



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 04:46 pm BST

PDB ID : 2IJ5  
Title : Crystal structure of cytochrome P450 CYP121, P212121 space group  
Authors : Roujeinikova, A.; Leys, D.  
Deposited on : 2006-09-29  
Resolution : 1.60 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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

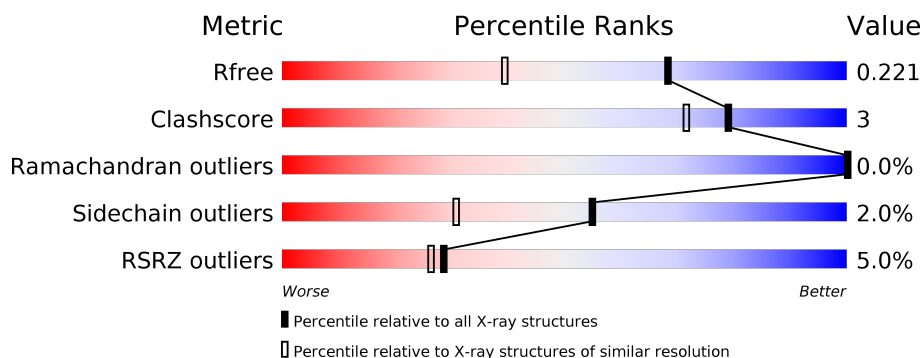
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.60 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))
$R_{free}$	130704	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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 on 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	396	
1	B	396	
1	C	396	
1	D	396	
1	E	396	
1	F	396	

## 2 Entry composition [i](#)

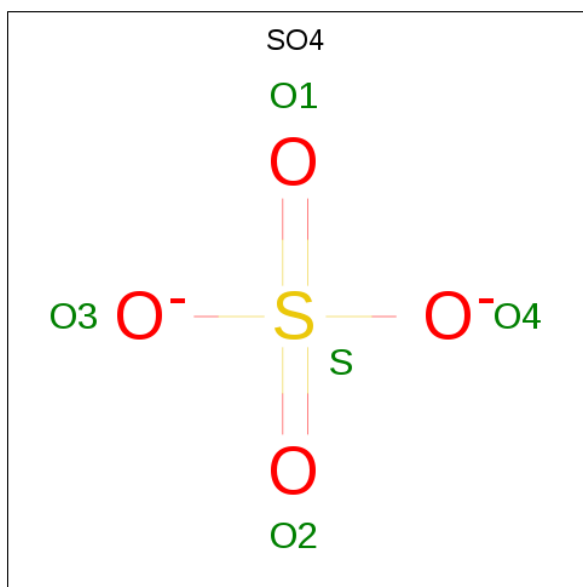
There are 4 unique types of molecules in this entry. The entry contains 20721 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cytochrome P450 121.

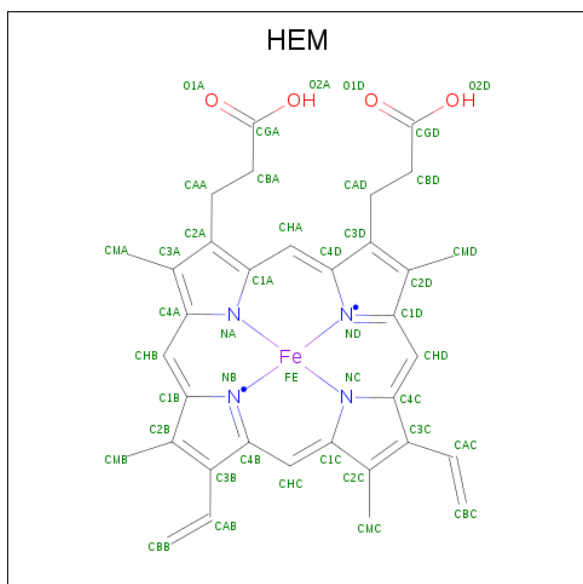
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	392	Total	C	N	O	S	0	2	0
			2974	1893	525	546	10			
1	B	390	Total	C	N	O	S	0	4	0
			2947	1877	521	539	10			
1	C	394	Total	C	N	O	S	0	4	0
			3008	1912	531	555	10			
1	D	391	Total	C	N	O	S	0	0	0
			2972	1891	524	547	10			
1	E	387	Total	C	N	O	S	0	8	0
			2974	1895	516	551	12			
1	F	384	Total	C	N	O	S	0	3	0
			2924	1864	510	540	10			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0

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



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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

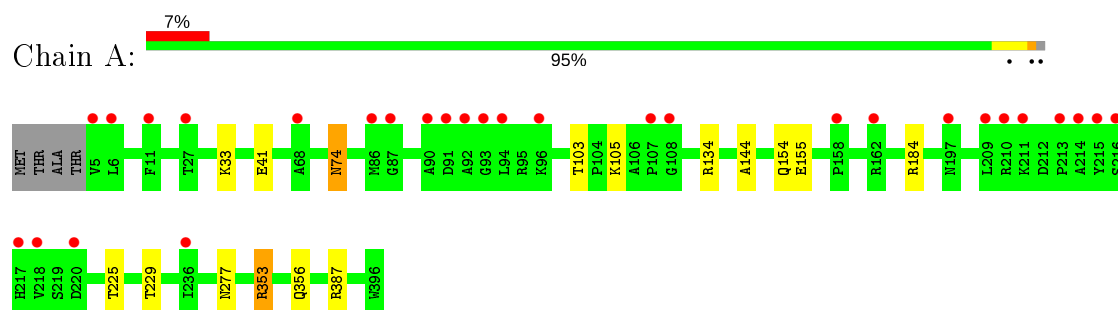
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	404	Total	O	0	0
			404	404		
4	B	389	Total	O	0	0
			389	389		
4	C	420	Total	O	0	0
			420	420		
4	D	454	Total	O	0	0
			454	454		
4	E	537	Total	O	0	0
			537	537		
4	F	430	Total	O	0	0
			430	430		

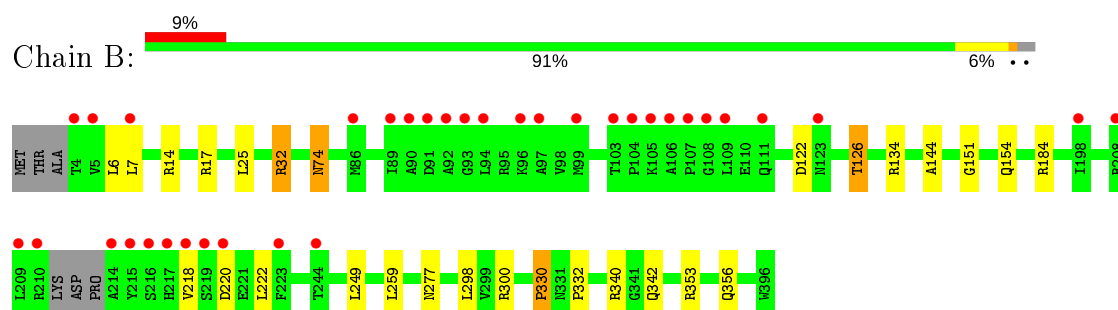
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

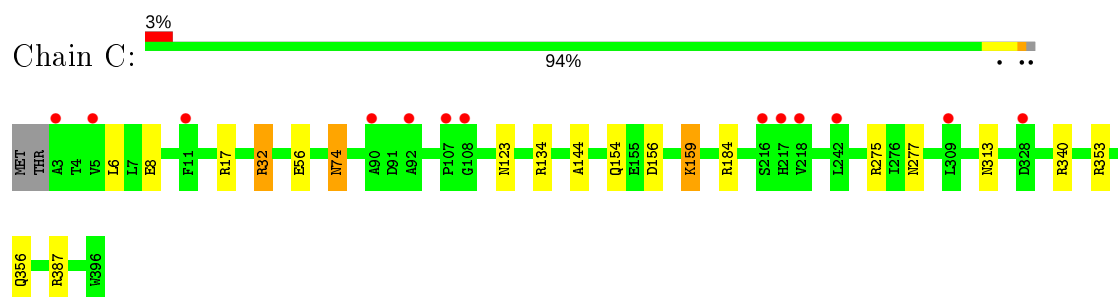
#### • Molecule 1: Cytochrome P450 121



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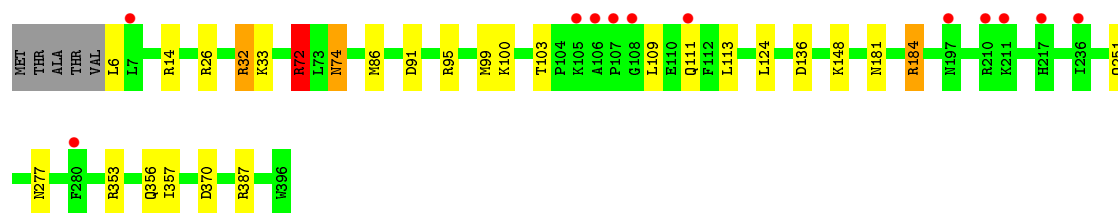


