



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 25, 2025 – 01:57 am BST

PDB ID : 9IA9 / pdb\_00009ia9  
Title : DtpB in complex with photocaged nitric oxide, 1.24 s, 8.05 microjoule, SSX  
Authors : Smyth, P.; Williams, L.J.; Hough, M.A.; Worrall, J.A.R.; Owen, R.L.  
Deposited on : 2025-02-08  
Resolution : 2.40 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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0rc1  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.45.1

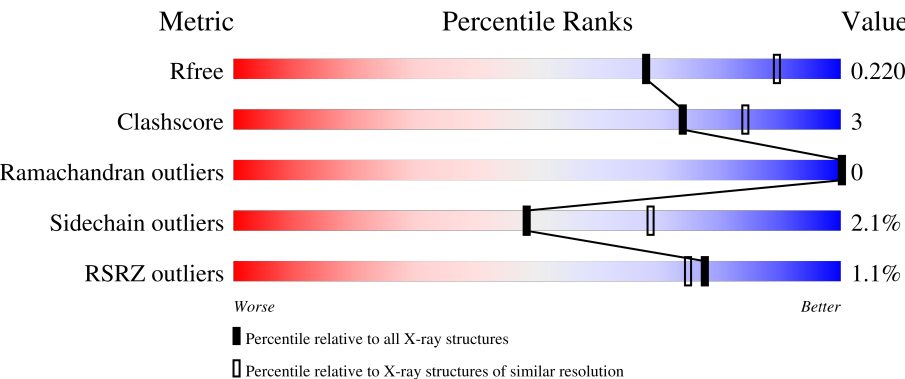
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
$R_{free}$	164625	4642 (2.40-2.40)
Clashscore	180529	5218 (2.40-2.40)
Ramachandran outliers	177936	5158 (2.40-2.40)
Sidechain outliers	177891	5159 (2.40-2.40)
RSRZ outliers	164620	4642 (2.40-2.40)

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	329	
1	B	329	
1	C	329	
1	D	329	
1	E	329	

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Mol	Chain	Length	Quality of chain
1	F	329	<div><div><div>%</div><div><div></div></div><div>84%</div><div>9%</div><div>• 7%</div></div></div>

## 2 Entry composition [i](#)

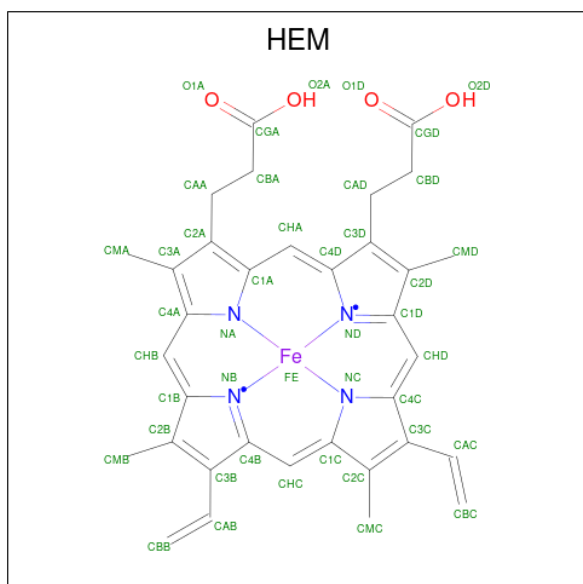
There are 4 unique types of molecules in this entry. The entry contains 15077 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

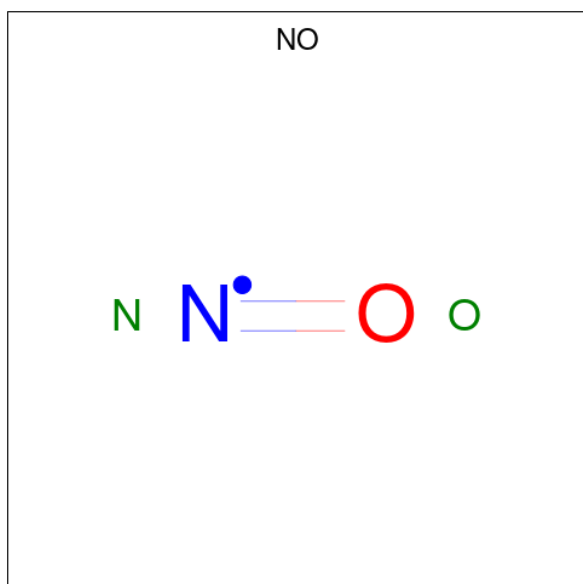
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	F	307	Total	C	N	O	S	0	7	1
			2392	1498	415	469	10			
1	A	306	Total	C	N	O	S	0	9	0
			2425	1518	424	472	11			
1	B	306	Total	C	N	O	S	0	3	0
			2359	1483	411	456	9			
1	C	307	Total	C	N	O	S	0	6	0
			2387	1495	412	471	9			
1	D	306	Total	C	N	O	S	0	8	0
			2405	1508	420	467	10			
1	E	305	Total	C	N	O	S	0	7	0
			2382	1495	412	466	9			

- 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	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	E	1	Total	C	Fe	N	O	0	0
			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	F	1	Total	N	O	0	0
			2	1	1		
3	A	1	Total	N	O	0	0
			2	1	1		
3	B	1	Total	N	O	0	0
			2	1	1		
3	C	1	Total	N	O	0	0
			2	1	1		
3	D	1	Total	N	O	0	0
			2	1	1		

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


- Molecule 4 is water.

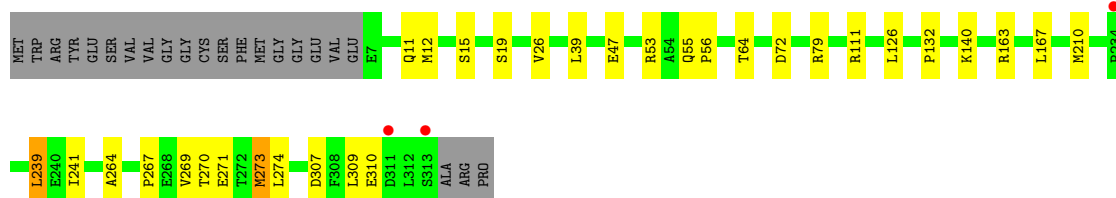
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	F	82	Total	O	0	0
			82	82		
4	A	91	Total	O	0	0
			91	91		
4	B	64	Total	O	0	0
			64	64		
4	C	58	Total	O	0	0
			58	58		
4	D	104	Total	O	0	0
			104	104		
4	E	58	Total	O	0	0
			58	58		

### 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.

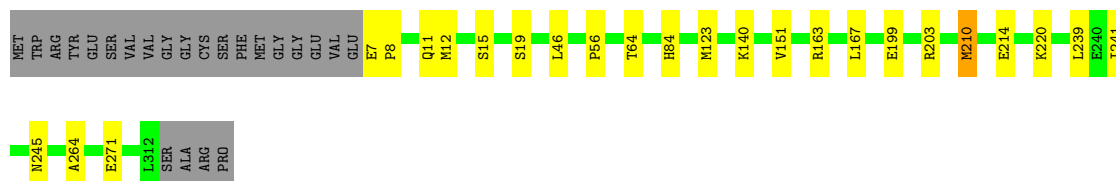
- Molecule 1: Dyp-type peroxidase family

Chain F: 




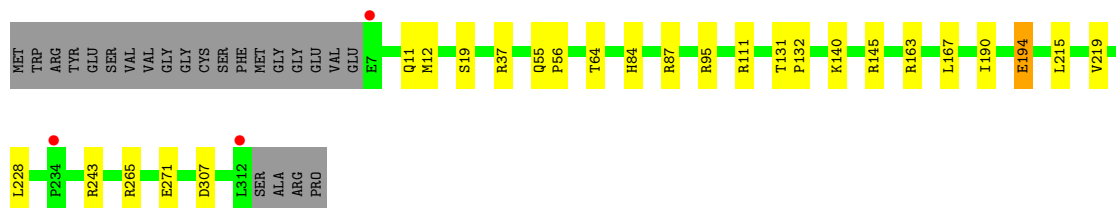
- Molecule 1: Dyp-type peroxidase family

Chain A: 




- Molecule 1: Dyp-type peroxidase family

Chain B: 



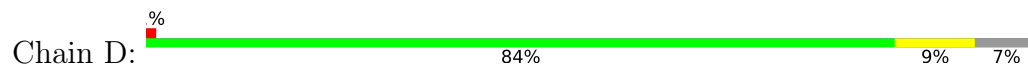
- Molecule 1: Dyp-type peroxidase family

Chain C: 

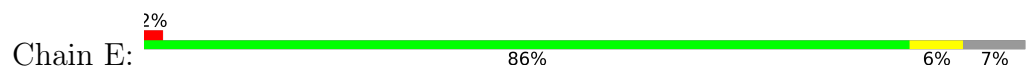




- Molecule 1: Dyp-type peroxidase family



- 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, $\alpha$ , $\beta$ , $\gamma$	87.10Å 122.91Å 195.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	79.66 – 2.40 79.66 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (79.66-2.40) 99.9 (79.66-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.04 (at 2.40Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, $R_{free}$	0.177 , 0.220 0.177 , 0.220	Depositor DCC
$R_{free}$ test set	4175 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.9	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 40.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	15077	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% 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 [i](#)

### 5.1 Standard geometry [i](#)

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	0.45	0/2475	0.98	1/3357 (0.0%)
1	B	0.46	0/2409	1.01	0/3271
1	C	0.46	0/2437	1.02	2/3310 (0.1%)
1	D	0.46	0/2454	0.98	1/3329 (0.0%)
1	E	0.45	0/2431	0.99	0/3299
1	F	0.45	0/2442	0.99	1/3315 (0.0%)
All	All	0.45	0/14648	0.99	5/19881 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	55	GLN	CB-CA-C	7.04	120.47	109.42
1	C	219	VAL	N-CA-C	-6.74	107.31	113.71
1	A	56	PRO	N-CA-CB	-6.00	96.00	102.60
1	D	56	PRO	N-CA-CB	-5.79	96.23	102.60
1	F	56	PRO	N-CA-CB	-5.30	96.77	102.60

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	2425	0	2341	15	0
1	B	2359	0	2280	13	0
1	C	2387	0	2296	12	0
1	D	2405	0	2326	19	0
1	E	2382	0	2300	11	0
1	F	2392	0	2305	17	0
2	A	43	0	30	0	0
2	B	43	0	30	2	0
2	C	43	0	30	0	0
2	D	43	0	30	1	0
2	E	43	0	30	0	0
2	F	43	0	30	1	0
3	A	2	0	0	1	0
3	B	2	0	0	1	0
3	C	2	0	0	0	0
3	D	2	0	0	1	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
4	A	91	0	0	0	2
4	B	64	0	0	0	0
4	C	58	0	0	0	0
4	D	104	0	0	4	2
4	E	58	0	0	0	0
4	F	82	0	0	0	0
All	All	15077	0	14028	86	2

