



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 5, 2026 – 01:50 PM EDT

PDB ID : 1BGY / pdb_00001bgry
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)	:	2.50

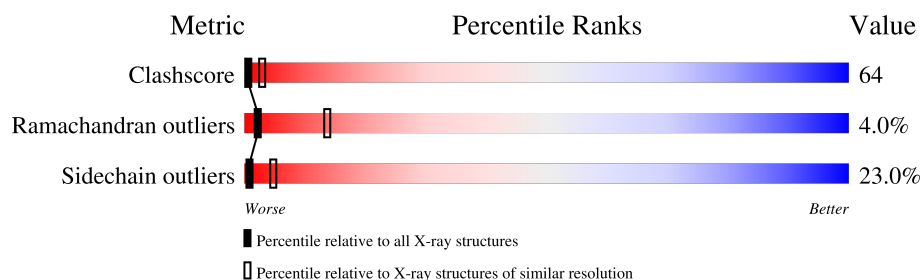
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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)

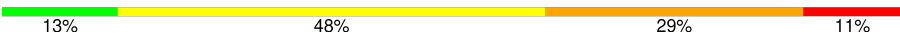
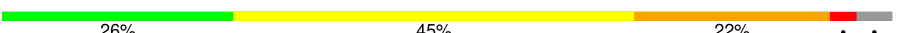
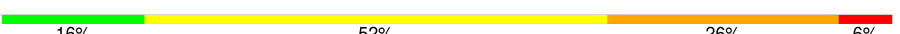
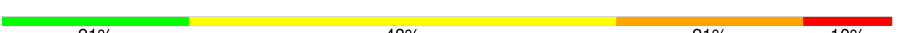
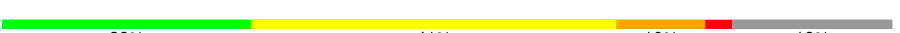
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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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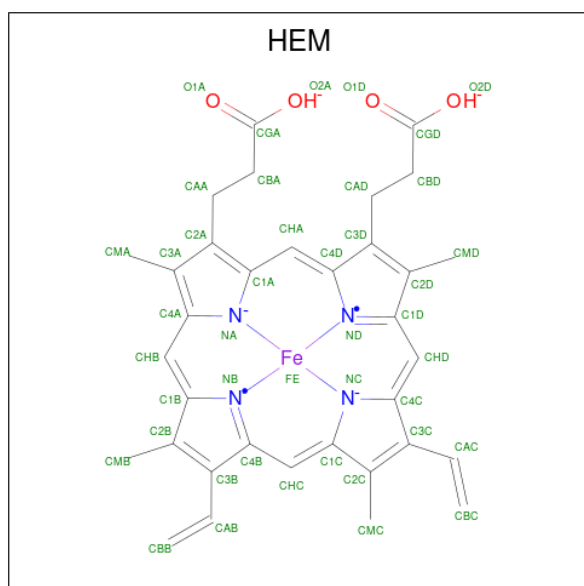
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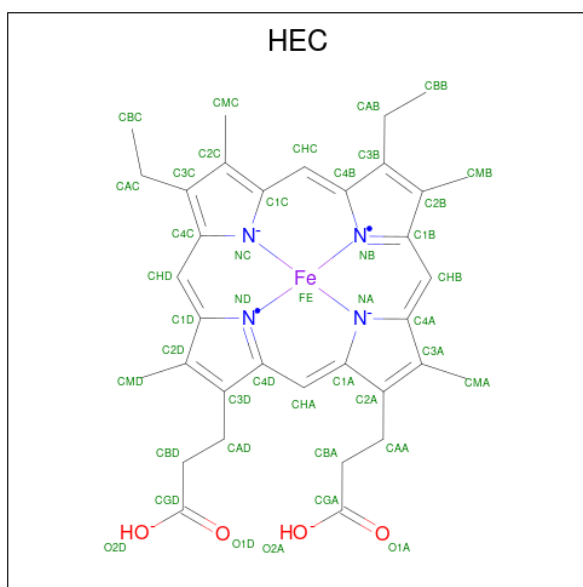
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	V	62	Total	C	N	O	0	0	0
			512	335	89	88			

- 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			

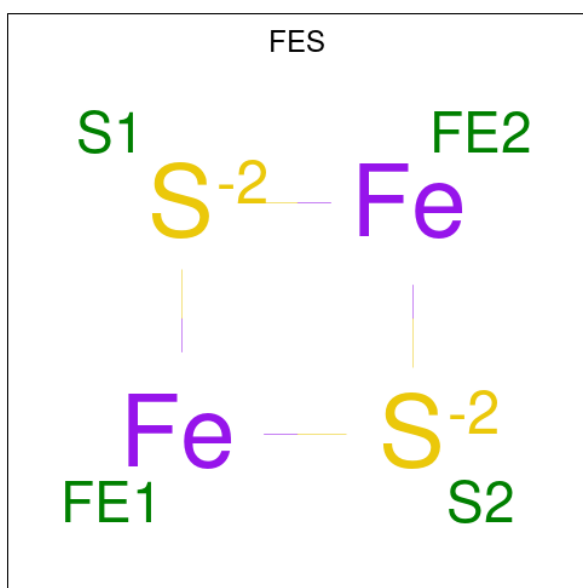
- Molecule 12 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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).



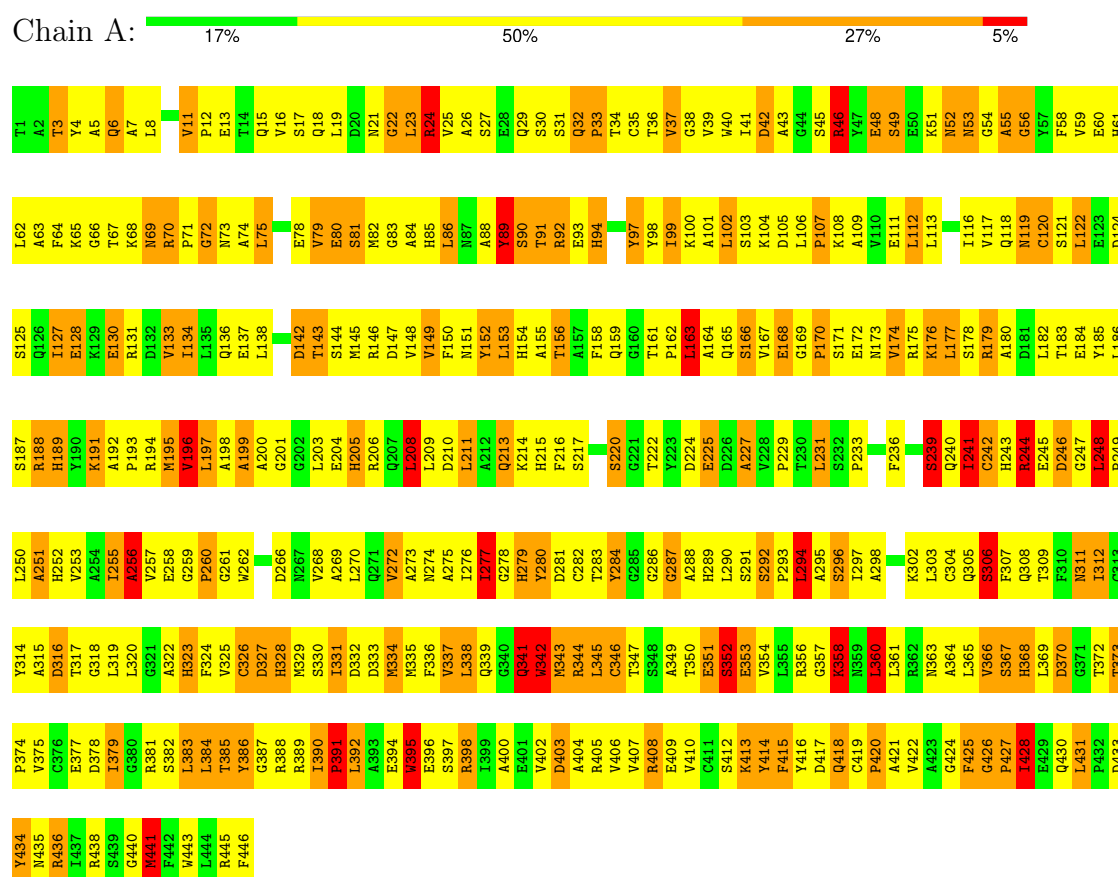
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	Q	1	Total	Fe	S	0	0
			4	2	2		

