



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 06:09 AM UTC

PDB ID : 1BGY / pdb_00001bg
Title : CYTOCHROME BC1 COMPLEX FROM BOVINE
Authors : Iwata, S.; Lee, J.W.; Okada, K.; Lee, J.K.; Iwata, M.; Ramaswamy, S.; Jap, B.K.
Deposited on : 1998-06-02
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

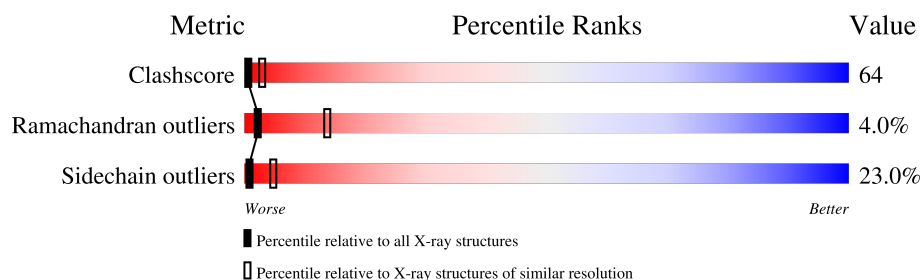
1 Overall quality at a glance

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)

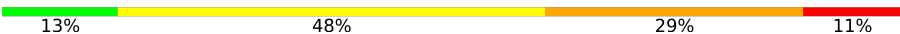
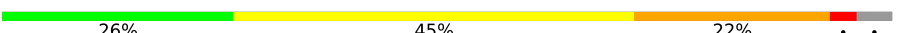
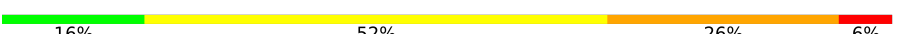
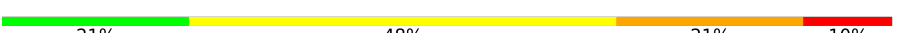
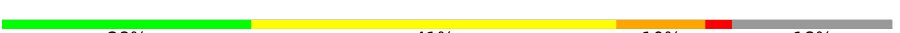
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	17% 50% 27% 5%
1	M	446	18% 53% 26% .
2	B	439	20% 51% 21% . 5%
2	N	439	22% 51% 21% . 5%
3	C	379	15% 51% 28% 6%
3	O	379	18% 53% 26% .
4	D	241	22% 51% 21% 6%
4	P	241	21% 54% 23% .

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Mol	Chain	Length	Quality of chain
5	E	196	
5	Q	196	
6	F	110	
6	R	110	
7	G	81	
7	S	81	
8	H	78	
8	T	78	
9	I	78	
9	U	78	
10	J	62	
10	V	62	
11	K	56	
11	W	56	

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 31486 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called CYTOCHROME BC1 COMPLEX.

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

- Molecule 2 is a protein called CYTOCHROME BC1 COMPLEX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	419	Total	C	N	O	S	0	0	0
			3141	1972	556	606	7			
2	N	419	Total	C	N	O	S	0	0	0
			3141	1972	556	606	7			

- Molecule 3 is a protein called CYTOCHROME BC1 COMPLEX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	379	Total	C	N	O	S	0	0	0
			3011	2018	472	502	19			
3	O	379	Total	C	N	O	S	0	0	0
			3011	2018	472	502	19			

- Molecule 4 is a protein called CYTOCHROME BC1 COMPLEX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	241	Total	C	N	O	S	0	0	0
			1919	1225	330	349	15			
4	P	241	Total	C	N	O	S	0	0	0
			1919	1225	330	349	15			

- Molecule 5 is a protein called CYTOCHROME BC1 COMPLEX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	75	Total	C	N	O	S	0	0	0
			566	352	94	118	2			
5	Q	196	Total	C	N	O	S	0	0	0
			1518	956	263	291	8			

- Molecule 6 is a protein called CYTOCHROME BC1 COMPLEX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	106	Total	C	N	O	S	0	0	0
			916	579	166	169	2			
6	R	106	Total	C	N	O	S	0	0	0
			916	579	166	169	2			

- Molecule 7 is a protein called CYTOCHROME BC1 COMPLEX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	81	Total	C	N	O	S	0	0	0
			682	441	128	112	1			
7	S	81	Total	C	N	O	S	0	0	0
			682	441	128	112	1			

- Molecule 8 is a protein called CYTOCHROME BC1 COMPLEX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	64	Total	C	N	O	S	0	0	0
			524	316	96	107	5			
8	T	64	Total	C	N	O	S	0	0	0
			524	316	96	107	5			

- Molecule 9 is a protein called CYTOCHROME BC1 COMPLEX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	33	Total	C	N	O	S	0	0	0
			248	152	51	44	1			
9	U	33	Total	C	N	O	S	0	0	0
			248	152	51	44	1			

- Molecule 10 is a protein called CYTOCHROME BC1 COMPLEX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	62	Total	C	N	O	0	0	0
			512	335	89	88			

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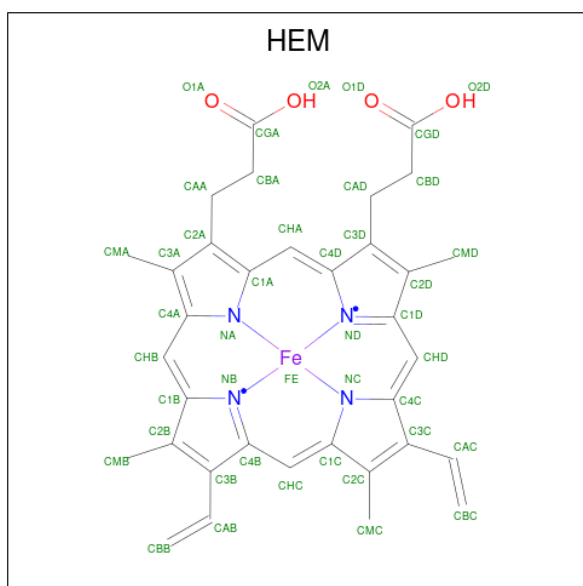
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	V	62	Total	C	N	O	0	0	0
			512	335	89	88			

- Molecule 11 is a protein called CYTOCHROME BC1 COMPLEX.

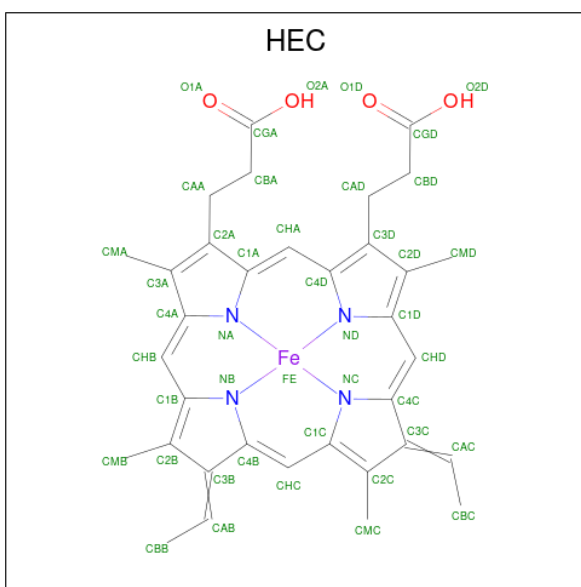
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	K	22	Total	C	N	O	0	0	0
			159	103	29	27			
11	W	22	Total	C	N	O	0	0	0
			159	103	29	27			

- Molecule 12 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



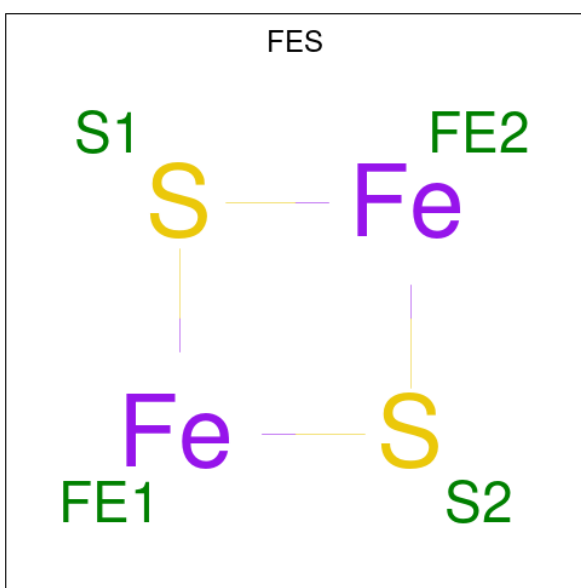
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	0
12	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	0
12	O	1	Total	C	Fe	N	O	0
			43	34	1	4	4	0
12	O	1	Total	C	Fe	N	O	0
			43	34	1	4	4	0