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

All (86) 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:D:26:VAL:HG11	1:D:123:MET:HE1	1.60	0.84
1:E:11:GLN:HE22	1:E:64:THR:H	1.26	0.83
1:C:11:GLN:HE22	1:C:64:THR:H	1.27	0.80
1:D:11:GLN:HE22	1:D:64:THR:H	1.28	0.79
1:F:11:GLN:HE22	1:F:64:THR:H	1.32	0.77
1:A:210[B]:MET:SD	1:D:210[B]:MET:HE3	2.24	0.76
1:B:11:GLN:HE22	1:B:64:THR:H	1.37	0.71
1:A:11:GLN:HE22	1:A:64:THR:H	1.39	0.70
1:D:7:GLU:N	1:D:8:PRO:HD2	2.07	0.69
1:C:84:HIS:HE1	1:C:271:GLU:OE2	1.78	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:191:ASP:OD2	4:D:501:HOH:O	2.14	0.66
1:B:84:HIS:HE1	1:B:271:GLU:OE2	1.80	0.65
1:D:147:MET:HG2	1:D:256:PHE:HB3	1.78	0.65
1:B:37[B]:ARG:HG2	1:B:37[B]:ARG:HH11	1.63	0.63
1:D:84:HIS:HE1	1:D:271:GLU:OE2	1.81	0.63
1:A:245:ASN:ND2	3:A:402:NO:O	2.35	0.59
2:B:401:HEM:HBC2	2:B:401:HEM:HMC2	1.85	0.59
1:A:163[A]:ARG:HG3	1:A:167:LEU:HD12	1.86	0.57
1:A:12:MET:HG3	1:A:15:SER:OG	2.05	0.57
1:C:241:ILE:HG22	1:C:264:ALA:HB2	1.86	0.57
1:C:199[A]:GLU:H	1:C:199[A]:GLU:CD	2.14	0.56
1:F:26:VAL:HG12	1:F:132:PRO:HA	1.88	0.56
1:D:199:GLU:O	1:D:203[B]:ARG:HG2	2.06	0.55
1:C:19:SER:HA	1:C:140:LYS:HB2	1.89	0.55
1:E:163[A]:ARG:HG3	1:E:167:LEU:HD12	1.88	0.54
1:D:7:GLU:N	1:D:8:PRO:CD	2.72	0.53
1:C:11:GLN:NE2	1:C:64:THR:H	2.03	0.53
1:E:253[A]:ARG:HG2	1:E:253[A]:ARG:HH11	1.74	0.52
1:F:239:LEU:HB3	1:F:269:VAL:HG13	1.92	0.52
1:F:39:LEU:HD22	1:F:126:LEU:HD11	1.91	0.52
1:A:199:GLU:O	1:A:203[A]:ARG:HG3	2.09	0.52
1:B:243:ARG:NH1	3:B:402:NO:O	2.37	0.52
1:F:267:PRO:O	1:F:271:GLU:HG3	2.10	0.51
1:F:274:LEU:HD13	2:F:401:HEM:HBC2	1.91	0.51
1:C:7:GLU:HB3	1:C:8:PRO:HD3	1.91	0.51
1:C:70:ALA:O	1:C:74:LEU:HB2	2.11	0.51
1:A:214:GLU:OE2	1:A:220:LYS:NZ	2.44	0.50
1:C:199[A]:GLU:CD	1:C:199[A]:GLU:N	2.69	0.50
1:D:245:ASN:ND2	3:D:402:NO:O	2.44	0.50
1:F:270:THR:HA	1:F:273:MET:HE2	1.93	0.50
1:A:84:HIS:HE1	1:A:271:GLU:OE2	1.94	0.50
1:C:26:VAL:HG12	1:C:132:PRO:HA	1.94	0.50
1:E:123:MET:HA	1:E:123:MET:CE	2.43	0.49
1:B:37[B]:ARG:HG2	1:B:37[B]:ARG:NH1	2.27	0.48
1:B:19:SER:HA	1:B:140:LYS:HB2	1.95	0.48
1:D:307:ASP:HA	1:D:310:GLU:HG2	1.96	0.48
2:D:401:HEM:HMC2	2:D:401:HEM:HBC2	1.96	0.47
1:F:12:MET:HE3	1:F:15[B]:SER:HB2	1.95	0.47
1:D:13:VAL:HG13	1:D:263:TYR:CD1	2.49	0.47
1:F:210:MET:HE1	1:B:145:ARG:HD3	1.97	0.47
1:B:163:ARG:HG3	1:B:167:LEU:HD12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:241:ILE:HG22	1:F:264:ALA:HB2	1.99	0.45
1:E:241:ILE:HG22	1:E:264:ALA:HB2	1.97	0.45
1:D:241:ILE:HG22	1:D:264:ALA:HB2	1.99	0.44
1:E:12:MET:HG3	1:E:15:SER:HB2	2.00	0.44
1:E:79:ARG:NH2	1:E:83:LEU:O	2.51	0.44
1:F:163:ARG:HG3	1:F:167:LEU:HD12	2.00	0.44
1:A:123:MET:HG3	1:C:251:VAL:HG12	2.00	0.44
1:E:26:VAL:HG12	1:E:132:PRO:HA	2.00	0.44
1:E:163[B]:ARG:HG3	1:E:167:LEU:HD12	1.99	0.43
1:F:72:ASP:OD1	1:F:79:ARG:HD2	2.19	0.43
1:D:11:GLN:NE2	1:D:64:THR:H	2.05	0.43
1:D:147:MET:CG	1:D:256:PHE:HB3	2.47	0.43
1:F:19:SER:HA	1:F:140:LYS:HB2	2.01	0.42
1:B:131:THR:HA	1:B:132:PRO:HD3	1.92	0.42
1:F:307:ASP:HA	1:F:310:GLU:HG2	2.01	0.42
1:D:26:VAL:HG11	1:D:123:MET:CE	2.42	0.42
1:A:210[B]:MET:HG3	4:D:549:HOH:O	2.18	0.42
1:B:12:MET:HA	1:B:12:MET:HE2	2.02	0.42
1:A:11:GLN:NE2	1:A:64:THR:H	2.12	0.42
1:A:19:SER:HA	1:A:140:LYS:HB2	2.02	0.42
1:D:47:GLU:HG3	4:D:586:HOH:O	2.19	0.42
1:F:53:ARG:HG2	1:A:151:VAL:HG21	2.02	0.42
1:A:7:GLU:HA	1:A:8:PRO:HD3	1.87	0.42
1:A:241:ILE:HG22	1:A:264:ALA:HB2	2.02	0.42
1:D:11:GLN:NE2	4:D:503:HOH:O	2.52	0.42
1:F:273:MET:HE2	1:F:273:MET:HB2	1.85	0.41
1:D:302:PHE:O	1:D:304:PRO:HD3	2.21	0.41
1:E:55:GLN:N	1:E:56:PRO:CD	2.83	0.41
1:B:55:GLN:HA	1:B:56:PRO:HA	1.84	0.41
2:B:401:HEM:HBC2	2:B:401:HEM:CMC	2.49	0.41
1:C:284:ALA:HA	1:C:285:PRO:HD3	1.94	0.41
1:E:39:LEU:HD22	1:E:126:LEU:HD11	2.03	0.41
1:F:47[B]:GLU:CD	1:F:47[B]:GLU:C	2.89	0.40
1:B:190:ILE:O	1:B:194:GLU:HB2	2.22	0.40
1:B:215:LEU:HB3	1:B:219:VAL:HG23	2.03	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:567:HOH:O	4:D:501:HOH:O[4_445]	2.13	0.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:505:HOH:O	4:D:501:HOH:O[4_445]	2.15	0.05

## 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	314/329 (95%)	309 (98%)	5 (2%)	0	100	100
1	B	307/329 (93%)	299 (97%)	8 (3%)	0	100	100
1	C	311/329 (94%)	304 (98%)	7 (2%)	0	100	100
1	D	311/329 (94%)	306 (98%)	5 (2%)	0	100	100
1	E	309/329 (94%)	300 (97%)	9 (3%)	0	100	100
1	F	312/329 (95%)	303 (97%)	9 (3%)	0	100	100
All	All	1864/1974 (94%)	1821 (98%)	43 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	255/263 (97%)	250 (98%)	5 (2%)	50	70
1	B	245/263 (93%)	237 (97%)	8 (3%)	33	53
1	C	252/263 (96%)	246 (98%)	6 (2%)	44	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	253/263 (96%)	246 (97%)	7 (3%)	38	59
1	E	250/263 (95%)	245 (98%)	5 (2%)	50	70
1	F	252/263 (96%)	247 (98%)	5 (2%)	50	70
All	All	1507/1578 (96%)	1471 (98%)	36 (2%)	48	64

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	55	GLN
1	F	111	ARG
1	F	239	LEU
1	F	273	MET
1	F	309	LEU
1	A	46	LEU
1	A	210[A]	MET
1	A	210[B]	MET
1	A	210[C]	MET
1	A	239	LEU
1	B	87	ARG
1	B	95	ARG
1	B	111	ARG
1	B	194	GLU
1	B	228	LEU
1	B	265[A]	ARG
1	B	265[B]	ARG
1	B	307	ASP
1	C	46	LEU
1	C	55	GLN
1	C	87[A]	ARG
1	C	87[B]	ARG
1	C	265	ARG
1	C	311	ASP
1	D	39	LEU
1	D	114	LEU
1	D	265[A]	ARG
1	D	265[B]	ARG
1	D	268	GLU
1	D	274	LEU
1	D	279	LEU
1	E	17	LEU
1	E	114	LEU

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Mol	Chain	Res	Type
1	E	123	MET
1	E	239	LEU
1	E	274	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	11	GLN
1	F	55	GLN
1	F	84	HIS
1	A	11	GLN
1	A	84	HIS
1	A	133	GLN
1	B	11	GLN
1	B	84	HIS
1	B	133	GLN
1	C	11	GLN
1	C	84	HIS
1	C	201	GLN
1	C	286	HIS
1	D	11	GLN
1	D	84	HIS
1	D	286	HIS
1	E	11	GLN
1	E	84	HIS

