



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 02:48 AM UTC

PDB ID : 1M56 / pdb_00001m56
Title : Structure of cytochrome c oxidase from Rhodobactor sphaeroides (Wild Type)
Authors : Svensson-Ek, M.; Abramson, J.; Larsson, G.; Tornroth, S.; Brezezinski, P.; Iwata, S.
Deposited on : 2002-07-08
Resolution : 2.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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A user guide is available at

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

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:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

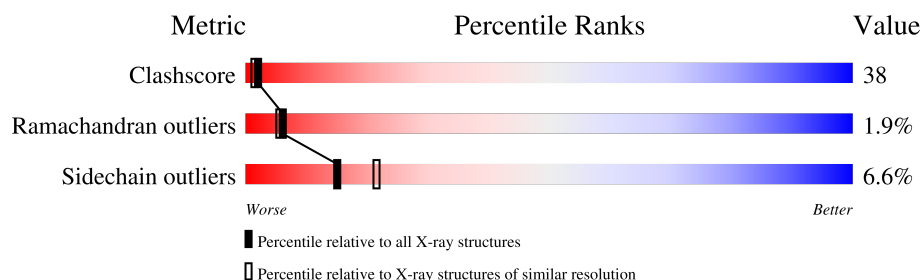
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	566	28% 45% 20% . .
1	G	566	29% 44% 20% . .
2	B	264	36% 46% 15% . .
2	H	264	37% 41% 19% . .
3	C	266	39% 46% 12% .
3	I	266	37% 48% 14% .
4	D	51	41% 24% 14% . 18%
4	J	51	27% 41% 10% . 18%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	3PE	C	2013	-	-	X	-
9	3PE	D	2011	-	-	X	-
9	3PE	I	3010	-	-	X	-
9	3PE	I	3013	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 18934 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 CYTOCHROME C OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	547	Total	C	N	O	S	0	0	0
			4322	2892	684	715	31			
1	G	547	Total	C	N	O	S	0	0	0
			4322	2892	684	715	31			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	436	ILE	SER	SEE REMARK 999	UNP P33517
A	437	TYR	THR	SEE REMARK 999	UNP P33517
A	438	PHE	SER	SEE REMARK 999	UNP P33517
A	439	TRP	GLY	SEE REMARK 999	UNP P33517
A	518	THR	SER	SEE REMARK 999	UNP P33517
A	520	THR	SER	SEE REMARK 999	UNP P33517
A	521	ARG	-	SEE REMARK 999	UNP P33517
G	436	ILE	SER	SEE REMARK 999	UNP P33517
G	437	TYR	THR	SEE REMARK 999	UNP P33517
G	438	PHE	SER	SEE REMARK 999	UNP P33517
G	439	TRP	GLY	SEE REMARK 999	UNP P33517
G	518	THR	SER	SEE REMARK 999	UNP P33517
G	520	THR	SER	SEE REMARK 999	UNP P33517
G	521	ARG	-	SEE REMARK 999	UNP P33517

- Molecule 2 is a protein called CYTOCHROME C OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	260	Total	C	N	O	S	0	0	0
			2046	1334	332	374	6			
2	H	260	Total	C	N	O	S	0	0	0
			2046	1334	332	374	6			

- Molecule 3 is a protein called CYTOCHROME C OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	265	Total	C	N	O	S	0	0	0
			2139	1448	342	337	12			
3	I	265	Total	C	N	O	S	0	0	0
			2139	1448	342	337	12			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	30	PHE	ASN	SEE REMARK 999	UNP P84153
C	92	MET	ILE	SEE REMARK 999	UNP P84153
C	244	ILE	MET	SEE REMARK 999	UNP P84153
I	30	PHE	ASN	SEE REMARK 999	UNP P84153
I	92	MET	ILE	SEE REMARK 999	UNP P84153
I	244	ILE	MET	SEE REMARK 999	UNP P84153

- Molecule 4 is a protein called CYTOCHROME C OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	42	Total	C	N	O	S	0	0	0
			311	203	52	54	2			
4	J	42	Total	C	N	O	S	0	0	0
			311	203	52	54	2			

- Molecule 5 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Cu	0	0
			1	1		
5	B	2	Total	Cu	0	0
			2	2		
5	G	1	Total	Cu	0	0
			1	1		
5	H	2	Total	Cu	0	0
			2	2		

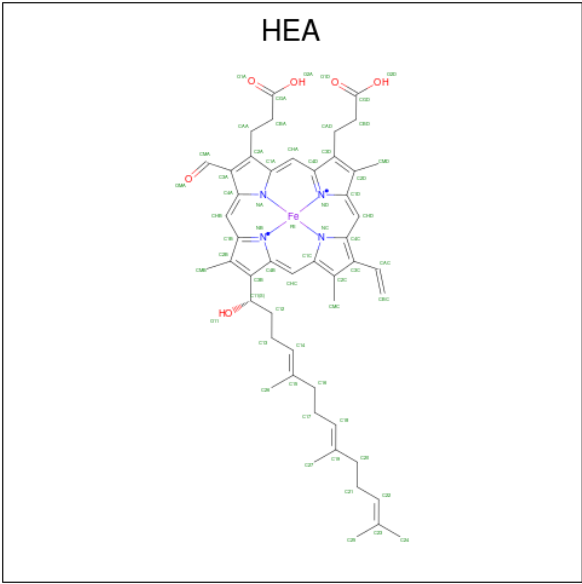
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mg	0	0
			1	1		
6	G	1	Total	Mg	0	0
			1	1		

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

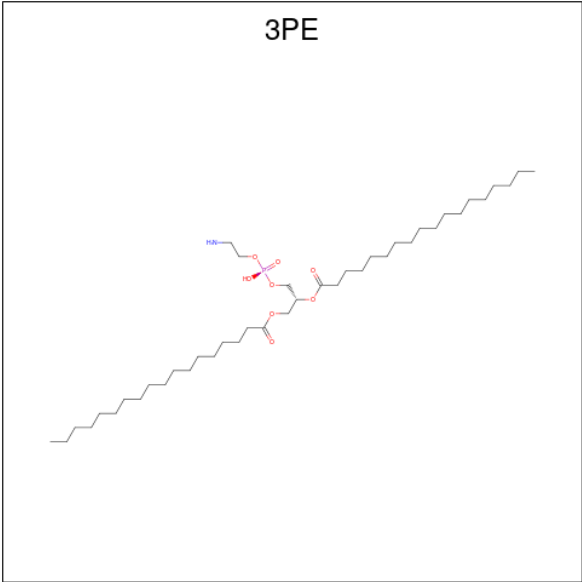
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		
7	G	1	Total	Ca	0	0
			1	1		

