



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 10:13 PM UTC

PDB ID : 2FMY / pdb_00002fmy
Title : CO-dependent transcription factor CooA from Carboxydotherrmus hydrogenofomans (Imidazole-bound form)
Authors : Higuchi, Y.; Komori, H.
Deposited on : 2006-01-10
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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) : 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 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

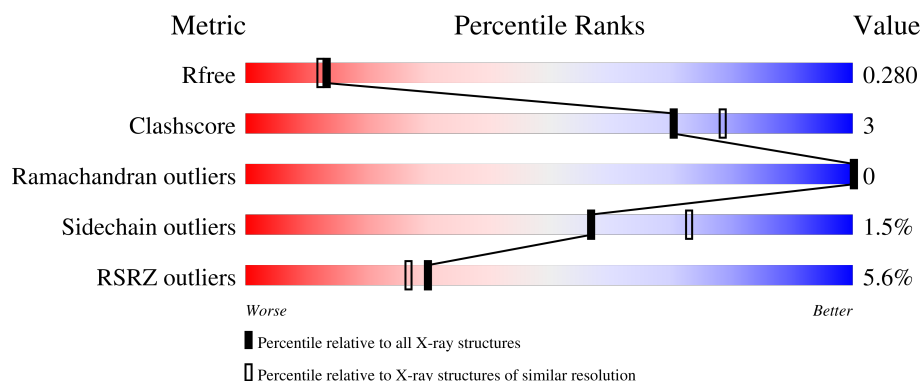
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	220	2% 92% 7%
1	B	220	9% 87% 12%
1	C	220	4% 88% 11%
1	D	220	7% 92% 7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7446 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 carbon monoxide oxidation system transcription regulator CooA-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	218	Total	C	N	O	S	0	0	0
			1750	1122	295	326	7			
1	B	218	Total	C	N	O	S	0	0	0
			1750	1122	295	326	7			
1	C	218	Total	C	N	O	S	0	0	0
			1750	1122	295	326	7			
1	D	218	Total	C	N	O	S	0	0	0
			1750	1122	295	326	7			

There are 12 discrepancies between the modelled and reference sequences:

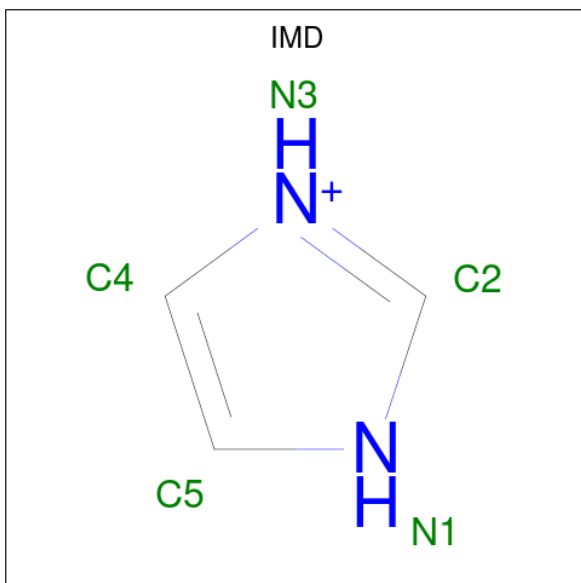
Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	-	cloning artifact	GB 77996136
A	3	THR	-	cloning artifact	GB 77996136
A	4	GLN	-	cloning artifact	GB 77996136
B	1002	ALA	-	cloning artifact	GB 77996136
B	1003	THR	-	cloning artifact	GB 77996136
B	1004	GLN	-	cloning artifact	GB 77996136
C	2002	ALA	-	cloning artifact	GB 77996136
C	2003	THR	-	cloning artifact	GB 77996136
C	2004	GLN	-	cloning artifact	GB 77996136
D	3002	ALA	-	cloning artifact	GB 77996136
D	3003	THR	-	cloning artifact	GB 77996136
D	3004	GLN	-	cloning artifact	GB 77996136

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 3 is IMIDAZOLE (CCD ID: IMD) (formula: $\text{C}_3\text{H}_5\text{N}_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N 5 3 2	0	0
3	B	1	Total C N 5 3 2	0	0
3	C	1	Total C N 5 3 2	0	0
3	D	1	Total C N 5 3 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	87	Total O 87 87	0	0
4	B	57	Total O 57 57	0	0
4	C	66	Total O 66 66	0	0
4	D	44	Total O 44 44	0	0

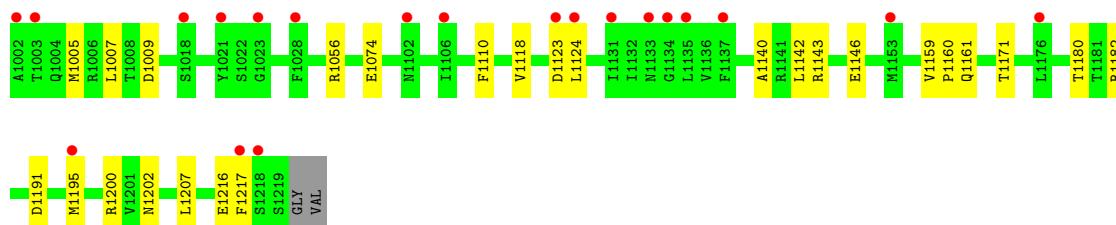
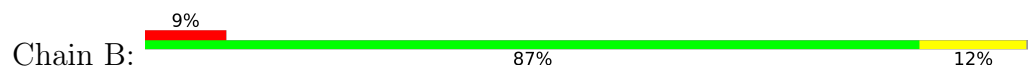
3 Residue-property plots [i](#)

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.

