



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 5, 2026 – 02:53 PM EDT

PDB ID : 1P84 / pdb_00001p84
Title : HDBT inhibited Yeast Cytochrome bc1 Complex
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Deposited on : 2003-05-06
Resolution : 2.50 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	:	4-5-2 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

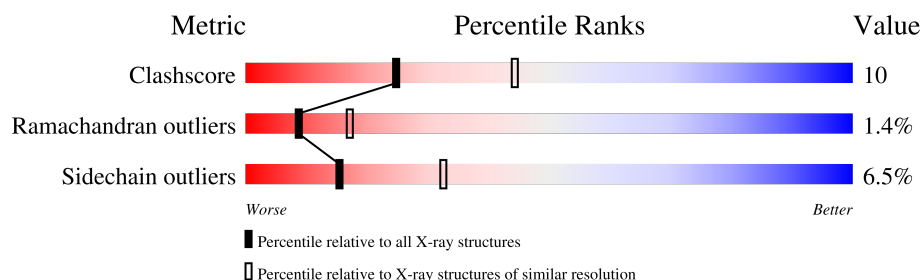
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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	
2	B	352	
3	C	385	
4	D	246	
5	E	185	
6	F	74	
7	G	125	
8	H	93	

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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
14	HEC	C	701	X	-	-	-
14	HEC	C	702	X	-	-	-
14	HEC	D	703	X	-	-	-

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 18069 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
			3344	2109	576	653	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
			2735	1747	453	534	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
			3089	2080	484	504	21			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	122	THR	ILE	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
			1941	1237	334	361	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
			1411	893	242	266	10			

- Molecule 6 is a protein called Ubiquinol-cytochrome C reductase complex 17 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	74	Total	C	N	O	S	0	0	0
			624	391	108	123	2			

- Molecule 7 is a protein called Ubiquinol-cytochrome C reductase complex 14 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	125	Total	C	N	O	S	0	0	0
			1012	648	172	190	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
			773	510	131	130	2			

- Molecule 9 is a protein called Ubiquinol-cytochrome C reductase complex 7.3 kDa protein.

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

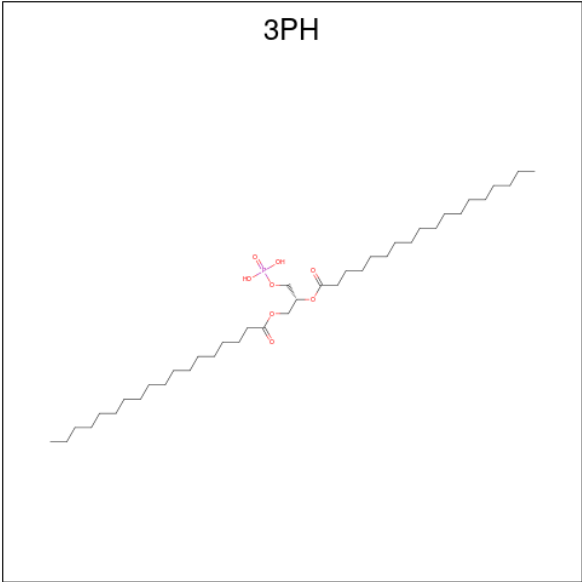
- Molecule 10 is a protein called Heavy Chain (Vh) Of Fv-Fragment.

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.

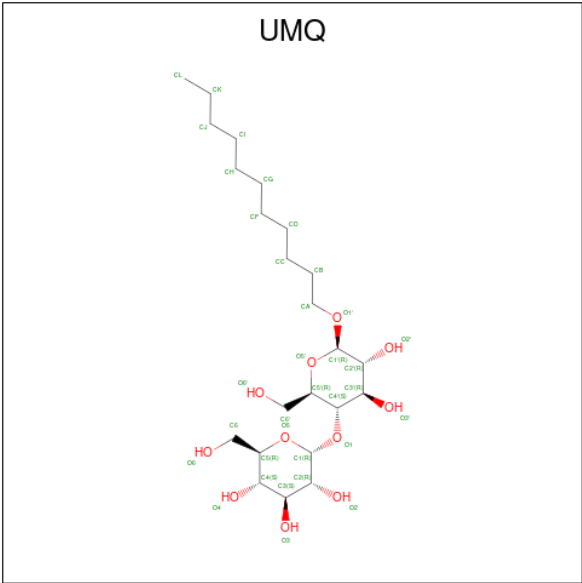
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	107	Total	C	N	O	S	0	0	0
			842	536	141	163	2			

- Molecule 12 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (CCD ID: 3PH) (formula: C₃₉H₇₇O₈P).



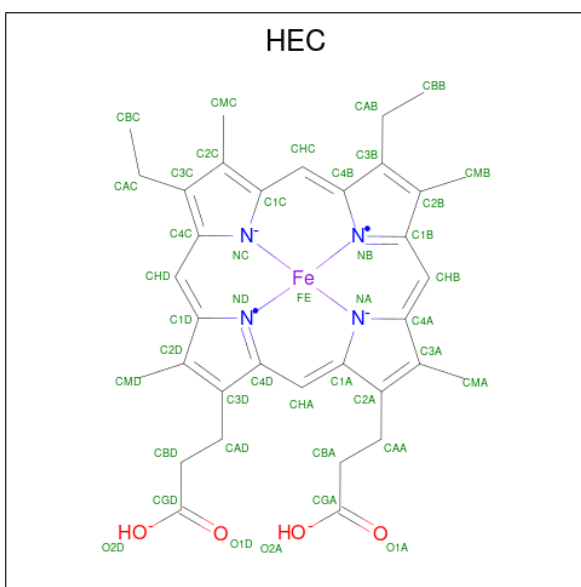
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	A	1	Total	C	O	P	0	0
			40	31	8	1		
12	D	1	Total	C	O	P	0	0
			38	29	8	1		

- Molecule 13 is UNDECYL-MALTOSIDE (CCD ID: UMQ) (formula: C₂₃H₄₄O₁₁).



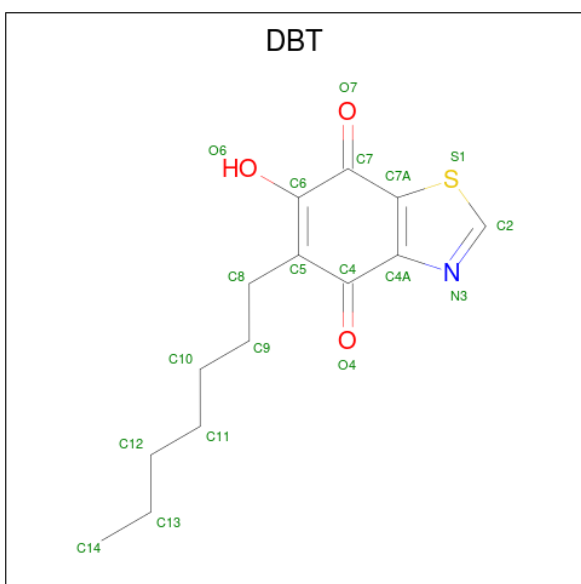
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	A	1	Total	C	O	0	0
			34	23	11		

- Molecule 14 is HEME C (CCD ID: HEC) (formula: C₃₄H₃₆FeN₄O₄).



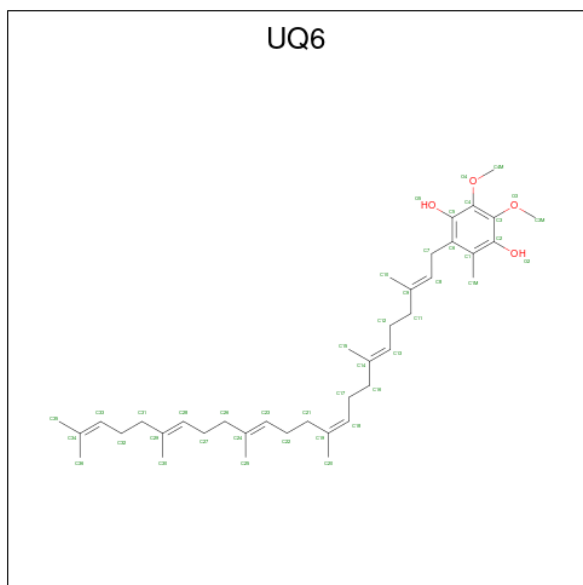
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
14	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
14	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 15 is 5-HEPTYL-6-HYDROXY-1,3-BENZOTHIAZOLE-4,7-DIONE (CCD ID: DBT) (formula: $C_{14}H_{17}NO_3S$).