- Molecule 8 is HEME-A (CCD ID: HEA) (formula: C₄₉H₅₆FeN₄O₆).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
8	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
8	G	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
8	G	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		

- Molecule 9 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: C₄₁H₈₂NO₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	A	1	Total	C	N	O	P	0	0
			51	41	1	8	1		
9	A	1	Total	C	N	O	P	0	0
			51	41	1	8	1		
9	C	1	Total	C	N	O	P	0	0
			51	41	1	8	1		
9	C	1	Total	C	N	O	P	0	0
			51	41	1	8	1		
9	C	1	Total	C	N	O	P	0	0
			51	41	1	8	1		
9	D	1	Total	C	N	O	P	0	0
			51	41	1	8	1		
9	G	1	Total	C	N	O	P	0	0
			51	41	1	8	1		
9	G	1	Total	C	N	O	P	0	0
			51	41	1	8	1		
9	I	1	Total	C	N	O	P	0	0
			51	41	1	8	1		
9	I	1	Total	C	N	O	P	0	0
			51	41	1	8	1		
9	I	1	Total	C	N	O	P	0	0
			51	41	1	8	1		
9	J	1	Total	C	N	O	P	0	0
			51	41	1	8	1		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	101	Total 101	O 101	0	0
10	B	68	Total 68	O 68	0	0
10	C	39	Total 39	O 39	0	0
10	D	12	Total 12	O 12	0	0
10	G	106	Total 106	O 106	0	0
10	H	64	Total 64	O 64	0	0
10	I	38	Total 38	O 38	0	0
10	J	8	Total 8	O 8	0	0

3 Residue-property plots

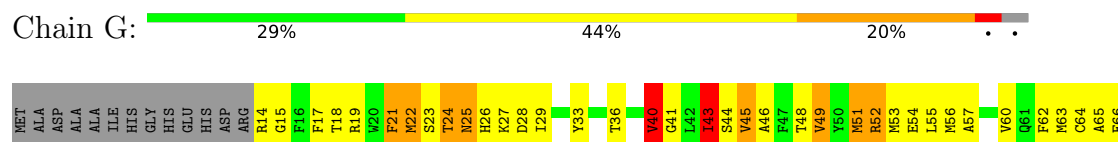
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

• Molecule 1: CYTOCHROME C OXIDASE



• Molecule 1: CYTOCHROME C OXIDASE

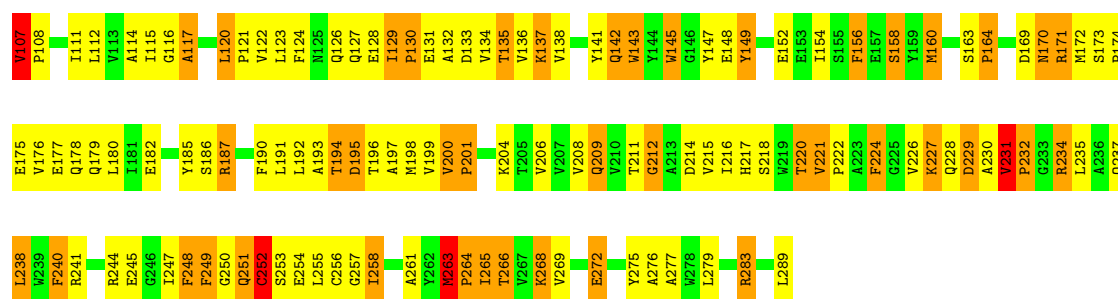




A230	G162	P99	GLN
V231	S163	L100	GLN
P232	P164	E101	GLN
G233	A165	I102	SER
R234		A103	L30
L235	D169	W104	
A236	N170	I105	G34
Q237	R171	I106	R35
L238	M172	V107	P36
W239	S173	P108	Q37
F240	P174	I109	P38
R241	E175		
E245	V176	W113	T41
G246	E177	I114	G42
I247	Q178	I115	F43
F248	Q179	G116	
F249	L180	A117	S48
	I181	F118	P49
Q250	E182	S119	
G251		L120	T52
C252	Y185	P121	
S253	S186	V122	H55
E254	L187	L123	W56
L255		F124	L57
C256	F190	M125	D58
G257	L191	Q126	G59
L258	L192	Q127	F60
S259	A193	I128	I61
H260	L194	I129	L62
A261	D195	P130	
V262	T196	E131	I65
M263	A197	A132	A66
P264	M198	D133	A67
L265	V199	V134	I68
T266	V200	T135	T69
V267	P201	V136	I70
K268	V202	K137	F71
V269			V72
A276	V207	G140	T73
A277	V208	Y141	L74
Q277	G209	Q142	L75
W278	V210	R143	I76
L279	T211	Y144	L77
	G212	W145	Y78
	A213	G146	A79
R283	D214	Y147	V80
		E148	W81
L289	H217	Y149	R82
	S218	P150	F83
	W219	D151	H84
	T220	E152	E85
	V221	E153	K86
	P222	I154	R87
	A223	S155	N88
	G224	F156	K89
	F225	E157	V90
	V226	S158	
	K227	Y159	T95
	Q228	W160	S98
	P230	T161	