### 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$
3	NO	B	402	2	0,1,1	-	-	-		
3	NO	F	402	2	0,1,1	-	-	-		
3	NO	A	402	2	0,1,1	-	-	-		
2	HEM	B	401	3,1	41,50,50	1.27	5 (12%)	45,82,82	1.65	8 (17%)
2	HEM	F	401	3,1	41,50,50	1.27	5 (12%)	45,82,82	1.64	8 (17%)
3	NO	E	402	2	0,1,1	-	-	-		
2	HEM	C	401	3,1	41,50,50	1.27	4 (9%)	45,82,82	1.67	8 (17%)
2	HEM	D	401	3,1	41,50,50	1.27	4 (9%)	45,82,82	1.65	8 (17%)
2	HEM	A	401	3,1	41,50,50	1.27	4 (9%)	45,82,82	1.72	8 (17%)
3	NO	C	402	2	0,1,1	-	-	-		
2	HEM	E	401	3,1	41,50,50	1.28	4 (9%)	45,82,82	1.68	7 (15%)
3	NO	D	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	3,1	-	6/12/54/54	-
2	HEM	F	401	3,1	-	6/12/54/54	-
2	HEM	C	401	3,1	-	6/12/54/54	-
2	HEM	D	401	3,1	-	6/12/54/54	-
2	HEM	A	401	3,1	-	6/12/54/54	-
2	HEM	E	401	3,1	-	6/12/54/54	-

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	401	HEM	C1B-NB	-3.22	1.34	1.40
2	C	401	HEM	C1B-NB	-3.15	1.34	1.40
2	B	401	HEM	C1B-NB	-3.10	1.35	1.40
2	A	401	HEM	C1B-NB	-3.09	1.35	1.40
2	F	401	HEM	C1B-NB	-3.08	1.35	1.40
2	F	401	HEM	FE-NB	2.99	2.11	1.96
2	C	401	HEM	C4D-ND	-2.97	1.35	1.40
2	B	401	HEM	FE-NB	2.96	2.11	1.96
2	A	401	HEM	FE-NB	2.95	2.11	1.96
2	D	401	HEM	FE-NB	2.94	2.11	1.96
2	B	401	HEM	C4D-ND	-2.94	1.35	1.40
2	C	401	HEM	FE-NB	2.93	2.11	1.96
2	E	401	HEM	C4D-ND	-2.93	1.35	1.40
2	D	401	HEM	C1B-NB	-2.92	1.35	1.40
2	E	401	HEM	FE-NB	2.81	2.10	1.96
2	A	401	HEM	C4D-ND	-2.80	1.35	1.40
2	D	401	HEM	C4D-ND	-2.79	1.35	1.40
2	F	401	HEM	C4D-ND	-2.67	1.35	1.40
2	D	401	HEM	CHB-C1B	2.42	1.41	1.35
2	B	401	HEM	C3B-C4B	2.32	1.49	1.44
2	A	401	HEM	CHB-C1B	2.26	1.40	1.35
2	F	401	HEM	CHB-C1B	2.16	1.40	1.35
2	E	401	HEM	CHB-C1B	2.16	1.40	1.35
2	F	401	HEM	C3B-C4B	2.13	1.49	1.44
2	B	401	HEM	CHB-C1B	2.10	1.40	1.35
2	C	401	HEM	CHB-C1B	2.10	1.40	1.35

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	401	HEM	CHC-C4B-NB	4.92	129.78	124.43
2	C	401	HEM	CHC-C4B-NB	4.82	129.67	124.43
2	D	401	HEM	CHC-C4B-NB	4.81	129.66	124.43
2	A	401	HEM	CHC-C4B-NB	4.79	129.64	124.43
2	F	401	HEM	CHC-C4B-NB	4.60	129.43	124.43
2	A	401	HEM	C1B-NB-C4B	4.05	109.26	105.07
2	B	401	HEM	C1B-NB-C4B	4.00	109.21	105.07
2	B	401	HEM	CHC-C4B-NB	3.91	128.68	124.43
2	A	401	HEM	CHD-C1D-ND	3.88	128.64	124.43
2	C	401	HEM	C1B-NB-C4B	3.85	109.05	105.07
2	D	401	HEM	C1B-NB-C4B	3.82	109.02	105.07
2	E	401	HEM	CHD-C1D-ND	3.81	128.56	124.43
2	F	401	HEM	C1B-NB-C4B	3.80	109.00	105.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	401	HEM	C1B-NB-C4B	3.74	108.94	105.07
2	C	401	HEM	CHD-C1D-ND	3.67	128.42	124.43
2	B	401	HEM	CHD-C1D-ND	3.64	128.39	124.43
2	D	401	HEM	CHD-C1D-ND	3.41	128.13	124.43
2	A	401	HEM	CHB-C1B-NB	3.25	128.40	124.38
2	F	401	HEM	CHD-C1D-ND	3.25	127.96	124.43
2	A	401	HEM	CHA-C4D-ND	3.18	128.31	124.38
2	B	401	HEM	CHB-C1B-NB	3.13	128.25	124.38
2	F	401	HEM	CHA-C4D-ND	3.08	128.19	124.38
2	C	401	HEM	CHA-C4D-ND	3.04	128.14	124.38
2	C	401	HEM	CHB-C1B-NB	2.99	128.07	124.38
2	B	401	HEM	CHA-C4D-ND	2.91	127.98	124.38
2	D	401	HEM	CHB-C1B-NB	2.91	127.98	124.38
2	E	401	HEM	CHD-C1D-C2D	-2.87	120.50	124.98
2	D	401	HEM	CHA-C4D-ND	2.86	127.92	124.38
2	E	401	HEM	CHB-C1B-NB	2.86	127.92	124.38
2	F	401	HEM	CHB-C1B-NB	2.86	127.92	124.38
2	A	401	HEM	CHD-C1D-C2D	-2.68	120.79	124.98
2	E	401	HEM	CHA-C4D-ND	2.65	127.66	124.38
2	B	401	HEM	CHD-C1D-C2D	-2.63	120.88	124.98
2	D	401	HEM	CHD-C1D-C2D	-2.49	121.09	124.98
2	C	401	HEM	CHD-C1D-C2D	-2.40	121.24	124.98
2	F	401	HEM	CHA-C4D-C3D	-2.32	120.98	125.33
2	D	401	HEM	CHA-C4D-C3D	-2.28	121.05	125.33
2	B	401	HEM	O2A-CGA-CBA	2.28	121.34	114.03
2	A	401	HEM	O2A-CGA-CBA	2.21	121.13	114.03
2	F	401	HEM	O2D-CGD-CBD	2.21	121.12	114.03
2	B	401	HEM	CHA-C4D-C3D	-2.13	121.33	125.33
2	F	401	HEM	CHD-C1D-C2D	-2.13	121.66	124.98
2	A	401	HEM	CHA-C4D-C3D	-2.10	121.39	125.33
2	C	401	HEM	CHA-C4D-C3D	-2.08	121.43	125.33
2	C	401	HEM	O2D-CGD-CBD	2.07	120.67	114.03
2	E	401	HEM	O2D-CGD-CBD	2.05	120.63	114.03
2	D	401	HEM	CMC-C2C-C3C	2.03	128.48	124.68

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	401	HEM	C2B-C3B-CAB-CBB
2	F	401	HEM	C4B-C3B-CAB-CBB
2	A	401	HEM	C2B-C3B-CAB-CBB

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

There are no ring outliers.

6 monomers are involved in 7 short contacts:

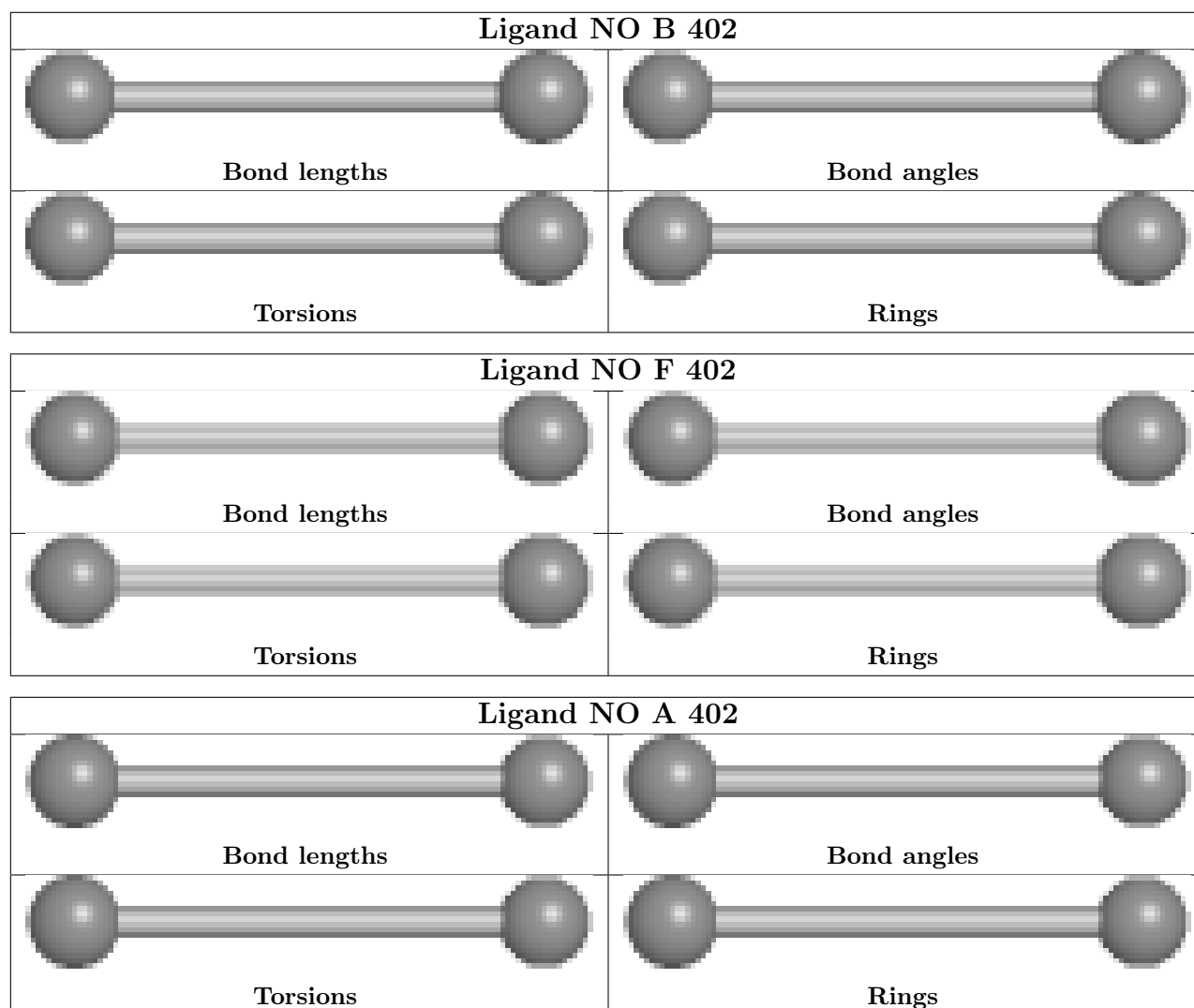
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	402	NO	1	0
3	A	402	NO	1	0
2	B	401	HEM	2	0
2	F	401	HEM	1	0

