



wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 13, 2026 – 04:52 pm BST

PDB ID : 9RWY / pdb_00009rwy
Title : Crystal structure of bifunctional catalase-phenol oxidase from a marine-derived Cladosporium species complexed with catechol
Authors : Kosinas, C.; Ferousi, C.; Pantelakis, O.I.; Topakas, E.; Dimarogona, M.
Deposited on : 2025-07-10
Resolution : 1.95 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 : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

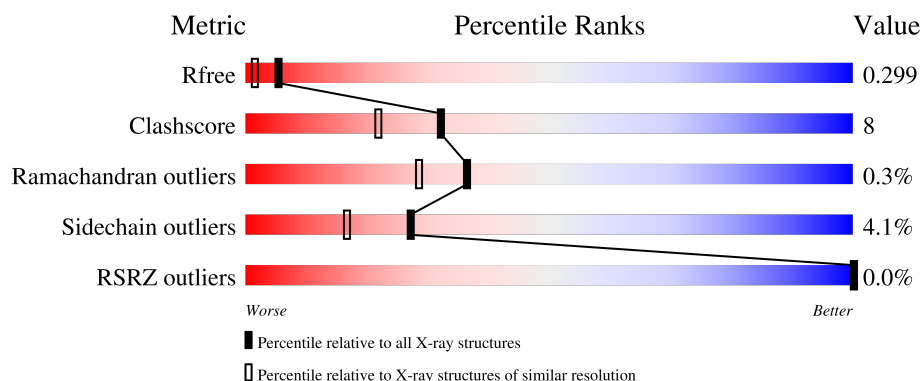
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

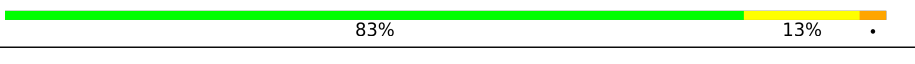
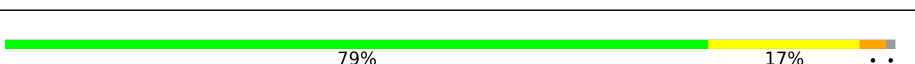
The reported resolution of this entry is 1.95 Å.

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))
R_{free}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	509	
1	B	509	
1	C	509	
1	D	509	
1	E	509	

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Mol	Chain	Length	Quality of chain
1	F	509	
1	G	509	
1	H	509	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	G	603	-	-	X	-
6	PEG	F	602	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 35420 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 catalase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	507	Total	C	N	O	S	0	0	0
			4088	2571	721	787	9			
1	B	507	Total	C	N	O	S	0	2	0
			4104	2581	724	790	9			
1	D	505	Total	C	N	O	S	0	1	0
			4084	2569	723	783	9			
1	C	507	Total	C	N	O	S	0	2	0
			4104	2583	726	786	9			
1	E	502	Total	C	N	O	S	0	3	0
			4084	2570	722	783	9			
1	F	504	Total	C	N	O	S	0	1	0
			4076	2566	720	781	9			
1	G	498	Total	C	N	O	S	0	1	0
			4039	2541	712	777	9			
1	H	507	Total	C	N	O	S	0	3	0
			4115	2589	730	787	9			

There are 16 discrepancies between the modelled and reference sequences:

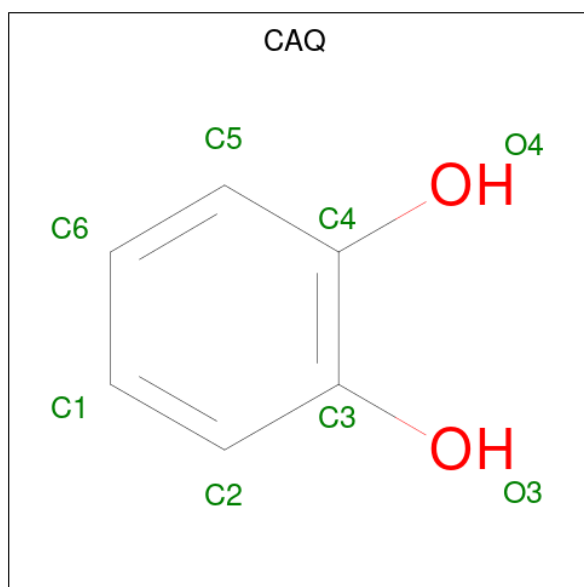
Chain	Residue	Modelled	Actual	Comment	Reference
A	508	ALA	-	expression tag	UNP A0AB34KRF0
A	509	LEU	-	expression tag	UNP A0AB34KRF0
B	508	ALA	-	expression tag	UNP A0AB34KRF0
B	509	LEU	-	expression tag	UNP A0AB34KRF0
D	508	ALA	-	expression tag	UNP A0AB34KRF0
D	509	LEU	-	expression tag	UNP A0AB34KRF0
C	508	ALA	-	expression tag	UNP A0AB34KRF0
C	509	LEU	-	expression tag	UNP A0AB34KRF0
E	508	ALA	-	expression tag	UNP A0AB34KRF0
E	509	LEU	-	expression tag	UNP A0AB34KRF0
F	508	ALA	-	expression tag	UNP A0AB34KRF0
F	509	LEU	-	expression tag	UNP A0AB34KRF0
G	508	ALA	-	expression tag	UNP A0AB34KRF0

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Chain	Residue	Modelled	Actual	Comment	Reference
G	509	LEU	-	expression tag	UNP A0AB34KRF0
H	508	ALA	-	expression tag	UNP A0AB34KRF0
H	509	LEU	-	expression tag	UNP A0AB34KRF0

- Molecule 2 is CATECHOL (CCD ID: CAQ) (formula: $C_6H_6O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			8	6	2		

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	G	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	H	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



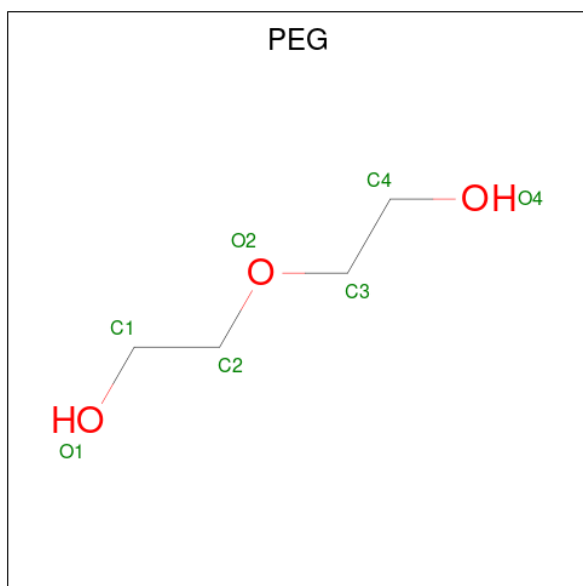
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	H	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	E	1	Total	C	O	0	0
			7	4	3		
6	F	1	Total	C	O	0	0
			7	4	3		

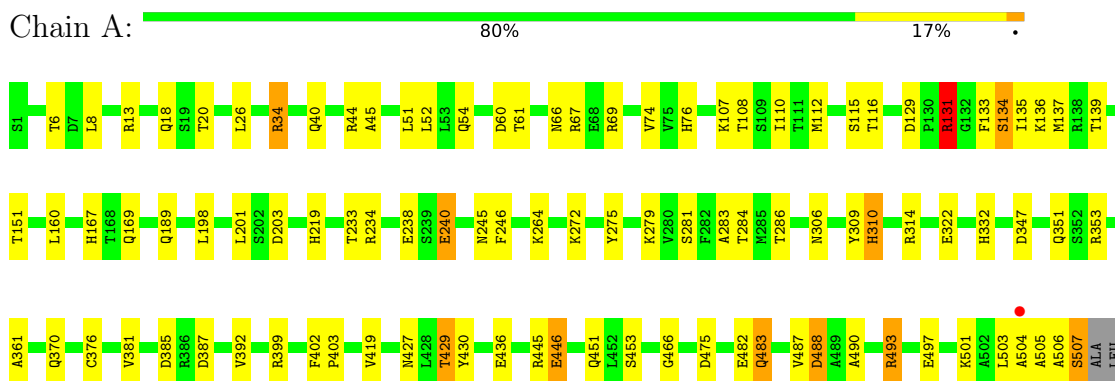
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	250	Total 252	O 252	0	2
7	B	258	Total 264	O 264	0	6
7	D	211	Total 213	O 213	0	2
7	C	225	Total 226	O 226	0	1
7	E	345	Total 348	O 348	0	3
7	F	324	Total 327	O 327	0	3
7	G	319	Total 321	O 321	0	2
7	H	305	Total 307	O 307	0	2

