



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 6, 2024 – 01:05 AM EDT

PDB ID : 1KB9
Title : YEAST CYTOCHROME BC1 COMPLEX
Authors : Lange, C.; Nett, J.H.; Trumpower, B.L.; Hunte, C.
Deposited on : 2001-11-05
Resolution : 2.30 Å(reported)

This is a wwPDB X-ray Structure 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/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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

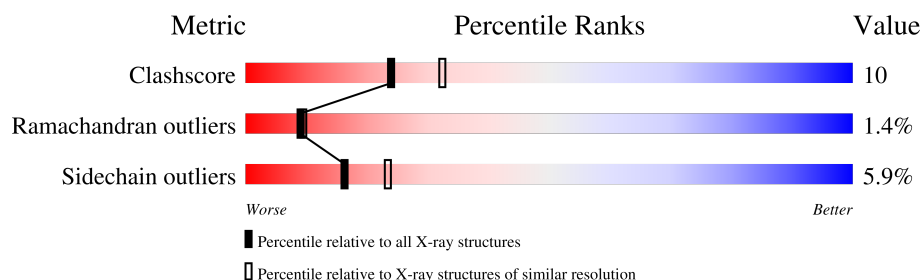
1 Overall quality at a glance

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	180529	6698 (2.30-2.30)
Ramachandran outliers	177936	6640 (2.30-2.30)
Sidechain outliers	177891	6640 (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	431	72% 26% .
2	B	352	63% 32% .
3	C	385	84% 14% .
4	D	246	84% 15% .
5	E	185	79% 20% .
6	F	74	78% 20% .
7	G	125	86% 12% .
8	H	93	74% 22% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	I	55	
10	J	127	
11	K	107	

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
15	SMA	C	505	X	-	-	-

2 Entry composition [i](#)

There are 21 unique types of molecules in this entry. The entry contains 18040 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 UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX CORE PROTEIN I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	431	Total	C	N	O	S	0	0	0
			3343	2109	576	652	6			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	153	ASP	GLU	conflict	UNP P07256

- Molecule 2 is a protein called UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX CORE PROTEIN 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	352	Total	C	N	O	S	0	0	0
			2734	1747	453	533	1			

- Molecule 3 is a protein called CYTOCHROME B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	385	Total	C	N	O	S	0	0	0
			3088	2080	484	503	21			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	270	VAL	ASP	conflict	UNP P00163

- Molecule 4 is a protein called CYTOCHROME C1, HEME PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	246	Total	C	N	O	S	0	0	0
			1940	1237	334	360	9			

- Molecule 5 is a protein called UBIQUINOL-CYTOCHROME C REDUCTASE IRON-SULFUR SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	185	Total	C	N	O	S	0	0	0
			1410	893	242	265	10			

- Molecule 6 is a protein called UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 17 KD PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	74	Total	C	N	O	S	0	0	0
			623	391	108	122	2			

- Molecule 7 is a protein called UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 14 KD PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	125	Total	C	N	O	S	0	0	0
			1011	648	172	189	2			

- Molecule 8 is a protein called UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX UBIQUINONE-BINDING PROTEIN QP-C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	93	Total	C	N	O	S	98	0	0
			772	510	131	129	2			

- Molecule 9 is a protein called UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 7.3 KD PROTEIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	I	55	Total	C	N	O	0	0	0
			449	298	75	76			

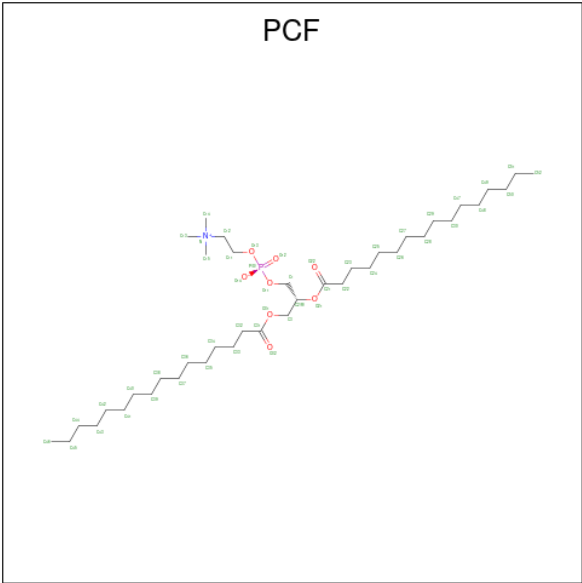
- Molecule 10 is a protein called HEAVY CHAIN (VH) OF FV-FRAGMENT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	127	Total	C	N	O	S	0	0	0
			1015	644	167	201	3			

- Molecule 11 is a protein called LIGHT CHAIN (VL) OF FV-FRAGMENT.

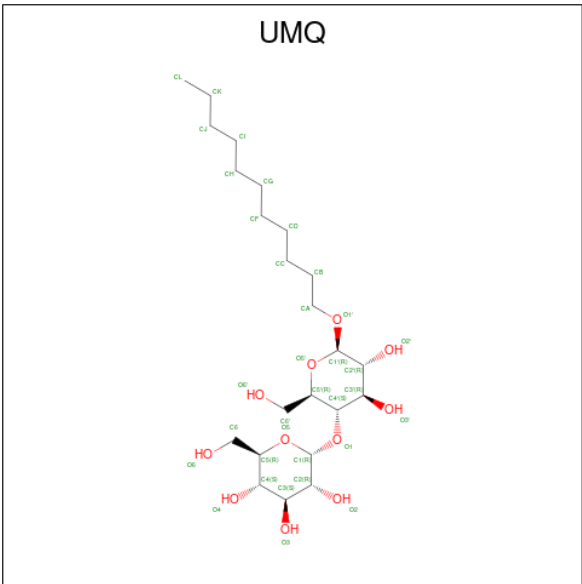
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	107	Total	C	N	O	S	0	0	0
			842	536	141	163	2			

- Molecule 12 is 1,2-DIACYL-SN-GLYCERO-3-PHOSHOCHOLINE (three-letter code: PCF) (formula: C₄₀H₈₀NO₈P).



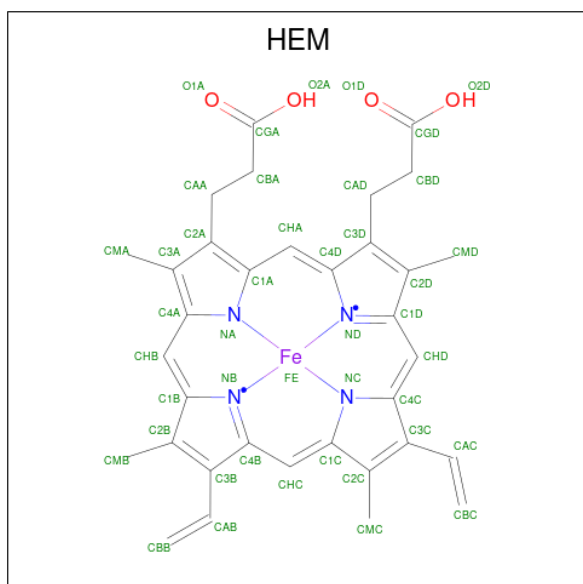
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	A	1	Total	C	N	O	P	0	0
			37	27	1	8	1		

- Molecule 13 is UNDECYL-MALTOSIDE (three-letter code: UMQ) (formula: C₂₃H₄₄O₁₁).