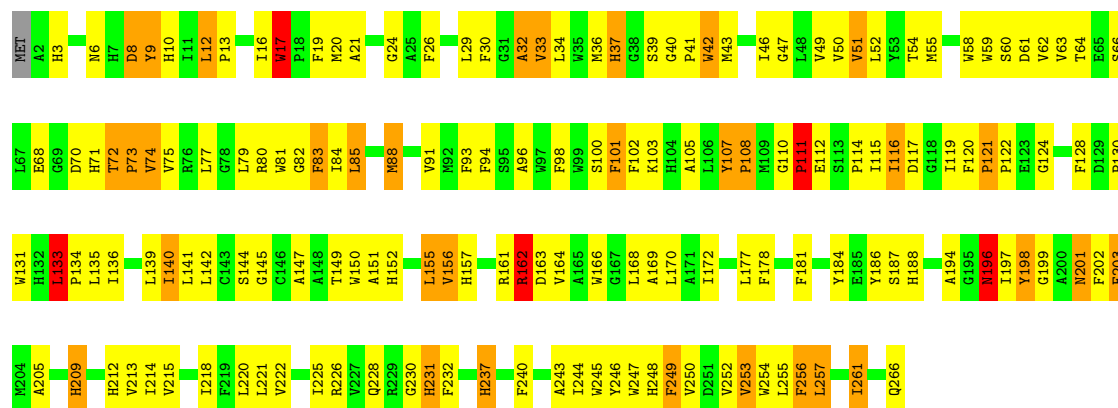
- Molecule 2: CYTOCHROME C OXIDASE

GLN	GLN	GLN	SER	L30		R35		T41	G42	F43	Q44	P45		S48		H55	W56	L57		F60	I61	L62		I65	A66	A67	I68	T69	I70	V71	V72	T73	L74	L75	I76	L77	V78	A79	V80		F83	H84	E85	K86	R87	N88	K89	V90		N97	S98	P99	L100	E101		W104	T105	I106
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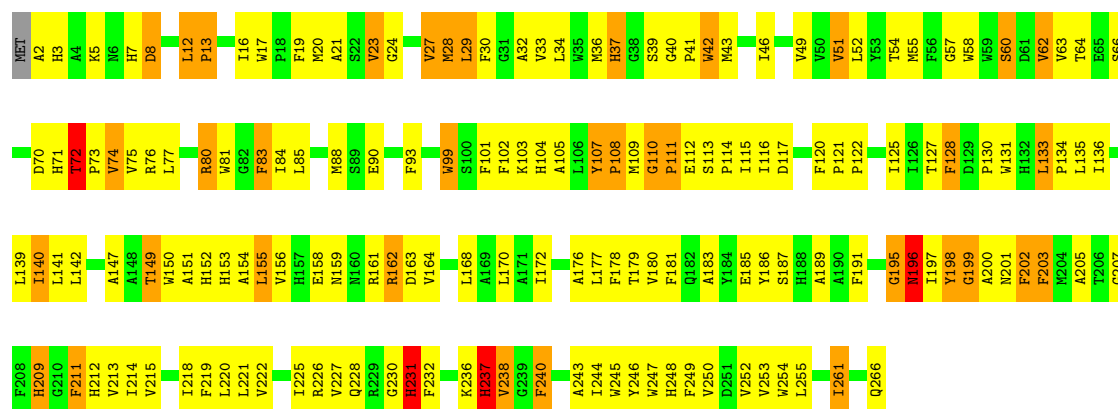
• Molecule 3: CYTOCHROME C OXIDASE

Chain C: 39% 46% 12%



• Molecule 3: CYTOCHROME C OXIDASE

Chain I: 37% 48% 14%



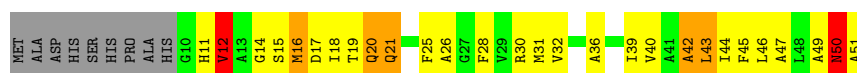
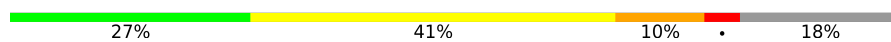
• Molecule 4: CYTOCHROME C OXIDASE

Chain D: 41% 24% 14% 18%



• Molecule 4: CYTOCHROME C OXIDASE

Chain J:



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	340.36 Å 340.36 Å 89.67 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (40.00-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.236 , 0.275	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	18934	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 3PE, HEA, MG, CU, CA

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	0.91	5/4482 (0.1%)	2.42	289/6114 (4.7%)
1	G	0.91	3/4482 (0.1%)	2.37	256/6114 (4.2%)
2	B	0.74	0/2105	2.16	83/2879 (2.9%)
2	H	0.74	0/2105	2.17	102/2879 (3.5%)
3	C	0.65	0/2232	1.93	78/3054 (2.6%)
3	I	0.69	0/2232	2.00	77/3054 (2.5%)
4	D	0.67	0/316	2.09	13/428 (3.0%)
4	J	0.68	0/316	2.09	15/428 (3.5%)
All	All	0.81	8/18270 (0.0%)	2.23	913/24950 (3.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	12
1	G	0	15
2	B	0	6
2	H	0	5
3	C	0	3
3	I	0	2
4	D	0	1
All	All	0	44

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	543	THR	C-O	7.80	1.34	1.23
1	G	544	SER	N-CA	-7.28	1.35	1.46
1	A	544	SER	N-CA	-7.23	1.35	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	543	THR	CA-C	-6.42	1.44	1.53
1	G	543	THR	CA-C	-6.16	1.44	1.53

The worst 5 of 913 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	543	THR	CA-C-N	21.62	174.56	121.80
1	G	543	THR	C-N-CA	21.62	174.56	121.80
1	A	420	PHE	CA-CB-CG	19.87	133.67	113.80
1	G	420	PHE	CA-CB-CG	19.21	133.01	113.80
1	G	333	HIS	CA-CB-CG	17.59	131.38	113.80

There are no chirality outliers.

5 of 44 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	108	PHE	Mainchain
1	A	112	ILE	Mainchain
1	A	157	LEU	Mainchain
1	A	202	ILE	Mainchain
1	A	257	ARG	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4322	0	4238	349	0
1	G	4322	0	4238	353	0
2	B	2046	0	2011	144	0
2	H	2046	0	2011	159	0
3	C	2139	0	2056	165	0
3	I	2139	0	2056	162	0
4	D	311	0	319	28	0
4	J	311	0	319	46	0
5	A	1	0	0	0	0
5	B	2	0	0	0	0
5	G	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	H	2	0	0	0	0
6	A	1	0	0	0	0
6	G	1	0	0	0	0
7	A	1	0	0	0	0
7	G	1	0	0	0	0
8	A	120	0	108	25	0
8	G	120	0	108	17	0
9	A	102	0	164	34	0
9	C	153	0	246	48	0
9	D	51	0	82	21	0
9	G	102	0	164	28	0
9	I	153	0	246	51	0
9	J	51	0	82	16	0
10	A	101	0	0	7	0
10	B	68	0	0	4	0
10	C	39	0	0	5	0
10	D	12	0	0	0	0
10	G	106	0	0	8	0
10	H	64	0	0	6	0
10	I	38	0	0	4	0
10	J	8	0	0	2	0
All	All	18934	0	18448	1397	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 38.

The worst 5 of 1397 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)
3:I:8:ASP:HB3	3:I:72:THR:HG21	1.27	1.12
1:A:520:THR:HG22	1:A:521:ARG:HG2	1.32	1.12
9:I:3013:3PE:O14	9:I:3013:3PE:H121	1.51	1.11
9:I:3013:3PE:C3H	9:I:3013:3PE:H2D2	1.78	1.11
9:C:2013:3PE:O14	9:C:2013:3PE:H121	1.48	1.06

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 X-ray entries followed by that with respect to entries of similar resolution.