- Molecule 13 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

- Molecule 14 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



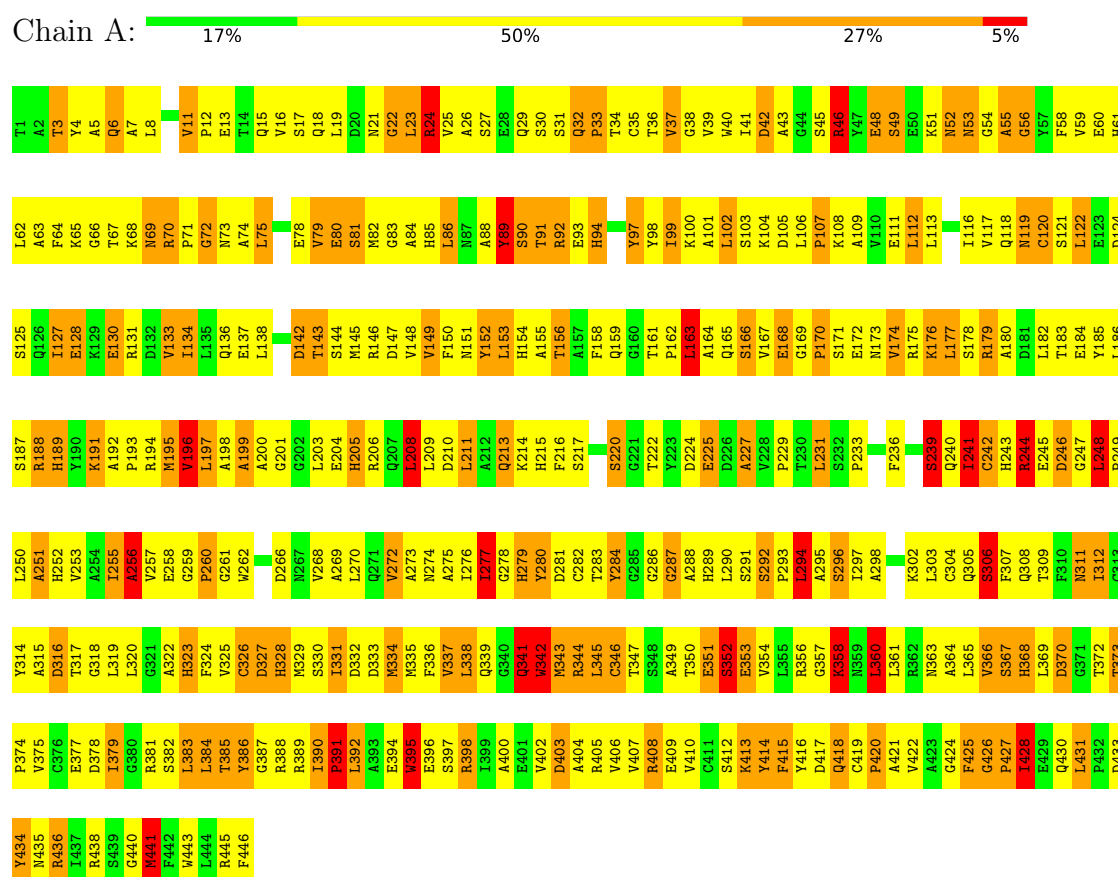
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	Q	1	Total	Fe	S	0	0
			4	2	2		

3 Residue-property plots

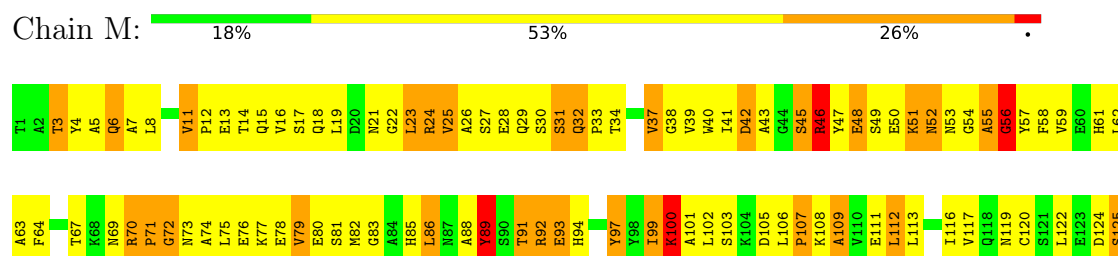
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

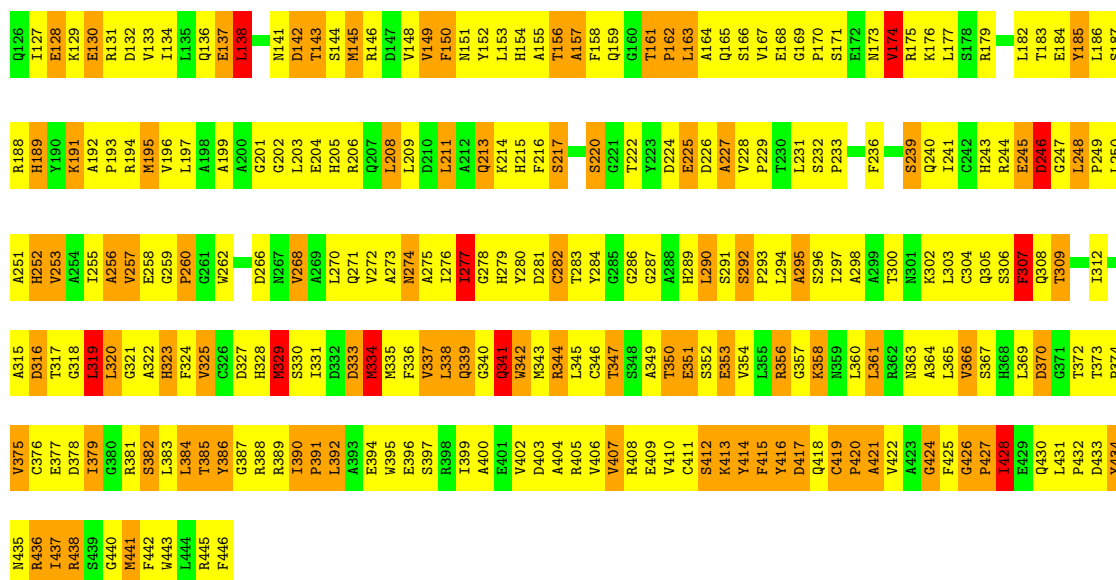
Note EDS was not executed.