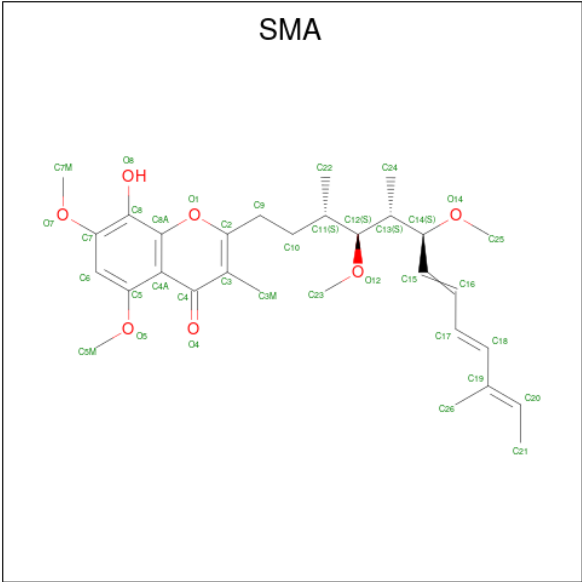
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	A	1	Total	C	O	0	0
			34	23	11		

- Molecule 14 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



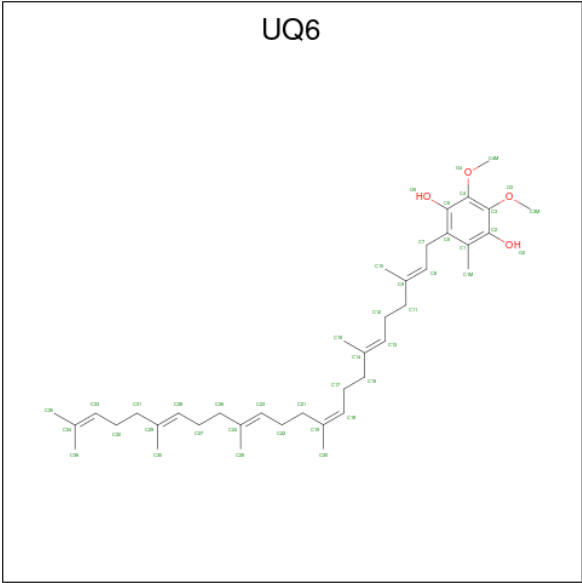
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
14	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
14	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 15 is STIGMATELLIN A (three-letter code: SMA) (formula: $\text{C}_{30}\text{H}_{42}\text{O}_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	C	1	Total	C	O	0	0
			37	30	7		

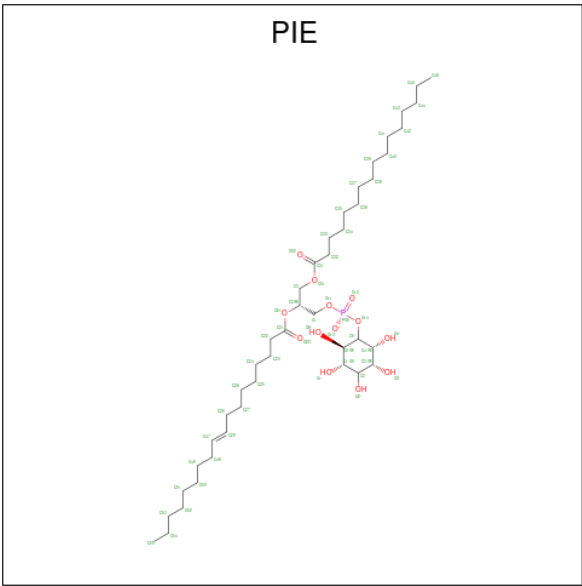
- Molecule 16 is 5-(3,7,11,15,19,23-HEXAMETHYL-TETRACOSA-2,6,10,14,18,22-HEX AENYL)-2,3-DIMETHOXY-6-METHYL-BENZENE-1,4-DIOL (three-letter code: UQ6) (formula: C₃₉H₆₀O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	C	1	Total	C	O	0	0
			43	39	4		

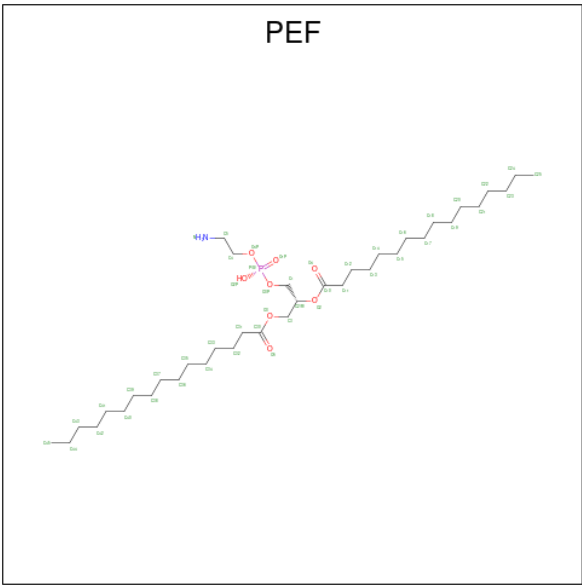
- Molecule 17 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOINOSITOL (three-letter code:

PIE) (formula: C₄₃H₈₀O₁₃P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	C	1	Total	C	O	P	0	0
			49	35	13	1		

- Molecule 18 is DI-PALMITOYL-3-SN-PHOSPHATIDYLETHANOLAMINE (three-letter code: PEF) (formula: C₃₇H₇₄NO₈P).



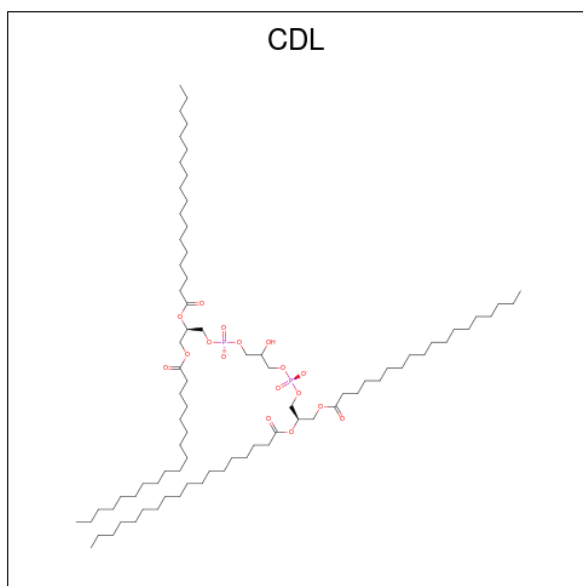
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	C	1	Total	C	N	O	P	0	0
			45	35	1	8	1		

Continued on next page...

Continued from previous page...

