



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 27, 2021 – 08:58 PM EST

PDB ID : 1SQX
Title : Crystal Structure Analysis of Bovine Bcl with Stigmatellin A
Authors : Esser, L.; Quinn, B.; Li, Y.F.; Zhang, M.; Elberry, M.; Yu, L.; Yu, C.A.; Xia, D.
Deposited on : 2004-03-21
Resolution : 2.60 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : NOT EXECUTED
EDS : NOT EXECUTED
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.17.1

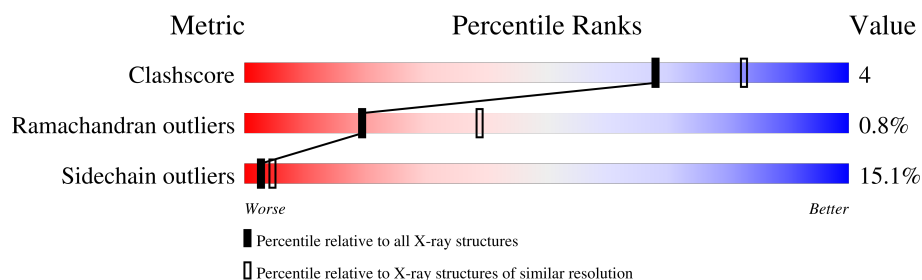
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)




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	E	196	
5	D	241	
6	G	81	
7	I	78	
8	F	110	

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Mol	Chain	Length	Quality of chain
9	K	56	 70% 25% 5%
10	H	78	 59% 26% • 14%
11	J	62	 77% 18% • •

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 16978 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	E	196	Total	C	N	O	S	0	0	0
			1519	957	263	291	8			

- 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	D	241	Total	C	N	O	S	0	0	0
			1919	1225	330	349	15			

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

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

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

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

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

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

- 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	K	53	Total	C	N	O	S	0	0	0
			438	293	78	66	1			

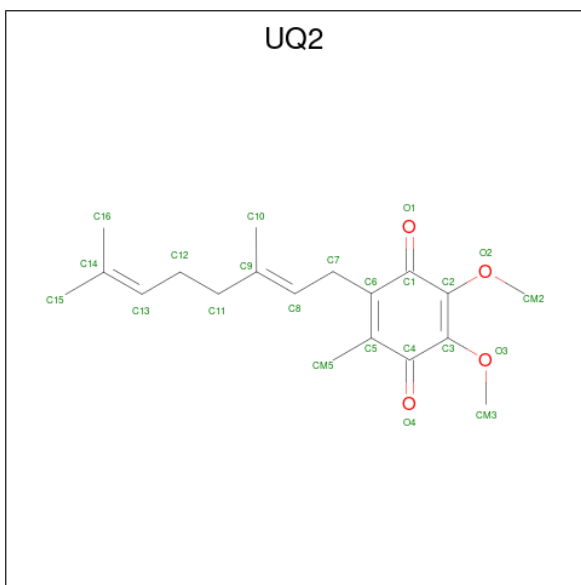
- Molecule 10 is a protein called Ubiquinol-cytochrome C reductase complex 7.2 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	H	67	Total	C	N	O	S	0	0	0
			548	332	99	112	5			

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

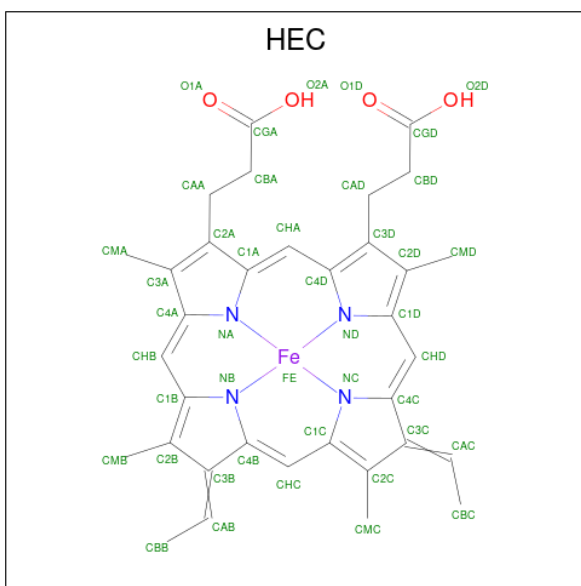
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	J	60	Total	C	N	O	0	0	0
			495	324	86	85			

- Molecule 12 is UBIQUINONE-2 (three-letter code: UQ2) (formula: C₁₉H₂₆O₄).



