



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:27 AM UTC

PDB ID : 9HL1 / pdb\_00009hl1  
Title : DtpB in complex with photocaged nitric oxide, 10 ms, 10 microjoule, SFX  
Authors : Smyth, P.; Williams, L.J.; Hough, M.A.; Worrall, J.A.R.; Owen, R.L.  
Deposited on : 2024-12-04  
Resolution : 1.56 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](mailto: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

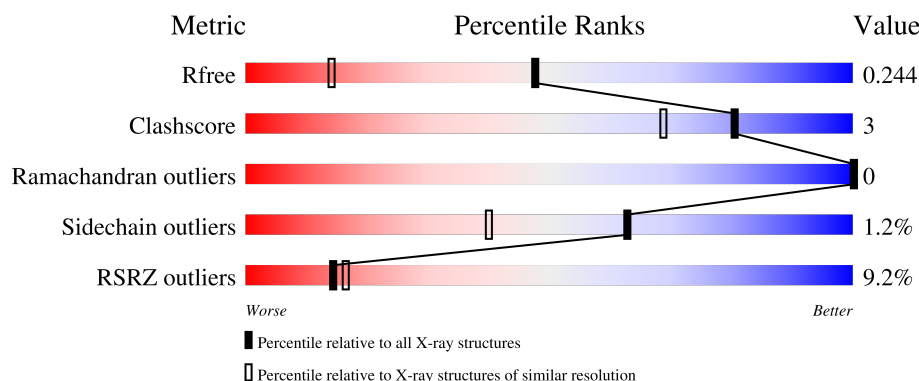
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.56 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.



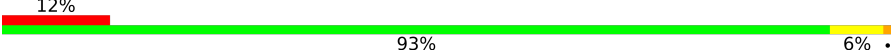
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	2145 (1.56-1.56)
Clashscore	190562	2189 (1.56-1.56)
Ramachandran outliers	187476	2153 (1.56-1.56)
Sidechain outliers	187428	2150 (1.56-1.56)
RSRZ outliers	180081	2146 (1.56-1.56)

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  $\geq 3$ , 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	306	<div> <div>6%</div> <div> <div></div> <div>94%</div> <div>5%</div> </div> </div>
1	B	306	<div> <div>12%</div> <div> <div></div> <div>92%</div> <div>7%</div> </div> </div>
1	C	306	<div> <div>9%</div> <div> <div></div> <div>89%</div> <div>10%</div> </div> </div>
1	D	306	<div> <div>8%</div> <div> <div></div> <div>93%</div> <div>7%</div> </div> </div>
1	E	306	<div> <div>8%</div> <div> <div></div> <div>93%</div> <div>7%</div> </div> </div>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	F	306	

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
3	NO	B	402	-	-	X	-
3	NO	E	402	-	-	X	-
3	NO	F	402	-	-	X	-

## 2 Entry composition [i](#)

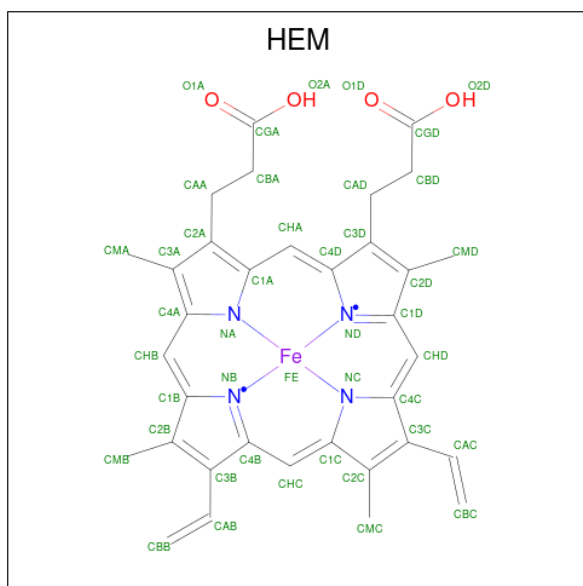
There are 4 unique types of molecules in this entry. The entry contains 15490 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Dyp-type peroxidase family.

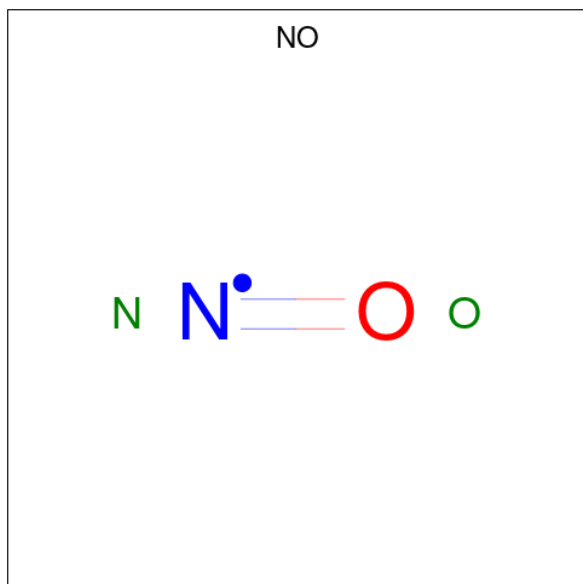
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	306	Total	C	N	O	S	0	3	0
			2352	1477	405	460	10			
1	B	306	Total	C	N	O	S	0	1	0
			2338	1471	403	455	9			
1	C	306	Total	C	N	O	S	0	5	0
			2367	1486	410	462	9			
1	D	305	Total	C	N	O	S	0	7	0
			2371	1488	411	463	9			
1	E	305	Total	C	N	O	S	0	5	0
			2350	1477	406	458	9			
1	F	305	Total	C	N	O	S	0	3	0
			2340	1471	403	456	10			

- 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	C	Fe	N	O	
			43	34	1	4	4	
2	B	1	Total	C	Fe	N	O	
			43	34	1	4	4	
2	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	
2	D	1	Total	C	Fe	N	O	
			43	34	1	4	4	
2	E	1	Total	C	Fe	N	O	
			43	34	1	4	4	
2	F	1	Total	C	Fe	N	O	
			43	34	1	4	4	

- Molecule 3 is NITRIC OXIDE (CCD ID: NO) (formula: NO) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	N	O		
			2	1	1		
3	B	1	Total	N	O		
			2	1	1		
3	C	1	Total	N	O		
			2	1	1		
3	D	1	Total	N	O		
			2	1	1		
3	E	1	Total	N	O		
			2	1	1		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	F	1	Total	N	O	0	0
			2	1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	198	Total	O	0	0
			198	198		
4	B	157	Total	O	0	0
			157	157		
4	C	171	Total	O	0	0
			171	171		
4	D	214	Total	O	0	0
			214	214		
4	E	203	Total	O	0	0
			203	203		
4	F	159	Total	O	0	0
			159	159		

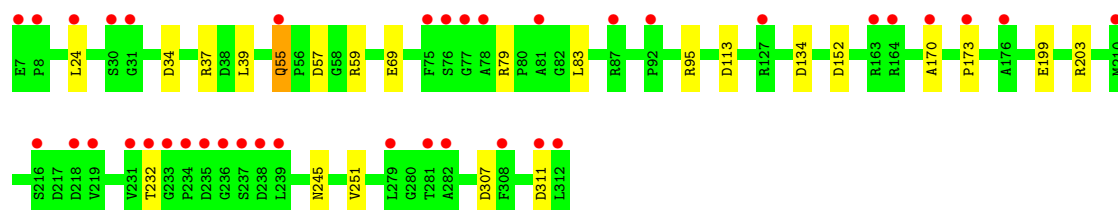
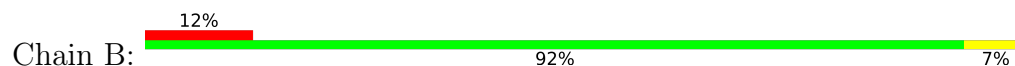
### 3 Residue-property plots [i](#)

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.

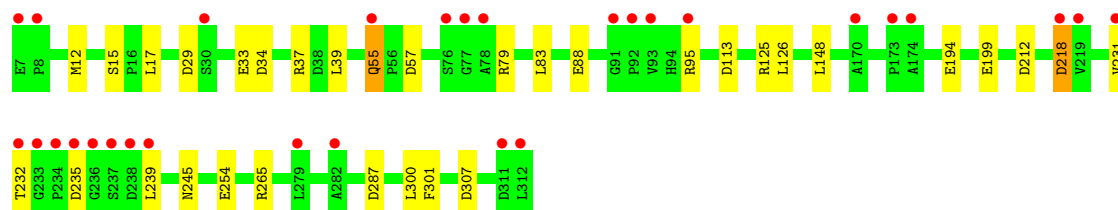
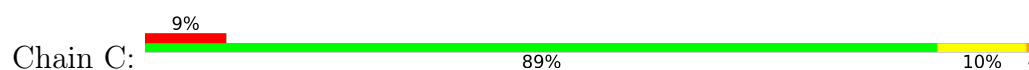
- Molecule 1: Dyp-type peroxidase family



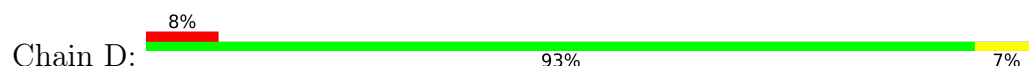
- Molecule 1: Dyp-type peroxidase family



- Molecule 1: Dyp-type peroxidase family

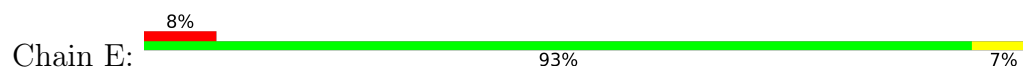


- Molecule 1: Dyp-type peroxidase family

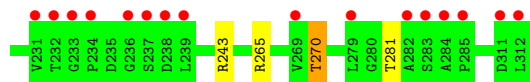
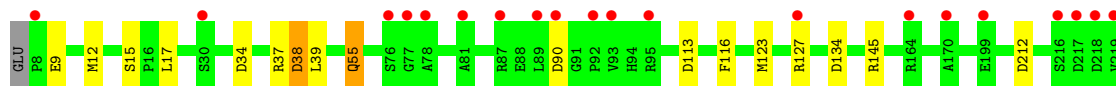
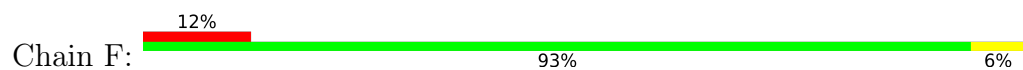




- Molecule 1: Dyp-type peroxidase family



- Molecule 1: Dyp-type peroxidase family





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.07Å 122.88Å 194.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.68 – 1.56 44.68 – 1.56	Depositor EDS
% Data completeness (in resolution range)	99.9 (44.68-1.56) 99.9 (44.68-1.56)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.68 (at 1.56Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, $R_{free}$	0.209 , 0.234 0.220 , 0.244	Depositor DCC
$R_{free}$ test set	2027 reflections (0.69%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.9	Xtriage
Anisotropy	0.009	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 32.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	15490	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: HEM, NO

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	0.80	0/2402	1.14	3/3262 (0.1%)
1	B	0.74	0/2388	1.18	9/3245 (0.3%)
1	C	0.72	0/2417	1.16	12/3284 (0.4%)
1	D	0.79	0/2421	1.16	5/3287 (0.2%)
1	E	0.77	0/2400	1.17	5/3261 (0.2%)
1	F	0.76	0/2390	1.21	8/3246 (0.2%)
All	All	0.76	0/14418	1.17	42/19585 (0.2%)

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	3
1	B	0	2
1	C	0	1
1	D	0	1
1	F	0	1
All	All	0	8

There are no bond length outliers.