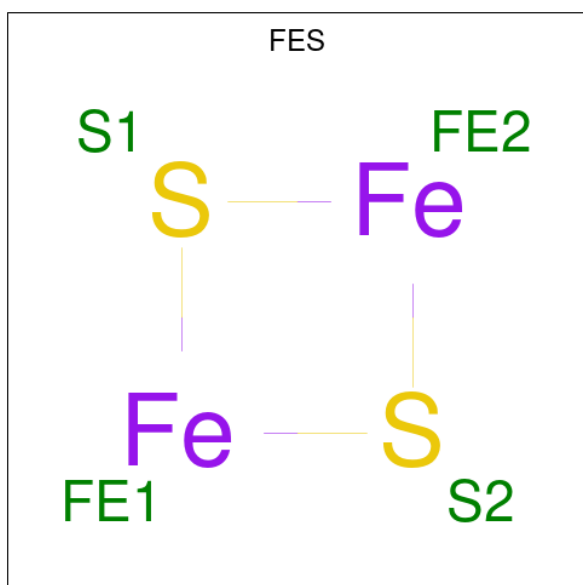
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	C	1	Total	C	N	O	P	0	0
			38	28	1	8	1		

- Molecule 19 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	C	1	Total	C	O	P	0	0
			76	57	17	2		

- Molecule 20 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	E	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 21 is water.

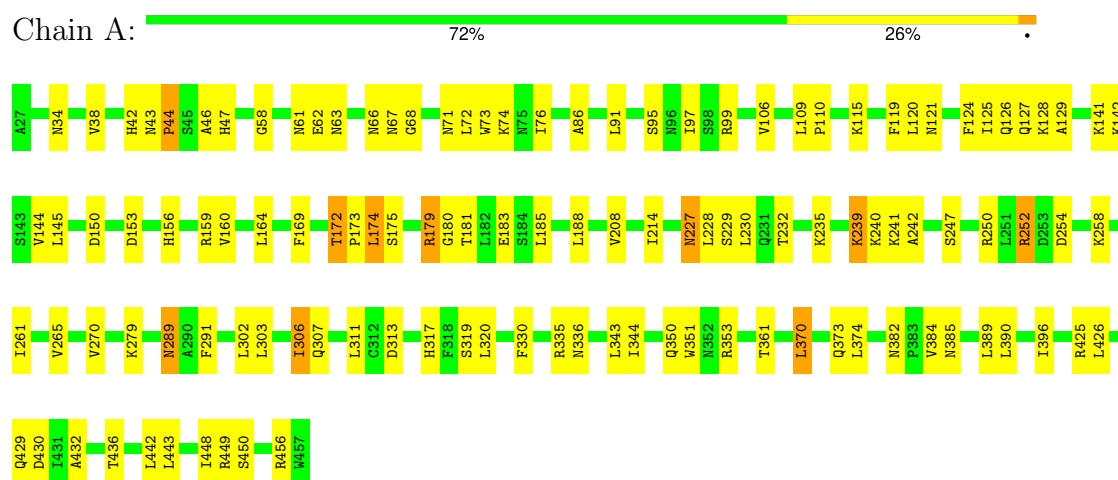
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	A	45	Total	O	0	0
			45	45		
21	B	9	Total	O	0	0
			9	9		
21	C	106	Total	O	0	0
			106	106		
21	D	67	Total	O	0	0
			67	67		
21	E	28	Total	O	0	0
			28	28		
21	F	7	Total	O	0	0
			7	7		
21	G	36	Total	O	0	0
			36	36		
21	H	14	Total	O	0	0
			14	14		
21	I	2	Total	O	0	0
			2	2		
21	J	5	Total	O	0	0
			5	5		
21	K	2	Total	O	0	0
			2	2		

3 Residue-property plots

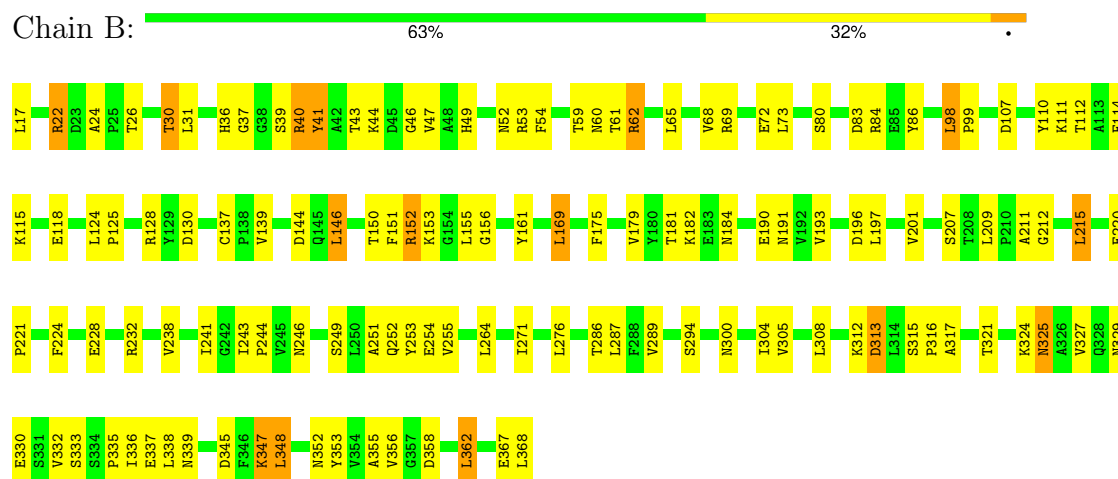
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

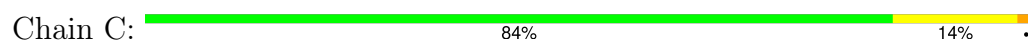
- Molecule 1: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX CORE PROTEIN I

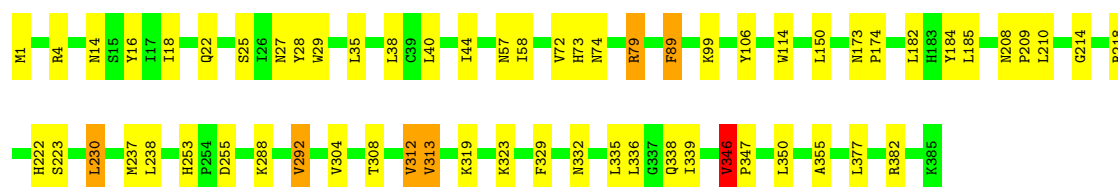


- Molecule 2: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX CORE PROTEIN 2



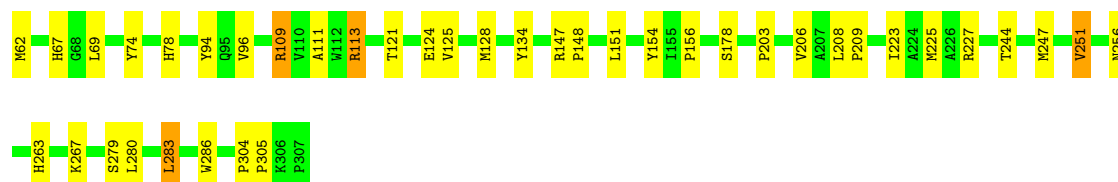
- Molecule 3: CYTOCHROME B





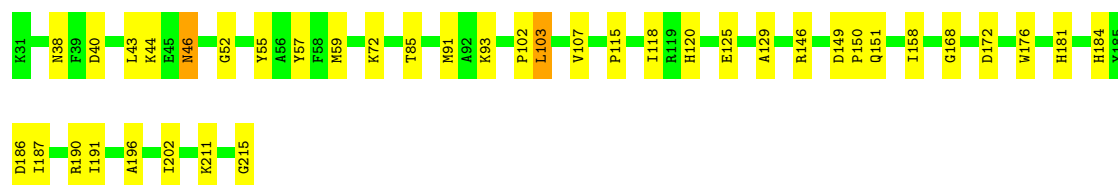
• Molecule 4: CYTOCHROME C1, HEME PROTEIN

Chain D: 84% 15% .