• Molecule 1: CYTOCHROME BC1 COMPLEX



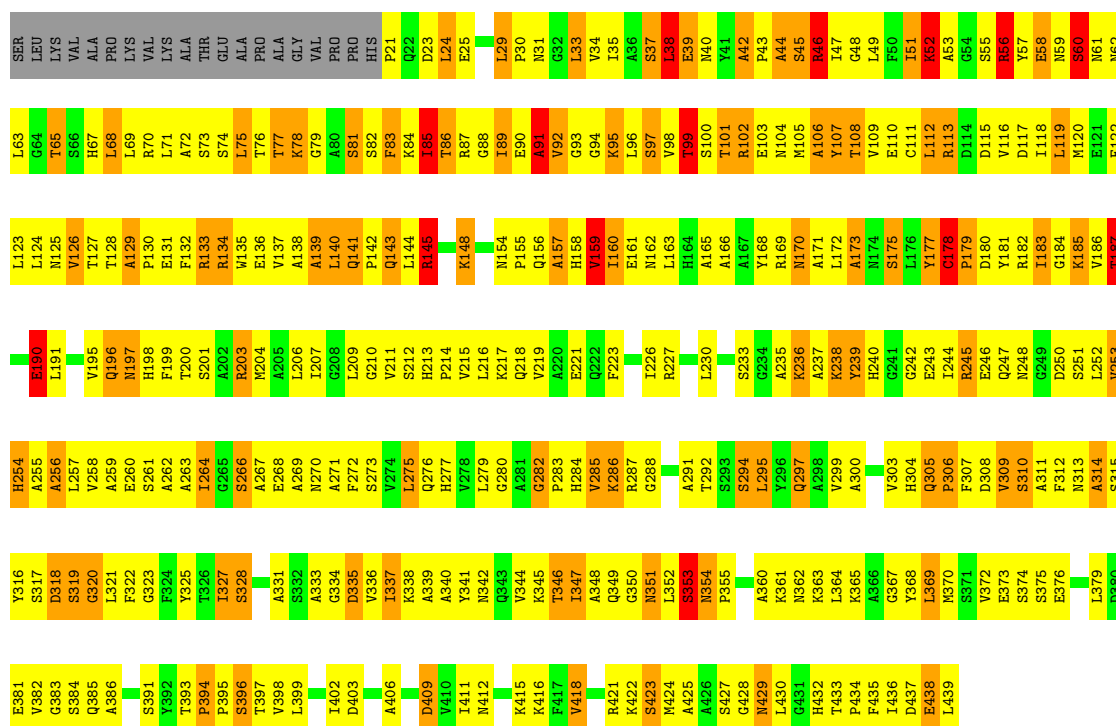
• Molecule 1: CYTOCHROME BC1 COMPLEX





• Molecule 2: CYTOCHROME BC1 COMPLEX

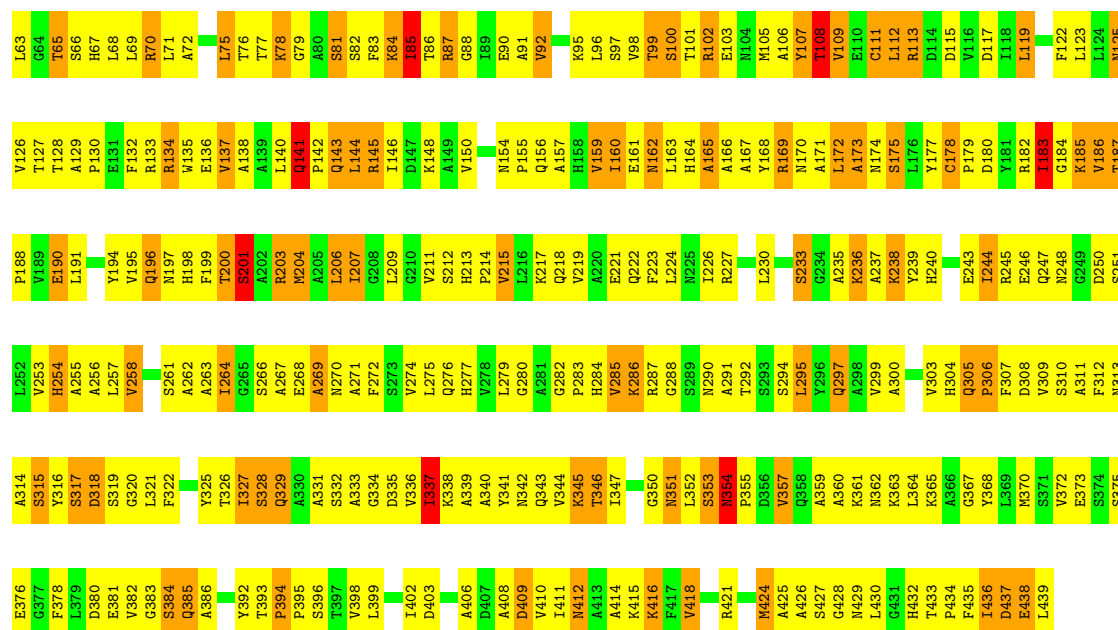
Chain B: 20% 51% 21% 5%



• Molecule 2: CYTOCHROME BC1 COMPLEX

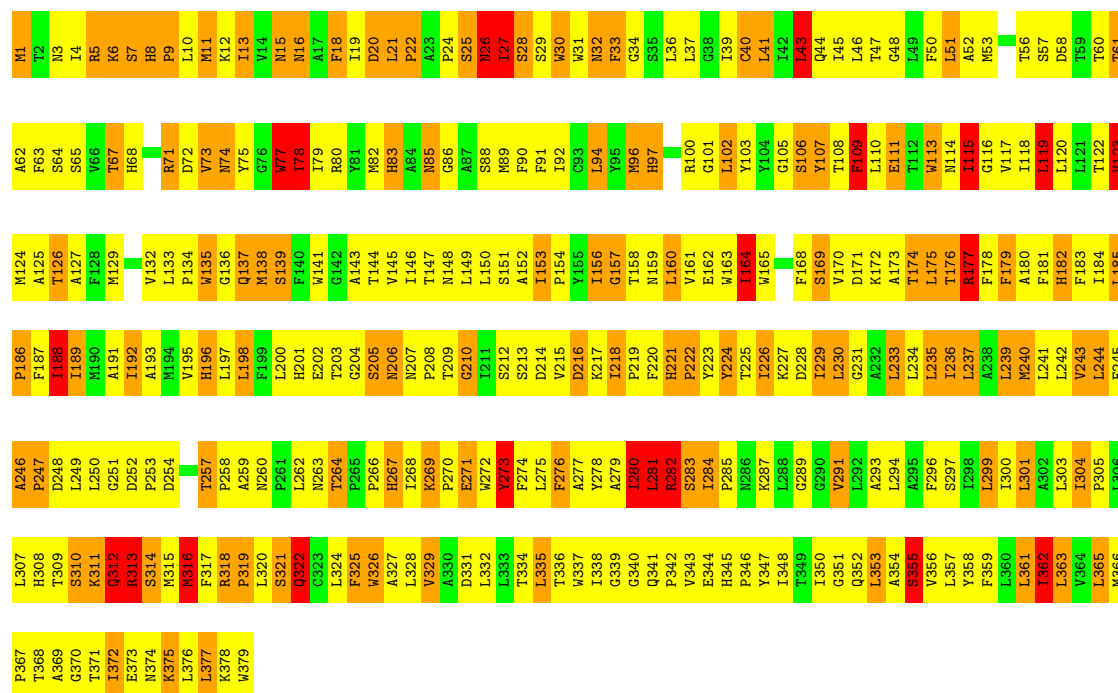
Chain N: 22% 51% 21% 5%





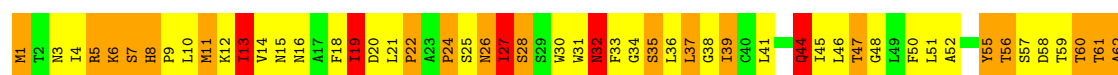
• Molecule 3: CYTOCHROME BC1 COMPLEX

Chain C: 15% 51% 28% 6%



• Molecule 3: CYTOCHROME BC1 COMPLEX

Chain O: 18% 53% 26%





Chain E:

Residue	State
S1	10%
H2	17%
T3	17%
D4	10%
I5	17%
K6	17%
V7	17%
P8	17%
S11	10%
D12	17%
Y13	17%
R14	17%
R15	17%
P16	17%
E17	17%
V18	17%
L19	17%
D20	17%
S21	17%
K22	17%
K23	17%
S24	17%
S25	17%
S28	17%
S29	17%
E30	17%
A31	17%
R32	17%
K33	17%
G34	17%
L38	10%
V39	17%
T40	17%
A41	17%
V45	17%
G46	10%
V47	17%
A48	17%
V49	17%
A50	17%
A51	17%
K52	17%
V53	17%
V54	17%
V55	17%
S56	17%
D57	17%
F58	17%
V59	17%
S60	17%
S61	17%
N62	17%
S63	17%
A64	17%
S65	17%
A66	17%