3 Residue-property plots

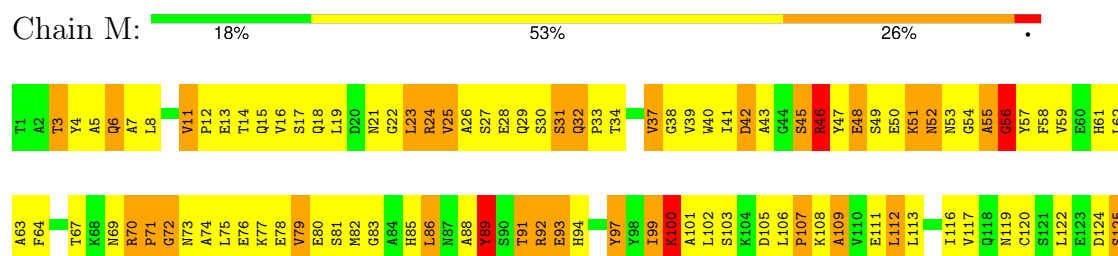
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

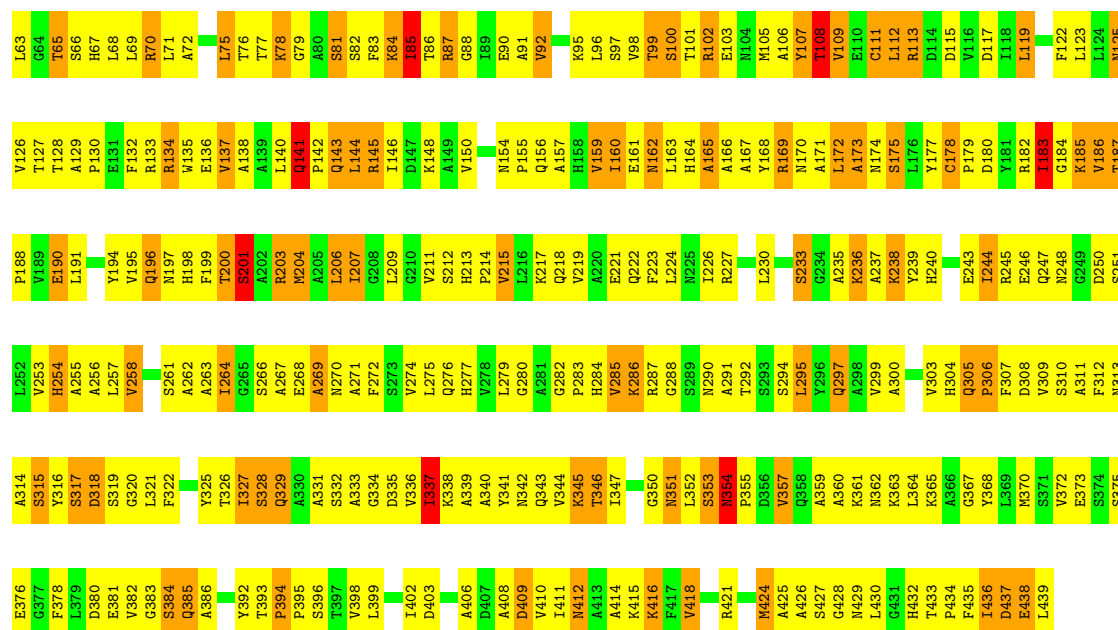




E381	V316	H254	L123	L63	SER
V382	S317	A255	L124	G64	LEU
G383	D318	A256	L125	T65	LYS
S384	S319	L257	V126	S66	VAL
Q385	G320	V258	L127	H67	ALA
A386	L321	A259	T128	L68	PRO
	F322	E260	A129	L69	LYS
S391	G323	S261	P130	R70	VAL
V392	F324	A262	F131	R71	LYS
T393	V325	A263	T200	F132	ALA
	T326	I264	S201	S73	THR
G394	I327	G265	A202	R134	GLU
P395	S328	S266	R203	L75	ALA
S396		A267	H204	T76	PRO
V397	A331	E268	V137	T77	ALA
V398	S332	A269	L206	K78	GLY
L399	A333	N270	T207	G79	VAL
	A334	A271	G208	A80	PRO
I402	G334	F272	L209	S81	PRO
D403	D335	S273	P142	S82	PRO
	V336	L279	L216	G88	HIS
A406	Q343	G280	N154	L29	
	V344	A281	P155	E90	P30
D409	K338	G282	Q218	A91	N31
K416	A339	Q276	S212	L144	
V410	A340	H277	H213	V92	G32
	T346	P283	A220	G93	L33
F417	I347	H284	E221	G94	V34
V418	A348	V285	Q222	K95	I35
	Q349	K286	F223	L96	A36
R421	G350	R287	L160	E161	S97
K422		G288	N162	L63	S37
S423	N351		T226	V98	L38
M424	L352		R227	T99	E39
	S353	A291	H164	S100	M40
A425	N354	T292	L230	T101	Y41
S427	P355	S293	A166	R102	E42
M428		S294	A167	E103	P43
M429	A360	L295	G234	E104	A44
L430	K361	V296	A235	M105	S45
G431	N362	Q297	R236	N170	
H432	K363	A298	A237	A106	R46
T433	L364	V299	R238	L172	I47
P434	K365	A300	V239	T108	G48
F435	A366		H240	V109	L49
	G367	V303	G241	E110	F50
I436	V368	H304	G242	C111	I51
E438	L369	Q305	E243	L112	K52
L439	M370	P306	T244	R113	A53
				D114	G54
	S371	F307	R245	D115	S55
V372	V372	D308	E246	D180	R56
E373	E373	V309	Q247	V116	
S374	S374	A311	M248	D117	Y57
S375	E376		G249	L118	E58
				L119	N59
				K185	S60
				M120	
				F121	N61
				V186	N62
	L379	G345	T252	E122	
	N386				