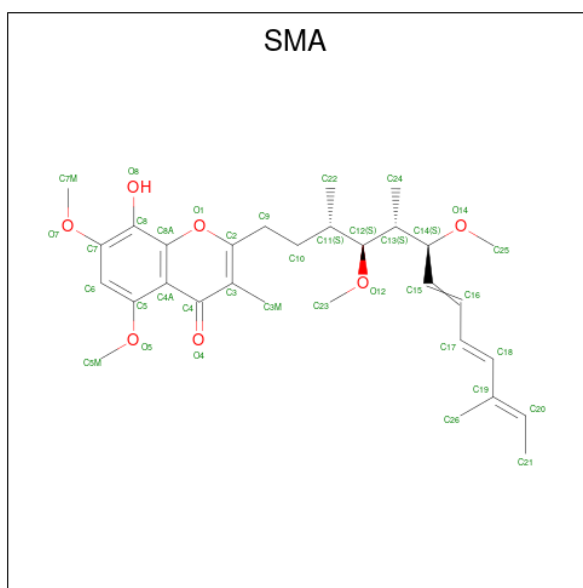
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	C	1	Total	C	O	0	0
			23	19	4		

- Molecule 13 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



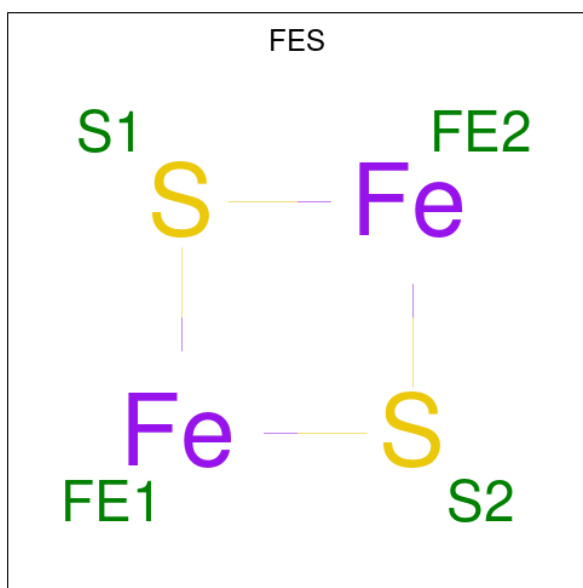
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
13	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
13	D	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 14 is STIGMATELLIN A (three-letter code: SMA) (formula: $C_{30}H_{42}O_7$).



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

- Molecule 15 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: 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.

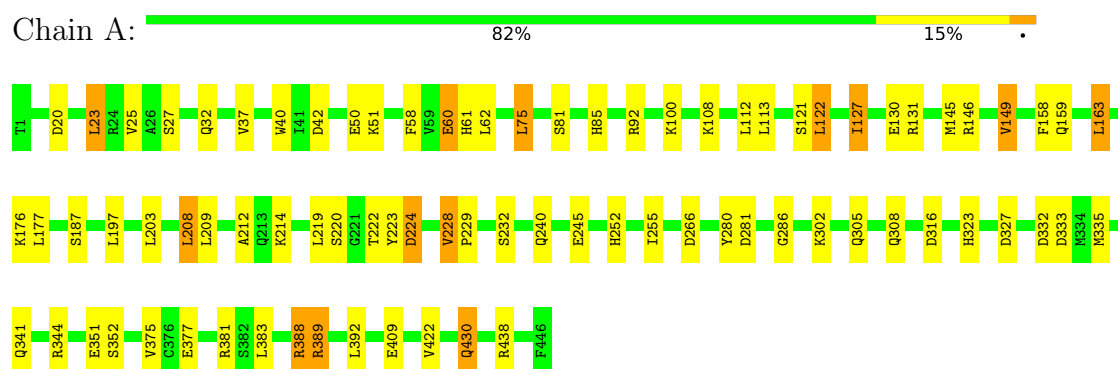
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	65	Total 65	O 65	0	0
16	B	99	Total 99	O 99	0	0
16	C	36	Total 36	O 36	0	0
16	E	8	Total 8	O 8	0	0
16	D	19	Total 19	O 19	0	0
16	G	19	Total 19	O 19	0	0
16	I	2	Total 2	O 2	0	0
16	F	32	Total 32	O 32	0	0
16	K	2	Total 2	O 2	0	0
16	H	6	Total 6	O 6	0	0

3 Residue-property plots

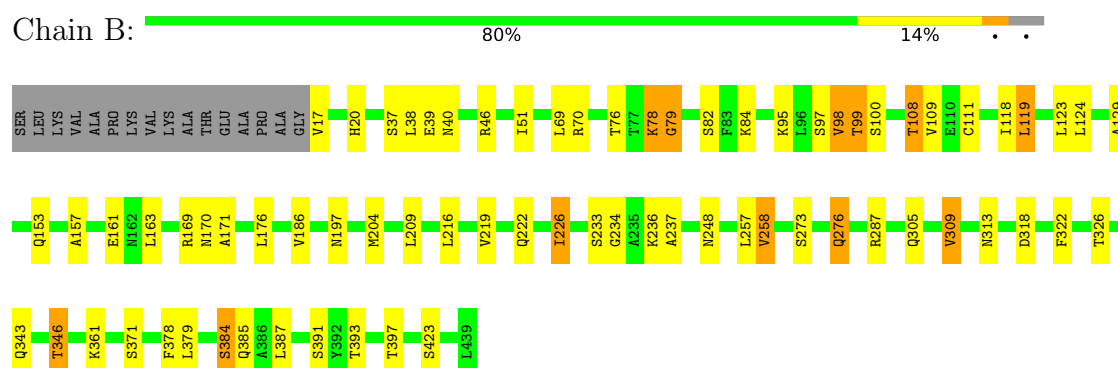
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