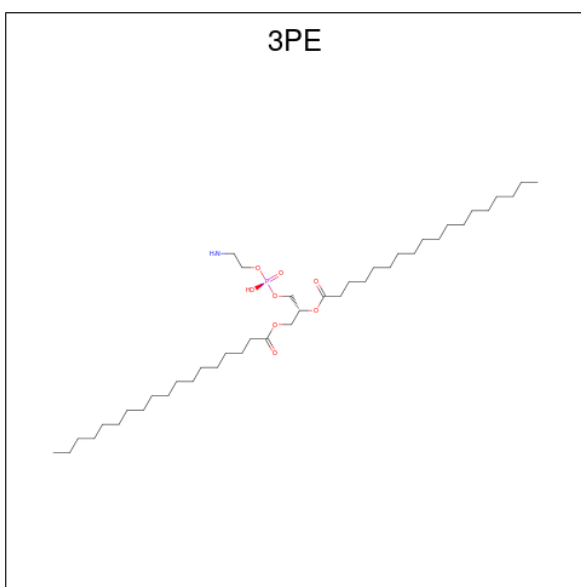
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	C	1	Total	C	N	O	S	0	0
			19	14	1	3	1		

- Molecule 16 is 5-(3,7,11,15,19,23-HEXAMETHYL-TETRACOSA-2,6,10,14,18,22-HEXA ENYL)-2,3-DIMETHOXY-6-METHYL-BENZENE-1,4-DIOL (CCD ID: UQ6) (formula: $C_{39}H_{60}O_4$).



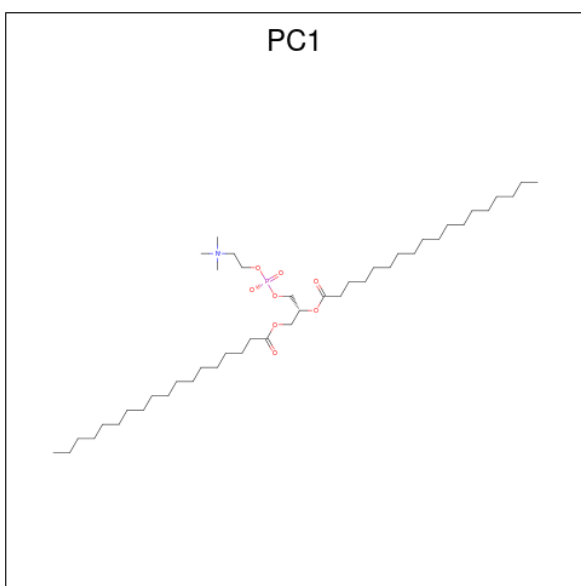
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	C	1	Total	C	O	0	0
			43	39	4		

- Molecule 17 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



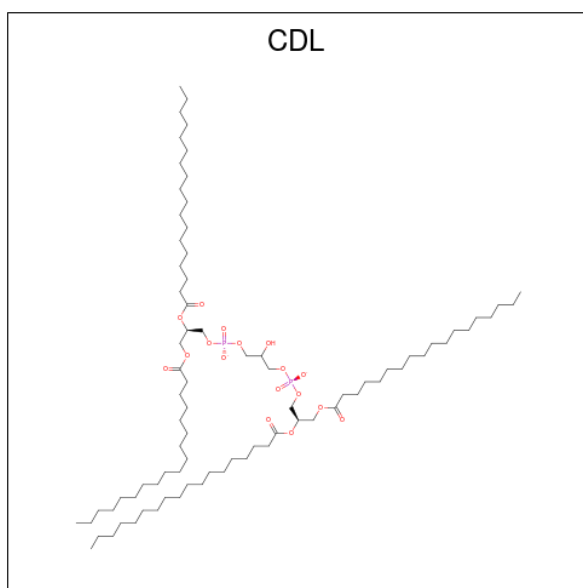
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	C	1	Total	C	N	O	P	0	0
			47	37	1	8	1		
17	C	1	Total	C	N	O	P	0	0
			40	30	1	8	1		

- Molecule 18 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



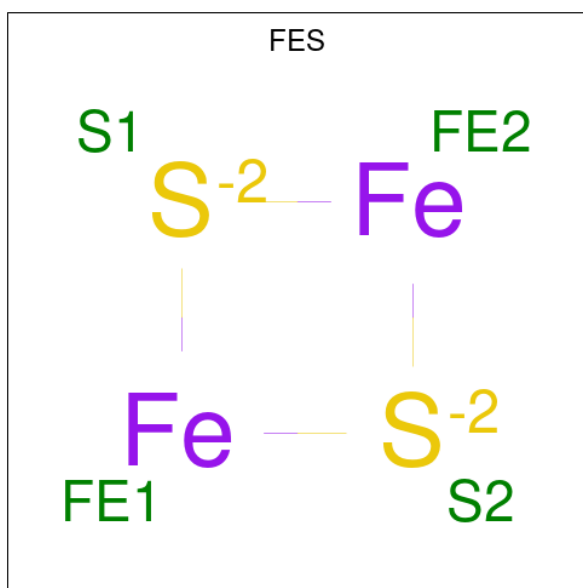
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	D	1	Total	C	N	O	P	0	0
			38	28	1	8	1		

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



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

- Molecule 20 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: 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.

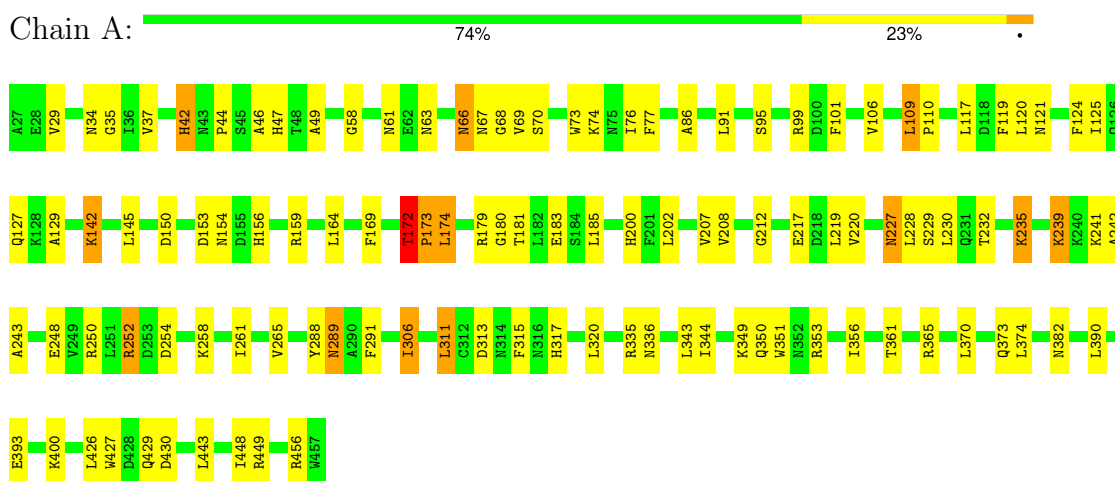
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	A	55	Total 55	O 55	0	0
21	B	11	Total 11	O 11	0	0
21	C	110	Total 110	O 110	0	0
21	D	62	Total 62	O 62	0	0
21	E	25	Total 25	O 25	0	0
21	F	4	Total 4	O 4	0	0
21	G	32	Total 32	O 32	0	0
21	H	20	Total 20	O 20	0	0
21	I	2	Total 2	O 2	0	0
21	J	3	Total 3	O 3	0	0
21	K	2	Total 2	O 2	0	0