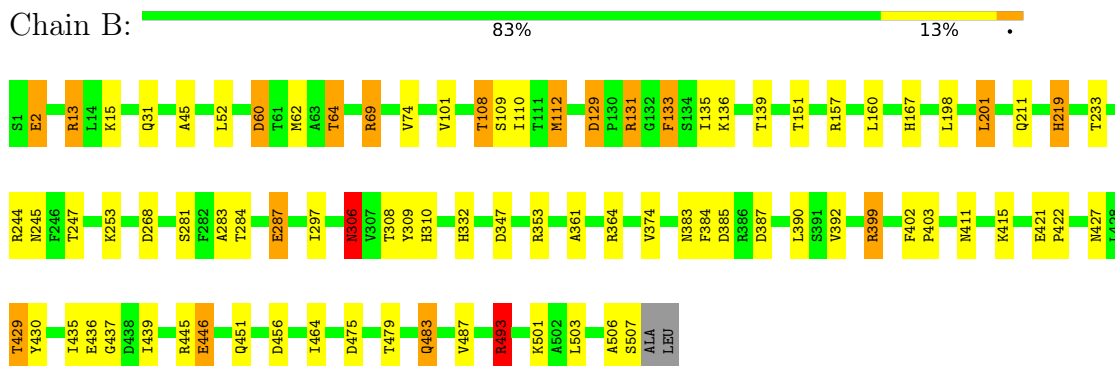
3 Residue-property plots

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

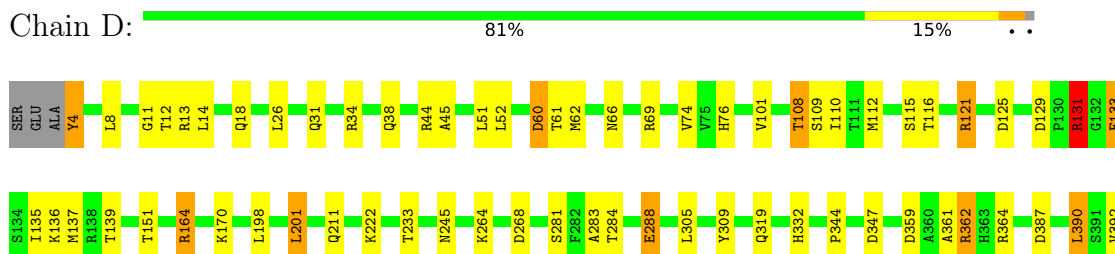
- Molecule 1: catalase



- Molecule 1: catalase



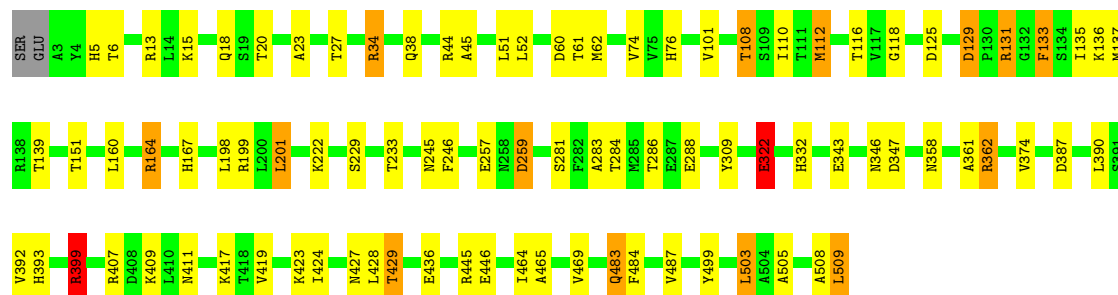
- Molecule 1: catalase





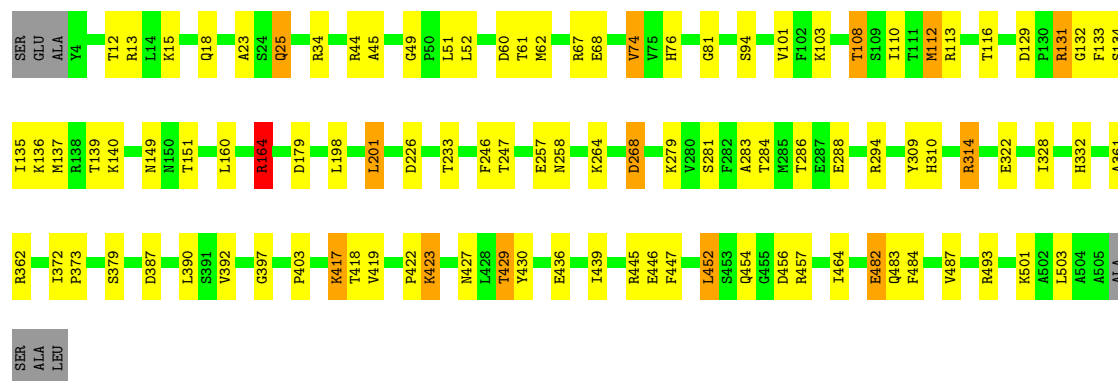
- Molecule 1: catalase

Chain C: 82% 15%



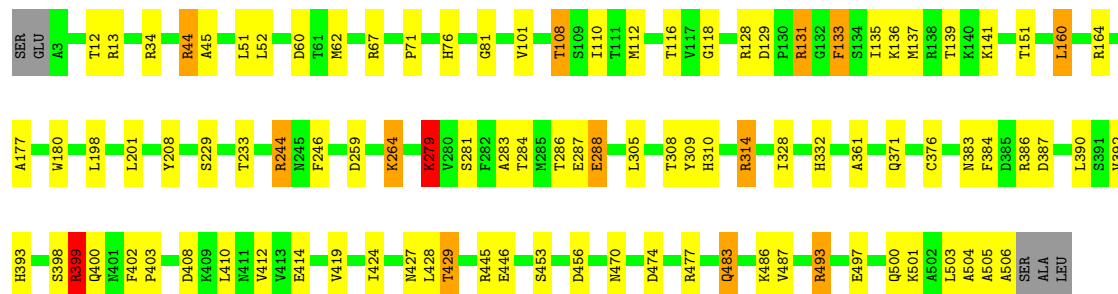
- Molecule 1: catalase

Chain E: 79% 17%



- Molecule 1: catalase

Chain F: 80% 17%



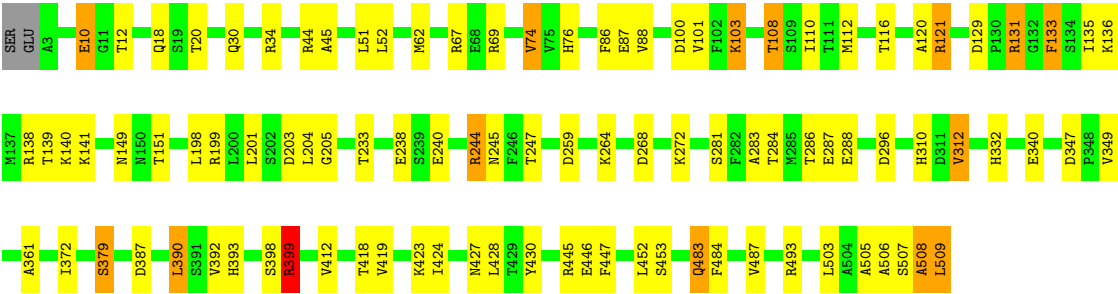
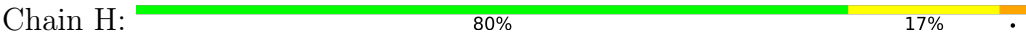
- Molecule 1: catalase

Chain G: 79% 17%





● Molecule 1: catalase



4 Data and refinement statistics

Property	Value
Space group	P 1
Cell constants a, b, c, α , β , γ	91.87Å 92.08Å 168.81Å 83.00° 77.94° 60.10°
Resolution (Å)	79.93 – 1.95 79.93 – 1.95
% Data completeness (in resolution range)	90.5 (79.93-1.95) 89.1 (79.93-1.95)
R_{merge}	0.13
R_{sym}	(Not available)
$\langle I/\sigma(I) \rangle$ ¹	1.22 (at 1.95Å)
Refinement program	REFMAC 5.8.0430 (refmacat 0.4.105), REFMAC 5.8.0430 (refmacat 0.4.105)
R, R_{free}	0.256 , 0.295 0.261 , 0.299
R_{free} test set	15664 reflections (4.58%)
Wilson B-factor (Å ²)	30.5
Anisotropy	0.414
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 49.7
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$
Estimated twinning fraction	0.034 for -h,-h+k,-l
F_o, F_c correlation	0.94
Total number of atoms	35420
Average B, all atoms (Å ²)	37.0

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, PEG, HEM, CAQ, EDO

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	0.69	0/4197	1.16	15/5700 (0.3%)
1	B	0.70	2/4213 (0.0%)	1.18	21/5722 (0.4%)
1	C	0.67	0/4213	1.15	22/5722 (0.4%)
1	D	0.67	0/4193	1.14	17/5694 (0.3%)
1	E	0.76	1/4193 (0.0%)	1.23	23/5694 (0.4%)
1	F	0.74	0/4185	1.20	21/5683 (0.4%)
1	G	0.73	0/4148	1.21	22/5634 (0.4%)
1	H	0.72	0/4224	1.22	20/5736 (0.3%)
All	All	0.71	3/33566 (0.0%)	1.19	161/45585 (0.4%)

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
1	B	0	3
1	C	0	3
1	D	0	7
1	E	0	5
1	F	0	6
1	G	0	8
1	H	0	7
All	All	0	43

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	457	ARG	NE-CZ	6.24	1.40	1.33
1	B	219	HIS	CE1-NE2	-5.45	1.27	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	399	ARG	NE-CZ	-5.19	1.27	1.33

The worst 5 of 161 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	131	ARG	CD-NE-CZ	18.01	149.61	124.40
1	G	131	ARG	NE-CZ-NH2	-14.98	105.72	119.20
1	H	131	ARG	NE-CZ-NH2	-14.85	105.83	119.20
1	F	131	ARG	NE-CZ-NH2	-14.81	105.87	119.20
1	E	131	ARG	CD-NE-CZ	14.06	144.09	124.40

There are no chirality outliers.

5 of 43 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	131	ARG	Sidechain
1	A	34	ARG	Sidechain
1	A	67	ARG	Sidechain
1	A	69	ARG	Sidechain
1	B	69	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4088	0	3859	71	0
1	B	4104	0	3874	68	0
1	C	4104	0	3881	77	0
1	D	4084	0	3857	62	0
1	E	4084	0	3855	83	0
1	F	4076	0	3852	84	0
1	G	4039	0	3801	74	0
1	H	4115	0	3893	65	0
2	A	8	0	5	2	0
3	A	43	0	30	6	0
3	B	43	0	30	4	0
3	C	43	0	30	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	43	0	30	1	0
3	E	43	0	30	7	0
3	F	43	0	30	3	0
3	G	43	0	30	6	0
3	H	43	0	30	3	0
4	A	14	0	13	5	0
4	B	14	0	13	6	0
4	C	14	0	13	2	0
4	D	14	0	13	3	0
4	G	28	0	26	9	0
4	H	14	0	13	3	0
5	A	4	0	6	1	0
6	E	7	0	10	0	0
6	F	7	0	10	17	0
7	A	252	0	0	11	0
7	B	264	0	0	13	0
7	C	226	0	0	12	1
7	D	213	0	0	11	1
7	E	348	0	0	15	0
7	F	327	0	0	20	0
7	G	321	0	0	24	0
7	H	307	0	0	16	0
All	All	35420	0	31234	517	1

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 8.