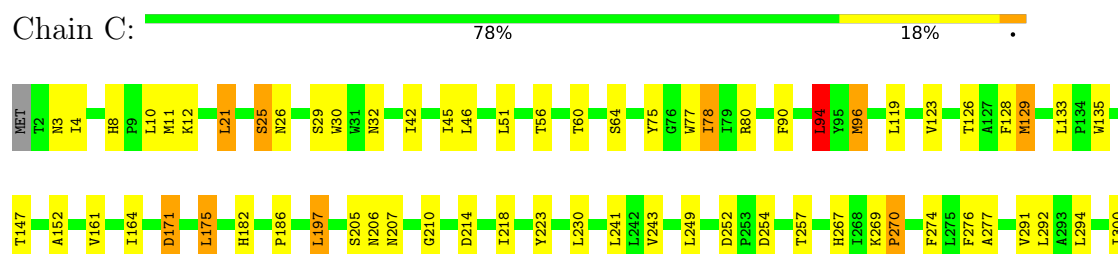
- Molecule 1: Ubiquinol-cytochrome-c reductase complex core protein I, mitochondrial precursor



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



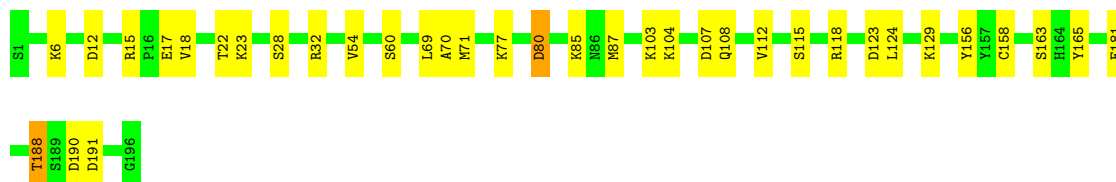
- Molecule 3: Cytochrome b





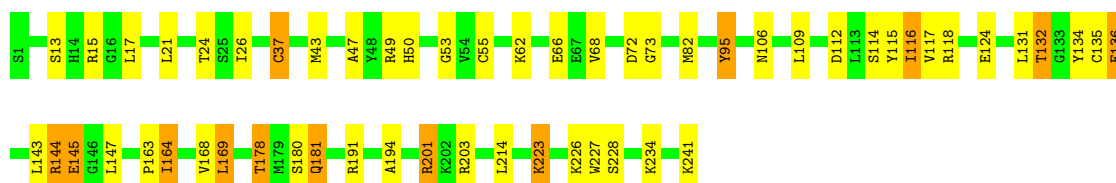
- Molecule 4: Cytochrome c1, heme protein, mitochondrial

Chain E: 82% 17%



- 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)]

Chain D: 77% 18% 5%



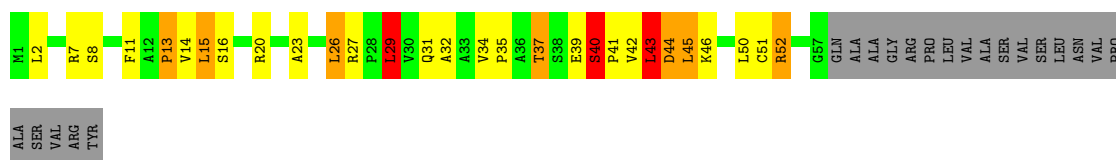
- Molecule 6: Ubiquinol-cytochrome C reductase complex 14 kDa protein

Chain G: 74% 16% 7%



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

Chain I: 36% 24% 9% 27%



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

Chain F: 79% 14% 5%



- 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 K: 




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

Chain H: 



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

Chain J: 



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	154.38Å 154.38Å 590.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.60	Depositor
% Data completeness (in resolution range)	94.2 (40.00-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.233 , 0.281	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	16978	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SMA, HEC, UQ2, FES

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	0.84	1/3531 (0.0%)	0.81	8/4792 (0.2%)
2	B	0.85	0/3232	0.80	1/4386 (0.0%)
3	C	0.97	0/3100	0.80	5/4242 (0.1%)
4	E	0.89	0/1553	0.78	4/2100 (0.2%)
5	D	0.90	0/1978	0.79	1/2684 (0.0%)
6	G	1.07	0/649	0.75	0/878
7	I	1.03	0/411	0.95	1/558 (0.2%)
8	F	0.95	0/930	0.84	0/1246
9	K	1.01	0/454	0.76	0/621
10	H	0.77	0/553	0.85	1/741 (0.1%)
11	J	1.00	0/508	0.78	0/686
All	All	0.91	1/16899 (0.0%)	0.80	21/22934 (0.1%)

