



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 5, 2026 – 09:38 PM EDT

PDB ID : 1M57 / pdb_00001m57
Title : Structure of cytochrome c oxidase from Rhodobacter sphaeroides (EQ(I-286 mutant))
Authors : Svensson-Ek, M.; Abramson, J.; Larsson, G.; Tornroth, S.; Brezezinski, P.; Iwata, S.
Deposited on : 2002-07-08
Resolution : 3.00 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)	:	2.50

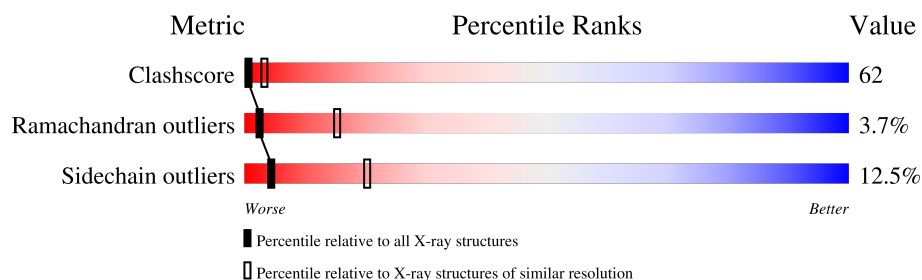
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)

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	12% 47% 32% 6% .
1	G	566	11% 43% 36% 7% .
2	B	264	23% 47% 23% 6% .
2	H	264	20% 48% 26% 5% .
3	C	266	24% 52% 20% .
3	I	266	26% 46% 24% .
4	D	51	22% 39% 22% 18%
4	J	51	20% 43% 16% . 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
8	HEA	G	1001	-	-	X	-
9	3PE	C	2010	-	-	X	-
9	3PE	C	2013	-	-	X	-
9	3PE	G	3012	-	-	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	685	714	31			
1	G	547	Total	C	N	O	S	0	0	0
			4322	2892	685	714	31			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	286	GLN	GLU	engineered mutation	UNP P33517
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	286	GLN	GLU	engineered mutation	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		

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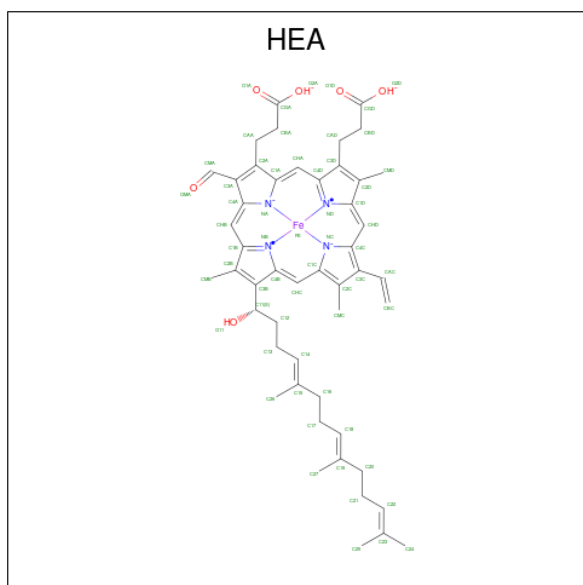
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	1	Total	Mg	0	0
			1	1		

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

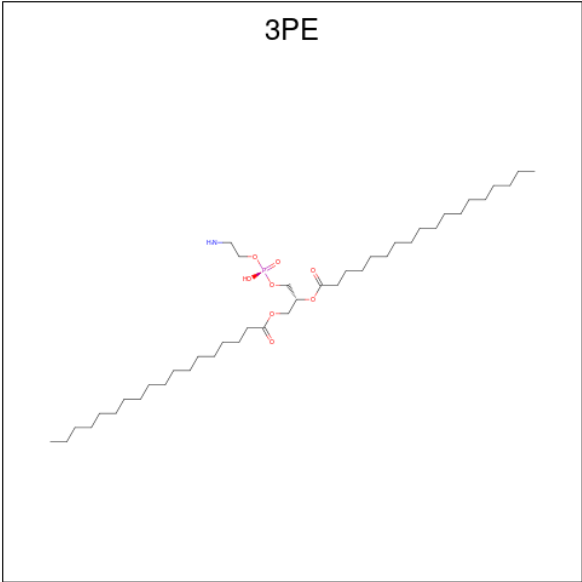
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		
7	G	1	Total	Ca	0	0
			1	1		

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



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

- 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.

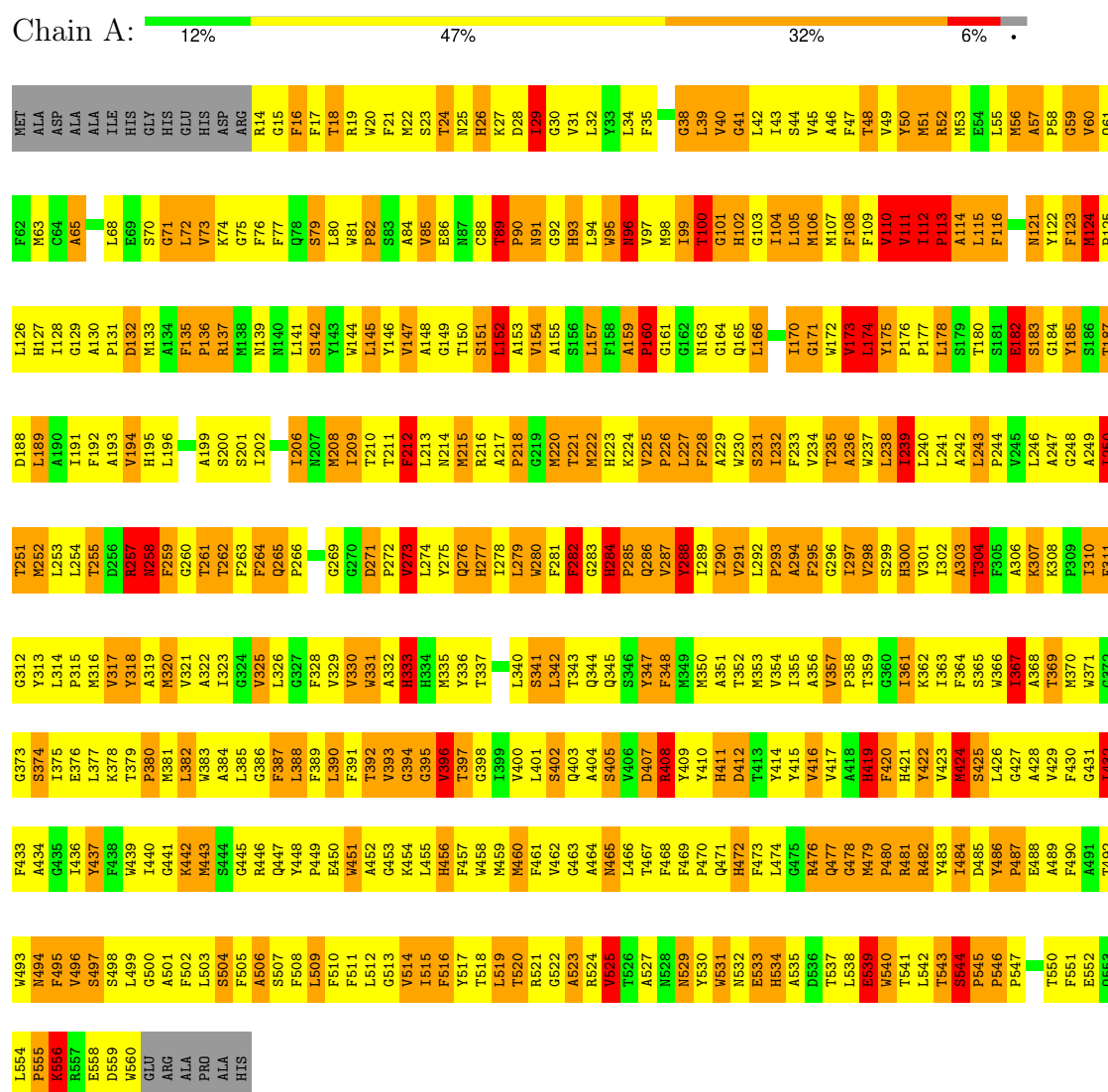
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	97	Total 97	O 97	0	0
10	B	70	Total 70	O 70	0	0
10	C	38	Total 38	O 38	0	0
10	D	13	Total 13	O 13	0	0
10	G	107	Total 107	O 107	0	0
10	H	64	Total 64	O 64	0	0
10	I	37	Total 37	O 37	0	0
10	J	10	Total 10	O 10	0	0