Chain Q: 13% 48% 29% 11%

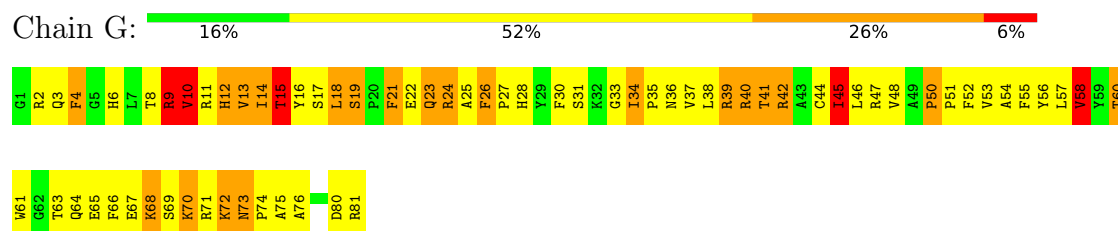
Category	Chain Q	Percentage
S1	Green	13%
H2	Green	13%
T3	Green	13%
D4	Green	13%
I5	Green	13%
K6	Green	13%
V7	Green	13%
P8	Green	13%
D9	Green	13%
F10	Green	13%
S11	Green	13%
D12	Green	13%
Y13	Green	13%
R14	Orange	48%
R15	Orange	48%
P16	Orange	48%
E17	Orange	48%
V18	Orange	48%
L19	Orange	48%
D20	Orange	48%
S21	Orange	48%
T22	Orange	48%
K23	Orange	48%
S24	Orange	48%
S25	Orange	48%
S28	Orange	48%
S29	Orange	48%
E30	Orange	48%
A31	Orange	48%
R32	Red	29%
K33	Red	29%
G34	Red	29%
F35	Red	29%
S36	Red	29%
Y37	Red	29%
L38	Red	29%
V39	Red	29%
T40	Red	29%
A41	Red	29%
T42	Red	29%
T43	Red	29%
T44	Red	29%
G46	Red	29%
V47	Red	29%
A48	Red	29%
Y49	Red	29%
A50	Red	29%
A51	Red	29%
K52	Red	29%
V55	Grey	11%
S56	Grey	11%
Q57	Grey	11%
V59	Grey	11%
S60	Grey	11%
S61	Grey	11%
S62	Grey	11%
S65	Green	13%
S66	Green	13%
Q67	Green	13%
S68	Green	13%
V69	Green	13%
S70	Green	13%
S71	Green	13%
S72	Green	13%
S75	Green	13%
A76	Green	13%
R77	Orange	48%
T78	Orange	48%
S79	Orange	48%
D80	Orange	48%
L81	Orange	48%
P82	Orange	48%
E83	Orange	48%
G84	Orange	48%
K85	Orange	48%
N86	Orange	48%
M87	Orange	48%
A88	Orange	48%
F89	Orange	48%
K90	Orange	48%
W91	Orange	48%
R92	Orange	48%
G93	Orange	48%
K94	Orange	48%
P95	Orange	48%
L96	Orange	48%
F97	Orange	48%
V98	Orange	48%
R99	Orange	48%
H100	Orange	48%
R101	Orange	48%
T102	Orange	48%
K103	Orange	48%
K104	Orange	48%
E105	Orange	48%
I106	Orange	48%
D107	Orange	48%
Q108	Orange	48%
E109	Orange	48%
A110	Orange	48%
E113	Orange	48%
V114	Orange	48%
S115	Orange	48%
Q116	Orange	48%
L117	Orange	48%
R118	Orange	48%
D119	Orange	48%
F120	Orange	48%
Q121	Orange	48%
S122	Orange	48%
D123	Orange	48%
L124	Green	13%
E125	Green	13%
R126	Green	13%
F127	Green	13%
T128	Green	13%
K129	Green	13%
P130	Green	13%
E131	Green	13%
W132	Green	13%
V133	Green	13%
L134	Green	13%
L135	Green	13%
T136	Green	13%
G137	Green	13%
V138	Green	13%
C139	Green	13%
T140	Green	13%
H141	Green	13%
L142	Green	13%
G143	Green	13%
C144	Green	13%
V145	Green	13%
P146	Green	13%
L147	Green	13%
A148	Green	13%
N149	Green	13%
A150	Green	13%
G151	Green	13%
D152	Green	13%
F153	Green	13%
Y156	Orange	48%
Y157	Orange	48%
C158	Orange	48%
P159	Orange	48%
C160	Orange	48%
G162		

Chain F:

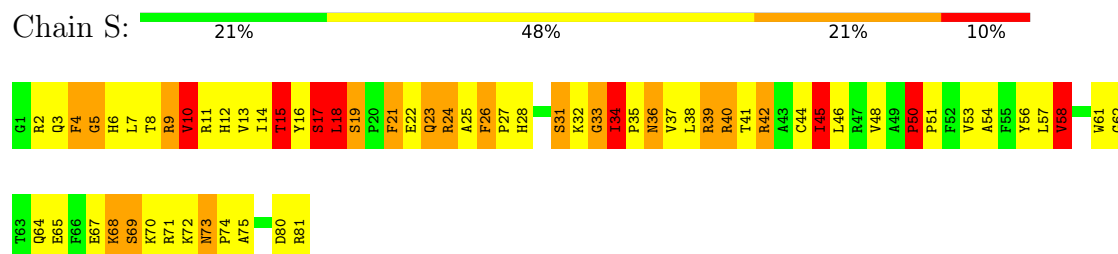
Chain R:

Residue	Category
ALA	Green
GLY	Green
ARG	Green
PRO	Green
A5	Green
V6	Green
S7	Green
S10	Yellow
R11	Yellow
W12	Yellow
L13	Yellow
I16	Yellow
Y20	Yellow
Y21	Yellow
N22	Yellow
A23	Yellow
A24	Yellow
G25	Yellow
F26	Yellow
N27	Yellow
K28	Yellow
L29	Yellow
M32	Yellow
R33	Yellow
D34	Yellow
D35	Yellow
T36	Yellow
I37	Yellow
H38	Yellow
E39	Yellow
N40	Yellow
D41	Yellow
D42	Yellow
V43	Yellow
K44	Yellow
E45	Yellow
A46	Yellow
I47	Yellow
R48	Yellow
R49	Yellow
L50	Yellow
P51	Yellow
E52	Yellow
N53	Yellow
L54	Yellow
Y55	Yellow
R58	Yellow
V59	Yellow
F60	Yellow
R61	Yellow
I62	Yellow
K63	Yellow
R64	Yellow
A65	Yellow
L66	Yellow
D67	Orange
L68	Orange
S69	Orange
M70	Orange
R71	Orange
K72	Orange
K73	Orange
I74	Orange
L75	Orange
P76	Orange
K77	Orange
E78	Orange
Q79	Orange
W80	Orange
E84	Orange
K87	Orange
S88	Orange
Y89	Orange
L90	Orange
E91	Orange
P92	Orange
Y93	Orange
L94	Orange
K95	Orange
E96	Orange
Y97	Orange
I98	Orange
R99	Orange
E100	Orange
R101	Orange
K102	Orange
E103	Orange
R104	Orange
E105	Orange
E106	Orange
K109	Orange
K110	Orange

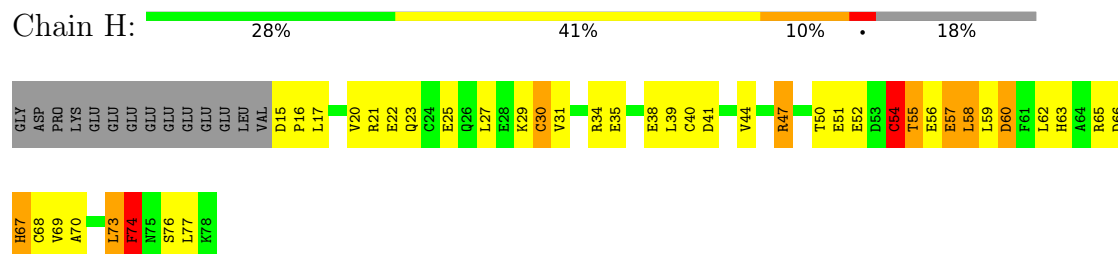
• Molecule 7: CYTOCHROME BC1 COMPLEX



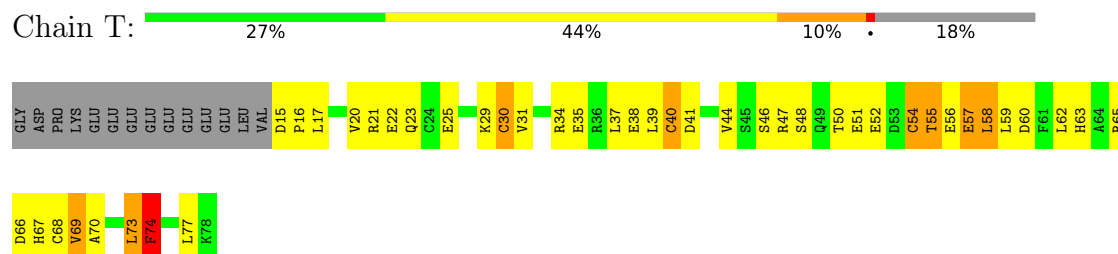
• Molecule 7: CYTOCHROME BC1 COMPLEX



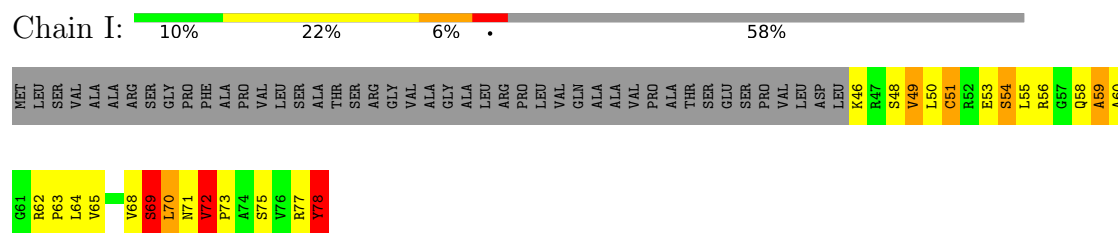
• Molecule 8: CYTOCHROME BC1 COMPLEX



• Molecule 8: CYTOCHROME BC1 COMPLEX

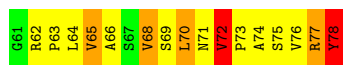
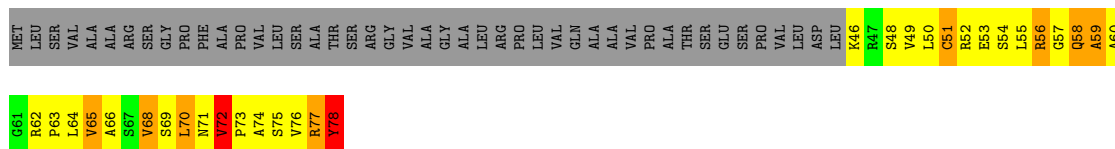


