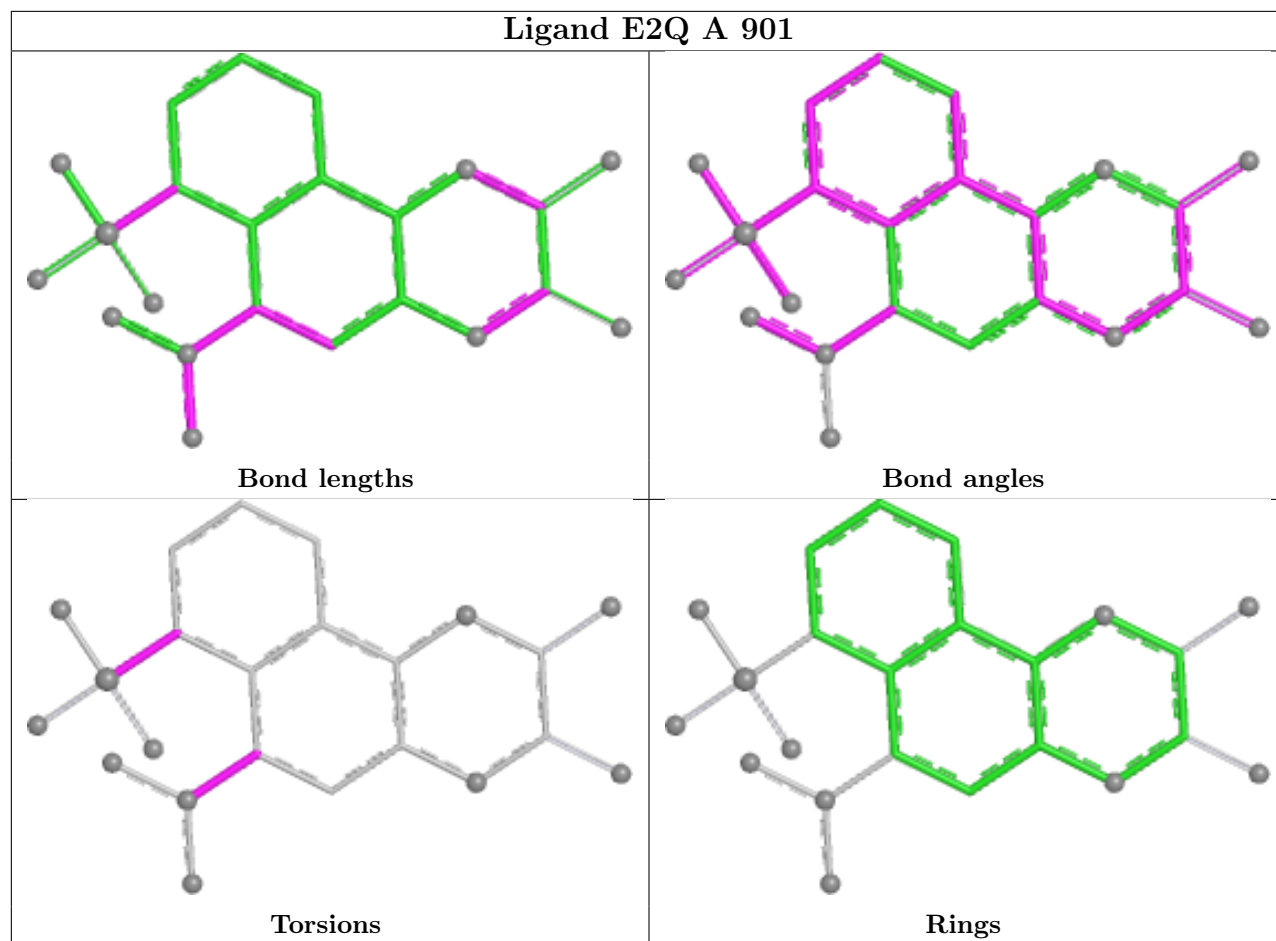
Mol	Chain	Res	Type	Atoms
7	A	901	E2Q	C06-C07-N15-O16
7	A	901	E2Q	C08-C07-N15-O16
7	B	2902	E2Q	C06-C07-N15-O16
7	B	2902	E2Q	C08-C07-N15-O16
7	D	901	E2Q	C06-C07-N15-O16

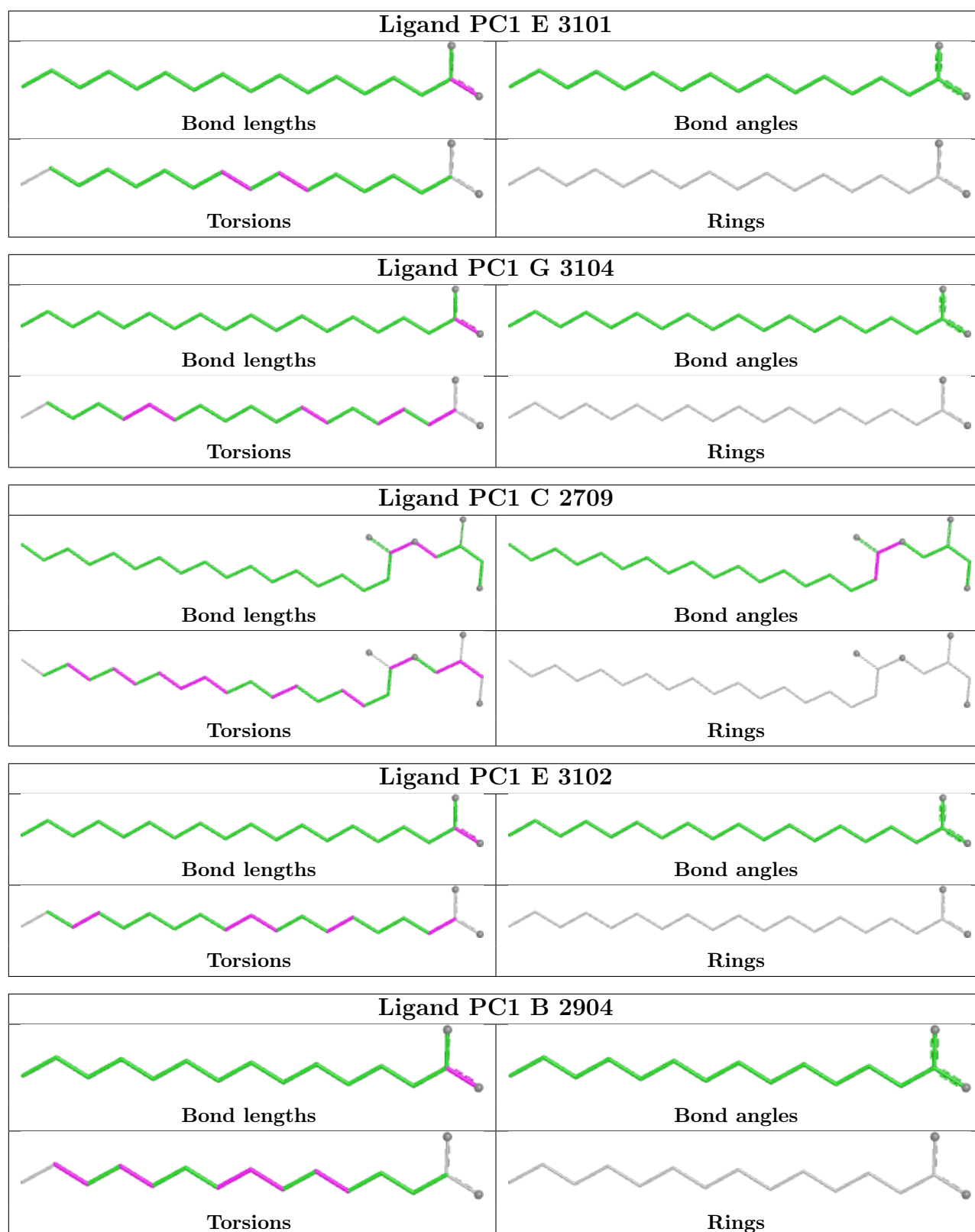
There are no ring outliers.

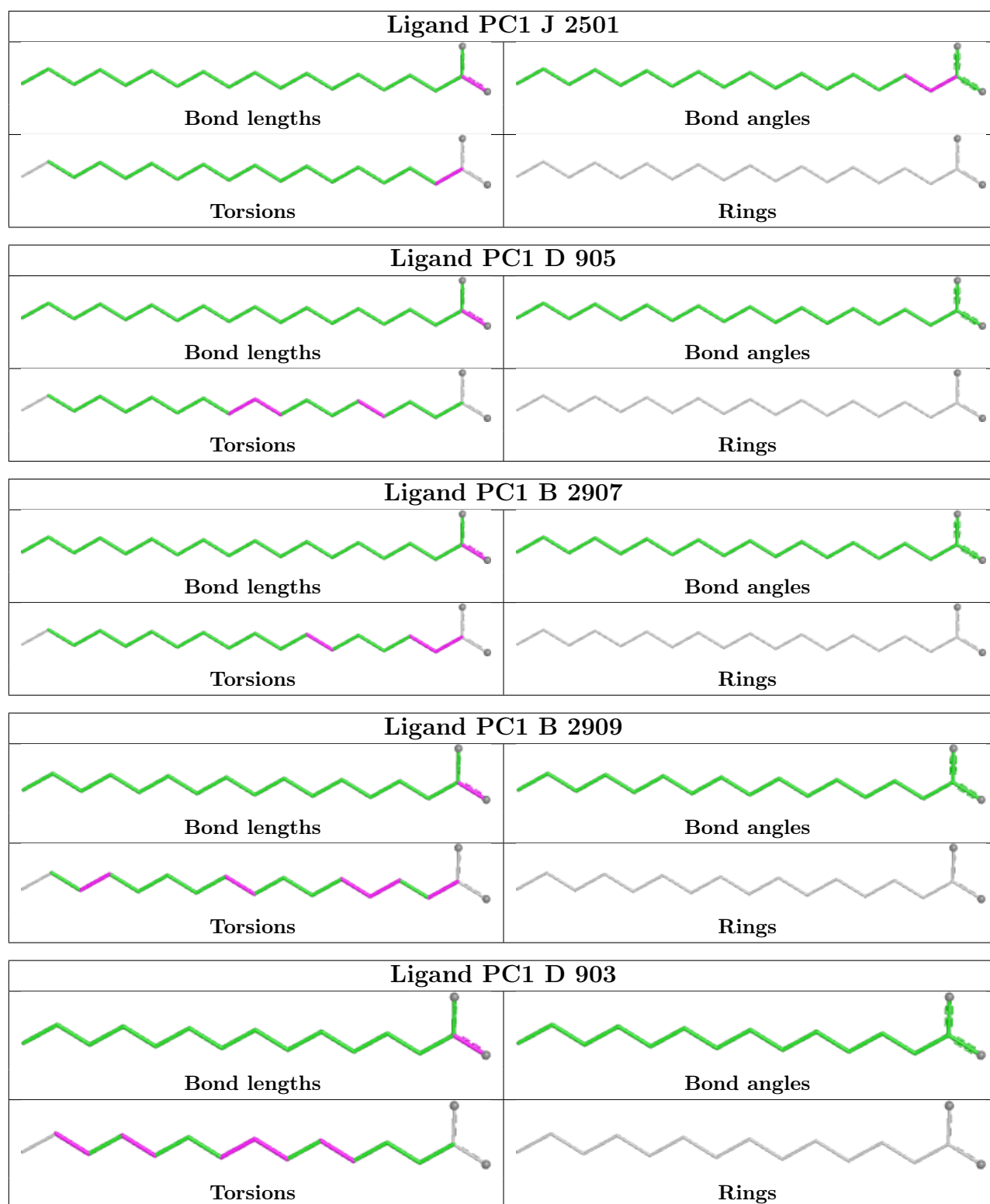
9 monomers are involved in 13 short contacts:

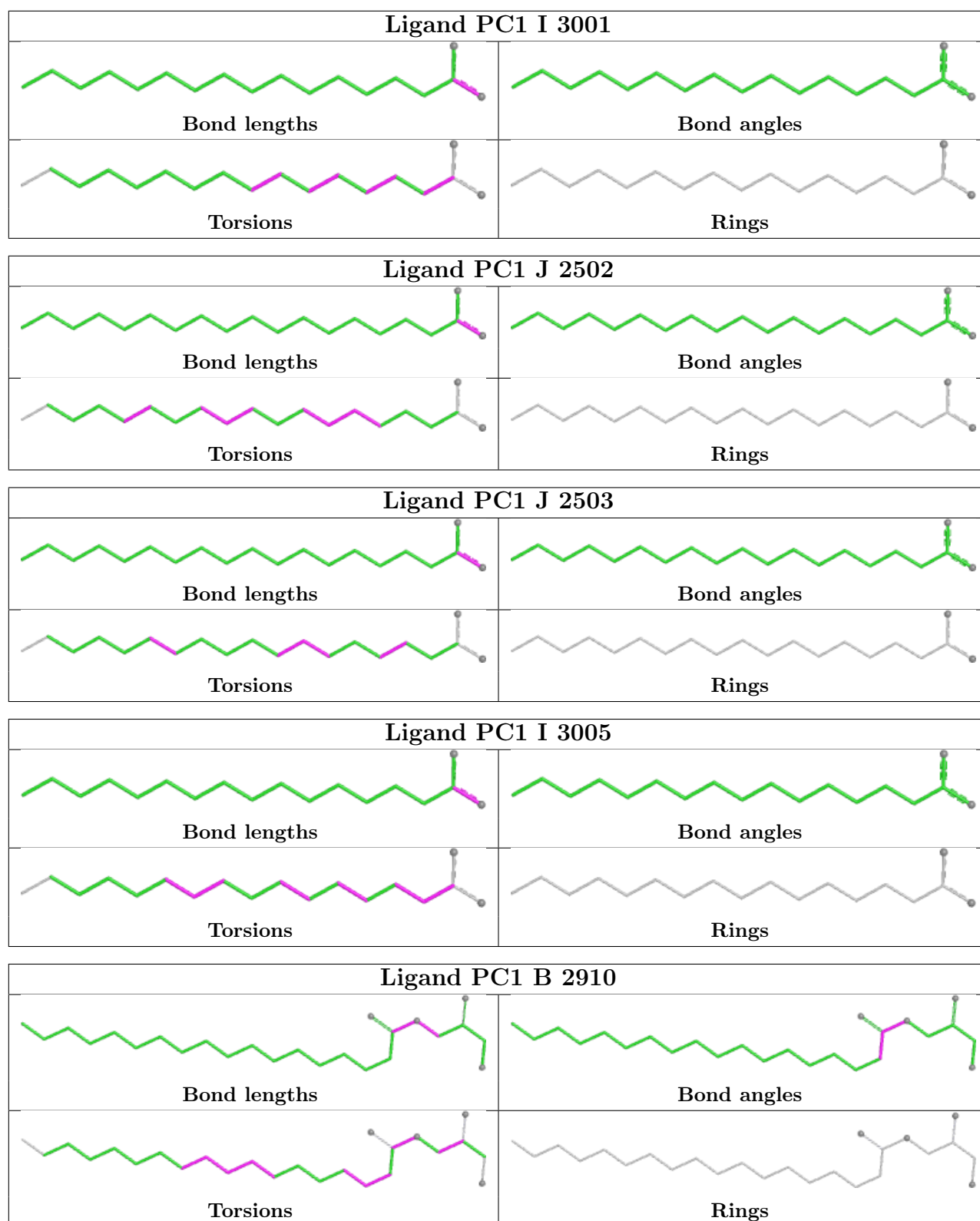
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	902	NAG	1	0
9	J	2502	PC1	1	0
10	E	3103	CLR	3	0
9	B	2901	PC1	1	0
8	B	2903	NAG	1	0
7	D	901	E2Q	1	0
9	D	909	PC1	1	0
10	G	3103	CLR	3	0
7	B	2902	E2Q	1	0

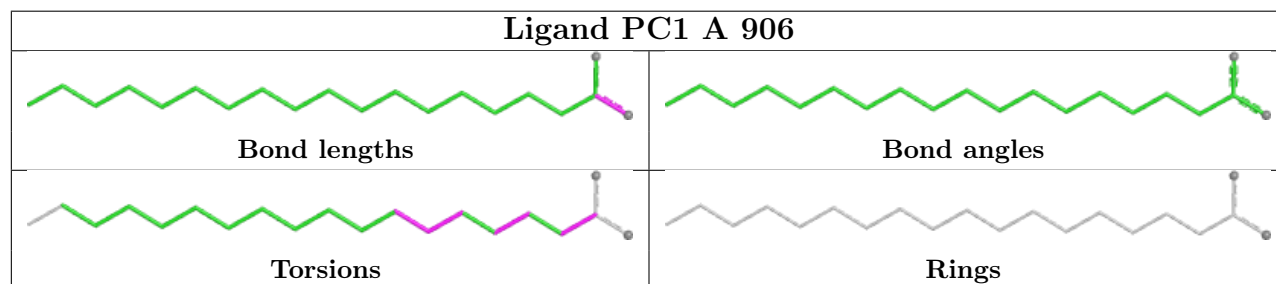
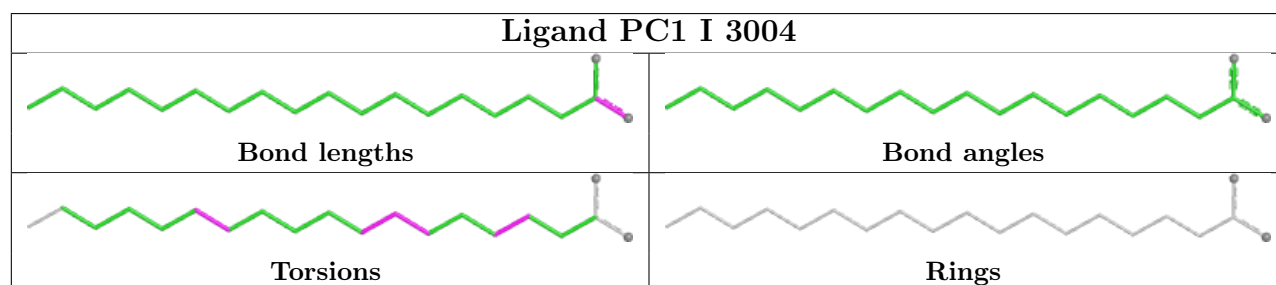
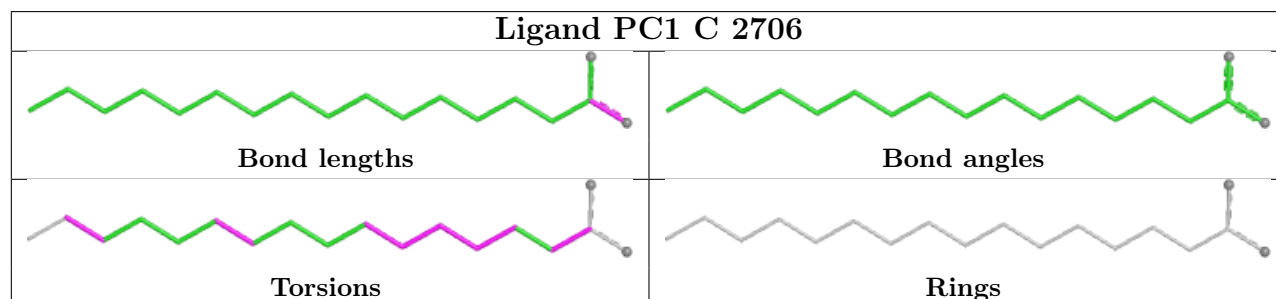
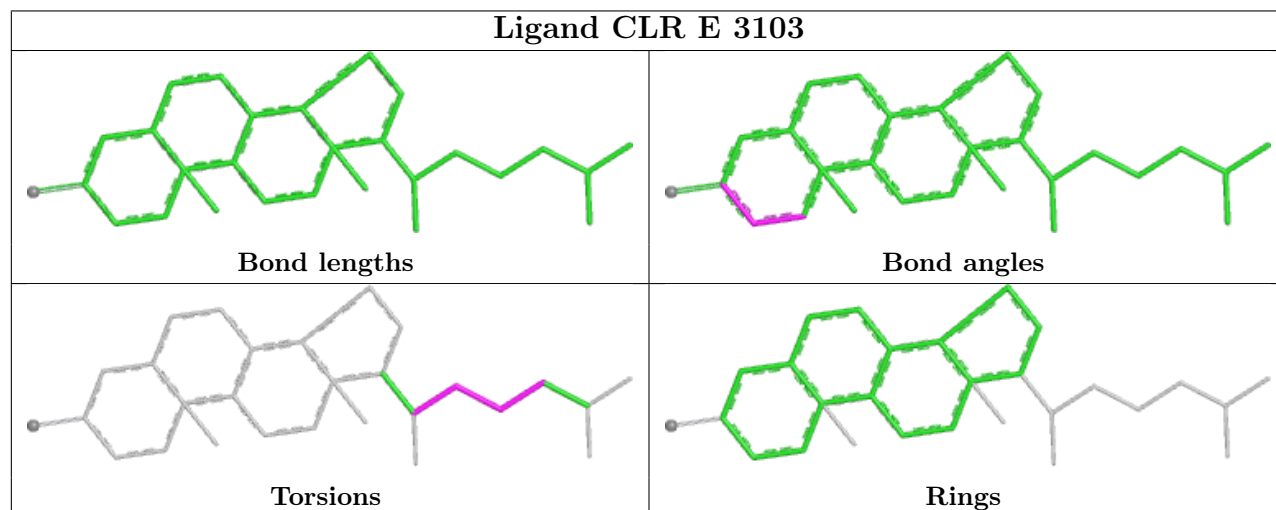
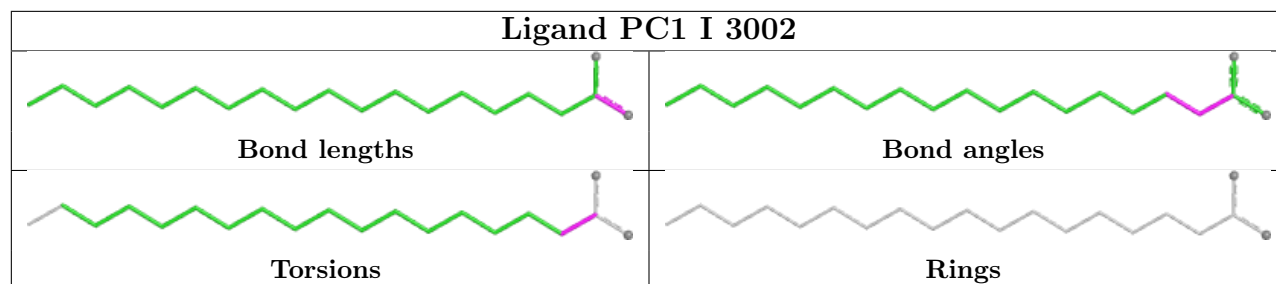
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