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	4
2	B	0	7
3	C	0	2
4	E	0	1
5	D	0	5
7	I	0	8
11	J	0	1
All	All	0	28

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	127	ILE	CA-CB	5.14	1.66	1.54

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	266	ASP	CB-CG-OD1	7.48	125.03	118.30
3	C	94	LEU	CA-CB-CG	6.08	129.28	115.30
1	A	224	ASP	CB-CG-OD1	5.98	123.69	118.30
7	I	44	ASP	CB-CG-OD2	5.65	123.38	118.30
4	E	123	ASP	CB-CG-OD2	5.63	123.37	118.30

There are no chirality outliers.

5 of 28 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	158	PHE	Peptide
1	A	228	VAL	Peptide
1	A	280	TYR	Peptide
1	A	388	ARG	Peptide
2	B	39	GLU	Peptide

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	3458	0	3356	23	0
2	B	3172	0	3152	25	0
3	C	3003	0	3065	35	0
4	E	1519	0	1503	4	0
5	D	1919	0	1870	17	0
6	G	628	0	636	2	0
7	I	406	0	437	11	0
8	F	911	0	904	4	0
9	K	438	0	447	6	0
10	H	548	0	530	2	0
11	J	495	0	493	3	0
12	C	23	0	26	4	0
13	C	86	0	64	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	D	43	0	32	4	0
14	C	37	0	41	3	0
15	E	4	0	0	0	0
16	A	65	0	0	0	0
16	B	99	0	0	2	0
16	C	36	0	0	0	0
16	D	19	0	0	1	0
16	E	8	0	0	0	0
16	F	32	0	0	0	0
16	G	19	0	0	0	0
16	H	6	0	0	0	0
16	I	2	0	0	0	0
16	K	2	0	0	0	0
All	All	16978	0	16556	124	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 4.

The worst 5 of 124 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)
2:B:385:GLN:HE22	2:B:393:THR:H	1.11	0.93
5:D:37:CYS:SG	13:D:242:HEC:HAB	2.19	0.82
12:C:380:UQ2:H2M3	13:C:381:HEC:HBA2	1.64	0.78
9:K:38:TRP:CE3	9:K:41:ILE:HD13	2.22	0.74
3:C:94:LEU:HD21	3:C:123:VAL:HG11	1.72	0.72

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%)	425 (96%)	15 (3%)	4 (1%)	17	35
2	B	421/439 (96%)	403 (96%)	16 (4%)	2 (0%)	29	52
3	C	376/379 (99%)	361 (96%)	15 (4%)	0	100	100
4	E	194/196 (99%)	184 (95%)	9 (5%)	1 (0%)	29	52
5	D	239/241 (99%)	223 (93%)	14 (6%)	2 (1%)	19	39
6	G	73/81 (90%)	66 (90%)	5 (7%)	2 (3%)	5	8
7	I	55/78 (70%)	35 (64%)	14 (26%)	6 (11%)	0	0
8	F	103/110 (94%)	102 (99%)	1 (1%)	0	100	100
9	K	51/56 (91%)	47 (92%)	4 (8%)	0	100	100
10	H	65/78 (83%)	63 (97%)	2 (3%)	0	100	100
11	J	58/62 (94%)	53 (91%)	5 (9%)	0	100	100
All	All	2079/2166 (96%)	1962 (94%)	100 (5%)	17 (1%)	19	39

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	159	GLN
1	A	229	PRO
7	I	40	SER
7	I	43	LEU
1	A	286	GLY

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%)	329 (89%)	41 (11%)	6	11
2	B	332/343 (97%)	294 (89%)	38 (11%)	5	10
3	C	326/327 (100%)	282 (86%)	44 (14%)	4	6
4	E	168/168 (100%)	144 (86%)	24 (14%)	3	5
5	D	206/206 (100%)	165 (80%)	41 (20%)	1	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	G	66/71 (93%)	55 (83%)	11 (17%)	2	3
7	I	44/60 (73%)	26 (59%)	18 (41%)	0	0
8	F	96/98 (98%)	81 (84%)	15 (16%)	2	4
9	K	43/46 (94%)	35 (81%)	8 (19%)	1	2
10	H	64/74 (86%)	45 (70%)	19 (30%)	0	0
11	J	50/52 (96%)	42 (84%)	8 (16%)	2	4
All	All	1765/1815 (97%)	1498 (85%)	267 (15%)	3	4