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	55	GLN	CB-CA-C	13.24	128.97	109.11
1	D	55	GLN	CB-CA-C	8.60	123.11	109.27
1	A	232	THR	CA-CB-OG1	-8.41	96.98	109.60
1	F	55	GLN	CB-CA-C	7.79	121.83	109.52
1	E	232	THR	CA-CB-OG1	-7.55	98.28	109.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	194	GLU	CB-CG-CD	7.03	124.55	112.60
1	F	212	ASP	CA-CB-CG	6.98	119.58	112.60
1	D	113	ASP	CA-CB-CG	6.67	119.28	112.60
1	D	232	THR	CA-CB-OG1	-6.59	99.71	109.60
1	C	113	ASP	CA-CB-CG	6.54	119.14	112.60
1	F	9	GLU	CB-CA-C	6.50	117.26	109.85
1	B	232	THR	CA-CB-OG1	-6.37	100.04	109.60
1	C	55	GLN	CB-CA-C	6.37	119.91	109.46
1	E	281	THR	CA-CB-OG1	-6.16	100.36	109.60
1	F	113	ASP	CA-CB-CG	6.14	118.74	112.60
1	C	55	GLN	N-CA-CB	-6.11	100.81	110.03
1	C	265	ARG	N-CA-CB	-6.04	100.91	110.28
1	C	199	GLU	CB-CG-CD	5.96	122.74	112.60
1	B	311	ASP	CB-CA-C	-5.62	104.31	111.22
1	D	145	ARG	CA-CB-CG	-5.59	102.93	114.10
1	B	134	ASP	CA-CB-CG	5.56	118.16	112.60
1	B	113	ASP	CA-CB-CG	5.53	118.13	112.60
1	B	152	ASP	CA-CB-CG	5.48	118.08	112.60
1	F	281	THR	CA-CB-OG1	-5.48	101.38	109.60
1	C	212	ASP	CA-CB-CG	5.43	118.03	112.60
1	C	232	THR	CA-CB-OG1	-5.43	101.46	109.60
1	C	29	ASP	CA-CB-CG	5.42	118.02	112.60
1	F	38	ASP	CA-CB-CG	5.38	117.98	112.60
1	B	95	ARG	N-CA-CB	-5.29	101.43	111.00
1	A	154	THR	CA-CB-OG1	-5.22	101.76	109.60
1	B	69	GLU	CB-CA-C	-5.21	101.99	110.85
1	E	175	PHE	CA-CB-CG	-5.21	108.59	113.80
1	A	88	GLU	N-CA-CB	5.19	117.67	109.83
1	E	113	ASP	CA-CB-CG	5.13	117.73	112.60
1	E	212	ASP	CA-CB-CG	5.13	117.73	112.60
1	D	212	ASP	CA-CB-CG	5.13	117.73	112.60
1	C	218	ASP	CB-CA-C	-5.11	99.96	110.38
1	C	218	ASP	CA-CB-CG	5.08	117.68	112.60
1	F	134	ASP	CA-CB-CG	5.08	117.68	112.60
1	C	287	ASP	CA-CB-CG	5.07	117.67	112.60
1	F	265	ARG	N-CA-CB	-5.05	102.01	110.39
1	B	199	GLU	CB-CG-CD	5.00	121.11	112.60

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	108	ARG	Sidechain
1	A	127	ARG	Sidechain
1	A	95	ARG	Sidechain
1	B	203	ARG	Sidechain
1	B	59	ARG	Sidechain
1	C	125	ARG	Sidechain
1	D	163	ARG	Sidechain
1	F	145	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	2352	0	2273	10	0
1	B	2338	0	2262	7	0
1	C	2367	0	2287	14	0
1	D	2371	0	2295	15	0
1	E	2350	0	2263	15	0
1	F	2340	0	2264	9	0
2	A	43	0	30	1	0
2	B	43	0	30	1	0
2	C	43	0	30	1	0
2	D	43	0	30	1	0
2	E	43	0	30	1	0
2	F	43	0	30	3	0
3	A	2	0	0	1	0
3	B	2	0	0	2	0
3	C	2	0	0	1	0
3	D	2	0	0	1	0
3	E	2	0	0	2	0
3	F	2	0	0	2	0
4	A	198	0	0	5	0
4	B	157	0	0	1	0
4	C	171	0	0	1	0
4	D	214	0	0	4	0
4	E	203	0	0	3	0
4	F	159	0	0	2	0
All	All	15490	0	13824	73	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 (73) 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:245:ASN:ND2	3:B:402:NO:O	1.86	1.08
1:D:312:LEU:HA	4:D:547:HOH:O	1.67	0.93
1:C:245:ASN:ND2	3:C:402:NO:O	2.05	0.89
1:C:57:ASP:HB2	4:C:581:HOH:O	1.74	0.85
1:D:245:ASN:ND2	3:D:402:NO:O	2.17	0.78
1:A:34:ASP:OD1	1:A:37:ARG:NH2	2.20	0.74
1:E:245[A]:ASN:ND2	3:E:402:NO:O	2.21	0.74
1:F:270[A]:THR:HG21	4:F:571:HOH:O	1.89	0.71
1:E:57:ASP:HB2	4:E:513:HOH:O	1.90	0.70
1:A:245:ASN:ND2	3:A:402:NO:O	2.24	0.69
1:F:243:ARG:NH1	3:F:402:NO:O	2.25	0.69
2:F:401:HEM:HBC2	2:F:401:HEM:HMC2	1.77	0.67
1:D:255:GLU:OE2	4:D:501:HOH:O	2.14	0.66
1:E:55:GLN:HB3	4:F:652:HOH:O	1.98	0.64
1:B:34:ASP:OD1	1:B:37:ARG:NH2	2.31	0.63
1:B:57:ASP:HB2	4:B:614:HOH:O	2.01	0.59
1:C:34:ASP:OD1	1:C:37[A]:ARG:NH1	2.37	0.57
2:E:401:HEM:NB	3:E:402:NO:N	2.52	0.57
1:E:12:MET:HE3	1:E:15[A]:SER:HB3	1.87	0.57
1:A:55:GLN:HB3	4:A:684:HOH:O	2.04	0.57
1:B:79:ARG:NH2	1:B:83:LEU:O	2.37	0.57
1:A:127:ARG:CZ	1:C:254:GLU:HG2	2.34	0.56
1:D:300[B]:LEU:HD13	1:D:300[B]:LEU:C	2.30	0.56
1:D:312:LEU:CD1	1:D:312:LEU:O	2.54	0.55
4:A:686:HOH:O	1:F:55:GLN:CB	2.57	0.53
1:D:312:LEU:O	1:D:312:LEU:HD12	2.08	0.53
1:A:55:GLN:CB	4:A:684:HOH:O	2.56	0.53
1:D:312:LEU:HG	4:D:614:HOH:O	2.09	0.52
1:D:251:VAL:HG12	1:F:123:MET:HG3	1.90	0.51
1:C:231:VAL:HG23	1:C:239:LEU:HB2	1.93	0.51
1:C:39:LEU:HD22	1:C:126:LEU:HD11	1.93	0.50
1:E:34:ASP:OD1	1:E:37:ARG:NH2	2.45	0.50
1:D:84:HIS:O	1:D:300[B]:LEU:HD12	2.12	0.49
1:E:37:ARG:CD	4:E:630:HOH:O	2.60	0.49
1:E:300:LEU:C	1:E:300:LEU:HD23	2.37	0.49
1:A:55:GLN:HG3	4:A:684:HOH:O	2.13	0.48
1:E:214:GLU:OE2	1:E:220:LYS:NZ	2.25	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:401:HEM:NB	3:F:402:NO:N	2.62	0.47
1:D:231:VAL:HG23	1:D:239:LEU:HB2	1.95	0.47
1:E:90:ASP:OD1	1:E:95:ARG:HD2	2.15	0.47
1:C:12:MET:HE3	1:C:15[A]:SER:HB3	1.97	0.47
1:B:39:LEU:C	1:B:39:LEU:HD13	2.39	0.46
1:D:255:GLU:CD	4:D:501:HOH:O	2.55	0.46
2:D:401:HEM:HMC2	2:D:401:HEM:HBC2	1.97	0.46
1:C:33:GLU:O	1:C:37[B]:ARG:HG3	2.16	0.46
2:A:401:HEM:HMC2	2:A:401:HEM:HBC2	1.97	0.45
1:E:12:MET:HE3	1:E:15[B]:SER:HB3	1.97	0.45
1:E:37:ARG:HD2	4:E:630:HOH:O	2.17	0.45
1:D:90:ASP:OD1	1:D:95:ARG:HG3	2.17	0.44
2:C:401:HEM:HMC2	2:C:401:HEM:HBC2	1.99	0.44
1:E:300:LEU:HD23	1:E:301:PHE:N	2.33	0.44
2:F:401:HEM:HBC2	2:F:401:HEM:CMC	2.45	0.44
1:E:12:MET:HE3	1:E:12:MET:HB3	1.90	0.43
1:C:300:LEU:HD23	1:C:301:PHE:N	2.34	0.43
1:F:39:LEU:O	1:F:39:LEU:HG	2.15	0.43
1:B:170:ALA:O	1:B:173:PRO:HD3	2.19	0.42
2:B:401:HEM:NB	3:B:402:NO:N	2.67	0.42
1:C:12:MET:HE3	1:C:15[B]:SER:HB3	2.00	0.42
1:A:187:LEU:HD22	1:A:255:GLU:HG3	2.01	0.42
1:F:12:MET:HE3	1:F:15:SER:HB3	2.01	0.42
1:A:123:MET:O	1:A:127:ARG:HG2	2.19	0.42
1:A:26:VAL:HG12	1:A:132:PRO:HA	2.00	0.41
1:C:79:ARG:NH2	1:C:83:LEU:O	2.51	0.41
1:C:88:GLU:OE2	1:C:95:ARG:NH2	2.53	0.41
1:A:55:GLN:CG	4:A:684:HOH:O	2.68	0.41
1:C:231:VAL:CG2	1:C:239:LEU:HB2	2.50	0.41
1:D:147:MET:HE1	1:F:116:PHE:CE2	2.55	0.41
1:D:214:GLU:OE2	1:D:220:LYS:NZ	2.33	0.41
1:D:254:GLU:HG2	1:F:127:ARG:CZ	2.51	0.41
1:F:34:ASP:OD1	1:F:37:ARG:NH1	2.53	0.41
1:E:152:ASP:CG	1:E:245[B]:ASN:HD21	2.29	0.41
1:B:251[A]:VAL:HG12	1:E:123:MET:HG3	2.03	0.40
1:C:300:LEU:HD23	1:C:300:LEU:C	2.47	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	307/306 (100%)	302 (98%)	5 (2%)	0	100	100
1	B	305/306 (100%)	300 (98%)	5 (2%)	0	100	100
1	C	309/306 (101%)	303 (98%)	6 (2%)	0	100	100
1	D	310/306 (101%)	304 (98%)	6 (2%)	0	100	100
1	E	308/306 (101%)	302 (98%)	6 (2%)	0	100	100
1	F	306/306 (100%)	300 (98%)	6 (2%)	0	100	100
All	All	1845/1836 (100%)	1811 (98%)	34 (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	248/245 (101%)	246 (99%)	2 (1%)	73	56
1	B	245/245 (100%)	242 (99%)	3 (1%)	63	40
1	C	249/245 (102%)	243 (98%)	6 (2%)	43	15
1	D	251/245 (102%)	249 (99%)	2 (1%)	73	56
1	E	245/245 (100%)	244 (100%)	1 (0%)	84	73
1	F	246/245 (100%)	241 (98%)	5 (2%)	48	20
All	All	1484/1470 (101%)	1465 (99%)	19 (1%)	63	36

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LEU
1	A	307	ASP
1	B	24	LEU
1	B	55	GLN
1	B	307	ASP
1	C	17	LEU
1	C	55	GLN
1	C	148	LEU
1	C	218	ASP
1	C	235	ASP
1	C	307	ASP
1	D	55	GLN
1	D	285	PRO
1	E	17	LEU
1	F	17	LEU
1	F	38	ASP
1	F	90	ASP
1	F	270[A]	THR
1	F	270[B]	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	184	GLN
1	F	245	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.



## 5.6 Ligand geometry

12 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	B	401	1,3	50,50,50	1.54	10 (20%)	67,82,82	1.54	11 (16%)
3	NO	E	402	2	0,1,1	-	-	-	-	-
2	HEM	F	401	1,3	50,50,50	1.46	8 (16%)	67,82,82	1.91	14 (20%)
3	NO	C	402	2	0,1,1	-	-	-	-	-
3	NO	D	402	2	0,1,1	-	-	-	-	-
2	HEM	A	401	1,3	50,50,50	1.30	7 (14%)	67,82,82	2.00	23 (34%)
2	HEM	C	401	1,3	50,50,50	1.53	11 (22%)	67,82,82	1.81	16 (23%)
3	NO	F	402	2	0,1,1	-	-	-	-	-
2	HEM	E	401	1,3	50,50,50	1.31	6 (12%)	67,82,82	1.74	15 (22%)
3	NO	B	402	2	0,1,1	-	-	-	-	-
2	HEM	D	401	1,3	50,50,50	1.27	5 (10%)	67,82,82	1.72	12 (17%)
3	NO	A	402	2	0,1,1	-	-	-	-	-

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	B	401	1,3	-	5/14/54/54	-
2	HEM	F	401	1,3	-	5/14/54/54	-
2	HEM	A	401	1,3	-	6/14/54/54	-
2	HEM	C	401	1,3	-	6/14/54/54	-
2	HEM	E	401	1,3	-	7/14/54/54	-
2	HEM	D	401	1,3	-	6/14/54/54	-

