



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 7, 2026 – 01:42 AM UTC

PDB ID : 1SQQ / pdb_00001sqq
Title : Crystal Structure Analysis of Bovine Bcl with Methoxy Acrylate Stilbene (MOAS)
Authors : Esser, L.; Quinn, B.; Li, Y.F.; Zhang, M.; Elberry, M.; Yu, L.; Yu, C.A.; Xia, D.
Deposited on : 2004-03-19
Resolution : 3.00 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)	:	2.49

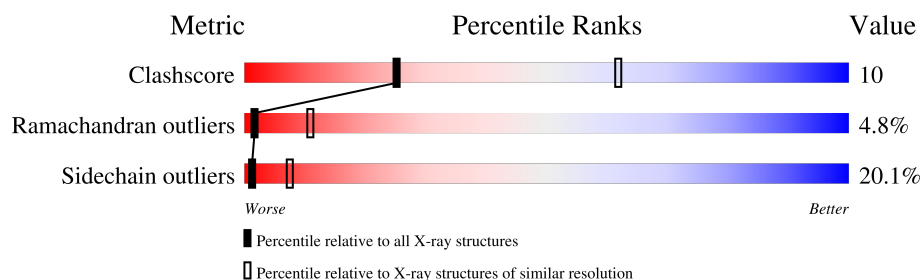
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	446	
2	B	439	
3	C	379	
4	D	241	
5	E	196	
6	F	110	
7	G	81	
8	H	78	

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Mol	Chain	Length	Quality of chain
9	I	78	8% 23% 28% 14% 27%
10	J	62	44% 35% 15% • 5%
11	K	56	57% 25% 11% • •

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 16887 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, mitochondrial precursor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	446	Total	C	N	O	S	0	0	0
			3458	2161	609	668	20			

- Molecule 2 is a protein called Ubiquinol-cytochrome-c reductase complex core protein 2, mitochondrial precursor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	423	Total	C	N	O	S	0	0	0
			3172	1993	562	610	7			

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	378	Total	C	N	O	S	0	0	0
			3003	2013	471	501	18			

- Molecule 4 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	241	Total	C	N	O	S	0	0	0
			1918	1225	330	348	15			

- Molecule 5 is a protein called Ubiquinol-cytochrome c reductase iron-sulfur subunit, mitochondrial precursor (EC 1.10.2.2) (Rieske iron-sulfur protein) (RISP) [Contains: Ubiquinol-cytochrome c reductase 8 kDa protein (Complex III subunit IX)].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	196	Total	C	N	O	S	0	0	0
			1519	957	263	291	8			

- Molecule 6 is a protein called Ubiquinol-cytochrome c reductase complex 14 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	105	Total	C	N	O	S	0	0	0
			911	576	165	168	2			

- Molecule 7 is a protein called Ubiquinol-cytochrome c reductase complex ubiquinone-binding protein QP-C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	75	Total	C	N	O	S	0	0	0
			628	410	118	99	1			

- Molecule 8 is a protein called Ubiquinol-cytochrome c reductase complex 11 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	70	Total	C	N	O	S	0	0	0
			575	347	102	121	5			

- Molecule 9 is a protein called Ubiquinol-cytochrome c reductase iron-sulfur subunit, mitochondrial precursor (EC 1.10.2.2) (Rieske iron-sulfur protein) (RISP) [Contains: Ubiquinol-cytochrome c reductase 8 kDa protein (Complex III subunit IX)].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	57	Total	C	N	O	S	0	0	0
			406	253	77	74	2			

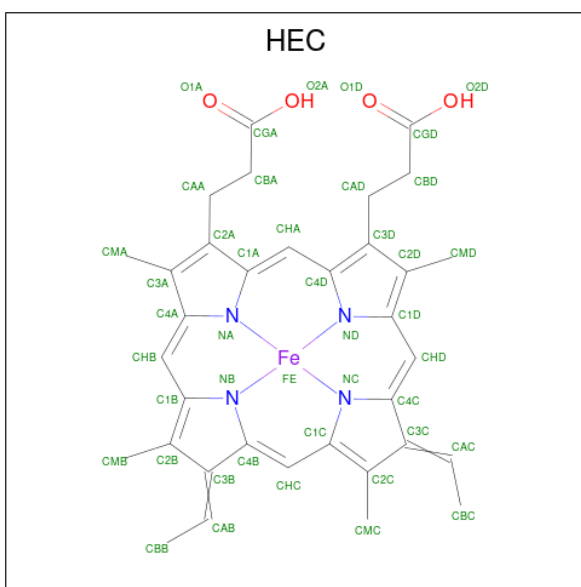
- Molecule 10 is a protein called Ubiquinol-cytochrome c reductase complex 7.2 kDa protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	59	Total	C	N	O	0	0	0
			490	321	85	84			

- Molecule 11 is a protein called Ubiquinol-cytochrome c reductase complex 6.4 kDa protein.

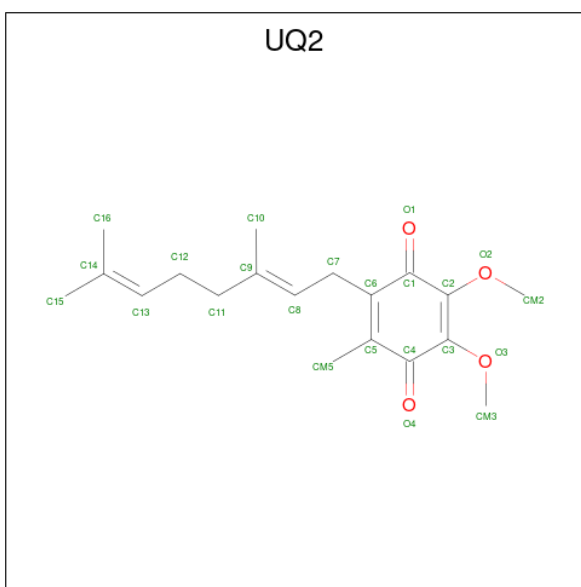
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	54	Total	C	N	O	S	0	0	0
			447	299	80	67	1			