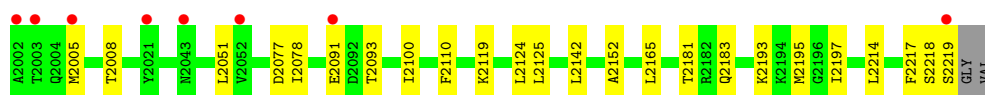
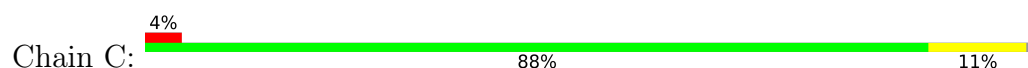
- Molecule 1: carbon monoxide oxidation system transcription regulator CoxA-1



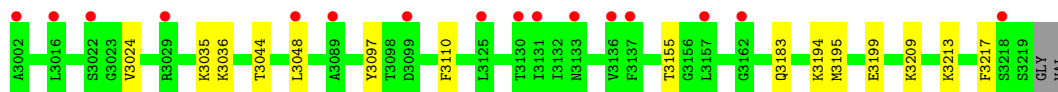
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- Molecule 1: carbon monoxide oxidation system transcription regulator CoxA-1



- Molecule 1: carbon monoxide oxidation system transcription regulator CoxA-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	61.65Å 93.93Å 91.90Å 90.00° 104.73° 90.00°	Depositor
Resolution (Å)	32.33 – 2.20 32.33 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (32.33-2.20) 99.5 (32.33-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	9.07 (at 2.20Å)	Xtriage
Refinement program	CNS 1.1, REFMAC 5.2.0019	Depositor
R, R_{free}	0.207 , 0.247 0.245 , 0.280	Depositor DCC
R_{free} test set	2563 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	35.4	Xtriage
Anisotropy	0.955	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 38.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7446	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 33.30 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.1831e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: IMD, 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	0.56	0/1771	0.79	0/2387
1	B	0.55	0/1771	0.84	2/2387 (0.1%)
1	C	0.57	1/1771 (0.1%)	0.84	2/2387 (0.1%)
1	D	0.52	0/1771	0.83	2/2387 (0.1%)
All	All	0.55	1/7084 (0.0%)	0.83	6/9548 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	2091	GLU	CD-OE2	5.29	1.35	1.25

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1110	PHE	CA-C-N	6.47	126.98	119.47
1	B	1110	PHE	C-N-CA	6.47	126.98	119.47
1	C	2110	PHE	CA-C-N	5.95	126.10	119.32
1	C	2110	PHE	C-N-CA	5.95	126.10	119.32
1	D	3110	PHE	CA-C-N	5.17	124.96	119.28
1	D	3110	PHE	C-N-CA	5.17	124.96	119.28

There are no chirality outliers.

There are no planarity outliers.

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	1750	0	1825	10	0
1	B	1750	0	1825	18	0
1	C	1750	0	1825	15	0
1	D	1750	0	1825	6	0
2	A	43	0	30	1	0
2	B	43	0	30	2	0
2	C	43	0	30	1	0
2	D	43	0	30	4	0
3	A	5	0	4	2	0
3	B	5	0	4	0	0
3	C	5	0	4	0	0
3	D	5	0	4	2	0
4	A	87	0	0	0	0
4	B	57	0	0	0	0
4	C	66	0	0	1	0
4	D	44	0	0	0	0
All	All	7446	0	7436	50	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (50) 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:B:1195:MET:HE1	1:B:1217:PHE:CZ	2.09	0.87
1:C:2195:MET:HE1	1:C:2217:PHE:HZ	1.42	0.85
1:C:2195:MET:HE1	1:C:2217:PHE:CZ	2.13	0.82
1:C:2181:THR:HG22	1:C:2183:GLN:H	1.46	0.80
1:A:195:MET:HE1	1:A:217:PHE:CZ	2.17	0.78
1:B:1195:MET:HE1	1:B:1217:PHE:HZ	1.47	0.77
1:A:195:MET:HE1	1:A:217:PHE:HZ	1.50	0.75
1:B:1143:ARG:HH21	1:B:1180:THR:HG23	1.54	0.71
1:C:2125:LEU:HD23	2:D:3300:HEM:CMD	2.24	0.67
1:D:3048:LEU:HD13	1:D:3097:TYR:HB2	1.78	0.65
1:B:1005:MET:HE3	1:B:1123:ASP:HA	1.83	0.61
1:C:2005:MET:HB2	3:D:3301:IMD:C2	2.33	0.59
4:C:4067:HOH:O	1:D:3194:LYS:HE3	2.02	0.59
1:D:3195:MET:HE1	1:D:3217:PHE:CZ	2.40	0.57
1:A:158:LYS:HE3	1:A:159:VAL:O	2.06	0.55
1:B:1143:ARG:HH21	1:B:1180:THR:CG2	2.20	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2125:LEU:HD23	2:D:3300:HEM:HMD2	1.90	0.54
1:B:1161:GLN:HB3	1:B:1207:LEU:HD21	1.91	0.53
1:A:121:LEU:HA	1:A:124:LEU:HD12	1.90	0.53
1:A:72:ILE:HD12	1:A:90:MET:SD	2.50	0.52
1:C:2077:ASP:OD1	1:C:2119:LYS:NZ	2.44	0.50
1:A:104:GLN:HA	2:A:300:HEM:HBB1	1.93	0.50
1:B:1171:THR:HG22	1:B:1182:ARG:HD2	1.94	0.50
1:C:2152:ALA:HA	1:C:2165:LEU:CD2	2.41	0.50
1:C:2051:LEU:HB2	1:C:2078:ILE:HD13	1.94	0.49
1:C:2181:THR:HG22	1:C:2183:GLN:N	2.22	0.48
3:A:301:IMD:H5	1:B:1118:VAL:O	2.14	0.48
1:B:1200:ARG:HD3	1:B:1202:ASN:O	2.13	0.48
1:B:1007:LEU:HD11	1:B:1118:VAL:HG11	1.96	0.47
1:A:7:LEU:HD22	2:B:1300:HEM:HBB2	1.96	0.47
1:B:1142:LEU:O	1:B:1146:GLU:HG3	2.15	0.47
1:C:2152:ALA:HA	1:C:2165:LEU:HD21	1.96	0.47
1:B:1143:ARG:NH2	1:B:1180:THR:CG2	2.78	0.47
1:C:2125:LEU:HD23	2:D:3300:HEM:HMD1	1.97	0.46
1:B:1191:ASP:O	1:B:1195:MET:HG3	2.17	0.45
1:C:2197:ILE:HG21	1:C:2214:LEU:HD13	1.99	0.44
1:B:1140:ALA:CB	1:B:1180:THR:HG21	2.48	0.44
1:B:1140:ALA:HB2	1:B:1180:THR:HG21	2.01	0.43
1:A:125:LEU:HD23	2:B:1300:HEM:HMD2	2.01	0.43
1:A:66:LYS:CG	1:A:67:GLU:H	2.32	0.42
1:D:3199:GLU:HG3	1:D:3209:LYS:HD2	2.00	0.42
3:A:301:IMD:N1	1:B:1005:MET:HG3	2.35	0.42
1:C:2100:ILE:HD11	2:C:2300:HEM:C2B	2.55	0.42
1:B:1159:VAL:HB	1:B:1160:PRO:HD2	2.03	0.41
1:D:3035:LYS:HG2	1:D:3036:LYS:HG2	2.02	0.41
2:D:3300:HEM:CHD	3:D:3301:IMD:H4	2.51	0.41
1:C:2142:LEU:HD11	1:C:2219:SER:HB2	2.02	0.41
1:A:165:LEU:HD22	1:A:208:LEU:HD13	2.03	0.41
1:D:3183:GLN:H	1:D:3183:GLN:CD	2.29	0.40
1:B:1056:ARG:HG2	1:B:1074:GLU:OE1	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	216/220 (98%)	211 (98%)	5 (2%)	0	100	100
1	B	216/220 (98%)	212 (98%)	4 (2%)	0	100	100
1	C	216/220 (98%)	212 (98%)	4 (2%)	0	100	100
1	D	216/220 (98%)	211 (98%)	5 (2%)	0	100	100
All	All	864/880 (98%)	846 (98%)	18 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	195/196 (100%)	195 (100%)	0	100	100
1	B	195/196 (100%)	192 (98%)	3 (2%)	57	73
1	C	195/196 (100%)	190 (97%)	5 (3%)	40	55
1	D	195/196 (100%)	191 (98%)	4 (2%)	47	63
All	All	780/784 (100%)	768 (98%)	12 (2%)	57	73