• Molecule 5: UBIQUINOL-CYTOCHROME C REDUCTASE IRON-SULFUR SUBUNIT

Chain E: 79% 20% .



• Molecule 6: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 17 KD PROTEIN

Chain F: 78% 20% .



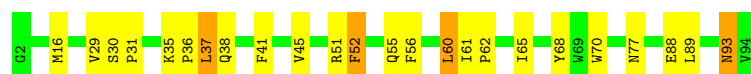
• Molecule 7: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 14 KD PROTEIN

Chain G: 86% 12% .



• Molecule 8: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX UBIQUINONE-BINDING PROTEIN QP-C

Chain H: 74% 22% .



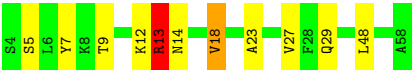
• Molecule 9: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 7.3 KD PROTEIN

Chain I:

80%

16%

• •



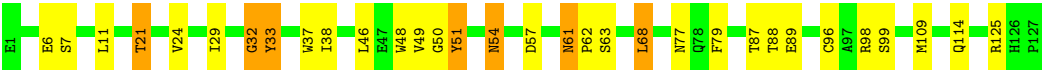
• Molecule 10: HEAVY CHAIN (VH) OF FV-FRAGMENT

Chain J:

75%

20%

6%



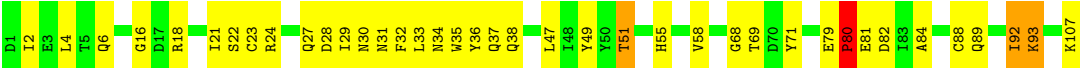
• Molecule 11: LIGHT CHAIN (VL) OF FV-FRAGMENT

Chain K:

64%

33%

• •



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	214.47Å 163.92Å 147.28Å 90.00° 117.50° 90.00°	Depositor
Resolution (Å)	14.96 – 2.30	Depositor
% Data completeness (in resolution range)	84.7 (14.96-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.218 , 0.249	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	18040	wwPDB-VP
Average B, all atoms (Å ²)	69.0	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: HEM, PCF, FES, UQ6, PEF, SMA, CDL, PIE, UMQ

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	0.34	0/3404	0.58	0/4614
2	B	0.31	0/2780	0.57	0/3764
3	C	0.45	0/3190	0.65	2/4353 (0.0%)
4	D	0.35	0/2001	0.60	0/2726
5	E	0.34	0/1443	0.61	0/1957
6	F	0.33	0/637	0.51	0/858
7	G	0.35	0/1031	0.62	1/1397 (0.1%)
8	H	0.39	0/803	0.52	0/1088
9	I	0.40	0/462	0.48	0/622
10	J	0.33	0/1043	0.61	1/1422 (0.1%)
11	K	0.31	0/863	0.53	0/1172
All	All	0.36	0/17657	0.59	4/23973 (0.0%)

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
4	D	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	32	GLY	N-CA-C	5.55	126.98	113.10
3	C	79	ARG	NE-CZ-NH1	-5.46	117.57	120.30
7	G	71	ARG	NE-CZ-NH1	-5.33	117.63	120.30
3	C	346	VAL	N-CA-C	5.12	124.83	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	94	TYR	Sidechain

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	3343	0	3321	72	0
2	B	2734	0	2774	80	0
3	C	3088	0	3125	40	0
4	D	1940	0	1862	22	0
5	E	1410	0	1386	30	0
6	F	623	0	581	11	0
7	G	1011	0	1026	14	0
8	H	772	0	736	16	0
9	I	449	0	445	9	0
10	J	1015	0	959	25	0
11	K	842	0	820	24	0
12	A	37	0	48	9	0
13	A	34	0	44	4	0
14	C	86	0	60	4	0
14	D	43	0	30	0	0
15	C	37	0	40	4	0
16	C	43	0	58	11	0
17	C	49	0	58	2	0
18	C	83	0	118	3	0
19	C	76	0	99	5	0
20	E	4	0	0	1	0
21	A	45	0	0	0	0
21	B	9	0	0	0	0
21	C	106	0	0	1	0
21	D	67	0	0	1	0
21	E	28	0	0	0	0
21	F	7	0	0	0	0
21	G	36	0	0	2	0
21	H	14	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	I	2	0	0	0	0
21	J	5	0	0	0	0
21	K	2	0	0	0	0
All	All	18040	0	17590	348	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

The worst 5 of 348 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)
6:F:77:GLN:H	6:F:77:GLN:HE21	1.03	1.01
11:K:31:ASN:HD22	11:K:51:THR:HG21	1.31	0.95
16:C:506:UQ6:H103	16:C:506:UQ6:H1M1	1.51	0.92
2:B:347:LYS:H	2:B:347:LYS:HD3	1.37	0.88
1:A:317:HIS:HE1	1:A:351:TRP:HE1	1.25	0.85

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	429/431 (100%)	397 (92%)	28 (6%)	4 (1%)	14 17
2	B	350/352 (99%)	311 (89%)	31 (9%)	8 (2%)	5 4
3	C	383/385 (100%)	369 (96%)	12 (3%)	2 (0%)	25 32
4	D	244/246 (99%)	237 (97%)	7 (3%)	0	100 100
5	E	183/185 (99%)	171 (93%)	9 (5%)	3 (2%)	8 7
6	F	72/74 (97%)	69 (96%)	3 (4%)	0	100 100
7	G	123/125 (98%)	121 (98%)	2 (2%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	H	91/93 (98%)	79 (87%)	7 (8%)	5 (6%)	1	0
9	I	53/55 (96%)	50 (94%)	1 (2%)	2 (4%)	2	1
10	J	125/127 (98%)	111 (89%)	12 (10%)	2 (2%)	8	7
11	K	105/107 (98%)	89 (85%)	11 (10%)	5 (5%)	2	1
All	All	2158/2180 (99%)	2004 (93%)	123 (6%)	31 (1%)	9	9

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	335	PRO
3	C	223	SER
5	E	103	LEU
8	H	93	ASN
2	B	153	LYS