- Molecule 12 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



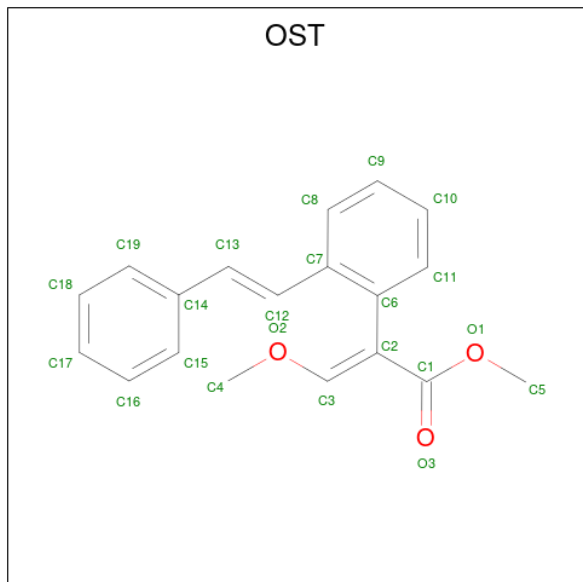
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
12	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
12	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 13 is UBIQUINONE-2 (CCD ID: UQ2) (formula: $\text{C}_{19}\text{H}_{26}\text{O}_4$).



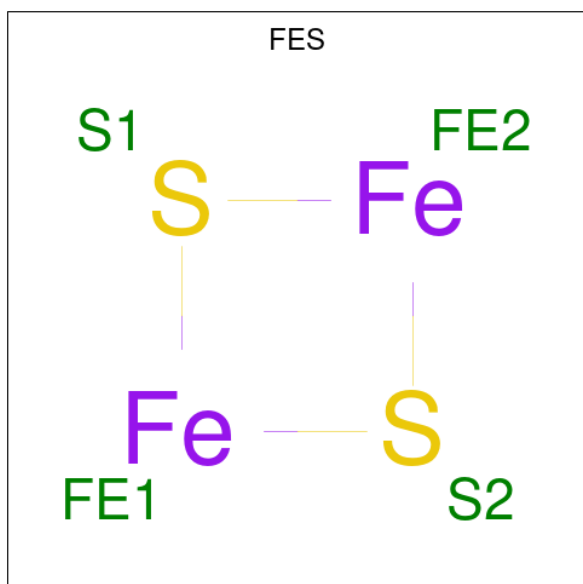
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	C	1	Total	C	O	0	0
			23	19	4		

- Molecule 14 is METHYL (2Z)-3-METHOXY-2-{2-[(E)-2-PHENYLVINYL]PHENYL}ACRYLATE (CCD ID: OST) (formula: $C_{19}H_{18}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	C	1	Total	C	O	0	0
			22	19	3		

- Molecule 15 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



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

- Molecule 16 is water.

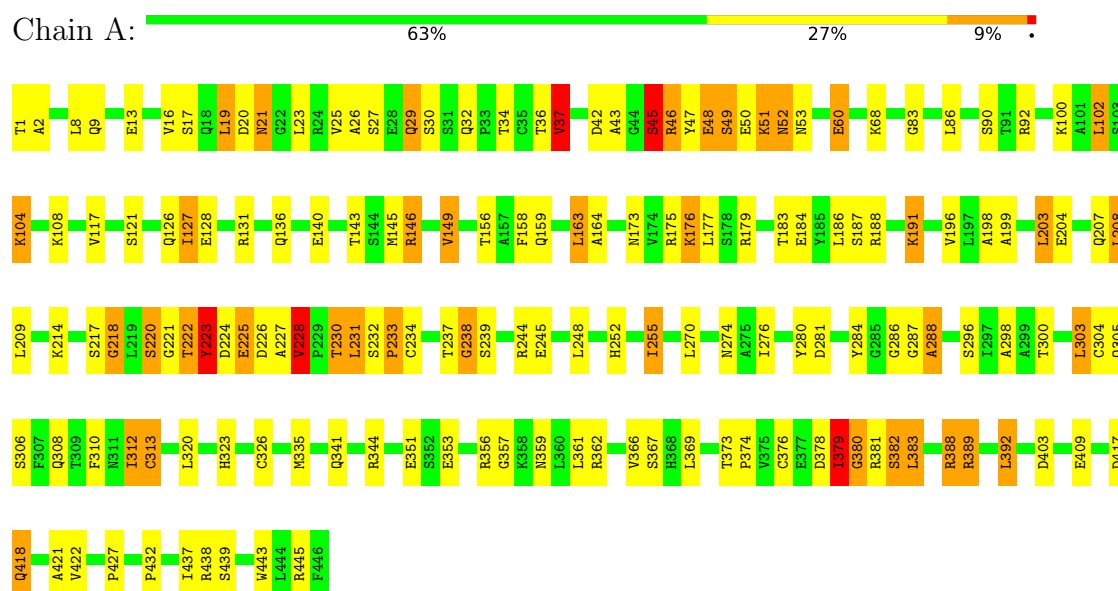
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	31	Total 31	O 31	0	0
16	B	78	Total 78	O 78	0	0
16	C	21	Total 21	O 21	0	0
16	D	5	Total 5	O 5	0	0
16	E	1	Total 1	O 1	0	0
16	F	25	Total 25	O 25	0	0
16	G	12	Total 12	O 12	0	0
16	H	2	Total 2	O 2	0	0
16	I	4	Total 4	O 4	0	0
16	J	1	Total 1	O 1	0	0
16	K	2	Total 2	O 2	0	0