#### • Molecule 1: Cytochrome P450 121

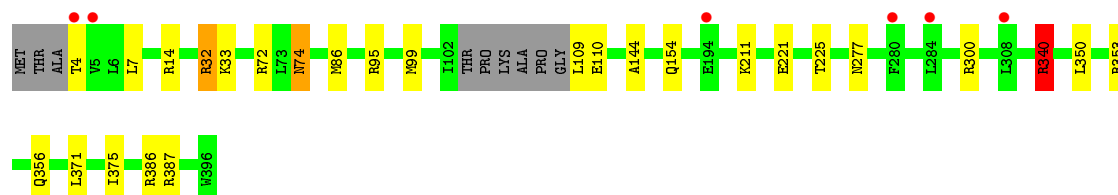
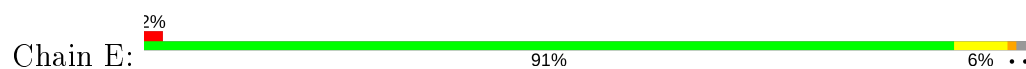


#### • Molecule 1: Cytochrome P450 121

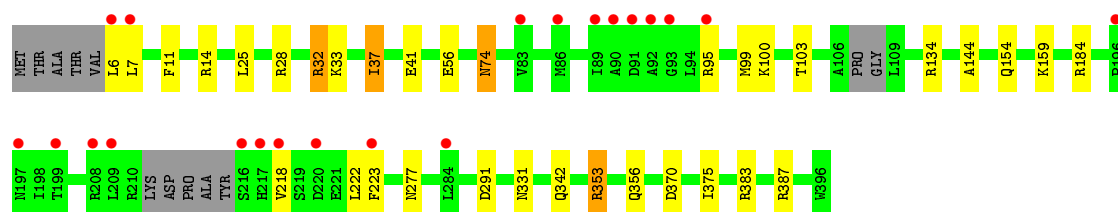
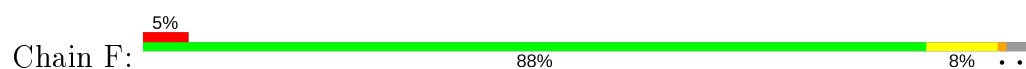




● Molecule 1: Cytochrome P450 121



● Molecule 1: Cytochrome P450 121



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.63Å 129.76Å 323.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.60 29.80 – 1.60	Depositor EDS
% Data completeness (in resolution range)	93.2 (20.00-1.60) 98.4 (29.80-1.60)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.37 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.165 , 0.210 0.178 , 0.221	Depositor DCC
$R_{free}$ test set	16700 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.6	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 51.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	20721	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% 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, SO4

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	0.65	0/3045	0.76	7/4152 (0.2%)
1	B	0.69	0/3020	0.78	3/4119 (0.1%)
1	C	0.68	0/3083	0.78	5/4200 (0.1%)
1	D	0.70	0/3035	0.83	10/4136 (0.2%)
1	E	0.77	1/3062 (0.0%)	0.83	6/4170 (0.1%)
1	F	0.70	0/2993	0.82	8/4076 (0.2%)
All	All	0.70	1/18238 (0.0%)	0.80	39/24853 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	110	GLU	CB-CG	-5.11	1.42	1.52

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	387	ARG	NE-CZ-NH1	10.34	125.47	120.30
1	D	72	ARG	NE-CZ-NH1	10.28	125.44	120.30
1	D	86	MET	CG-SD-CE	9.42	115.27	100.20
1	E	387	ARG	NE-CZ-NH1	8.91	124.75	120.30
1	B	134	ARG	NE-CZ-NH1	-8.71	115.94	120.30
1	D	72	ARG	NE-CZ-NH2	-8.56	116.02	120.30
1	F	387	ARG	NE-CZ-NH2	-8.31	116.14	120.30
1	C	387	ARG	NE-CZ-NH1	8.18	124.39	120.30
1	C	387	ARG	NE-CZ-NH2	-8.15	116.22	120.30
1	A	387	ARG	NE-CZ-NH2	-8.12	116.24	120.30
1	D	387	ARG	NE-CZ-NH1	7.85	124.22	120.30
1	D	184	ARG	NE-CZ-NH2	-7.83	116.38	120.30
1	F	134	ARG	NE-CZ-NH1	-7.79	116.40	120.30
1	A	353	ARG	NE-CZ-NH2	7.46	124.03	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	184	ARG	NE-CZ-NH2	-7.38	116.61	120.30
1	D	26	ARG	NE-CZ-NH2	7.21	123.91	120.30
1	A	134	ARG	NE-CZ-NH2	7.20	123.90	120.30
1	E	387	ARG	NE-CZ-NH2	-7.09	116.75	120.30
1	D	184	ARG	NE-CZ-NH1	6.98	123.79	120.30
1	A	134	ARG	NE-CZ-NH1	-6.89	116.86	120.30
1	B	134	ARG	NE-CZ-NH2	6.87	123.74	120.30
1	D	26	ARG	NE-CZ-NH1	-6.83	116.88	120.30
1	F	353	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	F	134	ARG	NE-CZ-NH2	6.63	123.62	120.30
1	A	387	ARG	NE-CZ-NH1	6.53	123.56	120.30
1	C	134	ARG	NE-CZ-NH1	-6.46	117.07	120.30
1	A	353	ARG	NE-CZ-NH1	-6.05	117.27	120.30
1	E	300	ARG	NE-CZ-NH1	-5.82	117.39	120.30
1	C	134	ARG	NE-CZ-NH2	5.67	123.14	120.30
1	B	184	ARG	NE-CZ-NH2	-5.51	117.55	120.30
1	D	370	ASP	CB-CG-OD1	5.45	123.20	118.30
1	C	184	ARG	NE-CZ-NH1	-5.40	117.60	120.30
1	E	72	ARG	NE-CZ-NH1	-5.40	117.60	120.30
1	E	350	LEU	CA-CB-CG	5.36	127.62	115.30
1	A	184	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	D	387	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	F	291	ASP	CB-CG-OD1	5.24	123.01	118.30
1	E	340	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	F	370	ASP	CB-CG-OD1	5.06	122.86	118.30

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	2974	0	2991	8	1
1	B	2947	0	2945	16	0
1	C	3008	0	3026	11	0
1	D	2972	0	2993	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2974	0	2982	22	1
1	F	2924	0	2936	18	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
3	A	43	0	30	4	0
3	B	43	0	30	2	0
3	C	43	0	30	0	0
3	D	43	0	30	1	0
3	E	43	0	30	2	0
3	F	43	0	30	1	0
4	A	404	0	0	0	0
4	B	389	0	0	5	0
4	C	420	0	0	4	0
4	D	454	0	0	7	1
4	E	537	0	0	11	2
4	F	430	0	0	5	1
All	All	20721	0	18053	102	3