• Molecule 9: CYTOCHROME BC1 COMPLEX

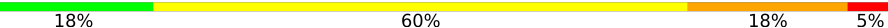


• Molecule 9: CYTOCHROME BC1 COMPLEX

Chain U:  26% 10% 58%

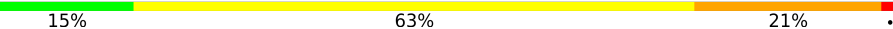


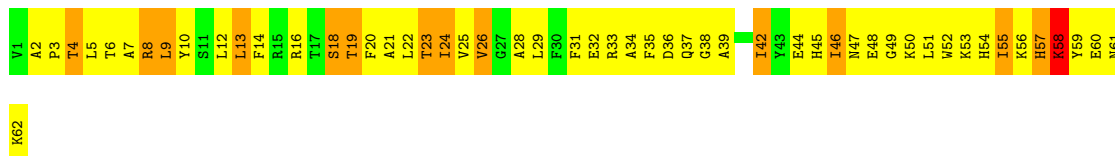
• Molecule 10: CYTOCHROME BC1 COMPLEX

Chain J:  18% 60% 18% 5%



• Molecule 10: CYTOCHROME BC1 COMPLEX

Chain V:  15% 63% 21% .



• Molecule 11: CYTOCHROME BC1 COMPLEX

Chain K:  16% 18% 5% 61%



• Molecule 11: CYTOCHROME BC1 COMPLEX

Chain W:  11% 18% 9% . 61%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	130.11Å 130.11Å 720.94Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.00	Depositor
% Data completeness (in resolution range)	74.0 (20.00-3.00)	Depositor
R_{merge}	0.92	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.320 , 0.360	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	31486	wwPDB-VP
Average B, all atoms (Å ²)	30.0	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: HEC, FES, HEM

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	0.77	3/3531 (0.1%)	2.02	137/4792 (2.9%)
1	M	0.82	4/3531 (0.1%)	2.03	114/4792 (2.4%)
2	B	0.66	2/3198 (0.1%)	1.89	85/4336 (2.0%)
2	N	0.65	0/3198	1.81	71/4336 (1.6%)
3	C	0.92	2/3108 (0.1%)	2.20	135/4252 (3.2%)
3	O	0.93	6/3108 (0.2%)	2.07	109/4252 (2.6%)
4	D	0.68	0/1978	1.88	57/2684 (2.1%)
4	P	0.70	2/1978 (0.1%)	1.83	50/2684 (1.9%)
5	E	0.76	0/574	2.02	17/775 (2.2%)
5	Q	0.80	1/1551 (0.1%)	2.16	61/2097 (2.9%)
6	F	0.74	1/935 (0.1%)	1.84	22/1253 (1.8%)
6	R	0.74	0/935	1.94	23/1253 (1.8%)
7	G	0.73	0/704	1.89	25/951 (2.6%)
7	S	0.74	0/704	1.77	23/951 (2.4%)
8	H	0.57	0/529	1.61	10/708 (1.4%)
8	T	0.50	0/529	1.51	4/708 (0.6%)
9	I	0.61	0/250	1.88	5/335 (1.5%)
9	U	0.63	0/250	1.85	7/335 (2.1%)
10	J	0.61	0/525	1.61	8/707 (1.1%)
10	V	0.63	0/525	1.71	7/707 (1.0%)
11	K	0.54	0/163	1.34	0/225
11	W	0.59	0/163	1.52	1/225 (0.4%)
All	All	0.76	21/31967 (0.1%)	1.95	971/43358 (2.2%)

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	13

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	M	0	3
2	B	0	9
2	N	0	5
3	C	0	14
3	O	0	6
4	D	0	5
4	P	0	4
5	E	0	1
5	Q	0	9
6	F	0	2
7	G	0	2
7	S	0	3
8	T	0	1
9	I	0	1
9	U	0	1
10	J	0	1
11	W	0	1
All	All	0	81

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	253	VAL	C-O	11.10	1.36	1.24
3	O	37	LEU	C-N	-8.13	1.24	1.33
3	O	221	HIS	CD2-NE2	-7.11	1.30	1.37
4	P	202	LYS	C-O	6.46	1.31	1.24
3	O	19	ILE	CA-C	-6.38	1.44	1.52

The worst 5 of 971 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	253	VAL	O-C-N	-23.35	98.90	123.18
1	M	253	VAL	CA-C-O	16.99	137.43	120.27
3	C	196	HIS	CA-CB-CG	16.17	129.97	113.80
3	O	196	HIS	CA-CB-CG	15.62	129.42	113.80
3	O	44	GLN	CA-C-N	15.26	139.78	120.70

There are no chirality outliers.

5 of 81 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	118	GLN	Mainchain
1	A	122	LEU	Mainchain
1	A	196	VAL	Mainchain
1	A	210	ASP	Mainchain
1	A	53	ASN	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3458	0	3356	487	0
1	M	3458	0	3356	476	0
2	B	3141	0	3123	417	0
2	N	3141	0	3123	428	1
3	C	3011	0	3077	467	0
3	O	3011	0	3077	431	0
4	D	1919	0	1868	307	0
4	P	1919	0	1868	298	0
5	E	566	0	564	67	0
5	Q	1518	0	1499	269	1
6	F	916	0	909	97	0
6	R	916	0	909	96	1
7	G	682	0	679	107	0
7	S	682	0	679	99	0
8	H	524	0	504	70	1
8	T	524	0	504	76	0
9	I	248	0	265	52	0
9	U	248	0	265	66	0
10	J	512	0	518	70	0
10	V	512	0	518	79	0
11	K	159	0	159	26	0
11	W	159	0	159	27	0
12	C	86	0	60	20	0
12	O	86	0	60	25	0
13	D	43	0	30	5	0
13	P	43	0	30	3	0
14	Q	4	0	0	0	0
All	All	31486	0	31159	3993	2

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 64.

The worst 5 of 3993 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)
7:S:50:PRO:HB2	7:S:51:PRO:HD3	1.25	1.17
4:D:224:ARG:HB2	7:G:25:ALA:HB1	1.27	1.17
2:B:77:THR:HG22	2:B:130:PRO:HA	1.25	1.14
1:M:67:THR:HG23	1:M:70:ARG:H	1.13	1.14
1:M:426:GLY:CA	1:M:428:ILE:HG13	1.78	1.13

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:412:ASN:ND2	5:Q:122:HIS:NE2[6_554]	2.01	0.19
8:H:41:ASP:OD1	6:R:77:LYS:NZ[5_565]	2.19	0.01

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	444/446 (100%)	355 (80%)	66 (15%)	23 (5%)	1	9
1	M	444/446 (100%)	370 (83%)	54 (12%)	20 (4%)	2	12
2	B	417/439 (95%)	341 (82%)	67 (16%)	9 (2%)	5	26
2	N	417/439 (95%)	344 (82%)	62 (15%)	11 (3%)	4	23
3	C	377/379 (100%)	303 (80%)	60 (16%)	14 (4%)	2	15
3	O	377/379 (100%)	317 (84%)	49 (13%)	11 (3%)	3	20
4	D	239/241 (99%)	188 (79%)	36 (15%)	15 (6%)	1	6
4	P	239/241 (99%)	195 (82%)	32 (13%)	12 (5%)	1	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	73/196 (37%)	57 (78%)	14 (19%)	2 (3%)	4	22
5	Q	194/196 (99%)	148 (76%)	35 (18%)	11 (6%)	1	8
6	F	104/110 (94%)	89 (86%)	12 (12%)	3 (3%)	3	20
6	R	104/110 (94%)	86 (83%)	16 (15%)	2 (2%)	6	30
7	G	79/81 (98%)	63 (80%)	13 (16%)	3 (4%)	2	15
7	S	79/81 (98%)	60 (76%)	16 (20%)	3 (4%)	2	15
8	H	62/78 (80%)	52 (84%)	10 (16%)	0	100	100
8	T	62/78 (80%)	51 (82%)	10 (16%)	1 (2%)	7	34
9	I	31/78 (40%)	19 (61%)	10 (32%)	2 (6%)	1	5
9	U	31/78 (40%)	17 (55%)	11 (36%)	3 (10%)	0	2
10	J	60/62 (97%)	41 (68%)	13 (22%)	6 (10%)	0	2
10	V	60/62 (97%)	44 (73%)	12 (20%)	4 (7%)	1	5
11	K	20/56 (36%)	17 (85%)	2 (10%)	1 (5%)	1	10
11	W	20/56 (36%)	15 (75%)	3 (15%)	2 (10%)	0	2
All	All	3933/4332 (91%)	3172 (81%)	603 (15%)	158 (4%)	2	14