3 Residue-property plots

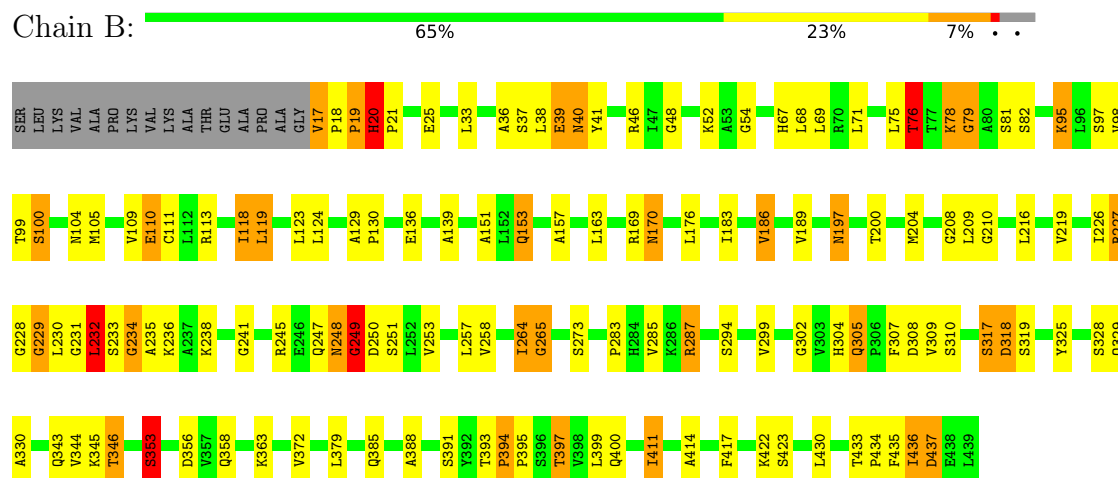
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



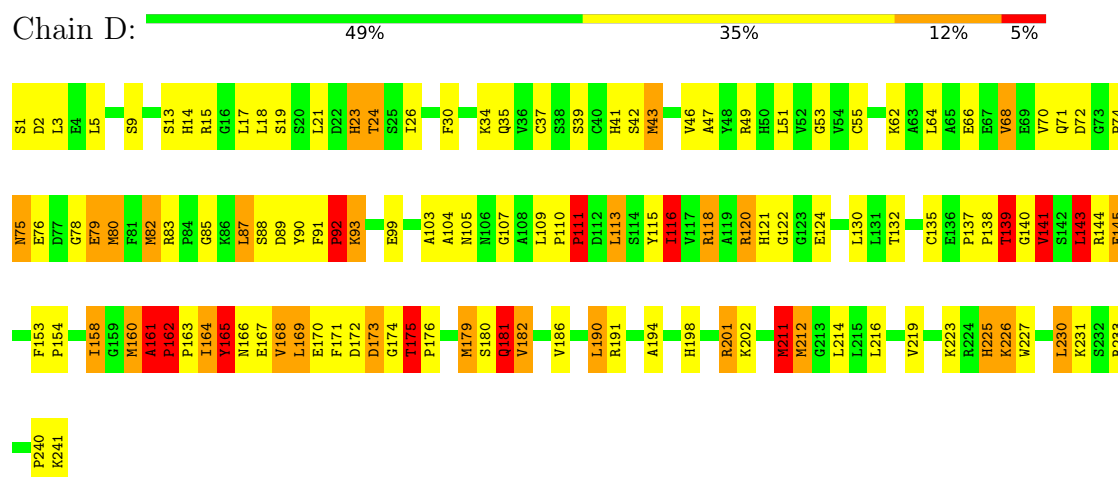
- Molecule 2: Ubiquinol-cytochrome-c reductase complex core protein 2, mitochondrial precursor



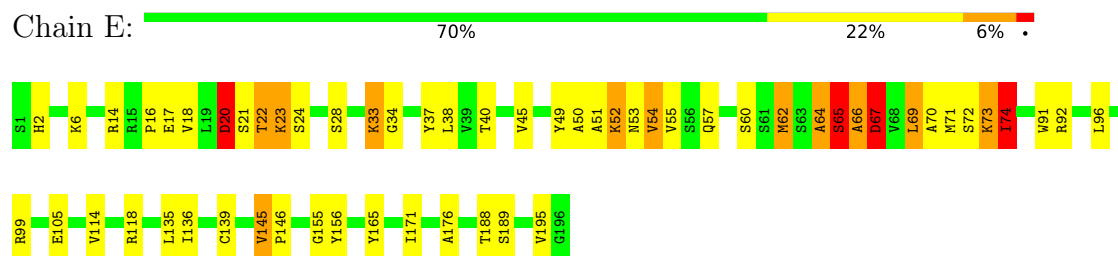
- Molecule 3: Cytochrome b



- Molecule 4: Cytochrome c1, heme protein, mitochondrial

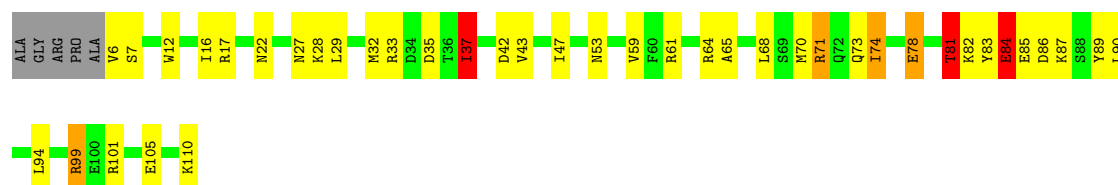


- Molecule 5: Ubiquinol-cytochrome c reductase iron-sulfur subunit, mitochondrial precursor (EC 1.10.2.2) (Rieske iron-sulfur protein) (RISP) [Contains: Ubiquinol-cytochrome c reductase 8 kDa protein (Complex III subunit IX)]