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	370/370 (100%)	342 (92%)	28 (8%)	11	14
2	B	301/301 (100%)	278 (92%)	23 (8%)	11	14
3	C	338/338 (100%)	320 (95%)	18 (5%)	19	28
4	D	204/204 (100%)	197 (97%)	7 (3%)	32	47
5	E	151/151 (100%)	148 (98%)	3 (2%)	50	68
6	F	67/67 (100%)	63 (94%)	4 (6%)	16	23
7	G	109/109 (100%)	104 (95%)	5 (5%)	23	33
8	H	77/77 (100%)	73 (95%)	4 (5%)	19	28
9	I	45/45 (100%)	41 (91%)	4 (9%)	8	10
10	J	112/112 (100%)	104 (93%)	8 (7%)	12	17
11	K	93/93 (100%)	86 (92%)	7 (8%)	11	15
All	All	1867/1867 (100%)	1756 (94%)	111 (6%)	16	23

5 of 111 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	182	LEU
11	K	107	LYS
4	D	113	ARG
11	K	93	LYS
10	J	57	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 60 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	14	ASN
11	K	31	ASN
4	D	78	HIS
10	J	114	GLN
11	K	91	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 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
13	UMQ	A	521	-	35,35,35	0.95	1 (2%)	46,46,46	1.45	7 (15%)
14	HEM	D	503	4	42,50,50	1.48	6 (14%)	46,82,82	1.07	4 (8%)
16	UQ6	C	506	-	43,43,43	2.49	14 (32%)	54,55,55	1.99	14 (25%)
19	CDL	C	511	-	75,75,99	1.09	5 (6%)	81,87,111	1.15	5 (6%)
15	SMA	C	505	-	38,38,38	1.59	7 (18%)	47,52,52	2.05	11 (23%)
18	PEF	C	513	-	37,37,46	0.72	0	40,42,51	0.98	1 (2%)
14	HEM	C	502	3	42,50,50	1.31	10 (23%)	46,82,82	1.04	3 (6%)
14	HEM	C	501	3	42,50,50	1.48	9 (21%)	46,82,82	1.07	1 (2%)
20	FES	E	504	5	0,4,4	-	-	-	-	-
18	PEF	C	510	-	44,44,46	0.72	0	47,49,51	1.08	2 (4%)
17	PIE	C	508	-	49,49,57	1.96	9 (18%)	58,61,69	1.40	9 (15%)
12	PCF	A	514	-	36,36,49	1.63	1 (2%)	42,44,57	1.29	2 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	UMQ	A	521	-	-	5/20/60/60	0/2/2/2
14	HEM	D	503	4	-	4/12/54/54	-
16	UQ6	C	506	-	-	14/39/39/39	0/1/1/1
19	CDL	C	511	-	-	36/86/86/110	-
15	SMA	C	505	-	2/2/5/10	21/34/34/34	0/2/2/2
18	PEF	C	513	-	-	13/41/41/50	-
14	HEM	C	502	3	-	4/12/54/54	-
14	HEM	C	501	3	-	5/12/54/54	-
20	FES	E	504	5	-	-	0/1/1/1
18	PEF	C	510	-	-	23/48/48/50	-
17	PIE	C	508	-	-	16/44/68/76	0/1/1/1
12	PCF	A	514	-	-	15/40/40/53	-

The worst 5 of 62 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	C	508	PIE	P-O14	-9.20	1.31	1.59
12	A	514	PCF	O13-C11	-8.76	1.09	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	C	506	UQ6	C7-C6	6.62	1.59	1.51
16	C	506	UQ6	O5-C5	-5.66	1.23	1.36
16	C	506	UQ6	O2-C2	-5.45	1.24	1.36

The worst 5 of 59 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	C	506	UQ6	C3M-O3-C3	6.90	133.47	114.74
15	C	505	SMA	O14-C14-C15	6.49	129.90	111.05
15	C	505	SMA	C26-C19-C18	-6.42	108.28	118.09
12	A	514	PCF	C3-C2-C1	-5.71	98.47	111.78
13	A	521	UMQ	CA-O1'-C1'	-5.28	104.66	113.68

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
15	C	505	SMA	C12
15	C	505	SMA	C14

5 of 156 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	A	514	PCF	C11-O13-P-O11
12	A	514	PCF	C11-O13-P-O12
15	C	505	SMA	C11-C12-C13-C24
15	C	505	SMA	O12-C12-C13-C14
15	C	505	SMA	O12-C12-C13-C24

There are no ring outliers.

10 monomers are involved in 39 short contacts:

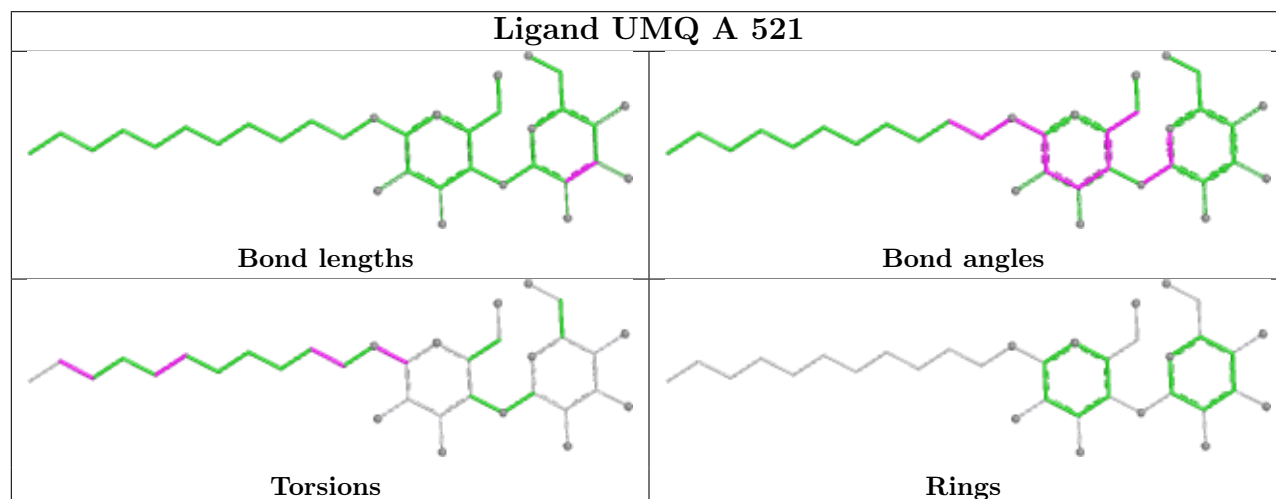
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	A	521	UMQ	4	0
16	C	506	UQ6	11	0
19	C	511	CDL	5	0
15	C	505	SMA	4	0
14	C	502	HEM	1	0
14	C	501	HEM	3	0
20	E	504	FES	1	0
18	C	510	PEF	3	0
17	C	508	PIE	2	0