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1009	ASP
1	B	1124	LEU

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Mol	Chain	Res	Type
1	B	1216	GLU
1	C	2008	THR
1	C	2093	THR
1	C	2124	LEU
1	C	2193	LYS
1	C	2218	SER
1	D	3024	VAL
1	D	3044	THR
1	D	3155	THR
1	D	3213	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	ASN
1	B	1017	ASN
1	B	1104	GLN
1	C	2150	GLN
1	D	3102	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](#)

8 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
2	HEM	C	2300	1,3	50,50,50	1.89	9 (18%)	67,82,82	1.40	8 (11%)
3	IMD	C	2301	2	5,5,5	0.66	0	5,5,5	0.27	0
3	IMD	A	301	2	5,5,5	0.59	0	5,5,5	0.39	0
3	IMD	D	3301	2	5,5,5	0.60	0	5,5,5	0.18	0
2	HEM	A	300	1,3	50,50,50	1.99	10 (20%)	67,82,82	1.46	7 (10%)
3	IMD	B	1301	2	5,5,5	0.62	0	5,5,5	0.17	0
2	HEM	D	3300	1,3	50,50,50	1.90	10 (20%)	67,82,82	1.42	5 (7%)
2	HEM	B	1300	1,3	50,50,50	1.91	11 (22%)	67,82,82	1.32	4 (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
2	HEM	C	2300	1,3	-	4/14/54/54	-
3	IMD	C	2301	2	-	-	0/1/1/1
3	IMD	A	301	2	-	-	0/1/1/1
3	IMD	D	3301	2	-	-	0/1/1/1
2	HEM	A	300	1,3	-	4/14/54/54	-
3	IMD	B	1301	2	-	-	0/1/1/1
2	HEM	D	3300	1,3	-	6/14/54/54	-
2	HEM	B	1300	1,3	-	6/14/54/54	-

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	3300	HEM	C3D-C2D	7.84	1.53	1.36
2	B	1300	HEM	C3D-C2D	7.82	1.53	1.36
2	A	300	HEM	C3D-C2D	7.80	1.53	1.36
2	C	2300	HEM	C3D-C2D	7.49	1.52	1.36
2	A	300	HEM	FE-NB	5.95	2.13	1.94
2	D	3300	HEM	FE-ND	5.29	2.11	1.94
2	C	2300	HEM	FE-ND	4.86	2.09	1.94
2	B	1300	HEM	FE-NA	4.60	2.10	1.95
2	B	1300	HEM	FE-NB	4.25	2.08	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	300	HEM	FE-NC	4.14	2.08	1.95
2	D	3300	HEM	FE-NA	4.13	2.08	1.95
2	A	300	HEM	FE-NA	3.94	2.08	1.95
2	C	2300	HEM	FE-NB	3.94	2.07	1.94
2	B	1300	HEM	FE-ND	3.84	2.06	1.94
2	C	2300	HEM	FE-NA	3.34	2.06	1.95
2	C	2300	HEM	FE-NC	3.26	2.05	1.95
2	D	3300	HEM	FE-NB	3.25	2.04	1.94
2	A	300	HEM	FE-ND	3.07	2.04	1.94
2	B	1300	HEM	CAC-C3C	3.03	1.55	1.47
2	C	2300	HEM	CAB-C3B	2.97	1.55	1.47
2	A	300	HEM	CAC-C3C	2.96	1.55	1.47
2	D	3300	HEM	CAC-C3C	2.95	1.55	1.47
2	B	1300	HEM	CAB-C3B	2.94	1.55	1.47
2	D	3300	HEM	CAB-C3B	2.74	1.54	1.47
2	A	300	HEM	CAB-C3B	2.73	1.54	1.47
2	C	2300	HEM	CMA-C3A	2.72	1.56	1.50
2	A	300	HEM	CMA-C3A	2.70	1.56	1.50
2	D	3300	HEM	FE-NC	2.69	2.04	1.95
2	C	2300	HEM	CAC-C3C	2.61	1.54	1.47
2	B	1300	HEM	CMB-C2B	2.58	1.56	1.50
2	B	1300	HEM	FE-NC	2.33	2.02	1.95
2	D	3300	HEM	CMA-C3A	2.29	1.55	1.50
2	D	3300	HEM	CMB-C2B	2.25	1.55	1.50
2	C	2300	HEM	CMB-C2B	2.21	1.55	1.50
2	A	300	HEM	CMB-C2B	2.19	1.55	1.50
2	B	1300	HEM	CMA-C3A	2.17	1.55	1.50
2	A	300	HEM	CMC-C2C	2.12	1.55	1.50
2	D	3300	HEM	CMC-C2C	2.06	1.55	1.50
2	B	1300	HEM	CMC-C2C	2.04	1.55	1.50
2	B	1300	HEM	CMD-C2D	2.01	1.54	1.50