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



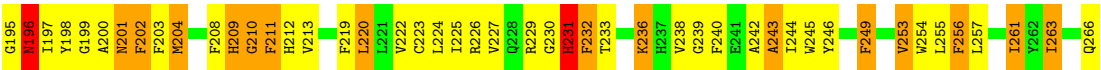
MET	Q61	F123	T187	G248	K308	M370	G431	T492	L554
ALA	P62	M124	D188	A249	P309	G373	T432	W493	P555
ASP	M63	P125	L189	I250	F311	G374	F433	W494	K556
ALA	C64	L126	A190	T251	G312	S374	A434	F495	K557
ALA	A65	H127	I191	M252	G312	I375	G435	W496	E558
ILE	E66	F128	F192	L254	Y313	E376	I436	S497	D559
HIS	H67	G129	A193	T255	L314	L377	Y437	S498	W560
GLY	L68	A130	H195	T256	P315	K378	F438	L499	GLU
HIS	P69	P131	H195	D256	M316	T379	G441	G500	ARG
GLU	S70	D132	G198	N258	V317	P380	A442	A501	ALA
HIS	G71	M133	A199	N258	Y318	M381	P443	F502	PRO
ASP	L72	D134	A199	F259	A319	L382	M443	F503	ALA
ARG	W73	F135	S200	G260	M320	H383	S444	S504	HIS
R14	K74	P136	S201	T261	V321	A384	G445	F505	
G15	G75	L137	I202	T262	A322	L385	R446	A506	
F16	F76	M138	L203	F263	I323	G386	Q447	S507	
F17	F77	M139	G204	F264	G387	F387	Y448	F508	
T18	G78	A205	Q265	Q265	V325	L388	P449	F509	
R19	S79	N140	T206	P266	L326	F389	E450	F510	
W20	L80	L141	N207	S267	G327	L390	W451	F511	
F21	W81	Y143	P208	G268	F328	F391	A452	L512	
M22	P82	M144	T209	G269	V329	T392	G453	G513	
S23	S83	L145	T210	G270	V330	V393	K454	V514	
T24	A84	Y146	T211	D271	W331	G394	L455	I515	
N25	H85	Y147	E212	P272	A332	G395	H456	F516	
H26	E86	A148	L213	V273	H333	V396	F457	Y517	
K27	N87		M214	L274	H334	T397	W458	T518	
T29	T89	L152	R216	Q276	M335	G398	M459	L519	
G30	P90		R217	H277	R236	V399	T520	F521	
V31	N91	A155	P218	L278	T337	V400	Y462	G522	
L32	G92	A156	G219	L279	S341	S402	G463	A523	
L33	H93	L157	M220	W280	L342	Q403	A464	G524	
F35	L94	F158	T221	F281	T343	A404	M465	V525	
T36	N95	A159	M222	F282	S405	S405	L466		
G37	N96	P160	H223	G283	Q345	V406	T467	N529	
G38	N97		K224	H284	S346	D407	F468	Y530	
L39	N98		V225	P285	Y347	R408	F469	M531	
V40	I99	G164	P226	Q286	F348	Y409	F470	M532	
L41	G101	Q165	L227	V287	M349	Y410	Q471	E533	
L42	H102		F228	Y288	H411	H411	H472	H534	
L43	G103	S168	A229	L289	A351	D412	F473	A535	
S44	I104	G169	W230	L290	T352	T413	L474	D536	
V45	L105	I170	S231	Y291	M353	Y414	G475	T537	
A46	M106	G171	L232	L292	V364	Y415	R476	L538	
F47	M107	W172	F233	P293	I355	V416	Q477	E539	
V48	F108	V173	V234	A294	A356	G478	G477	W540	
T49	L174	L174	T235	F295	V357	M479	M479	T541	
V49	Y175	Y175	A236	G296	P358	H419	P480	L542	
Y50	V110	P176	W237	I297	T359	F420	R481	T543	
M51	V111	P177	L238	V298	G360	H421	R482	S544	
R52	I112	L178	T239	S299	I361	Y422	Y483	P545	
M53	P113	S179	L240	H300	K362	Y423	I484	P546	
E54	A114	T180	L241	V301	L363	M424	D485	P547	
L55	L115	S181	A242	I302	S364	S425	Y486	E548	
M56	F116	E182	L243	A303	S365	L426	Y487	H549	
A57	G120	S183	P244	T304	W366	G427	E488	T550	
P58	M121	G184	V245	F305	I367	A428	A489	F551	
G59	Y122	A185	L246	A306	F368	V429	F490	E552	
V60		S186	A247	K307	T369	F430	A491	Q553	

• Molecule 2: CYTOCHROME C OXIDASE

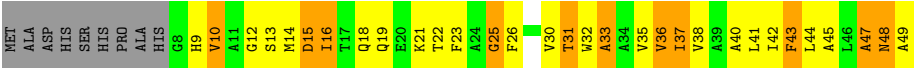
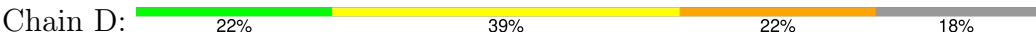
Chain B:  23% 47% 23% 6%