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	HEM	C1B-NB	-4.45	1.32	1.40
2	C	401	HEM	C1C-C2C	-3.77	1.37	1.45
2	F	401	HEM	FE-NB	3.76	2.06	1.94
2	C	401	HEM	FE-NB	3.57	2.05	1.94
2	F	401	HEM	C4D-C3D	3.48	1.50	1.45
2	B	401	HEM	FE-NC	3.39	2.06	1.95
2	F	401	HEM	C1B-NB	-3.35	1.34	1.40
2	B	401	HEM	C1C-C2C	-3.31	1.38	1.45
2	D	401	HEM	FE-NC	3.21	2.05	1.95
2	E	401	HEM	FE-NC	3.18	2.05	1.95
2	C	401	HEM	FE-NC	3.13	2.05	1.95
2	F	401	HEM	C1C-C2C	-3.09	1.39	1.45
2	A	401	HEM	FE-NB	3.08	2.04	1.94
2	D	401	HEM	FE-NB	3.01	2.04	1.94
2	E	401	HEM	C1B-NB	-3.01	1.35	1.40
2	C	401	HEM	C4B-NB	-2.99	1.33	1.38
2	C	401	HEM	C1B-NB	-2.94	1.35	1.40
2	A	401	HEM	FE-NC	2.90	2.04	1.95
2	E	401	HEM	C1C-C2C	-2.90	1.39	1.45
2	B	401	HEM	O2D-CGD	-2.84	1.21	1.30
2	B	401	HEM	C4C-NC	-2.83	1.34	1.39
2	E	401	HEM	FE-NB	2.83	2.03	1.94
2	A	401	HEM	C1B-NB	-2.75	1.35	1.40
2	C	401	HEM	C4D-C3D	2.71	1.49	1.45
2	B	401	HEM	FE-NB	2.68	2.03	1.94
2	F	401	HEM	C4D-ND	-2.60	1.35	1.40
2	F	401	HEM	FE-NC	2.60	2.03	1.95
2	E	401	HEM	C4B-NB	-2.55	1.33	1.38
2	F	401	HEM	FE-NA	2.47	2.03	1.95
2	B	401	HEM	C1A-C2A	-2.45	1.39	1.44
2	B	401	HEM	C3D-C2D	-2.43	1.31	1.36
2	C	401	HEM	C4C-NC	-2.42	1.35	1.39
2	D	401	HEM	C3D-C2D	-2.34	1.31	1.36
2	A	401	HEM	FE-NA	2.28	2.02	1.95
2	B	401	HEM	C3C-C4C	-2.23	1.42	1.46
2	C	401	HEM	C1D-C2D	2.21	1.49	1.44
2	A	401	HEM	C1D-C2D	2.18	1.48	1.44
2	C	401	HEM	O2D-CGD	-2.18	1.23	1.30
2	E	401	HEM	FE-NA	2.17	2.02	1.95
2	C	401	HEM	C1D-ND	-2.15	1.34	1.38
2	D	401	HEM	O2D-CGD	-2.13	1.23	1.30
2	D	401	HEM	C1C-C2C	-2.09	1.41	1.45
2	C	401	HEM	C4D-ND	-2.04	1.36	1.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	HEM	CHA-C4D	2.03	1.42	1.38
2	F	401	HEM	CBA-CAA	2.02	1.58	1.51
2	A	401	HEM	O1D-CGD	2.01	1.28	1.22
2	B	401	HEM	CBA-CGA	-2.00	1.45	1.50

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	401	HEM	CHC-C4B-NB	7.17	132.14	124.42
2	F	401	HEM	C3B-C4B-NB	-6.58	104.75	109.47
2	C	401	HEM	CHC-C4B-NB	5.63	130.48	124.42
2	A	401	HEM	CHD-C4C-NC	5.60	130.55	124.45
2	E	401	HEM	CHC-C4B-NB	5.41	130.24	124.42
2	F	401	HEM	C1B-NB-C4B	5.23	111.40	105.21
2	D	401	HEM	C2D-C1D-ND	5.03	115.71	109.90
2	A	401	HEM	C1B-NB-C4B	4.96	111.09	105.21
2	C	401	HEM	C1B-NB-C4B	4.93	111.05	105.21
2	B	401	HEM	CHC-C4B-NB	4.92	129.72	124.42
2	A	401	HEM	CHB-C1B-NB	4.67	130.14	124.37
2	D	401	HEM	C4D-ND-C1D	-4.64	99.71	105.21
2	A	401	HEM	CHC-C4B-NB	4.58	129.35	124.42
2	E	401	HEM	CHD-C4C-NC	4.45	129.30	124.45
2	C	401	HEM	CHB-C1B-NB	4.39	129.79	124.37
2	E	401	HEM	C1B-NB-C4B	3.90	109.82	105.21
2	D	401	HEM	C2A-C1A-NA	-3.84	105.89	110.15
2	D	401	HEM	CHA-C1A-NA	3.70	130.57	123.86
2	F	401	HEM	CHD-C4C-NC	3.66	128.44	124.45
2	D	401	HEM	C3B-C4B-NB	-3.65	106.85	109.47
2	C	401	HEM	C3B-C4B-NB	-3.64	106.85	109.47
2	A	401	HEM	C3B-C4B-NB	-3.29	107.10	109.47
2	D	401	HEM	CHD-C1D-C2D	-3.27	119.87	125.03
2	C	401	HEM	CMD-C2D-C1D	3.14	129.94	125.03
2	B	401	HEM	O2A-CGA-CBA	3.09	123.77	114.00
2	A	401	HEM	CHC-C1C-NC	3.00	127.72	124.45
2	F	401	HEM	CHB-C1B-NB	2.94	128.00	124.37
2	C	401	HEM	CHD-C4C-NC	2.90	127.61	124.45
2	E	401	HEM	C4D-ND-C1D	-2.89	101.78	105.21
2	D	401	HEM	C3D-C4D-ND	2.89	113.34	110.17
2	D	401	HEM	C1B-NB-C4B	2.87	108.61	105.21
2	B	401	HEM	C1B-NB-C4B	2.86	108.60	105.21
2	F	401	HEM	CHA-C4D-ND	2.83	127.87	124.37
2	D	401	HEM	CHD-C4C-NC	2.81	127.51	124.45

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	HEM	CHD-C1D-ND	2.81	127.45	124.42
2	B	401	HEM	CMA-C3A-C2A	2.81	131.58	125.62
2	A	401	HEM	CAB-C3B-C2B	-2.76	119.46	128.43
2	A	401	HEM	C4C-CHD-C1D	-2.76	120.15	126.02
2	E	401	HEM	C3B-C4B-NB	-2.75	107.49	109.47
2	C	401	HEM	CHA-C4D-ND	2.74	127.76	124.37
2	D	401	HEM	CHC-C4B-NB	2.67	127.29	124.42
2	E	401	HEM	CAD-C3D-C4D	2.64	129.31	124.70
2	A	401	HEM	CHD-C1D-C2D	-2.63	120.87	125.03
2	B	401	HEM	C3B-C4B-NB	-2.61	107.59	109.47
2	E	401	HEM	C3D-C4D-ND	2.61	113.03	110.17
2	B	401	HEM	CHD-C1D-C2D	-2.61	120.91	125.03
2	E	401	HEM	C2D-C1D-ND	2.60	112.91	109.90
2	E	401	HEM	CHA-C1A-NA	2.57	128.53	123.86
2	F	401	HEM	C4B-C3B-C2B	2.51	109.59	107.28
2	E	401	HEM	CHA-C4D-C3D	-2.51	120.60	125.23
2	B	401	HEM	O2A-CGA-O1A	-2.50	116.89	123.33
2	A	401	HEM	C1A-CHA-C4D	-2.49	120.40	126.25
2	C	401	HEM	O2A-CGA-CBA	2.48	121.84	114.00
2	A	401	HEM	C4C-NC-C1C	2.47	109.84	105.82
2	E	401	HEM	C2A-C1A-NA	-2.45	107.44	110.15
2	C	401	HEM	C4C-NC-C1C	2.41	109.75	105.82
2	A	401	HEM	CAD-CBD-CGD	-2.40	107.29	113.67
2	B	401	HEM	C2D-C1D-ND	2.39	112.67	109.90
2	A	401	HEM	CAD-C3D-C4D	2.38	128.85	124.70
2	A	401	HEM	CHA-C4D-ND	2.36	127.29	124.37
2	F	401	HEM	O2A-CGA-O1A	-2.34	117.32	123.33
2	A	401	HEM	C1C-CHC-C4B	-2.33	121.07	126.02
2	C	401	HEM	CHD-C1D-C2D	-2.30	121.39	125.03
2	C	401	HEM	CBB-CAB-C3B	-2.27	116.16	127.53
2	C	401	HEM	CHA-C1A-NA	2.26	127.96	123.86
2	C	401	HEM	CHC-C1C-NC	2.24	126.89	124.45
2	E	401	HEM	C1A-CHA-C4D	-2.22	121.02	126.25
2	B	401	HEM	C4C-CHD-C1D	-2.21	121.32	126.02
2	E	401	HEM	CAB-C3B-C2B	-2.18	121.34	128.43
2	D	401	HEM	C1A-C2A-C3A	2.18	110.24	106.87
2	F	401	HEM	C4A-C3A-C2A	-2.17	104.33	106.82
2	F	401	HEM	CMA-C3A-C2A	2.17	130.23	125.62
2	A	401	HEM	CAD-C3D-C2D	-2.17	123.81	127.87
2	E	401	HEM	CBB-CAB-C3B	-2.15	116.76	127.53
2	C	401	HEM	CHA-C4D-C3D	-2.15	121.27	125.23
2	A	401	HEM	CHA-C4D-C3D	-2.14	121.28	125.23

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	401	HEM	CAD-CBD-CGD	-2.14	108.00	113.67
2	A	401	HEM	CAB-C3B-C4B	2.11	133.73	124.39
2	F	401	HEM	C2D-C1D-ND	2.09	112.32	109.90
2	D	401	HEM	C1A-CHA-C4D	-2.08	121.35	126.25
2	C	401	HEM	C2D-C1D-ND	2.08	112.31	109.90
2	C	401	HEM	C4A-CHB-C1B	-2.07	121.39	126.25
2	F	401	HEM	CBB-CAB-C3B	-2.06	117.25	127.53
2	A	401	HEM	C4A-C3A-C2A	2.05	109.17	106.82
2	E	401	HEM	C4C-C3C-C2C	2.04	108.58	106.81
2	B	401	HEM	CHD-C4C-NC	2.02	126.65	124.45
2	F	401	HEM	CHD-C1D-C2D	-2.01	121.85	125.03
2	B	401	HEM	C3B-C2B-C1B	-2.01	104.90	106.41
2	A	401	HEM	CAA-C2A-C3A	2.01	131.57	127.07
2	A	401	HEM	CMA-C3A-C4A	-2.01	122.36	125.42
2	A	401	HEM	C2B-C1B-NB	-2.00	107.54	109.84

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	HEM	C2B-C3B-CAB-CBB
2	E	401	HEM	C2B-C3B-CAB-CBB
2	C	401	HEM	C4B-C3B-CAB-CBB
2	C	401	HEM	C2B-C3B-CAB-CBB
2	E	401	HEM	C4B-C3B-CAB-CBB
2	B	401	HEM	C4B-C3B-CAB-CBB
2	D	401	HEM	C4B-C3B-CAB-CBB
2	B	401	HEM	CAD-CBD-CGD-O2D
2	C	401	HEM	CAD-CBD-CGD-O2D
2	D	401	HEM	CAD-CBD-CGD-O2D
2	A	401	HEM	CAD-CBD-CGD-O1D
2	E	401	HEM	CAD-CBD-CGD-O1D
2	F	401	HEM	CAD-CBD-CGD-O2D
2	E	401	HEM	CAD-CBD-CGD-O2D
2	A	401	HEM	CAD-CBD-CGD-O2D
2	F	401	HEM	CAD-CBD-CGD-O1D
2	E	401	HEM	CAA-CBA-CGA-O2A
2	B	401	HEM	CAD-CBD-CGD-O1D
2	D	401	HEM	CAD-CBD-CGD-O1D
2	F	401	HEM	CAA-CBA-CGA-O2A
2	A	401	HEM	CAA-CBA-CGA-O2A
2	F	401	HEM	CAA-CBA-CGA-O1A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	C	401	HEM	CAA-CBA-CGA-O1A
2	E	401	HEM	CAA-CBA-CGA-O1A
2	C	401	HEM	CAA-CBA-CGA-O2A
2	C	401	HEM	CAD-CBD-CGD-O1D
2	D	401	HEM	CAA-CBA-CGA-O2A
2	A	401	HEM	C4B-C3B-CAB-CBB
2	F	401	HEM	C4B-C3B-CAB-CBB
2	B	401	HEM	CAA-CBA-CGA-O2A
2	D	401	HEM	CAA-CBA-CGA-O1A
2	A	401	HEM	CAA-CBA-CGA-O1A
2	B	401	HEM	CAA-CBA-CGA-O1A
2	D	401	HEM	C2B-C3B-CAB-CBB
2	E	401	HEM	C2C-C3C-CAC-CBC