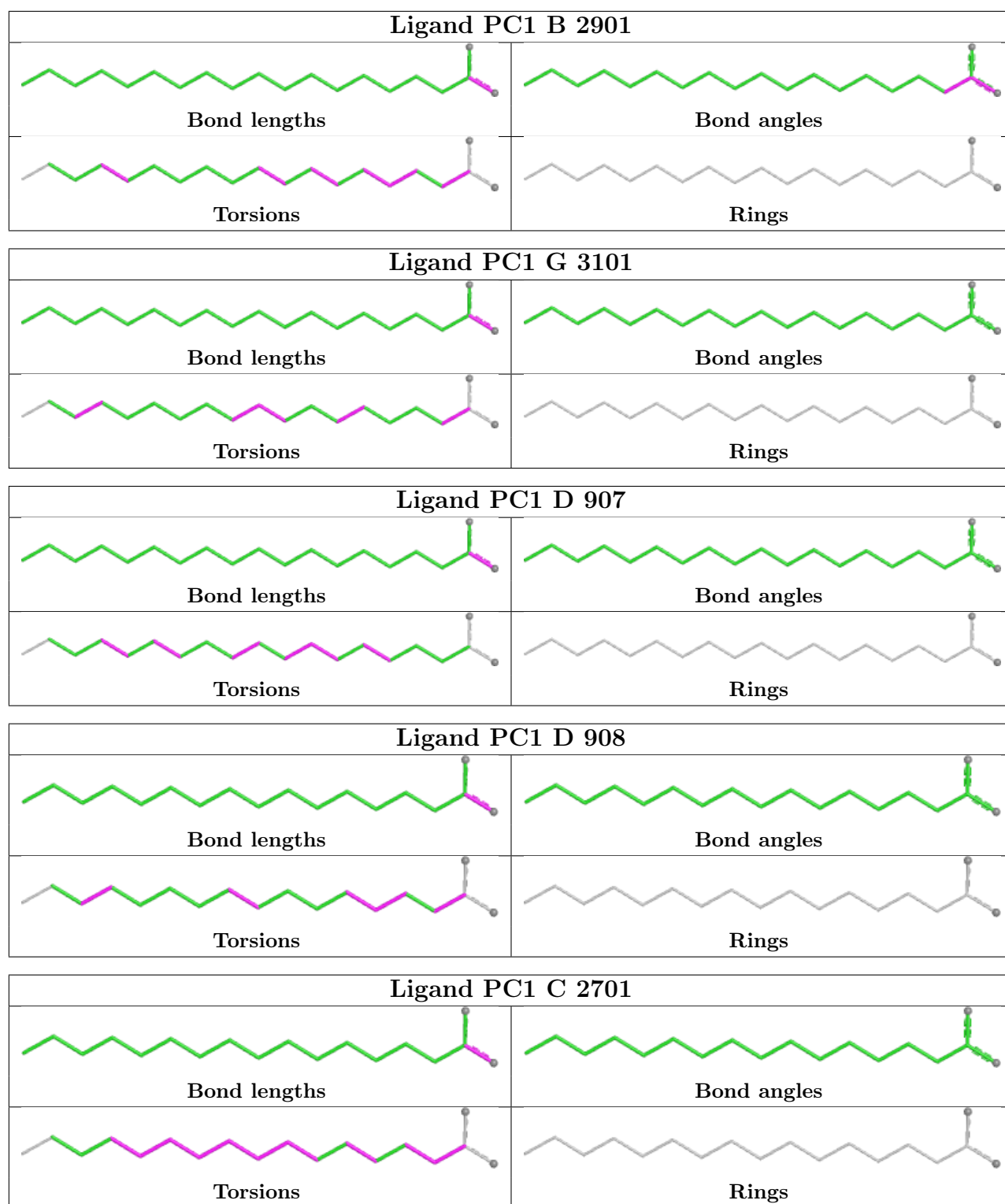


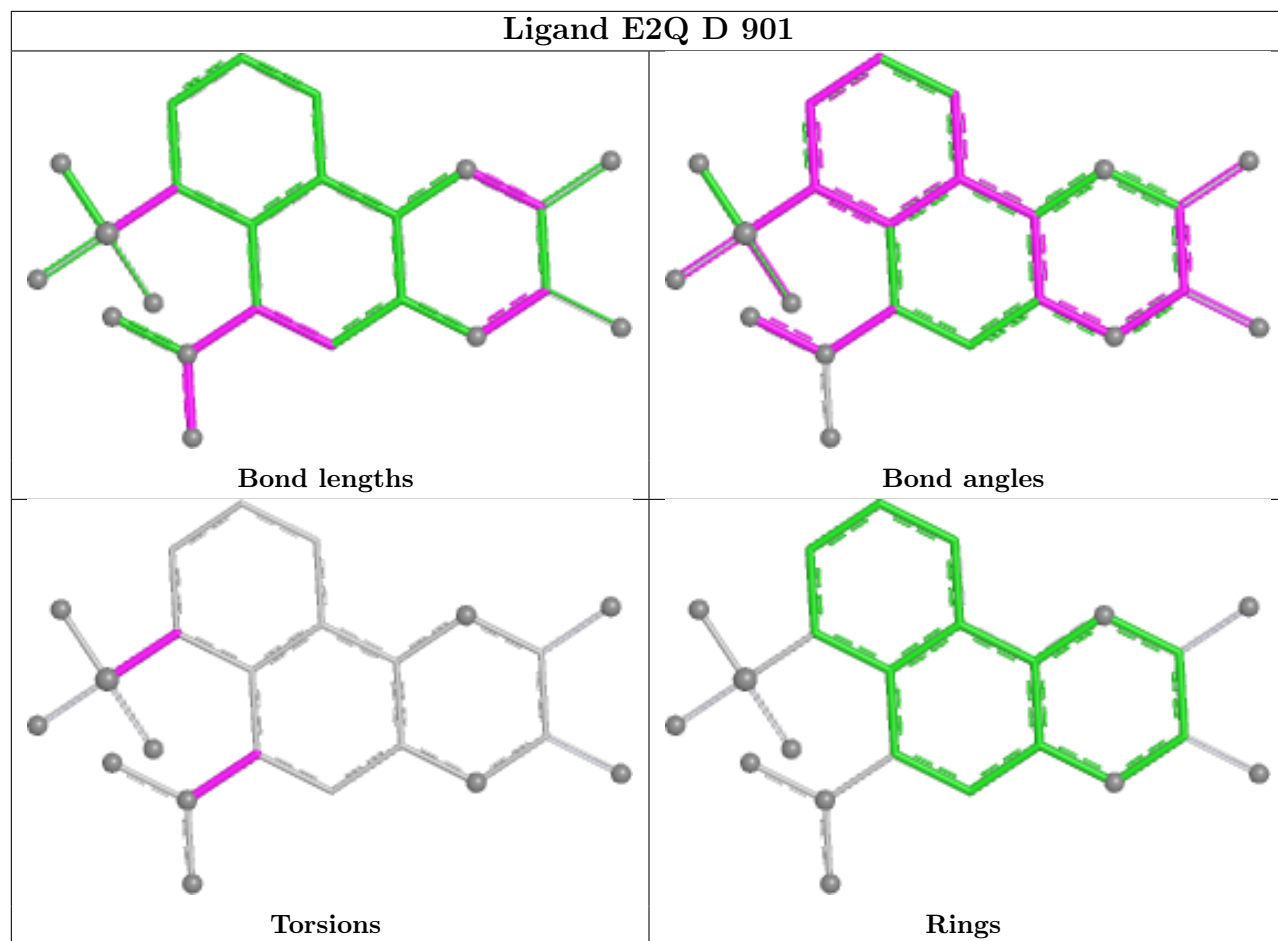


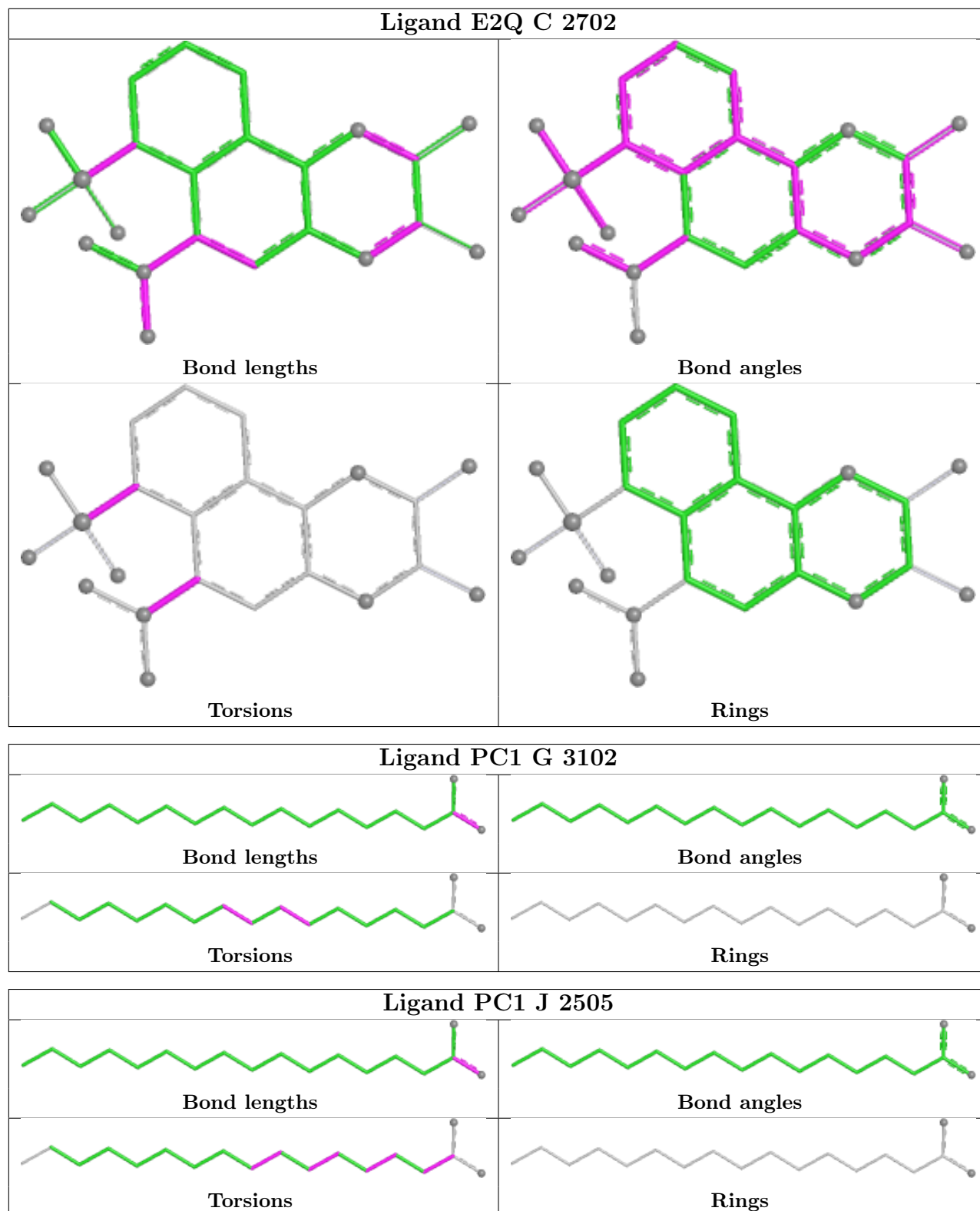