3 Residue-property plots

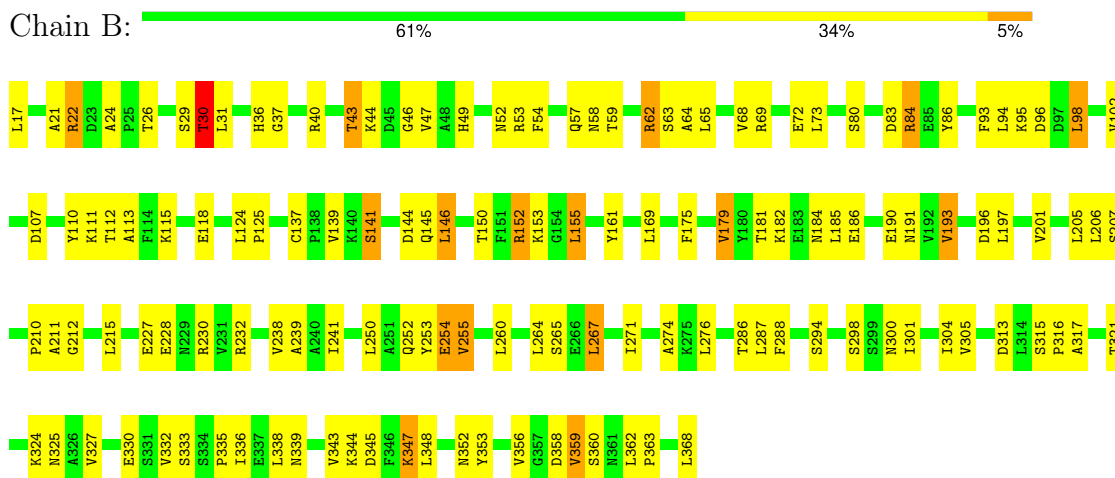
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

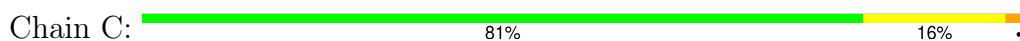
• Molecule 1: Ubiquinol-cytochrome C reductase complex core protein I

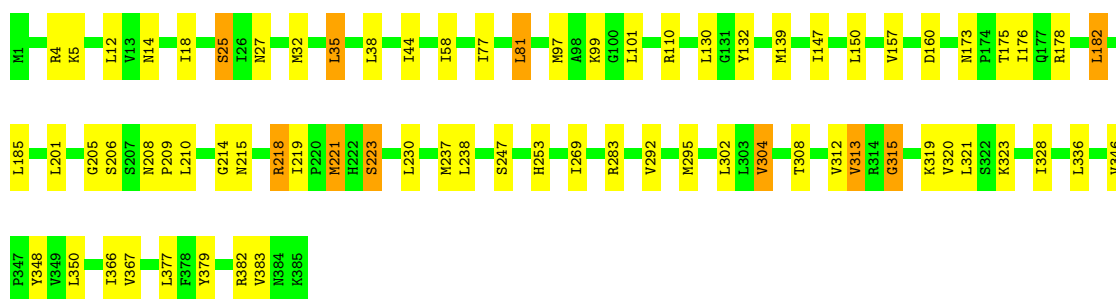


• Molecule 2: Ubiquinol-cytochrome C reductase complex core protein 2



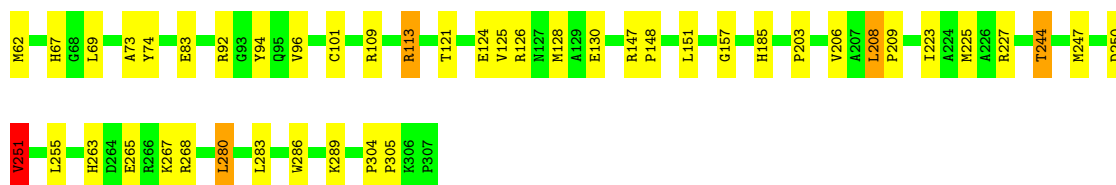
• Molecule 3: cytochrome b





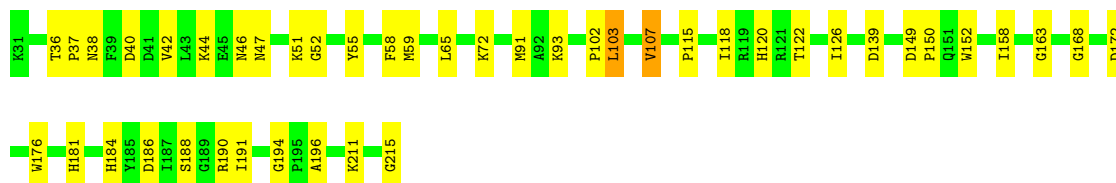
- Molecule 4: Cytochrome c1, heme protein

Chain D: 82% 16% .



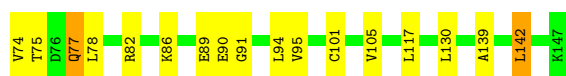
- Molecule 5: Ubiquinol-cytochrome C reductase iron-sulfur subunit

Chain E: 76% 23% .



- Molecule 6: Ubiquinol-cytochrome C reductase complex 17 kDa protein

Chain F: 77% 20% .



- Molecule 7: Ubiquinol-cytochrome C reductase complex 14 kDa protein

Chain G: 88% 11% .



- Molecule 8: Ubiquinol-cytochrome C reductase complex ubiquinone-binding protein QP-C

Chain H: 83% 14% .



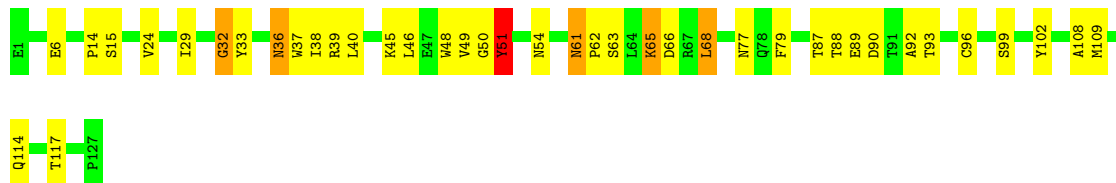
- Molecule 9: Ubiquinol-cytochrome C reductase complex 7.3 kDa protein

Chain I:  85% 11% .



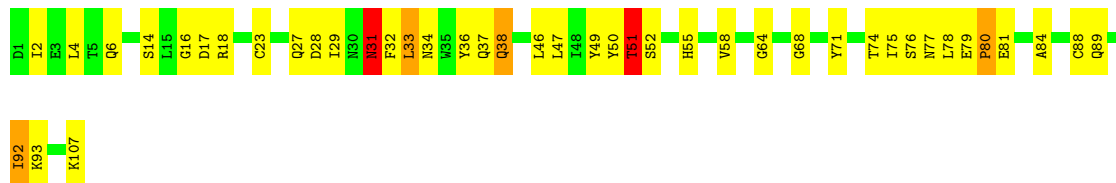
- Molecule 10: Heavy Chain (Vh) Of Fv-Fragment

Chain J:  69% 27% . .



- Molecule 11: Light Chain (Vl) Of Fv-Fragment

Chain K:  60% 35% . .