5 of 267 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	F	110	LYS
9	K	51	LYS
11	J	8	ARG
3	C	164	ILE
3	C	96	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	114	ASN
8	F	53	ASN
3	C	206	ASN
3	C	352	GLN
9	K	16	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 monosaccharides 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
12	UQ2	C	380	-	23,23,23	2.68	6 (26%)	28,31,31	1.24	3 (10%)
14	SMA	C	383	-	35,38,38	1.08	1 (2%)	46,52,52	2.07	14 (30%)
15	FES	E	200	4	0,4,4	0.00	-	-		
13	HEC	D	242	5	26,50,50	1.79	7 (26%)	18,82,82	1.05	0
13	HEC	C	381	3	26,50,50	1.59	6 (23%)	18,82,82	1.67	5 (27%)
13	HEC	C	382	3	26,50,50	1.59	6 (23%)	18,82,82	1.21	3 (16%)

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
12	UQ2	C	380	-	-	3/15/39/39	0/1/1/1
14	SMA	C	383	-	-	11/33/34/34	0/2/2/2
15	FES	E	200	4	-	-	0/1/1/1
13	HEC	D	242	5	-	0/6/54/54	-
13	HEC	C	381	3	-	2/6/54/54	-
13	HEC	C	382	3	-	1/6/54/54	-

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	380	UQ2	C6-C5	9.43	1.52	1.35
13	D	242	HEC	C3C-C2C	-4.50	1.36	1.40
13	D	242	HEC	C3B-C2B	-4.49	1.36	1.40
13	C	381	HEC	C3B-C2B	-4.06	1.36	1.40
12	C	380	UQ2	C8-C9	3.75	1.42	1.33

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	C	383	SMA	O7-C7-C8	6.76	121.36	114.54
14	C	383	SMA	O1-C2-C9	4.04	116.70	111.91
14	C	383	SMA	C22-C11-C10	3.93	116.52	110.36
14	C	383	SMA	O14-C14-C13	3.74	115.80	107.98
14	C	383	SMA	O5-C5-C4A	3.71	121.34	115.89

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	C	381	HEC	C1A-C2A-CAA-CBA
13	C	381	HEC	C3A-C2A-CAA-CBA
14	C	383	SMA	C4A-C5-O5-C5M
14	C	383	SMA	C6-C5-O5-C5M
14	C	383	SMA	C8-C7-O7-C7M

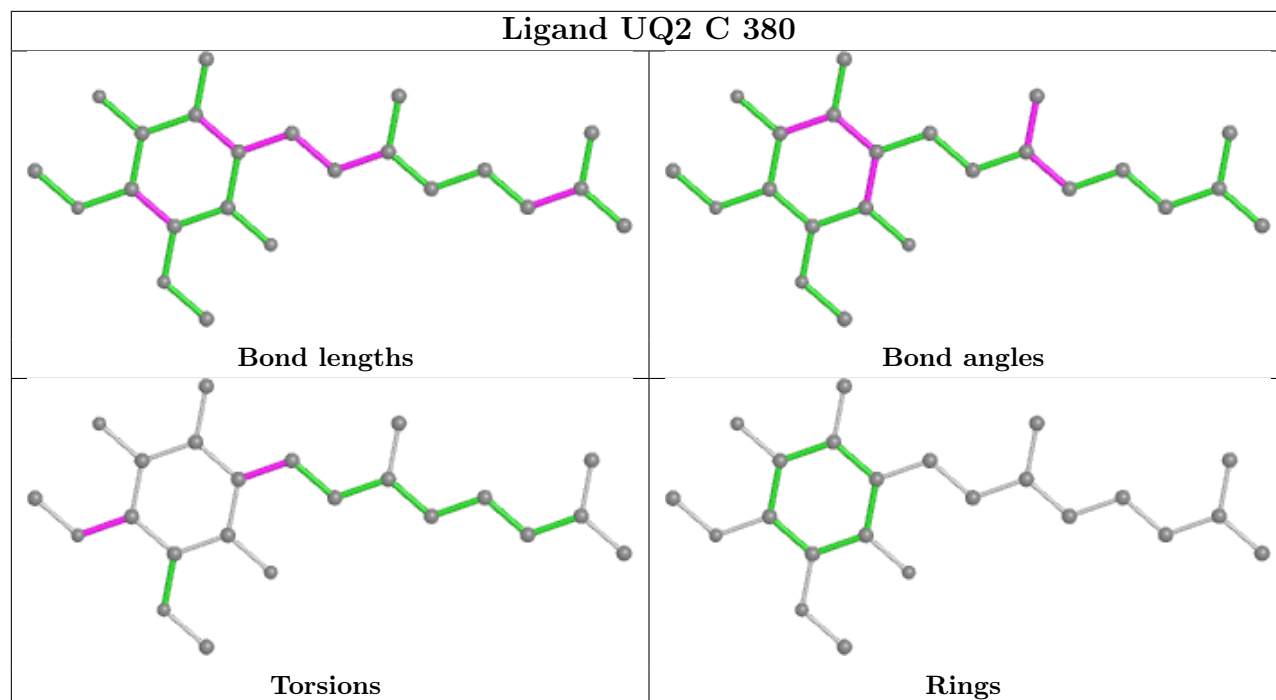
There are no ring outliers.