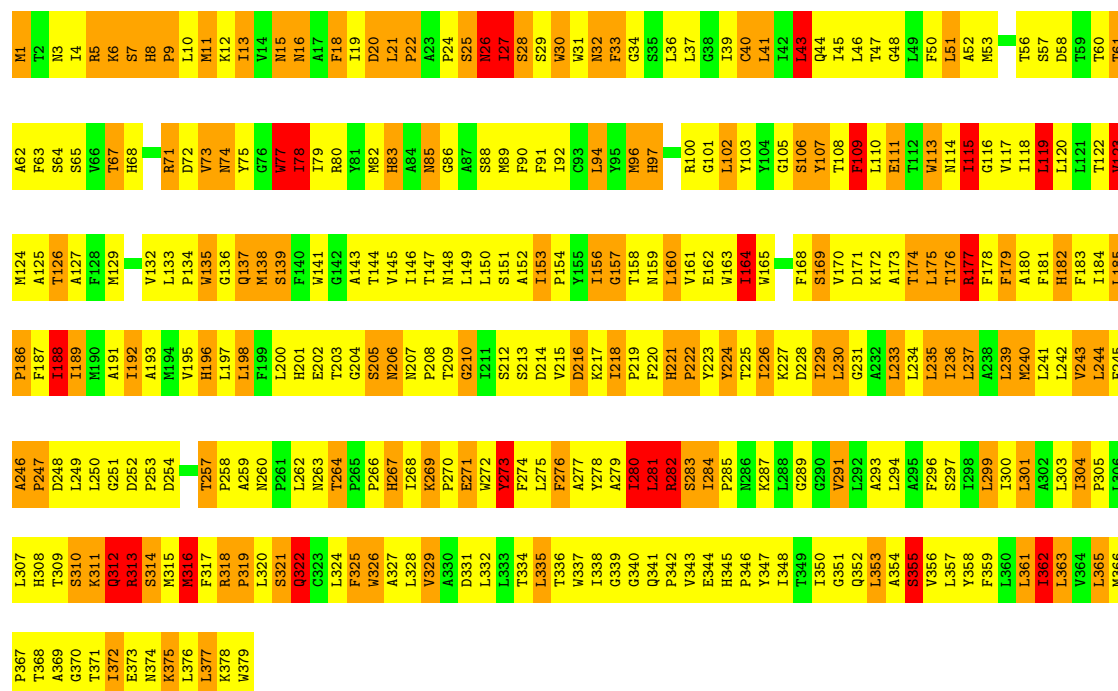
- Molecule 2: CYTOCHROME BC1 COMPLEX

SER	LEU	LYS	VAL	ALA	PRO	LYS	VAL	ALA	ALA	THR	GLU	ALA	PRO	ALA	GLY	VAL	PRO	PRO	HRG	P21	Q22	D23	L24	E25	L29	P30	N31	G32	L33	V34	I35	A36	S37	L38	E39	Y41	A42	P43	A44	S45	R46	I47	G48	L49	F50	I51	K52	A53	G54	S55	R56	E58	N59	S60	W61	R62
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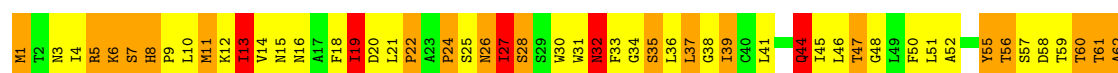
• Molecule 3: CYTOCHROME BC1 COMPLEX