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	215.00Å 165.09Å 147.53Å 90.00° 117.33° 90.00°	Depositor
Resolution (Å)	25.00 – 2.50	Depositor
% Data completeness (in resolution range)	92.5 (25.00-2.50)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.228 , 0.252	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	18069	wwPDB-VP
Average B, all atoms (Å ²)	71.0	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: UMQ, 3PH, PC1, UQ6, DBT, HEC, FES, CDL, 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	0.42	0/3405	0.92	9/4614 (0.2%)
2	B	0.41	0/2781	0.95	12/3764 (0.3%)
3	C	0.58	1/3191 (0.0%)	1.05	16/4353 (0.4%)
4	D	0.45	0/2002	1.01	8/2726 (0.3%)
5	E	0.46	0/1444	1.03	10/1957 (0.5%)
6	F	0.38	0/638	0.91	1/858 (0.1%)
7	G	0.46	0/1032	0.97	3/1397 (0.2%)
8	H	0.44	0/804	0.89	2/1088 (0.2%)
9	I	0.43	0/462	0.83	0/622
10	J	0.39	0/1043	0.90	4/1422 (0.3%)
11	K	0.40	0/863	0.84	1/1172 (0.1%)
All	All	0.46	1/17665 (0.0%)	0.97	66/23973 (0.3%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	367	VAL	CA-CB	5.62	1.57	1.54

The worst 5 of 66 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	47	ASN	N-CA-C	-9.38	102.34	113.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	346	VAL	N-CA-C	8.43	127.08	108.88
2	B	179	VAL	N-CA-C	8.30	119.08	110.62
5	E	163	GLY	N-CA-C	8.27	126.73	115.32
3	C	328	ILE	N-CA-C	-7.85	103.16	110.53

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	3344	0	3321	73	0
2	B	2735	0	2774	84	0
3	C	3089	0	3125	40	0
4	D	1941	0	1862	25	0
5	E	1411	0	1386	26	0
6	F	624	0	581	12	0
7	G	1012	0	1026	9	0
8	H	773	0	736	13	0
9	I	449	0	445	5	0
10	J	1015	0	959	30	0
11	K	842	0	820	26	0
12	A	40	0	53	4	0
12	D	38	0	49	3	0
13	A	34	0	44	2	0
14	C	86	0	64	3	0
14	D	43	0	30	0	0
15	C	19	0	17	1	0
16	C	43	0	58	11	0
17	C	87	0	128	3	0
18	D	38	0	50	3	0
19	D	76	0	99	6	0
20	E	4	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	A	55	0	0	1	0
21	B	11	0	0	0	0
21	C	110	0	0	5	0
21	D	62	0	0	0	0
21	E	25	0	0	0	0
21	F	4	0	0	1	0
21	G	32	0	0	1	0
21	H	20	0	0	1	0
21	I	2	0	0	0	0
21	J	3	0	0	0	0
21	K	2	0	0	0	0
All	All	18069	0	17627	345	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 345 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	1.01	0.98
17:C:710:3PE:H111	8:H:51:ARG:HD2	1.53	0.90
2:B:182:LYS:HB2	2:B:211:ALA:HB2	1.58	0.86
6:F:77:GLN:H	6:F:77:GLN:NE2	1.75	0.85
1:A:63:ASN:HB2	1:A:66:ASN:ND2	1.91	0.84

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%)	391 (91%)	33 (8%)	5 (1%)	10 20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	350/352 (99%)	304 (87%)	39 (11%)	7 (2%)	6	10
3	C	383/385 (100%)	368 (96%)	14 (4%)	1 (0%)	36	55
4	D	244/246 (99%)	233 (96%)	11 (4%)	0	100	100
5	E	183/185 (99%)	168 (92%)	12 (7%)	3 (2%)	7	14
6	F	72/74 (97%)	69 (96%)	3 (4%)	0	100	100
7	G	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
8	H	91/93 (98%)	78 (86%)	9 (10%)	4 (4%)	2	2
9	I	53/55 (96%)	49 (92%)	2 (4%)	2 (4%)	2	3
10	J	125/127 (98%)	114 (91%)	8 (6%)	3 (2%)	4	8
11	K	105/107 (98%)	88 (84%)	11 (10%)	6 (6%)	1	1
All	All	2158/2180 (99%)	1983 (92%)	144 (7%)	31 (1%)	9	17

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	152	ARG
2	B	335	PRO
3	C	223	SER
8	H	93	ASN
11	K	80	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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%)	339 (92%)	31 (8%)	10	22
2	B	301/301 (100%)	275 (91%)	26 (9%)	10	21
3	C	338/338 (100%)	314 (93%)	24 (7%)	13	29
4	D	204/204 (100%)	197 (97%)	7 (3%)	32	60
5	E	151/151 (100%)	146 (97%)	5 (3%)	33	61
6	F	67/67 (100%)	62 (92%)	5 (8%)	12	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	G	109/109 (100%)	105 (96%)	4 (4%)	30	57
8	H	77/77 (100%)	76 (99%)	1 (1%)	61	82
9	I	45/45 (100%)	42 (93%)	3 (7%)	15	31
10	J	112/112 (100%)	105 (94%)	7 (6%)	16	34
11	K	93/93 (100%)	85 (91%)	8 (9%)	10	21
All	All	1867/1867 (100%)	1746 (94%)	121 (6%)	15	32

5 of 121 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	5	LYS
10	J	68	LEU
3	C	292	VAL
10	J	66	ASP
11	K	92	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 72 such sidechains are listed below:

Mol	Chain	Res	Type
7	G	57	GLN
11	K	91	HIS
7	G	97	GLN
10	J	77	ASN
1	A	317	HIS

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

13 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
20	FES	E	704	5	0,4,4	-	-	-		
12	3PH	D	714	-	37,37,47	1.09	1 (2%)	40,42,52	1.46	8 (20%)
12	3PH	A	713	-	39,39,47	1.16	4 (10%)	42,44,52	1.42	4 (9%)
14	HEC	D	703	4	50,50,50	0.93	2 (4%)	68,82,82	0.96	4 (5%)
15	DBT	C	705	-	20,20,20	0.80	0	22,27,27	1.58	3 (13%)
17	3PE	C	711	-	39,39,50	0.85	1 (2%)	42,44,55	1.04	2 (4%)
18	PC1	D	715	-	37,37,53	2.05	9 (24%)	43,45,61	1.54	7 (16%)
19	CDL	D	731	-	75,75,99	1.68	13 (17%)	81,87,111	1.50	12 (14%)
13	UMQ	A	721	-	35,35,35	1.03	2 (5%)	46,46,46	1.71	8 (17%)
14	HEC	C	701	3	50,50,50	1.46	7 (14%)	68,82,82	1.46	7 (10%)
16	UQ6	C	706	-	43,43,43	3.23	19 (44%)	54,55,55	2.08	11 (20%)
14	HEC	C	702	3	50,50,50	1.25	4 (8%)	68,82,82	1.47	6 (8%)
17	3PE	C	710	-	46,46,50	1.17	5 (10%)	49,51,55	1.28	3 (6%)

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
20	FES	E	704	5	-	-	0/1/1/1
14	HEC	D	703	4	1/1/3/7	6/14/54/54	-
12	3PH	A	713	-	-	19/41/41/49	-
12	3PH	D	714	-	-	8/39/39/49	-
15	DBT	C	705	-	-	2/7/27/27	0/2/2/2
17	3PE	C	711	-	-	16/43/43/54	-
18	PC1	D	715	-	-	18/41/41/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CDL	D	731	-	-	37/86/86/110	-
13	UMQ	A	721	-	-	6/20/60/60	0/2/2/2
14	HEC	C	701	3	1/1/3/7	8/14/54/54	-
16	UQ6	C	706	-	-	18/39/39/39	0/1/1/1
14	HEC	C	702	3	1/1/3/7	8/14/54/54	-
17	3PE	C	710	-	-	19/50/50/54	-

The worst 5 of 67 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	C	706	UQ6	C7-C6	10.59	1.63	1.51
16	C	706	UQ6	C5-C6	8.05	1.51	1.40
16	C	706	UQ6	C5-C4	7.33	1.51	1.39
18	D	715	PC1	O21-C21	7.23	1.54	1.34
18	D	715	PC1	O31-C31	6.23	1.51	1.33