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 (102) 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:E:86[B]:MET:SD	4:E:3047:HOH:O	2.15	1.03
1:E:109:LEU:N	4:E:3243:HOH:O	1.92	1.01
1:D:91:ASP:HB3	4:D:3110:HOH:O	1.74	0.86
1:C:353:ARG:HH21	1:C:356:GLN:HE21	1.29	0.79
1:D:72:ARG:HD3	1:D:74:ASN:O	1.82	0.78
1:E:353:ARG:HH11	1:E:356:GLN:HE21	1.27	0.78
1:A:353:ARG:HH11	1:A:356:GLN:HE21	1.28	0.78
1:C:8:GLU:HB3	4:C:2906:HOH:O	1.83	0.77
1:E:86[A]:MET:HE1	1:E:386:ARG:HH12	1.50	0.77
1:D:353:ARG:HH11	1:D:356:GLN:HE21	1.33	0.77
1:E:99[A]:MET:HE2	4:E:3030:HOH:O	1.85	0.77
1:B:122:ASP:O	1:B:126:THR:HG23	1.86	0.76
1:E:86[A]:MET:CE	1:E:386:ARG:HH12	2.00	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:353:ARG:HH11	1:B:356:GLN:HE21	1.35	0.72
1:D:251:GLN:OE1	4:D:3038:HOH:O	2.09	0.71
1:F:56[A]:GLU:HG2	4:F:3024:HOH:O	1.91	0.70
1:D:100:LYS:O	1:D:103:THR:HG22	1.94	0.66
1:D:72:ARG:NH2	4:D:3104:HOH:O	2.11	0.66
1:F:353:ARG:HH11	1:F:356:GLN:HE21	1.42	0.66
1:E:221:GLU:O	1:E:225[A]:THR:HG23	1.96	0.65
1:B:144:ALA:HA	1:B:154:GLN:HE22	1.60	0.65
1:C:123:ASN:OD1	4:C:3040:HOH:O	2.15	0.65
1:D:91:ASP:OD2	4:D:3237:HOH:O	2.14	0.65
1:B:330:PRO:O	4:B:3205:HOH:O	2.14	0.65
1:F:95:ARG:O	1:F:99:MET:HG2	1.99	0.63
1:F:7:LEU:HG	1:F:11:PHE:CE2	2.35	0.60
1:E:95:ARG:NE	4:E:3277:HOH:O	2.34	0.59
1:D:181:ASN:OD1	1:D:184:ARG:NH2	2.30	0.59
3:E:462:HEM:HBC2	3:E:462:HEM:HMC1	1.86	0.58
1:A:155:GLU:CD	1:A:155:GLU:H	2.07	0.58
1:D:111:GLN:HG3	4:D:3069:HOH:O	2.04	0.57
1:E:99[A]:MET:CE	4:E:3030:HOH:O	2.47	0.57
1:C:144:ALA:HA	1:C:154:GLN:HE22	1.70	0.57
1:D:91:ASP:CG	4:D:3237:HOH:O	2.44	0.56
1:A:353:ARG:HH11	1:A:356:GLN:NE2	2.02	0.56
1:C:74:ASN:C	1:C:74:ASN:HD22	2.08	0.56
1:B:330:PRO:O	1:B:332:PRO:HD3	2.05	0.56
1:B:7:LEU:HD12	4:B:3085:HOH:O	2.05	0.56
1:C:353:ARG:HH21	1:C:356:GLN:NE2	2.01	0.56
1:E:144:ALA:HA	1:E:154:GLN:HE22	1.72	0.55
1:E:353:ARG:NH1	1:E:356:GLN:HE21	2.01	0.54
1:C:56:GLU:OE1	4:C:3001:HOH:O	2.17	0.53
1:D:353:ARG:HH11	1:D:356:GLN:NE2	2.04	0.52
3:B:462:HEM:HBC2	3:B:462:HEM:CMC	2.40	0.51
3:B:462:HEM:HMC2	3:B:462:HEM:HBC2	1.93	0.51
1:A:144:ALA:HA	1:A:154:GLN:HE22	1.76	0.51
3:A:462:HEM:HBC2	3:A:462:HEM:HMC1	1.91	0.51
1:C:32:ARG:NH1	4:C:3018:HOH:O	2.43	0.51
1:B:74:ASN:C	1:B:74:ASN:HD22	2.15	0.50
1:F:144:ALA:HA	1:F:154:GLN:HE22	1.76	0.50
1:F:159:LYS:C	4:F:3150:HOH:O	2.50	0.50
1:E:14:ARG:NH2	4:E:3174:HOH:O	2.43	0.49
1:F:28:ARG:CD	1:F:28:ARG:CZ	2.90	0.49
1:F:95:ARG:HD3	4:F:3084:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:14:ARG:NH2	4:F:3016:HOH:O	2.46	0.48
1:A:74:ASN:HD22	1:A:74:ASN:C	2.17	0.48
1:F:25:LEU:HD11	1:F:32:ARG:HG2	1.95	0.47
1:F:218:VAL:HG13	1:F:222:LEU:HD23	1.95	0.47
1:B:298:LEU:O	1:B:300:ARG:NH2	2.45	0.47
1:E:375:ILE:HD13	4:E:3351:HOH:O	2.14	0.47
1:E:99[A]:MET:HE3	4:E:3205:HOH:O	2.14	0.47
1:F:37:ILE:HD11	1:F:383:ARG:CZ	2.44	0.47
1:B:151:GLY:HA2	4:B:3014:HOH:O	2.13	0.47
1:D:74:ASN:C	1:D:74:ASN:HD22	2.19	0.47
1:D:95:ARG:O	1:D:99:MET:HG2	2.15	0.46
1:C:156:ASP:HA	1:C:159:LYS:HE2	1.98	0.46
1:B:218:VAL:CG1	1:B:222:LEU:HD23	2.45	0.46
1:B:218:VAL:HG13	1:B:222:LEU:HD23	1.97	0.46
1:F:33:LYS:HD2	1:F:41:GLU:HB3	1.97	0.46
1:E:340:ARG:HD3	4:E:2895:HOH:O	2.17	0.45
3:E:462:HEM:HBC2	3:E:462:HEM:CMC	2.46	0.45
3:A:462:HEM:HBC2	3:A:462:HEM:CMC	2.48	0.44
3:D:462:HEM:HBC2	3:D:462:HEM:HMC1	1.99	0.44
1:E:32:ARG:HD3	1:E:33:LYS:O	2.18	0.44
1:A:33:LYS:HE3	1:A:41:GLU:OE1	2.17	0.44
1:F:218:VAL:CG1	1:F:223:PHE:CE1	3.01	0.43
1:B:14:ARG:NH2	4:B:2981:HOH:O	2.51	0.43
3:A:462:HEM:HMB2	3:A:462:HEM:HBB2	2.00	0.43
1:E:74:ASN:C	1:E:74:ASN:HD22	2.22	0.43
1:E:86[B]:MET:HB2	4:E:2935:HOH:O	2.19	0.43
1:B:342:GLN:HG3	4:B:3209:HOH:O	2.18	0.42
1:D:113:LEU:HD13	1:D:357:ILE:HD12	2.01	0.42
1:E:353:ARG:HA	1:E:353:ARG:HE	1.84	0.42
1:F:375[A]:ILE:HD13	4:F:3052:HOH:O	2.18	0.42
1:F:7:LEU:HG	1:F:11:PHE:HE2	1.78	0.42
1:A:225:THR:O	1:A:229:THR:HG23	2.19	0.42
1:D:124:LEU:HD21	1:D:136:ASP:HB3	2.00	0.42
1:E:86[A]:MET:HE2	1:E:386:ARG:HH12	1.81	0.42
1:B:249:LEU:HD21	1:B:259:LEU:HD12	2.01	0.42
1:D:32:ARG:HD3	1:D:33:LYS:O	2.19	0.41
3:A:462:HEM:CMB	3:A:462:HEM:HBB2	2.50	0.41
1:C:353:ARG:HD2	1:C:356:GLN:NE2	2.35	0.41
1:F:100:LYS:O	1:F:103:THR:HG22	2.20	0.41
3:F:462:HEM:HBC2	3:F:462:HEM:HMC1	2.01	0.41
1:D:14:ARG:NH2	4:D:3003:HOH:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:74:ASN:HD22	1:F:74:ASN:C	2.23	0.41
1:B:353:ARG:HH11	1:B:356:GLN:NE2	2.09	0.41
1:E:353:ARG:HH11	1:E:356:GLN:NE2	2.07	0.41
1:A:103[B]:THR:HG22	1:A:105:LYS:H	1.86	0.41
1:B:25:LEU:HD11	1:B:32:ARG:HG2	2.03	0.41
1:C:275:ARG:O	1:C:313:ASN:HB3	2.20	0.40
1:E:371:LEU:HD11	4:E:3351:HOH:O	2.21	0.40