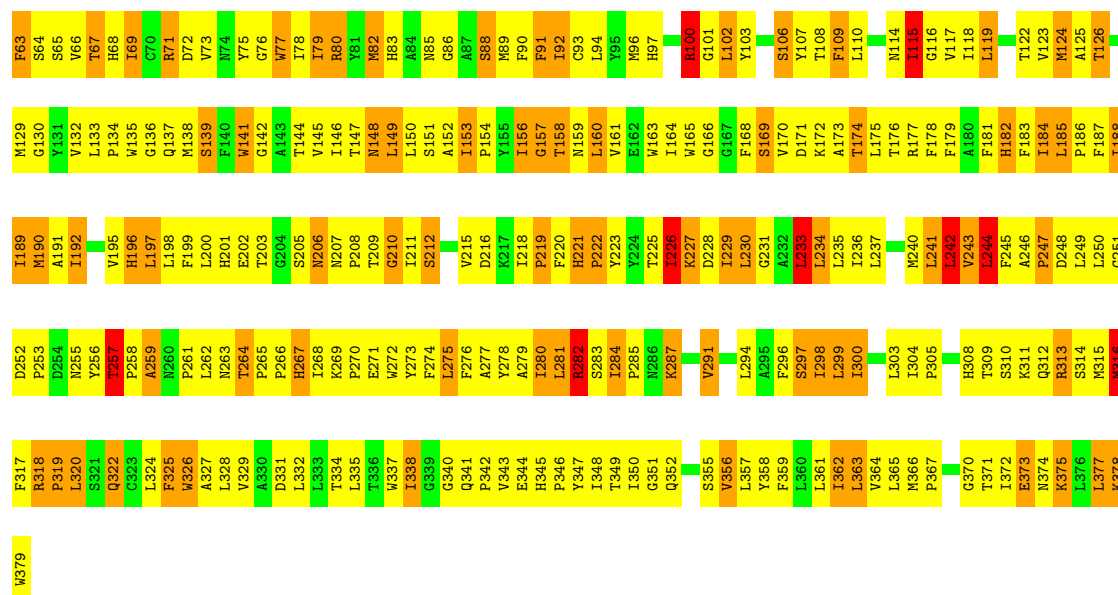
Chain C: 15% 51% 28% 6%



• Molecule 3: CYTOCHROME BC1 COMPLEX

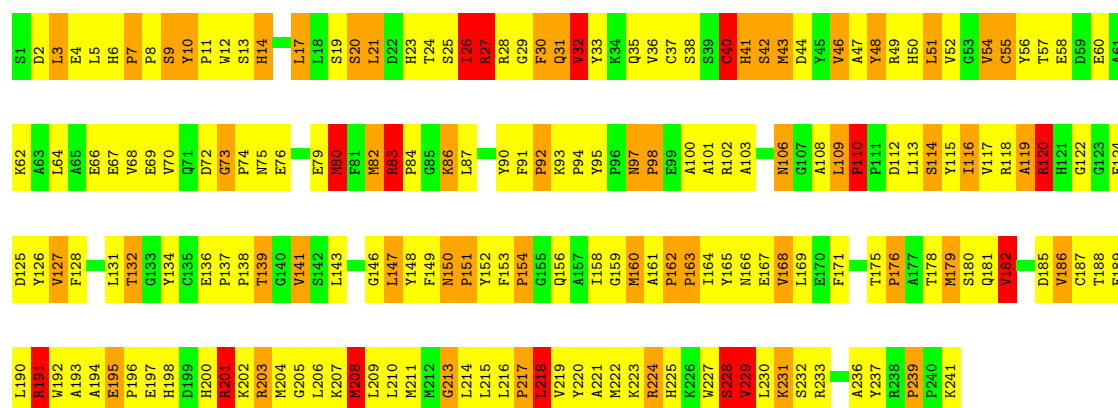
Chain O: 18% 53% 26% 1%





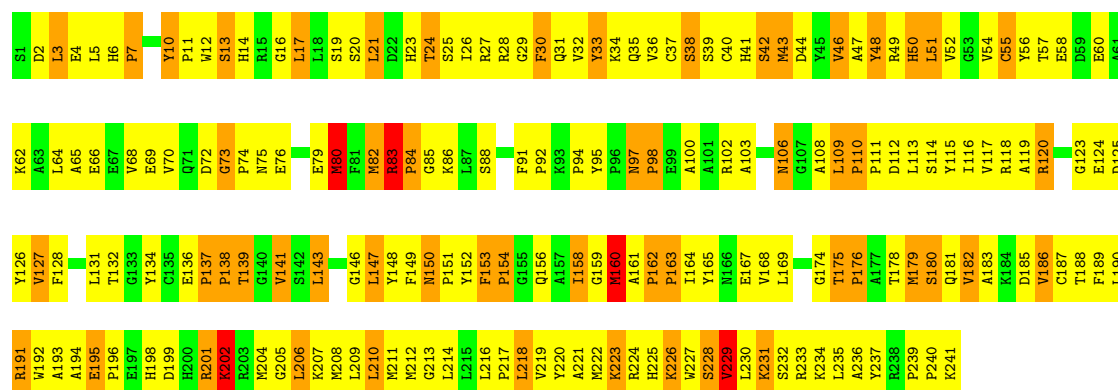
• Molecule 4: CYTOCHROME BC1 COMPLEX

Chain D: 22% 51% 21% 6%

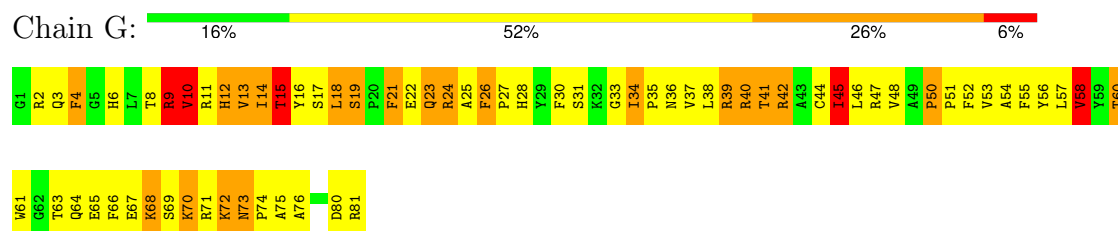


• Molecule 4: CYTOCHROME BC1 COMPLEX

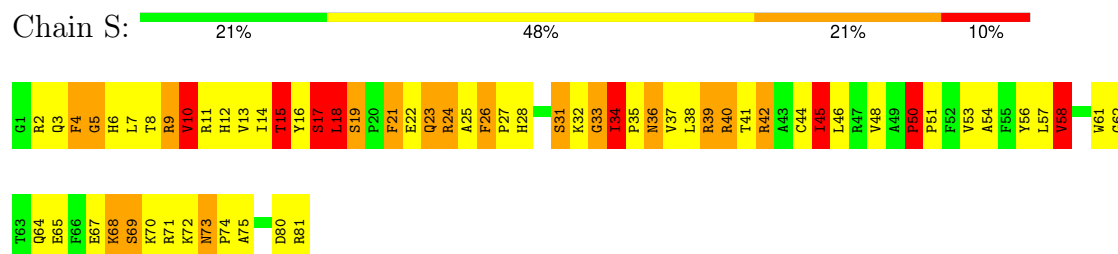
Chain P: 21% 54% 23% .