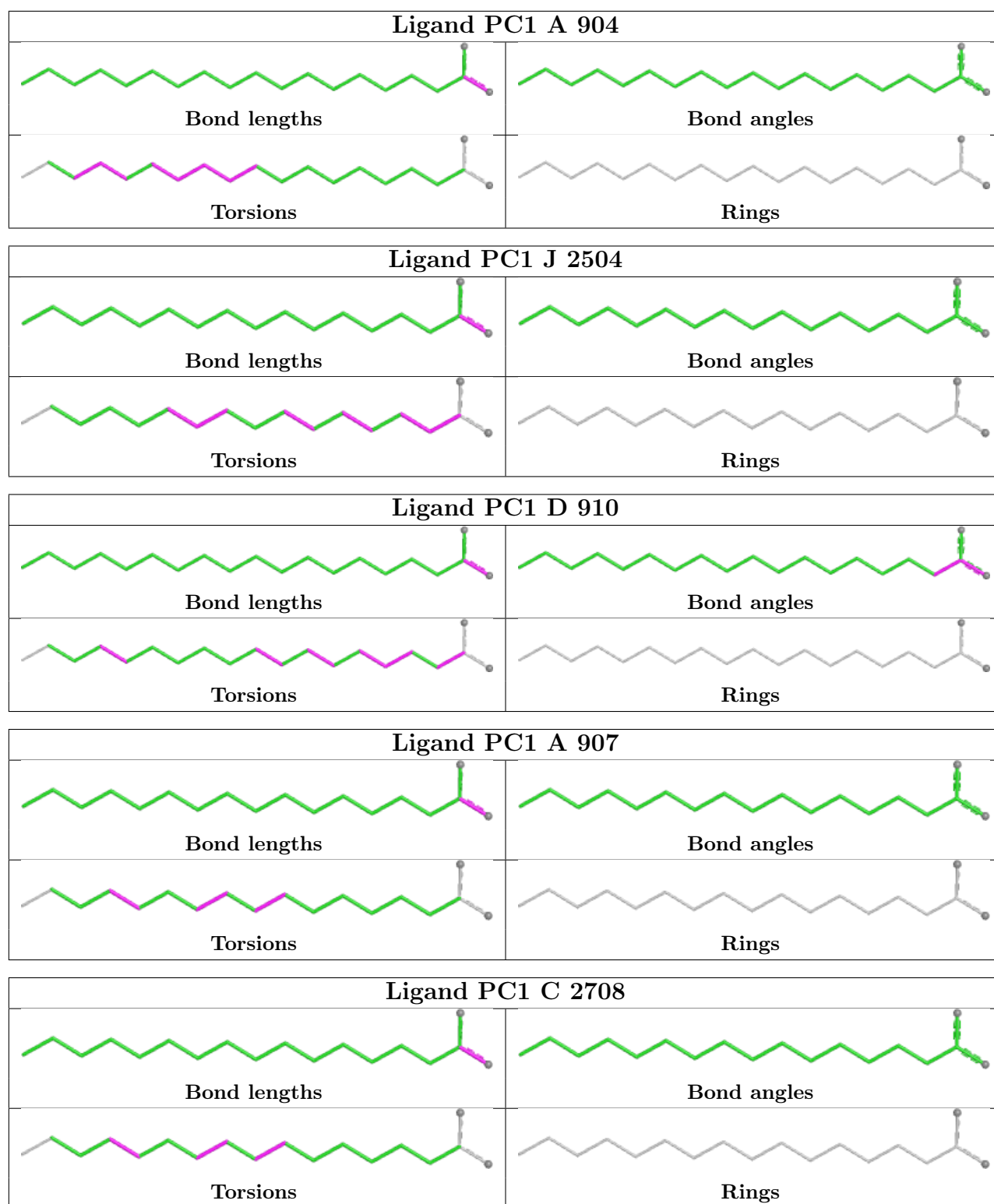


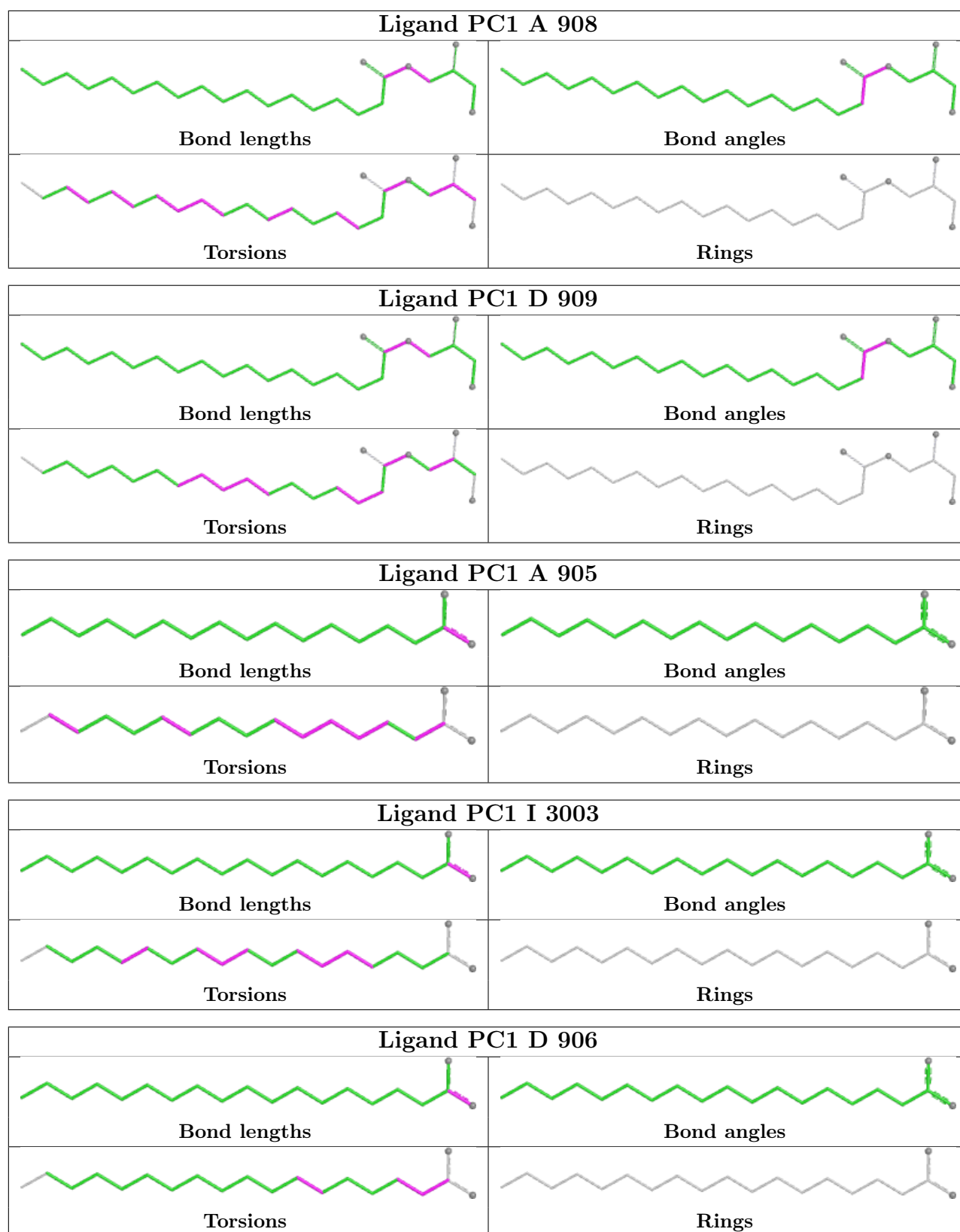


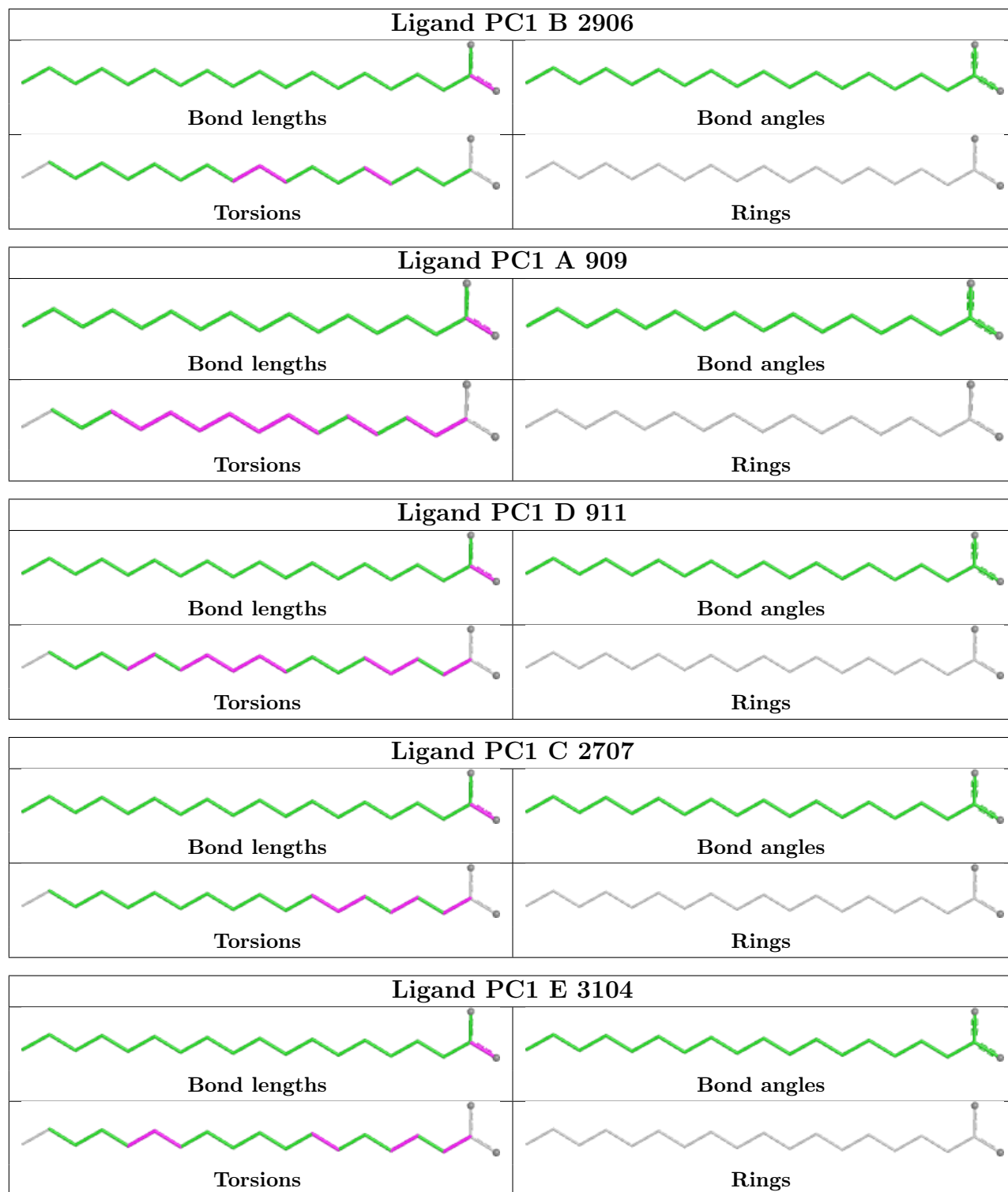