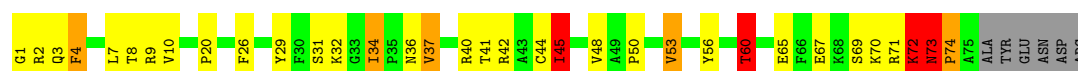
- Molecule 6: Ubiquinol-cytochrome c reductase complex 14 kDa protein

Chain F:  58% 31% • • 5%

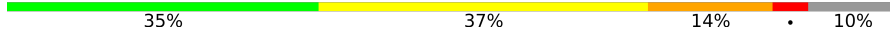


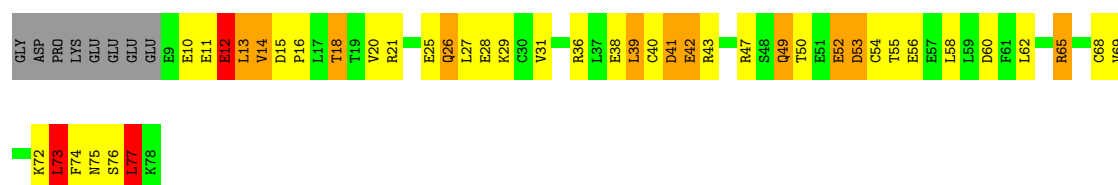
- Molecule 7: Ubiquinol-cytochrome c reductase complex ubiquinone-binding protein QP-C

Chain G:  51% 31% 6% 5% 7%



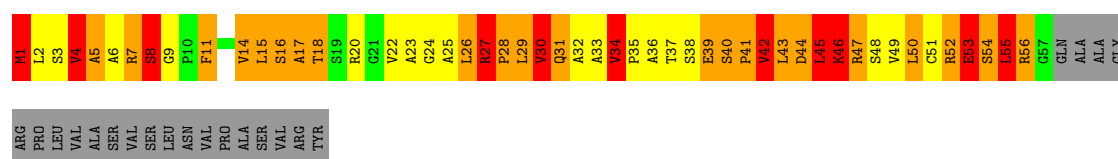
- Molecule 8: Ubiquinol-cytochrome c reductase complex 11 kDa protein

Chain H:  35% 37% 14% • 10%

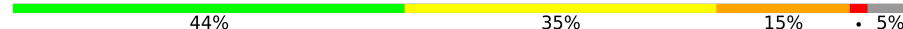


- Molecule 9: Ubiquinol-cytochrome c reductase iron-sulfur subunit, mitochondrial precursor (EC 1.10.2.2) (Rieske iron-sulfur protein) (RISP) [Contains: Ubiquinol-cytochrome c reductase 8 kDa protein (Complex III subunit IX)]

Chain I:  8% 23% 28% 14% 27%



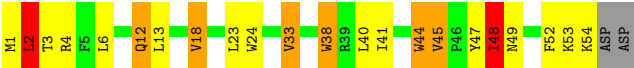
- Molecule 10: Ubiquinol-cytochrome c reductase complex 7.2 kDa protein

Chain J:  44% 35% 15% • 5%



- Molecule 11: Ubiquinol-cytochrome c reductase complex 6.4 kDa protein

Chain K:  57% 25% 11% • •



4 Data and refinement statistics

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

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	153.68Å 153.68Å 598.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00	Depositor
% Data completeness (in resolution range)	96.8 (50.00-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.228 , 0.295	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	16887	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: FES, HEC, OST, UQ2

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	1.18	6/3531 (0.2%)	1.10	2/4792 (0.0%)
2	B	1.38	13/3232 (0.4%)	1.17	4/4386 (0.1%)
3	C	1.28	16/3100 (0.5%)	1.21	8/4242 (0.2%)
4	D	1.24	11/1977 (0.6%)	1.12	7/2684 (0.3%)
5	E	0.90	3/1553 (0.2%)	1.08	7/2100 (0.3%)
6	F	1.26	4/930 (0.4%)	1.18	0/1246
7	G	1.56	7/649 (1.1%)	1.25	4/878 (0.5%)
8	H	1.27	3/580 (0.5%)	1.18	0/777
9	I	2.16	15/411 (3.6%)	1.53	8/558 (1.4%)
10	J	1.32	6/503 (1.2%)	1.18	1/678 (0.1%)
11	K	1.32	5/463 (1.1%)	1.12	0/632
All	All	1.29	89/16929 (0.5%)	1.16	41/22973 (0.2%)

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	28
2	B	0	33
3	C	0	20
4	D	0	50
6	F	0	4
7	G	0	4
8	H	0	15
9	I	0	33
10	J	0	8
11	K	0	8
All	All	0	203

The worst 5 of 89 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	34	ILE	CA-CB	19.05	1.63	1.54
4	D	211	MET	SD-CE	-10.77	1.52	1.79
3	C	124	MET	SD-CE	9.56	2.03	1.79
3	C	240	MET	SD-CE	-8.62	1.57	1.79
9	I	46	LYS	CA-C	8.62	1.61	1.53

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	226	ILE	N-CA-C	8.53	118.55	110.53
5	E	114	VAL	N-CA-C	8.31	119.09	110.62
7	G	34	ILE	N-CA-CB	8.23	116.03	110.52
2	B	197	ASN	N-CA-C	8.14	123.33	113.23
7	G	50	PRO	N-CA-C	7.56	119.92	110.70

There are no chirality outliers.