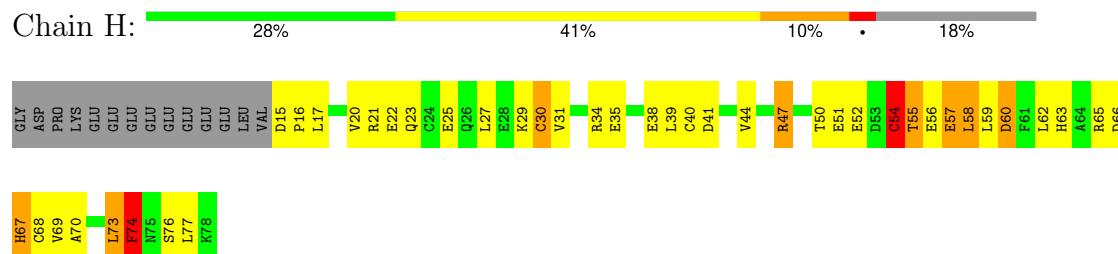
- Molecule 7: CYTOCHROME BC1 COMPLEX



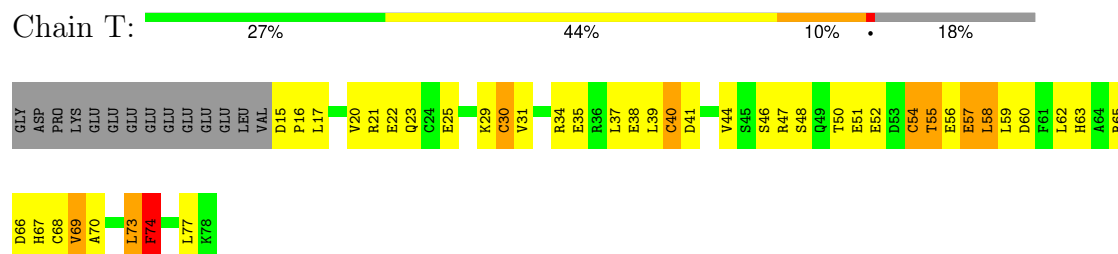
- Molecule 7: CYTOCHROME BC1 COMPLEX



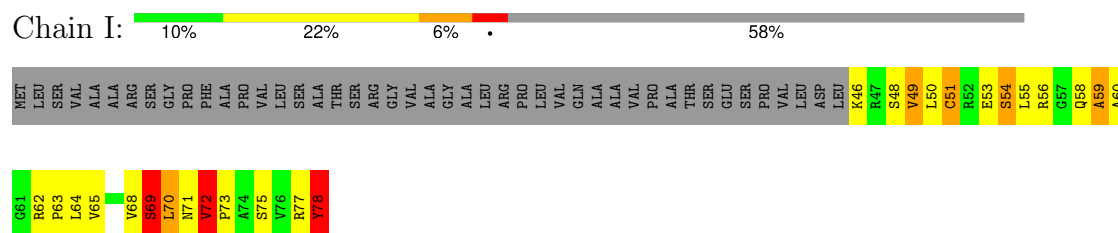
- Molecule 8: CYTOCHROME BC1 COMPLEX



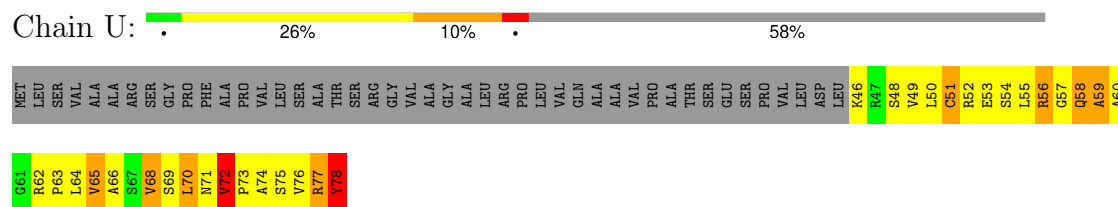
- Molecule 8: CYTOCHROME BC1 COMPLEX



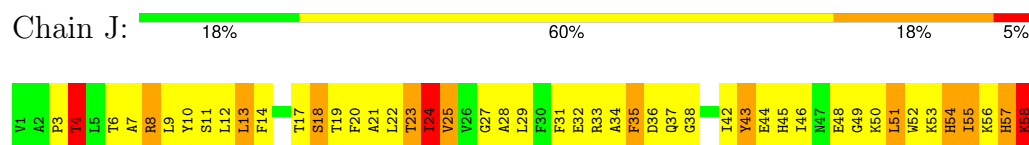
- Molecule 9: CYTOCHROME BC1 COMPLEX



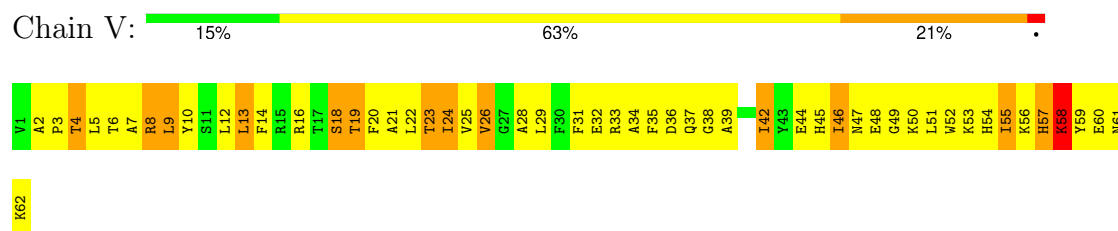
- Molecule 9: CYTOCHROME BC1 COMPLEX



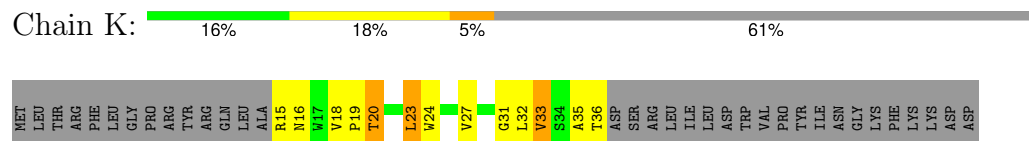
- Molecule 10: CYTOCHROME BC1 COMPLEX



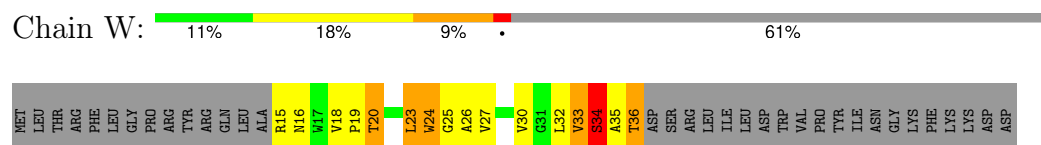
- Molecule 10: CYTOCHROME BC1 COMPLEX



- Molecule 11: CYTOCHROME BC1 COMPLEX



- Molecule 11: CYTOCHROME BC1 COMPLEX



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: FES, HEC, 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	$\# Z > 2$
12	HEM	O	381	3	50,50,50	1.37	7 (14%)	67,82,82	1.73	14 (20%)
12	HEM	C	381	3	50,50,50	1.27	6 (12%)	67,82,82	1.73	17 (25%)
13	HEC	P	242	4	50,50,50	1.34	5 (10%)	68,82,82	1.01	3 (4%)
12	HEM	O	380	3	50,50,50	1.41	8 (16%)	67,82,82	1.87	18 (26%)
12	HEM	C	380	3	50,50,50	1.31	7 (14%)	67,82,82	1.51	9 (13%)
14	FES	Q	197	5	0,4,4	-	-	-		
13	HEC	D	242	4	50,50,50	1.32	4 (8%)	68,82,82	1.11	5 (7%)

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

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	D	242	HEC	CBB-CAB	-3.72	1.35	1.51
13	P	242	HEC	CBC-CAC	-3.66	1.35	1.51
13	D	242	HEC	CBC-CAC	-3.56	1.36	1.51
13	P	242	HEC	CBB-CAB	-3.51	1.36	1.51
12	C	380	HEM	CAB-C3B	3.43	1.56	1.47

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	O	380	HEM	C3B-C2B-C1B	-5.36	102.39	106.41
12	O	381	HEM	C3B-C2B-C1B	4.97	110.14	106.41
12	O	380	HEM	CMA-C3A-C4A	-4.92	117.92	125.42
12	C	380	HEM	CBD-CAD-C3D	4.79	125.78	112.53
12	O	381	HEM	C2A-C1A-NA	-4.21	105.48	110.15

There are no chirality outliers.

5 of 36 torsion outliers are listed below:

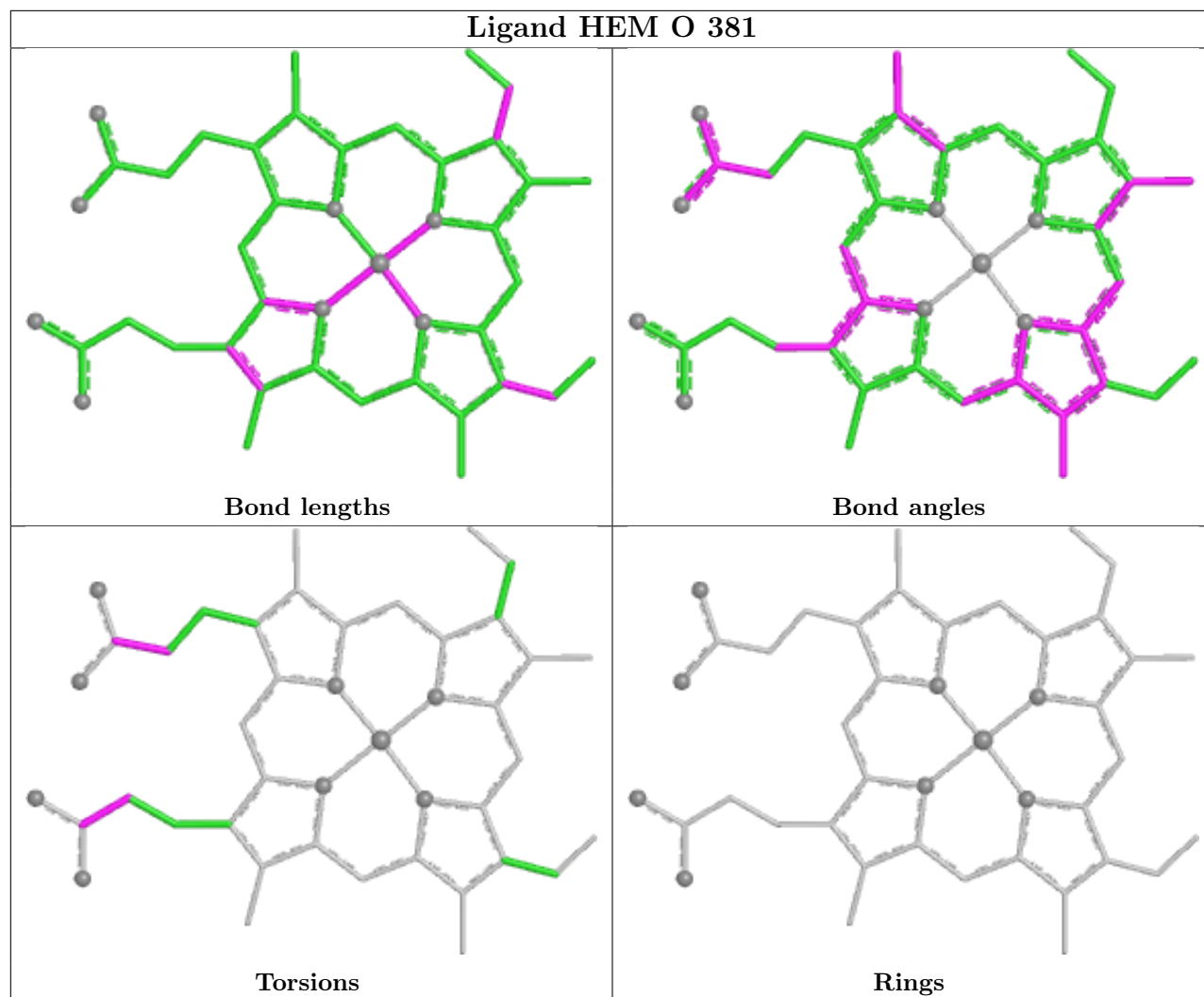
Mol	Chain	Res	Type	Atoms
12	O	380	HEM	C2B-C3B-CAB-CBB
13	P	242	HEC	C2C-C3C-CAC-CBC
13	D	242	HEC	C2B-C3B-CAB-CBB
13	D	242	HEC	C4B-C3B-CAB-CBB
13	P	242	HEC	C4C-C3C-CAC-CBC