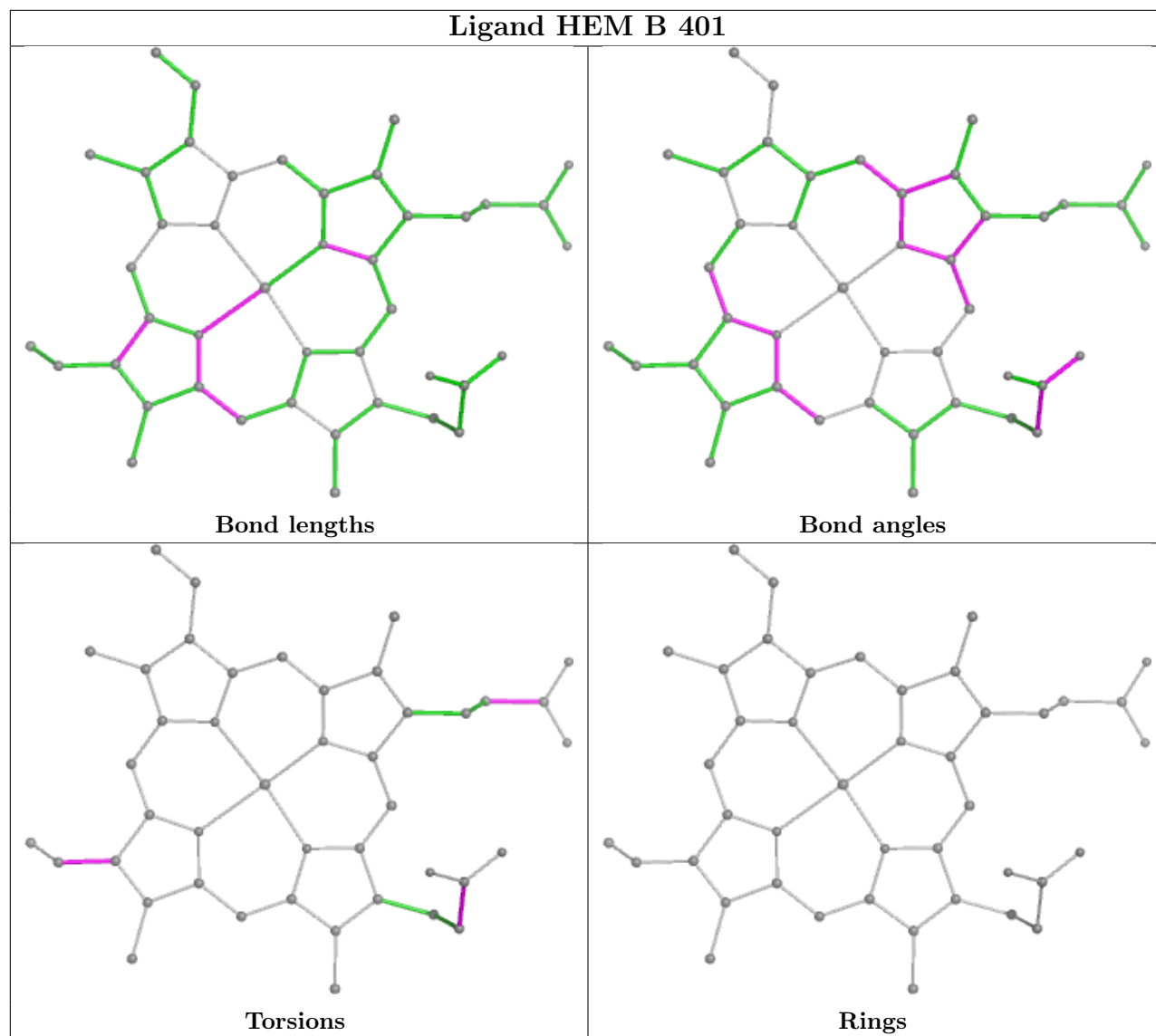
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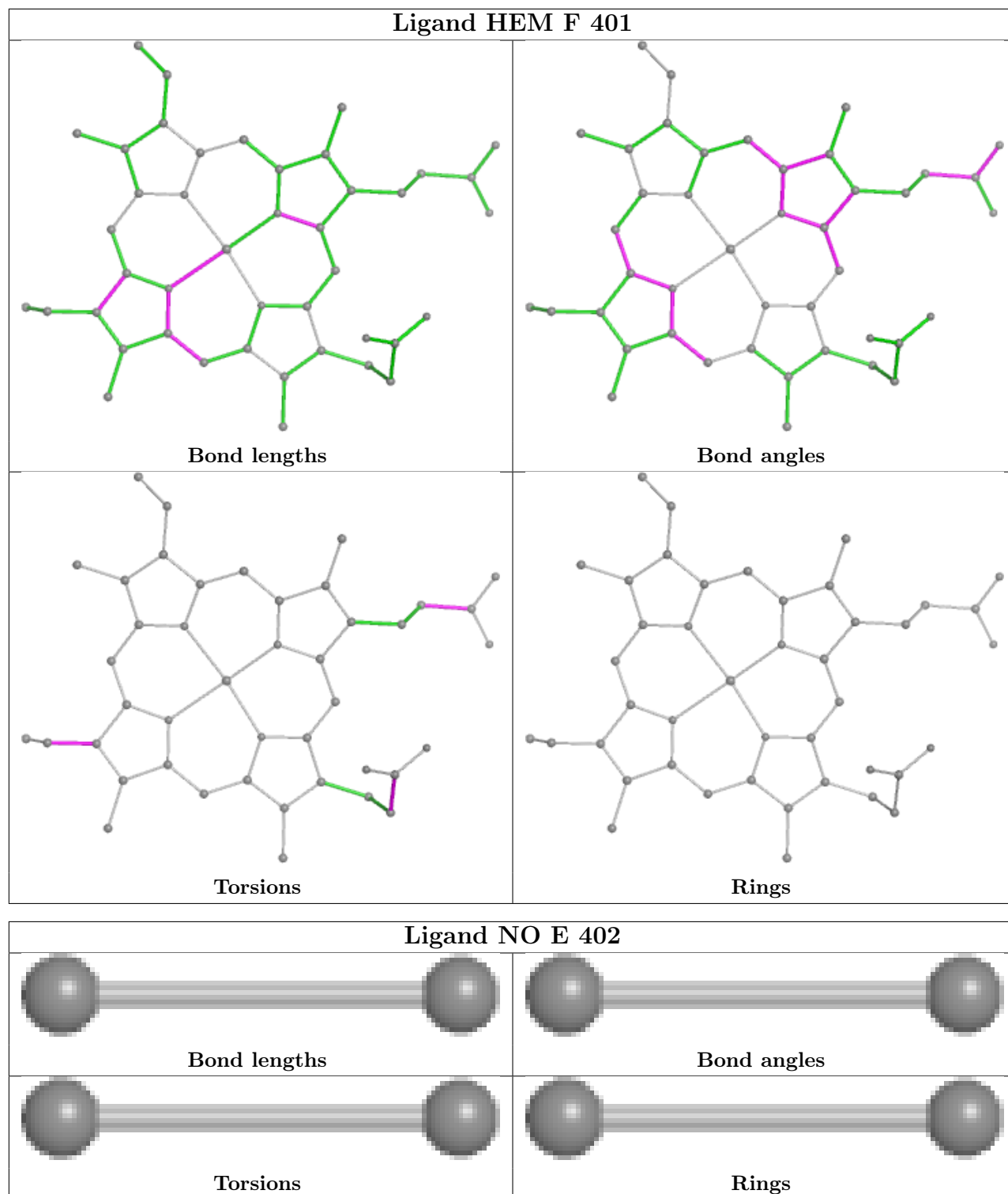
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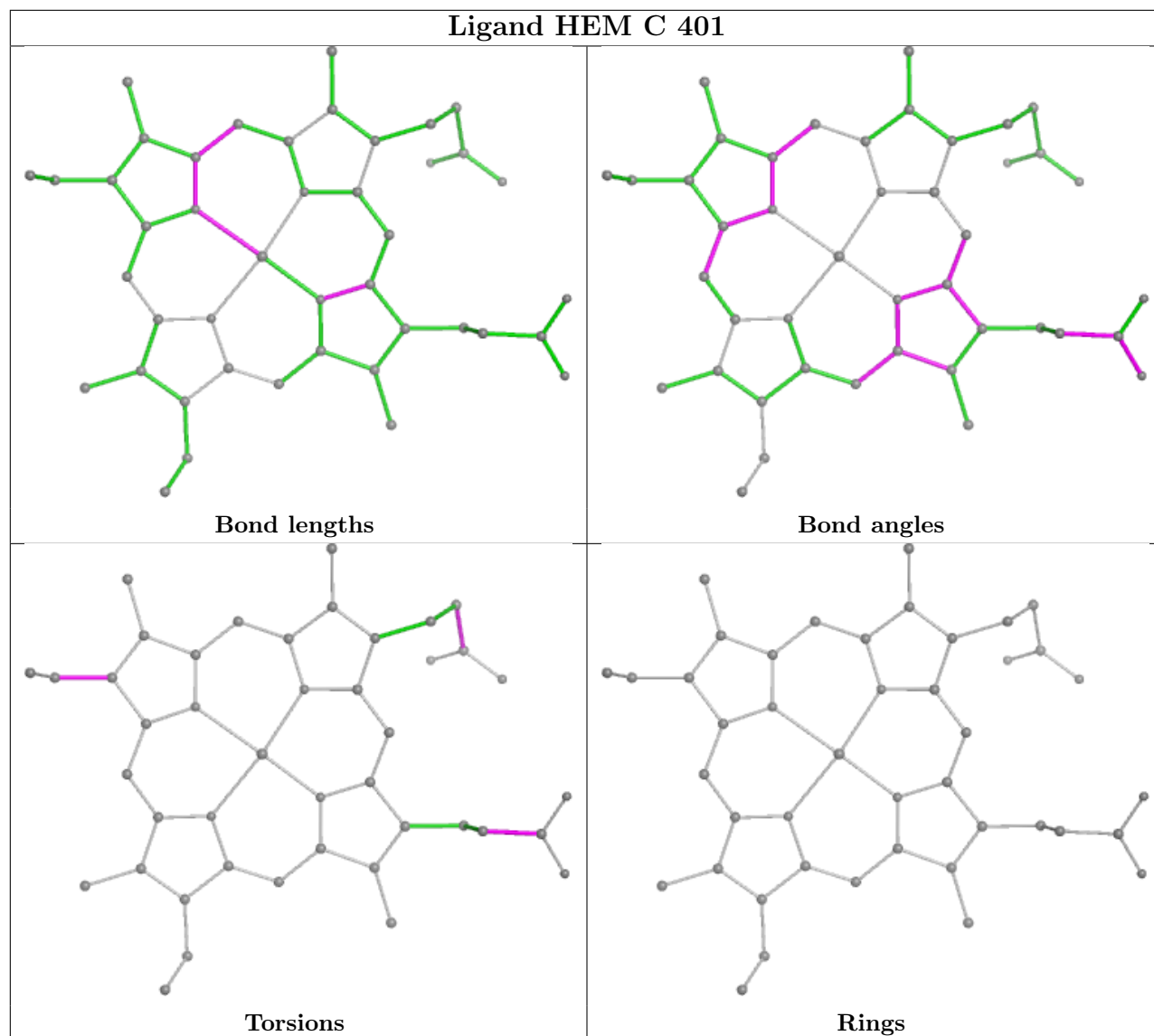
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	401	HEM	1	0
3	D	402	NO	1	0

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.