5 of 158 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	327	ASP
1	A	426	GLY
1	A	427	PRO
2	B	141	GLN
2	B	183	ILE

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%)	278 (75%)	92 (25%)	0	4
1	M	370/370 (100%)	284 (77%)	86 (23%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	328/343 (96%)	254 (77%)	74 (23%)	1	5
2	N	328/343 (96%)	254 (77%)	74 (23%)	1	5
3	C	327/327 (100%)	251 (77%)	76 (23%)	1	4
3	O	327/327 (100%)	259 (79%)	68 (21%)	1	7
4	D	206/206 (100%)	172 (84%)	34 (16%)	2	12
4	P	206/206 (100%)	170 (82%)	36 (18%)	2	10
5	E	65/168 (39%)	47 (72%)	18 (28%)	0	2
5	Q	167/168 (99%)	110 (66%)	57 (34%)	0	1
6	F	96/98 (98%)	68 (71%)	28 (29%)	0	2
6	R	96/98 (98%)	76 (79%)	20 (21%)	1	7
7	G	71/71 (100%)	53 (75%)	18 (25%)	0	3
7	S	71/71 (100%)	51 (72%)	20 (28%)	0	2
8	H	61/74 (82%)	50 (82%)	11 (18%)	2	10
8	T	61/74 (82%)	50 (82%)	11 (18%)	2	10
9	I	27/60 (45%)	19 (70%)	8 (30%)	0	2
9	U	27/60 (45%)	19 (70%)	8 (30%)	0	2
10	J	52/52 (100%)	43 (83%)	9 (17%)	2	10
10	V	52/52 (100%)	42 (81%)	10 (19%)	1	8
11	K	15/46 (33%)	11 (73%)	4 (27%)	0	3
11	W	15/46 (33%)	10 (67%)	5 (33%)	0	1
All	All	3338/3630 (92%)	2571 (77%)	767 (23%)	1	5

5 of 767 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	N	45	SER
3	O	233	LEU
2	N	99	THR
2	N	38	LEU
2	N	346	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 86 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	339	GLN
3	O	206	ASN
2	N	62	ASN
2	N	304	HIS
4	P	75	ASN

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](#)

7 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	HEC	P	242	4	46,50,50	1.89	7 (15%)	58,82,82	1.55	4 (6%)
12	HEM	C	381	3	50,50,50	1.27	6 (12%)	67,82,82	1.73	17 (25%)
13	HEC	D	242	4	46,50,50	1.85	7 (15%)	58,82,82	1.53	7 (12%)
12	HEM	O	381	3	50,50,50	1.37	7 (14%)	67,82,82	1.73	14 (20%)
14	FES	Q	197	5	0,4,4	-	-	-	-	-
12	HEM	C	380	3	50,50,50	1.31	7 (14%)	67,82,82	1.51	9 (13%)
12	HEM	O	380	3	50,50,50	1.41	8 (16%)	67,82,82	1.87	18 (26%)

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	HEC	P	242	4	-	10/14/54/54	-
12	HEM	C	381	3	-	6/14/54/54	-
13	HEC	D	242	4	-	8/14/54/54	-
12	HEM	O	381	3	-	4/14/54/54	-
14	FES	Q	197	5	-	-	0/1/1/1
12	HEM	C	380	3	-	4/14/54/54	-
12	HEM	O	380	3	-	6/14/54/54	-

The worst 5 of 42 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	P	242	HEC	CAB-C3B	6.65	1.56	1.35
13	P	242	HEC	CAC-C3C	6.46	1.56	1.35
13	D	242	HEC	CAB-C3B	6.46	1.56	1.35
13	D	242	HEC	CAC-C3C	6.30	1.55	1.35
13	D	242	HEC	CBB-CAB	-3.72	1.35	1.49

The worst 5 of 69 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	D	242	HEC	CBC-CAC-C3C	-6.70	114.05	127.43
13	P	242	HEC	CBB-CAB-C3B	-6.69	114.06	127.43
13	P	242	HEC	CBC-CAC-C3C	-6.11	115.23	127.43
12	O	380	HEM	C3B-C2B-C1B	-5.36	102.39	106.41
13	D	242	HEC	CBB-CAB-C3B	-4.98	117.47	127.43

There are no chirality outliers.

5 of 38 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	O	380	HEM	C2B-C3B-CAB-CBB
13	D	242	HEC	C2B-C3B-CAB-CBB
13	D	242	HEC	C4B-C3B-CAB-CBB
13	D	242	HEC	C2C-C3C-CAC-CBC
13	D	242	HEC	C4C-C3C-CAC-CBC

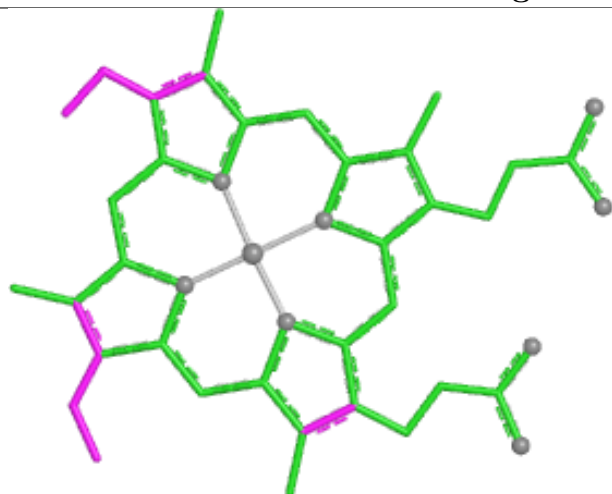
There are no ring outliers.

6 monomers are involved in 53 short contacts:

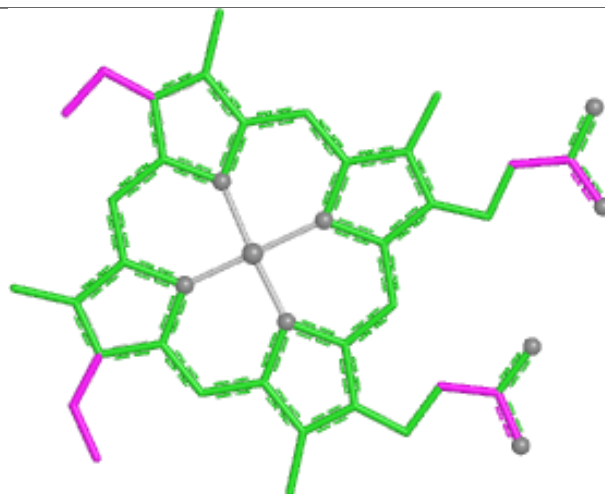
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	P	242	HEC	3	0
12	C	381	HEM	14	0
13	D	242	HEC	5	0
12	O	381	HEM	14	0
12	C	380	HEM	6	0
12	O	380	HEM	11	0

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.