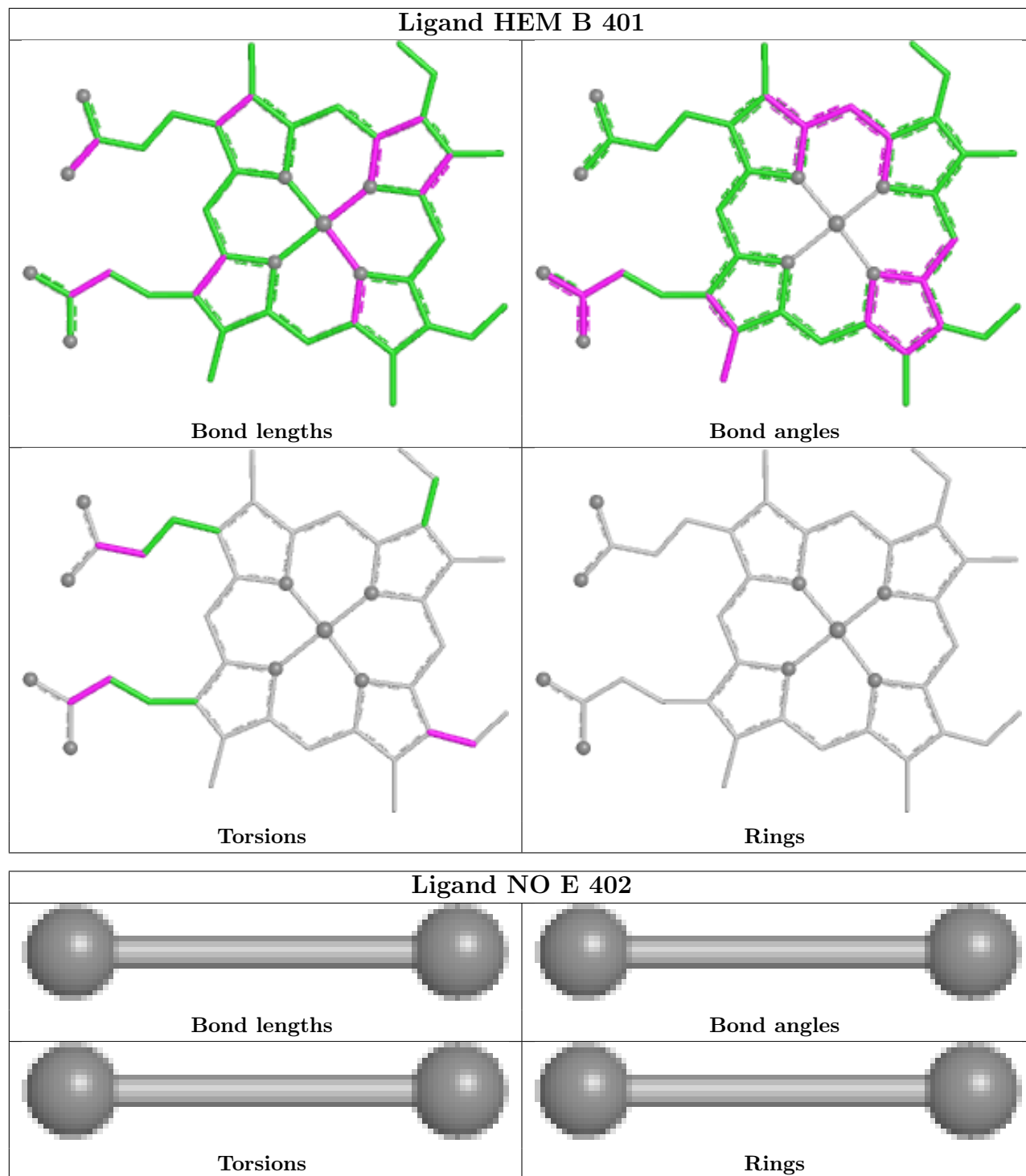
There are no ring outliers.

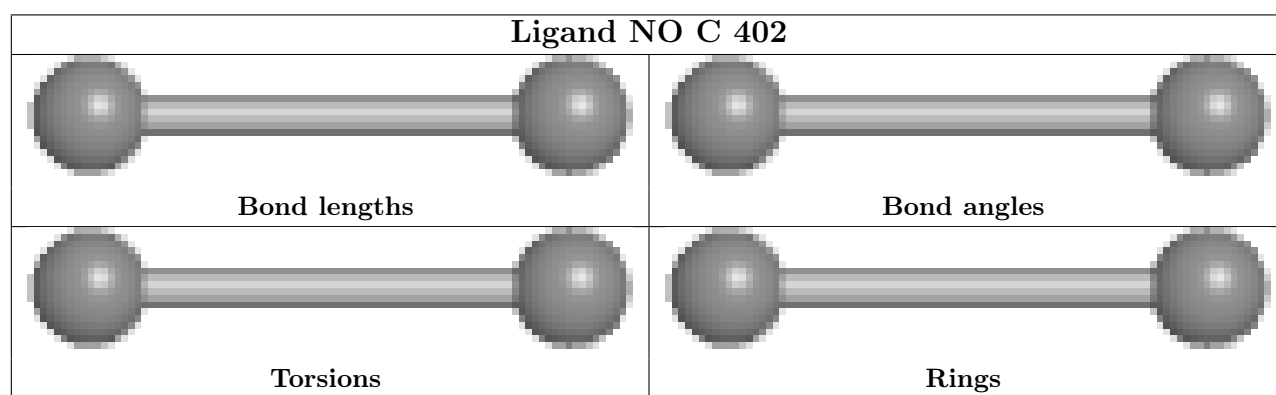
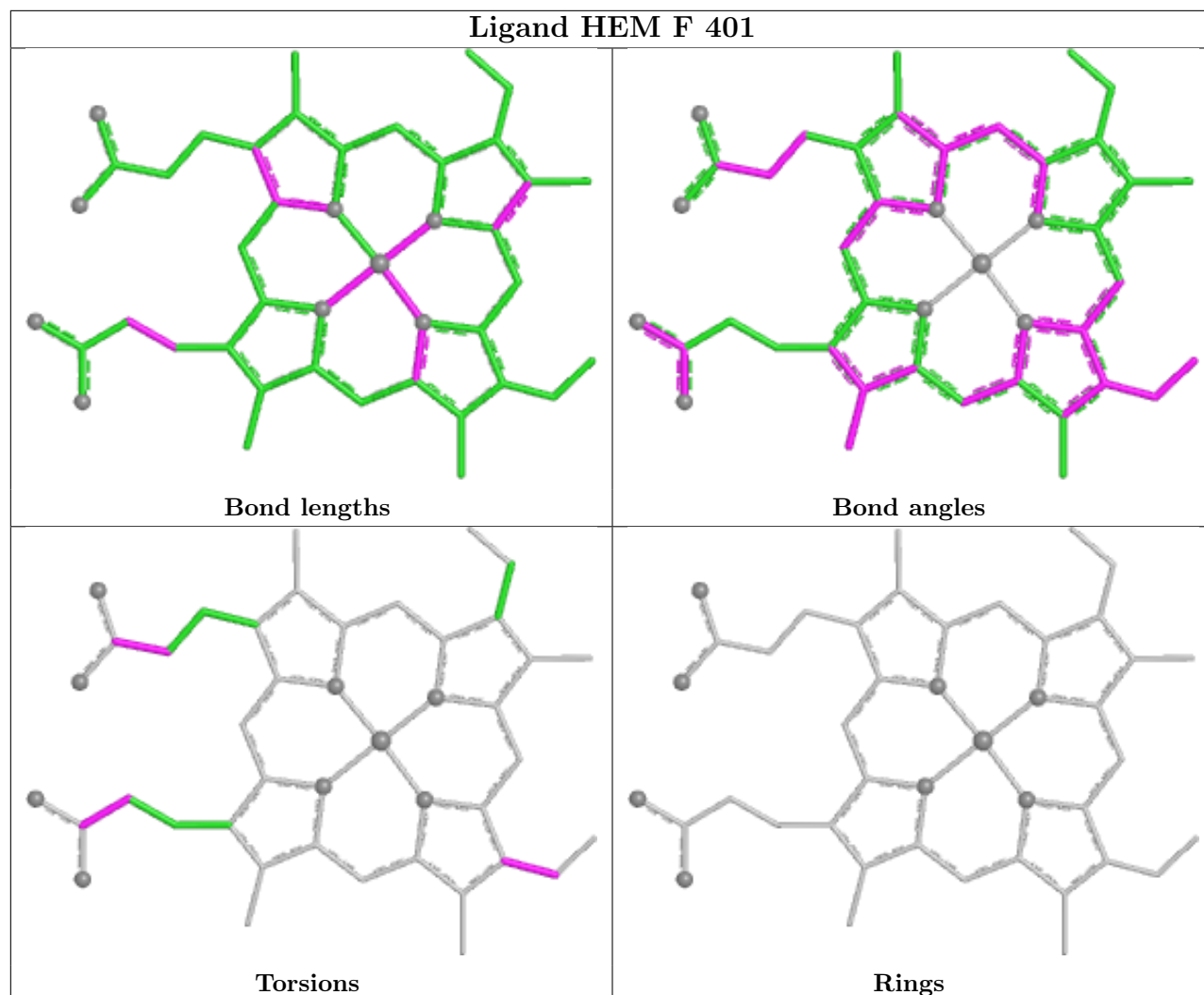
12 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	HEM	1	0
3	E	402	NO	2	0
2	F	401	HEM	3	0
3	C	402	NO	1	0
3	D	402	NO	1	0
2	A	401	HEM	1	0
2	C	401	HEM	1	0
3	F	402	NO	2	0
2	E	401	HEM	1	0
3	B	402	NO	2	0
2	D	401	HEM	1	0
3	A	402	NO	1	0

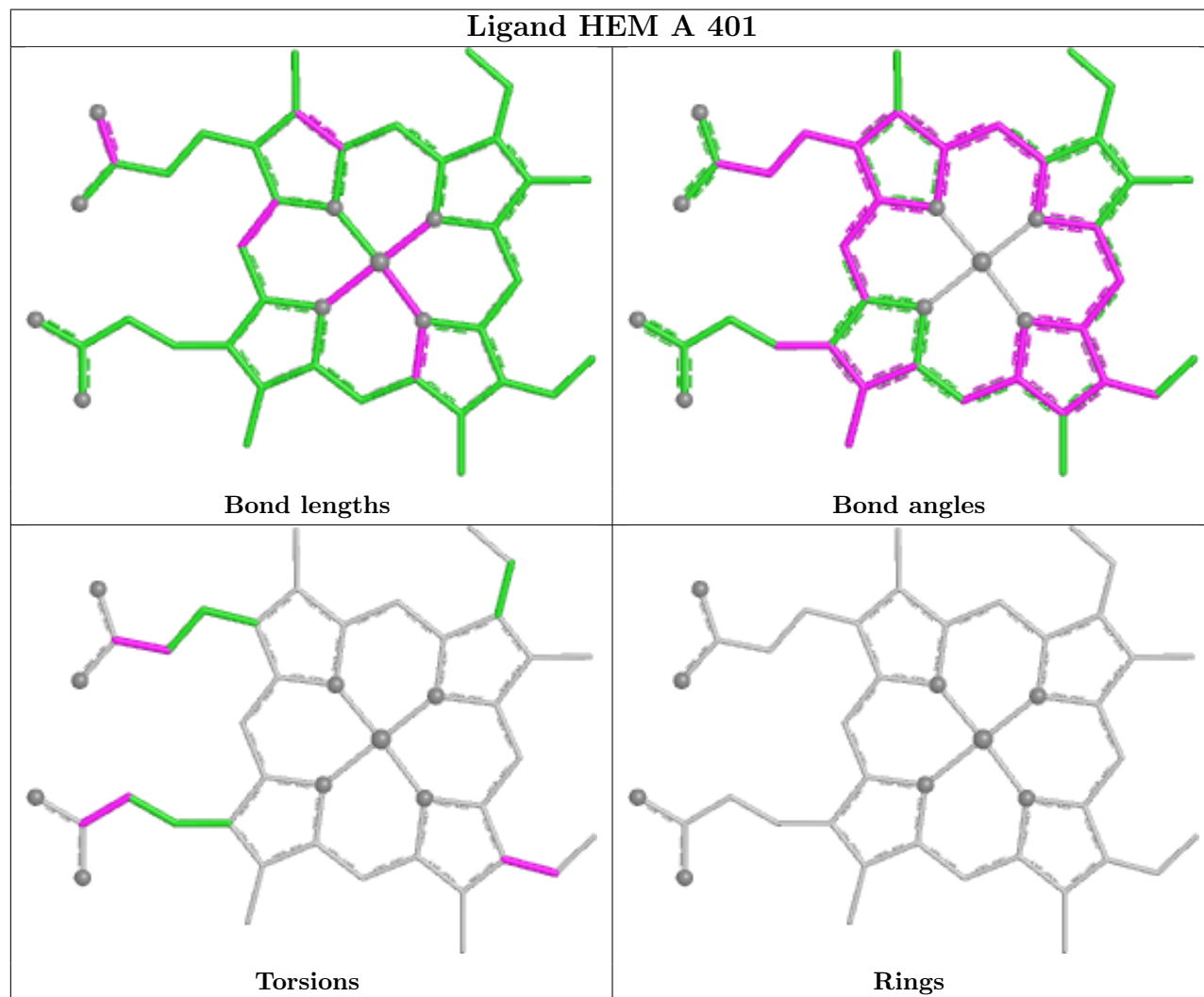
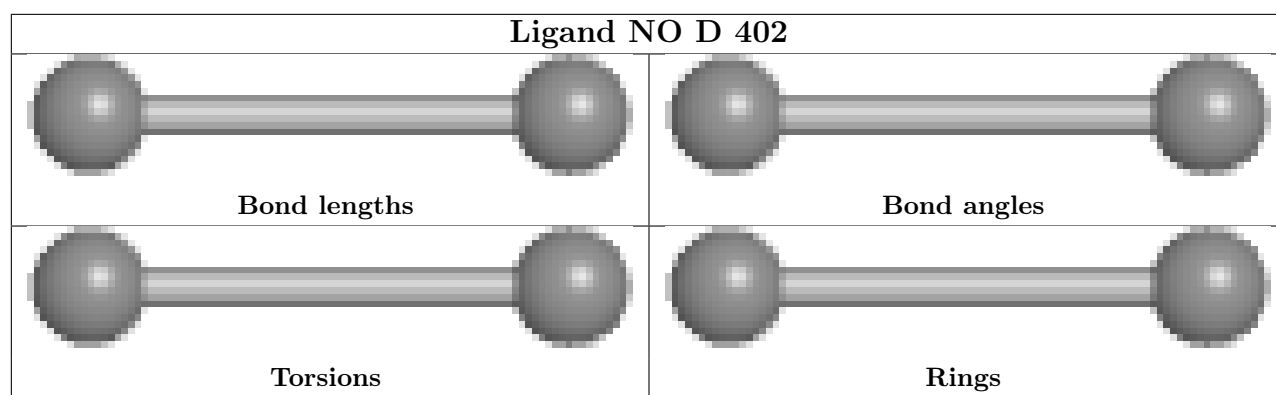
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