GLN	R87	D151	H217	W278
GLN	R88	E152	S218	L279
SER	R89	F156	W219	E280
L30	V90	T220	T220	Q281
E31	P91	S158	W221	A282
A92	R92	S159	P222	R283
R93	R93	M160	A223	
L32	L33	Y159	F224	T286
G34	G34	T161	G225	
R35	R35	S162	G226	L289
P36	P36	G162	K227	
L100	L100	P164	Q228	
Q37	Q37	A165	D229	
L503	L503	T166	A230	
G39	G39	G167	V231	
T40	T40	M104	P232	
A41	A41	D169	G233	
F43	F43	N170	R234	
Q44	Q44	R171	L235	
P45	P45	M172	A236	
S48	S48	S173	Q237	
P49	P49	E175	L238	
V110	V110	T176	W239	
L112	L112	E177	F240	
V113	V113	Q178	R241	
A51	A51	L180	A242	
T52	T52	G180	E243	
Q53	Q53	L181	R244	
H55	H55	S186	E245	
F118	F118	R187	G246	
L61	L61	D188	L247	
S119	S119	E189	F248	
L120	L120	F190	F249	
F60	F60	L121	G250	
I61	I61	L122	Q251	
F124	F124	L123	C252	
L62	L62	N125	S253	
V63	V63	I193	E254	
I64	I64	T194	L255	
L65	L65	D195	C256	
A66	A66	T196	G257	
A67	A67	M198	L258	
I68	I68	V199	S259	
T69	T69	W200	H260	
L70	L70	P201	A261	
F71	F71	T135	Y262	
V72	V72	M203	M263	
T73	T73	K204	P264	
L74	L74	T205	L265	
W138	W138	V206	T266	
L76	L76	V207	V267	
L77	L77	V208	K268	
Y141	Y141	Q142	W269	
Q142	Q142	V143	Q209	
V143	V143	W210	V270	
A79	A79	T211	S271	
V80	V80	G145	E272	
W81	W81	Y147	Y275	
E548	E548	E148	A276	
F83	F83	E55	A277	
H84	H84	V215		
R84	R84	I216		
K66	K66	P150		

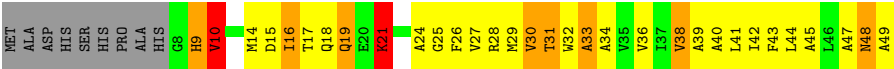
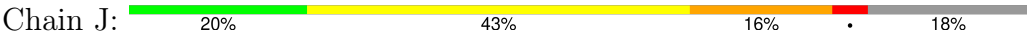
• Molecule 2: CYTOCHROME C OXIDASE



• Molecule 4: CYTOCHROME C OXIDASE



• Molecule 4: CYTOCHROME C OXIDASE



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	340.72 Å 340.72 Å 89.76 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	4.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (4.00-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.293 , 0.329	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	18934	wwPDB-VP
Average B, all atoms (Å ²)	26.0	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: HEA, MG, CA, CU, 3PE

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	0.90	2/4482 (0.0%)	2.58	345/6114 (5.6%)
1	G	0.94	4/4482 (0.1%)	2.62	381/6114 (6.2%)
2	B	0.75	0/2105	2.46	149/2879 (5.2%)
2	H	0.83	0/2105	2.52	159/2879 (5.5%)
3	C	0.68	0/2232	2.10	107/3054 (3.5%)
3	I	0.71	0/2232	2.11	104/3054 (3.4%)
4	D	0.70	0/316	2.15	15/428 (3.5%)
4	J	0.70	0/316	2.21	13/428 (3.0%)
All	All	0.83	6/18270 (0.0%)	2.45	1273/24950 (5.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	19
1	G	0	16
2	B	0	6
2	H	0	3
3	C	0	5
3	I	0	7
4	D	0	1
All	All	0	57

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	112	ILE	N-CA	8.07	1.56	1.46
1	A	111	VAL	C-N	-6.89	1.25	1.33
1	G	543	THR	C-N	-6.24	1.24	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	171	GLY	C-N	5.64	1.41	1.33
1	G	277	HIS	CE1-NE2	5.25	1.37	1.32

The worst 5 of 1273 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	543	THR	CA-C-N	26.72	169.80	121.70
1	A	543	THR	C-N-CA	26.72	169.80	121.70
1	G	543	THR	CA-C-N	22.95	163.02	121.70
1	G	543	THR	C-N-CA	22.95	163.02	121.70
1	G	170	ILE	CB-CA-C	-16.65	96.23	111.05

There are no chirality outliers.

5 of 57 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	108	PHE	Mainchain
1	A	112	ILE	Mainchain
1	A	114	ALA	Mainchain
1	A	29	ILE	Mainchain
1	A	96	ASN	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	4240	650	0
1	G	4322	0	4240	657	0
2	B	2046	0	2011	232	0
2	H	2046	0	2011	247	0
3	C	2139	0	2056	242	0
3	I	2139	0	2056	233	0
4	D	311	0	319	34	0
4	J	311	0	319	42	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	37	0
8	G	120	0	108	38	0
9	A	102	0	164	38	0
9	C	153	0	246	56	0
9	D	51	0	82	17	0
9	G	102	0	164	42	0
9	I	153	0	246	59	0
9	J	51	0	82	12	0
10	A	97	0	0	27	0
10	B	70	0	0	20	0
10	C	38	0	0	8	0
10	D	13	0	0	0	0
10	G	107	0	0	30	0
10	H	64	0	0	18	0
10	I	37	0	0	7	0
10	J	10	0	0	1	0
All	All	18934	0	18452	2278	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 62.

The worst 5 of 2278 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:G:379:THR:HB	1:G:380:PRO:HD3	1.18	1.17
1:A:106:MET:HG2	8:A:1001:HEA:HAC	1.17	1.16
9:C:2010:3PE:H3E2	9:C:2010:3PE:H3I2	1.22	1.13
9:I:3010:3PE:H3E2	9:I:3010:3PE:C3I	1.78	1.13
1:A:279:LEU:HD23	1:A:279:LEU:C	1.73	1.12

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%)	416 (76%)	106 (19%)	23 (4%)	2	13
1	G	545/566 (96%)	403 (74%)	112 (21%)	30 (6%)	1	8
2	B	258/264 (98%)	203 (79%)	47 (18%)	8 (3%)	3	19
2	H	258/264 (98%)	206 (80%)	44 (17%)	8 (3%)	3	19
3	C	263/266 (99%)	217 (82%)	41 (16%)	5 (2%)	6	30
3	I	263/266 (99%)	209 (80%)	49 (19%)	5 (2%)	6	30
4	D	40/51 (78%)	26 (65%)	13 (32%)	1 (2%)	4	23
4	J	40/51 (78%)	26 (65%)	12 (30%)	2 (5%)	1	10
All	All	2212/2294 (96%)	1706 (77%)	424 (19%)	82 (4%)	2	15

5 of 82 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	102	HIS
1	A	160	PRO
1	A	544	SER
1	A	545	PRO
2	B	254	GLU

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%)	388 (87%)	58 (13%)	4	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	446/459 (97%)	380 (85%)	66 (15%)	3	15
2	B	216/220 (98%)	188 (87%)	28 (13%)	4	19
2	H	216/220 (98%)	193 (89%)	23 (11%)	6	27
3	C	215/216 (100%)	197 (92%)	18 (8%)	10	37
3	I	215/216 (100%)	189 (88%)	26 (12%)	5	21
4	D	30/37 (81%)	26 (87%)	4 (13%)	4	18
4	J	30/37 (81%)	26 (87%)	4 (13%)	4	18
All	All	1814/1864 (97%)	1587 (88%)	227 (12%)	4	20