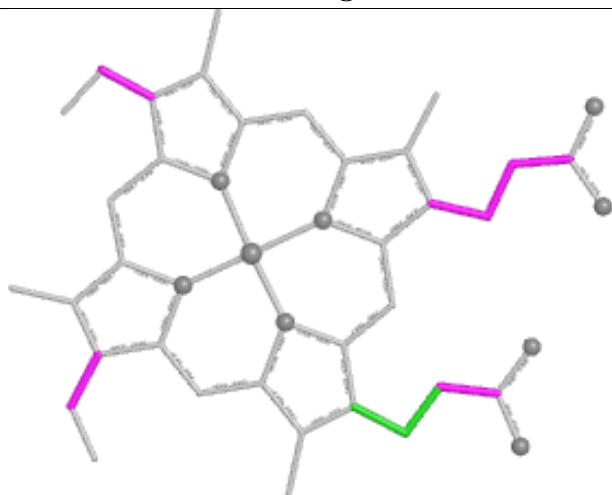
Ligand HEC P 242



Bond lengths



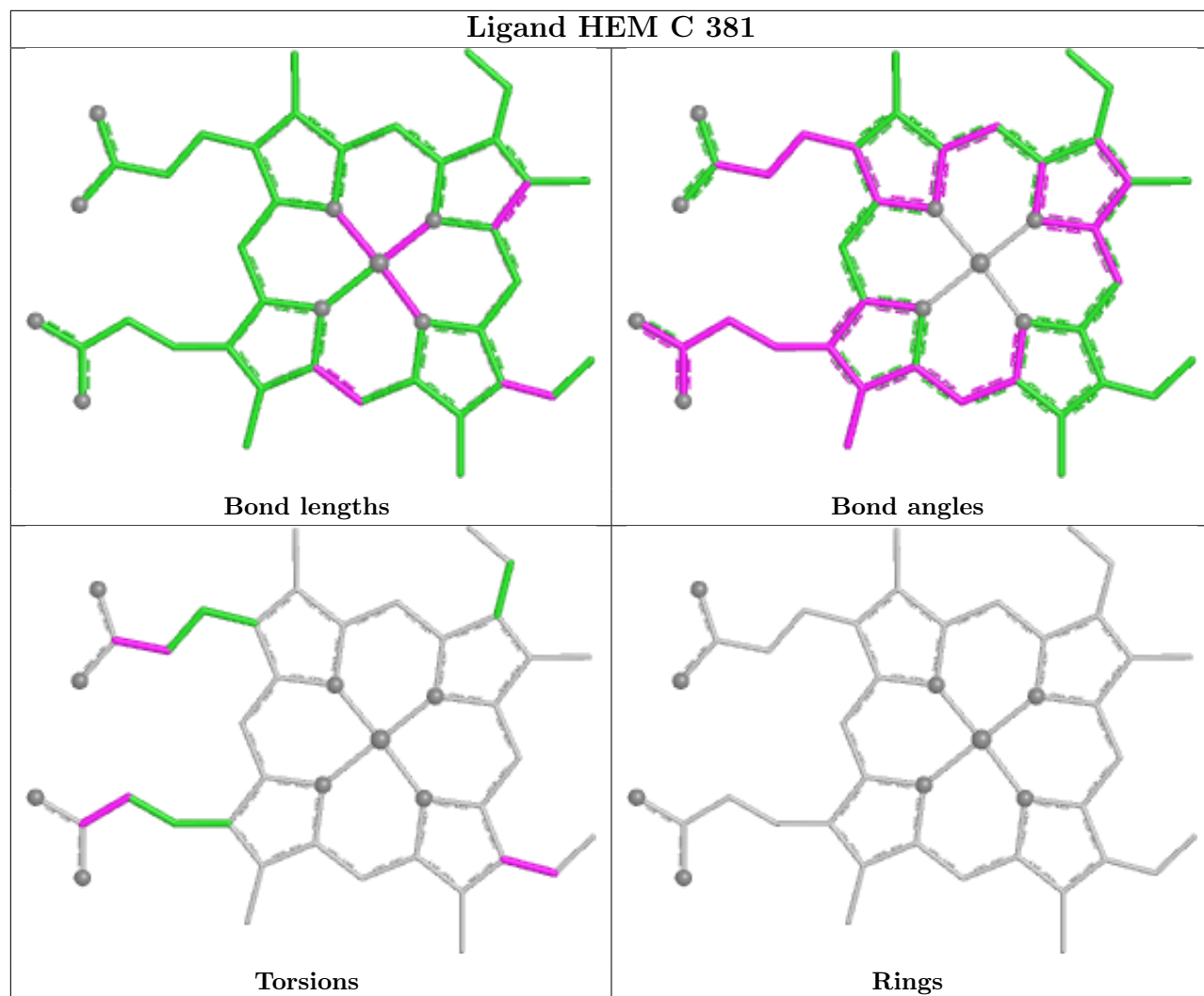
Bond angles



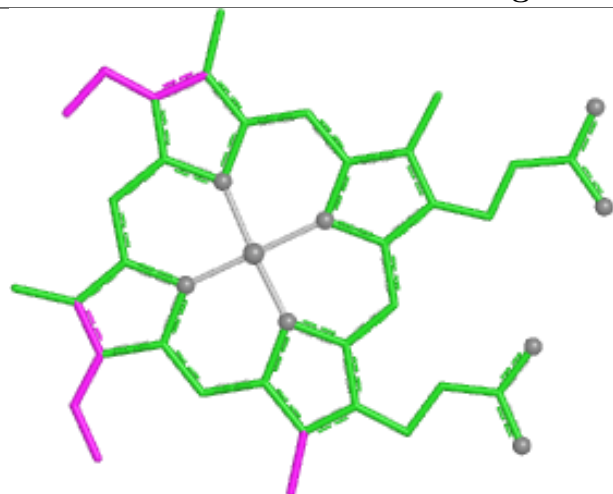
Torsions



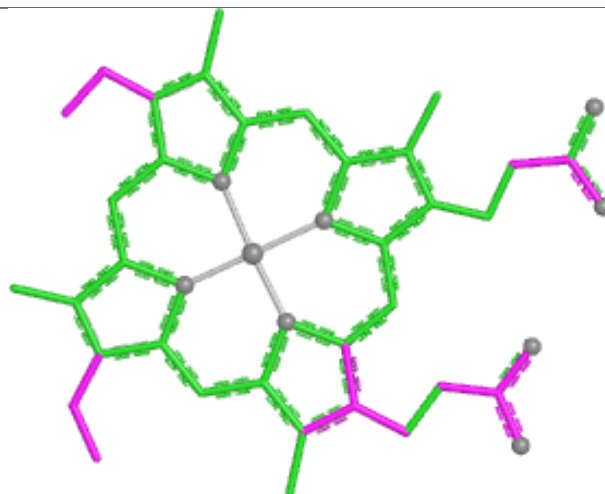
Rings



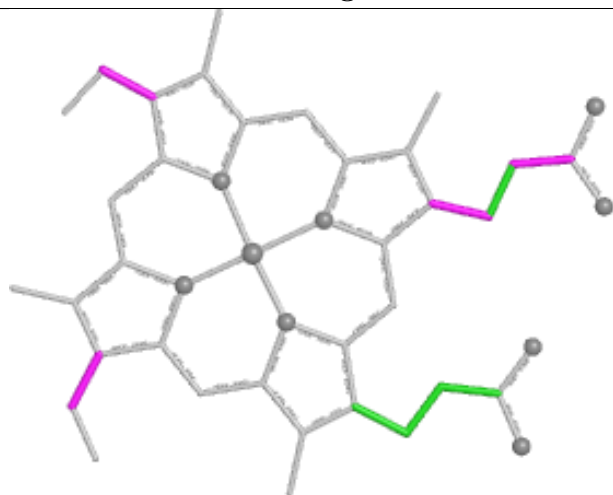