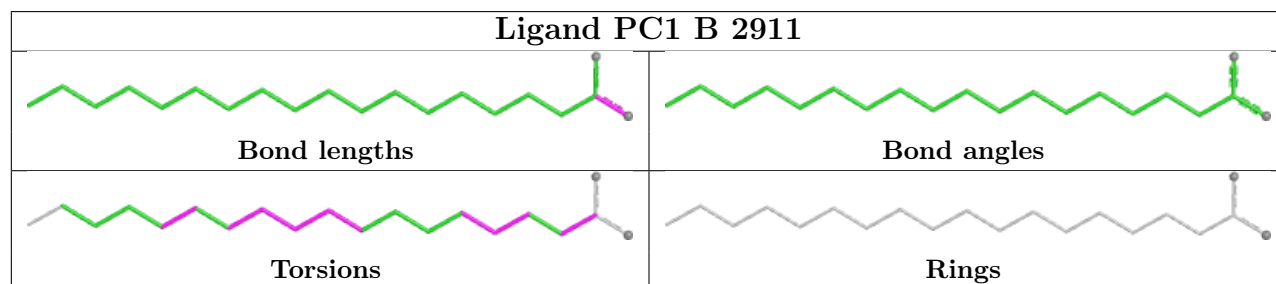
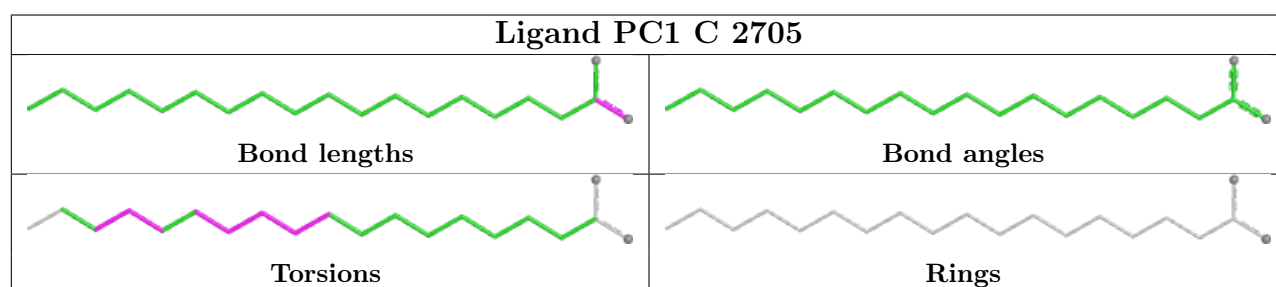
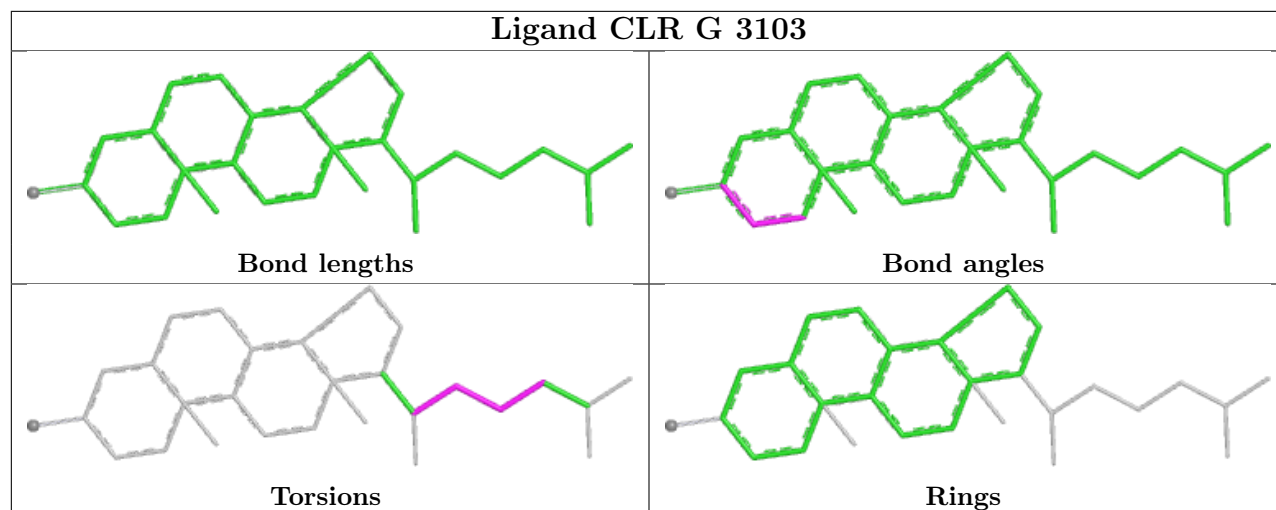