There are no ring outliers.

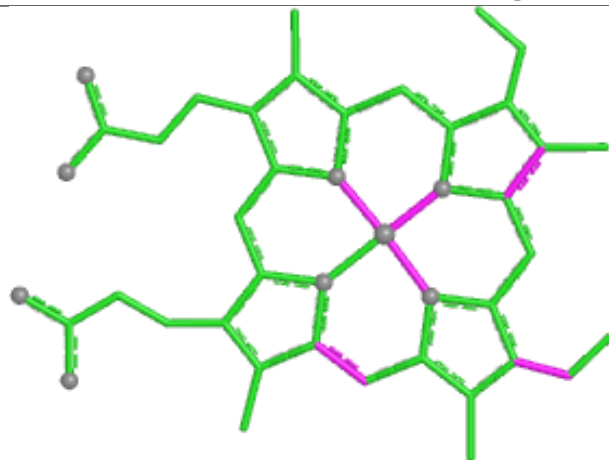
6 monomers are involved in 53 short contacts:

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

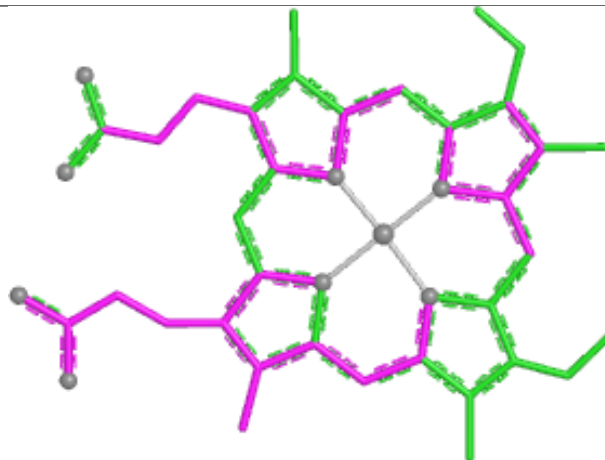
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