The worst 5 of 517 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)
1:H:245:ASN:HD22	4:H:602:NAG:C1	1.02	1.65
1:G:245:ASN:HD22	4:G:602:NAG:C1	1.12	1.61
1:B:245:ASN:HD22	4:B:602:NAG:C1	1.08	1.60
1:A:245:ASN:HD22	4:A:603:NAG:C1	1.01	1.59
1:C:245:ASN:HD22	4:C:602:NAG:C1	0.99	1.58

All (1) 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)
7:D:899:HOH:O	7:C:890:HOH:O[1_455]	2.00	0.20

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	505/509 (99%)	487 (96%)	16 (3%)	2 (0%)	30	21
1	B	507/509 (100%)	490 (97%)	16 (3%)	1 (0%)	43	36
1	C	507/509 (100%)	487 (96%)	19 (4%)	1 (0%)	43	36
1	D	504/509 (99%)	486 (96%)	17 (3%)	1 (0%)	43	36
1	E	503/509 (99%)	484 (96%)	18 (4%)	1 (0%)	43	36
1	F	503/509 (99%)	485 (96%)	16 (3%)	2 (0%)	30	21
1	G	497/509 (98%)	478 (96%)	17 (3%)	2 (0%)	30	21
1	H	508/509 (100%)	487 (96%)	17 (3%)	4 (1%)	16	8
All	All	4034/4072 (99%)	3884 (96%)	136 (3%)	14 (0%)	36	28

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	4	TYR
1	H	121[A]	ARG
1	H	121[B]	ARG
1	A	506	ALA
1	F	505	ALA

5.3.2 Protein sidechains [i](#)

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	429/430 (100%)	409 (95%)	20 (5%)	23	12
1	B	431/430 (100%)	414 (96%)	17 (4%)	28	18
1	C	430/430 (100%)	414 (96%)	16 (4%)	30	20
1	D	428/430 (100%)	411 (96%)	17 (4%)	28	17
1	E	429/430 (100%)	414 (96%)	15 (4%)	32	22
1	F	427/430 (99%)	405 (95%)	22 (5%)	21	9
1	G	425/430 (99%)	412 (97%)	13 (3%)	35	26
1	H	431/430 (100%)	408 (95%)	23 (5%)	20	9
All	All	3430/3440 (100%)	3287 (96%)	143 (4%)	27	16

5 of 143 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	288	GLU
1	G	483	GLN
1	H	272	LYS
1	D	288	GLU
1	D	284	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	245	ASN
1	G	351	GLN
1	H	212	HIS
1	D	245	ASN
1	D	196	GLN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

19 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$
3	HEM	E	601	1	50,50,50	2.34	18 (36%)	66,82,82	1.75	14 (21%)
3	HEM	G	601	1	50,50,50	2.50	12 (24%)	66,82,82	1.81	20 (30%)
6	PEG	E	602	-	6,6,6	0.22	0	5,5,5	0.07	0
3	HEM	B	601	1	50,50,50	2.27	12 (24%)	66,82,82	1.81	16 (24%)
4	NAG	G	602	-	14,14,15	0.58	0	17,19,21	1.72	3 (17%)
4	NAG	H	602	-	14,14,15	0.48	0	17,19,21	1.50	3 (17%)
3	HEM	D	601	1	50,50,50	2.72	17 (34%)	66,82,82	1.72	14 (21%)
4	NAG	B	602	-	14,14,15	0.39	0	17,19,21	1.27	3 (17%)
6	PEG	F	602	-	6,6,6	0.37	0	5,5,5	0.30	0
4	NAG	C	602	-	14,14,15	0.52	0	17,19,21	1.56	3 (17%)
3	HEM	H	601	1	50,50,50	2.14	15 (30%)	66,82,82	1.59	14 (21%)
4	NAG	A	603	-	14,14,15	0.53	0	17,19,21	1.48	1 (5%)
4	NAG	G	603	-	14,14,15	0.40	0	17,19,21	1.86	3 (17%)
5	EDO	A	604	-	3,3,3	0.16	0	2,2,2	0.29	0
3	HEM	A	602	1	50,50,50	1.75	14 (28%)	66,82,82	1.34	6 (9%)
3	HEM	C	601	1	50,50,50	2.16	14 (28%)	66,82,82	1.33	7 (10%)
2	CAQ	A	601	-	8,8,8	0.36	0	10,10,10	0.54	0
3	HEM	F	601	1	50,50,50	2.08	13 (26%)	66,82,82	1.40	10 (15%)
4	NAG	D	602	-	14,14,15	0.57	0	17,19,21	1.30	1 (5%)

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
3	HEM	E	601	1	-	4/14/54/54	-
3	HEM	G	601	1	-	4/14/54/54	-
6	PEG	E	602	-	-	3/4/4/4	-
3	HEM	B	601	1	-	2/14/54/54	-
4	NAG	G	602	-	-	2/6/23/26	0/1/1/1
4	NAG	H	602	-	-	2/6/23/26	0/1/1/1
3	HEM	D	601	1	-	2/14/54/54	-
4	NAG	B	602	-	-	2/6/23/26	0/1/1/1
6	PEG	F	602	-	-	4/4/4/4	-
4	NAG	C	602	-	-	1/6/23/26	0/1/1/1
3	HEM	H	601	1	-	2/14/54/54	-
4	NAG	A	603	-	-	2/6/23/26	0/1/1/1
4	NAG	G	603	-	-	5/6/23/26	0/1/1/1
5	EDO	A	604	-	-	1/1/1/1	-
3	HEM	A	602	1	-	2/14/54/54	-
3	HEM	C	601	1	-	4/14/54/54	-
2	CAQ	A	601	-	-	-	0/1/1/1
3	HEM	F	601	1	-	4/14/54/54	-
4	NAG	D	602	-	-	2/6/23/26	0/1/1/1

The worst 5 of 115 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	601	HEM	FE-NC	11.23	2.33	1.95
3	G	601	HEM	FE-NB	9.54	2.24	1.94
3	E	601	HEM	FE-NB	8.53	2.21	1.94
3	B	601	HEM	FE-NC	7.68	2.21	1.95
3	F	601	HEM	FE-NB	7.62	2.18	1.94

The worst 5 of 118 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	601	HEM	CHB-C1B-NB	-5.66	117.40	124.37
3	B	601	HEM	CHC-C1C-NC	-5.51	118.47	124.44
3	D	601	HEM	CHD-C1D-ND	5.11	129.97	124.42
3	C	601	HEM	CAA-CBA-CGA	4.96	124.28	113.60
4	A	603	NAG	C2-N2-C7	4.93	129.92	122.90

There are no chirality outliers.

5 of 48 torsion outliers are listed below:

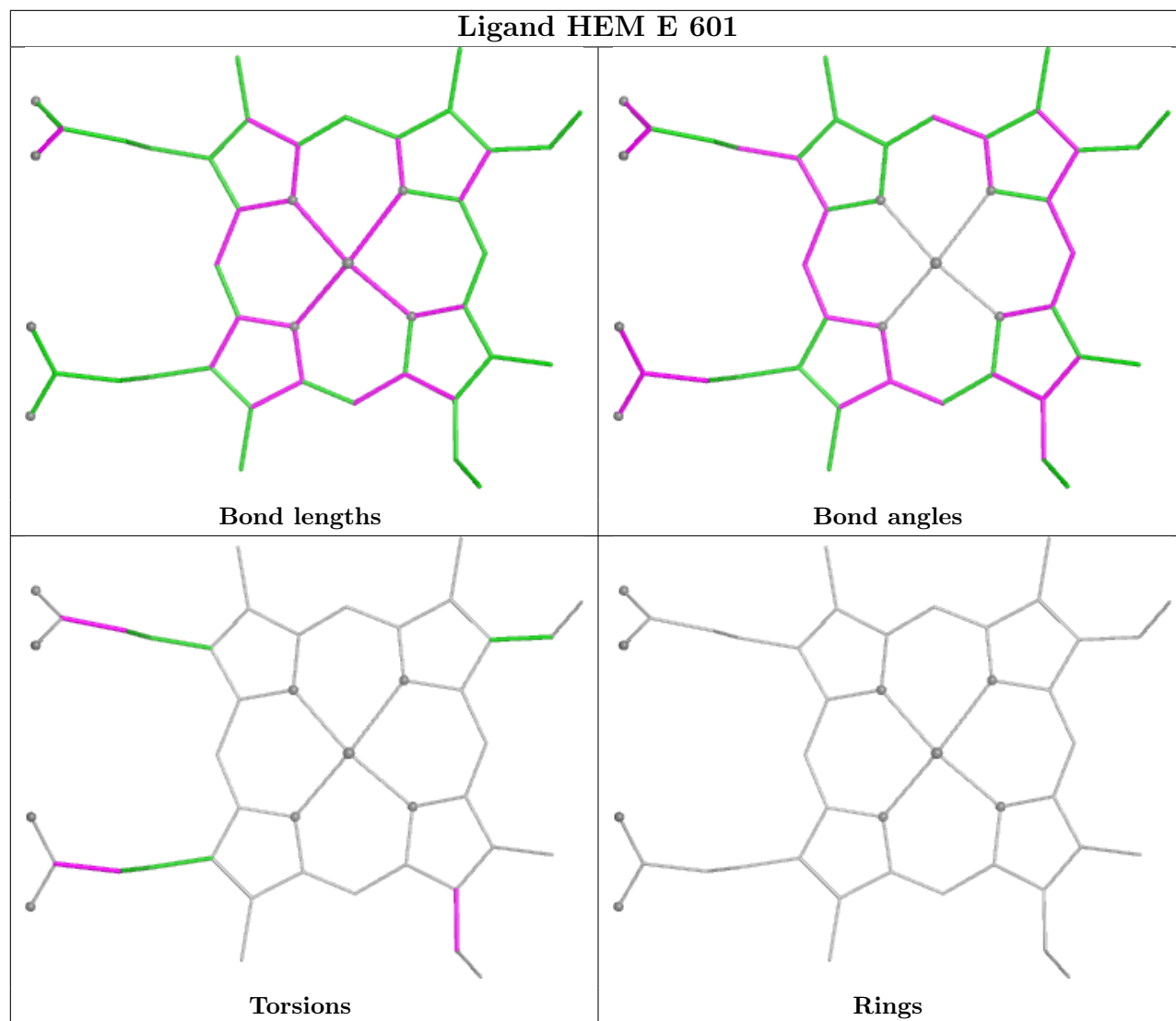
Mol	Chain	Res	Type	Atoms
4	G	603	NAG	C4-C5-C6-O6
4	G	603	NAG	O5-C5-C6-O6
4	A	603	NAG	C8-C7-N2-C2
4	A	603	NAG	O7-C7-N2-C2
4	B	602	NAG	C8-C7-N2-C2