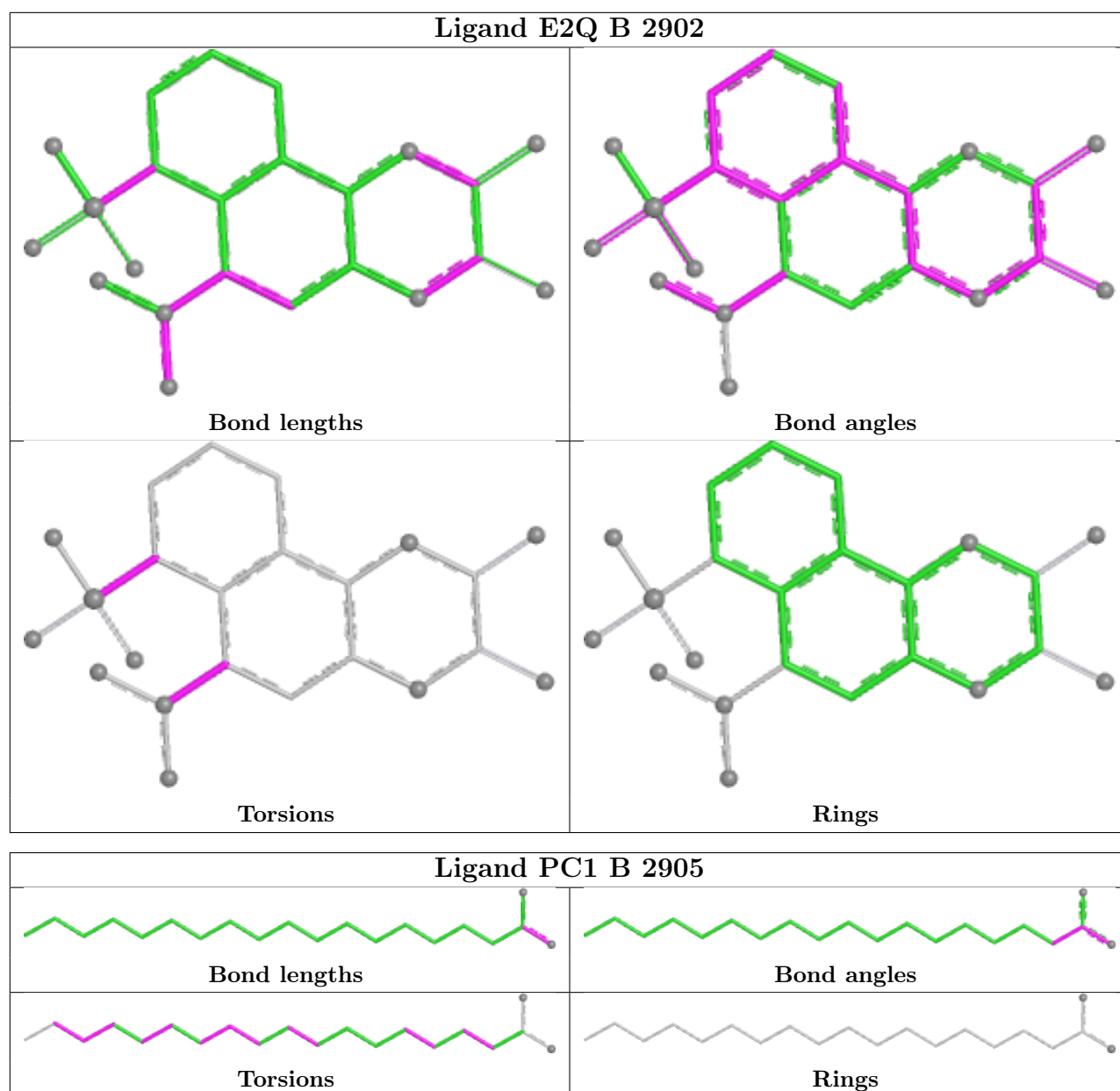












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

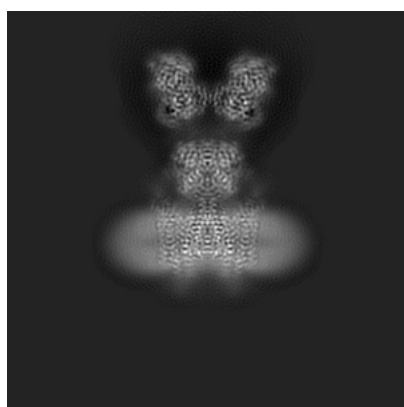
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12802. These allow visual inspection of the internal detail of the map and identification of artifacts.

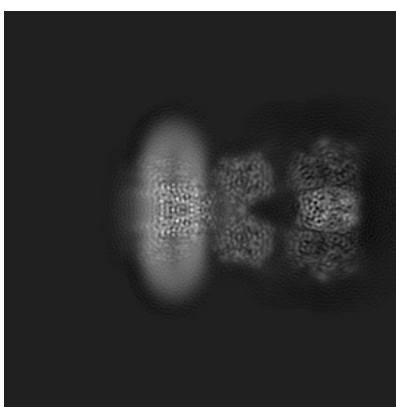
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

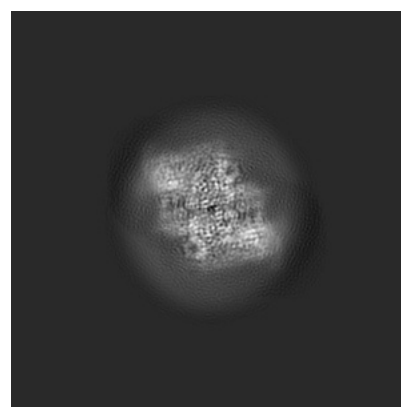
6.1.1 Primary map



X



Y

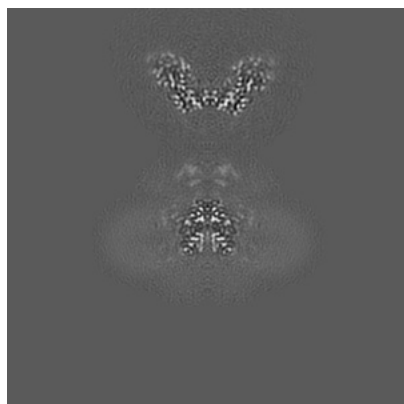


Z

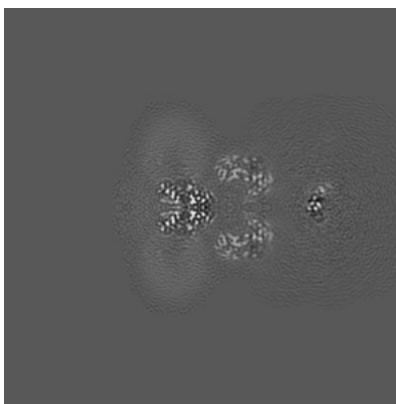
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

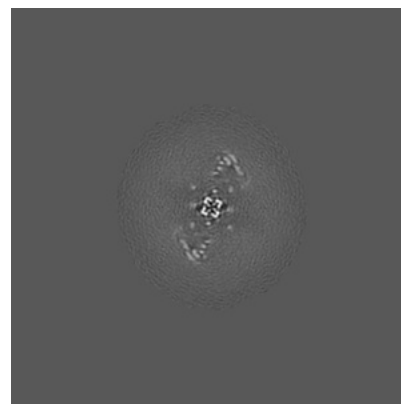
6.2.1 Primary map



X Index: 160



Y Index: 160

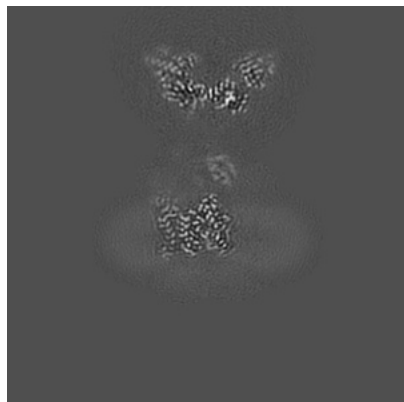


Z Index: 160

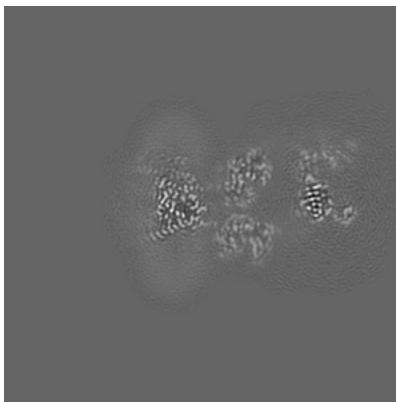
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

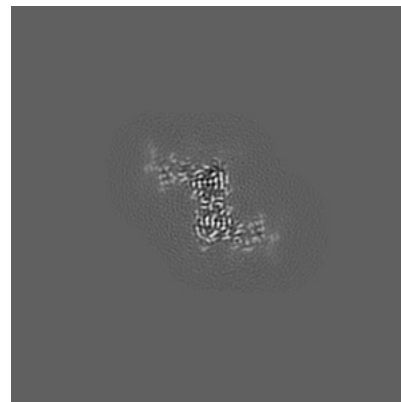
6.3.1 Primary map



X Index: 155



Y Index: 147

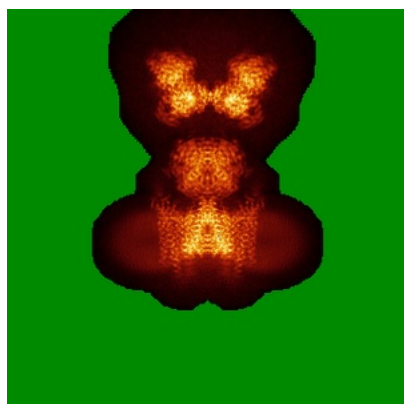


Z Index: 248

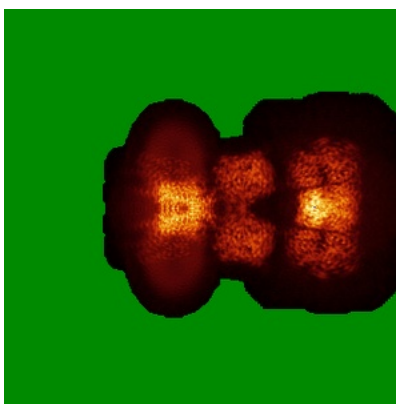
The images above show the largest variance slices of the map in three orthogonal directions.