5 of 203 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	20	ASP	Peptide
1	A	27	SER	Peptide
1	A	37	VAL	Peptide
1	A	43	ALA	Peptide
1	A	45	SER	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3458	0	3355	68	0
2	B	3172	0	3152	56	0
3	C	3003	0	3065	82	0
4	D	1918	0	1870	40	0
5	E	1519	0	1502	61	0
6	F	911	0	904	17	0
7	G	628	0	636	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	H	575	0	548	10	0
9	I	406	0	437	30	0
10	J	490	0	489	8	0
11	K	447	0	460	2	0
12	C	86	0	64	11	0
12	D	43	0	32	3	0
13	C	23	0	26	6	0
14	C	22	0	18	4	0
15	E	4	0	0	0	0
16	A	31	0	0	3	0
16	B	78	0	0	2	0
16	C	21	0	0	2	0
16	D	5	0	0	0	0
16	E	1	0	0	0	0
16	F	25	0	0	1	0
16	G	12	0	0	0	0
16	H	2	0	0	0	0
16	I	4	0	0	1	0
16	J	1	0	0	0	0
16	K	2	0	0	0	0
All	All	16887	0	16558	322	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 322 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:C:124:MET:SD	3:C:124:MET:CE	2.03	1.44
1:A:237:THR:OG1	5:E:14:ARG:NH2	1.85	1.09
3:C:53:MET:HE1	5:E:62:MET:HG2	1.37	1.05
2:B:310:SER:HB3	9:I:28:PRO:HD3	1.41	1.03
1:A:284:TYR:HE1	9:I:20:ARG:HG2	1.34	0.92

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	444/446 (100%)	393 (88%)	34 (8%)	17 (4%)	2	15
2	B	421/439 (96%)	377 (90%)	31 (7%)	13 (3%)	3	19
3	C	376/379 (99%)	321 (85%)	41 (11%)	14 (4%)	2	15
4	D	239/241 (99%)	187 (78%)	33 (14%)	19 (8%)	1	3
5	E	194/196 (99%)	174 (90%)	12 (6%)	8 (4%)	2	13
6	F	103/110 (94%)	91 (88%)	10 (10%)	2 (2%)	6	30
7	G	73/81 (90%)	66 (90%)	4 (6%)	3 (4%)	2	13
8	H	68/78 (87%)	56 (82%)	7 (10%)	5 (7%)	1	4
9	I	55/78 (70%)	24 (44%)	20 (36%)	11 (20%)	0	0
10	J	57/62 (92%)	45 (79%)	6 (10%)	6 (10%)	0	2
11	K	52/56 (93%)	45 (86%)	5 (10%)	2 (4%)	2	15
All	All	2082/2166 (96%)	1779 (85%)	203 (10%)	100 (5%)	2	11

5 of 100 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	46	ARG
1	A	121	SER
1	A	223	TYR
1	A	224	ASP

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%)	296 (80%)	74 (20%)	1	7
2	B	332/343 (97%)	285 (86%)	47 (14%)	3	16
3	C	326/327 (100%)	264 (81%)	62 (19%)	1	8
4	D	206/206 (100%)	153 (74%)	53 (26%)	0	3
5	E	168/168 (100%)	156 (93%)	12 (7%)	13	43
6	F	96/98 (98%)	76 (79%)	20 (21%)	1	7
7	G	66/71 (93%)	52 (79%)	14 (21%)	1	6
8	H	67/74 (90%)	45 (67%)	22 (33%)	0	1
9	I	44/60 (73%)	21 (48%)	23 (52%)	0	0
10	J	50/52 (96%)	36 (72%)	14 (28%)	0	2
11	K	44/46 (96%)	30 (68%)	14 (32%)	0	1
All	All	1769/1815 (98%)	1414 (80%)	355 (20%)	1	7

5 of 355 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	214	LEU
8	H	18	THR
5	E	22	THR
6	F	78	GLU
8	H	65	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 57 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	362	ASN
11	K	12	GLN
3	C	85	ASN
10	J	61	ASN
5	E	161	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 ⓘ

6 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	$\# Z > 2$
15	FES	E	197	5	0,4,4	-	-	-		
12	HEC	C	382	3	46,50,50	1.88	9 (19%)	58,82,82	2.26	17 (29%)
13	UQ2	C	383	-	23,23,23	2.90	8 (34%)	30,31,31	1.34	5 (16%)
12	HEC	D	242	4	46,50,50	1.62	8 (17%)	58,82,82	2.53	17 (29%)
12	HEC	C	381	3	46,50,50	1.64	6 (13%)	58,82,82	2.71	14 (24%)
14	OST	C	384	-	23,23,23	2.29	12 (52%)	29,29,29	1.46	6 (20%)

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
15	FES	E	197	5	-	-	0/1/1/1
12	HEC	C	382	3	-	13/14/54/54	-
13	UQ2	C	383	-	-	6/15/39/39	0/1/1/1
12	HEC	D	242	4	-	7/14/54/54	-
12	HEC	C	381	3	-	6/14/54/54	-
14	OST	C	384	-	-	6/18/18/18	0/2/2/2

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	C	383	UQ2	C6-C5	8.98	1.51	1.35
12	D	242	HEC	CAC-C3C	5.38	1.52	1.35
12	C	382	HEC	CAB-C3B	5.18	1.51	1.35
13	C	383	UQ2	C8-C9	5.06	1.44	1.33
12	C	382	HEC	CAC-C3C	4.96	1.51	1.35

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	C	381	HEC	CBB-CAB-C3B	-11.28	104.90	127.43
12	C	381	HEC	CBC-CAC-C3C	-9.31	108.83	127.43
12	D	242	HEC	CBC-CAC-C3C	-9.27	108.91	127.43
12	D	242	HEC	CBB-CAB-C3B	-8.75	109.94	127.43
12	C	382	HEC	CBB-CAB-C3B	-7.12	113.20	127.43

There are no chirality outliers.