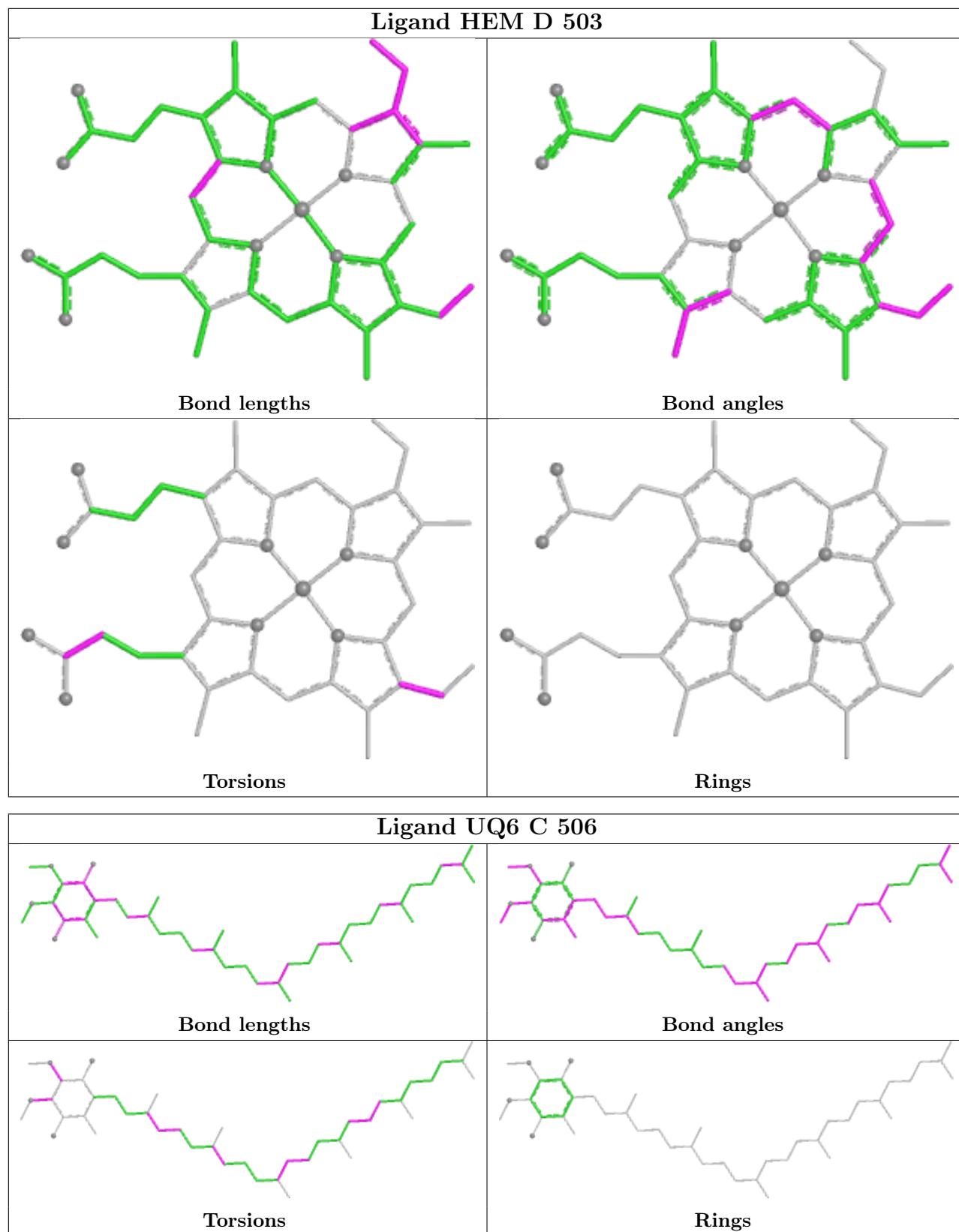
Continued on next page...

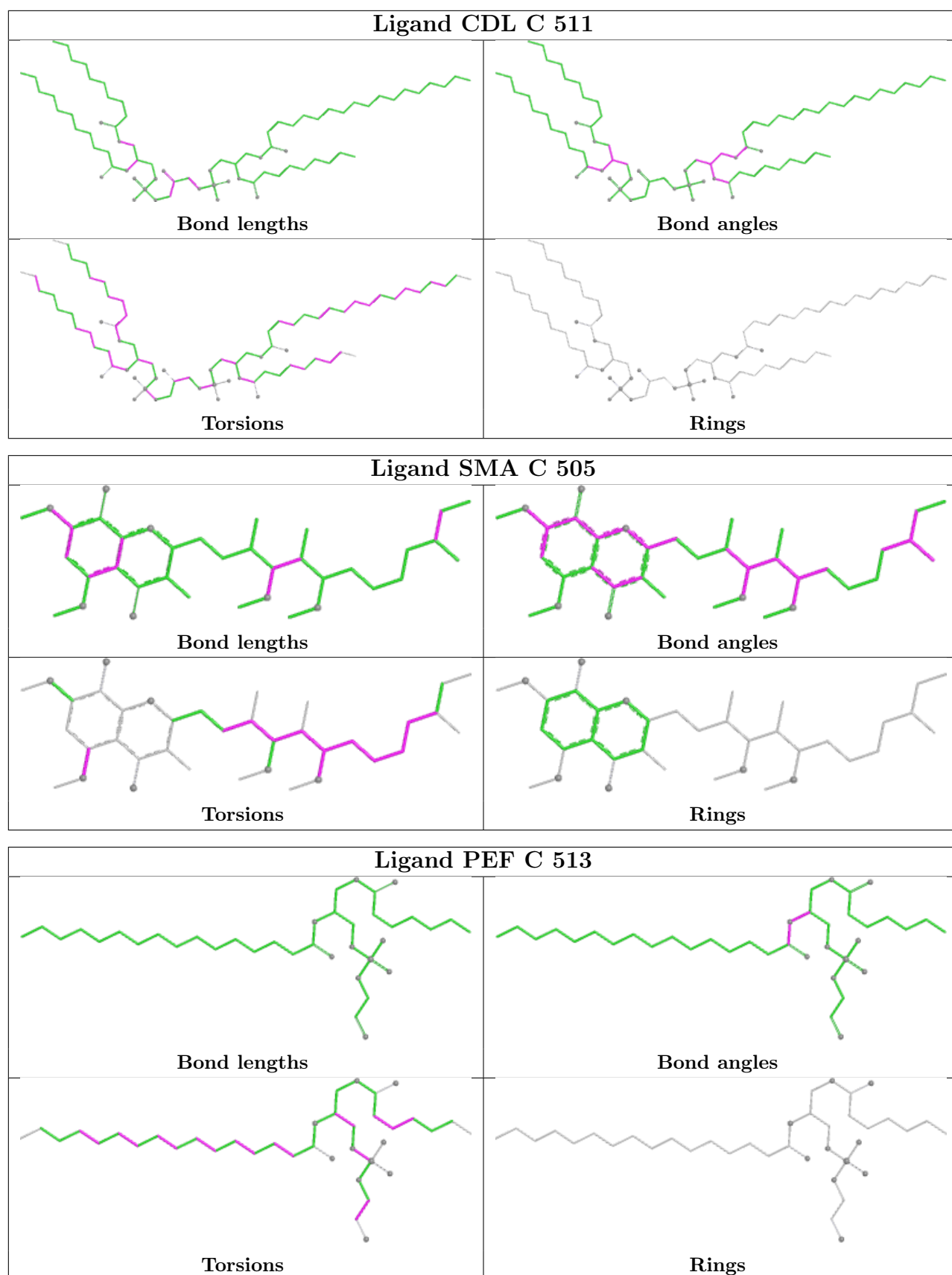
Continued from previous page...