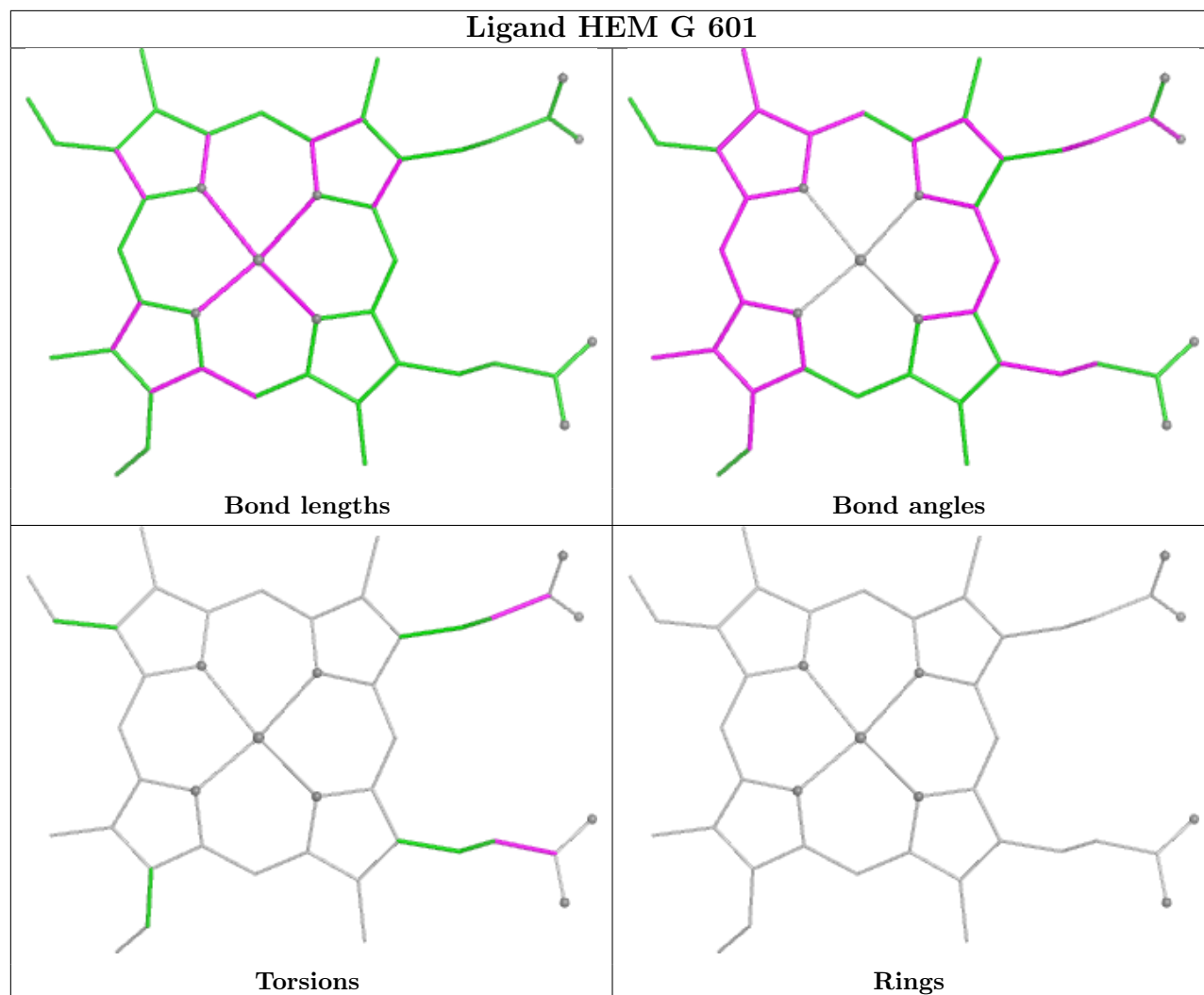
There are no ring outliers.

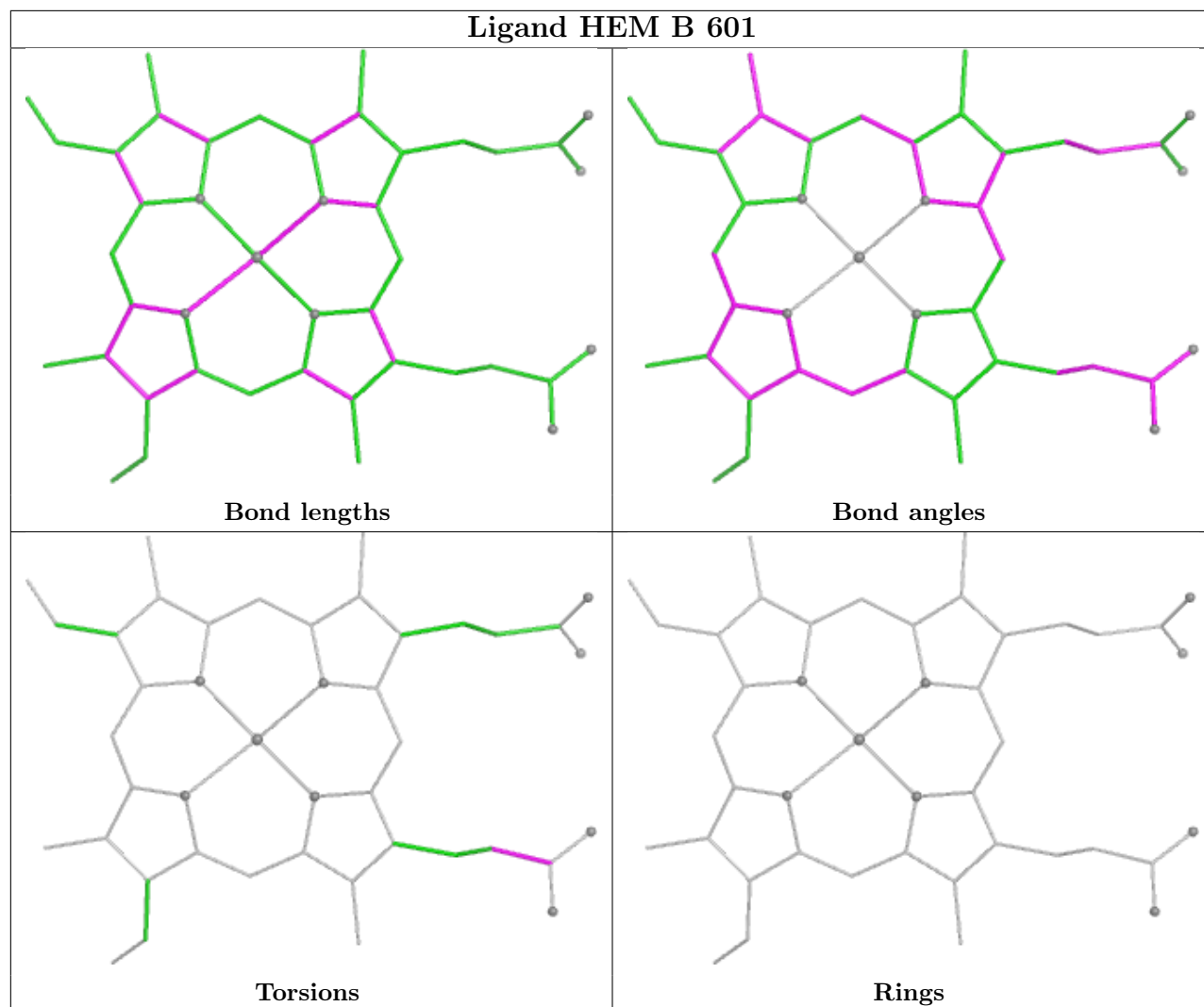
18 monomers are involved in 80 short contacts:

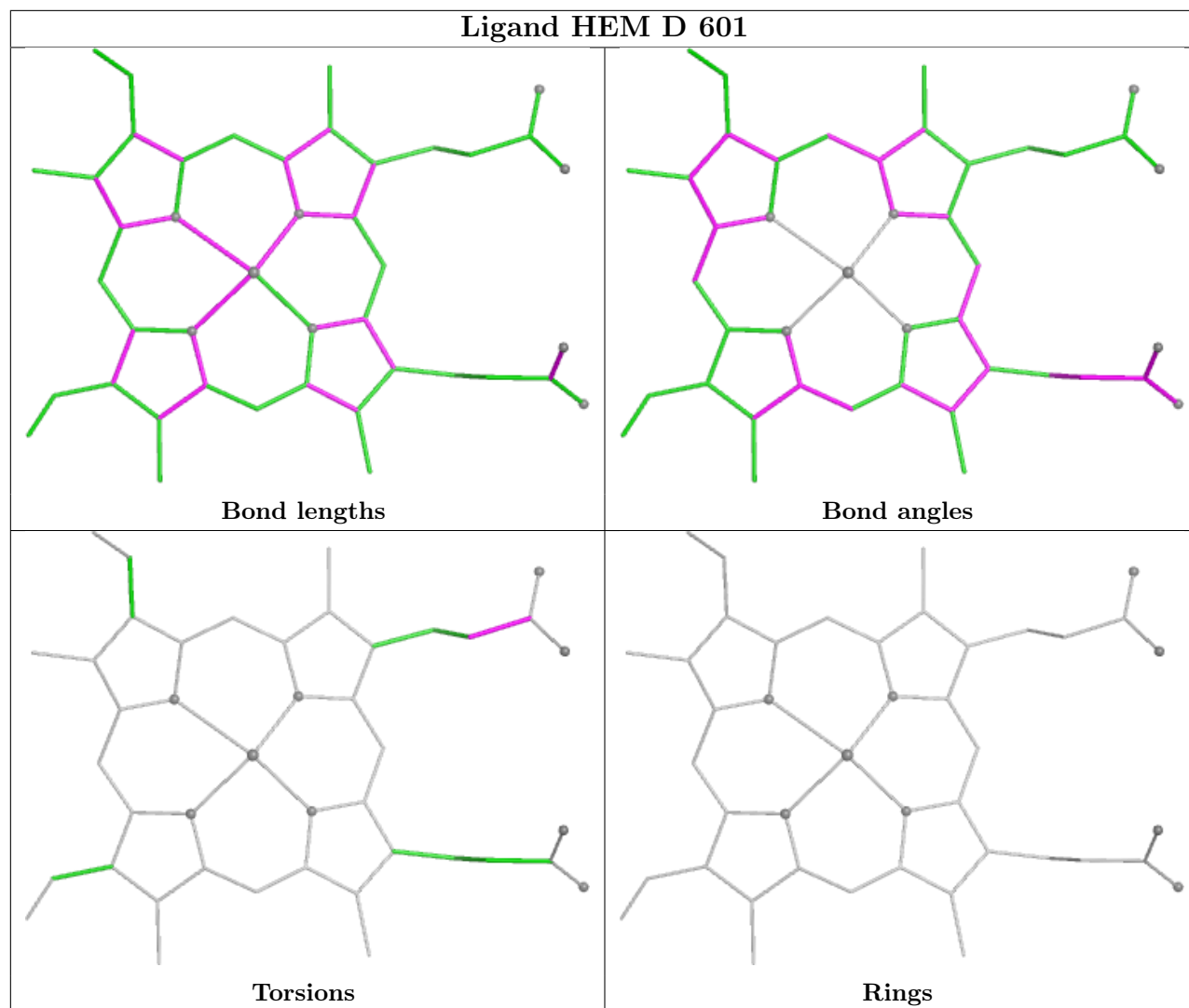
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	601	HEM	7	0
3	G	601	HEM	6	0
3	B	601	HEM	4	0
4	G	602	NAG	2	0
4	H	602	NAG	3	0
3	D	601	HEM	1	0
4	B	602	NAG	6	0
6	F	602	PEG	17	0
4	C	602	NAG	2	0
3	H	601	HEM	3	0
4	A	603	NAG	5	0
4	G	603	NAG	7	0
5	A	604	EDO	1	0
3	A	602	HEM	6	0
3	C	601	HEM	2	0
2	A	601	CAQ	2	0
3	F	601	HEM	3	0
4	D	602	NAG	3	0