5 of 38 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	C	382	HEC	C1A-C2A-CAA-CBA
12	C	382	HEC	C3A-C2A-CAA-CBA
12	C	382	HEC	C2B-C3B-CAB-CBB
12	C	382	HEC	C4B-C3B-CAB-CBB
12	C	382	HEC	C2C-C3C-CAC-CBC

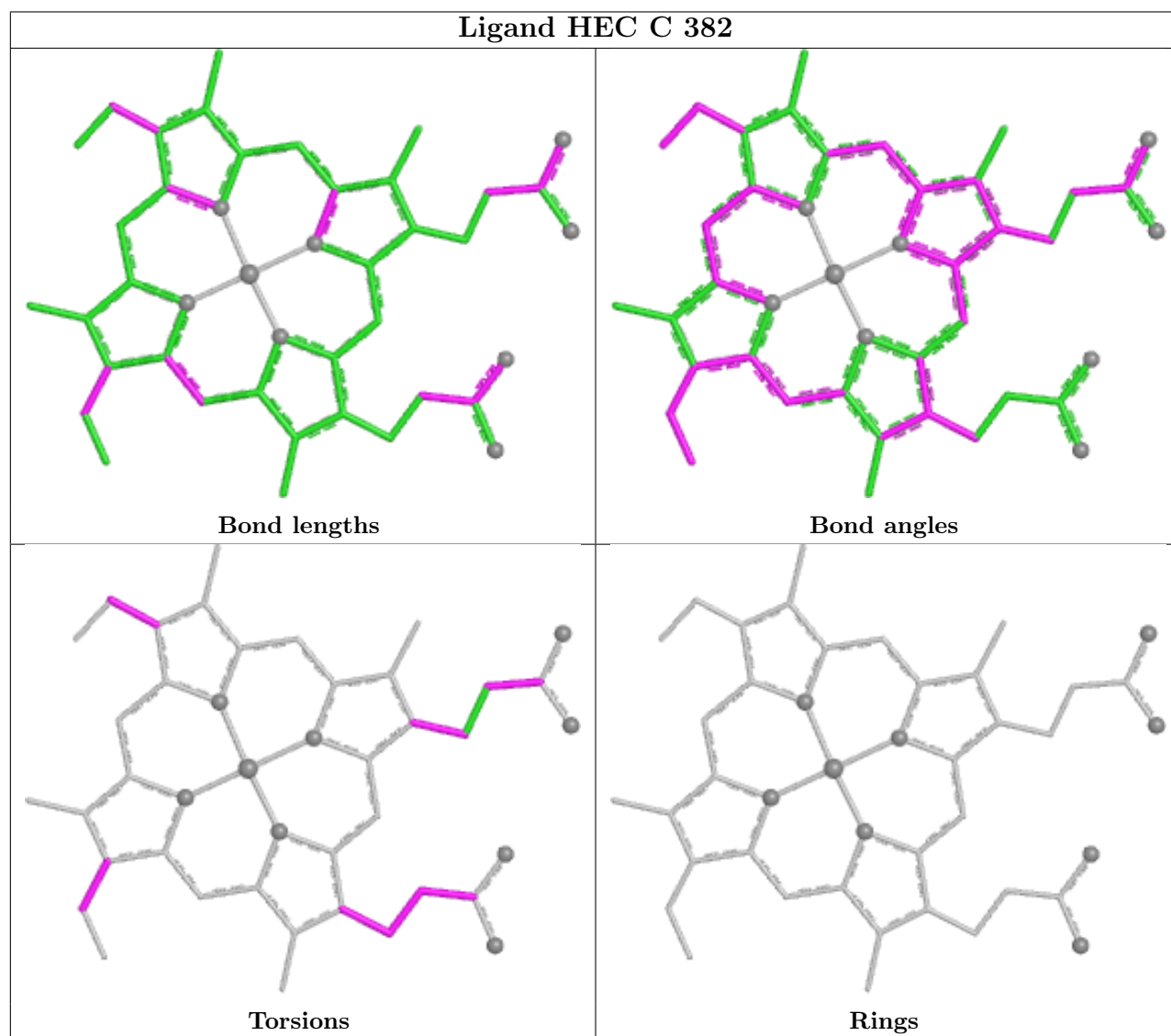
There are no ring outliers.

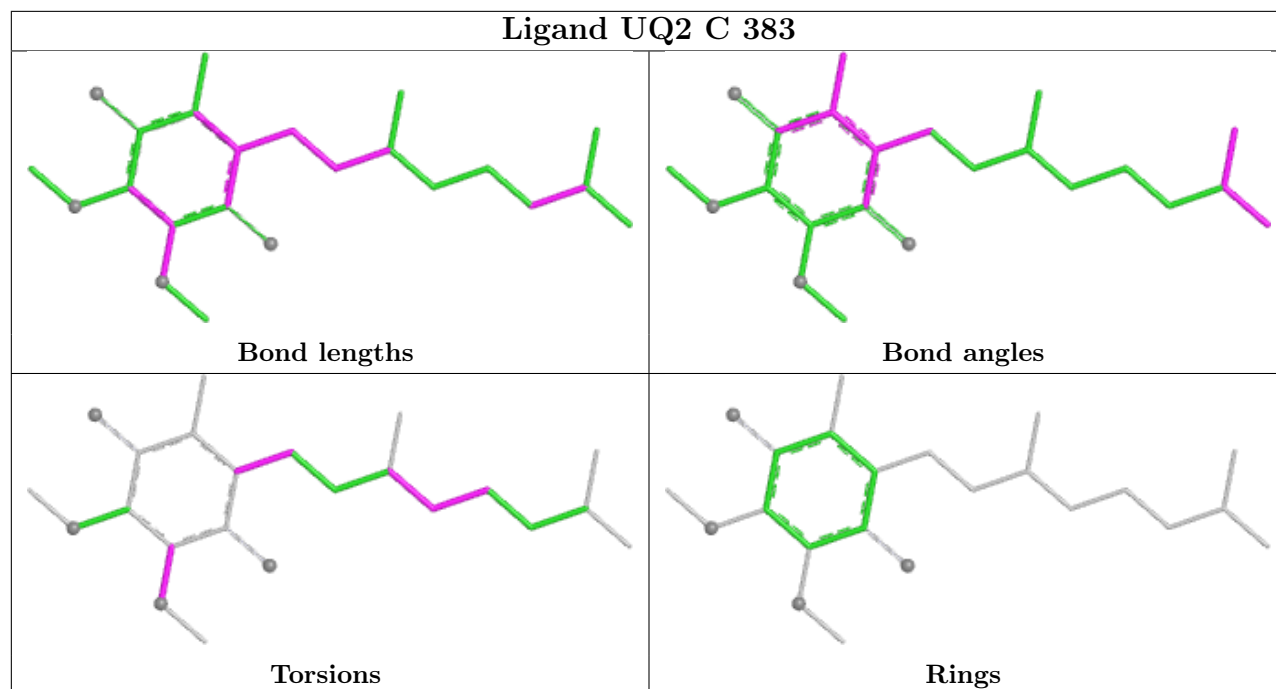
5 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	C	382	HEC	6	0
13	C	383	UQ2	6	0
12	D	242	HEC	3	0
12	C	381	HEC	5	0
14	C	384	OST	4	0