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	300	HEM	C4D-ND-C1D	6.22	112.58	105.21
2	C	2300	HEM	C4D-ND-C1D	6.06	112.38	105.21
2	D	3300	HEM	C4D-ND-C1D	5.67	111.92	105.21
2	B	1300	HEM	C4D-ND-C1D	5.61	111.85	105.21
2	C	2300	HEM	CBD-CAD-C3D	-4.20	100.92	112.53
2	D	3300	HEM	CBD-CAD-C3D	-4.11	101.18	112.53
2	D	3300	HEM	C3B-C4B-NB	-3.09	107.25	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3300	HEM	C1B-NB-C4B	3.07	108.85	105.21
2	B	1300	HEM	CBD-CAD-C3D	-3.01	104.20	112.53
2	A	300	HEM	CBD-CAD-C3D	-2.98	104.28	112.53
2	A	300	HEM	C3B-C4B-NB	-2.91	107.38	109.47
2	A	300	HEM	C1B-NB-C4B	2.89	108.63	105.21
2	C	2300	HEM	CBA-CAA-C2A	-2.89	104.56	112.53
2	A	300	HEM	CBA-CAA-C2A	-2.66	105.17	112.53
2	B	1300	HEM	CBA-CAA-C2A	-2.41	105.87	112.53
2	C	2300	HEM	CHA-C4D-ND	2.33	127.24	124.37
2	C	2300	HEM	C3D-C4D-ND	-2.31	107.64	110.17
2	A	300	HEM	C2A-C1A-NA	-2.24	107.67	110.15
2	B	1300	HEM	C2A-C1A-NA	-2.21	107.70	110.15
2	D	3300	HEM	CHD-C1D-ND	2.18	126.77	124.42
2	C	2300	HEM	C1B-NB-C4B	2.17	107.77	105.21
2	A	300	HEM	C4C-NC-C1C	2.06	109.18	105.82
2	C	2300	HEM	CHC-C1C-NC	2.04	126.67	124.45
2	C	2300	HEM	C3B-C2B-C1B	2.03	107.94	106.41

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	300	HEM	C2C-C3C-CAC-CBC
2	B	1300	HEM	C2B-C3B-CAB-CBB
2	B	1300	HEM	C2C-C3C-CAC-CBC
2	B	1300	HEM	C4C-C3C-CAC-CBC
2	C	2300	HEM	C2C-C3C-CAC-CBC
2	D	3300	HEM	C2B-C3B-CAB-CBB
2	D	3300	HEM	C2C-C3C-CAC-CBC
2	A	300	HEM	C4C-C3C-CAC-CBC
2	B	1300	HEM	C4B-C3B-CAB-CBB
2	C	2300	HEM	C4C-C3C-CAC-CBC
2	D	3300	HEM	C4C-C3C-CAC-CBC
2	D	3300	HEM	C4B-C3B-CAB-CBB
2	D	3300	HEM	CAA-CBA-CGA-O1A
2	D	3300	HEM	CAA-CBA-CGA-O2A
2	B	1300	HEM	CAA-CBA-CGA-O2A
2	A	300	HEM	CAA-CBA-CGA-O2A
2	A	300	HEM	CAA-CBA-CGA-O1A
2	B	1300	HEM	CAA-CBA-CGA-O1A
2	C	2300	HEM	CAA-CBA-CGA-O1A
2	C	2300	HEM	CAA-CBA-CGA-O2A

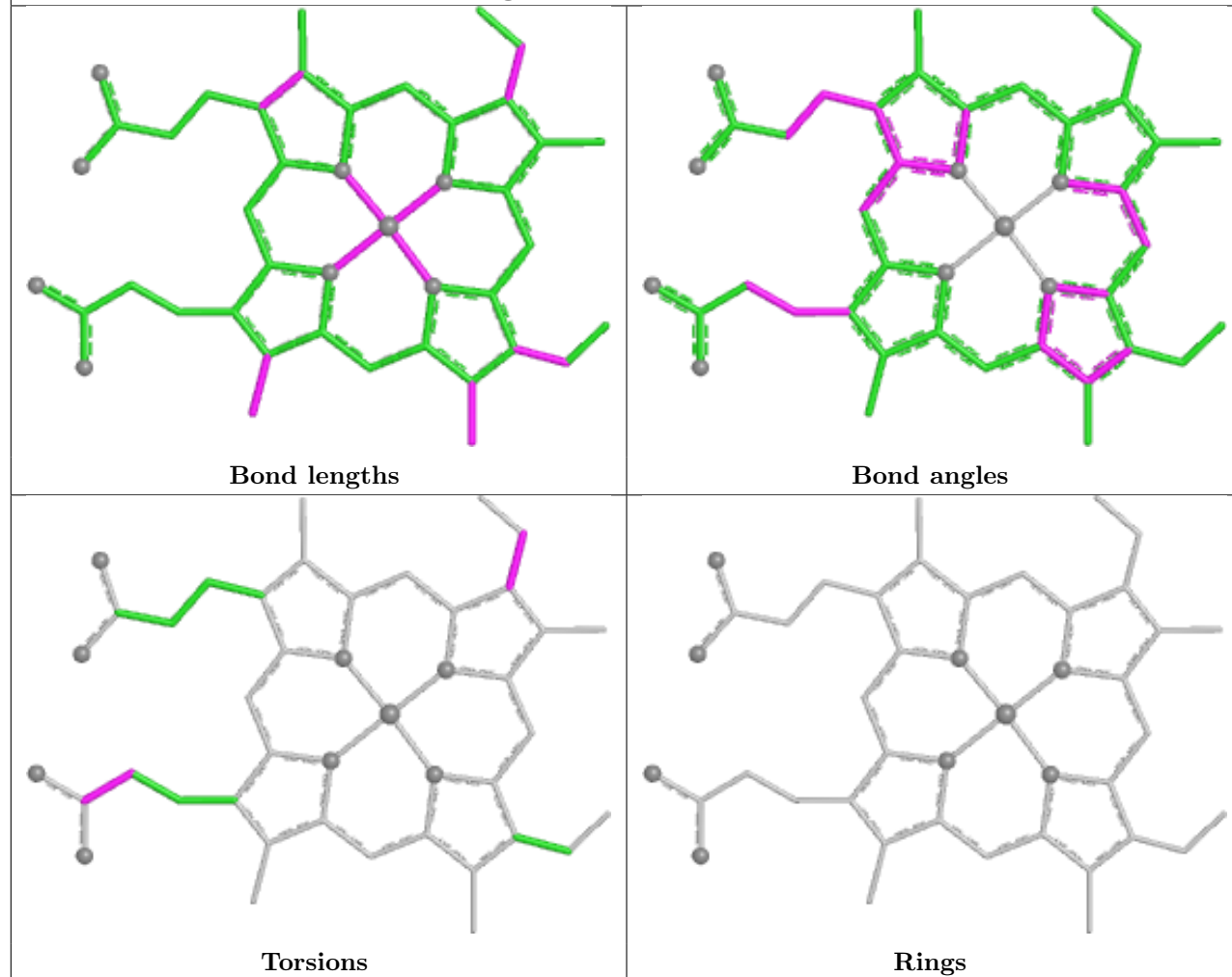
There are no ring outliers.