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	545/566 (96%)	479 (88%)	54 (10%)	12 (2%)	5	4
1	G	545/566 (96%)	466 (86%)	67 (12%)	12 (2%)	5	4
2	B	258/264 (98%)	222 (86%)	32 (12%)	4 (2%)	7	7
2	H	258/264 (98%)	220 (85%)	33 (13%)	5 (2%)	6	5
3	C	263/266 (99%)	229 (87%)	30 (11%)	4 (2%)	8	8
3	I	263/266 (99%)	234 (89%)	25 (10%)	4 (2%)	8	8
4	D	40/51 (78%)	37 (92%)	2 (5%)	1 (2%)	4	3
4	J	40/51 (78%)	32 (80%)	7 (18%)	1 (2%)	4	3
All	All	2212/2294 (96%)	1919 (87%)	250 (11%)	43 (2%)	6	5

5 of 43 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	544	SER
3	C	111	PRO
1	G	327	GLY
1	G	544	SER
2	H	264	PRO

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	446/459 (97%)	415 (93%)	31 (7%)	14	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	446/459 (97%)	405 (91%)	41 (9%)	8	11
2	B	216/220 (98%)	202 (94%)	14 (6%)	15	22
2	H	216/220 (98%)	207 (96%)	9 (4%)	26	40
3	C	215/216 (100%)	206 (96%)	9 (4%)	26	40
3	I	215/216 (100%)	206 (96%)	9 (4%)	26	40
4	D	30/37 (81%)	26 (87%)	4 (13%)	4	4
4	J	30/37 (81%)	27 (90%)	3 (10%)	7	9
All	All	1814/1864 (97%)	1694 (93%)	120 (7%)	15	21

5 of 120 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	50	ASN
3	I	72	THR
1	G	131	PRO
3	I	60	SER
4	J	19	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	494	ASN
2	H	170	ASN
1	G	534	HIS
2	H	84	HIS
2	H	209	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 10 are monoatomic - leaving 16 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$
9	3PE	A	2012	-	50,50,50	1.60	3 (6%)	53,55,55	1.08	5 (9%)
9	3PE	I	3013	-	50,50,50	1.55	4 (8%)	53,55,55	1.09	4 (7%)
8	HEA	G	1002	1	67,67,67	1.31	10 (14%)	81,103,103	2.21	28 (34%)
9	3PE	A	2009	-	50,50,50	1.53	2 (4%)	53,55,55	1.02	3 (5%)
8	HEA	G	1001	1	67,67,67	1.21	7 (10%)	81,103,103	1.99	24 (29%)
8	HEA	A	1002	1	67,67,67	1.31	9 (13%)	81,103,103	1.92	19 (23%)
9	3PE	C	2010	-	50,50,50	1.61	3 (6%)	53,55,55	1.00	3 (5%)
8	HEA	A	1001	1	67,67,67	1.36	8 (11%)	81,103,103	2.09	21 (25%)
9	3PE	C	2013	-	50,50,50	1.60	3 (6%)	53,55,55	1.13	3 (5%)
9	3PE	D	2011	-	50,50,50	1.55	2 (4%)	53,55,55	1.29	4 (7%)
9	3PE	J	3011	-	50,50,50	1.55	2 (4%)	53,55,55	1.32	4 (7%)
9	3PE	I	3010	-	50,50,50	1.61	2 (4%)	53,55,55	0.98	3 (5%)
9	3PE	G	3012	-	50,50,50	1.59	3 (6%)	53,55,55	1.12	4 (7%)
9	3PE	G	3009	-	50,50,50	1.56	2 (4%)	53,55,55	1.02	1 (1%)
9	3PE	C	2008	-	50,50,50	1.59	2 (4%)	53,55,55	1.19	5 (9%)
9	3PE	I	3008	-	50,50,50	1.55	2 (4%)	53,55,55	1.16	4 (7%)

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
9	3PE	A	2012	-	-	23/54/54/54	-
9	3PE	I	3013	-	-	27/54/54/54	-
8	HEA	G	1002	1	-	5/36/76/76	-
9	3PE	A	2009	-	-	31/54/54/54	-
8	HEA	G	1001	1	-	13/36/76/76	-
8	HEA	A	1002	1	-	10/36/76/76	-
9	3PE	C	2010	-	-	29/54/54/54	-
8	HEA	A	1001	1	-	17/36/76/76	-
9	3PE	C	2013	-	-	27/54/54/54	-
9	3PE	D	2011	-	-	22/54/54/54	-
9	3PE	J	3011	-	-	25/54/54/54	-
9	3PE	I	3010	-	-	24/54/54/54	-
9	3PE	G	3012	-	-	24/54/54/54	-
9	3PE	G	3009	-	-	27/54/54/54	-
9	3PE	C	2008	-	-	34/54/54/54	-
9	3PE	I	3008	-	-	34/54/54/54	-

The worst 5 of 64 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	2013	3PE	O21-C21	7.68	1.56	1.34
9	C	2010	3PE	O31-C31	7.67	1.55	1.33
9	G	3009	3PE	O21-C21	7.51	1.55	1.34
9	C	2008	3PE	O31-C31	7.49	1.55	1.33
9	C	2008	3PE	O21-C21	7.49	1.55	1.34

The worst 5 of 135 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1001	HEA	C13-C14-C15	-7.31	110.89	127.62
8	A	1001	HEA	CAA-C2A-C1A	6.36	137.78	124.85
8	G	1001	HEA	C13-C14-C15	-5.66	114.68	127.62
9	J	3011	3PE	C2-O21-C21	-5.62	104.36	117.80
8	A	1002	HEA	C12-C11-C3B	5.44	120.62	112.12

There are no chirality outliers.