All (3) 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)
1:A:105:LYS:NZ	4:F:3252:HOH:O[4_456]	1.93	0.27
1:E:4:THR:N	4:E:3334:HOH:O[1_655]	2.07	0.13
4:D:2958:HOH:O	4:E:3263:HOH:O[1_655]	2.11	0.09

## 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	392/396 (99%)	388 (99%)	4 (1%)	0	100	100
1	B	390/396 (98%)	385 (99%)	4 (1%)	1 (0%)	41	21
1	C	396/396 (100%)	393 (99%)	3 (1%)	0	100	100
1	D	389/396 (98%)	385 (99%)	4 (1%)	0	100	100
1	E	391/396 (99%)	387 (99%)	4 (1%)	0	100	100
1	F	381/396 (96%)	379 (100%)	2 (0%)	0	100	100
All	All	2339/2376 (98%)	2317 (99%)	21 (1%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	330	PRO

### 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	313/326 (96%)	311 (99%)	2 (1%)	86	77
1	B	305/326 (94%)	297 (97%)	8 (3%)	46	21
1	C	316/326 (97%)	309 (98%)	7 (2%)	52	27
1	D	313/326 (96%)	306 (98%)	7 (2%)	52	27
1	E	316/326 (97%)	310 (98%)	6 (2%)	57	34
1	F	308/326 (94%)	301 (98%)	7 (2%)	50	25
All	All	1871/1956 (96%)	1834 (98%)	37 (2%)	55	31

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
1	A	277	ASN
1	B	6	LEU
1	B	17	ARG
1	B	32	ARG
1	B	74	ASN
1	B	126	THR
1	B	220	ASP
1	B	277	ASN
1	B	340	ARG
1	C	6	LEU
1	C	17	ARG
1	C	32	ARG
1	C	74	ASN
1	C	159	LYS
1	C	277	ASN
1	C	340	ARG
1	D	6	LEU

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Mol	Chain	Res	Type
1	D	32	ARG
1	D	72	ARG
1	D	74	ASN
1	D	109	LEU
1	D	148	LYS
1	D	277	ASN
1	E	7	LEU
1	E	32	ARG
1	E	74	ASN
1	E	211	LYS
1	E	277	ASN
1	E	340	ARG
1	F	6	LEU
1	F	32	ARG
1	F	37	ILE
1	F	74	ASN
1	F	277	ASN
1	F	331	ASN
1	F	342	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
1	A	154	GLN
1	A	342	GLN
1	A	356	GLN
1	B	74	ASN
1	B	111	GLN
1	B	154	GLN
1	B	356	GLN
1	C	74	ASN
1	C	111	GLN
1	C	154	GLN
1	C	251	GLN
1	C	356	GLN
1	D	74	ASN
1	D	154	GLN
1	D	251	GLN
1	D	342	GLN
1	D	356	GLN
1	D	385	GLN

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Mol	Chain	Res	Type
1	E	74	ASN
1	E	85	ASN
1	E	123	ASN
1	E	154	GLN
1	E	342	GLN
1	E	356	GLN
1	E	385	GLN
1	F	74	ASN
1	F	111	GLN
1	F	154	GLN
1	F	251	GLN
1	F	331	ASN
1	F	342	GLN
1	F	356	GLN
1	F	385	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates 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	HEM	B	462	1,4	27,50,50	2.10	8 (29%)	17,82,82	1.45	2 (11%)
2	SO4	D	2823	-	4,4,4	0.45	0	6,6,6	0.56	0
2	SO4	C	2822	-	4,4,4	0.59	0	6,6,6	0.57	0
2	SO4	B	2821	-	4,4,4	0.13	0	6,6,6	0.38	0
3	HEM	C	462	1,4	27,50,50	1.89	7 (25%)	17,82,82	1.76	6 (35%)
3	HEM	F	462	1,4	27,50,50	1.92	7 (25%)	17,82,82	1.91	5 (29%)
3	HEM	A	462	1,4	27,50,50	2.06	9 (33%)	17,82,82	2.03	7 (41%)
2	SO4	A	2820	-	4,4,4	0.28	0	6,6,6	0.89	0
2	SO4	F	2825	-	4,4,4	0.45	0	6,6,6	1.19	0
3	HEM	E	462	1,4	27,50,50	1.83	8 (29%)	17,82,82	1.34	1 (5%)
2	SO4	E	2824	-	4,4,4	0.34	0	6,6,6	0.69	0
3	HEM	D	462	1,4	27,50,50	1.88	7 (25%)	17,82,82	1.79	4 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEM	B	462	1,4	-	0/6/54/54	-
3	HEM	F	462	1,4	-	0/6/54/54	-
3	HEM	C	462	1,4	-	0/6/54/54	-
3	HEM	A	462	1,4	-	0/6/54/54	-
3	HEM	E	462	1,4	-	0/6/54/54	-
3	HEM	D	462	1,4	-	0/6/54/54	-

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	462	HEM	C3D-C2D	4.57	1.51	1.37
3	B	462	HEM	C3D-C2D	4.56	1.51	1.37
3	E	462	HEM	C3C-C2C	-4.47	1.34	1.40
3	C	462	HEM	C3D-C2D	4.28	1.50	1.37
3	A	462	HEM	C3D-C2D	4.26	1.50	1.37
3	A	462	HEM	C3C-C2C	-4.19	1.34	1.40
3	B	462	HEM	C3C-C2C	-4.16	1.34	1.40
3	F	462	HEM	C3D-C2D	3.95	1.49	1.37
3	B	462	HEM	C3B-C2B	-3.85	1.35	1.40
3	B	462	HEM	C3C-CAC	3.83	1.55	1.47
3	F	462	HEM	C3B-C2B	-3.68	1.35	1.40
3	A	462	HEM	C3B-CAB	3.46	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	462	HEM	C3C-C2C	-3.46	1.35	1.40
3	C	462	HEM	C3C-CAC	3.41	1.54	1.47
3	E	462	HEM	C3D-C2D	3.39	1.47	1.37
3	A	462	HEM	C3C-CAC	3.39	1.54	1.47
3	F	462	HEM	C3B-CAB	3.37	1.54	1.47
3	E	462	HEM	C3C-CAC	3.37	1.54	1.47
3	C	462	HEM	C3C-C2C	-3.31	1.35	1.40
3	D	462	HEM	C3B-C2B	-3.15	1.36	1.40
3	A	462	HEM	CAA-C2A	3.10	1.56	1.52
3	D	462	HEM	C3C-CAC	2.97	1.53	1.47
3	D	462	HEM	CAA-C2A	2.91	1.56	1.52
3	B	462	HEM	C3B-CAB	2.79	1.53	1.47
3	C	462	HEM	C3B-C2B	-2.77	1.36	1.40
3	A	462	HEM	C3B-C2B	-2.71	1.36	1.40
3	E	462	HEM	C3B-C2B	-2.71	1.36	1.40
3	F	462	HEM	C3C-CAC	2.67	1.53	1.47
3	F	462	HEM	CAA-C2A	2.66	1.56	1.52
3	D	462	HEM	C3B-CAB	2.65	1.53	1.47
3	B	462	HEM	C1C-C2C	2.56	1.48	1.42
3	E	462	HEM	C3B-CAB	2.46	1.53	1.47
3	B	462	HEM	C4A-NA	2.43	1.41	1.36
3	D	462	HEM	C3C-C2C	-2.41	1.37	1.40
3	E	462	HEM	C1C-C2C	2.41	1.48	1.42
3	A	462	HEM	C1D-ND	2.39	1.41	1.36
3	A	462	HEM	C1D-CHD	-2.38	1.34	1.41
3	F	462	HEM	CMA-C3A	2.36	1.56	1.51
3	C	462	HEM	C3B-CAB	2.31	1.52	1.47
3	D	462	HEM	C1B-C2B	2.30	1.47	1.42
3	C	462	HEM	C1C-C2C	2.26	1.47	1.42
3	B	462	HEM	C1D-ND	2.21	1.40	1.36
3	E	462	HEM	C4D-C3D	2.19	1.47	1.42
3	A	462	HEM	C4A-NA	2.18	1.40	1.36
3	E	462	HEM	CAA-C2A	2.08	1.55	1.52
3	C	462	HEM	CAA-C2A	2.02	1.55	1.52