The worst 5 of 75 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	C	706	UQ6	C3M-O3-C3	7.80	135.91	114.74
13	A	721	UMQ	CA-O1'-C1'	-7.69	100.54	113.68
19	D	731	CDL	CB4-OB6-CB5	-6.41	102.45	117.80
14	C	702	HEC	CBC-CAC-C3C	6.38	129.72	112.42
14	C	702	HEC	CBB-CAB-C3B	6.29	129.47	112.42

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
14	C	701	HEC	NA
14	C	702	HEC	NA
14	D	703	HEC	NA

5 of 165 torsion outliers are listed below:

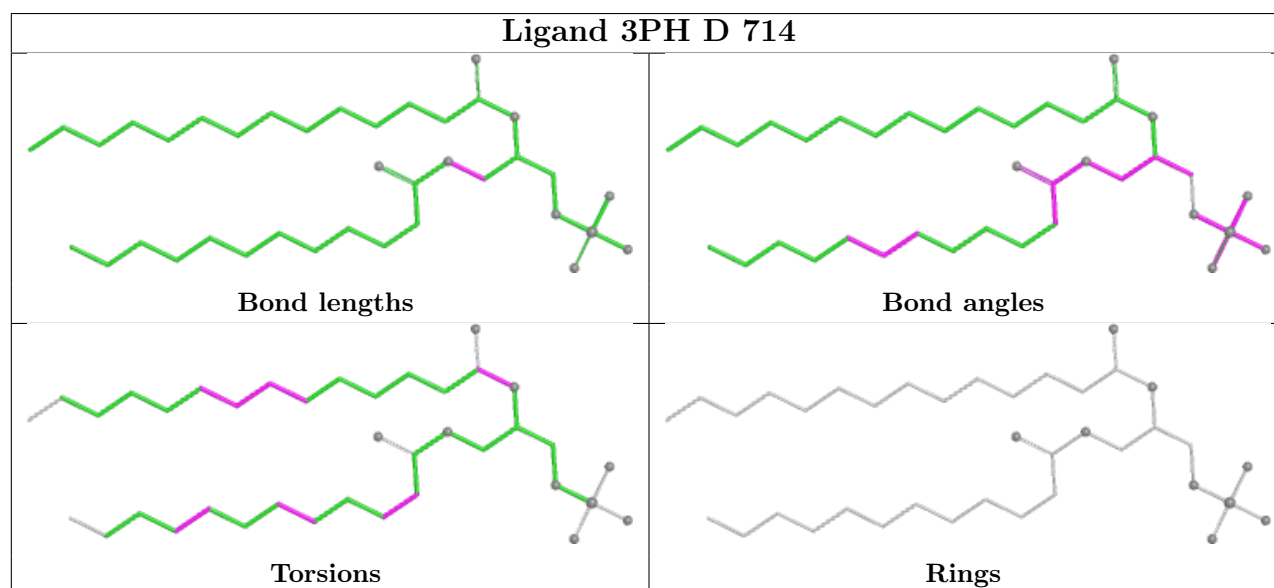
Mol	Chain	Res	Type	Atoms
17	C	710	3PE	O13-C11-C12-N
17	C	711	3PE	C1-O11-P-O12
17	C	711	3PE	C1-O11-P-O13
17	C	711	3PE	C1-O11-P-O14
18	D	715	PC1	C1-O11-P-O12

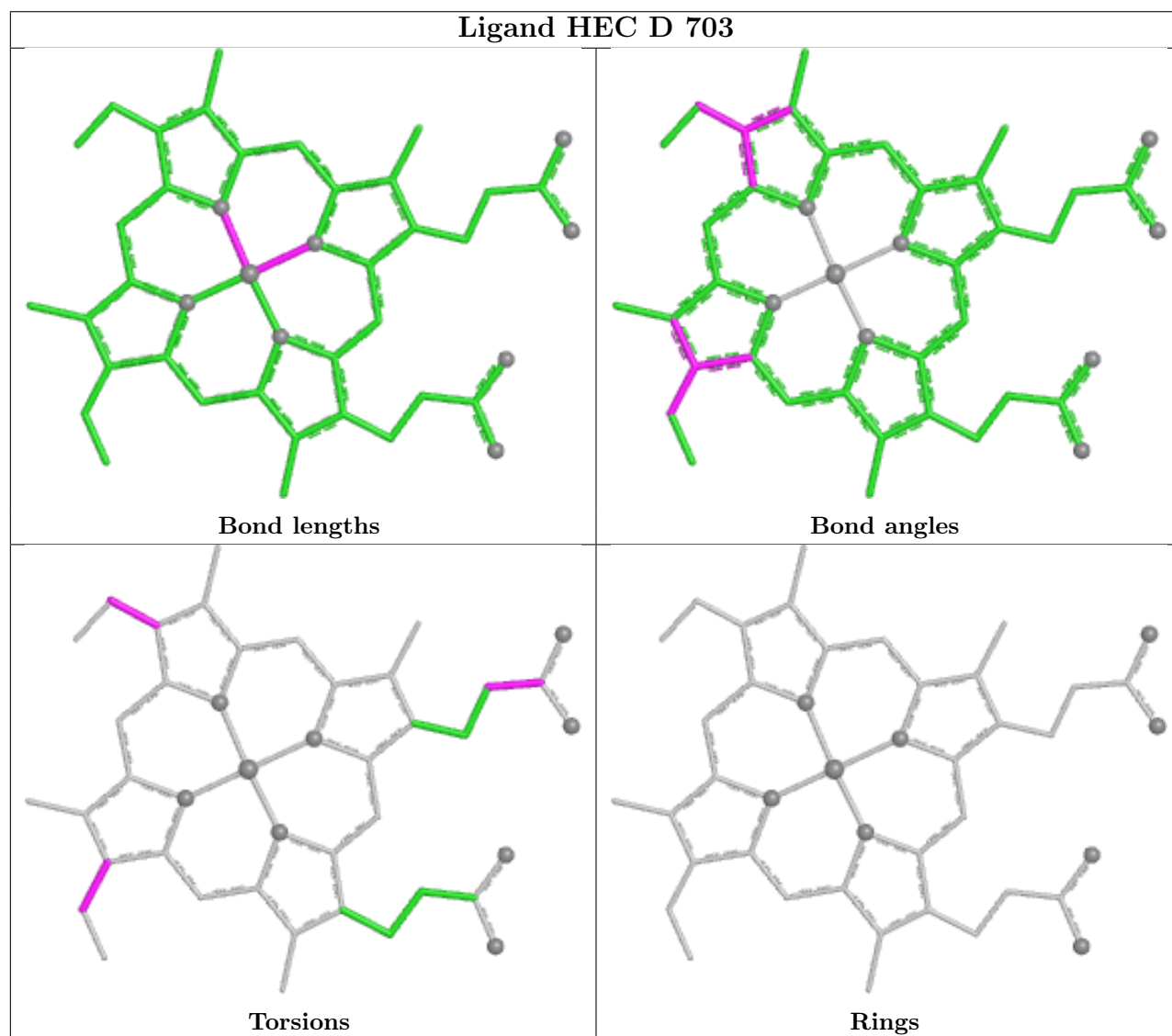
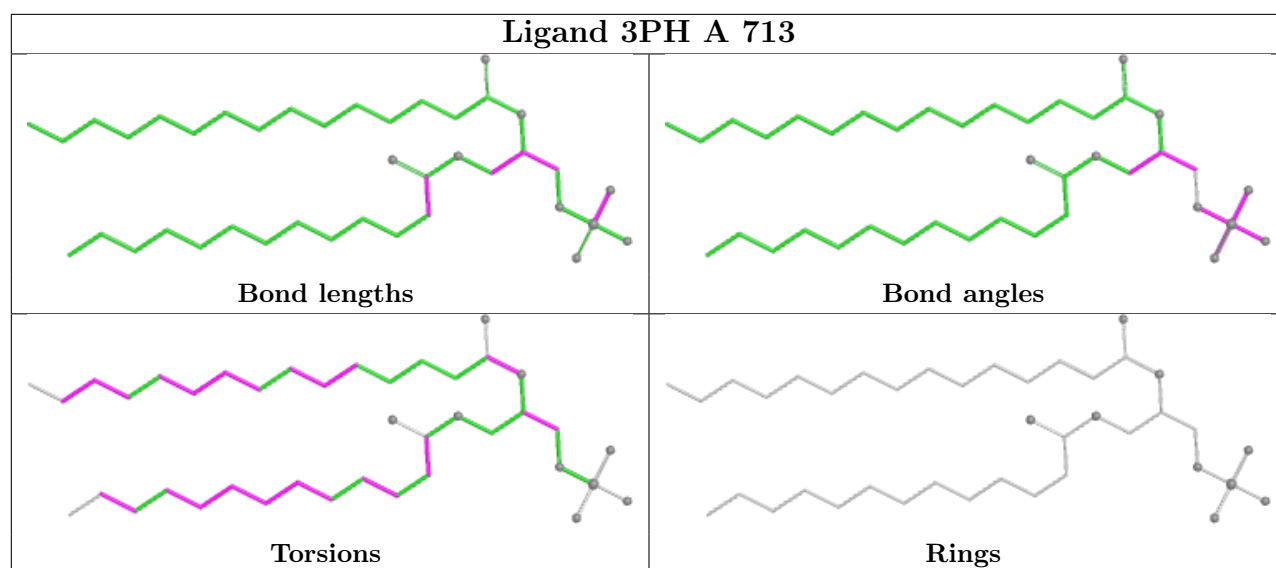
There are no ring outliers.