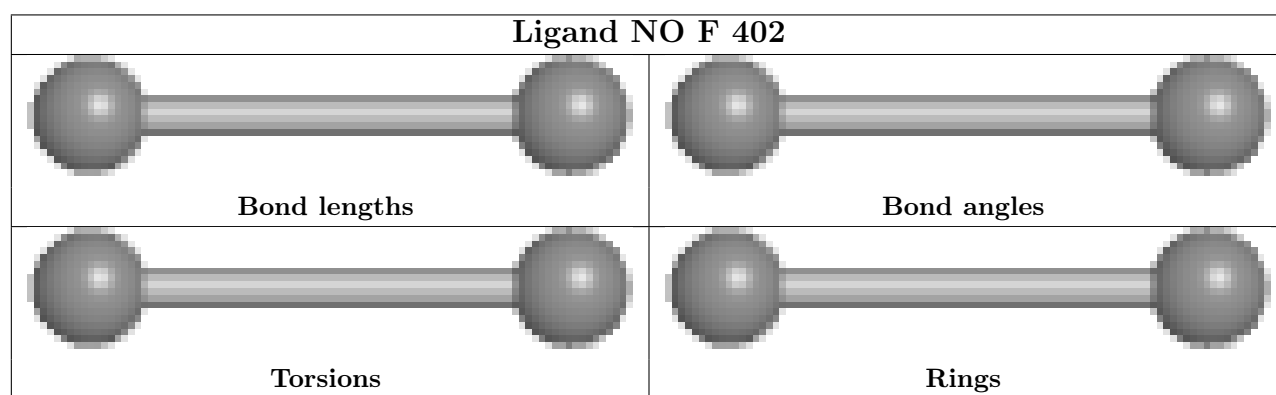
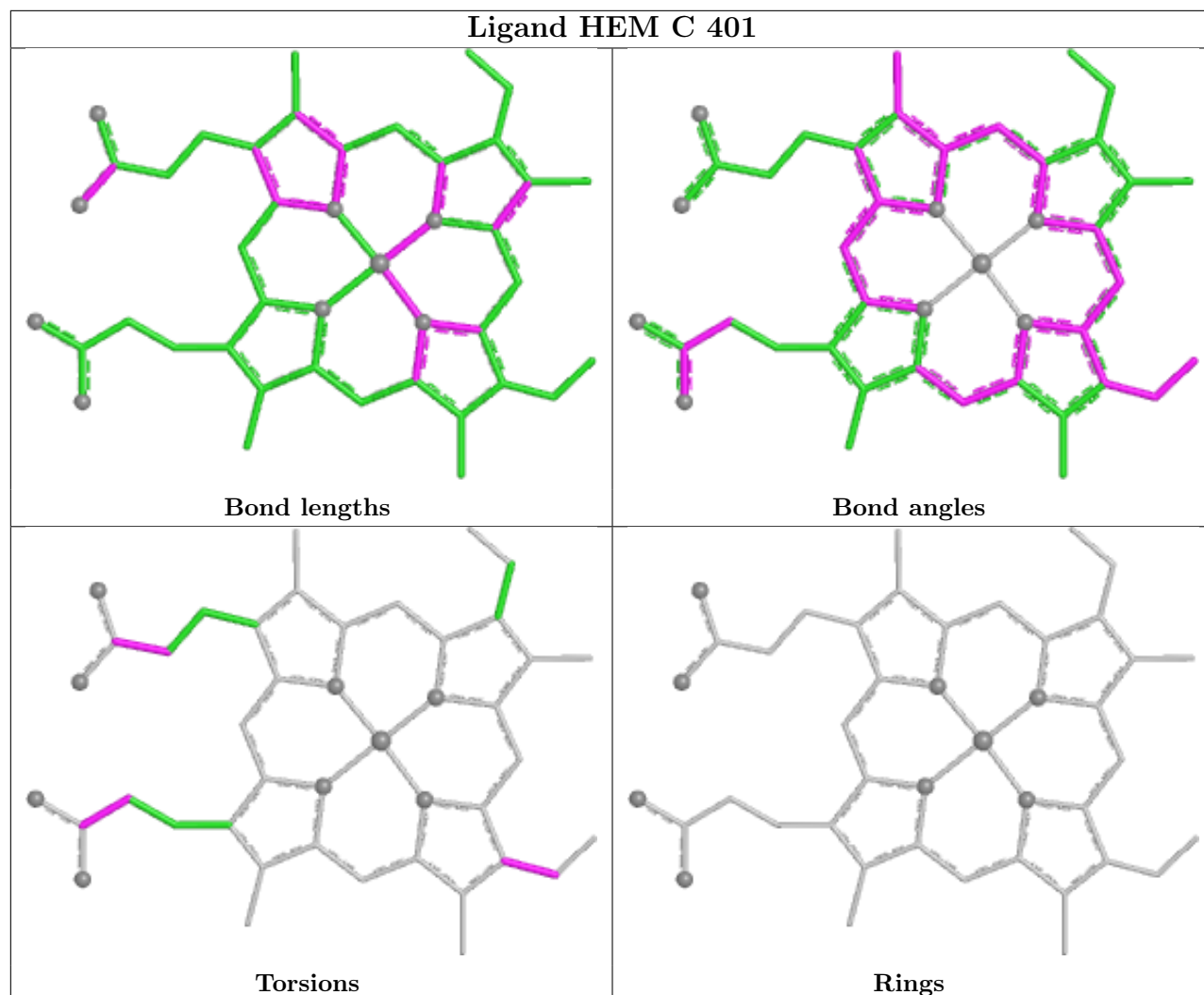
equivalents in the CSD to analyse the geometry.