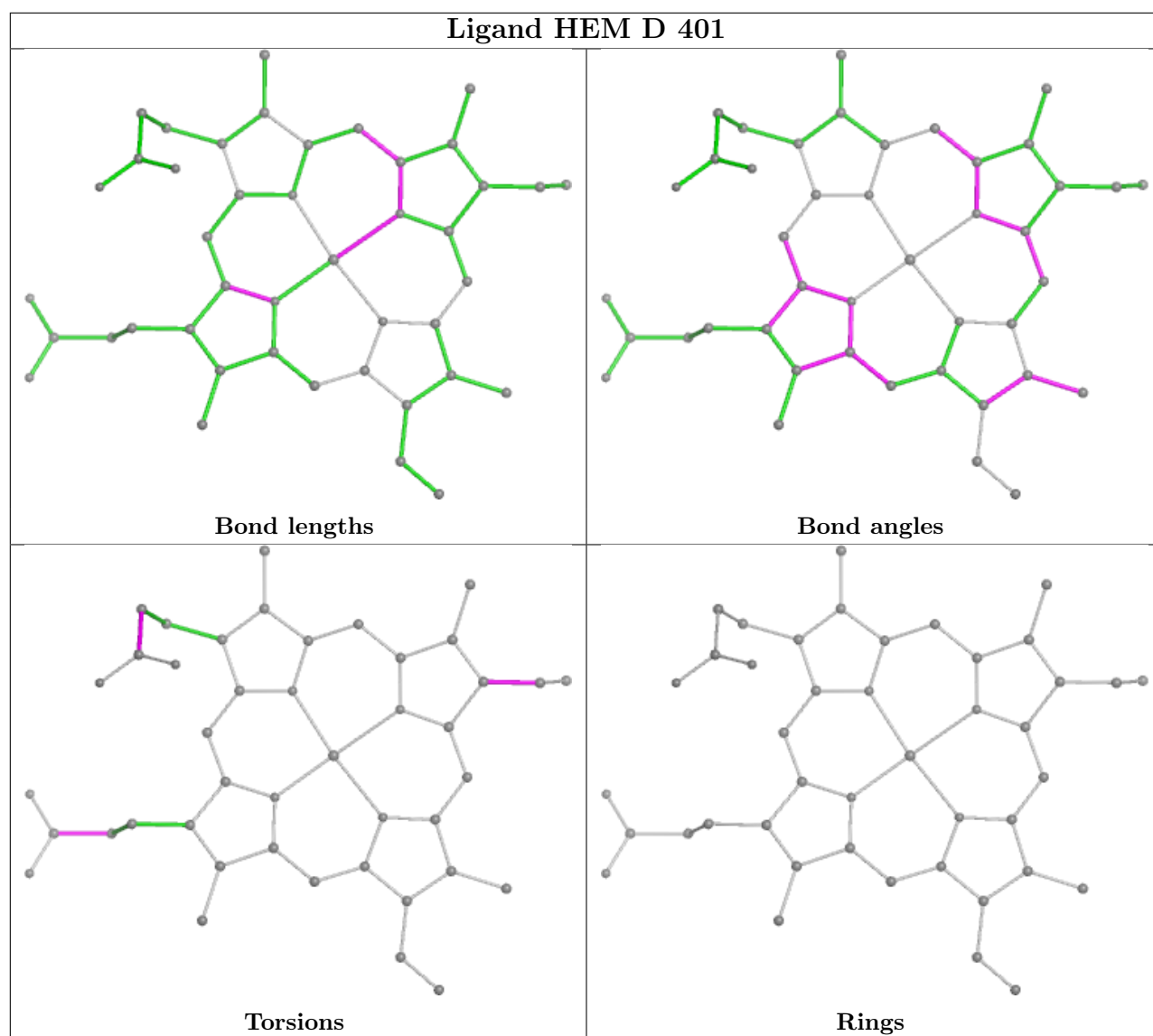


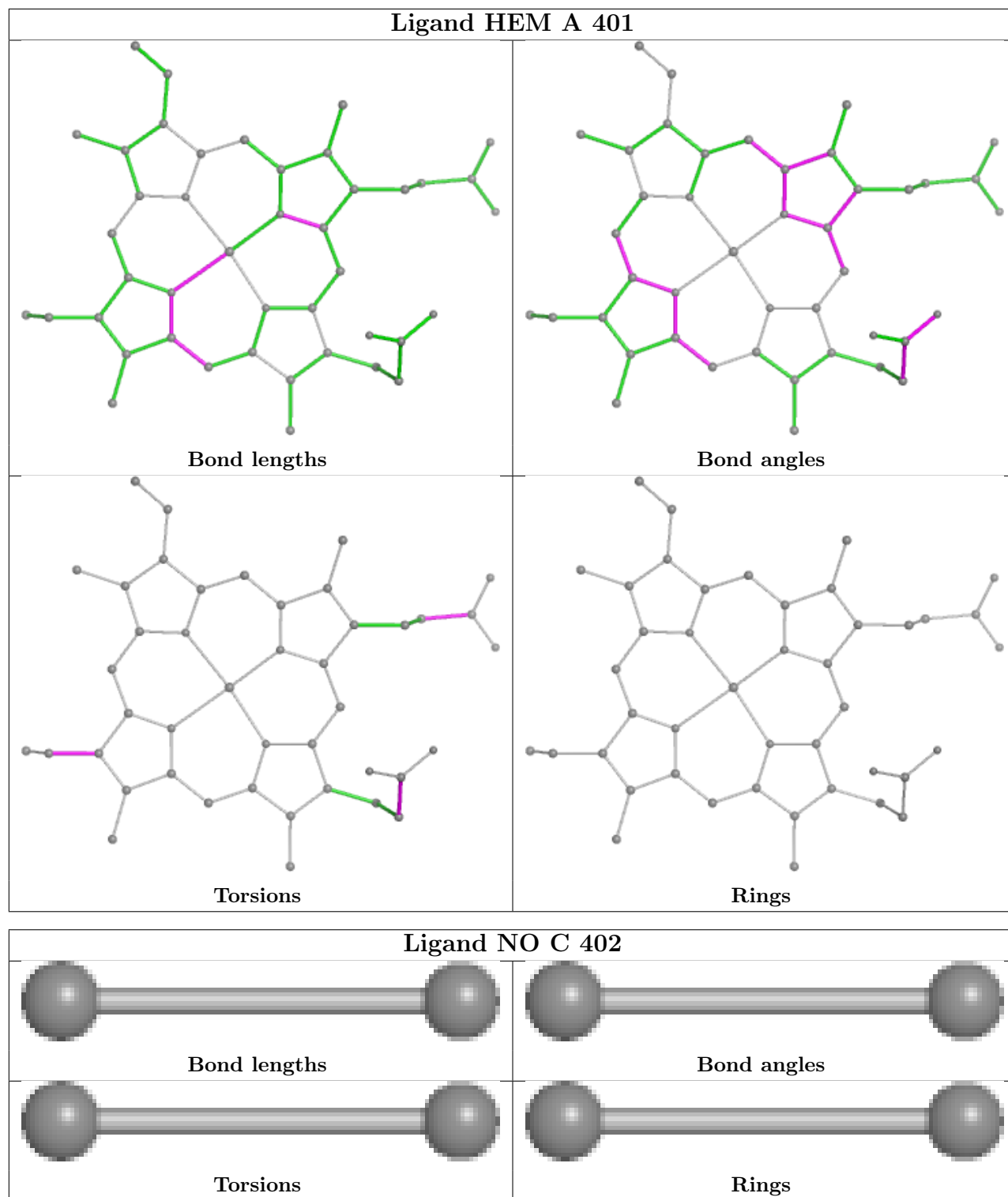


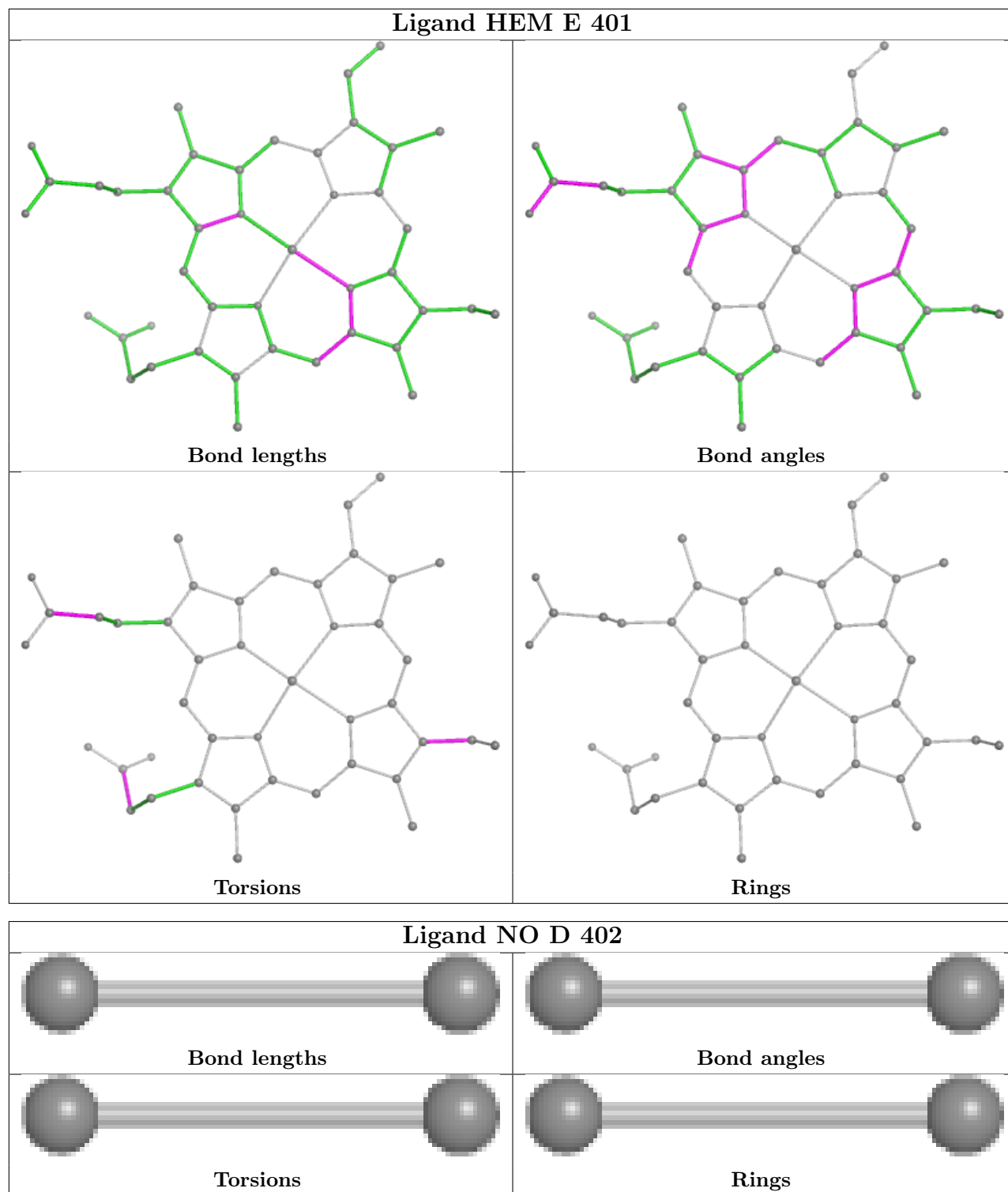












## 5.7 Other polymers [i](#)

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	306/329 (93%)	-0.50	0 <span>100</span> <span>100</span>	10, 32, 57, 98	9 (2%)
1	B	306/329 (93%)	-0.41	3 (0%) <span>79</span> <span>76</span>	16, 33, 60, 117	3 (0%)
1	C	307/329 (93%)	-0.28	5 (1%) <span>70</span> <span>67</span>	16, 37, 64, 113	6 (1%)
1	D	306/329 (93%)	-0.54	2 (0%) <span>84</span> <span>81</span>	15, 31, 53, 89	8 (2%)
1	E	305/329 (92%)	-0.28	7 (2%) <span>61</span> <span>58</span>	13, 37, 59, 108	7 (2%)
1	F	307/329 (93%)	-0.36	3 (0%) <span>79</span> <span>76</span>	15, 35, 61, 102	7 (2%)
All	All	1837/1974 (93%)	-0.39	20 (1%) <span>77</span> <span>75</span>	10, 34, 61, 117	40 (2%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	234	PRO	3.9
1	C	234	PRO	3.7
1	F	313	SER	3.7
1	E	55	GLN	3.3
1	F	234	PRO	3.0
1	E	8	PRO	2.9
1	E	56	PRO	2.9
1	C	232	THR	2.7
1	E	9[A]	GLU	2.7
1	B	234	PRO	2.5
1	B	312	LEU	2.4
1	E	312[A]	LEU	2.4
1	F	311[A]	ASP	2.3