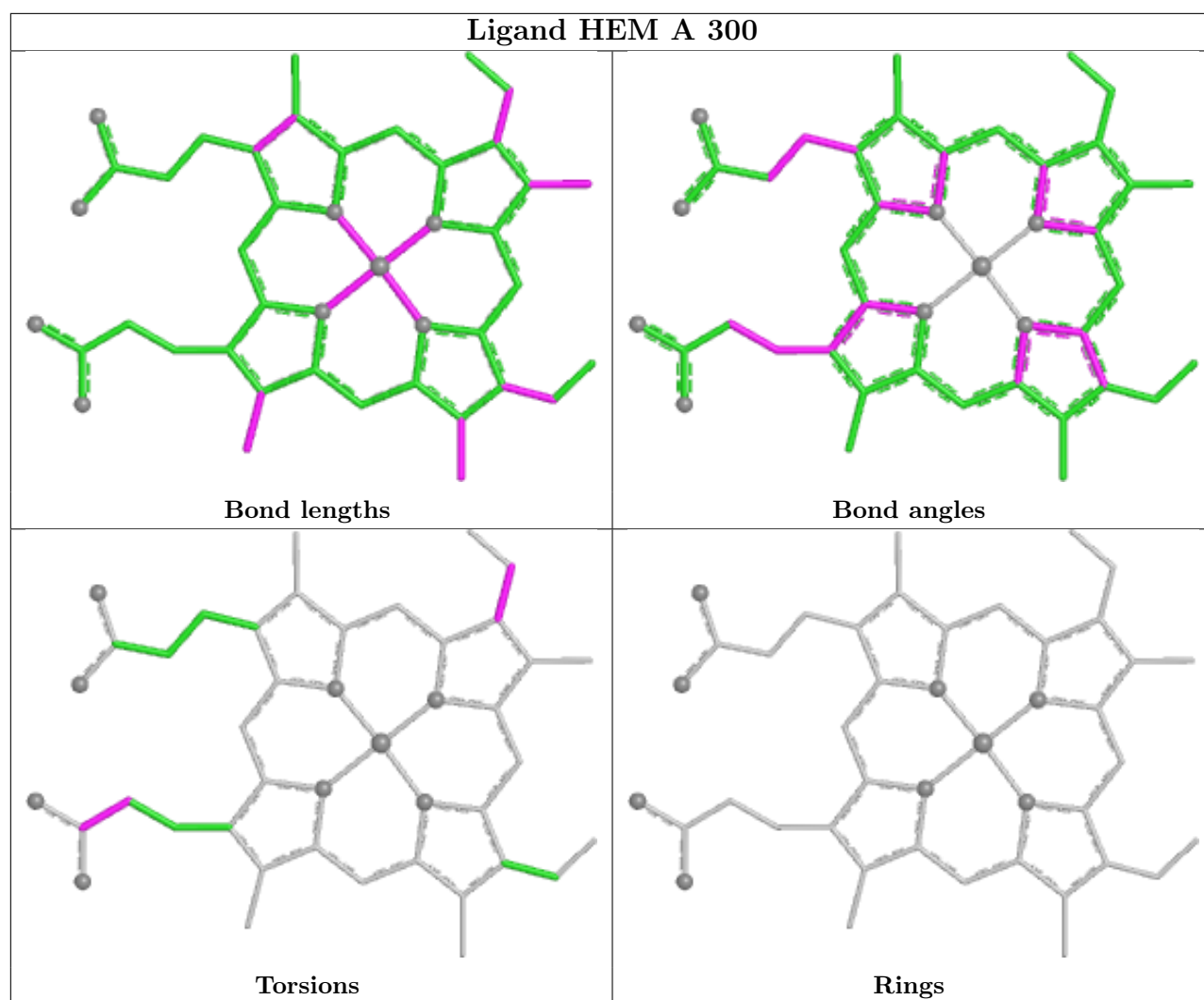
6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2300	HEM	1	0
3	A	301	IMD	2	0
3	D	3301	IMD	2	0
2	A	300	HEM	1	0
2	D	3300	HEM	4	0
2	B	1300	HEM	2	0