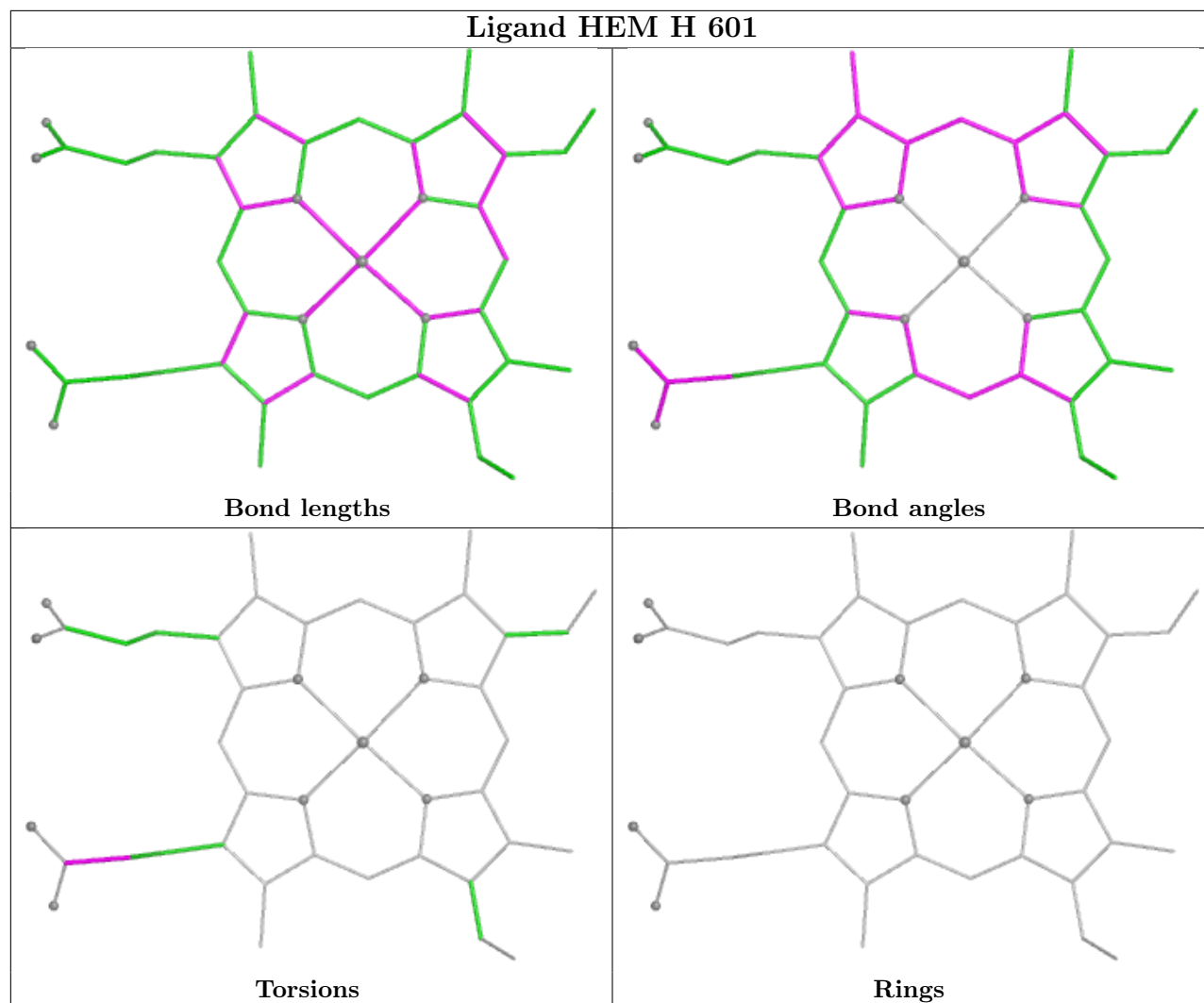
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