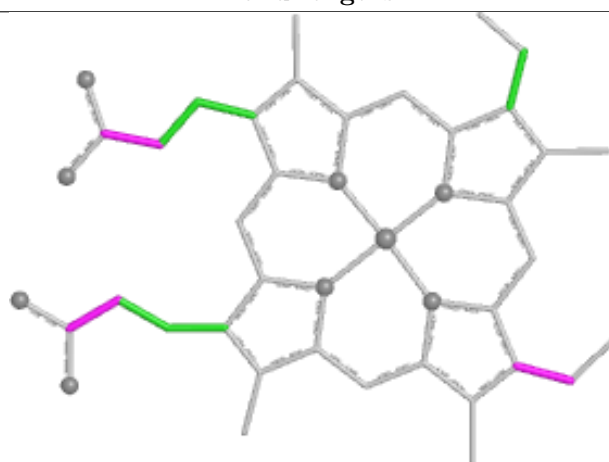
Ligand HEM C 381



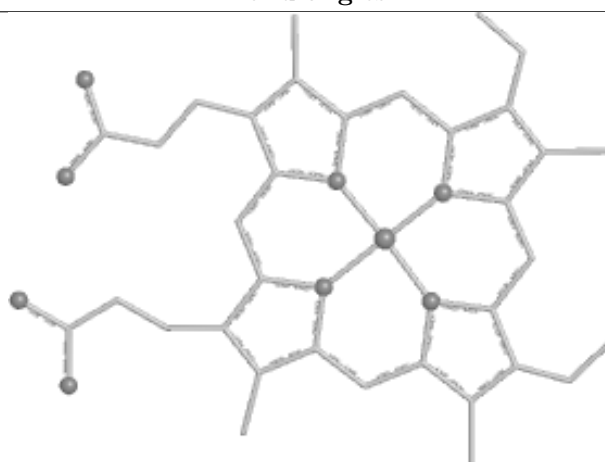
Bond lengths



Bond angles

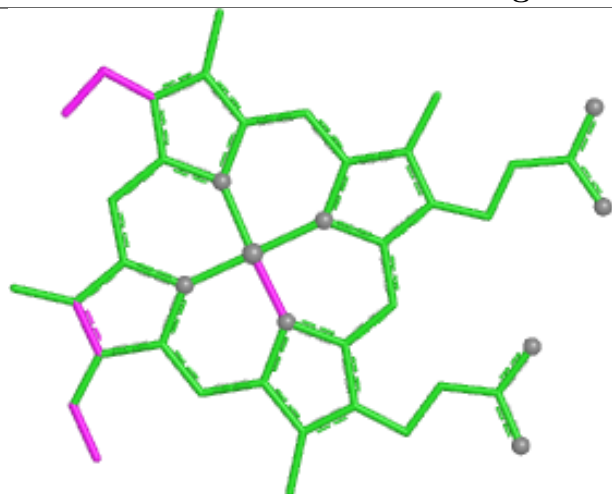


Torsions

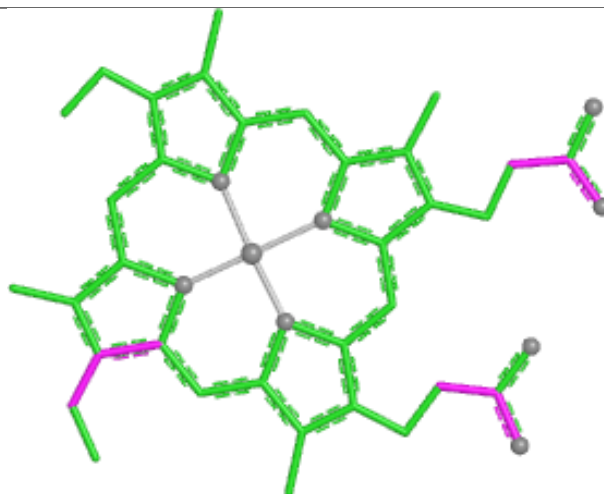


Rings

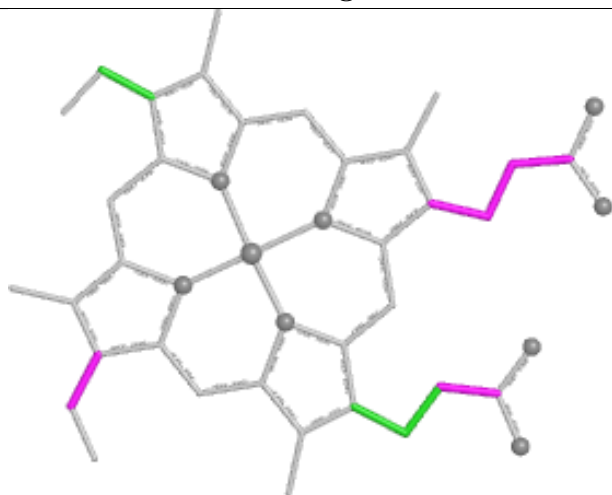