5 of 227 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	100	THR
3	I	236	LYS
1	G	307	LYS
3	I	204	MET
3	I	16	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 43 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	55	HIS
3	I	153	HIS
2	H	84	HIS
2	H	237	GLN
3	I	160	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	I	3008	-	50,50,50	1.65	2 (4%)	53,55,55	1.14	3 (5%)
8	HEA	G	1002	1	67,67,67	1.31	9 (13%)	81,103,103	2.00	20 (24%)
9	3PE	C	2008	-	50,50,50	1.58	2 (4%)	53,55,55	1.20	6 (11%)
9	3PE	G	3009	-	50,50,50	1.50	3 (6%)	53,55,55	0.99	2 (3%)
8	HEA	A	1002	1	67,67,67	1.41	11 (16%)	81,103,103	2.22	24 (29%)
9	3PE	I	3010	-	50,50,50	1.61	4 (8%)	53,55,55	1.03	2 (3%)
9	3PE	A	2009	-	50,50,50	1.62	3 (6%)	53,55,55	1.13	3 (5%)
8	HEA	A	1001	1	67,67,67	1.39	10 (14%)	81,103,103	2.41	35 (43%)
9	3PE	J	3011	-	50,50,50	1.70	2 (4%)	53,55,55	1.54	7 (13%)
9	3PE	I	3013	-	50,50,50	1.63	3 (6%)	53,55,55	1.20	3 (5%)
9	3PE	C	2010	-	50,50,50	1.54	2 (4%)	53,55,55	1.15	3 (5%)
9	3PE	D	2011	-	50,50,50	1.50	3 (6%)	53,55,55	1.31	7 (13%)
9	3PE	G	3012	-	50,50,50	1.63	3 (6%)	53,55,55	1.25	5 (9%)
9	3PE	A	2012	-	50,50,50	1.62	3 (6%)	53,55,55	1.41	6 (11%)
9	3PE	C	2013	-	50,50,50	1.58	3 (6%)	53,55,55	1.31	3 (5%)
8	HEA	G	1001	1	67,67,67	1.46	10 (14%)	81,103,103	2.62	35 (43%)

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	I	3008	-	-	32/54/54/54	-
8	HEA	G	1002	1	-	6/36/76/76	-
9	3PE	C	2008	-	-	35/54/54/54	-
9	3PE	G	3009	-	-	29/54/54/54	-
8	HEA	A	1002	1	-	9/36/76/76	-
9	3PE	I	3010	-	-	28/54/54/54	-
9	3PE	A	2009	-	-	28/54/54/54	-
8	HEA	A	1001	1	-	17/36/76/76	-
9	3PE	J	3011	-	-	22/54/54/54	-
9	3PE	I	3013	-	-	27/54/54/54	-
9	3PE	C	2010	-	-	22/54/54/54	-
9	3PE	D	2011	-	-	21/54/54/54	-
9	3PE	G	3012	-	-	22/54/54/54	-
9	3PE	A	2012	-	-	21/54/54/54	-
9	3PE	C	2013	-	-	26/54/54/54	-
8	HEA	G	1001	1	-	16/36/76/76	-

The worst 5 of 73 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	J	3011	3PE	O21-C21	8.32	1.57	1.34
9	I	3013	3PE	O31-C31	7.71	1.55	1.33
9	A	2009	3PE	O21-C21	7.63	1.55	1.34
9	I	3008	3PE	O21-C21	7.63	1.55	1.34
9	G	3012	3PE	O31-C31	7.57	1.55	1.33

The worst 5 of 164 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	G	1001	HEA	CHB-C1B-NB	-7.09	116.80	124.42
8	G	1001	HEA	CMB-C2B-C1B	6.94	135.88	125.03
8	A	1002	HEA	CMC-C2C-C1C	6.85	135.85	125.42
9	C	2013	3PE	C2-O21-C21	-6.63	101.93	117.80
8	A	1002	HEA	C13-C14-C15	-6.50	112.75	127.62

There are no chirality outliers.

5 of 361 torsion outliers are listed below:

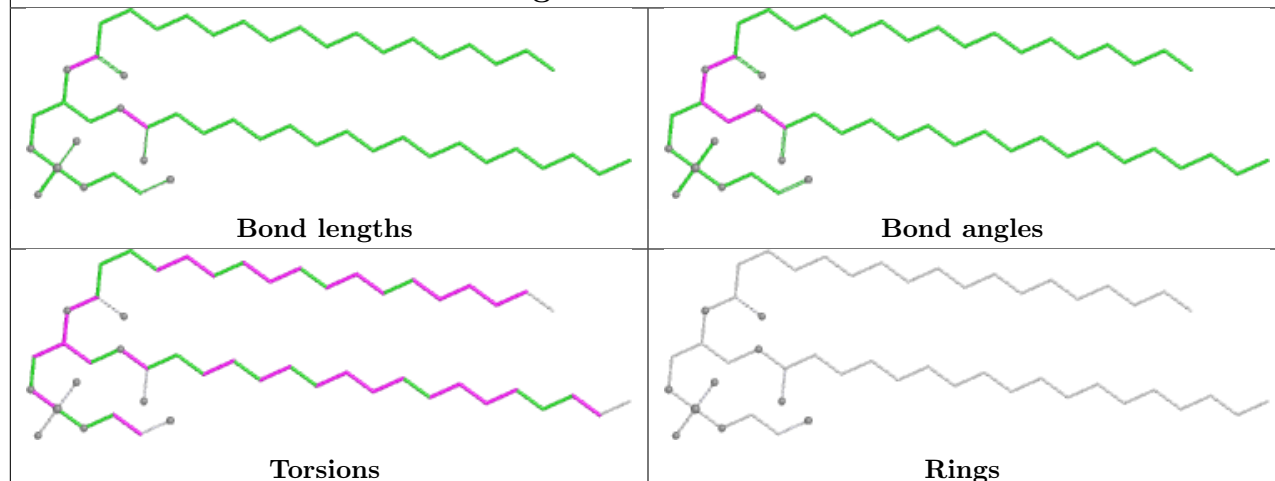
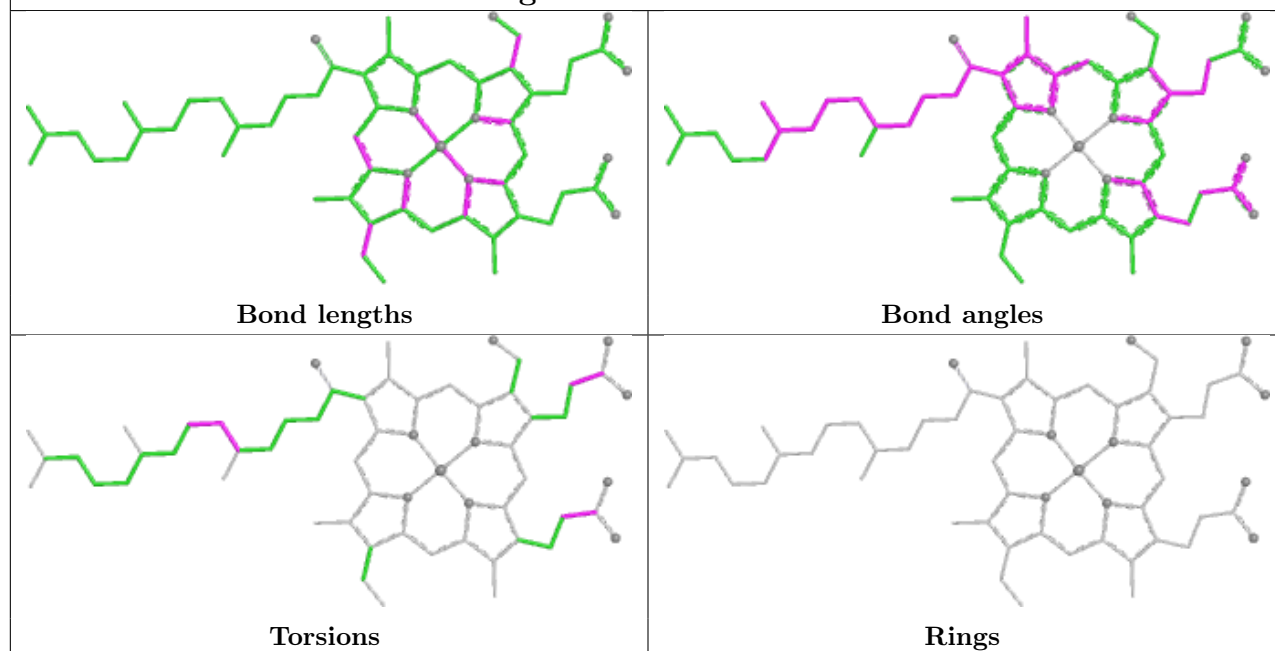
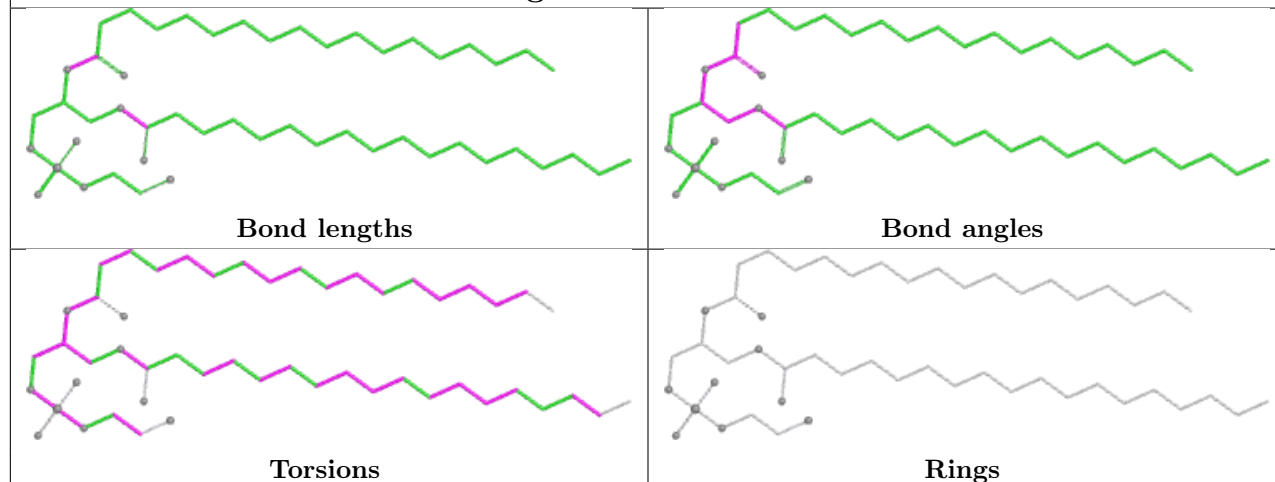
Mol	Chain	Res	Type	Atoms
8	A	1001	HEA	C11-C12-C13-C14
8	A	1002	HEA	C2A-C3A-CMA-OMA
8	G	1001	HEA	C12-C11-C3B-C2B
8	G	1001	HEA	C11-C12-C13-C14
9	A	2009	3PE	C1-O11-P-O12