5 of 372 torsion outliers are listed below:

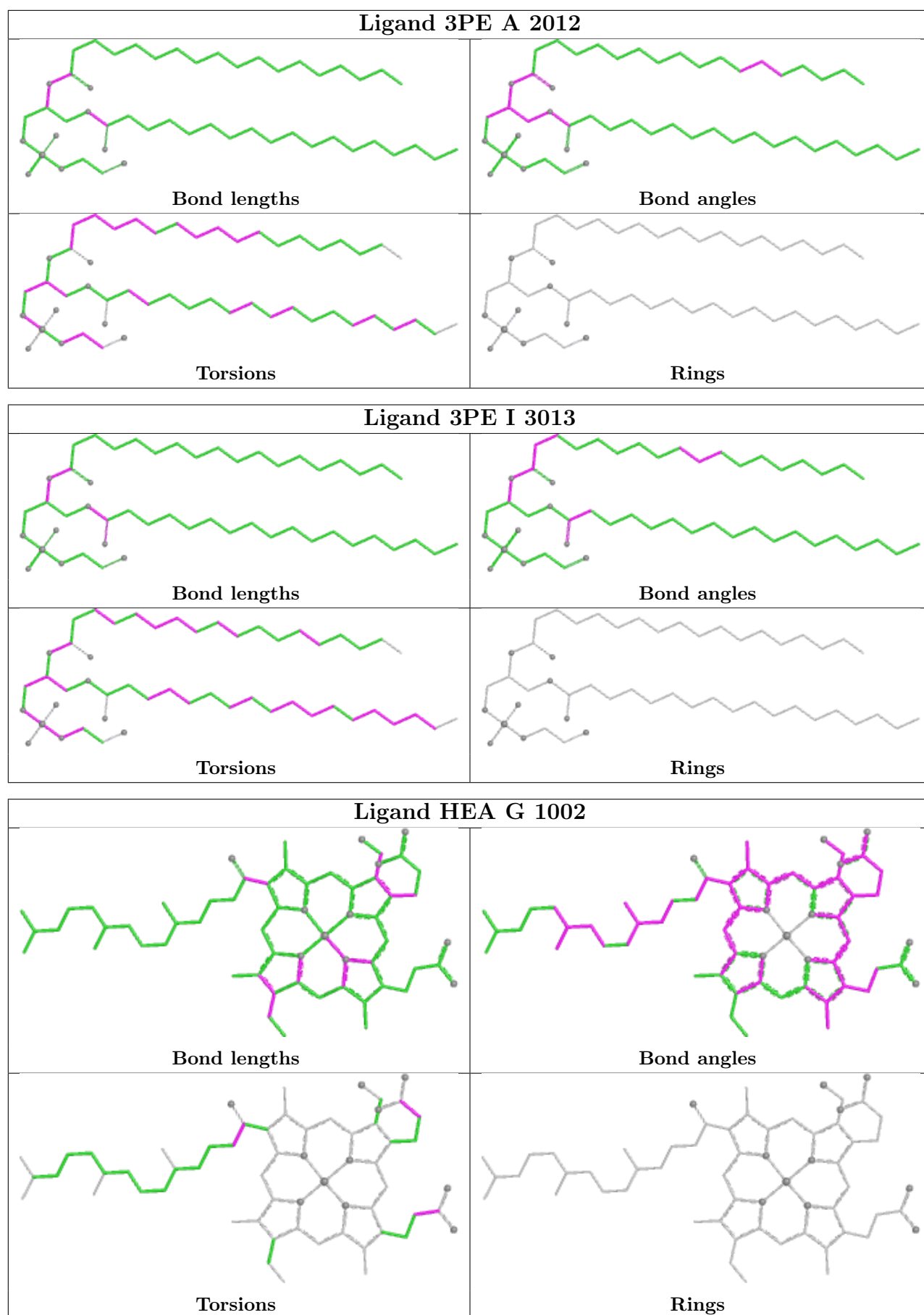
Mol	Chain	Res	Type	Atoms
8	A	1001	HEA	C2A-C3A-CMA-OMA
8	A	1001	HEA	C2C-C3C-CAC-CBC
8	A	1001	HEA	C4C-C3C-CAC-CBC
8	A	1001	HEA	C11-C12-C13-C14
8	A	1002	HEA	C2A-C3A-CMA-OMA