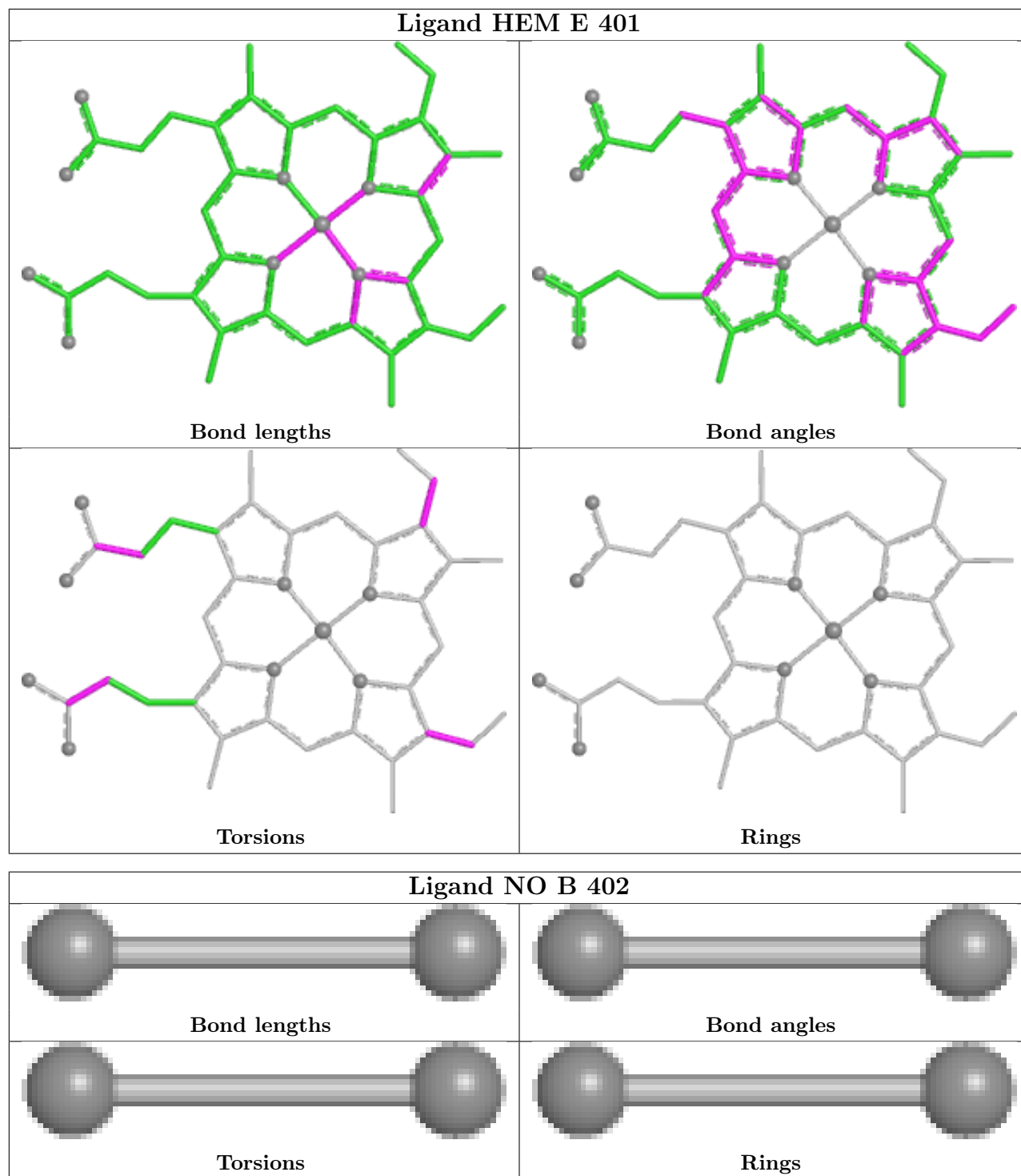


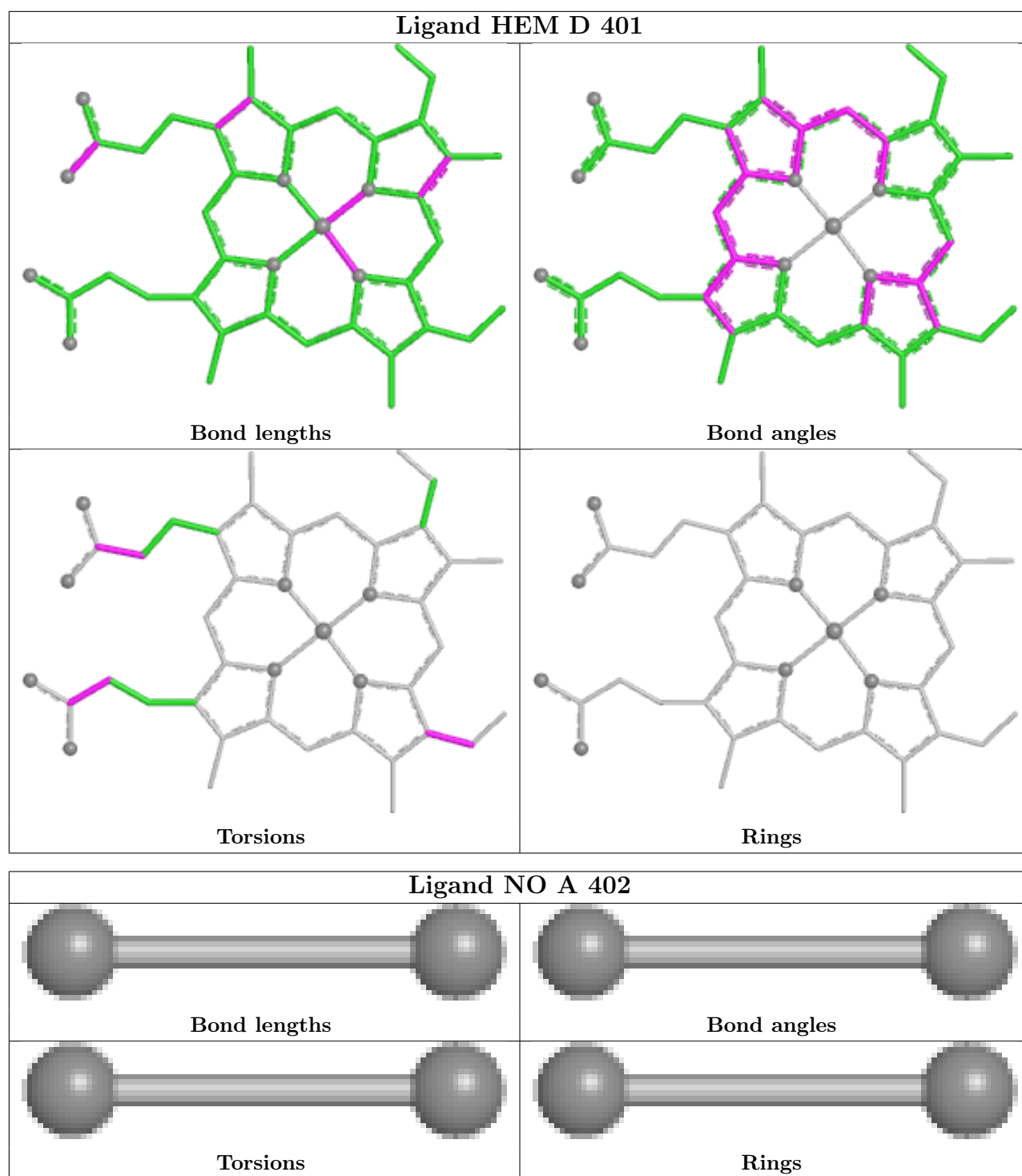












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	306/306 (100%)	0.15	19 (6%)	26	31	6, 16, 39, 75	3 (0%)
1	B	306/306 (100%)	0.67	38 (12%)	8	10	9, 23, 48, 92	1 (0%)
1	C	306/306 (100%)	0.56	29 (9%)	14	15	8, 21, 49, 86	5 (1%)
1	D	305/306 (99%)	0.26	23 (7%)	20	23	7, 17, 42, 77	7 (2%)
1	E	305/306 (99%)	0.35	24 (7%)	18	22	6, 19, 43, 88	5 (1%)
1	F	305/306 (99%)	0.73	36 (11%)	9	11	9, 23, 48, 89	3 (0%)
All	All	1833/1836 (99%)	0.45	169 (9%)	14	16	6, 20, 46, 92	24 (1%)

All (169) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	312	LEU	9.2
1	E	312	LEU	5.7
1	B	312	LEU	5.5
1	C	234	PRO	5.3
1	D	8	PRO	5.1
1	F	76	SER	4.9
1	B	233	GLY	4.6
1	F	282	ALA	4.6
1	F	234	PRO	4.5
1	B	234	PRO	4.4
1	C	312	LEU	4.3
1	C	7	GLU	4.2
1	E	234	PRO	4.1
1	F	8	PRO	4.1
1	E	8	PRO	4.1
1	E	170	ALA	4.0
1	F	93	VAL	4.0
1	F	312	LEU	4.0
1	B	76	SER	3.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	77	GLY	3.9
1	F	239	LEU	3.9
1	C	236	GLY	3.9
1	B	8	PRO	3.8
1	C	8	PRO	3.7
1	B	239	LEU	3.6
1	F	218	ASP	3.6
1	F	231	VAL	3.5
1	C	170	ALA	3.5
1	C	237	SER	3.5
1	E	233	GLY	3.4
1	F	236	GLY	3.4
1	C	218	ASP	3.4
1	D	234	PRO	3.4
1	B	236	GLY	3.3
1	E	237	SER	3.3
1	E	282	ALA	3.3
1	A	219	VAL	3.3
1	E	219	VAL	3.3
1	C	78	ALA	3.3
1	A	216	SER	3.2
1	D	238	ASP	3.2
1	A	312	LEU	3.2
1	F	77	GLY	3.2
1	F	219	VAL	3.2
1	B	237	SER	3.2
1	D	232	THR	3.2
1	C	93	VAL	3.2
1	F	216	SER	3.2
1	C	232	THR	3.1
1	C	233	GLY	3.1
1	D	77	GLY	3.1
1	C	239	LEU	3.1
1	E	239	LEU	3.1
1	F	30	SER	3.1
1	B	218	ASP	3.0
1	E	218	ASP	3.0
1	A	234	PRO	3.0
1	B	219	VAL	3.0
1	B	55	GLN	3.0
1	C	55	GLN	3.0
1	B	232	THR	2.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	78	ALA	2.9
1	D	170	ALA	2.9
1	C	173	PRO	2.9
1	F	279	LEU	2.9
1	B	235	ASP	2.8
1	B	238	ASP	2.8
1	F	233	GLY	2.8
1	A	217	ASP	2.8
1	C	231	VAL	2.8
1	F	170	ALA	2.8
1	E	78	ALA	2.7
1	D	311	ASP	2.7
1	B	279	LEU	2.7
1	B	30	SER	2.7
1	E	283	SER	2.7
1	E	232	THR	2.7
1	A	8	PRO	2.7
1	A	310	GLU	2.6
1	B	231	VAL	2.6
1	C	235	ASP	2.6
1	C	76	SER	2.6
1	A	218	ASP	2.6
1	B	176	ALA	2.6
1	B	75	PHE	2.6
1	B	210	MET	2.5
1	F	127	ARG	2.5
1	F	285	PRO	2.5
1	B	81	ALA	2.5
1	A	55	GLN	2.5
1	E	235	ASP	2.5
1	B	7	GLU	2.5
1	D	9	GLU	2.5
1	D	219	VAL	2.5
1	E	284	ALA	2.5
1	F	78	ALA	2.5
1	A	283	SER	2.5
1	D	76	SER	2.5
1	D	239	LEU	2.5
1	B	163	ARG	2.5
1	D	231	VAL	2.5
1	B	282	ALA	2.4
1	E	236	GLY	2.4

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	F	89	LEU	2.4
1	B	216	SER	2.4
1	B	31	GLY	2.4
1	C	279	LEU	2.4
1	D	237	SER	2.4
1	F	283	SER	2.4
1	F	87	ARG	2.4
1	B	170	ALA	2.4
1	E	222	ALA	2.4
1	F	81	ALA	2.4
1	D	56	PRO	2.4
1	F	92	PRO	2.4
1	B	127	ARG	2.4
1	F	199	GLU	2.4
1	F	284	ALA	2.3
1	F	90	ASP	2.3
1	A	127	ARG	2.3
1	C	92	PRO	2.3
1	C	30	SER	2.3
1	E	310	GLU	2.3
1	D	217	ASP	2.3
1	F	217	ASP	2.3
1	F	269	VAL	2.3
1	A	7	GLU	2.3
1	E	217	ASP	2.3
1	A	92	PRO	2.3
1	A	311	ASP	2.3
1	B	311	ASP	2.3
1	F	232	THR	2.3
1	F	164	ARG	2.3
1	C	311	ASP	2.2
1	D	235	ASP	2.2
1	E	311	ASP	2.2
1	B	308	PHE	2.2
1	D	310	GLU	2.2
1	B	78	ALA	2.2
1	B	281	THR	2.2
1	D	75	PHE	2.2
1	A	237	SER	2.2
1	E	238	ASP	2.2
1	C	174	ALA	2.2
1	A	236	GLY	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	30	SER	2.2
1	B	77	GLY	2.1
1	F	311	ASP	2.1
1	B	92	PRO	2.1
1	B	87	ARG	2.1
1	D	37	ARG	2.1
1	A	56	PRO	2.1
1	B	173	PRO	2.1
1	C	238	ASP	2.1
1	C	282	ALA	2.1
1	C	95	ARG	2.1
1	D	55	GLN	2.1
1	F	237	SER	2.1
1	D	218	ASP	2.1
1	C	219	VAL	2.0
1	F	95	ARG	2.0
1	B	24	LEU	2.0
1	E	307	ASP	2.0
1	F	238	ASP	2.0
1	C	91	GLY	2.0
1	B	164	ARG	2.0
1	E	127	ARG	2.0
1	E	55	GLN	2.0
1	A	239	LEU	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](#)

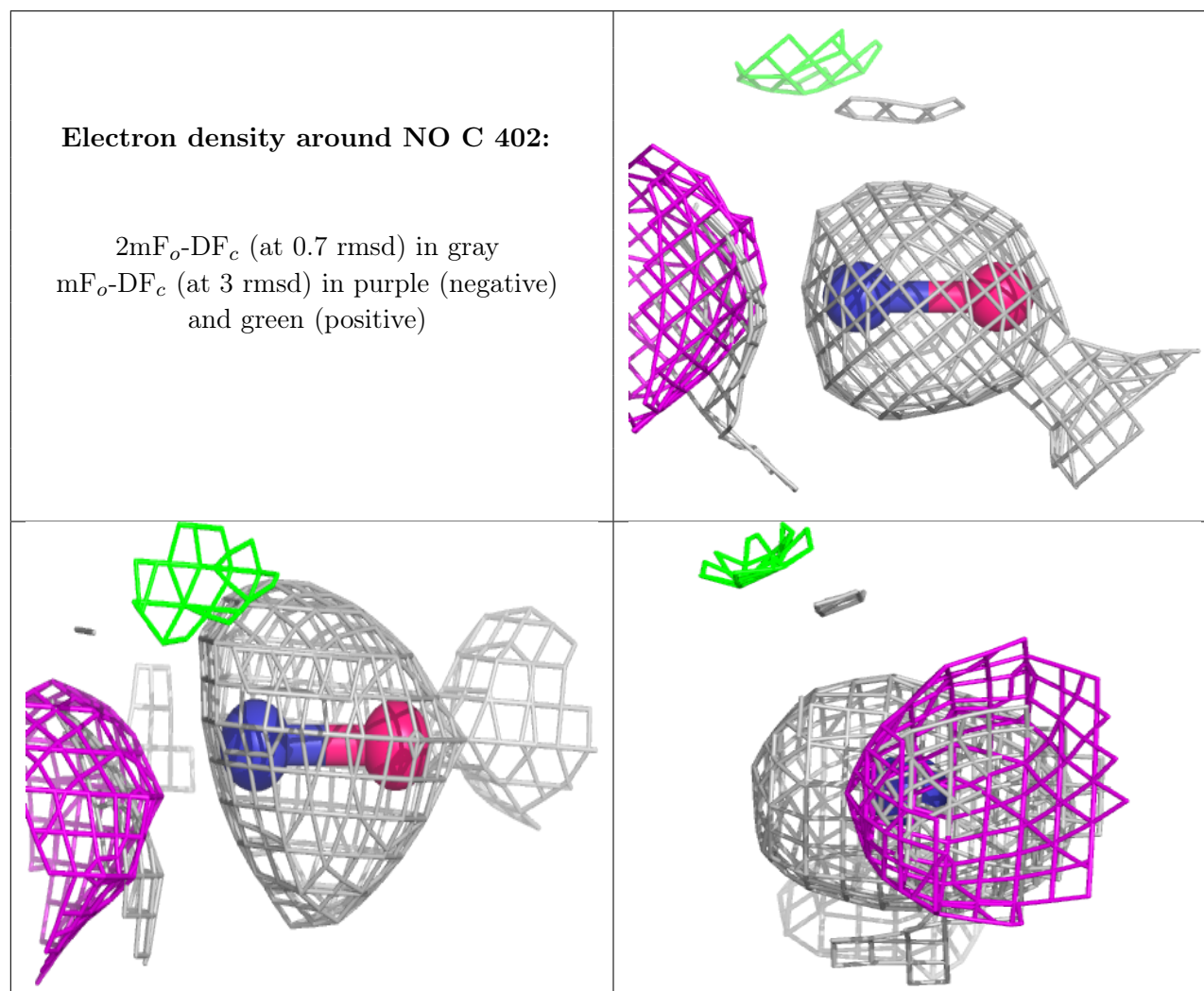
There are no oligosaccharides in this entry.

## 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, 95<sup>th</sup> 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.