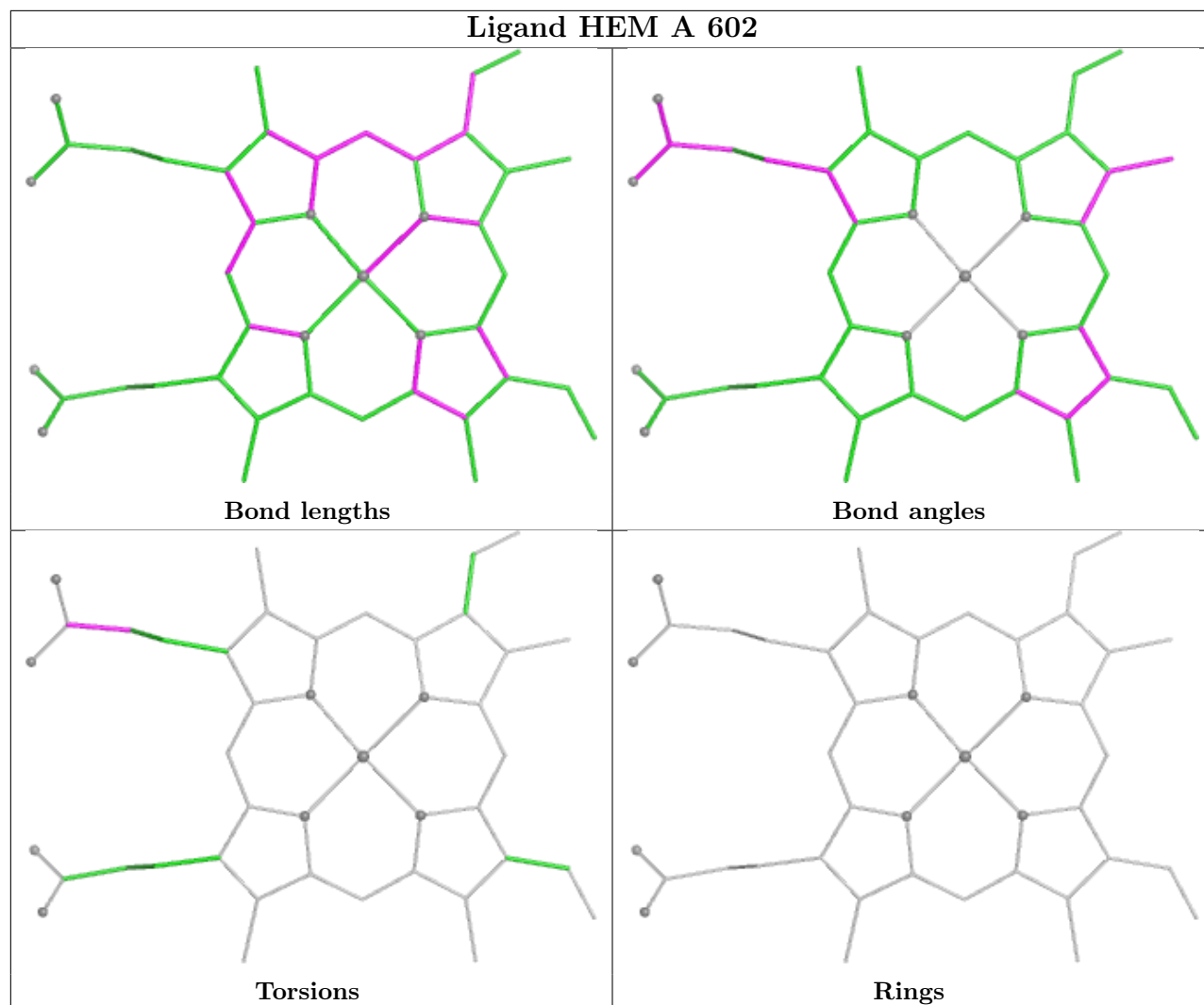


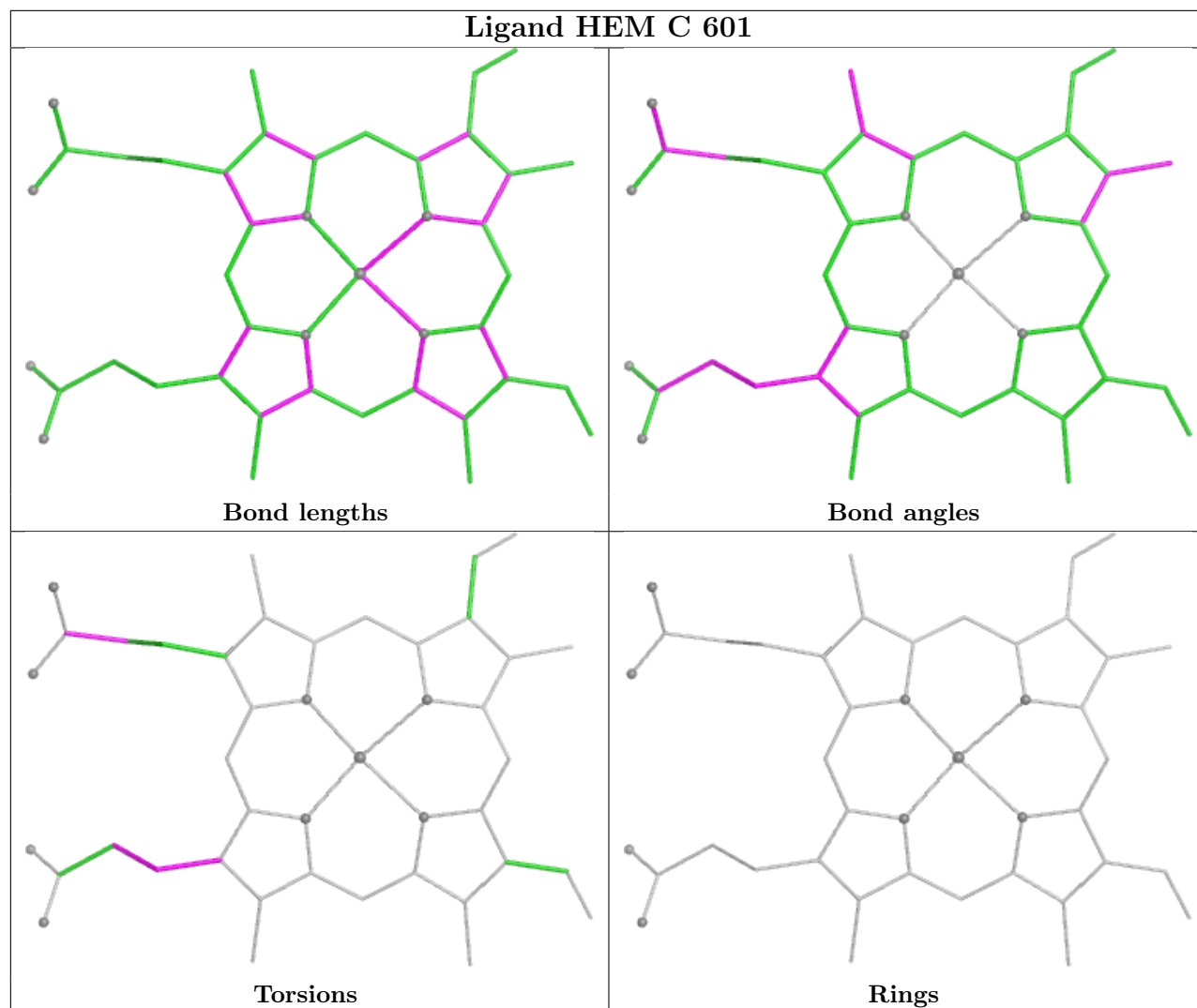


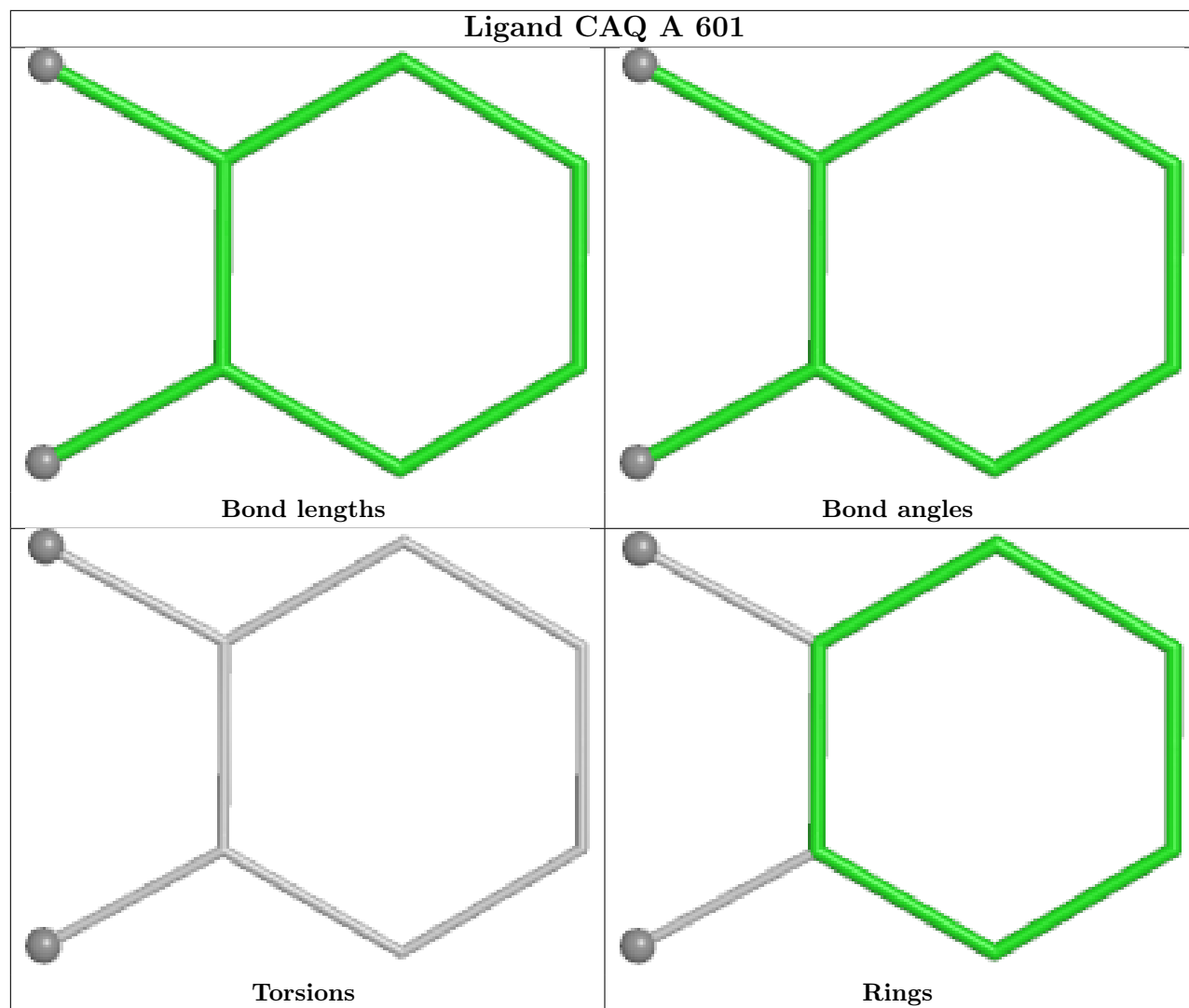


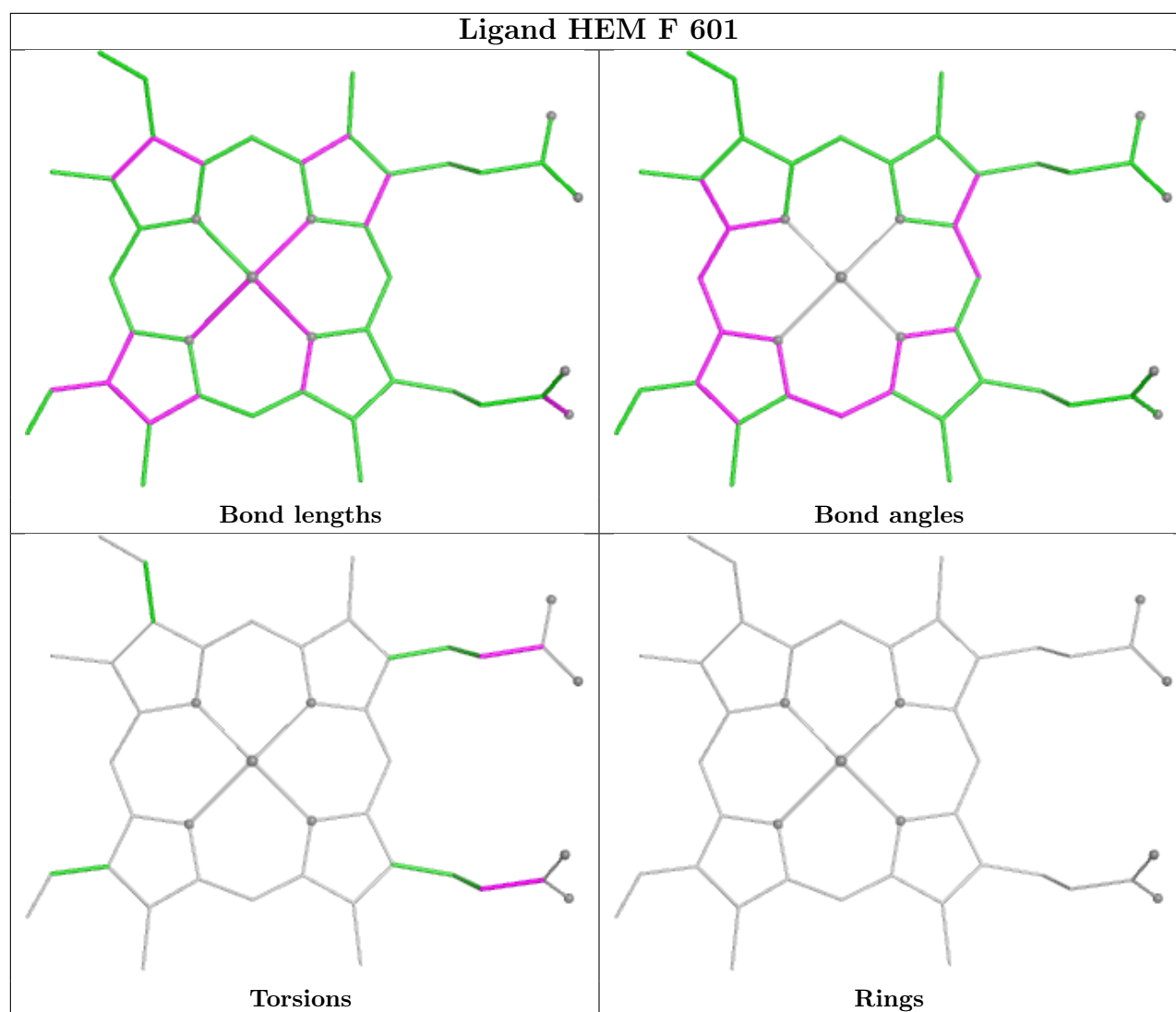












5.7 Other polymers [i](#)

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](#)