Ligand HEC D 242



Bond lengths



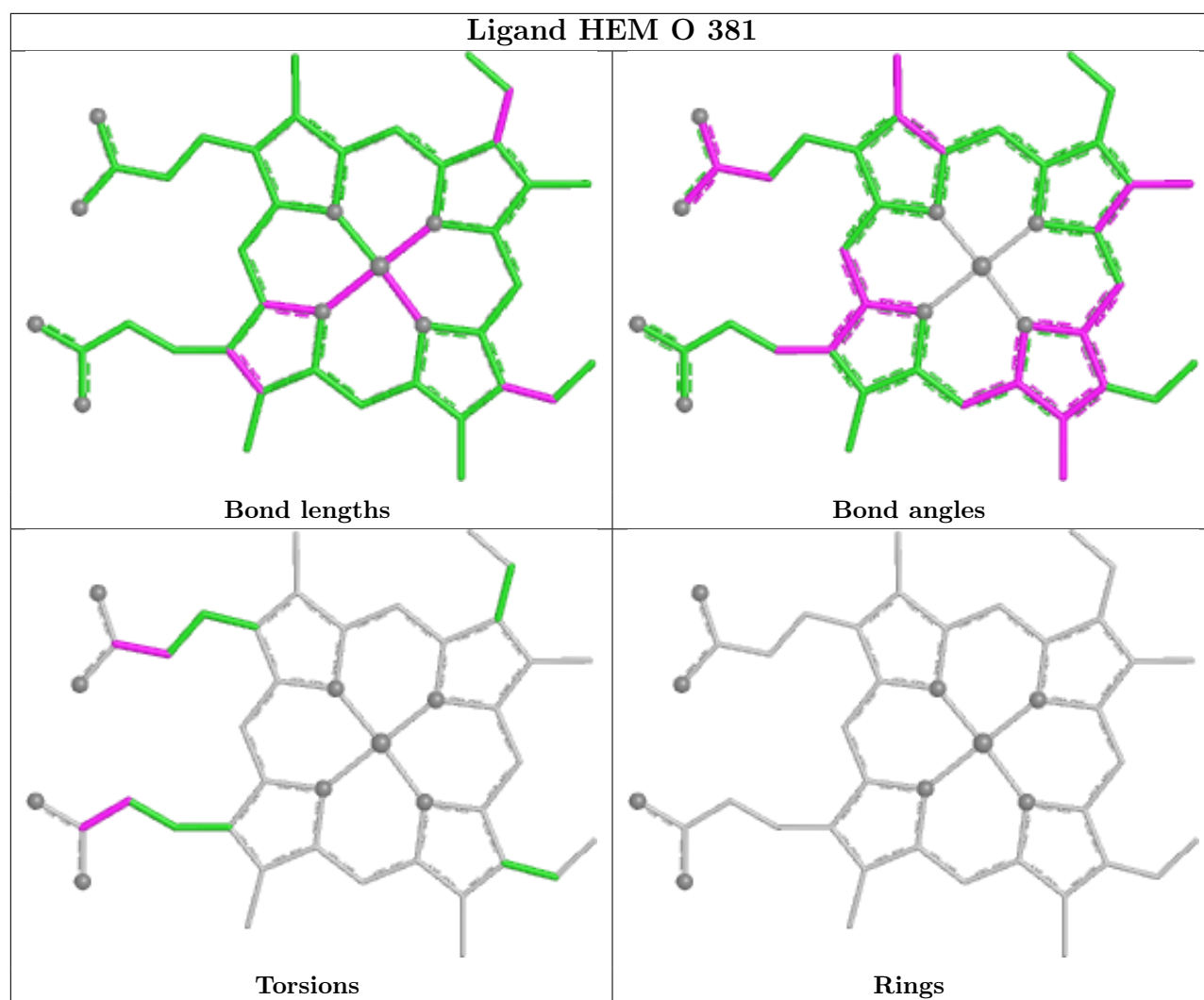
Bond angles

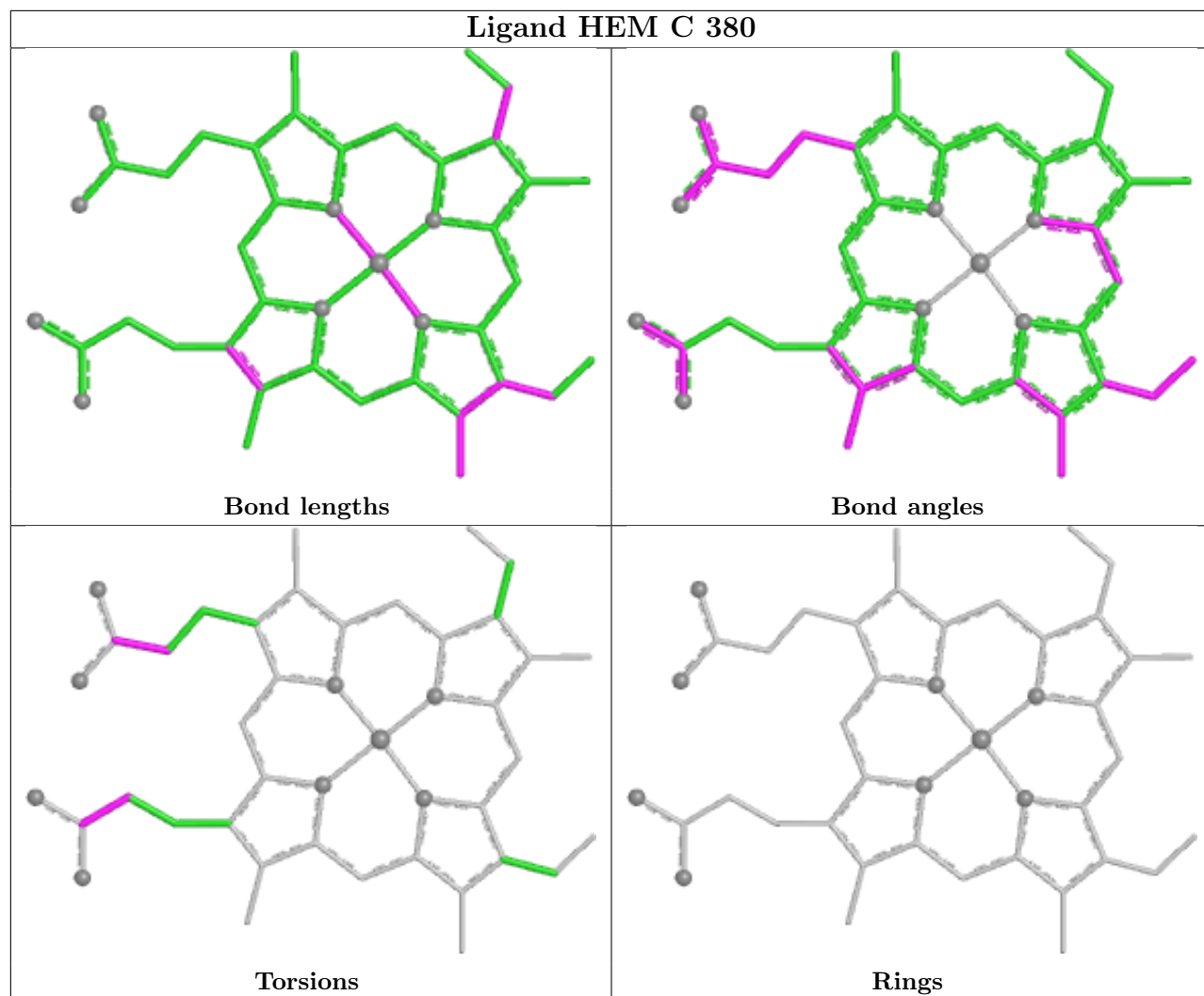


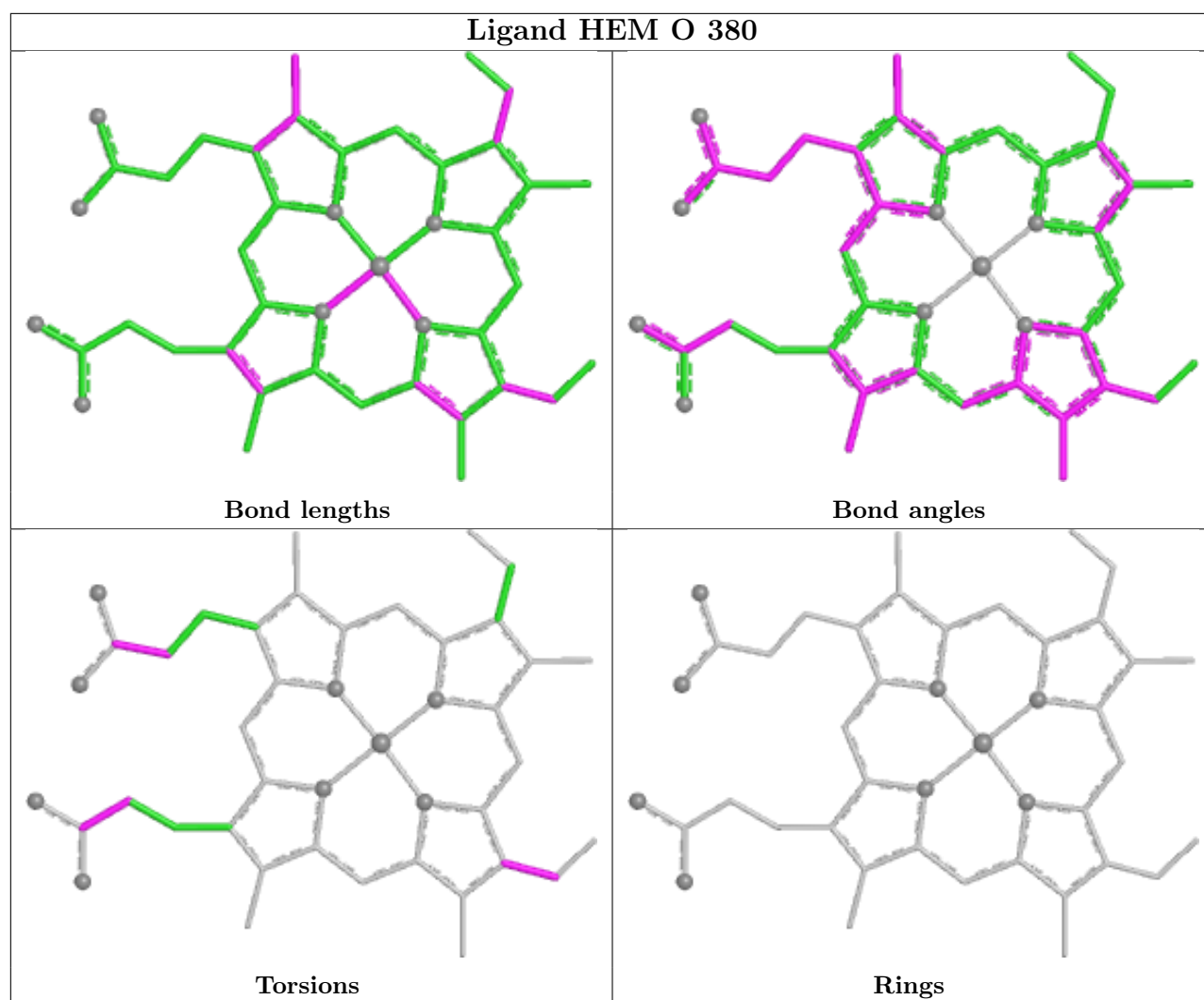
Torsions



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 [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.