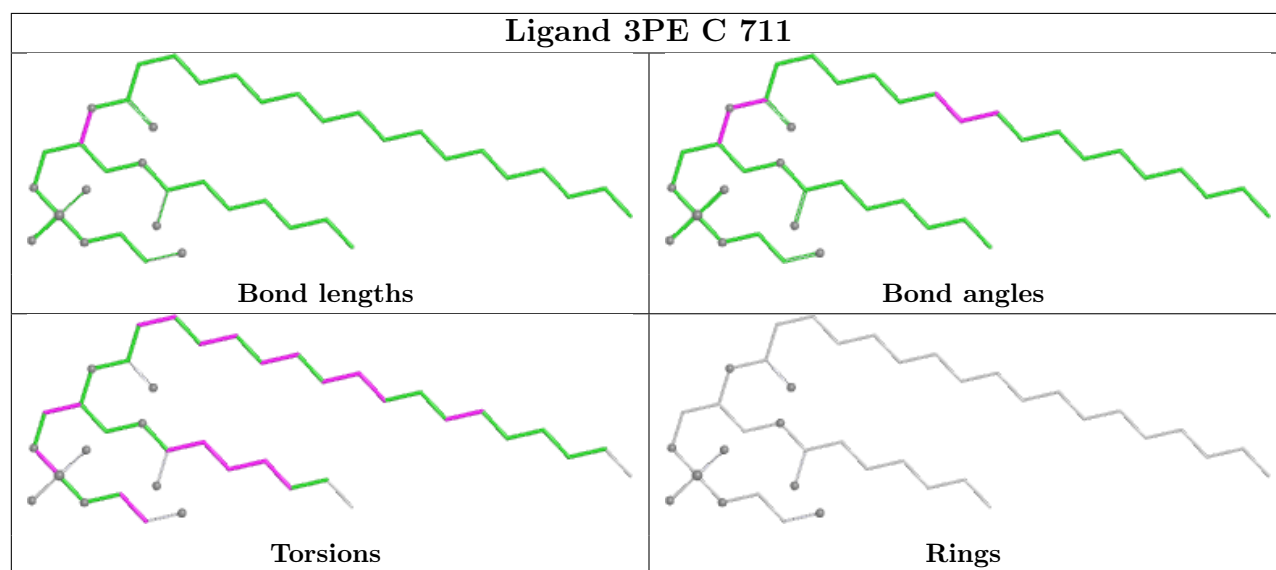
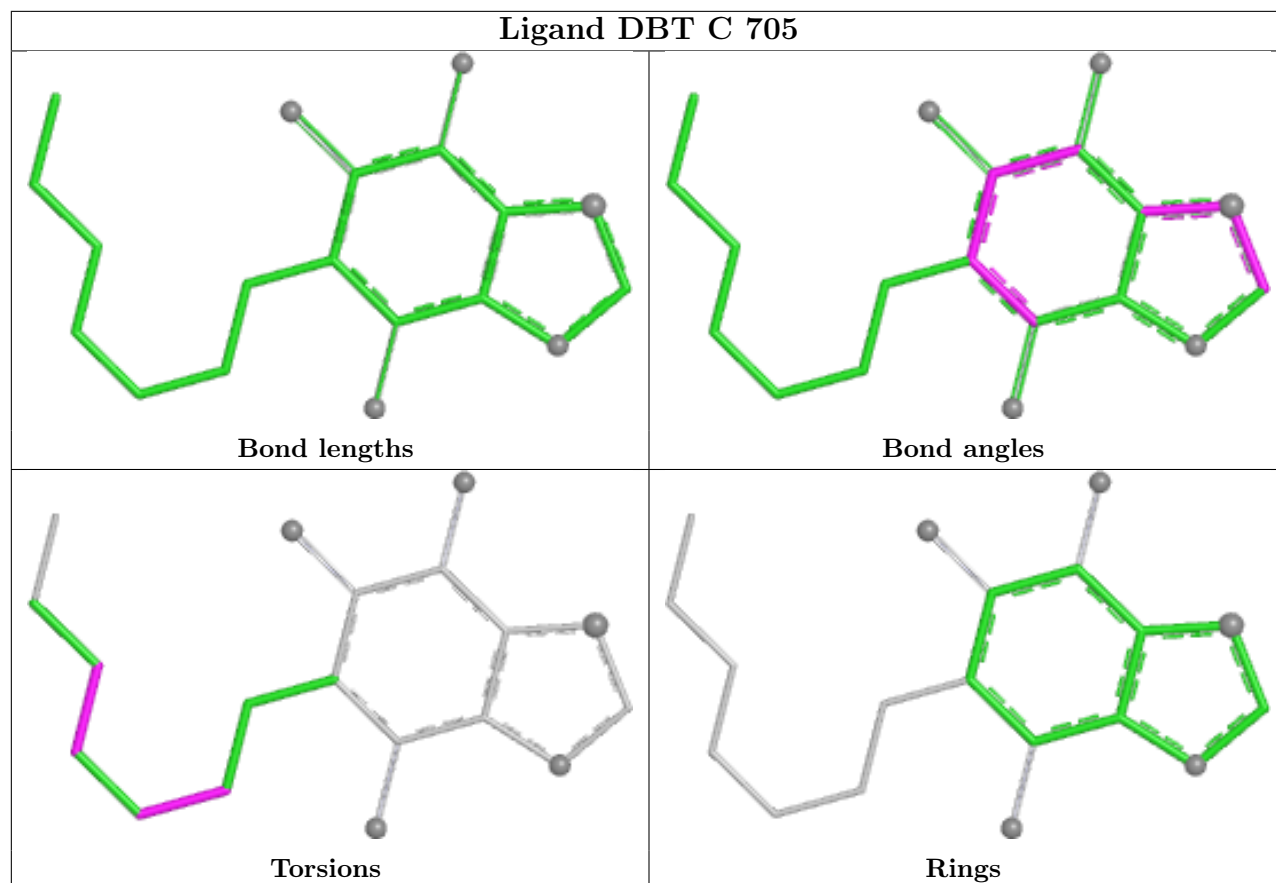
11 monomers are involved in 36 short contacts:

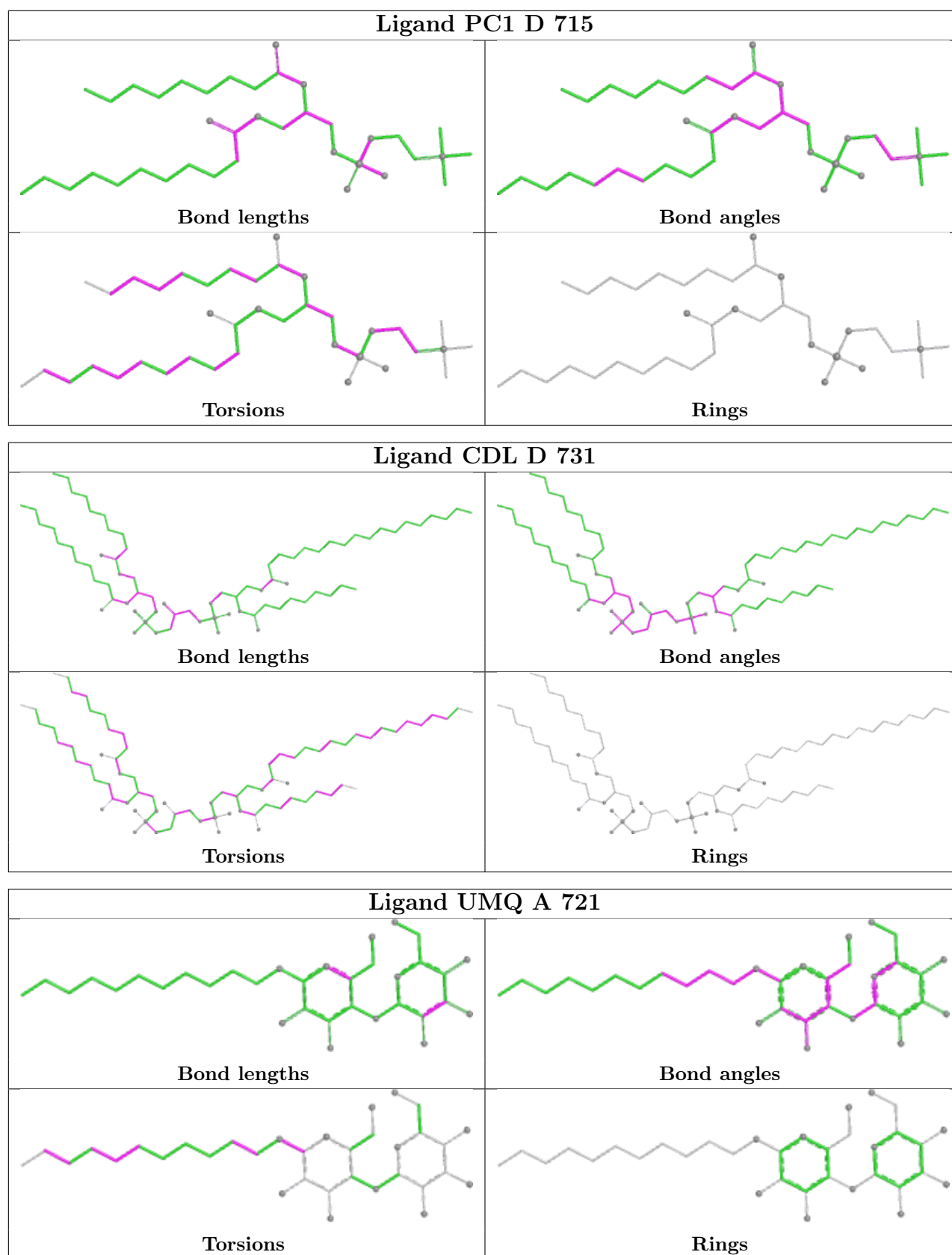
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	E	704	FES	1	0
12	D	714	3PH	3	0
12	A	713	3PH	4	0
15	C	705	DBT	1	0
18	D	715	PC1	3	0
19	D	731	CDL	6	0
13	A	721	UMQ	2	0
14	C	701	HEC	2	0
16	C	706	UQ6	11	0
14	C	702	HEC	1	0
17	C	710	3PE	3	0

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.