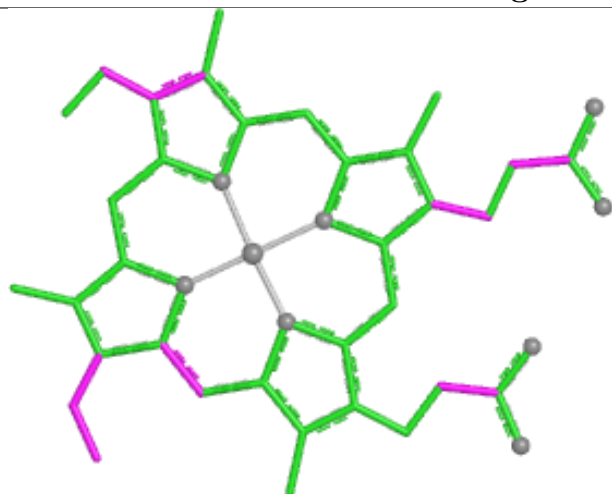
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

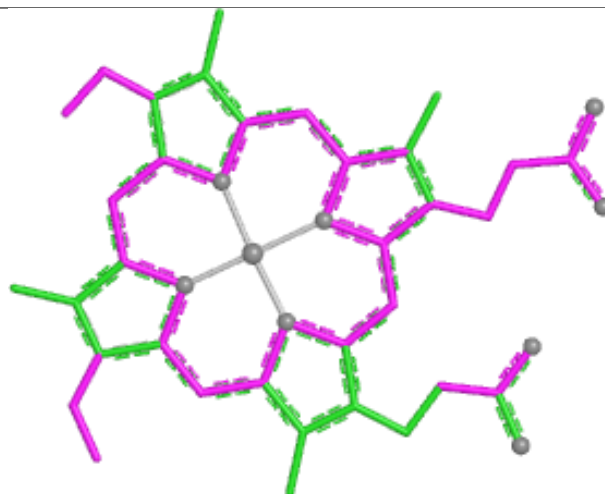




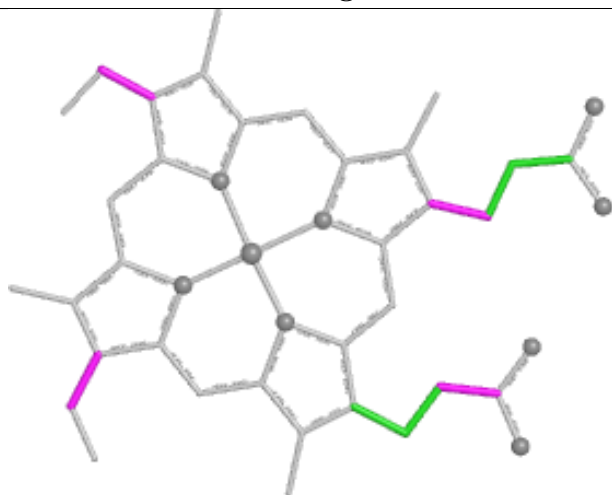
Ligand HEC D 242



Bond lengths



Bond angles

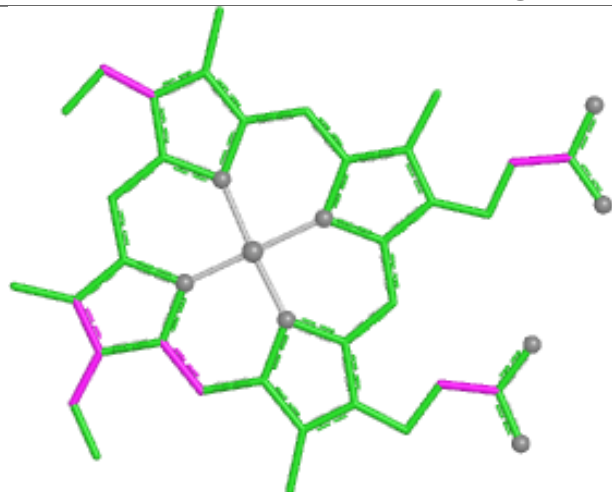