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

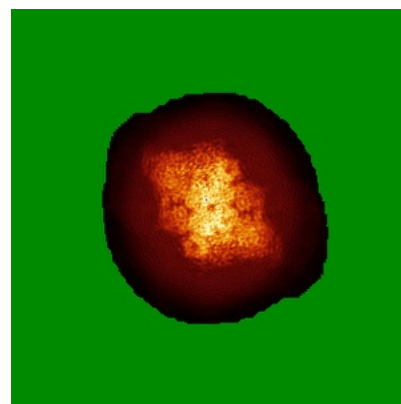
6.4.1 Primary map



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

This section was not generated.

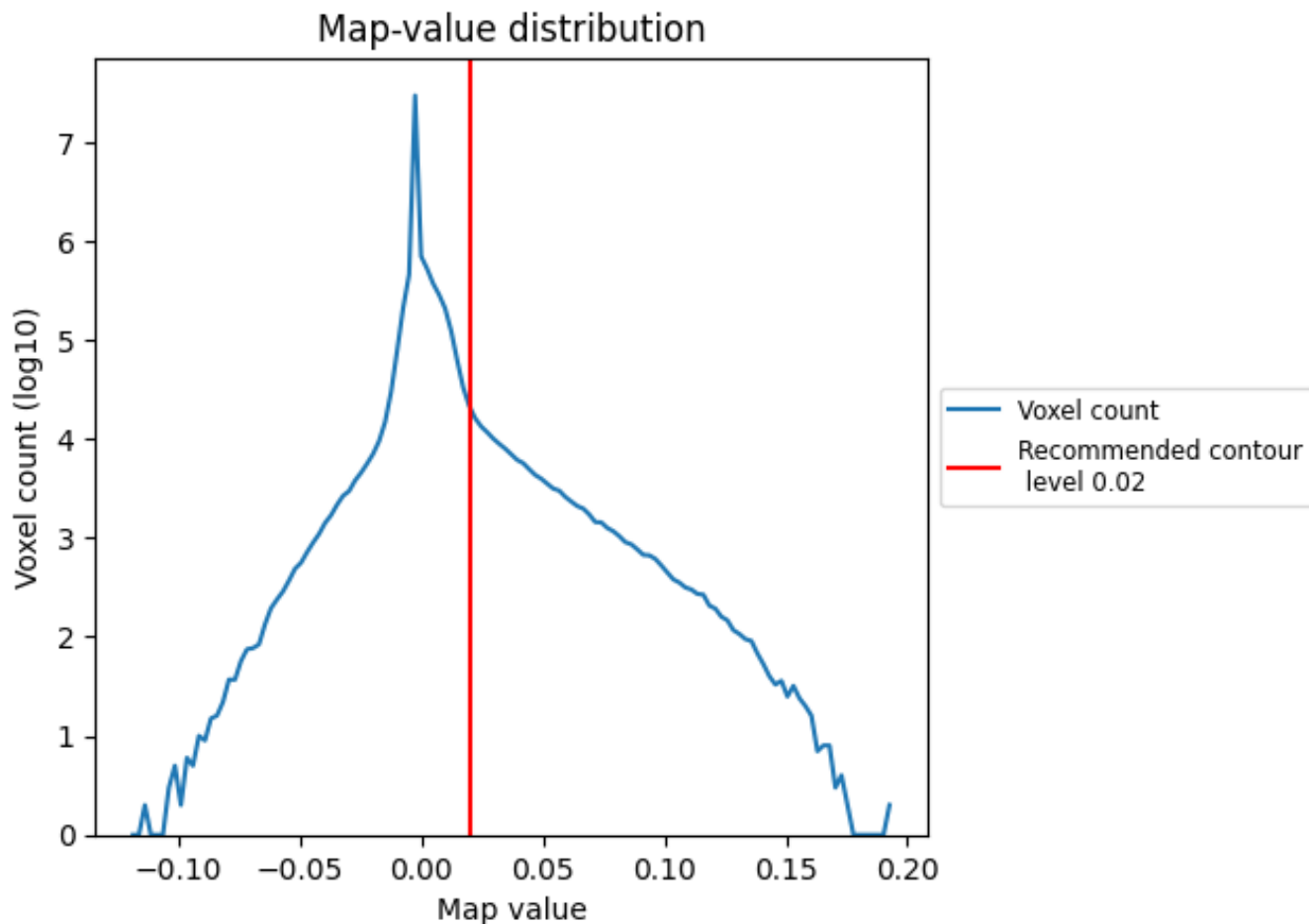
6.6 Mask visualisation

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

7 Map analysis [i](#)

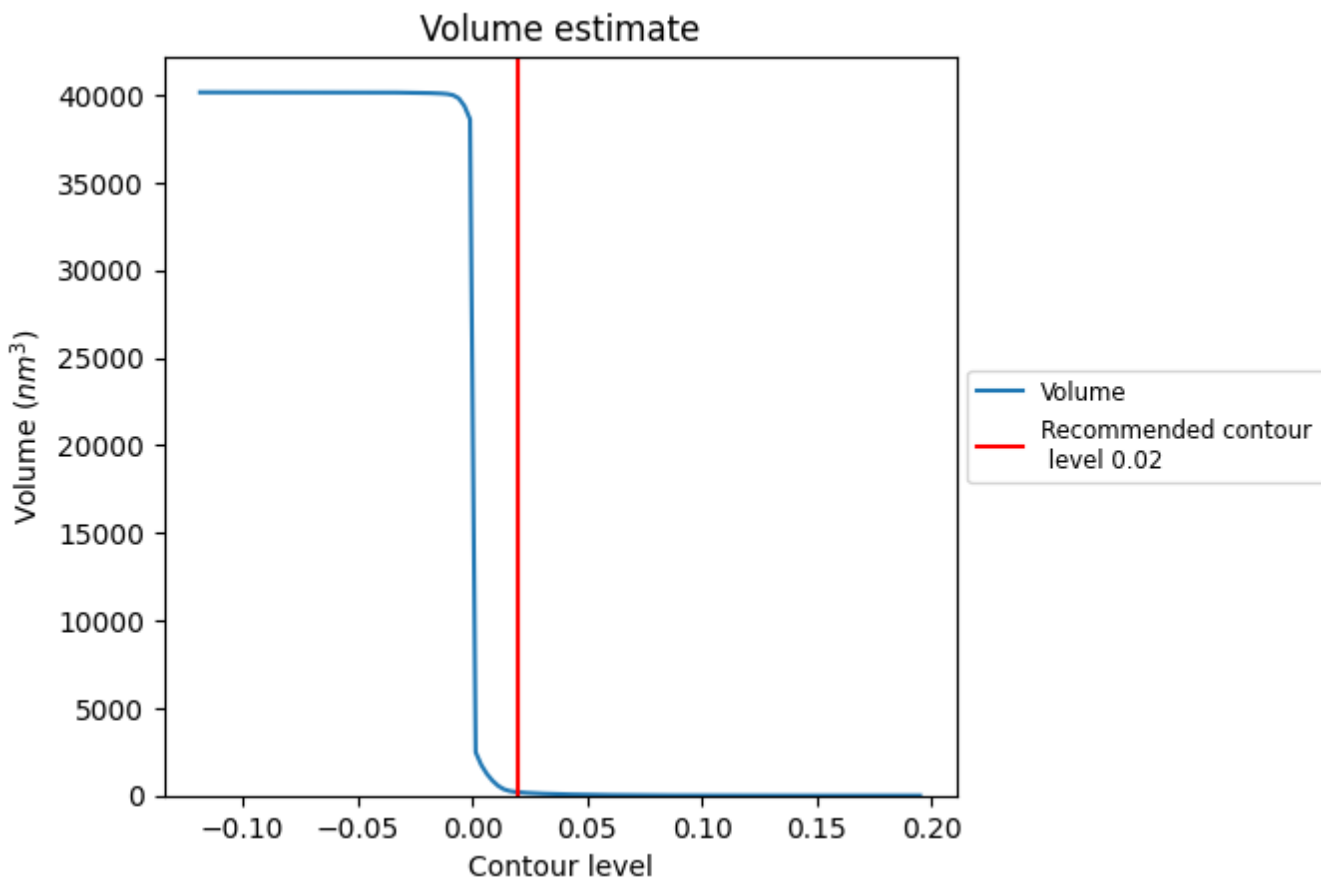
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