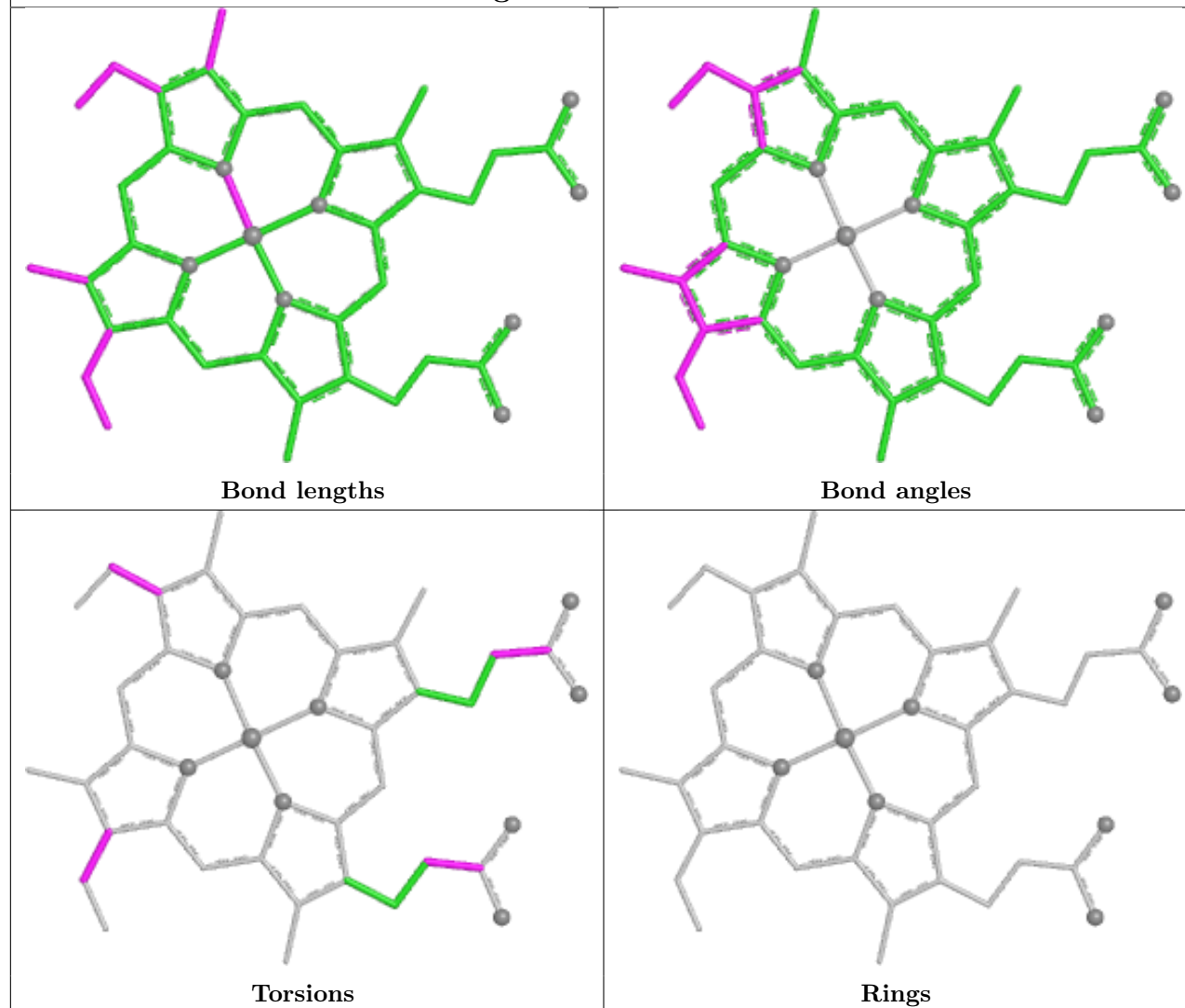




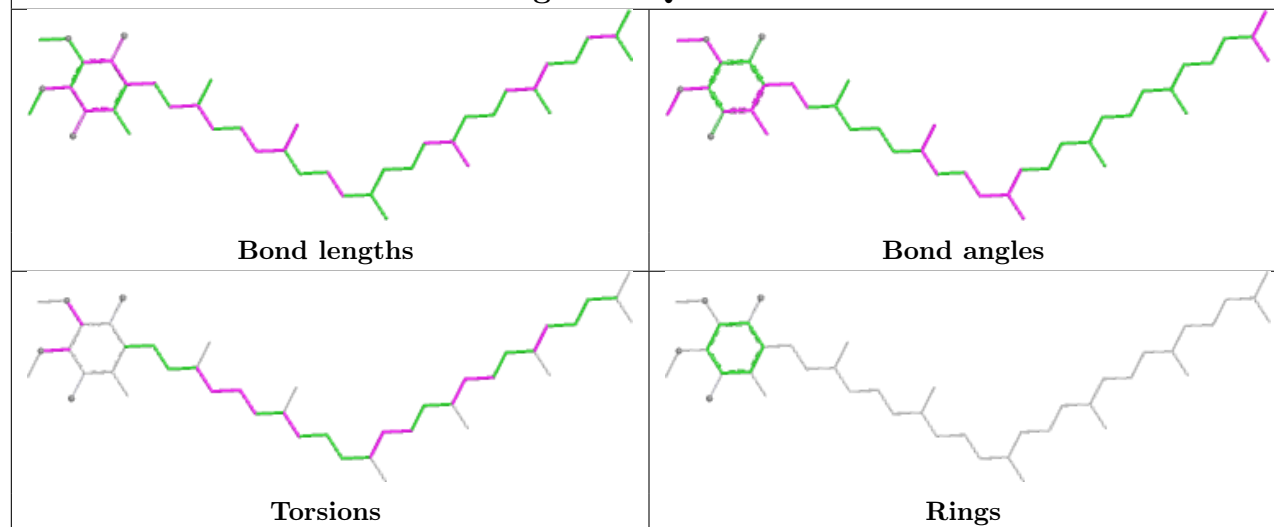




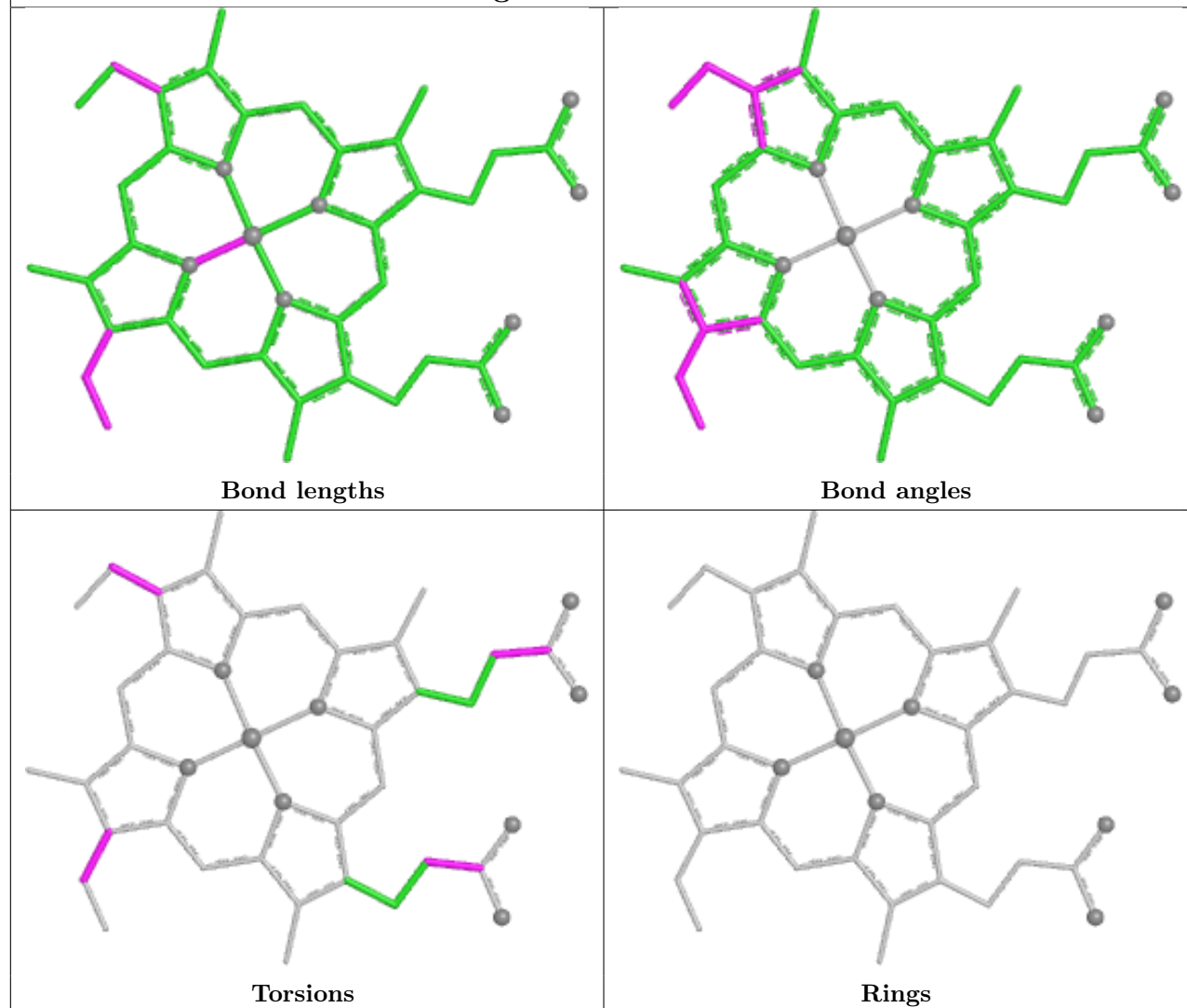
Ligand HEC C 701



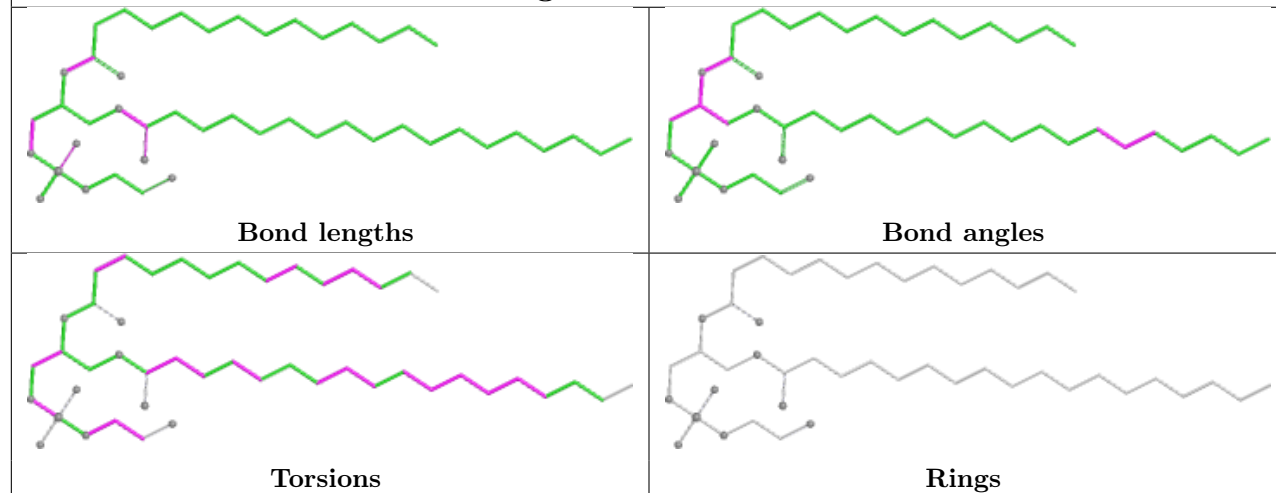
Ligand UQ6 C 706



Ligand HEC C 702



Ligand 3PE C 710



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.