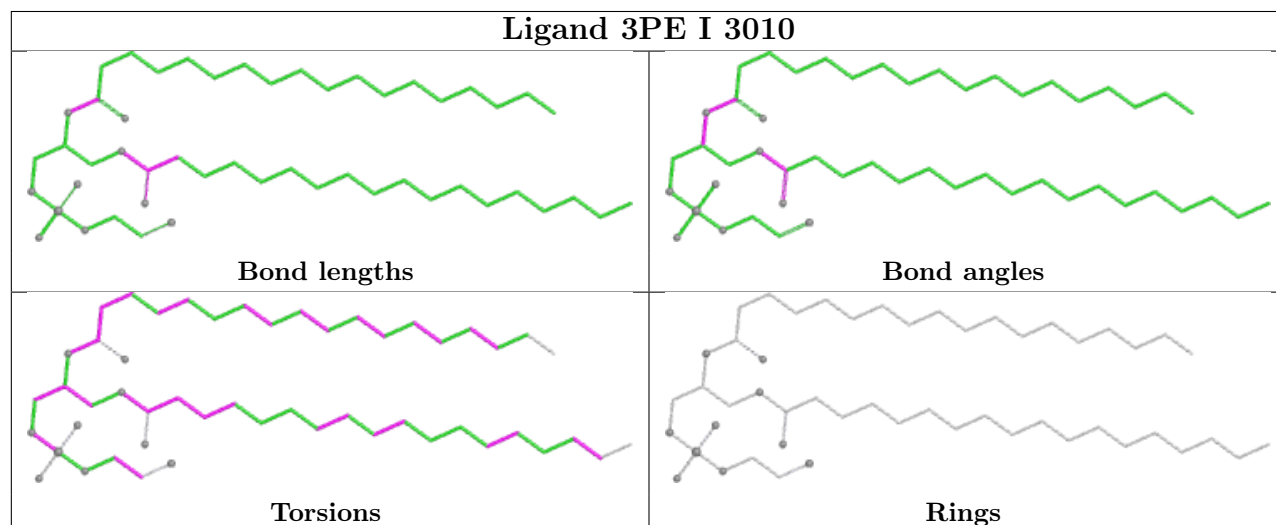
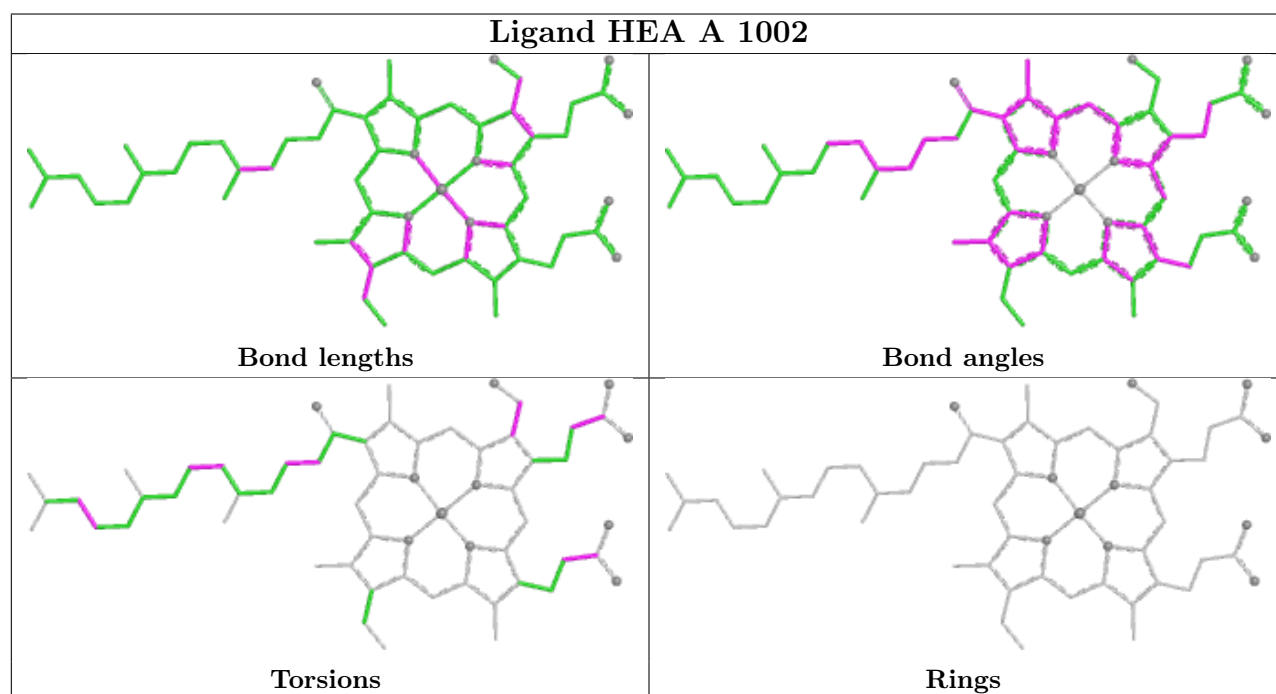
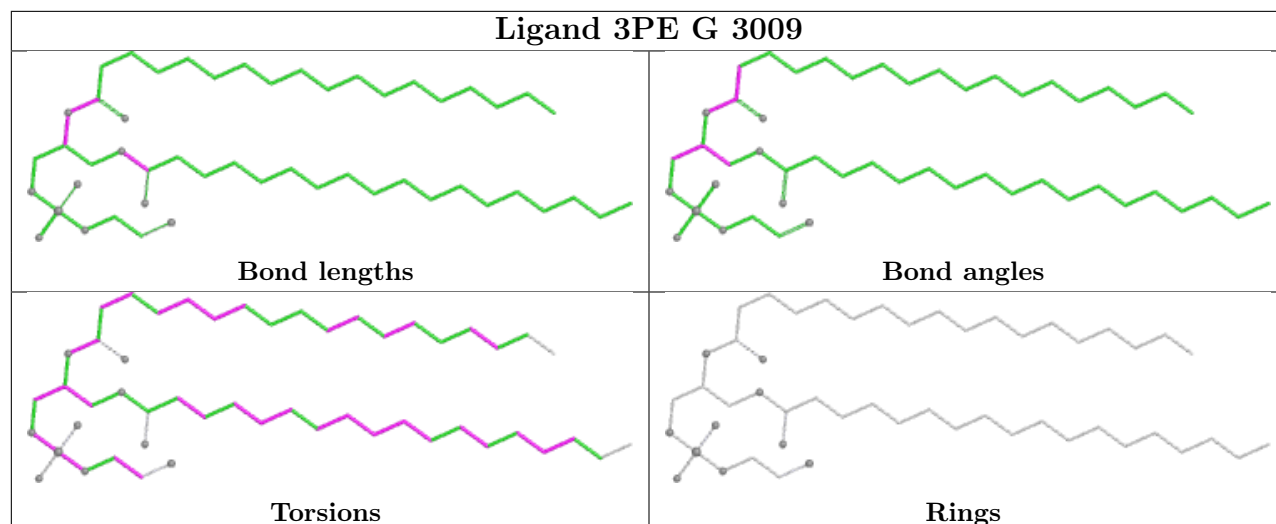
There are no ring outliers.

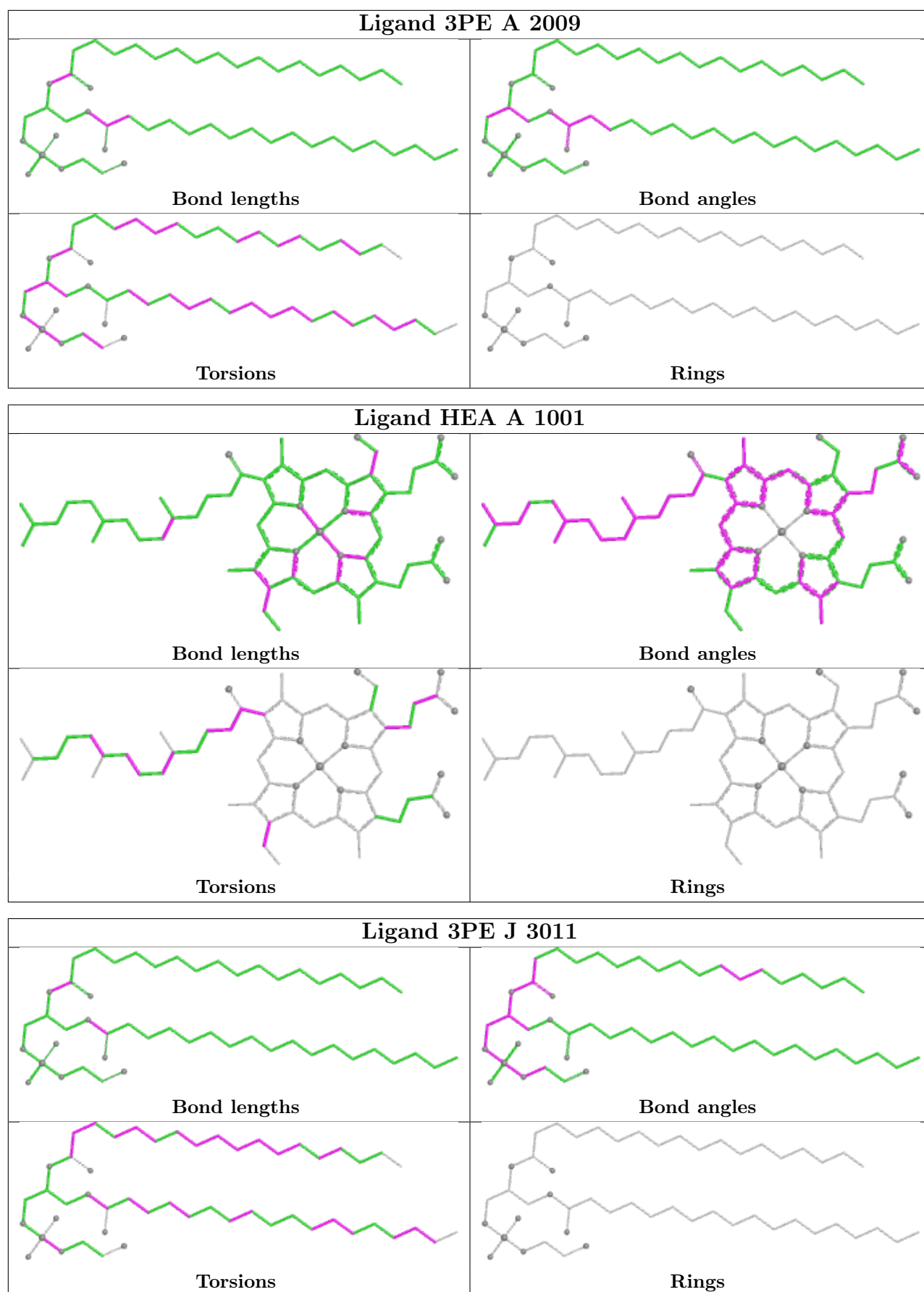
16 monomers are involved in 280 short contacts:

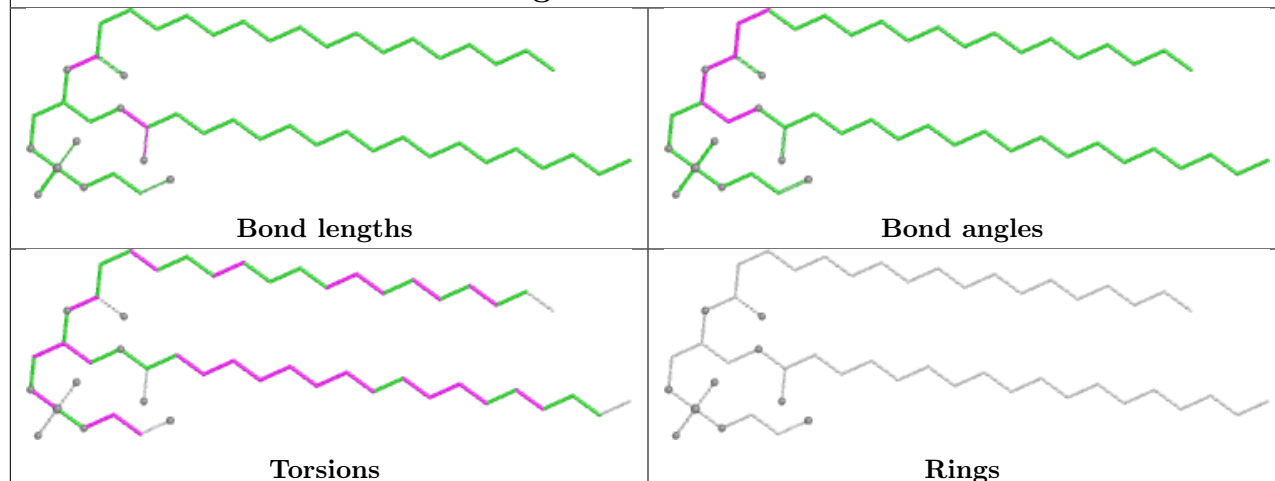
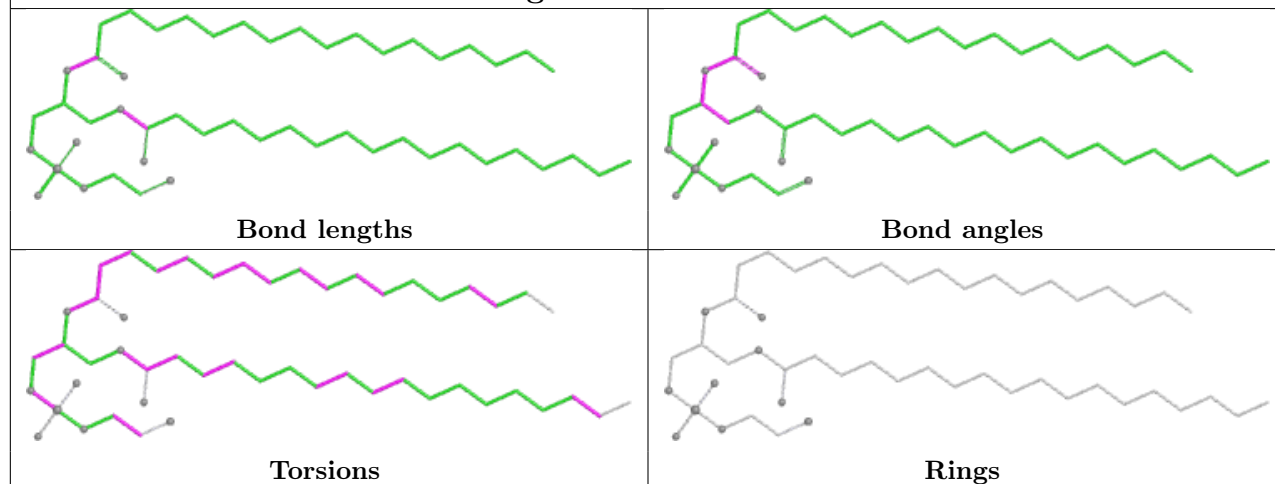
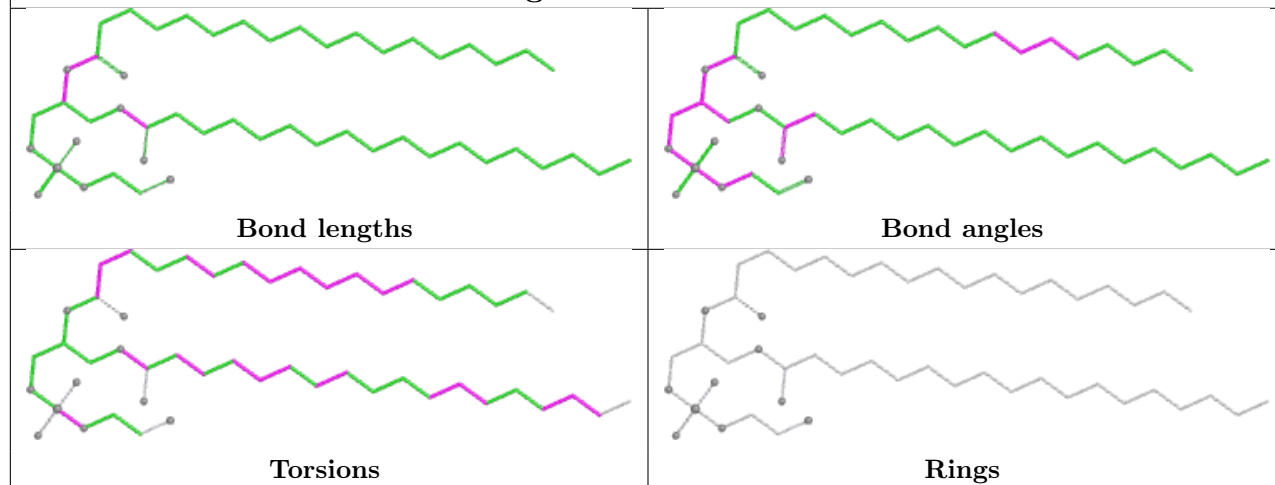
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	I	3008	3PE	13	0
8	G	1002	HEA	15	0
9	C	2008	3PE	13	0
9	G	3009	3PE	20	0
8	A	1002	HEA	19	0
9	I	3010	3PE	24	0
9	A	2009	3PE	18	0
8	A	1001	HEA	18	0
9	J	3011	3PE	12	0
9	I	3013	3PE	22	0
9	C	2010	3PE	24	0
9	D	2011	3PE	17	0
9	G	3012	3PE	22	0
9	A	2012	3PE	20	0
9	C	2013	3PE	21	0
8	G	1001	HEA	23	0