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	462	HEM	CMC-C2C-C3C	4.20	132.54	124.68
3	A	462	HEM	C1D-C2D-C3D	-4.17	104.10	107.00
3	F	462	HEM	C4C-C3C-C2C	3.92	109.64	106.90
3	B	462	HEM	C4C-C3C-C2C	3.45	109.31	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	462	HEM	CMB-C2B-C3B	3.31	130.87	124.68
3	F	462	HEM	CMC-C2C-C3C	3.27	130.79	124.68
3	A	462	HEM	C4A-C3A-C2A	3.21	109.23	107.00
3	D	462	HEM	CMA-C3A-C4A	-3.14	123.63	128.46
3	A	462	HEM	CMC-C2C-C3C	3.05	130.38	124.68
3	D	462	HEM	CMC-C2C-C3C	2.95	130.19	124.68
3	C	462	HEM	C1D-C2D-C3D	-2.79	105.05	107.00
3	C	462	HEM	CBD-CAD-C3D	-2.75	107.42	112.48
3	F	462	HEM	CMA-C3A-C4A	-2.66	124.38	128.46
3	A	462	HEM	C4C-C3C-C2C	2.52	108.66	106.90
3	F	462	HEM	CMB-C2B-C3B	2.50	129.36	124.68
3	E	462	HEM	CMB-C2B-C3B	2.45	129.27	124.68
3	D	462	HEM	CMB-C2B-C3B	2.36	129.10	124.68
3	D	462	HEM	C4C-C3C-C2C	2.31	108.51	106.90
3	A	462	HEM	CBD-CAD-C3D	-2.28	108.28	112.48
3	B	462	HEM	CMB-C2B-C3B	2.17	128.73	124.68
3	A	462	HEM	CMA-C3A-C4A	-2.15	125.15	128.46
3	F	462	HEM	CMA-C3A-C2A	2.13	128.97	124.94
3	C	462	HEM	C4A-C3A-C2A	2.12	108.47	107.00
3	C	462	HEM	CAD-CBD-CGD	-2.03	109.27	112.67
3	C	462	HEM	C4C-C3C-C2C	2.00	108.30	106.90

There are no chirality outliers.

There are no torsion outliers.

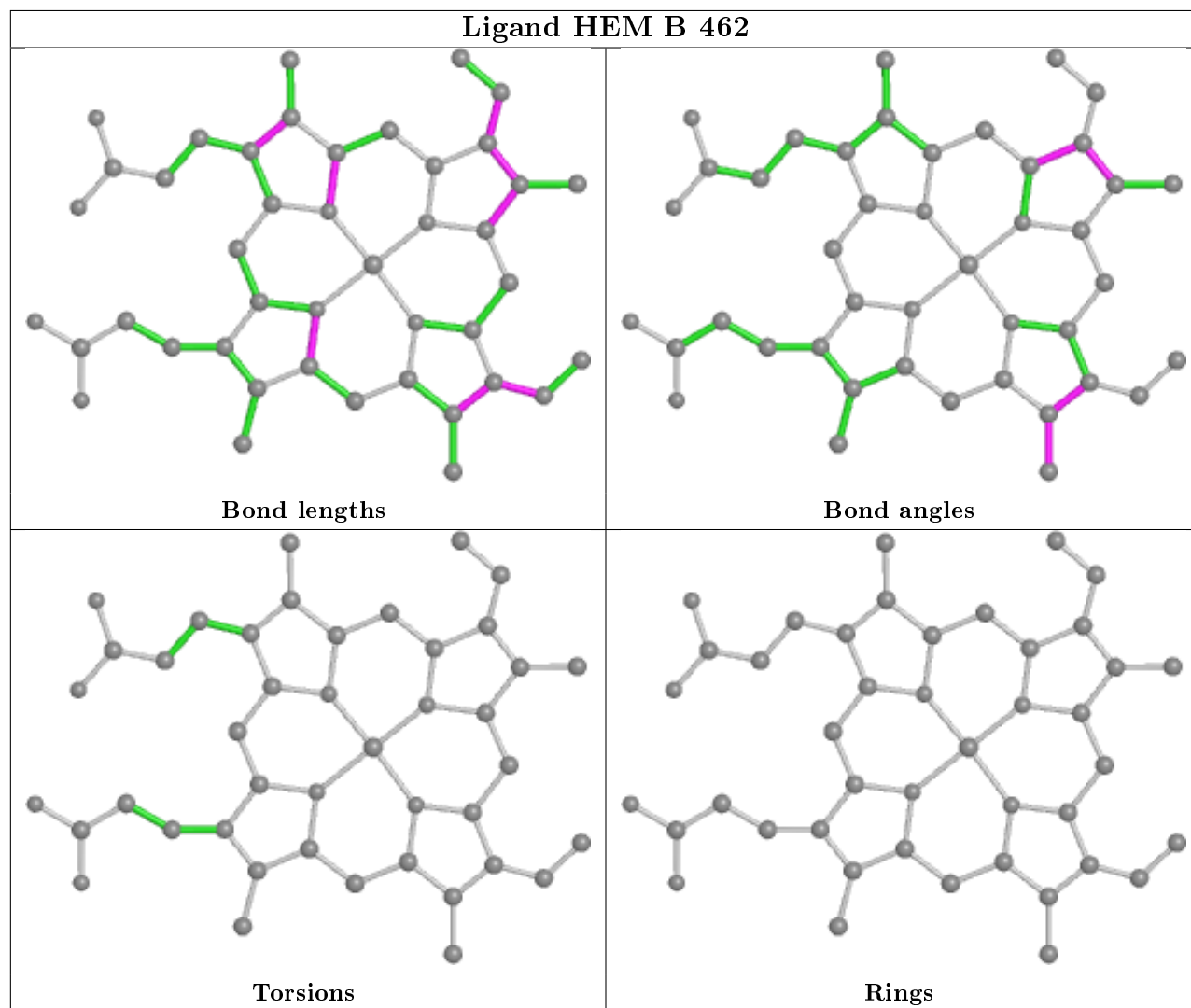
There are no ring outliers.

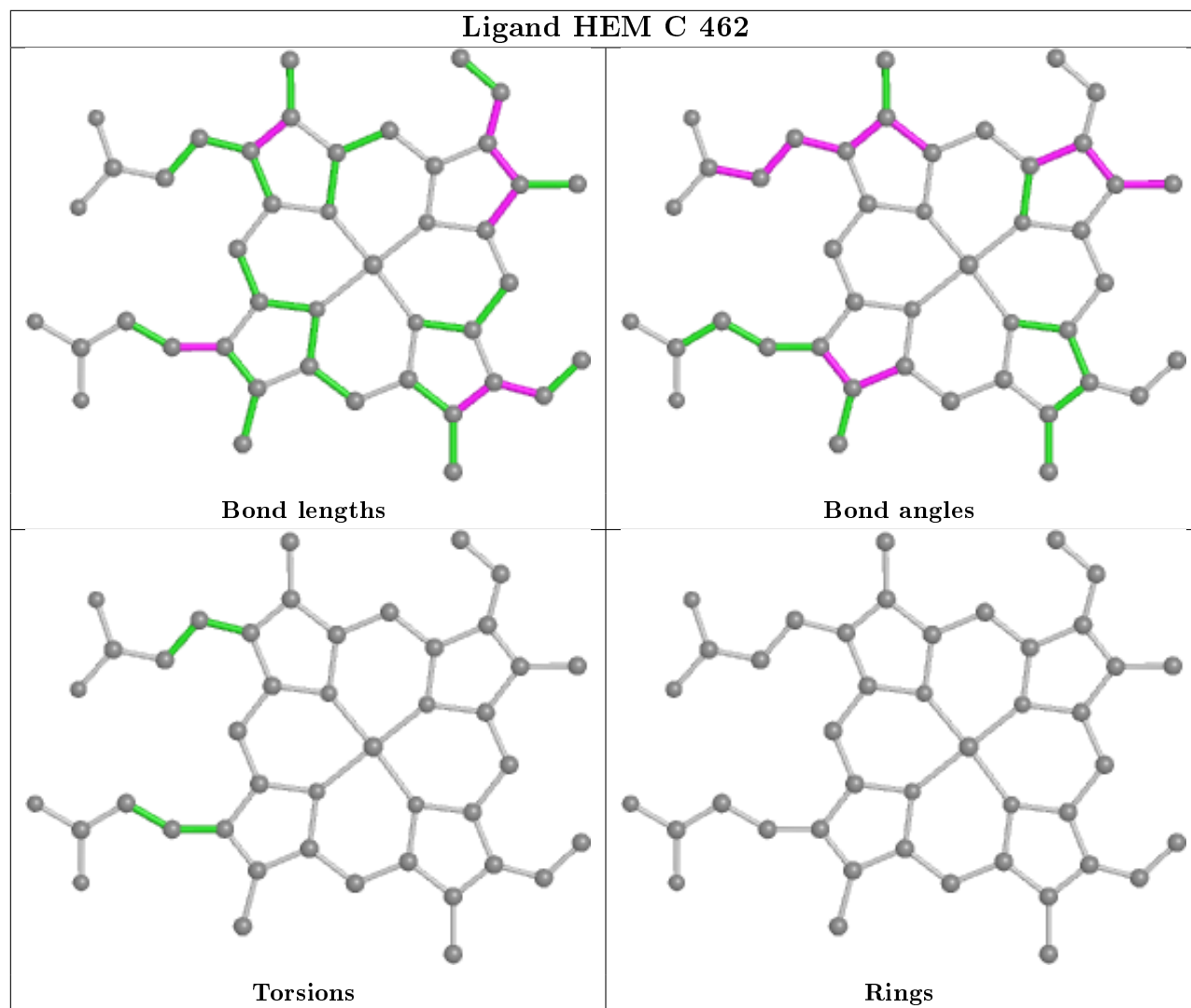
5 monomers are involved in 10 short contacts:

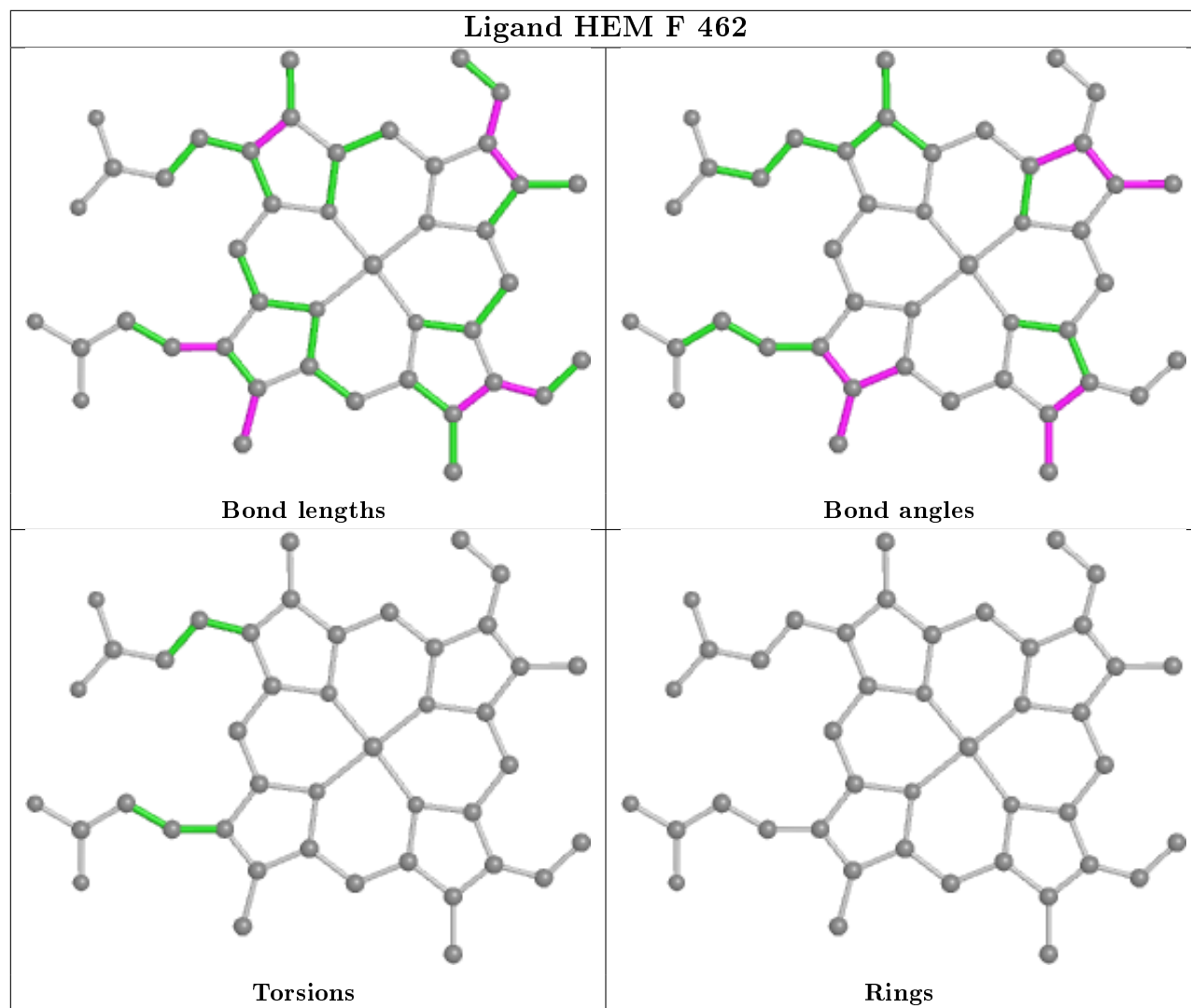
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	462	HEM	2	0
3	F	462	HEM	1	0
3	A	462	HEM	4	0
3	E	462	HEM	2	0
3	D	462	HEM	1	0

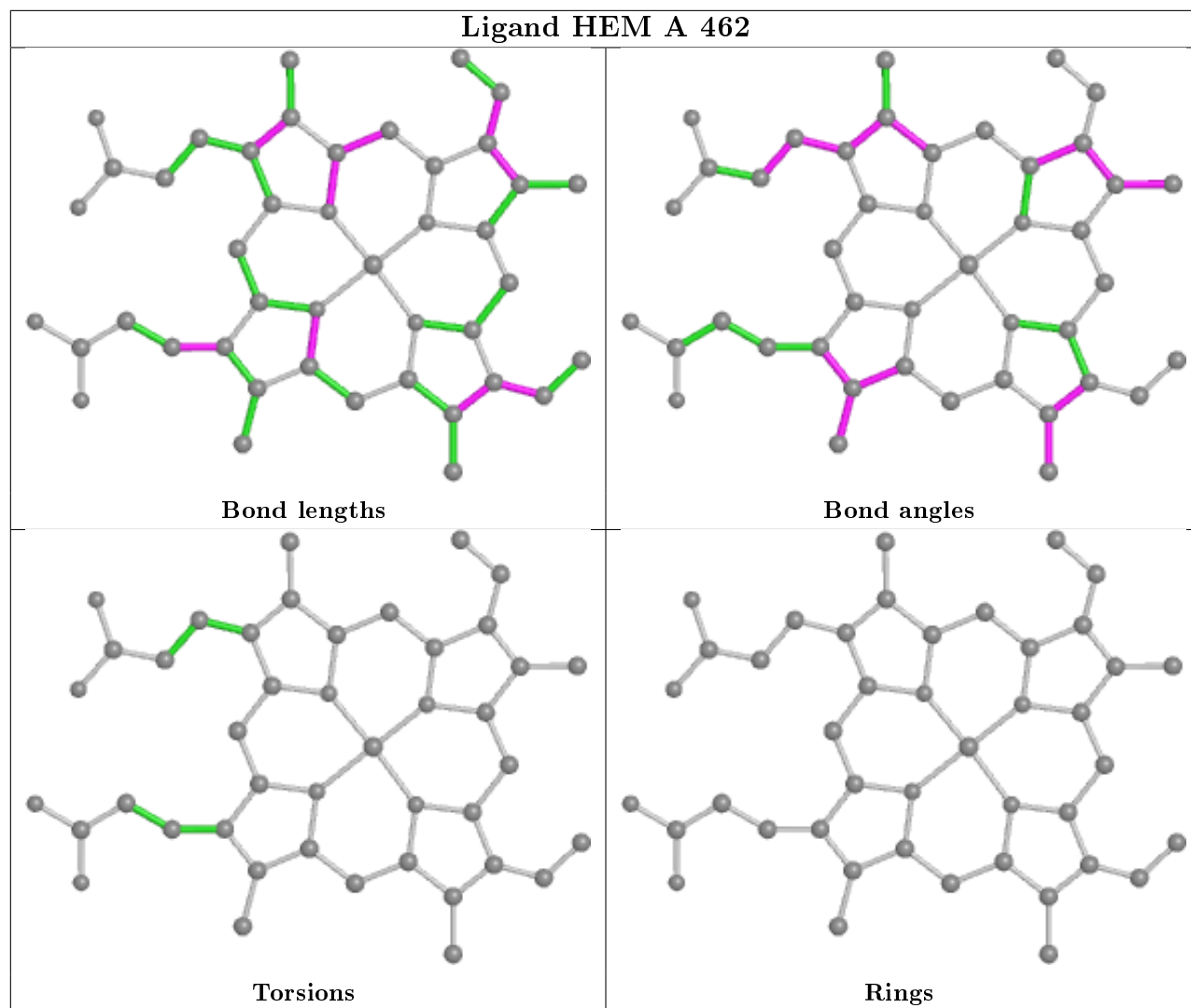
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