5 monomers are involved in 20 short contacts:

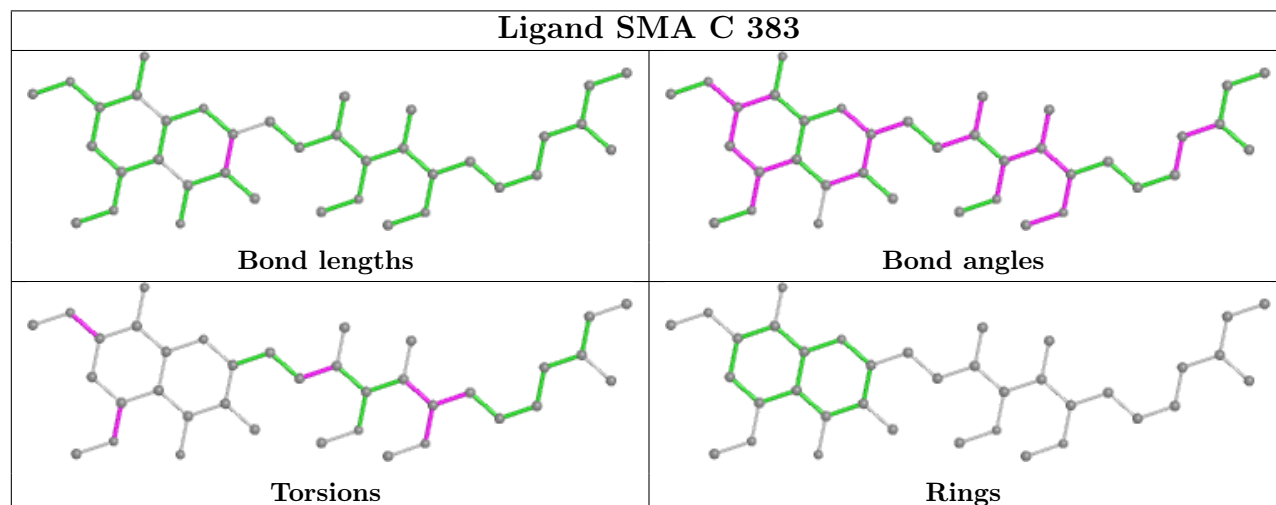
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	C	380	UQ2	4	0
14	C	383	SMA	3	0
13	D	242	HEC	4	0
13	C	381	HEC	4	0
13	C	382	HEC	6	0

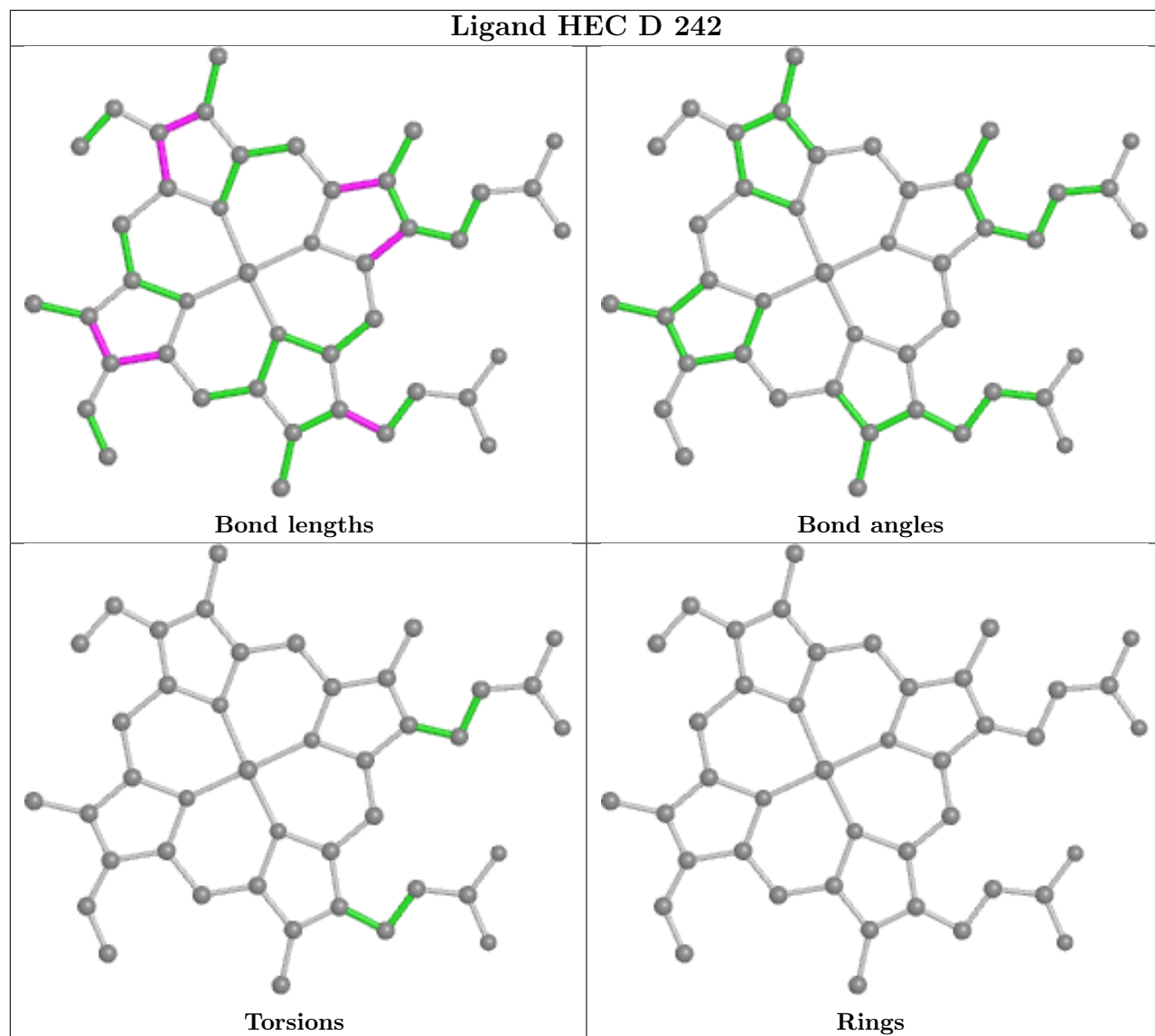
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 UQ2 C 380