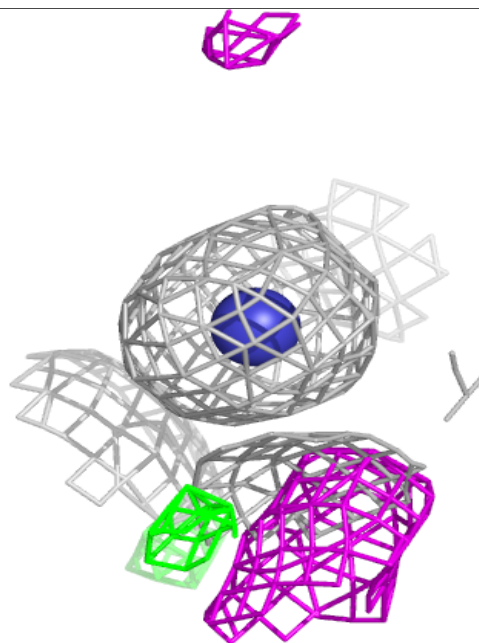
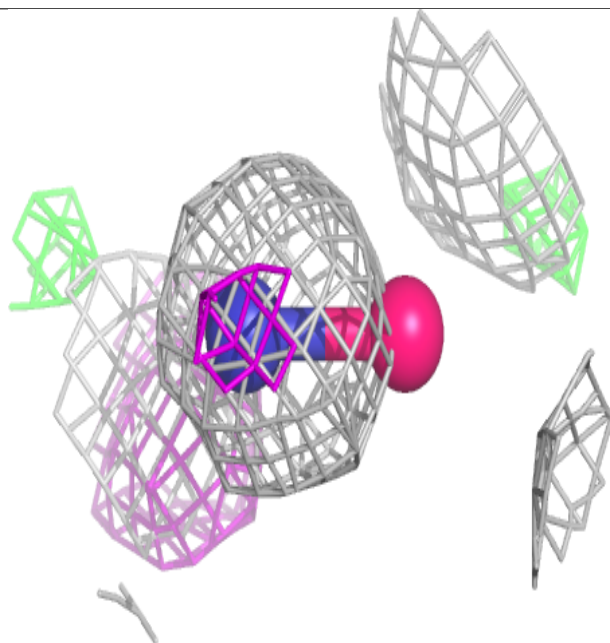
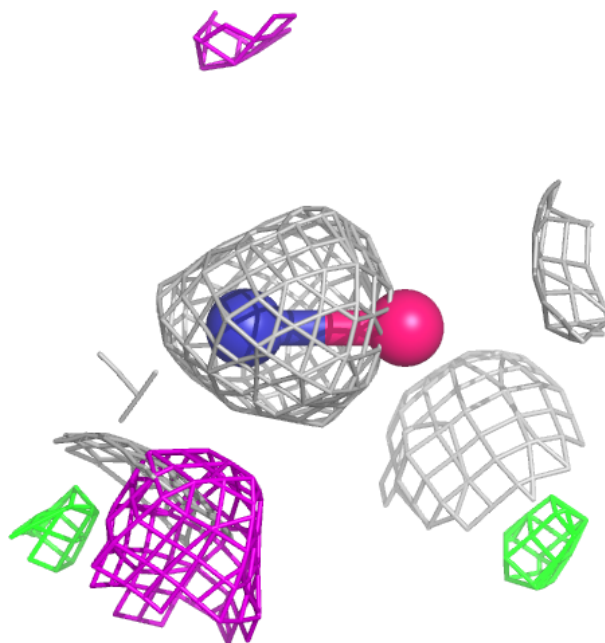
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NO	C	402	2/2	0.88	0.20	37,37,37,46	0
3	NO	F	402	2/2	0.88	0.32	37,37,37,63	0
3	NO	B	402	2/2	0.90	0.25	42,42,42,51	0
3	NO	E	402	2/2	0.93	0.22	37,37,37,41	0
3	NO	A	402	2/2	0.93	0.26	35,35,35,38	0
2	HEM	F	401	43/43	0.97	0.08	16,19,23,28	0
3	NO	D	402	2/2	0.97	0.13	37,37,37,40	0
2	HEM	B	401	43/43	0.98	0.06	13,15,21,28	0
2	HEM	C	401	43/43	0.98	0.07	14,18,22,27	0
2	HEM	A	401	43/43	0.98	0.06	12,16,20,26	0
2	HEM	E	401	43/43	0.99	0.05	12,14,20,22	0
2	HEM	D	401	43/43	0.99	0.05	10,12,18,22	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.



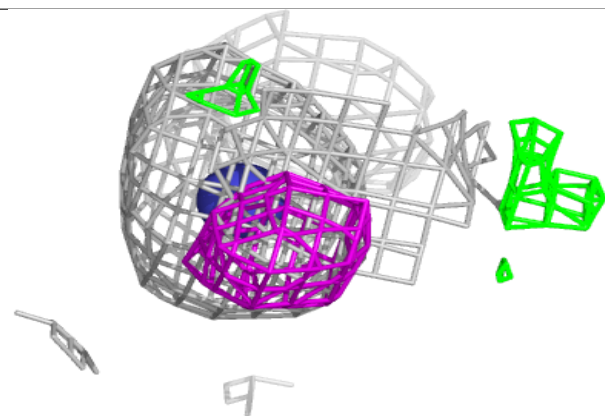
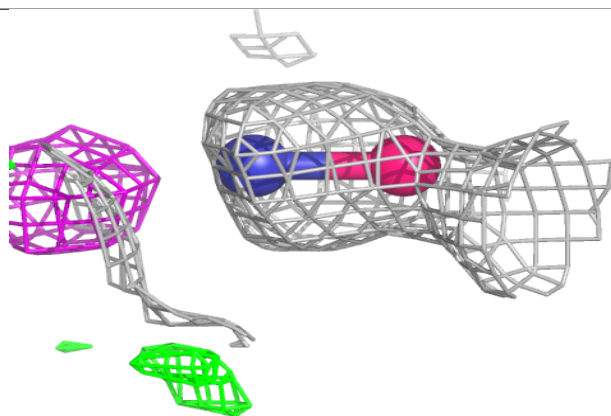
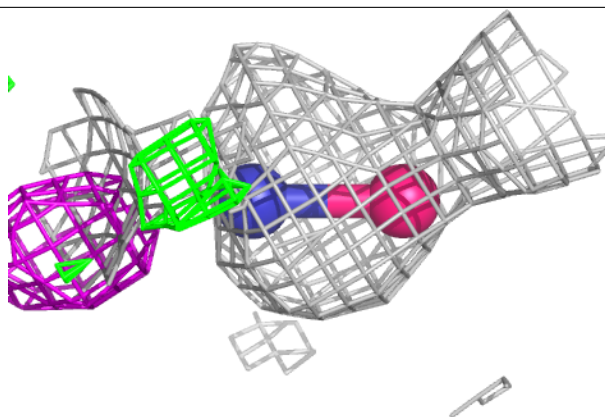
**Electron density around NO F 402:**

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



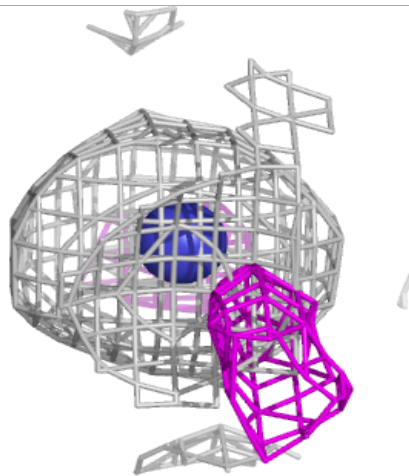
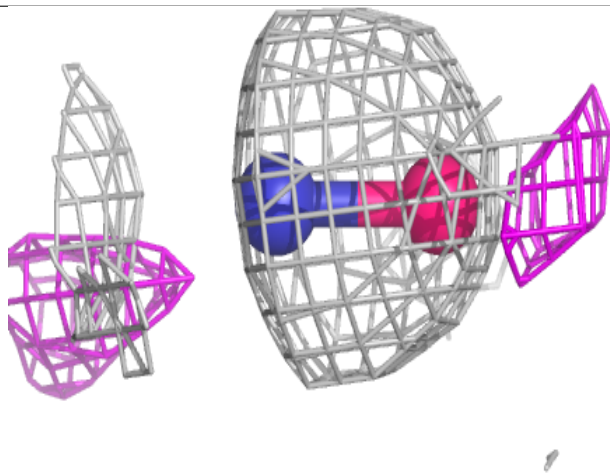
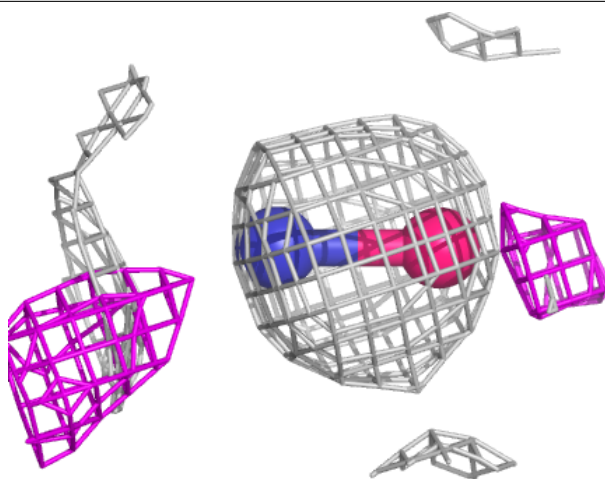
**Electron density around NO B 402:**

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



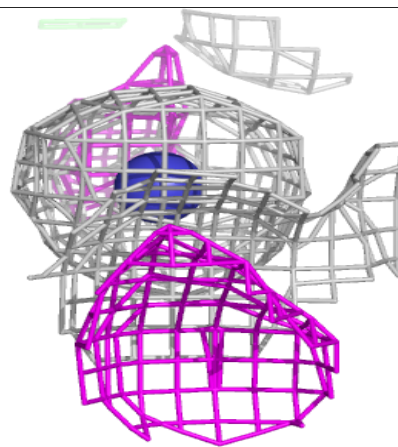
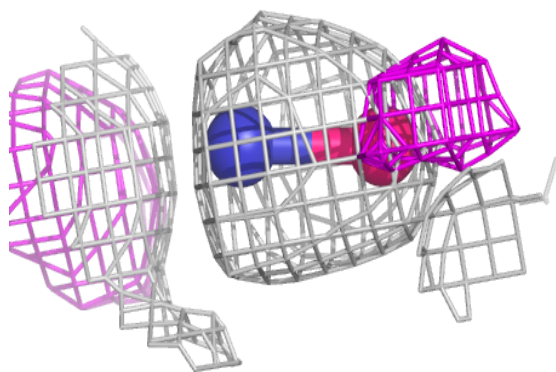
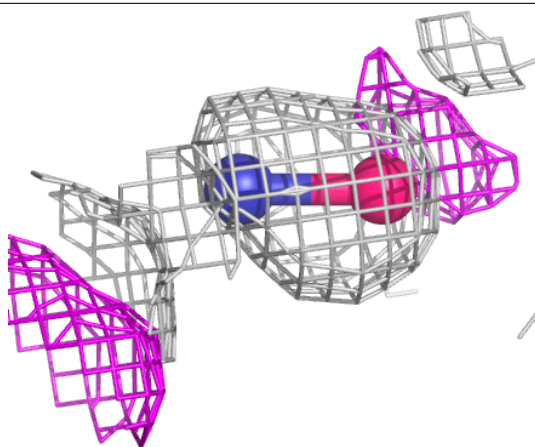
**Electron density around NO E 402:**

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



**Electron density around NO A 402:**

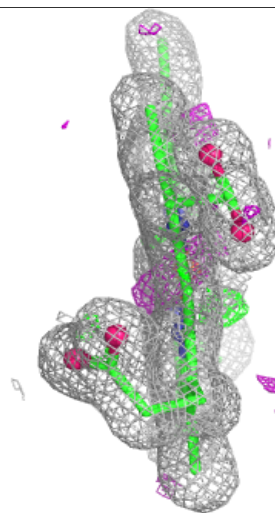
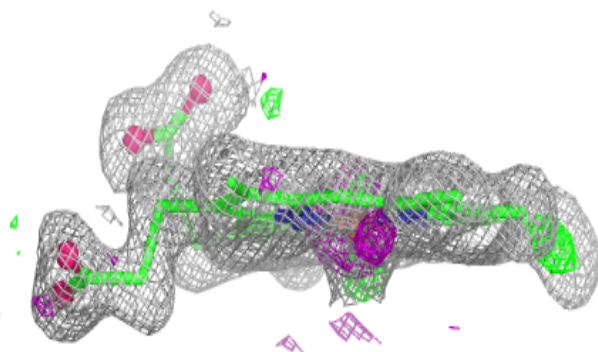
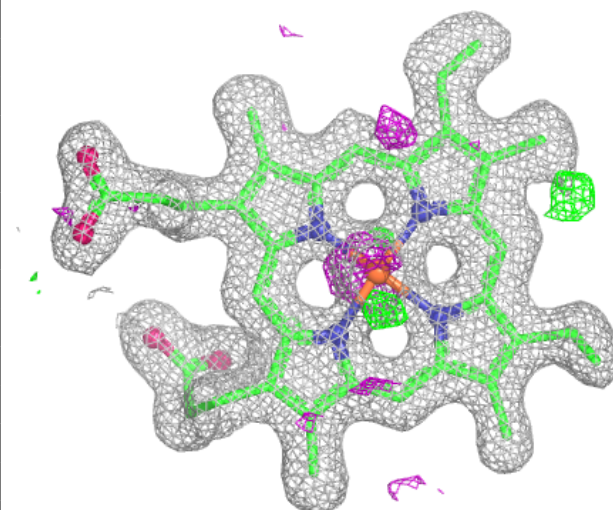
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around HEM F 401:**