Torsions

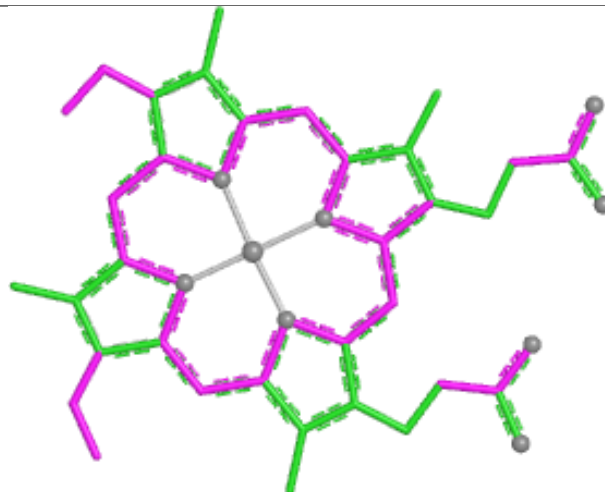


Rings

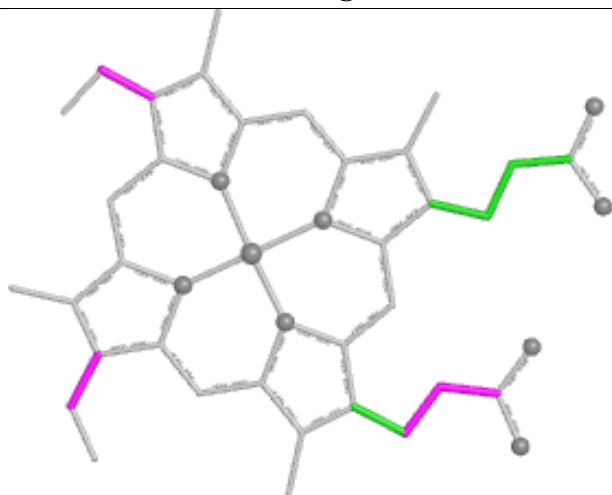
Ligand HEC C 381



Bond lengths



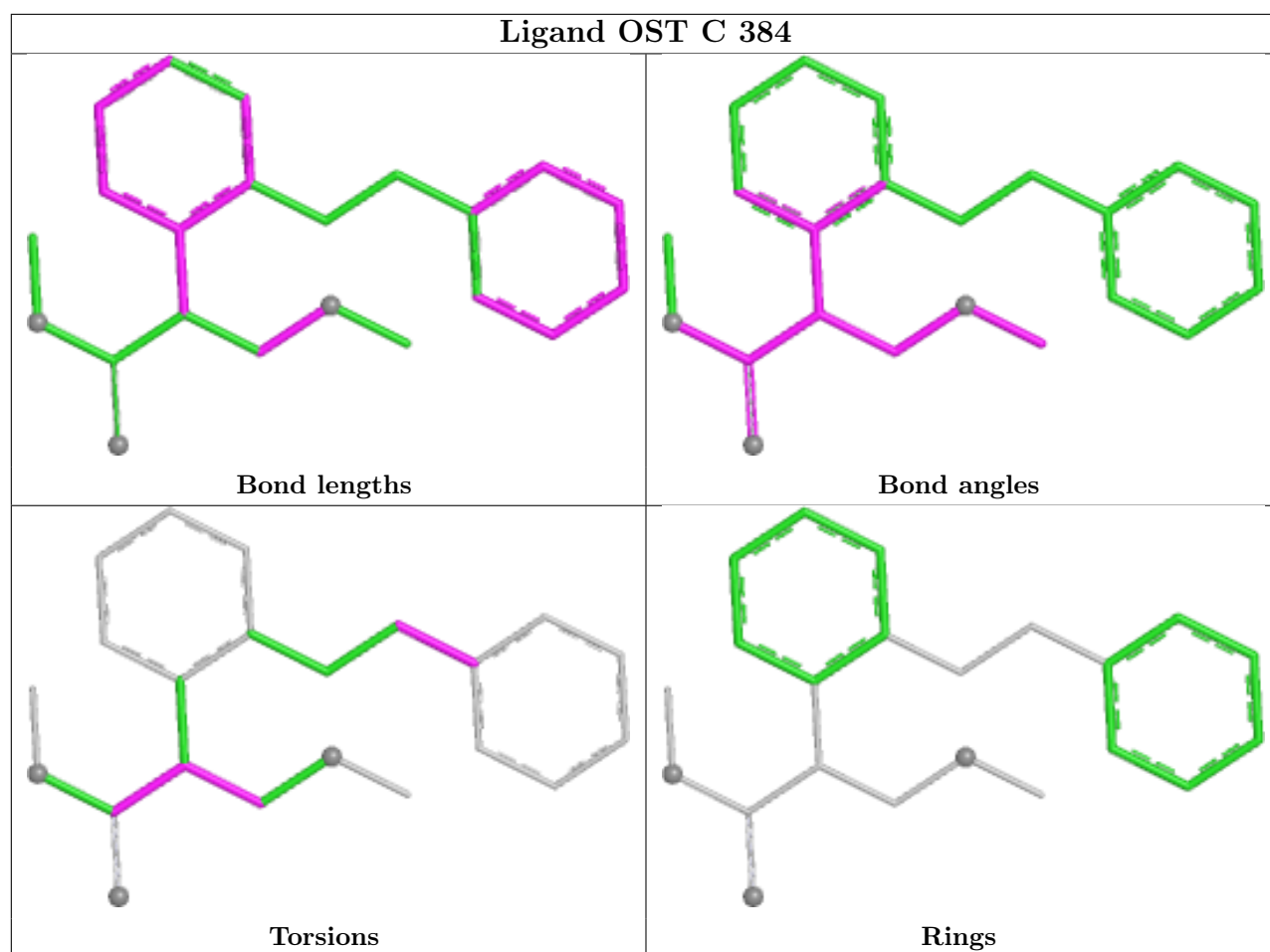
Bond angles



Torsions



Rings



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.