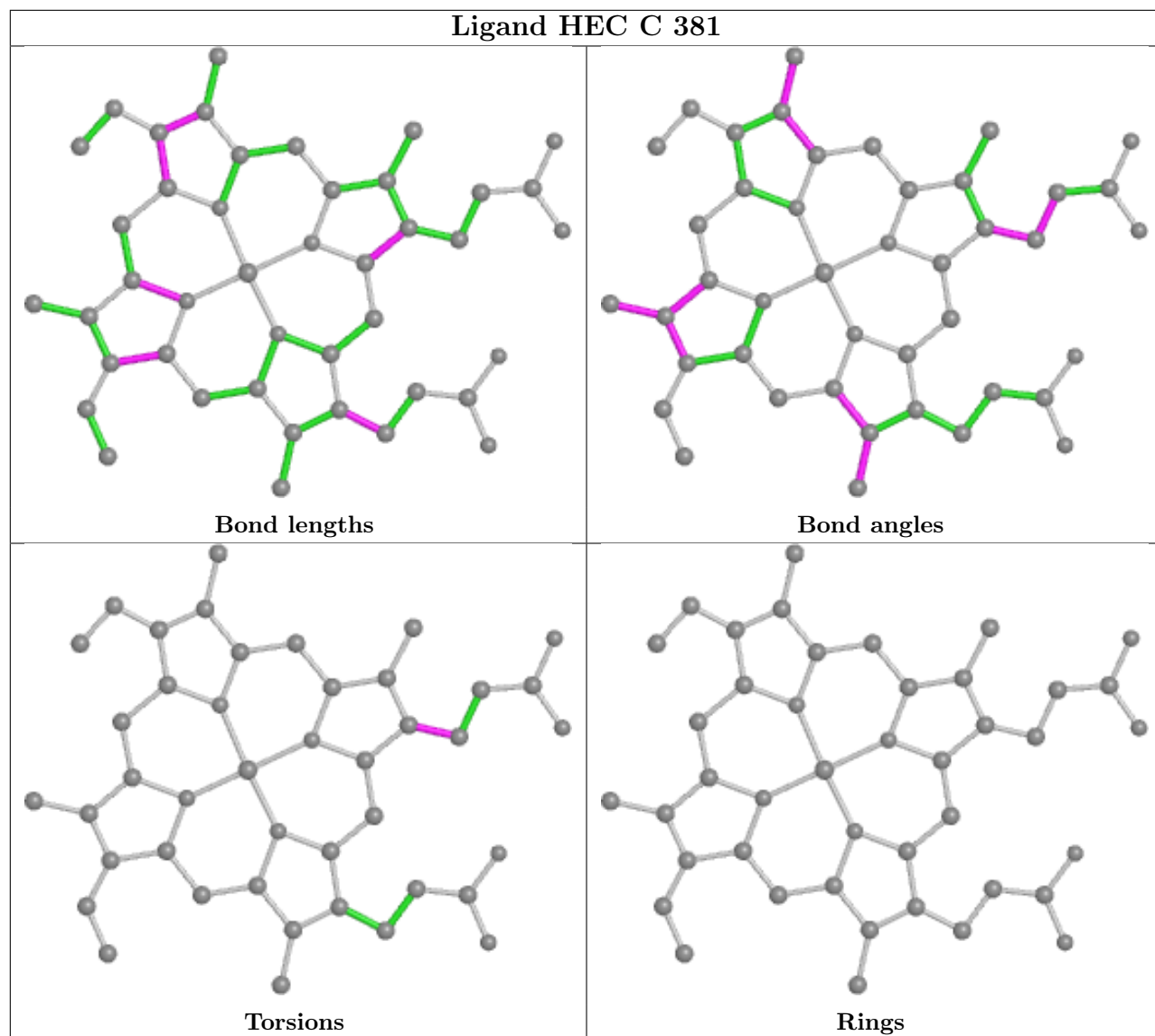


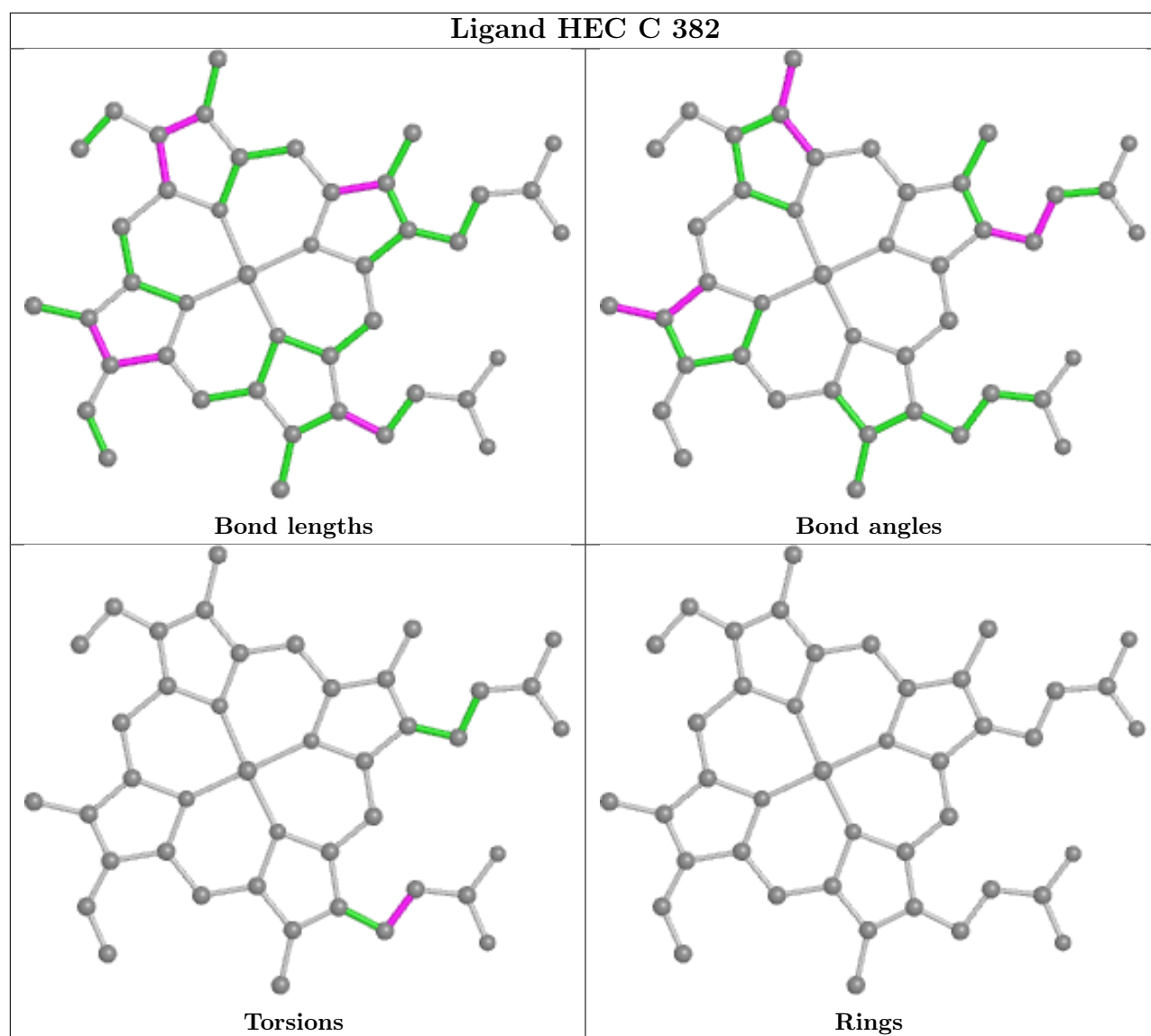
Ligand SMA C 383





Ligand HEC C 381





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.