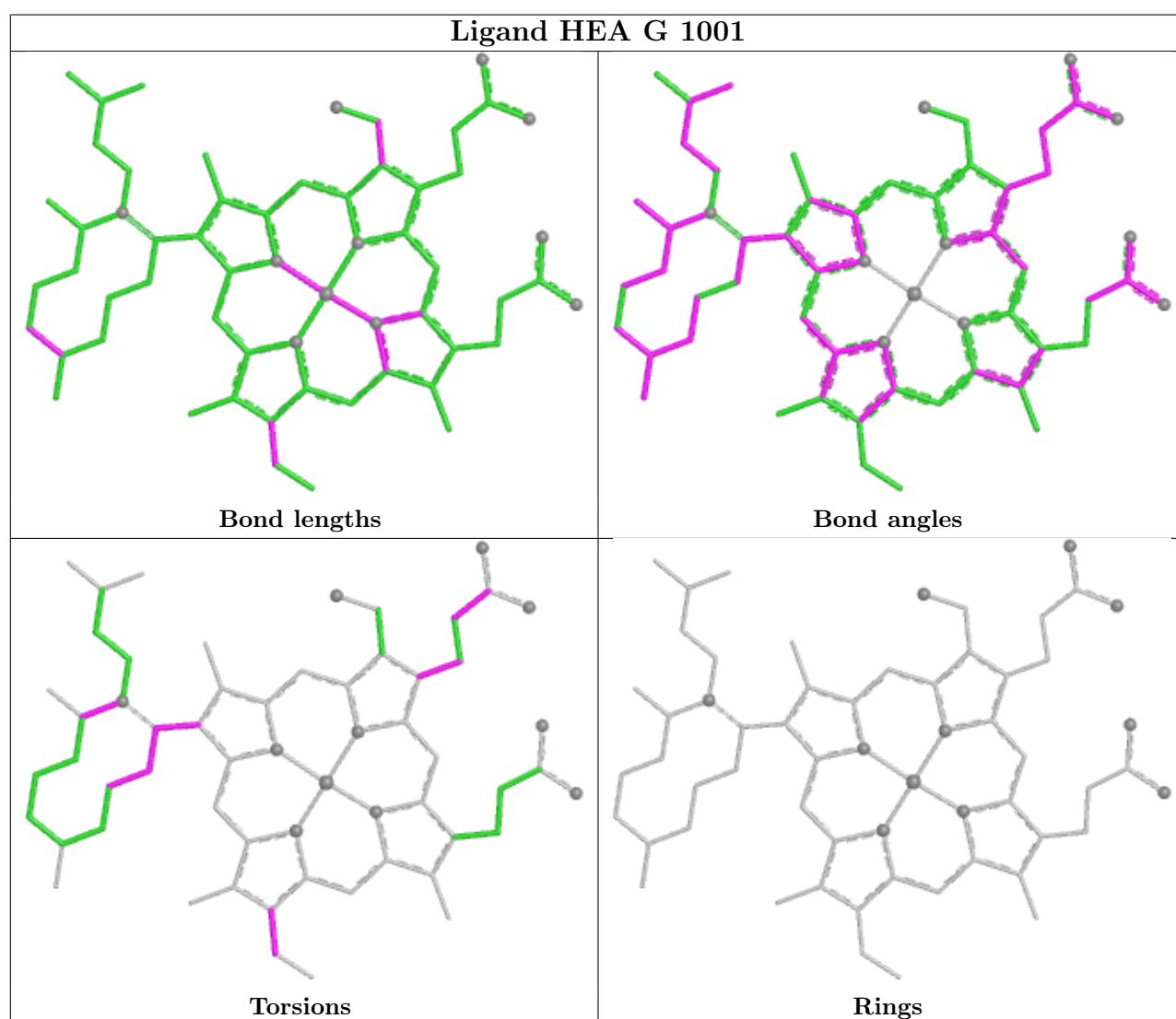
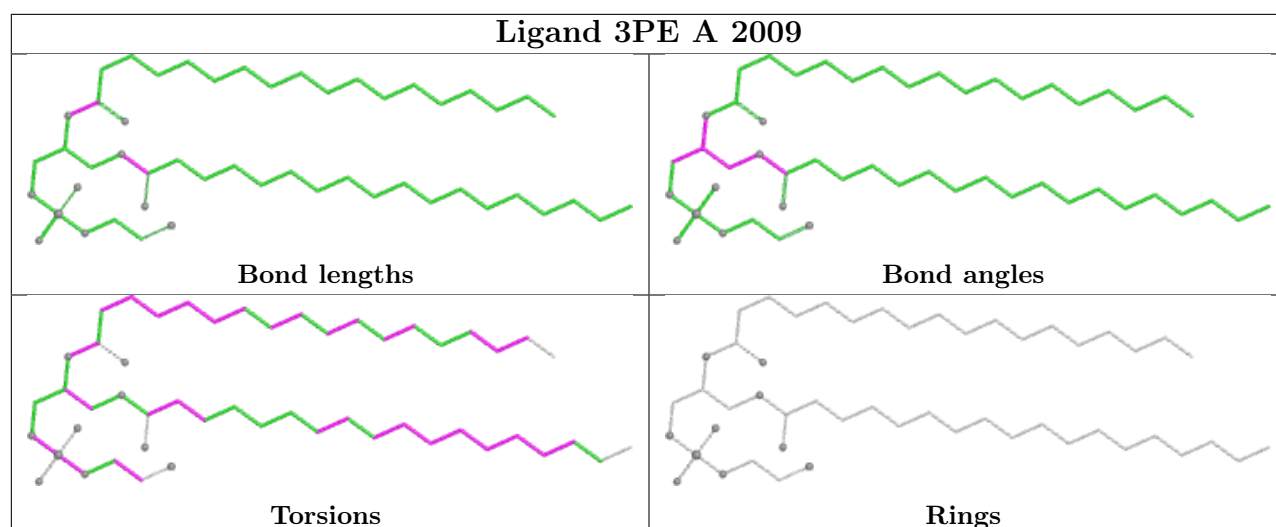
There are no ring outliers.

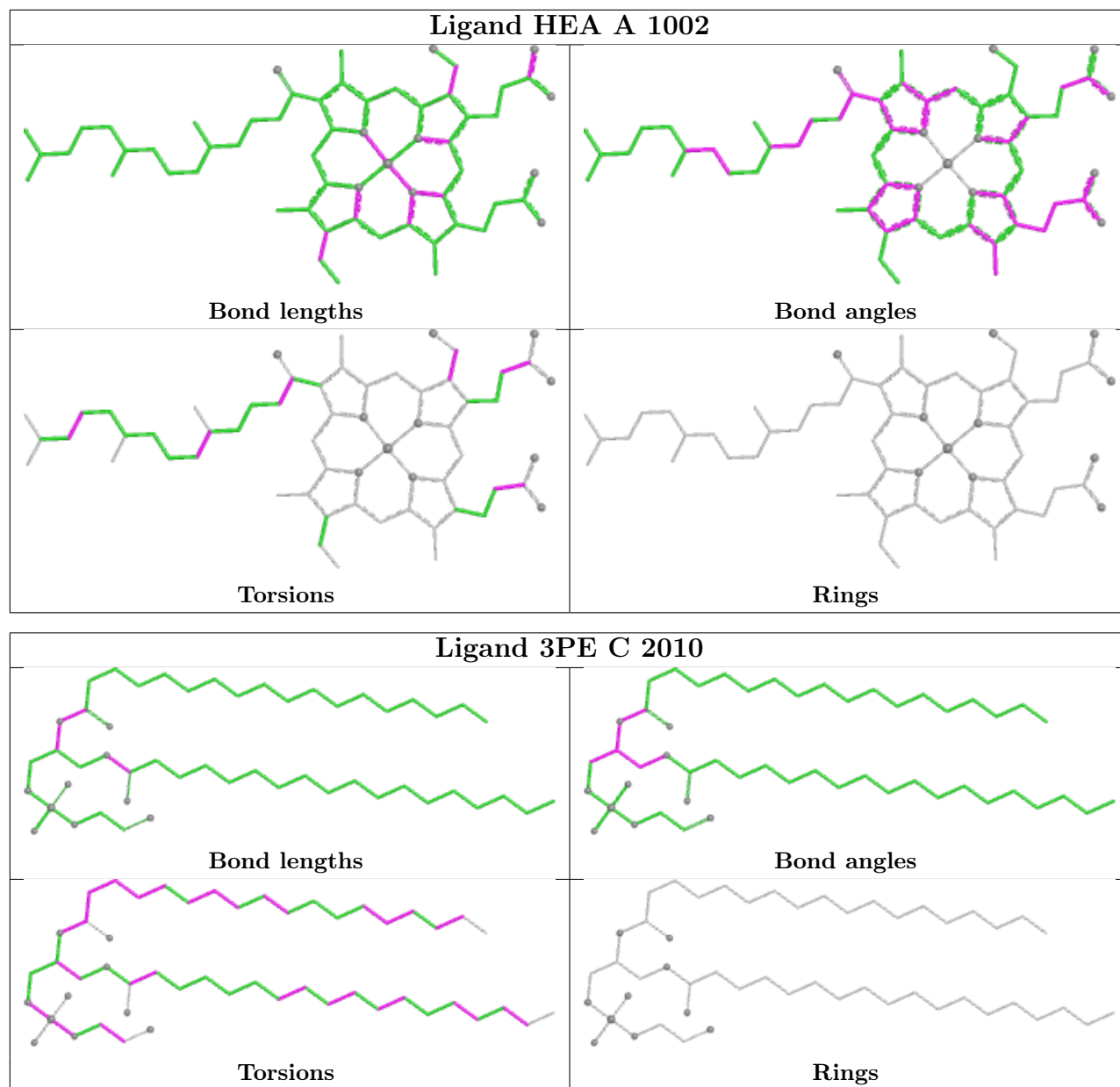
16 monomers are involved in 223 short contacts:

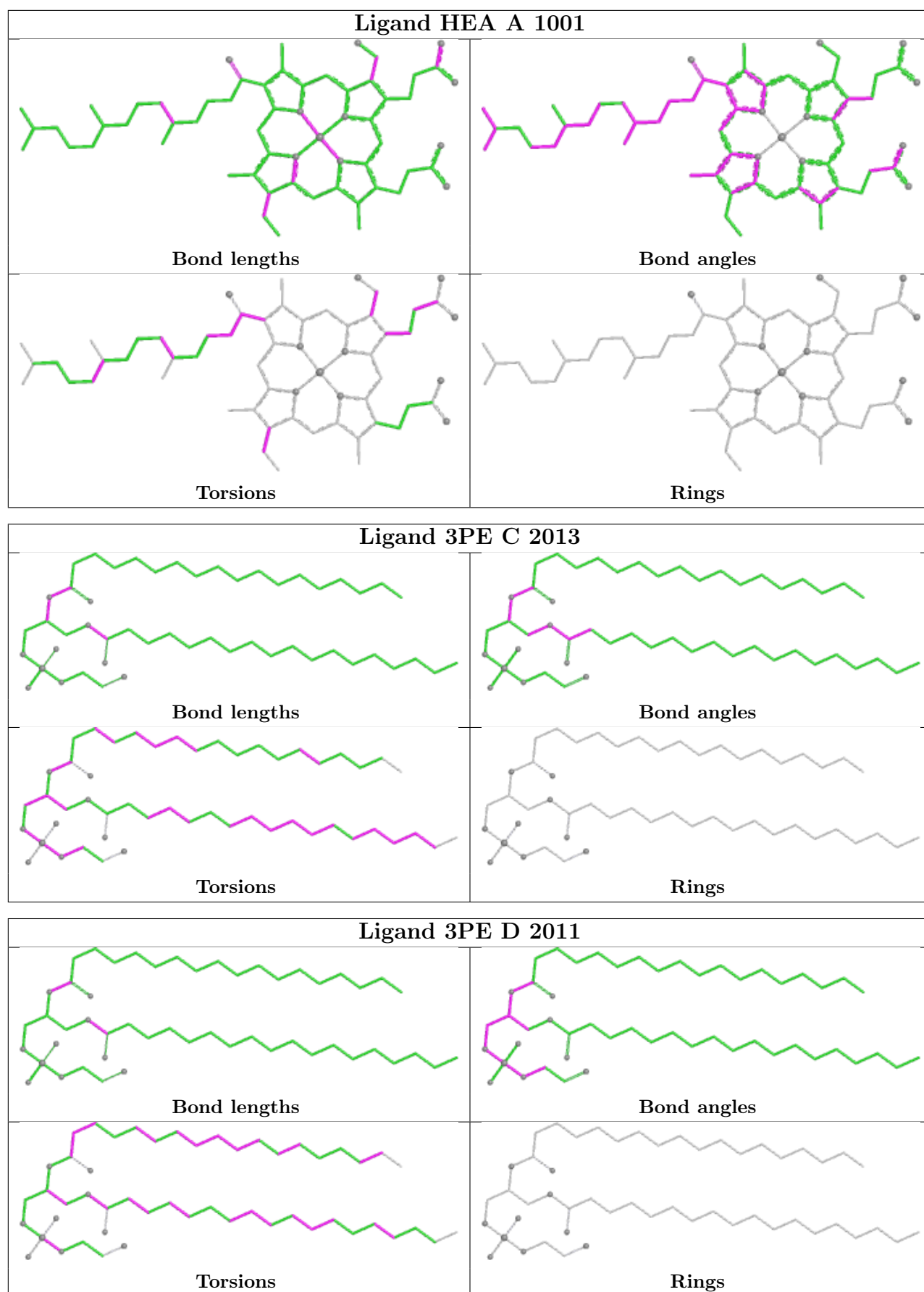
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	2012	3PE	14	0
9	I	3013	3PE	22	0
8	G	1002	HEA	7	0
9	A	2009	3PE	20	0
8	G	1001	HEA	10	0
8	A	1002	HEA	9	0
9	C	2010	3PE	20	0
8	A	1001	HEA	16	0
9	C	2013	3PE	21	0
9	D	2011	3PE	21	0
9	J	3011	3PE	16	0
9	I	3010	3PE	21	0
9	G	3012	3PE	12	0
9	G	3009	3PE	16	0
9	C	2008	3PE	7	0
9	I	3008	3PE	9	0