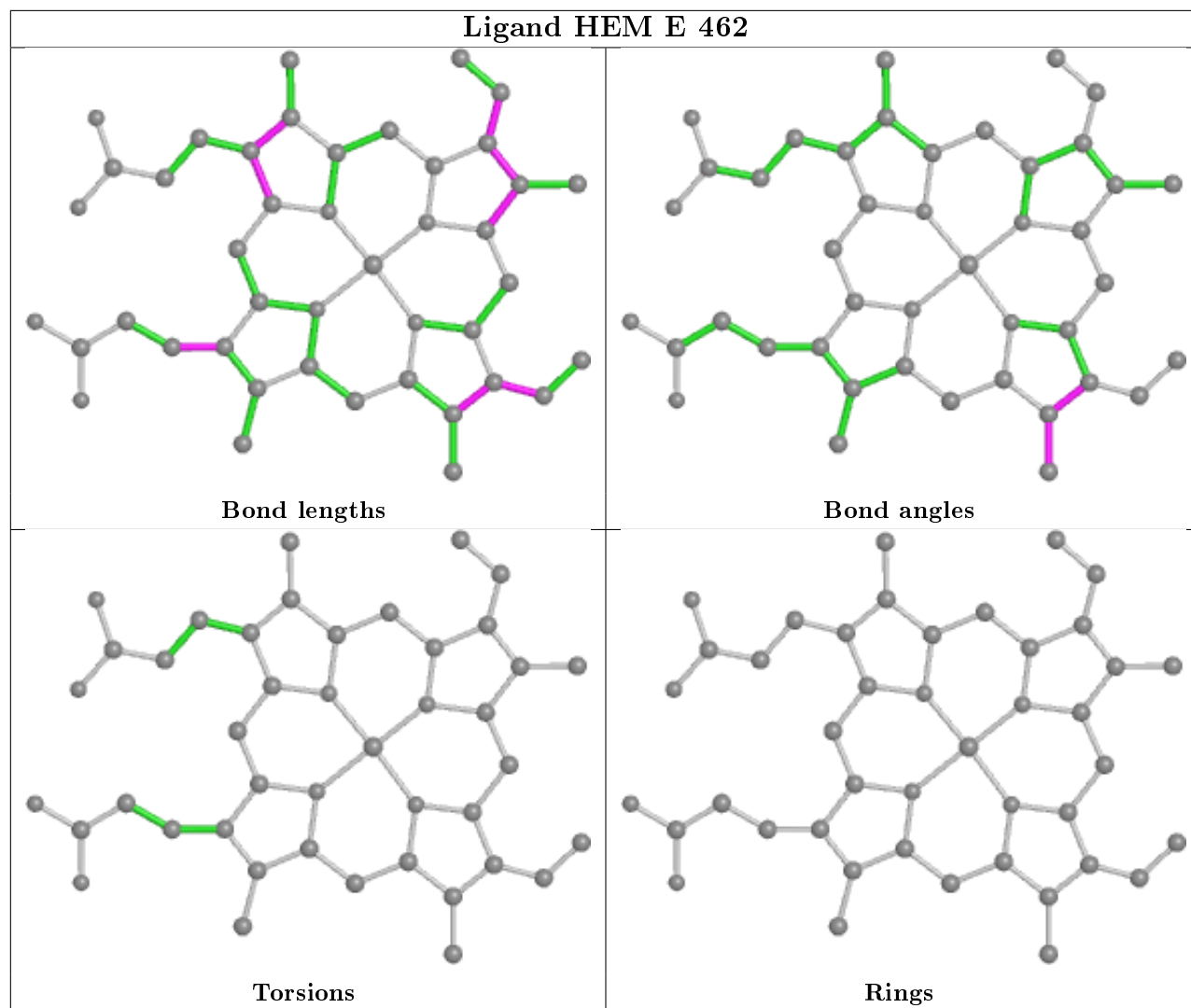


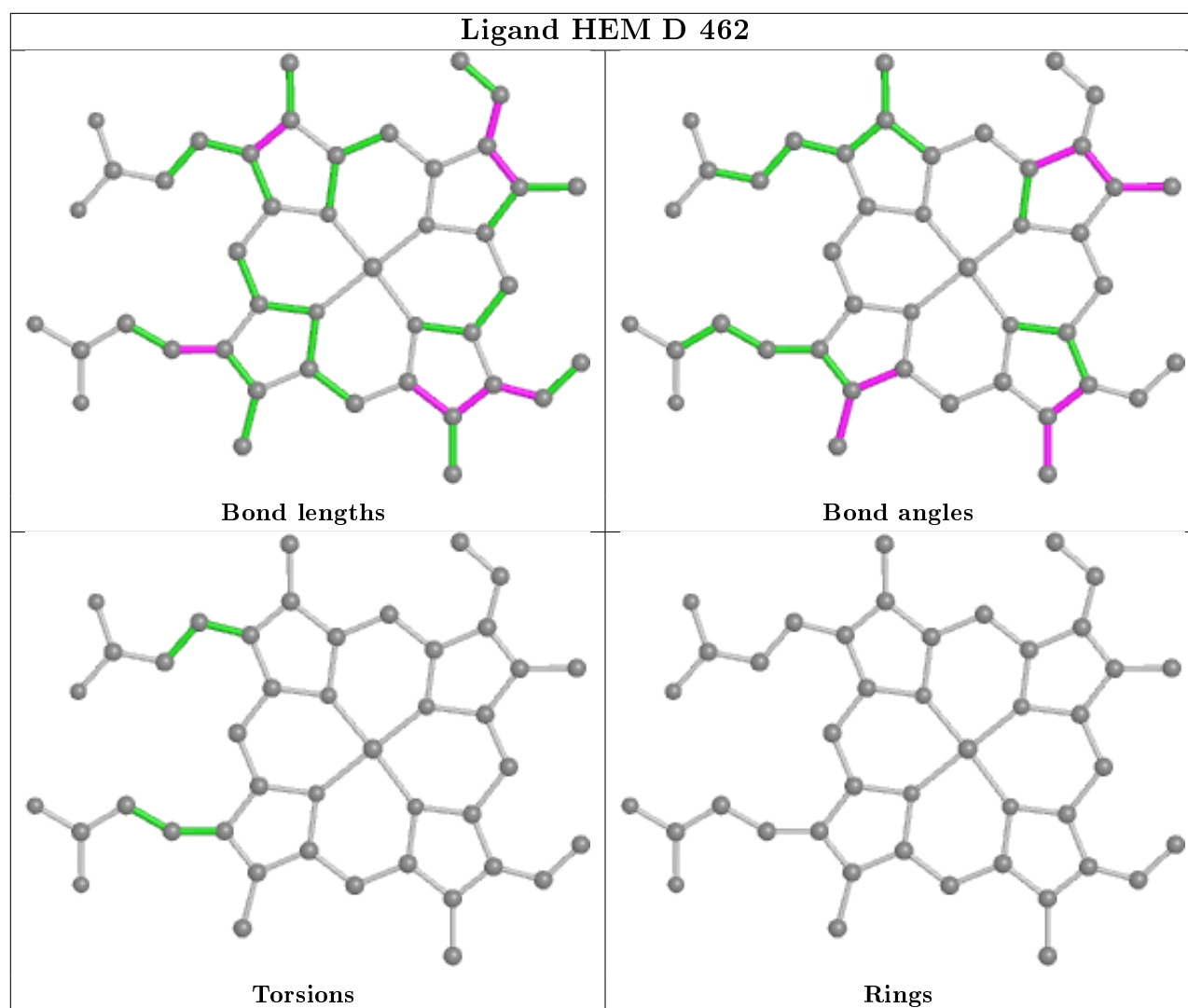












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [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, 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	392/396 (98%)	0.25	29 (7%) 14 13	16, 27, 47, 63	0
1	B	390/396 (98%)	0.40	35 (8%) 9 8	16, 28, 48, 67	0
1	C	394/396 (99%)	0.17	13 (3%) 46 43	17, 26, 39, 44	0
1	D	391/396 (98%)	-0.01	12 (3%) 49 46	16, 24, 41, 50	0
1	E	387/396 (97%)	-0.15	6 (1%) 72 71	14, 21, 31, 40	0
1	F	384/396 (96%)	0.07	21 (5%) 25 22	16, 24, 42, 62	0
All	All	2338/2376 (98%)	0.12	116 (4%) 28 26	14, 25, 42, 67	0