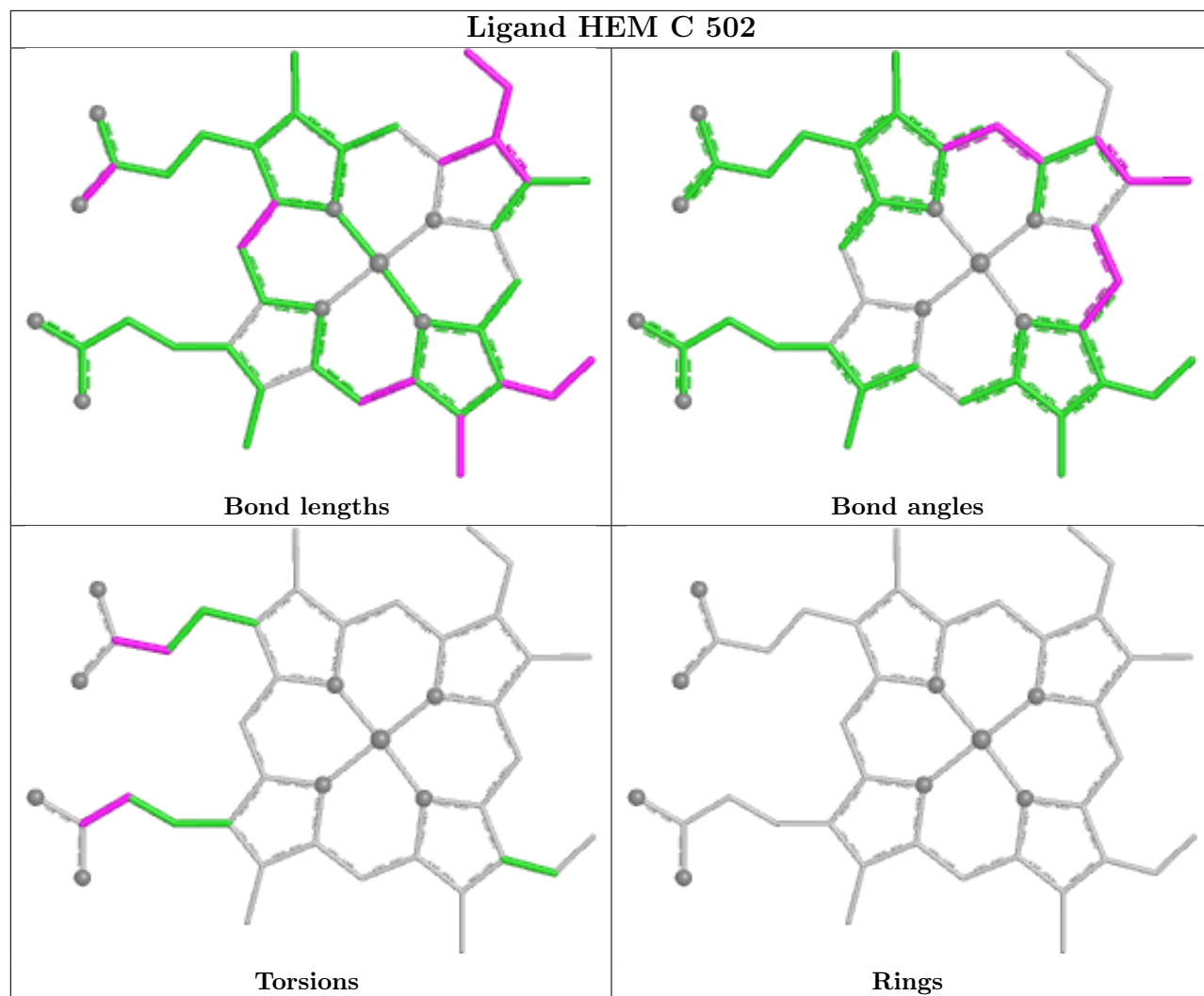
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	A	514	PCF	9	0