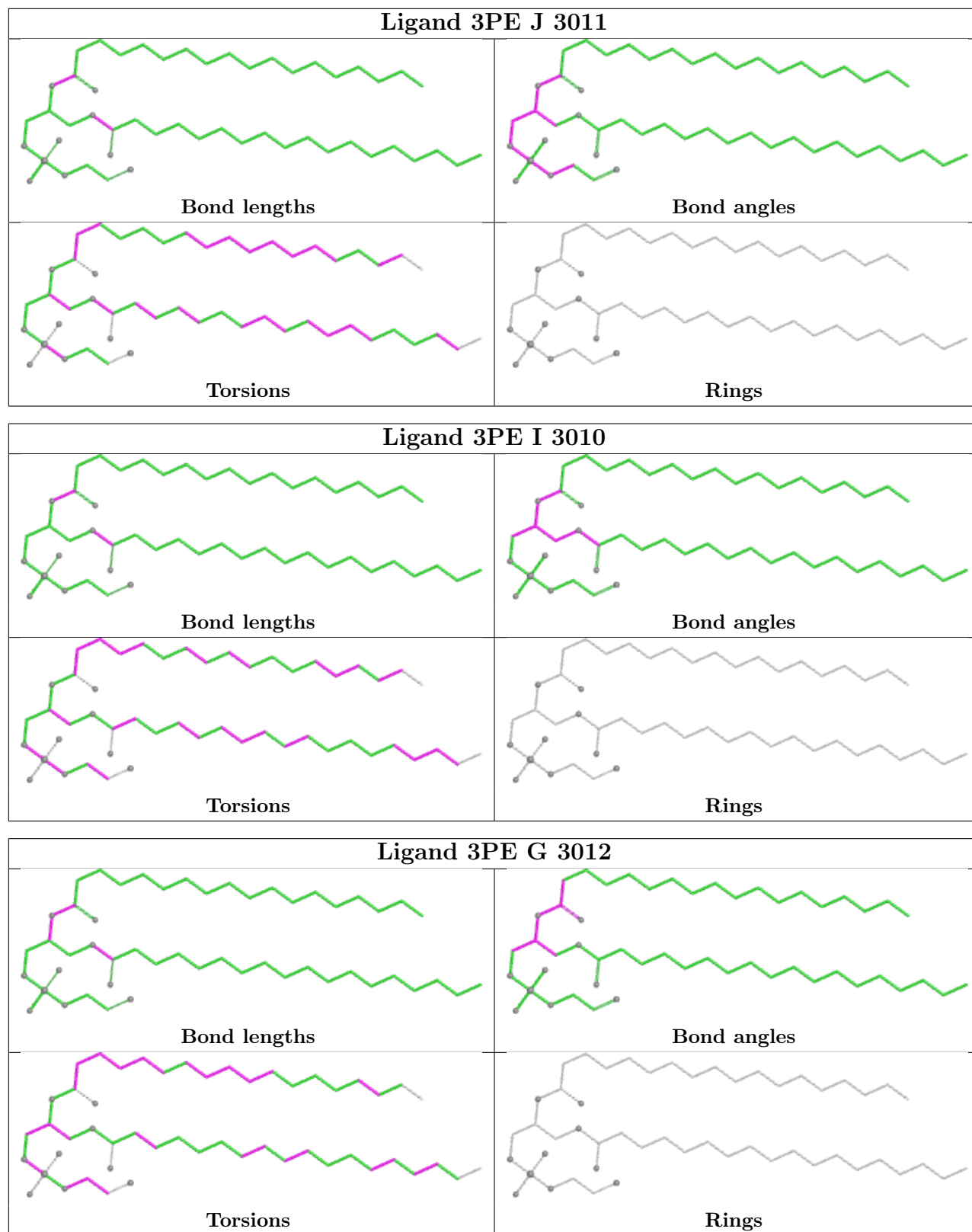
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

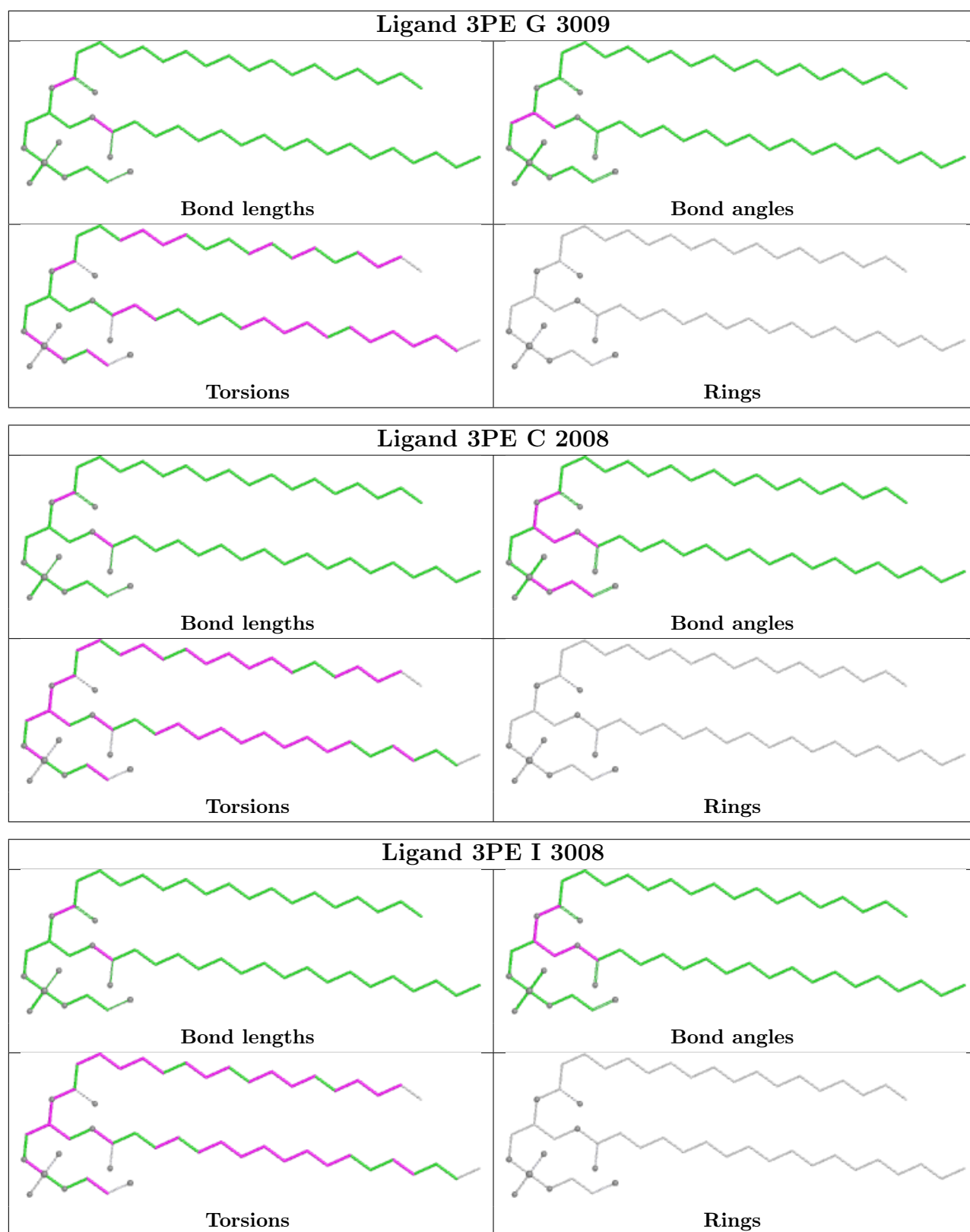












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.