1	D	312[A]	LEU	2.3
1	C	313	SER	2.2
1	B	7	GLU	2.2
1	D	8	PRO	2.2
1	E	236	GLY	2.1
1	C	236	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	127	ARG	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](#)

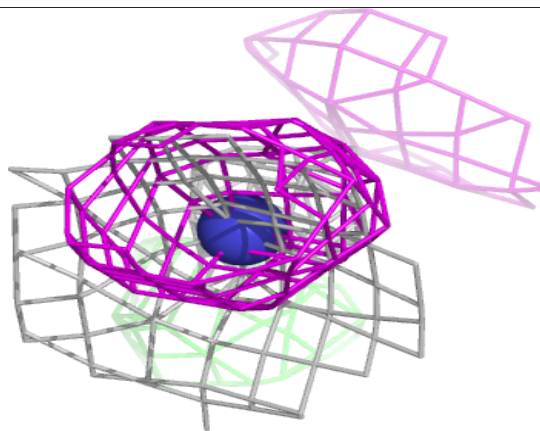
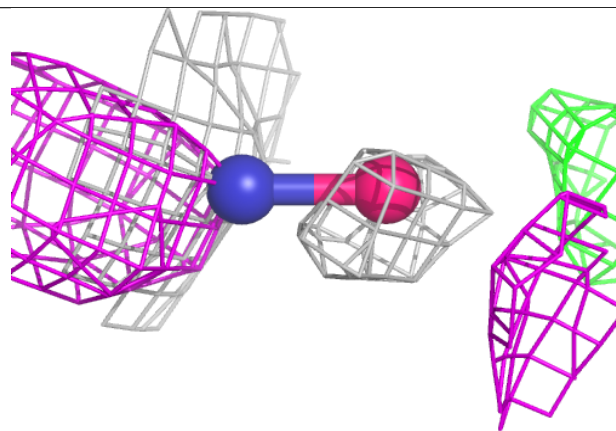
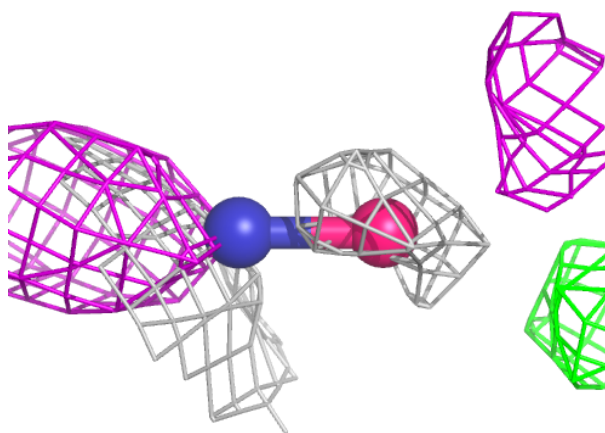
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	NO	F	402	2/2	0.80	0.22	31,31,31,32	2
3	NO	D	402	2/2	0.87	0.24	29,29,29,30	2
3	NO	B	402	2/2	0.90	0.16	28,28,28,29	2
3	NO	C	402	2/2	0.93	0.29	36,36,36,36	2
3	NO	E	402	2/2	0.93	0.21	32,32,32,32	2
3	NO	A	402	2/2	0.95	0.12	26,26,26,26	2
2	HEM	F	401	43/43	0.97	0.07	30,31,33,34	0
2	HEM	C	401	43/43	0.97	0.07	30,32,35,36	0
2	HEM	B	401	43/43	0.98	0.06	26,27,29,32	0
2	HEM	D	401	43/43	0.98	0.06	27,28,29,31	0
2	HEM	E	401	43/43	0.98	0.06	27,30,31,33	0
2	HEM	A	401	43/43	0.99	0.05	24,26,31,35	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.

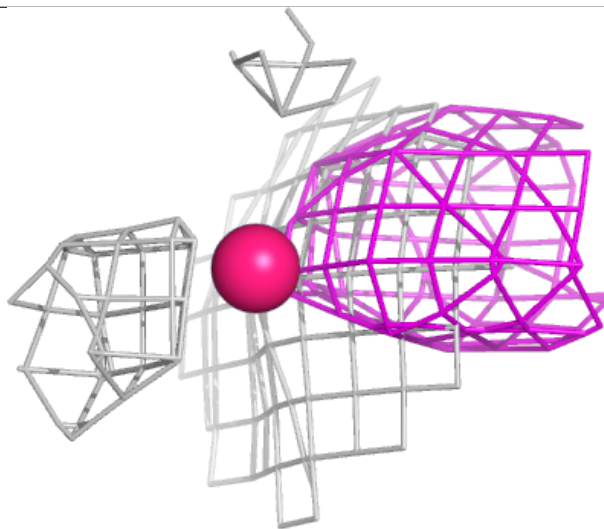
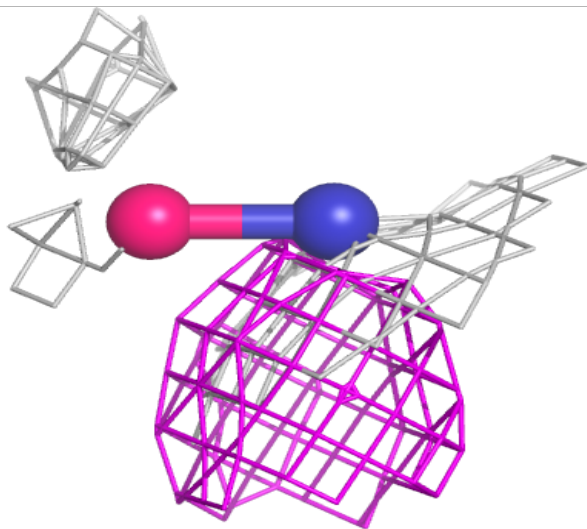
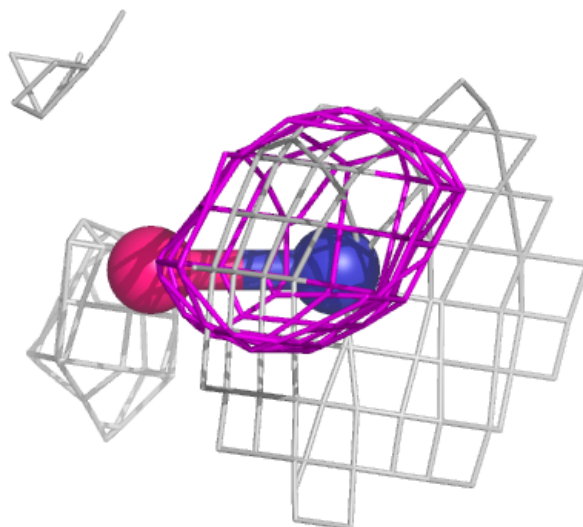
**Electron density around NO F 402:**