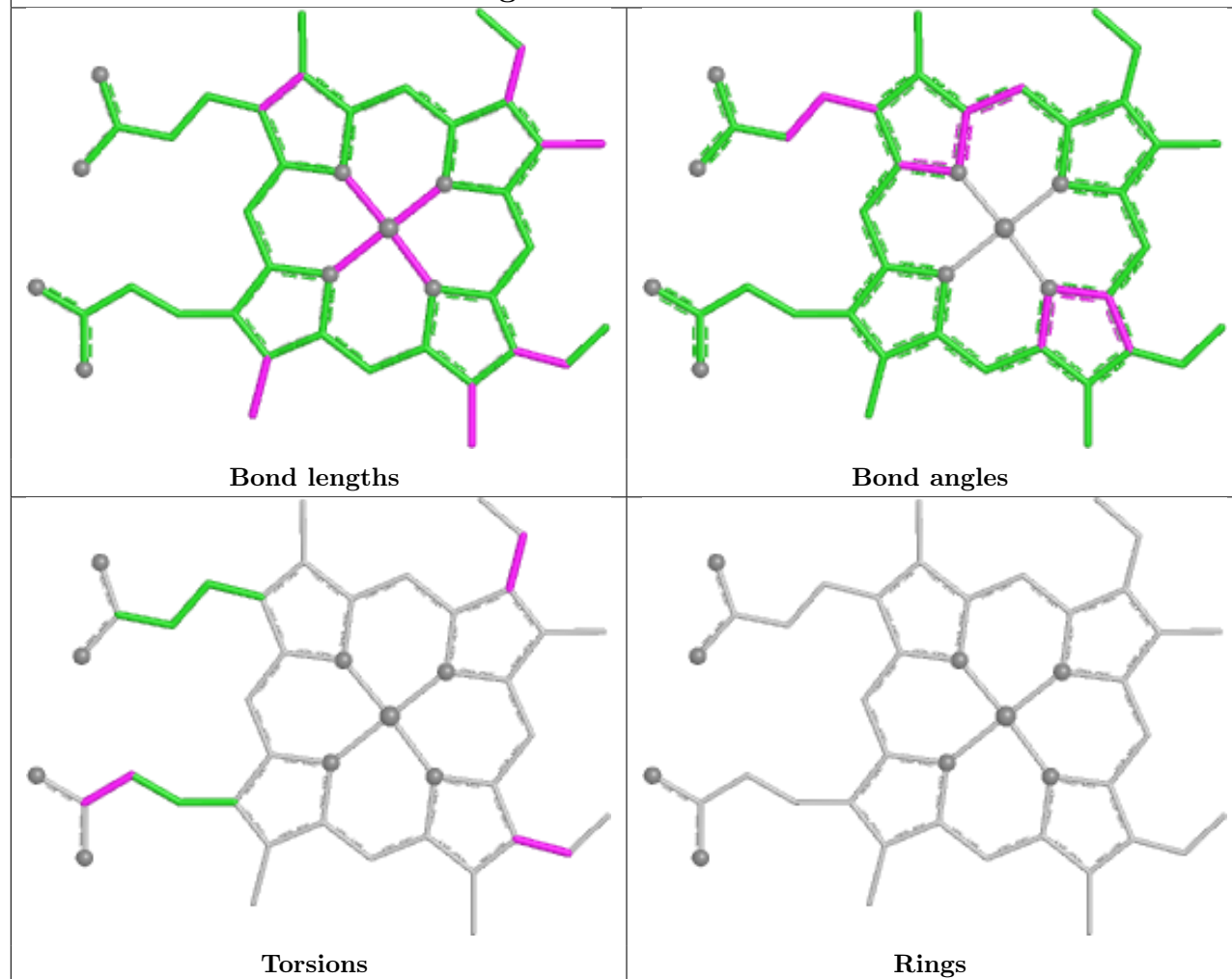
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