Ligand HEC P 242



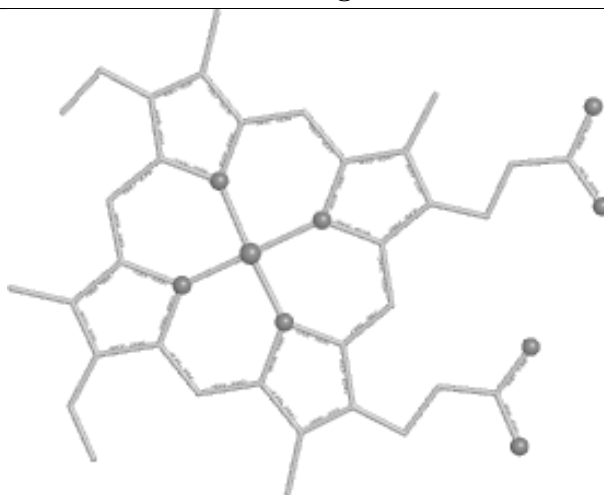
Bond lengths



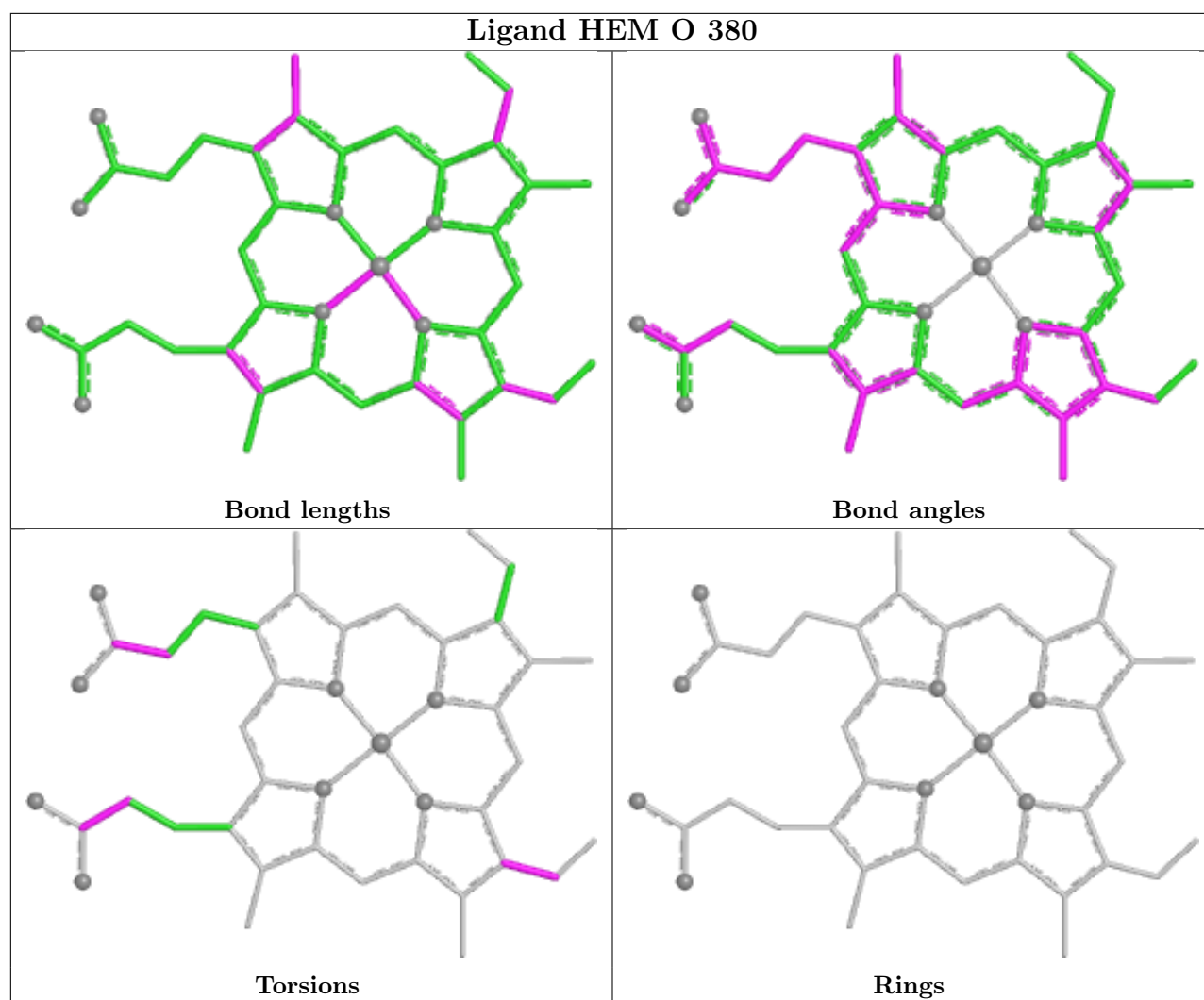
Bond angles

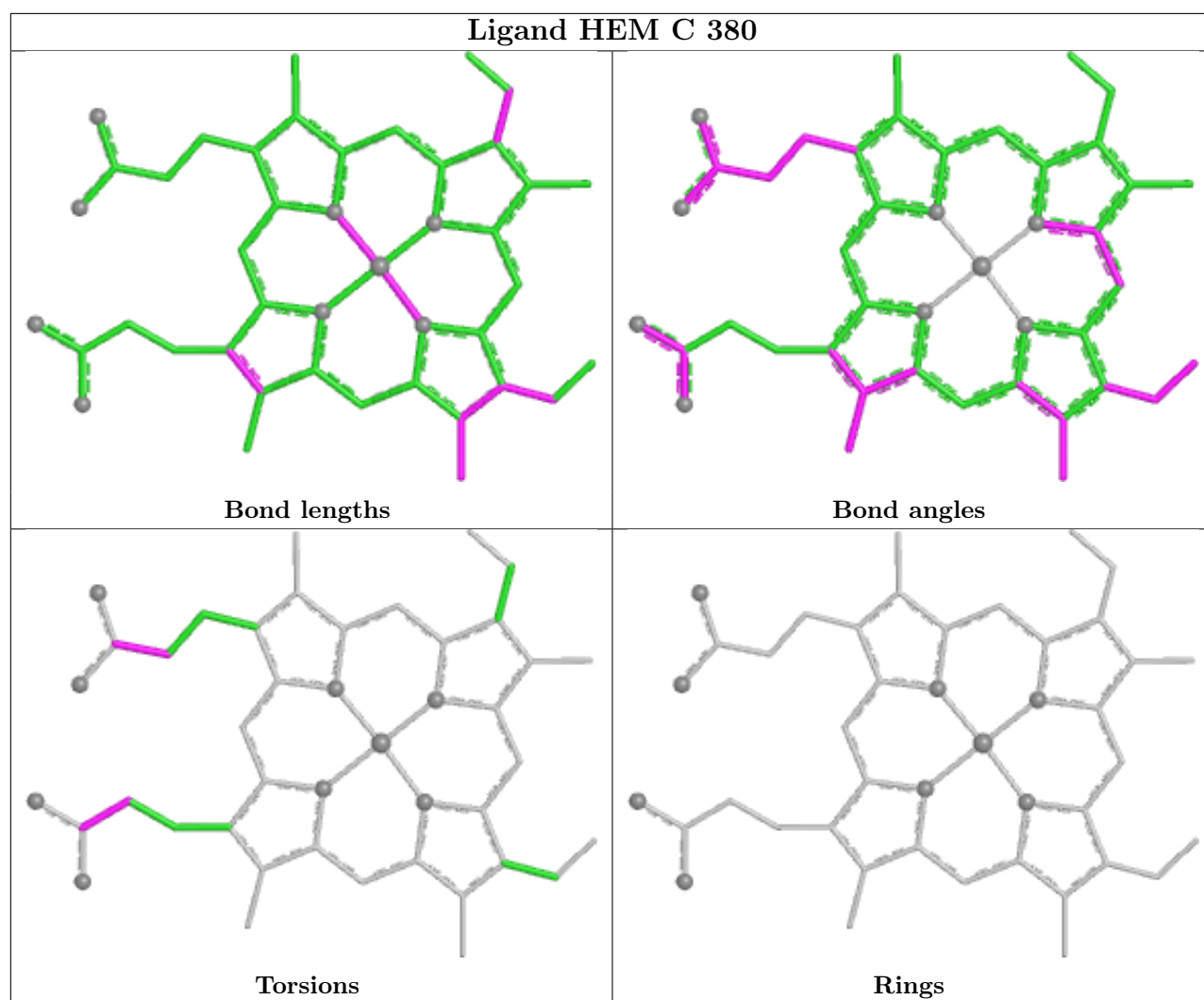


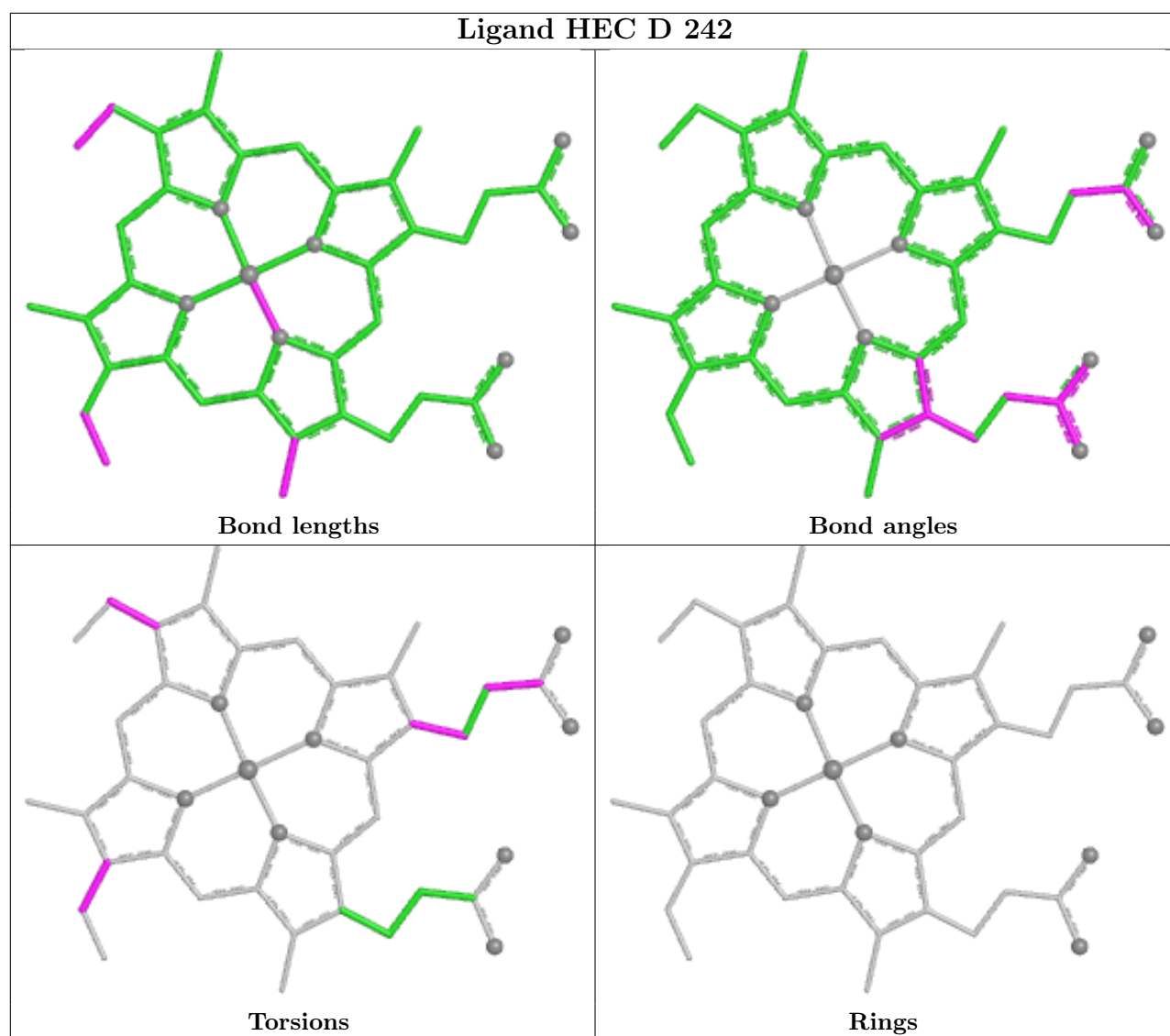
Torsions



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.