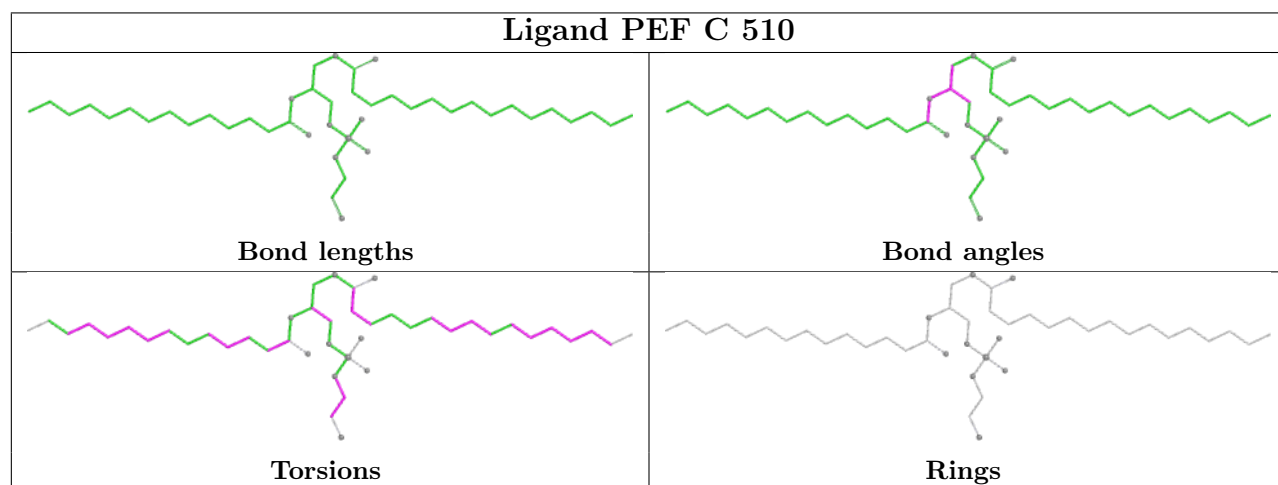
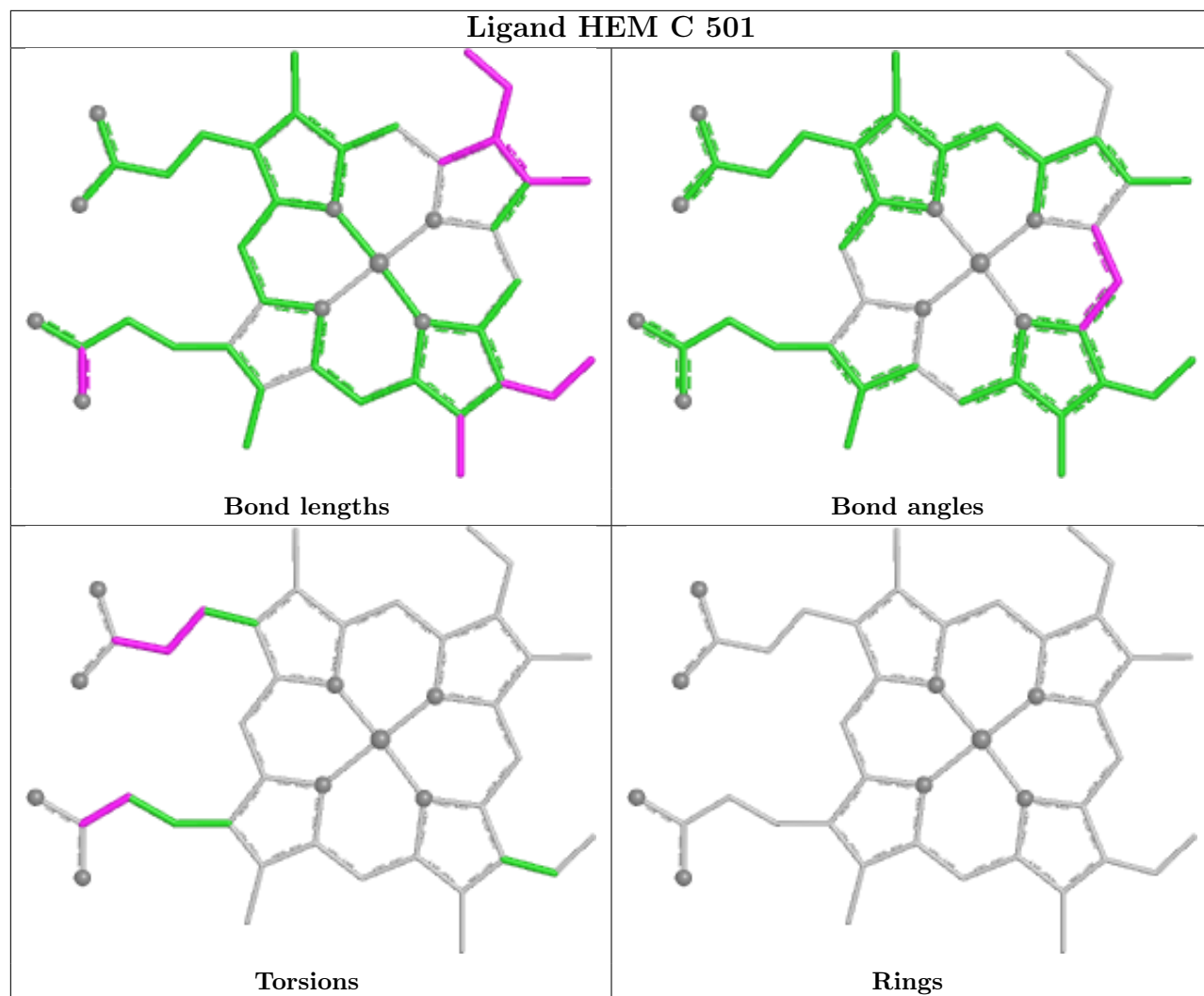
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

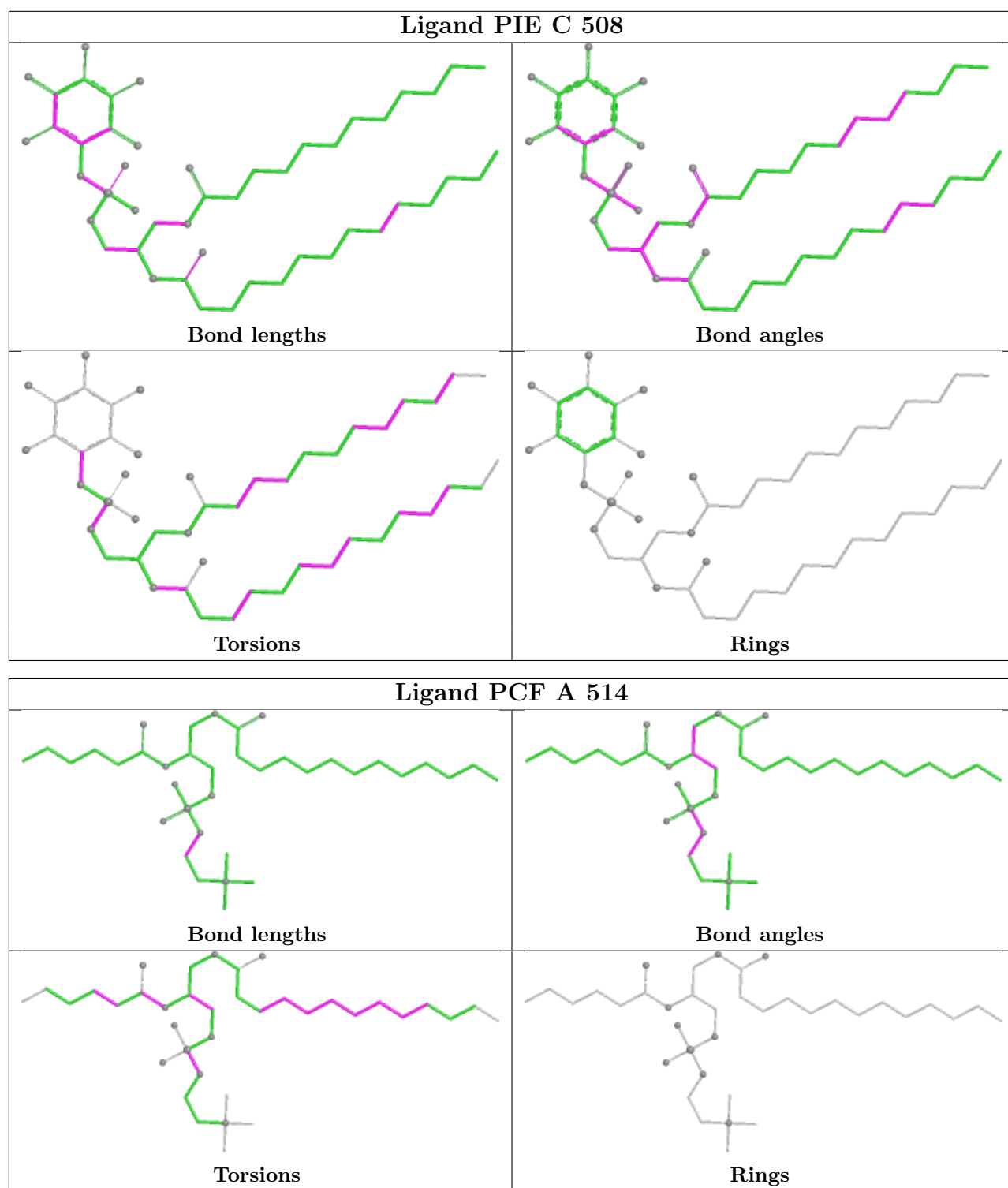












5.7 Other polymers ⓘ

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.