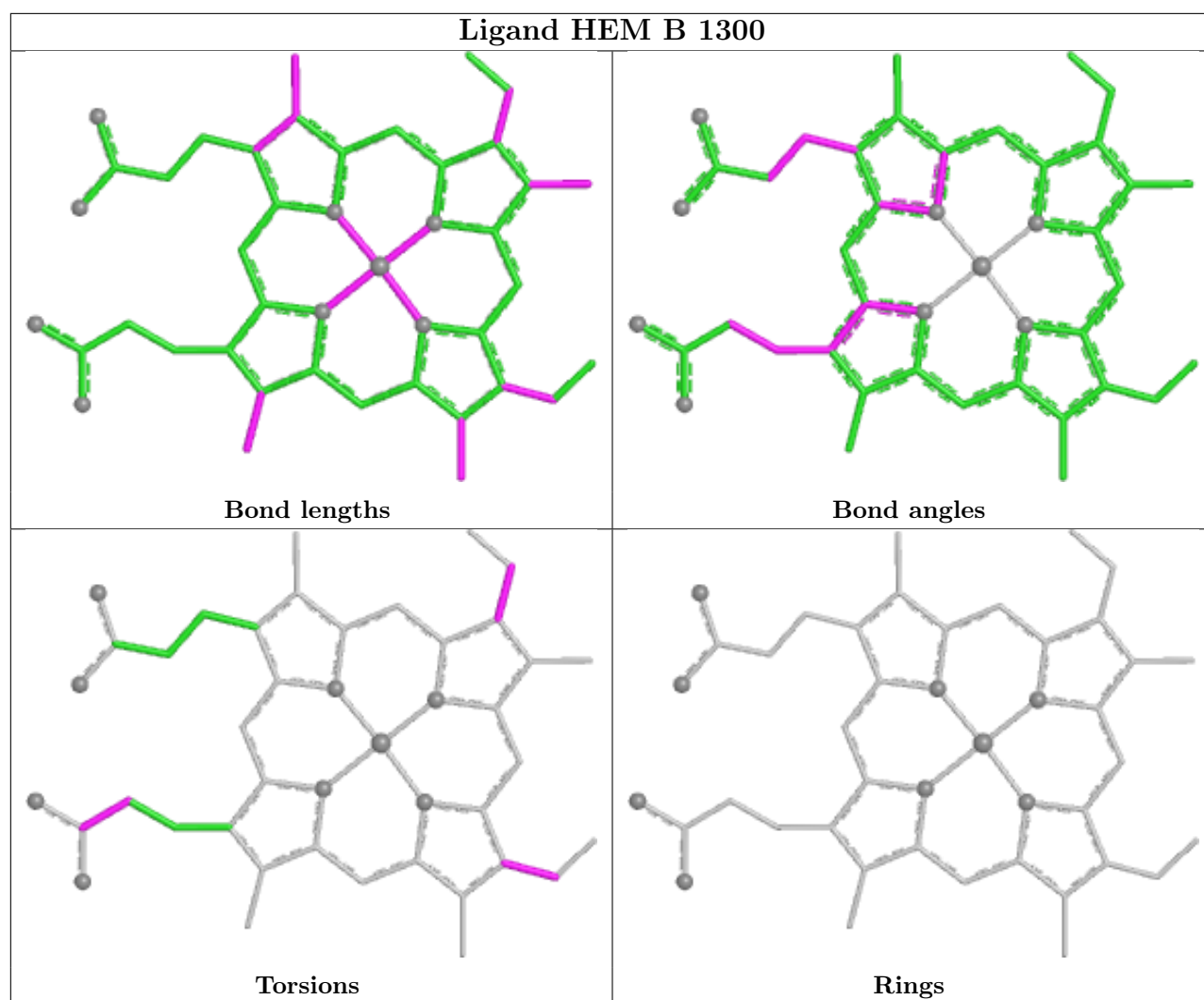
Ligand HEM C 2300





Ligand HEM D 3300





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	218/220 (99%)	0.23	5 (2%) 61 58	35, 40, 51, 59	0
1	B	218/220 (99%)	0.85	20 (9%) 14 12	30, 41, 51, 62	0
1	C	218/220 (99%)	0.66	8 (3%) 45 42	35, 41, 50, 70	0
1	D	218/220 (99%)	0.84	16 (7%) 21 18	32, 41, 53, 57	0
All	All	872/880 (99%)	0.64	49 (5%) 30 27	30, 41, 52, 70	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2003	THR	4.6
1	B	1002	ALA	4.3
1	C	2002	ALA	4.1
1	B	1217	PHE	4.0
1	D	3162	GLY	3.2
1	B	1135	LEU	3.1
1	D	3136	VAL	3.0
1	C	2219	SER	3.0
1	D	3099	ASP	2.8
1	D	3218	SER	2.8
1	B	1176	LEU	2.8
1	D	3137	PHE	2.8
1	B	1134	GLY	2.7
1	A	219	SER	2.7
1	B	1124	LEU	2.7
1	A	65	ASP	2.7
1	D	3002	ALA	2.7
1	B	1021	TYR	2.6
1	B	1131	ILE	2.6
1	B	1003	THR	2.6
1	D	3048	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	1102	ASN	2.5
1	C	2005	MET	2.5
1	D	3029	ARG	2.4
1	D	3130	THR	2.4
1	A	2	ALA	2.4
1	B	1018	SER	2.3
1	B	1137	PHE	2.3
1	D	3157	LEU	2.3
1	C	2052	VAL	2.3
1	A	43	ASN	2.3
1	C	2021	TYR	2.3
1	D	3125	LEU	2.2
1	D	3089	ALA	2.2
1	B	1106	ILE	2.2
1	C	2091	GLU	2.2
1	D	3016	LEU	2.2
1	C	2043	ASN	2.2
1	D	3133	ASN	2.2
1	B	1023	GLY	2.2
1	D	3131	ILE	2.2
1	B	1218	SER	2.2
1	B	1153	MET	2.1
1	B	1195	MET	2.1
1	B	1123	ASP	2.1
1	B	1028	PHE	2.1
1	D	3022	SER	2.0
1	B	1133	ASN	2.0
1	A	217	PHE	2.0

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,

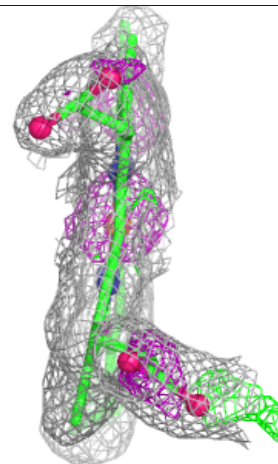
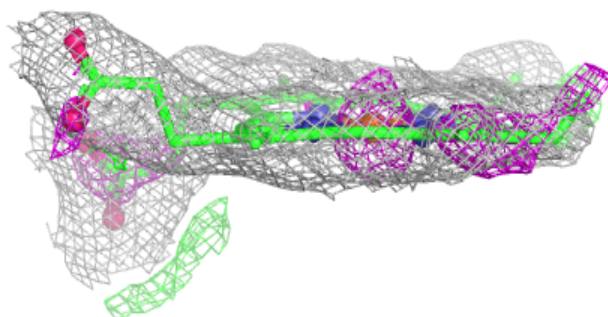
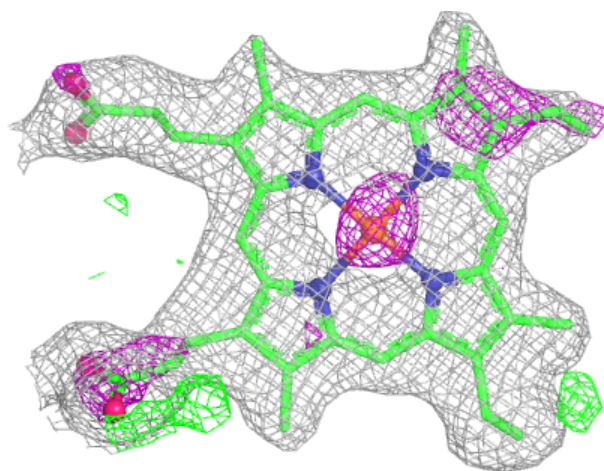
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	IMD	A	301	5/5	0.91	0.13	33,34,34,35	0
2	HEM	D	3300	43/43	0.92	0.12	40,45,51,55	0
3	IMD	D	3301	5/5	0.92	0.17	42,42,43,43	0
3	IMD	B	1301	5/5	0.93	0.13	31,32,33,33	0
2	HEM	A	300	43/43	0.95	0.10	26,34,45,51	0
2	HEM	B	1300	43/43	0.96	0.09	33,35,42,47	0
2	HEM	C	2300	43/43	0.96	0.09	29,32,39,44	0
3	IMD	C	2301	5/5	0.98	0.08	31,32,32,32	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.