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



**Electron density around NO D 402:**

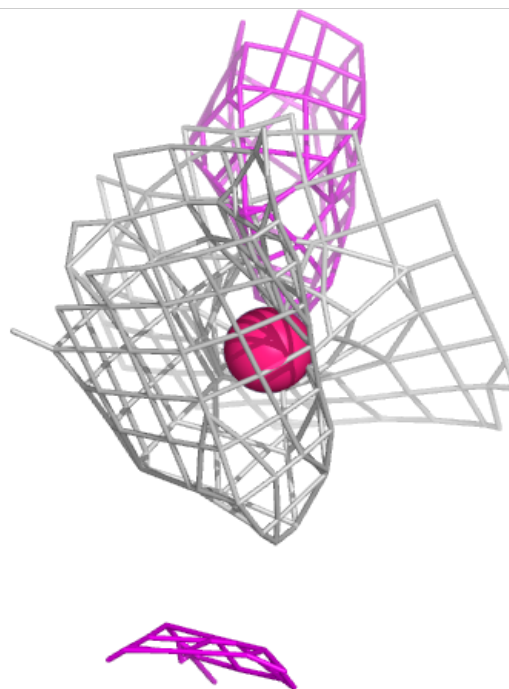
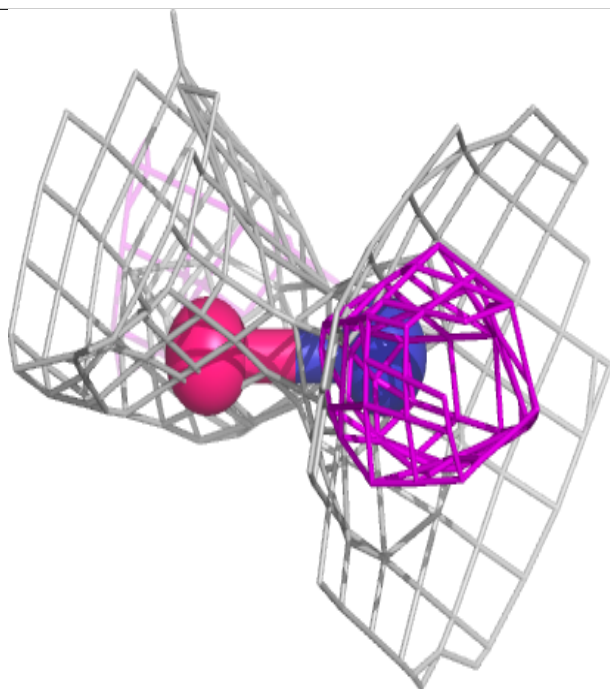
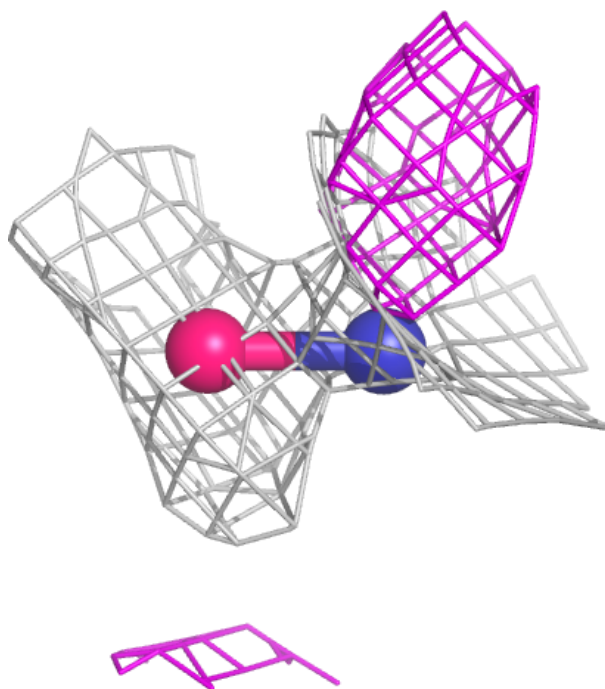
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





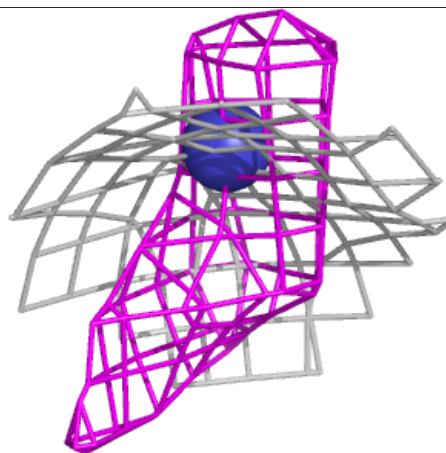
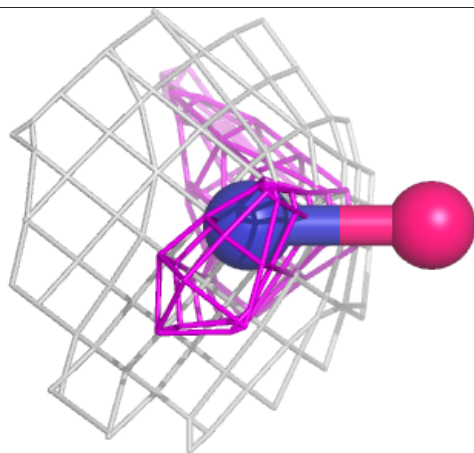
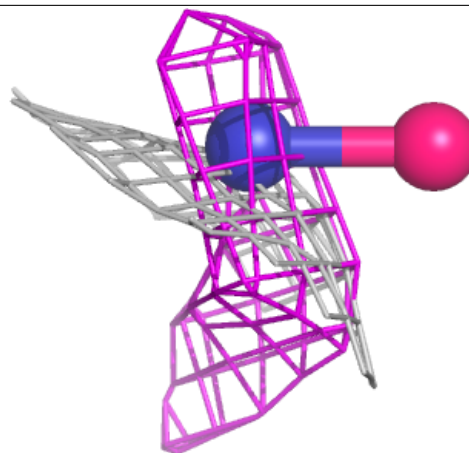
**Electron density around NO B 402:**

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



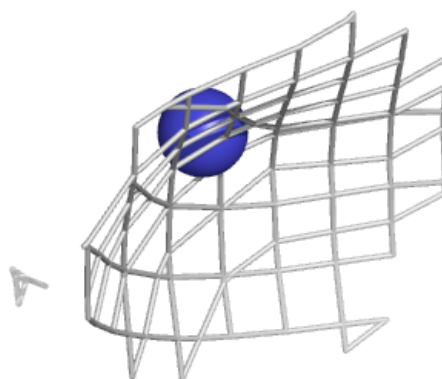
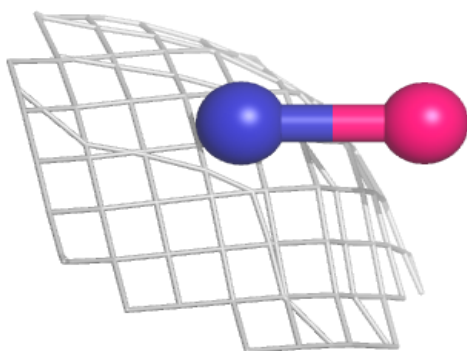
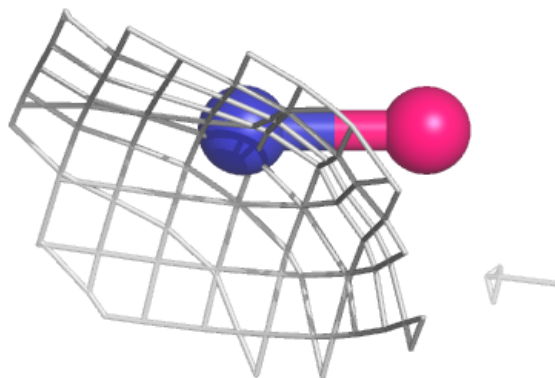
**Electron density around NO C 402:**

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



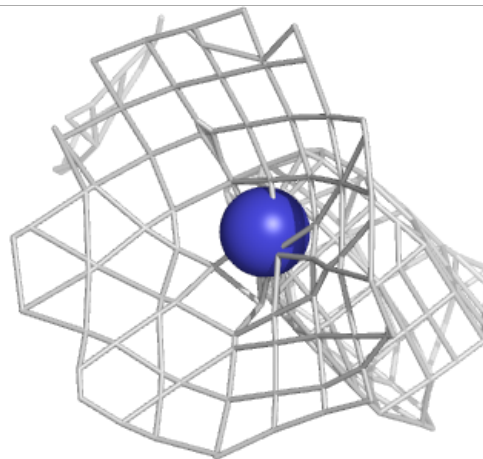
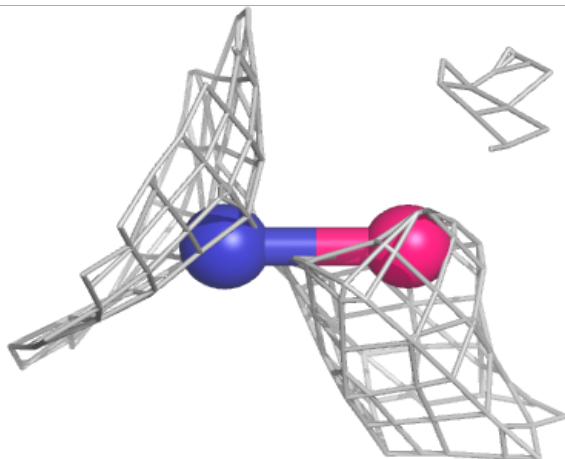
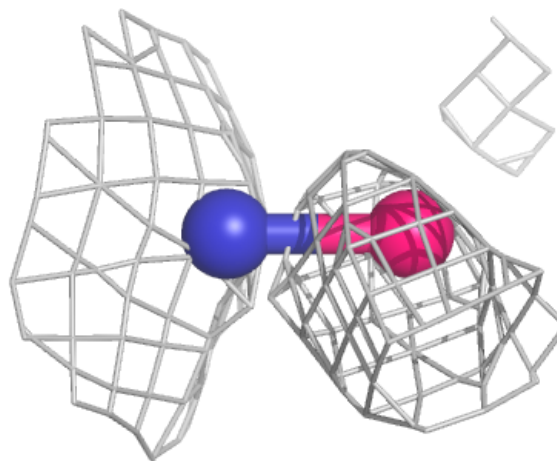
**Electron density around NO E 402:**

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



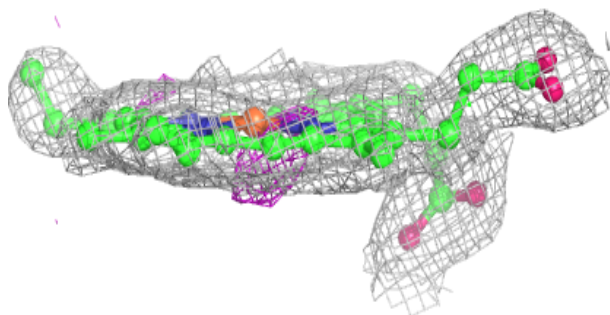
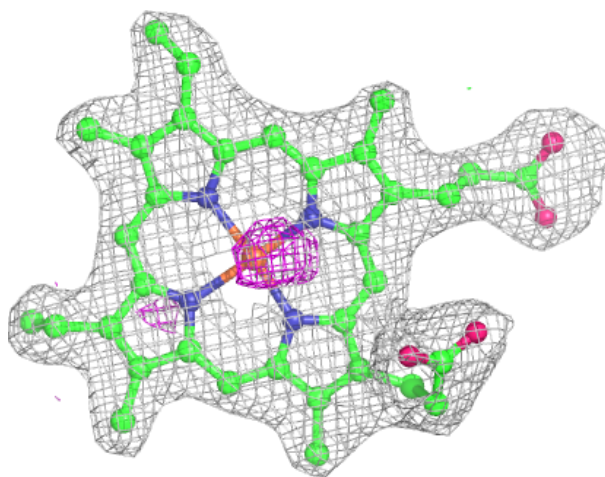
**Electron density around NO A 402:**