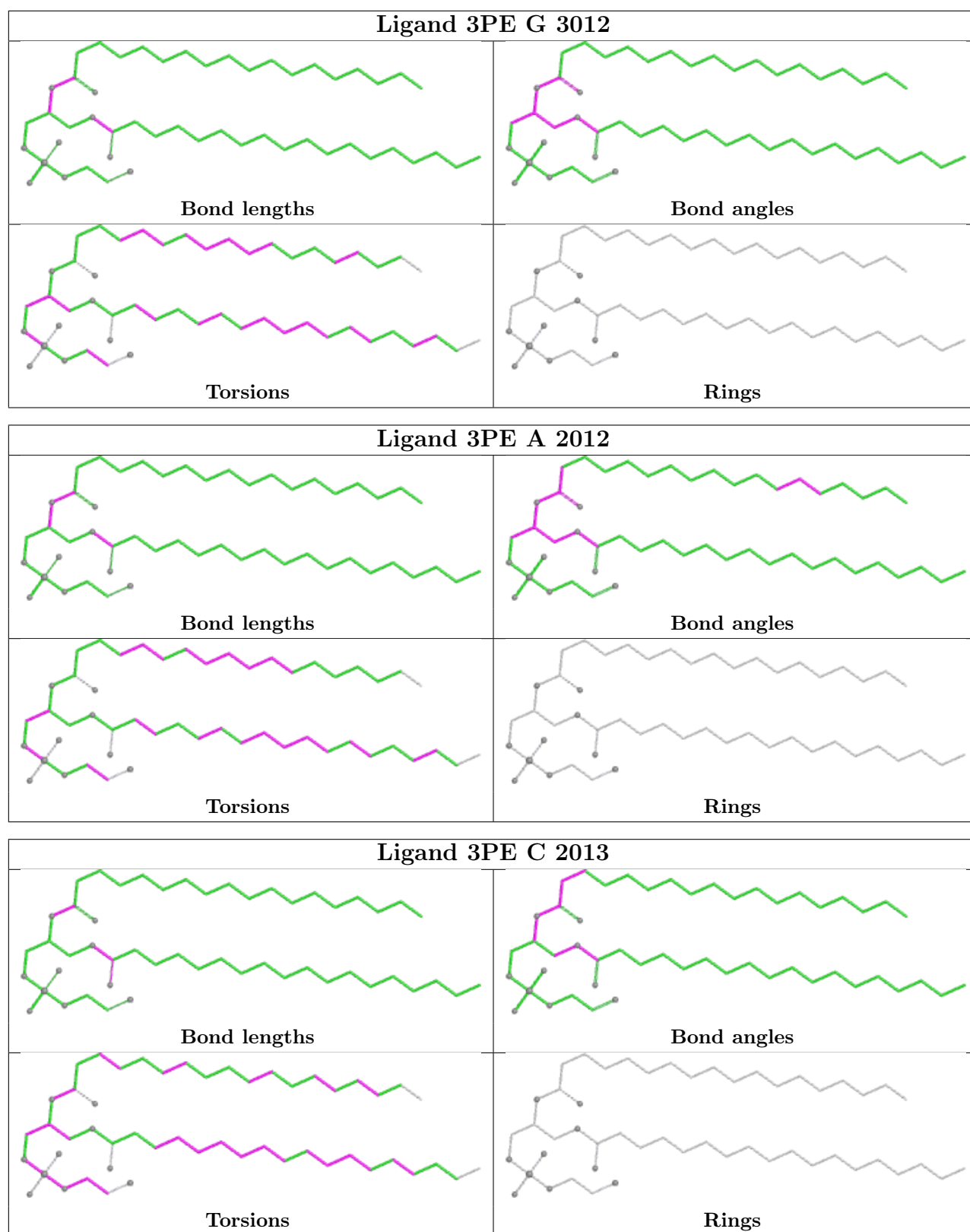
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

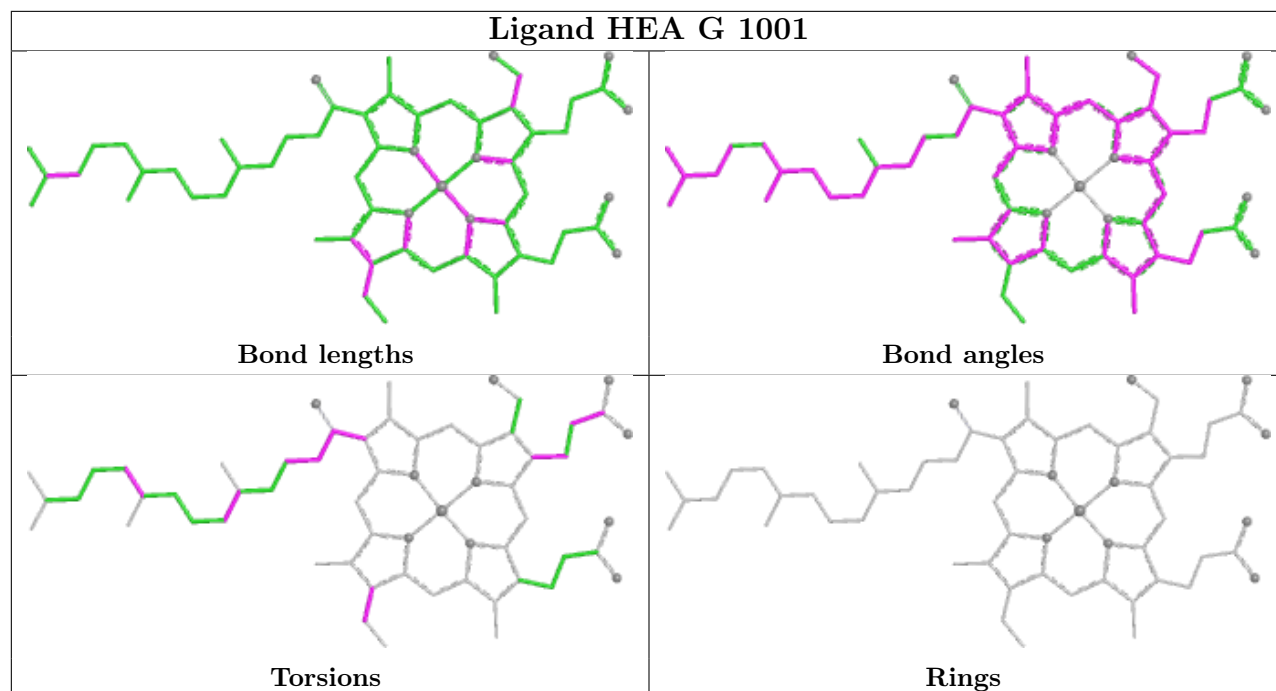
Ligand 3PE I 3008**Ligand HEA G 1002****Ligand 3PE C 2008**





Ligand 3PE I 3013**Ligand 3PE C 2010****Ligand 3PE D 2011**





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 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.