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	507/509 (99%)	-1.09	1 (0%) 91 92	22, 36, 58, 105	0
1	B	507/509 (99%)	-1.09	0 100 100	12, 38, 55, 79	2 (0%)
1	C	507/509 (99%)	-1.03	0 100 100	12, 40, 62, 82	2 (0%)
1	D	505/509 (99%)	-1.02	0 100 100	14, 41, 63, 86	1 (0%)
1	E	502/509 (98%)	-1.11	0 100 100	12, 32, 45, 65	3 (0%)
1	F	504/509 (99%)	-1.08	0 100 100	15, 34, 50, 87	1 (0%)
1	G	498/509 (97%)	-1.13	0 100 100	22, 34, 49, 74	1 (0%)
1	H	507/509 (99%)	-1.07	0 100 100	12, 35, 52, 85	3 (0%)
All	All	4037/4072 (99%)	-1.08	1 (0%) 100 100	12, 36, 57, 105	13 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	504	ALA	2.2

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

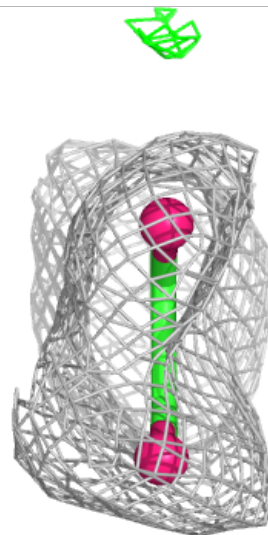
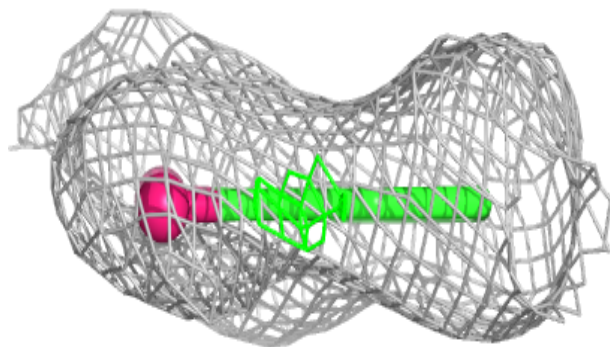
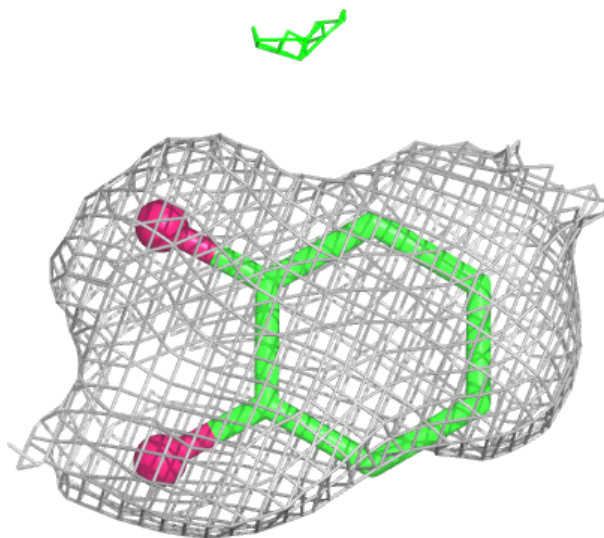
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CAQ	A	601	8/8	0.98	0.06	41,46,52,56	0
4	NAG	H	602	14/15	0.98	0.04	30,39,41,42	0
5	EDO	A	604	4/4	0.98	0.05	45,45,48,51	0
3	HEM	E	601	43/43	0.99	0.03	15,24,28,32	0
3	HEM	F	601	43/43	0.99	0.03	20,24,31,36	0
3	HEM	H	601	43/43	0.99	0.03	20,23,29,32	0
4	NAG	A	603	14/15	0.99	0.03	27,31,34,35	0
4	NAG	B	602	14/15	0.99	0.03	39,44,46,52	0
4	NAG	D	602	14/15	0.99	0.03	36,37,44,44	0
4	NAG	C	602	14/15	0.99	0.04	38,45,53,54	0
4	NAG	G	602	14/15	0.99	0.03	33,37,41,42	0
4	NAG	G	603	14/15	0.99	0.03	46,50,53,53	0
3	HEM	D	601	43/43	0.99	0.03	26,33,37,40	0
3	HEM	C	601	43/43	0.99	0.03	20,29,33,35	0
6	PEG	E	602	7/7	0.99	0.03	39,41,48,49	0
6	PEG	F	602	7/7	0.99	0.06	29,32,40,47	0
3	HEM	G	601	43/43	1.00	0.03	20,24,27,29	0
3	HEM	A	602	43/43	1.00	0.03	21,26,33,35	0
3	HEM	B	601	43/43	1.00	0.03	23,27,33,41	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

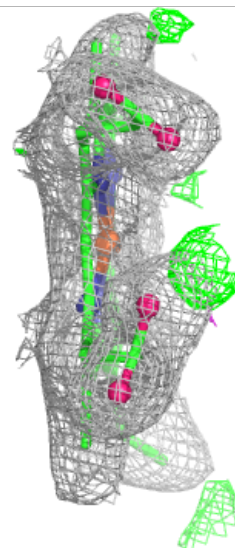
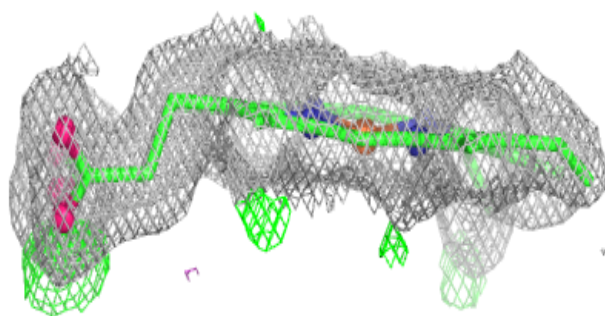
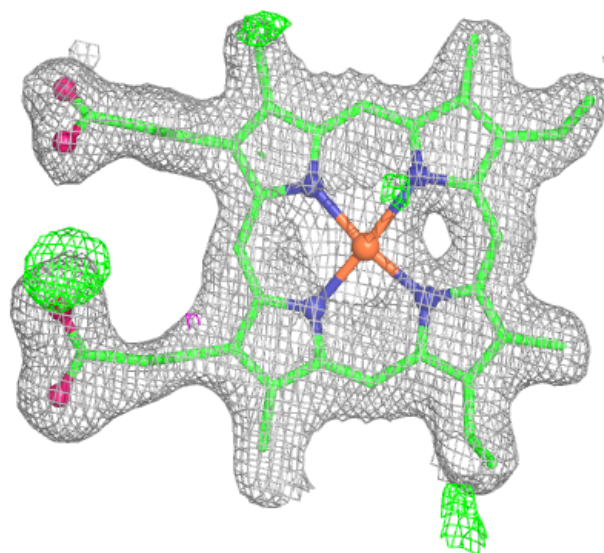
Electron density around CAQ A 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



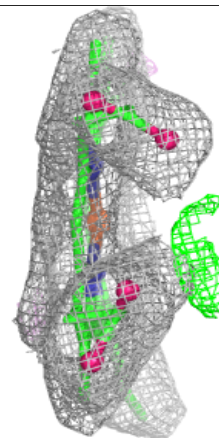
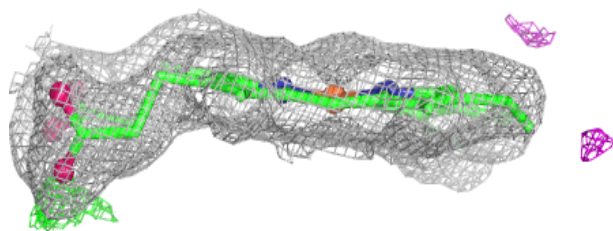
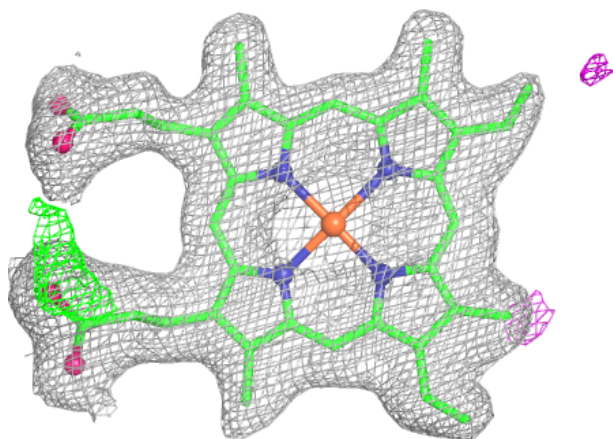
Electron density around HEM E 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



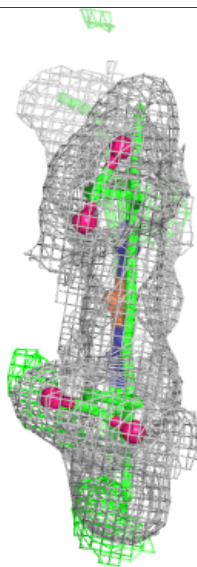
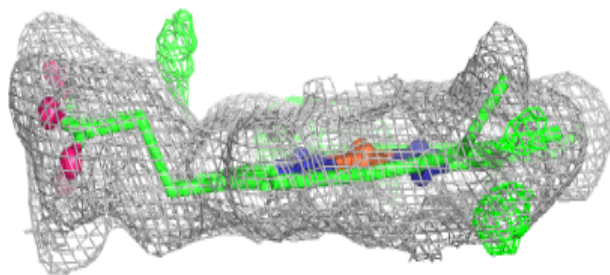
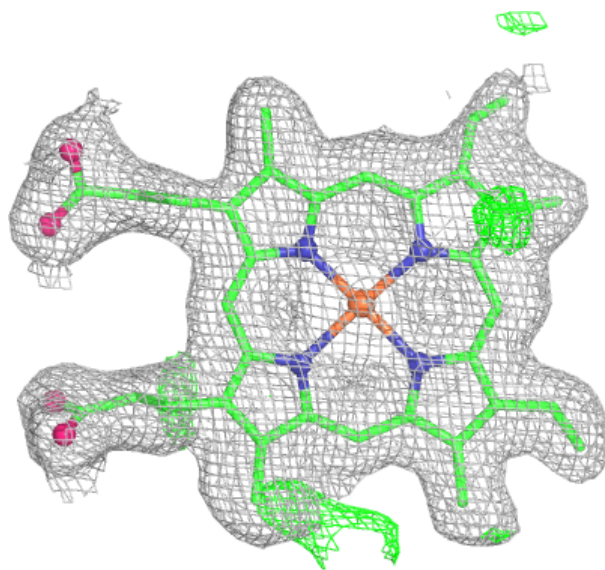
Electron density around HEM F 601:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