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



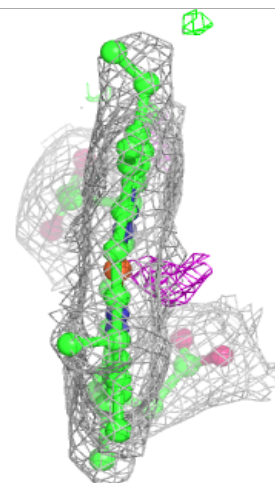
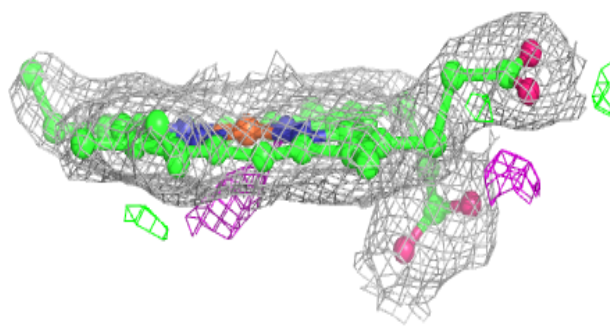
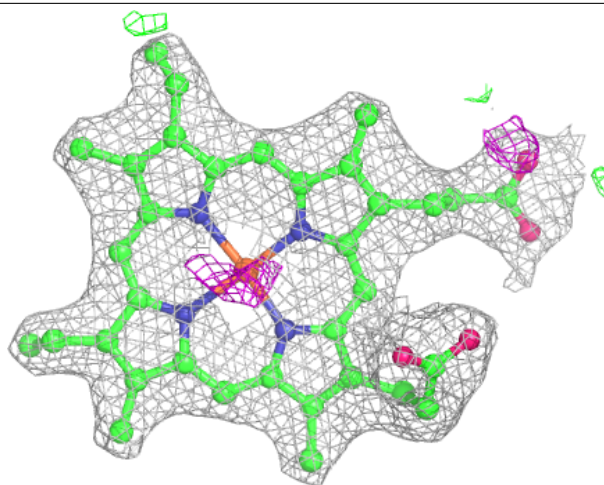
**Electron density around HEM F 401:**

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



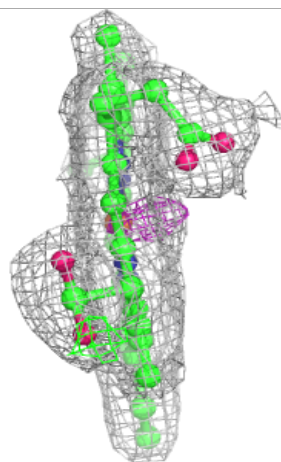
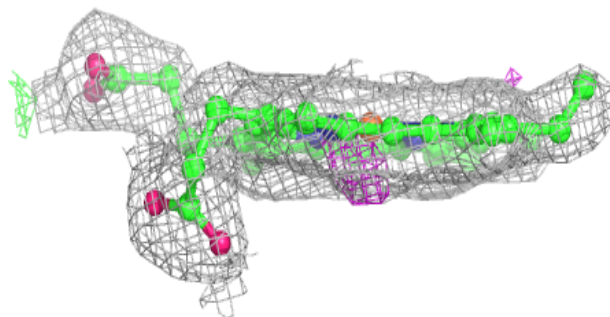
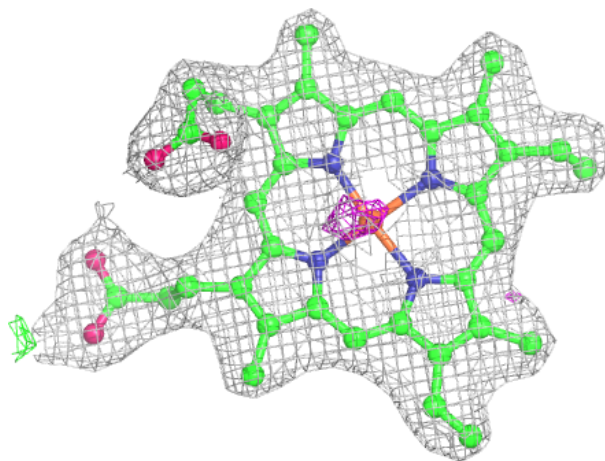
**Electron density around HEM C 401:**

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



**Electron density around HEM B 401:**

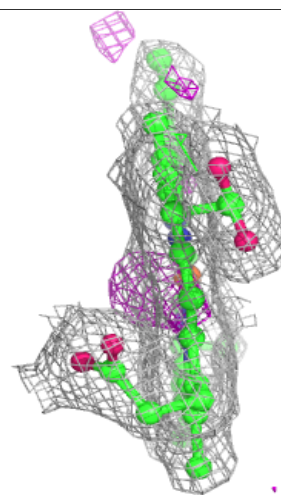
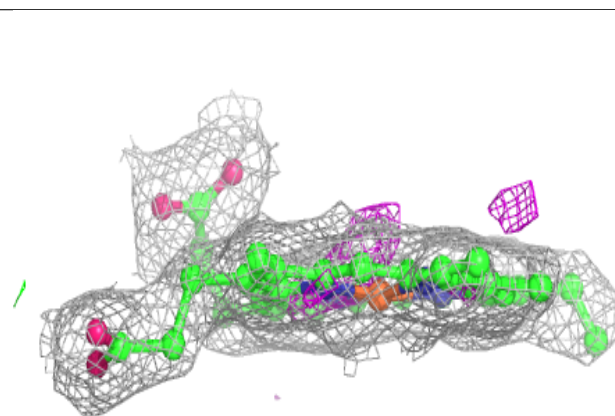
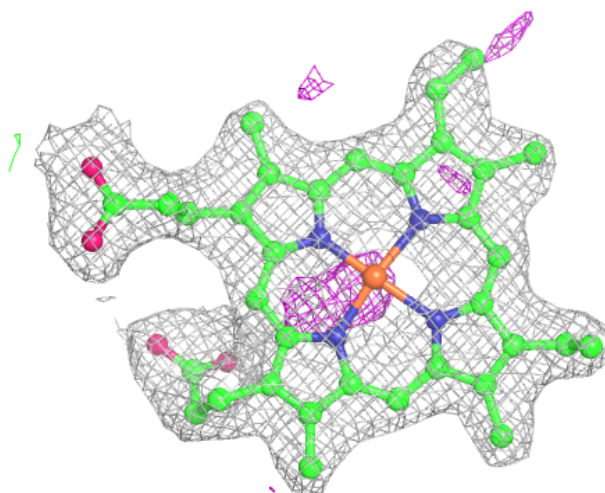
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around HEM D 401:**

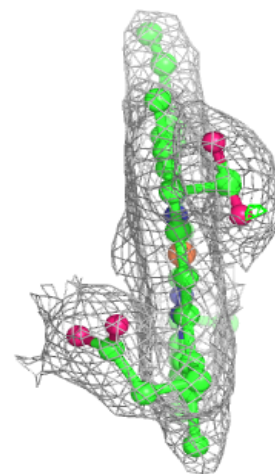
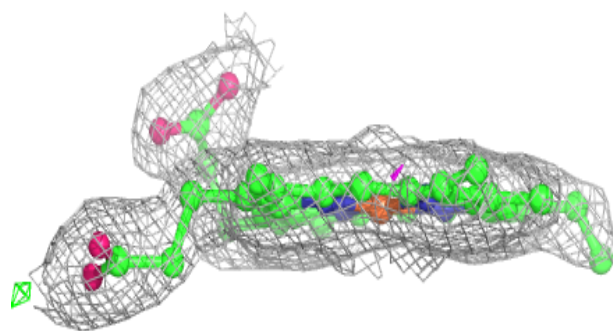
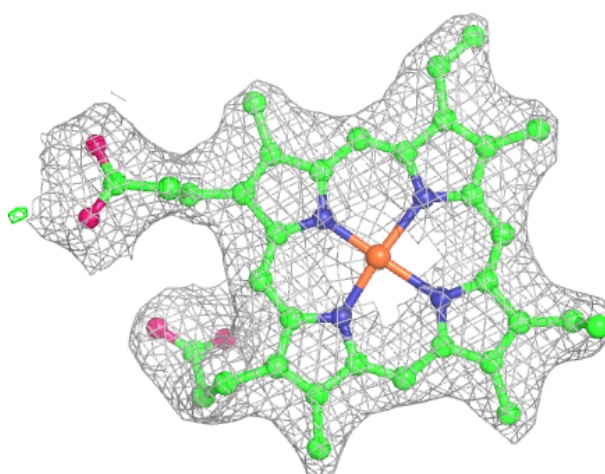
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





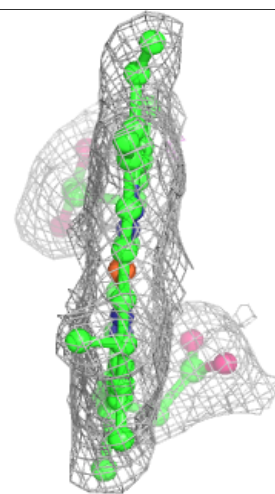
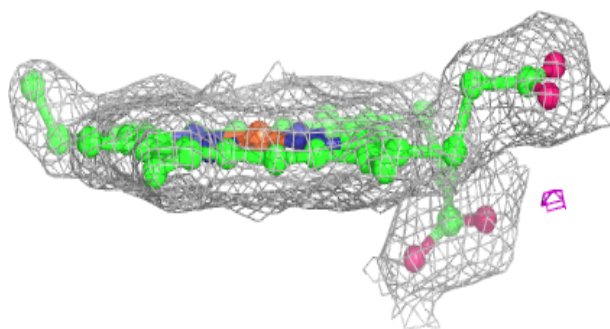
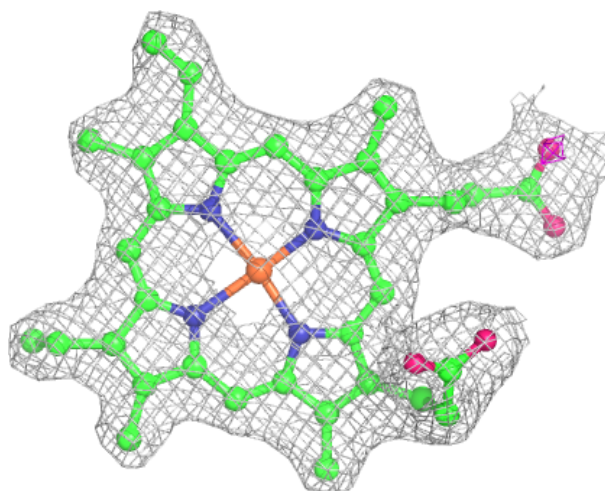
**Electron density around HEM E 401:**

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



**Electron density around HEM 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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.