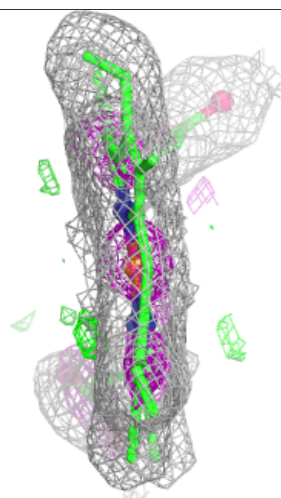
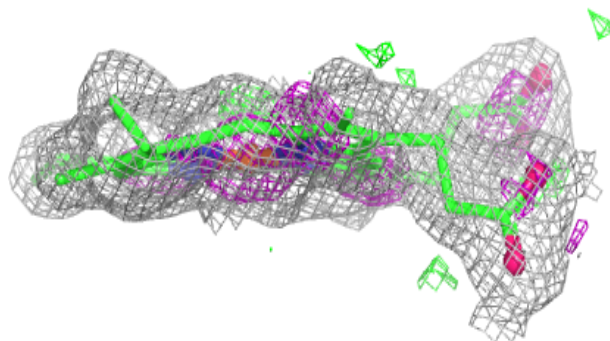
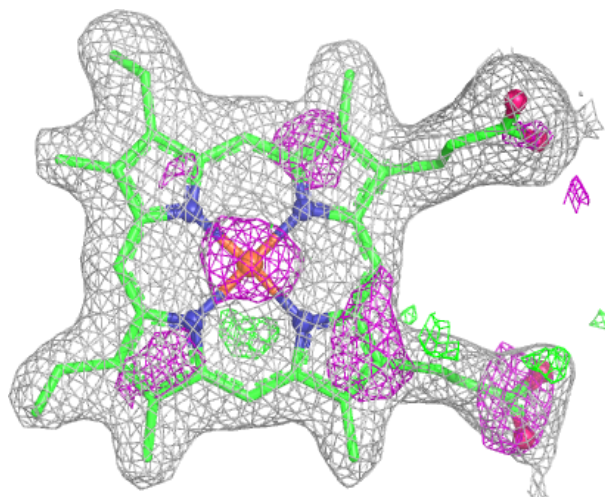
Electron density around HEM D 3300:

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



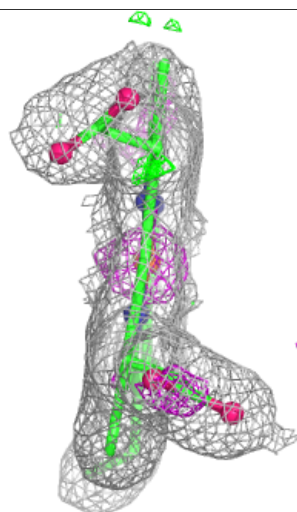
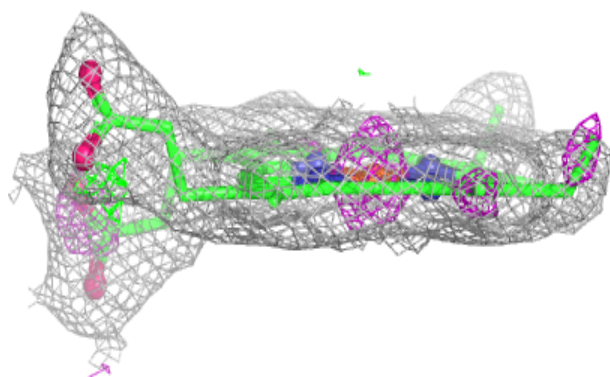
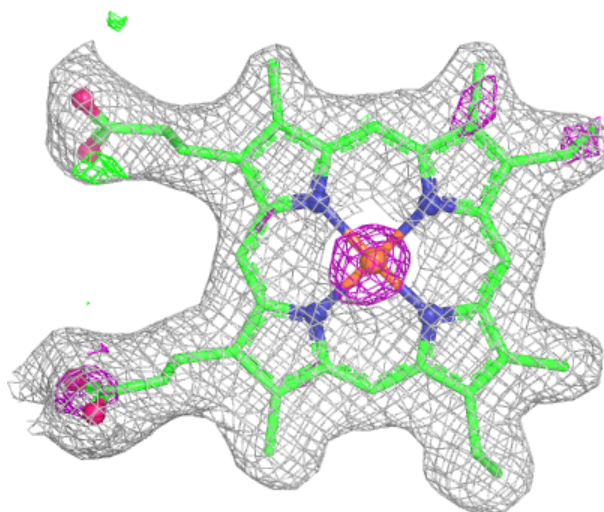
Electron density around HEM A 300:

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



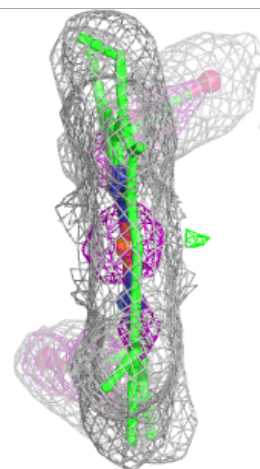
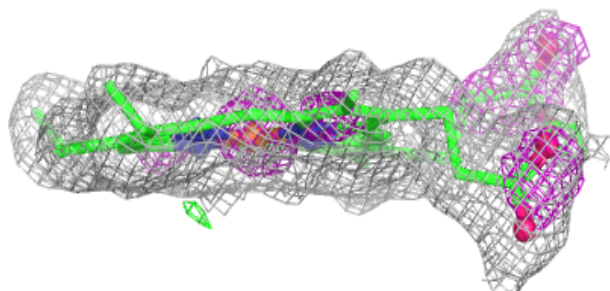
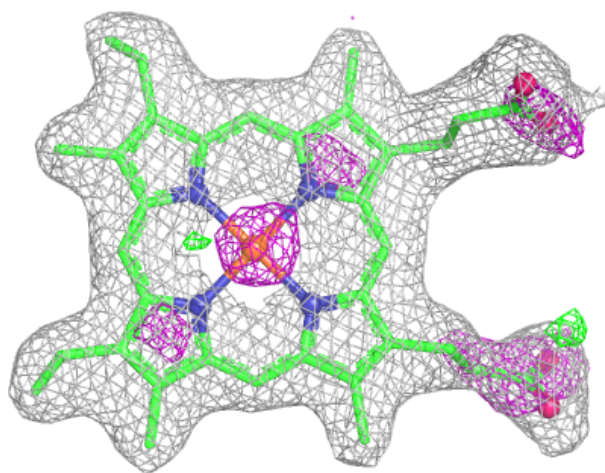
Electron density around HEM B 1300:

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



Electron density around HEM C 2300:

$2mF_o-DF_c$ (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.