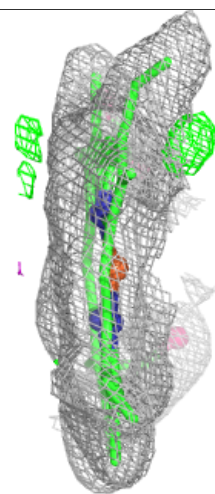
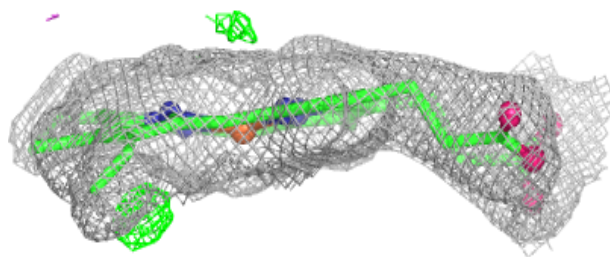
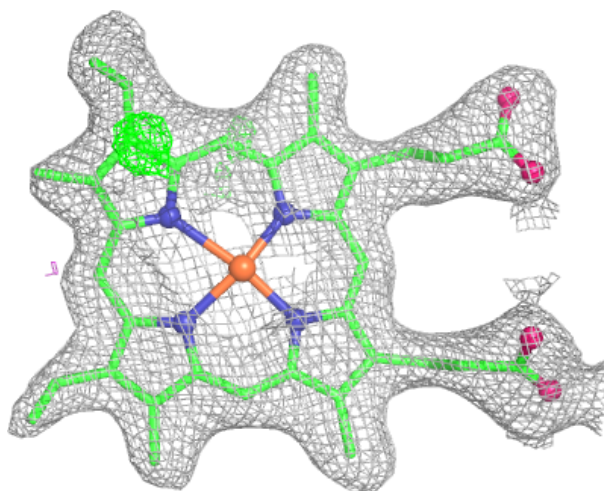
Electron density around HEM H 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



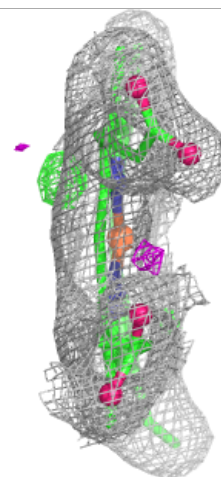
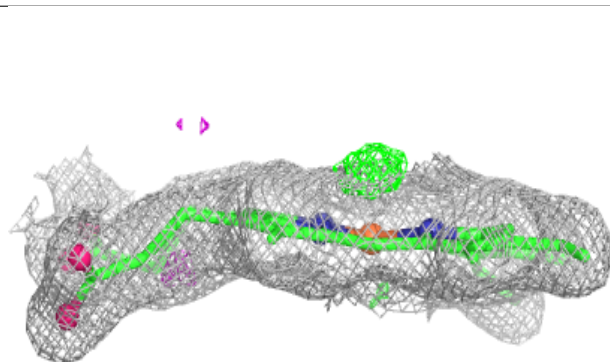
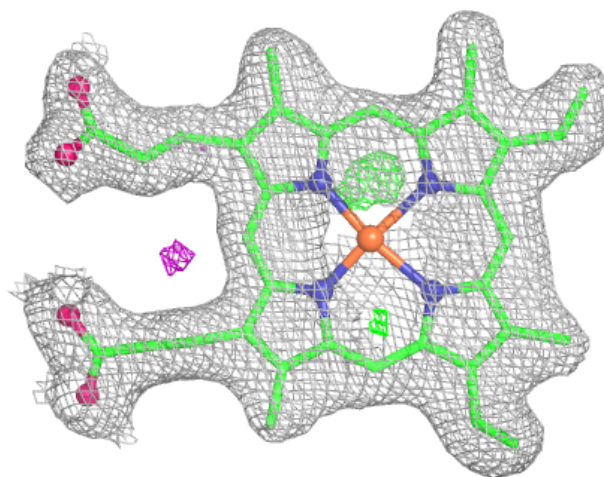
Electron density around HEM D 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



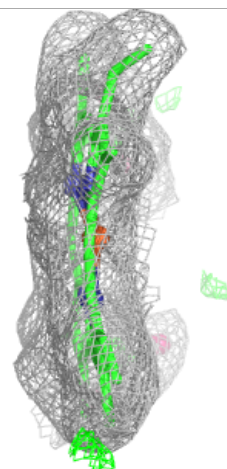
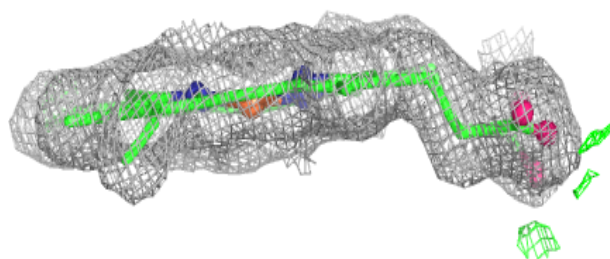
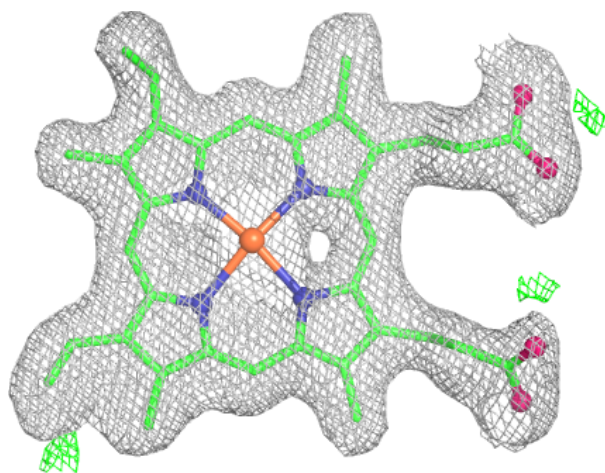
Electron density around HEM C 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



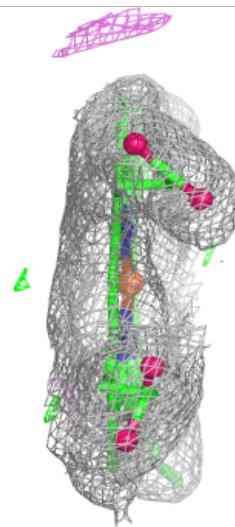
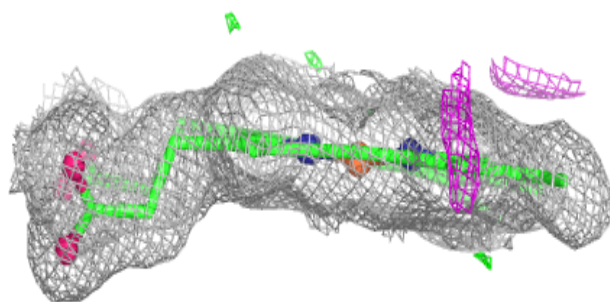
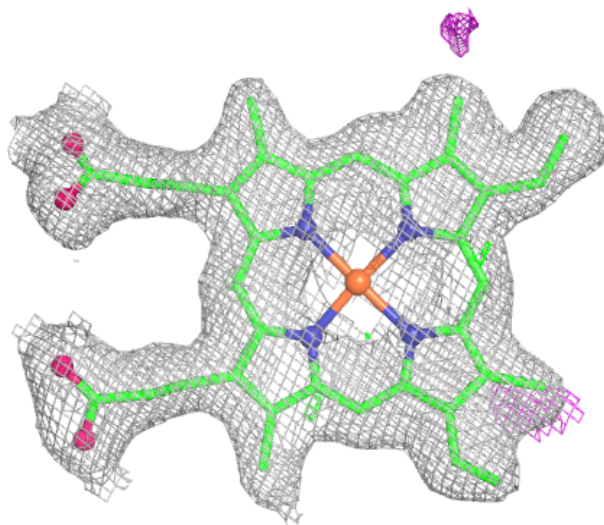
Electron density around HEM G 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



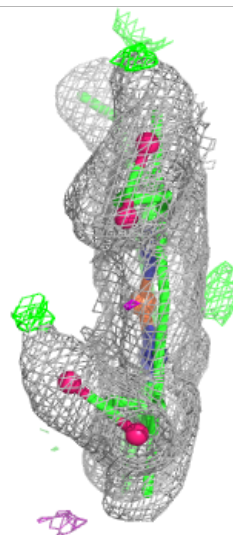
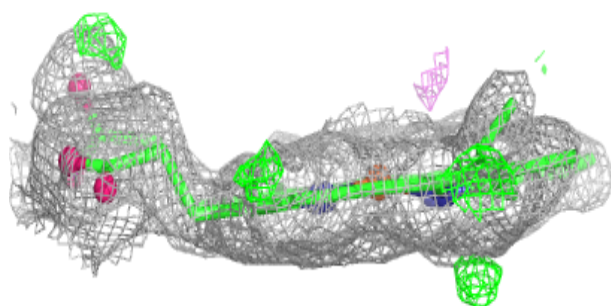
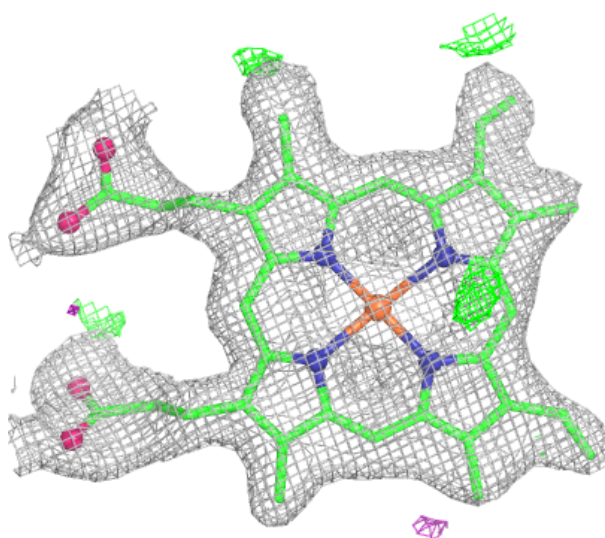
Electron density around HEM A 602:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM B 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.