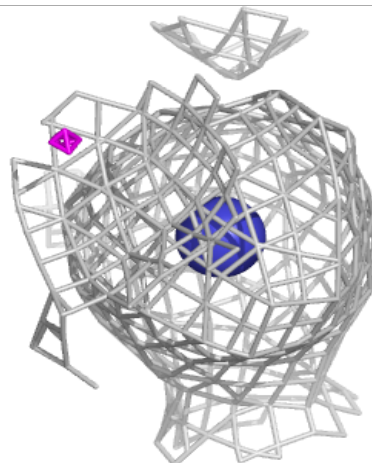
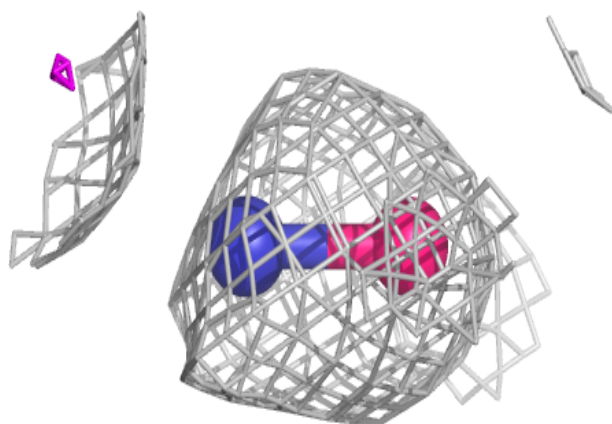
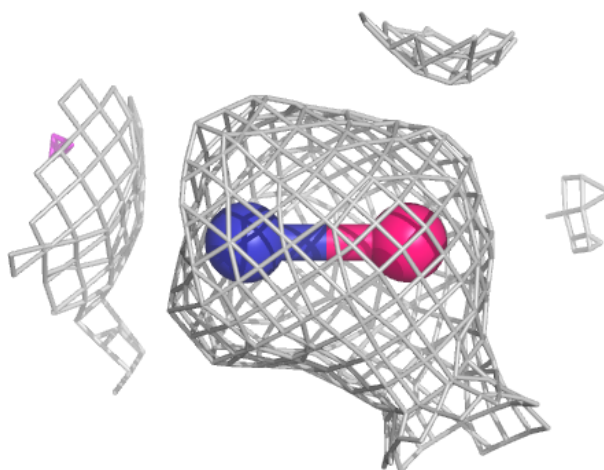
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





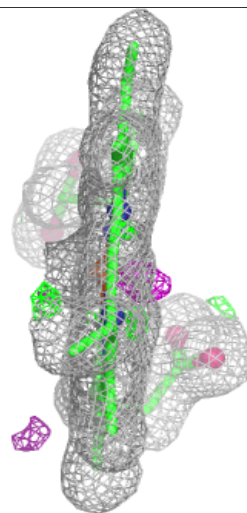
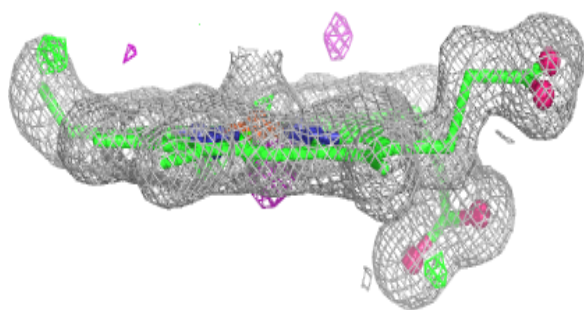
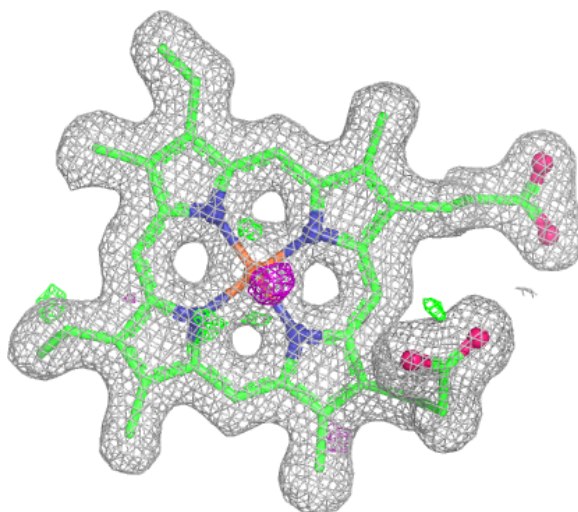
**Electron density around NO D 402:**

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



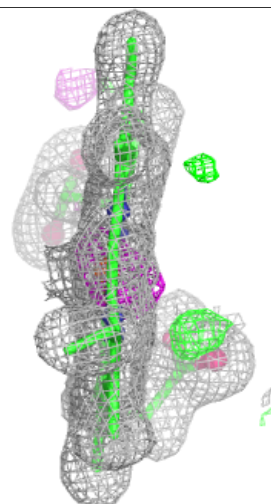
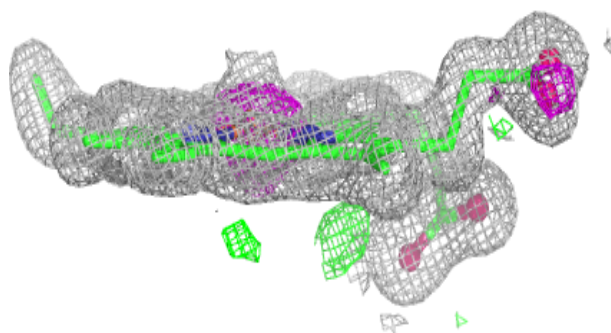
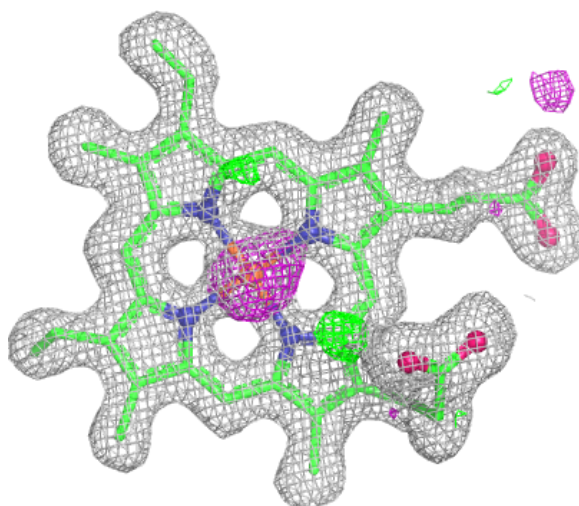
**Electron density around HEM B 401:**

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



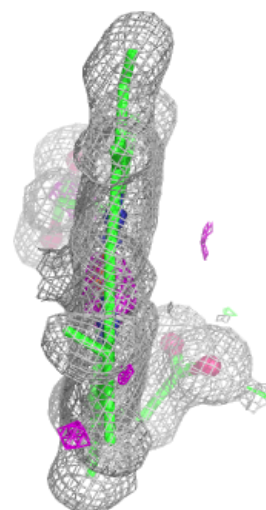
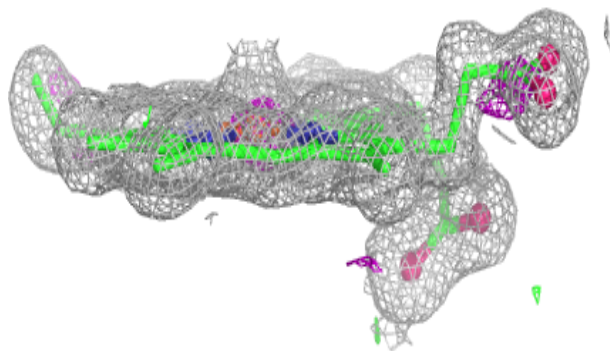
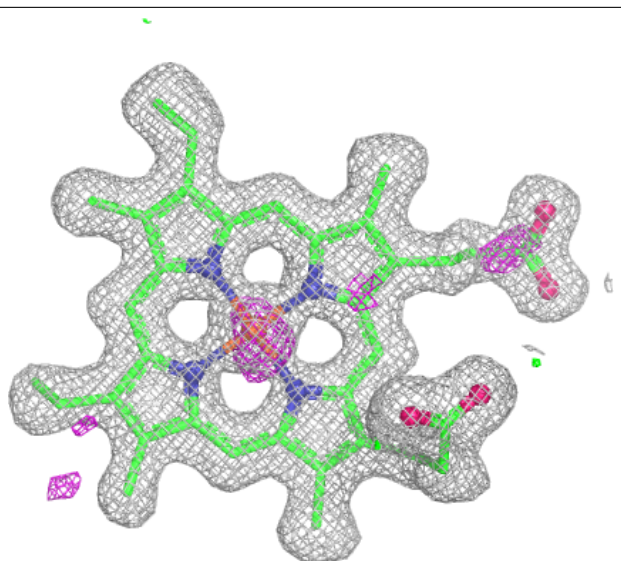
**Electron density around HEM C 401:**

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



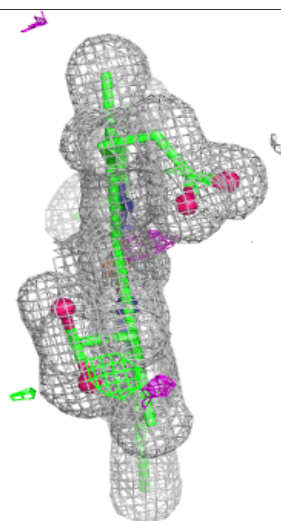
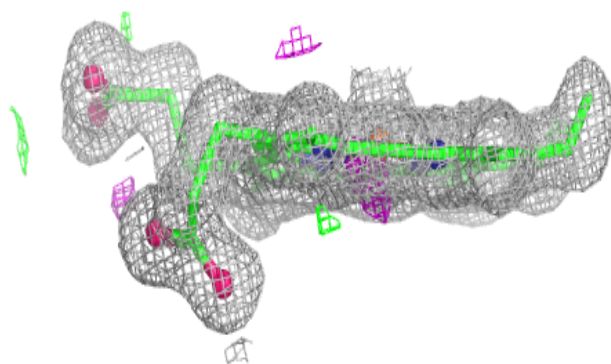
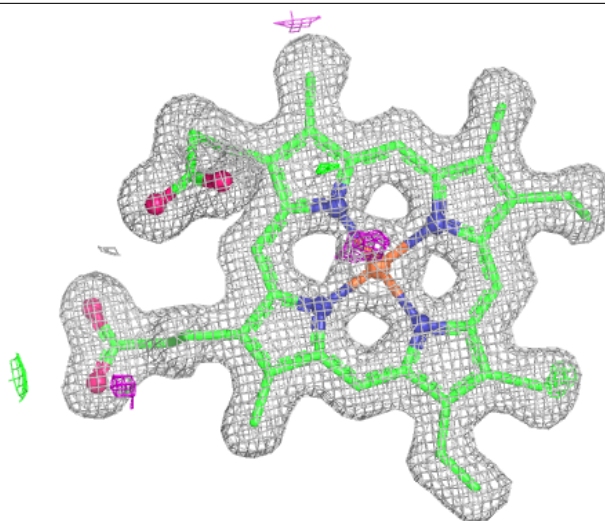
**Electron density around HEM A 401:**

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



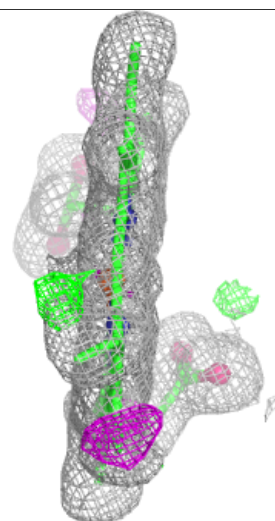
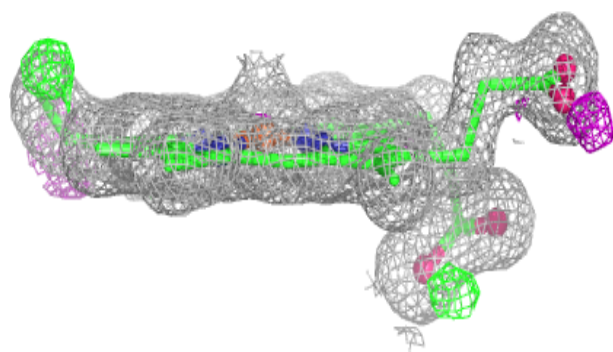
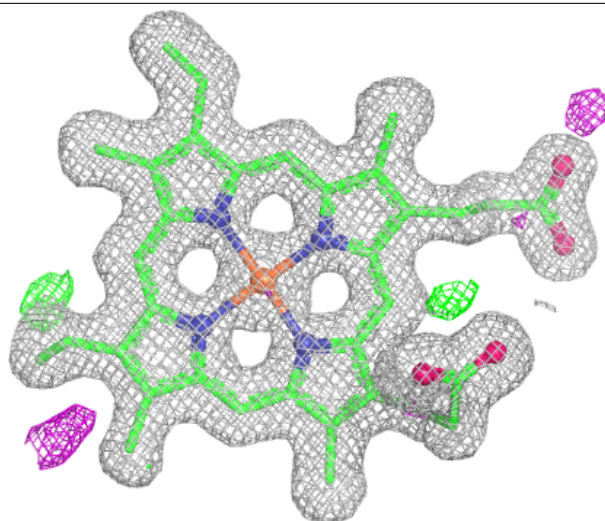
**Electron density around HEM E 401:**

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



**Electron density around HEM D 401:**

$2mF_o-DF_c$  (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.