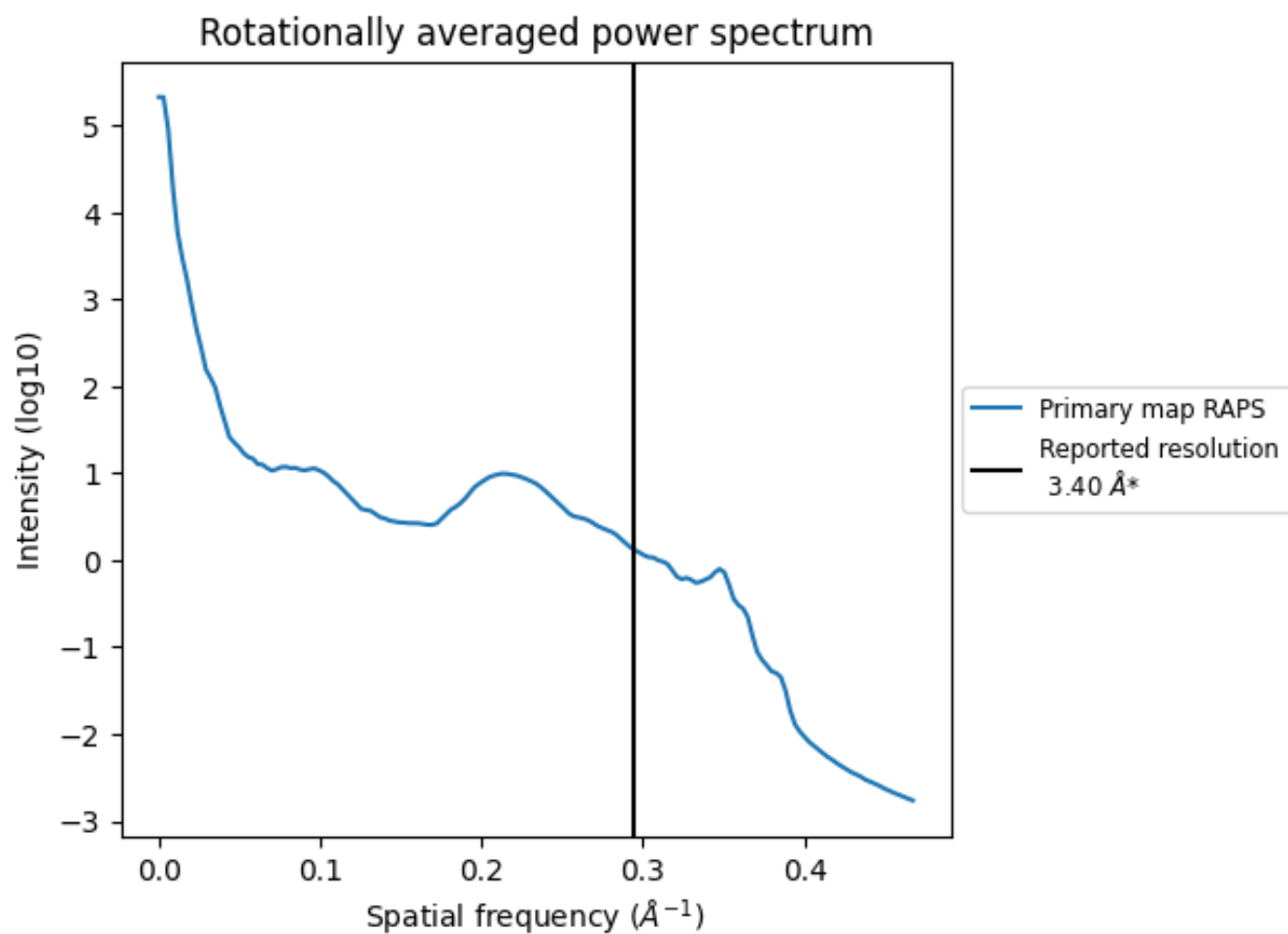
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 192 nm³; this corresponds to an approximate mass of 173 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum i



*Reported resolution corresponds to spatial frequency of 0.294 \AA^{-1}

8 Fourier-Shell correlation

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

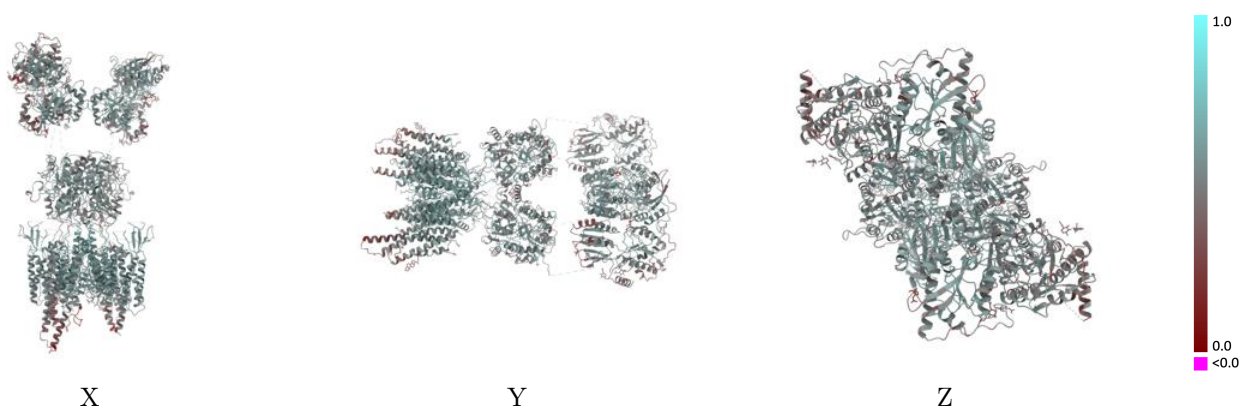
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-12802 and PDB model 7OCA. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay [i](#)

This section was not generated.

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

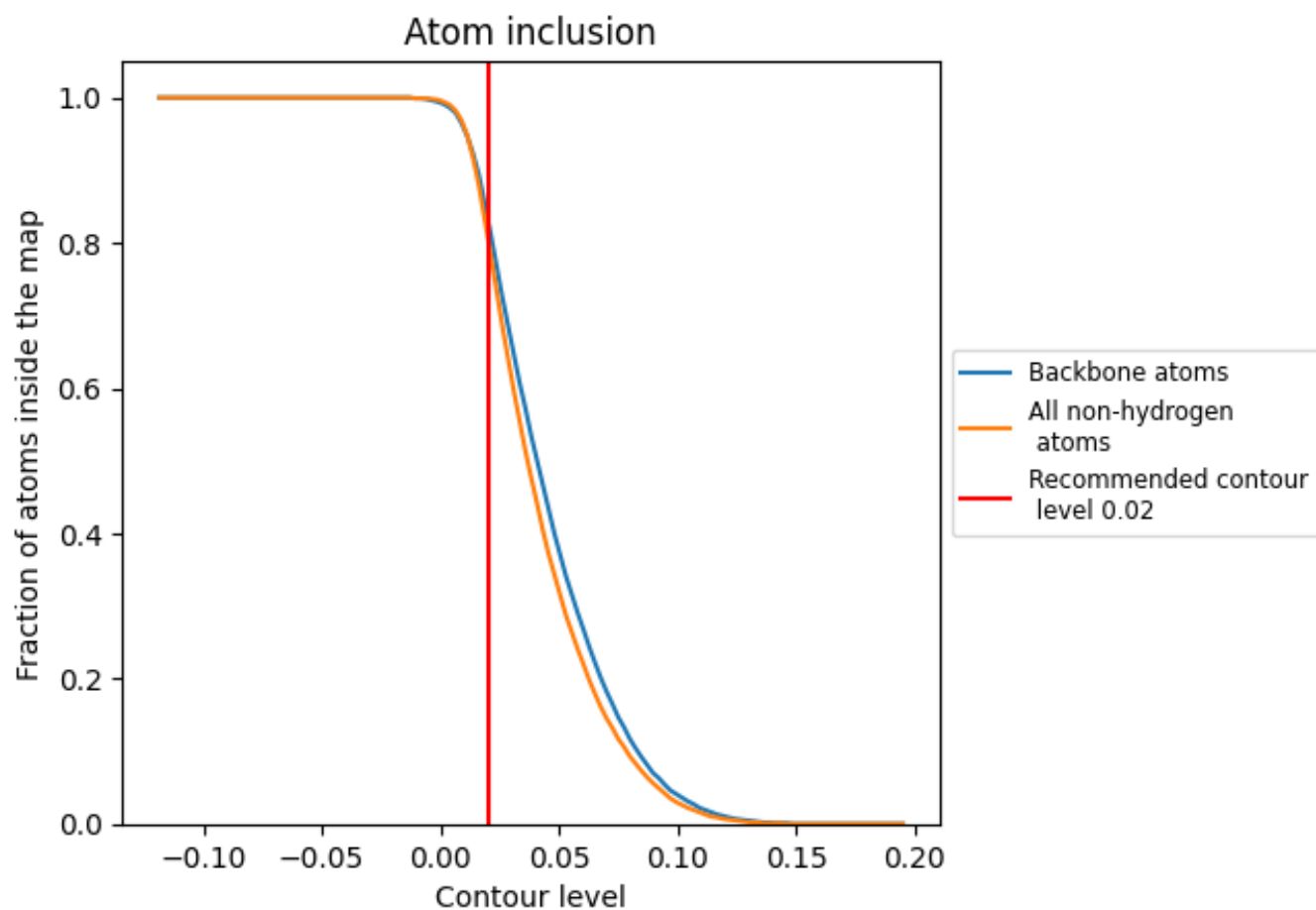


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.































9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 81% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8080	 0.5250
A	 0.8130	 0.5170
B	 0.8630	 0.5460
C	 0.8160	 0.5180
D	 0.8620	 0.5460
E	 0.5500	 0.4560
F	 0.2050	 0.3300
G	 0.5420	 0.4530
H	 0.4290	 0.3870
I	 0.8230	 0.5490
J	 0.8180	 0.5470
K	 0.7140	 0.4350
L	 0.6790	 0.4400
M	 0.2050	 0.3050
N	 0.3570	 0.4080