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	218	VAL	8.4
1	B	107	PRO	6.5
1	B	5	VAL	6.4
1	E	5	VAL	6.2
1	F	216	SER	6.1
1	B	218	VAL	5.7
1	F	217	HIS	5.6
1	F	92	ALA	5.5
1	B	216	SER	5.3
1	A	5	VAL	5.2
1	E	4	THR	5.1
1	D	107	PRO	5.0
1	B	4	THR	5.0
1	B	217	HIS	4.9
1	D	108	GLY	4.9
1	D	106	ALA	4.8
1	B	108	GLY	4.8
1	B	215	TYR	4.8
1	A	217	HIS	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	99	MET	4.6
1	B	214	ALA	4.5
1	A	215	TYR	4.4
1	A	214	ALA	4.4
1	C	216[A]	SER	4.3
1	C	107	PRO	4.3
1	C	217	HIS	4.3
1	A	213	PRO	4.1
1	C	92	ALA	4.0
1	A	211	LYS	4.0
1	B	92	ALA	4.0
1	B	106	ALA	4.0
1	F	93	GLY	3.9
1	A	91	ASP	3.9
1	B	109	LEU	3.8
1	A	93	GLY	3.8
1	B	93	GLY	3.8
1	A	92	ALA	3.8
1	C	5	VAL	3.6
1	B	104	PRO	3.5
1	A	218	VAL	3.5
1	B	86	MET	3.5
1	C	218	VAL	3.5
1	B	7	LEU	3.4
1	A	107	PRO	3.3
1	F	196	PRO	3.3
1	A	94	LEU	3.3
1	A	86	MET	3.3
1	A	210	ARG	3.3
1	F	197	ASN	3.2
1	B	105	LYS	3.1
1	D	105	LYS	3.1
1	A	216	SER	3.0
1	F	208	ARG	3.0
1	B	209	LEU	3.0
1	A	236	ILE	3.0
1	B	96	LYS	3.0
1	B	223	PHE	3.0
1	F	209	LEU	2.9
1	D	197	ASN	2.8
1	C	328	ASP	2.8
1	B	198	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	208	ARG	2.8
1	B	89	ILE	2.7
1	F	220	ASP	2.7
1	A	220	ASP	2.7
1	C	108	GLY	2.6
1	B	91	ASP	2.6
1	B	244[A]	THR	2.6
1	F	91	ASP	2.6
1	D	280	PHE	2.6
1	B	219	SER	2.6
1	F	83	VAL	2.5
1	A	96	LYS	2.5
1	A	6	LEU	2.5
1	D	236	ILE	2.5
1	E	308	LEU	2.5
1	A	162	ARG	2.4
1	A	11	PHE	2.4
1	B	94	LEU	2.4
1	B	97	ALA	2.4
1	B	111	GLN	2.4
1	F	6	LEU	2.4
1	F	199	THR	2.4
1	A	158	PRO	2.3
1	F	95	ARG	2.3
1	A	209	LEU	2.3
1	D	217	HIS	2.3
1	E	194	GLU	2.3
1	B	103	THR	2.3
1	B	210	ARG	2.3
1	F	7	LEU	2.2
1	A	27	THR	2.2
1	F	223	PHE	2.2
1	D	111	GLN	2.2
1	C	242	LEU	2.2
1	F	284	LEU	2.2
1	F	90	ALA	2.2
1	B	220	ASP	2.2
1	D	211	LYS	2.2
1	A	68	ALA	2.2
1	C	90	ALA	2.2
1	C	11	PHE	2.1
1	C	309	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	7	LEU	2.1
1	F	89	ILE	2.1
1	B	90	ALA	2.1
1	F	86	MET	2.1
1	C	3	ALA	2.1
1	E	280	PHE	2.1
1	A	108	GLY	2.1
1	A	197	ASN	2.1
1	D	210	ARG	2.0
1	A	87	GLY	2.0
1	B	123	ASN	2.0
1	A	90	ALA	2.0
1	E	284	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 carbohydrates 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
2	SO4	B	2821	5/5	0.93	0.20	51,53,55,56	0
2	SO4	C	2822	5/5	0.95	0.13	28,34,34,35	0
3	HEM	B	462	43/43	0.96	0.12	18,22,31,33	0
3	HEM	F	462	43/43	0.98	0.11	15,18,24,28	0
2	SO4	A	2820	5/5	0.98	0.18	38,38,41,42	0
3	HEM	C	462	43/43	0.98	0.09	17,20,27,29	0
3	HEM	D	462	43/43	0.98	0.12	15,18,23,25	0
3	HEM	A	462	43/43	0.98	0.12	15,17,24,26	0
3	HEM	E	462	43/43	0.98	0.10	12,15,20,24	0
2	SO4	D	2823	5/5	0.98	0.07	24,25,27,29	0

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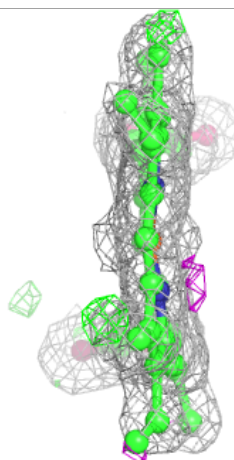
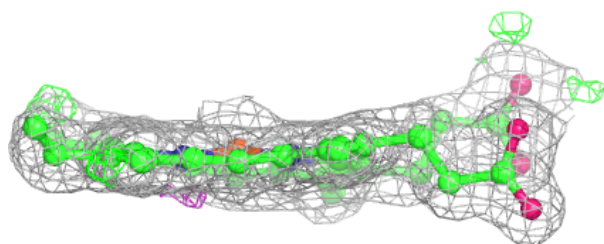
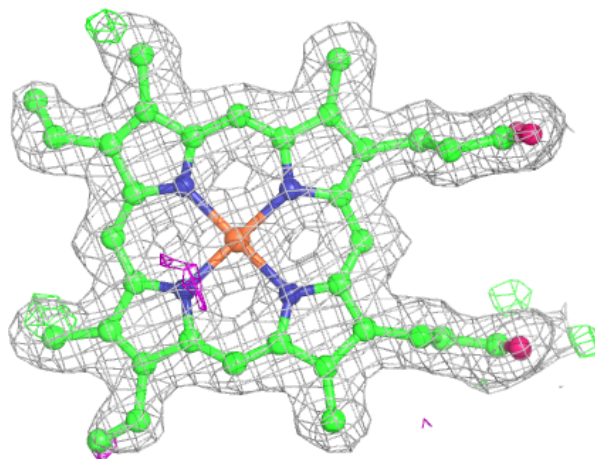
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	E	2824	5/5	0.99	0.04	23,23,24,25	0
2	SO4	F	2825	5/5	0.99	0.07	26,28,28,33	0

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.

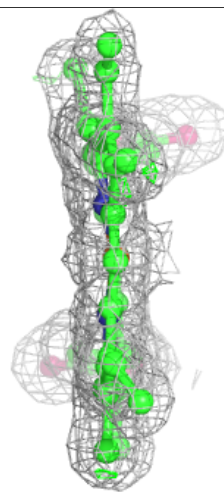
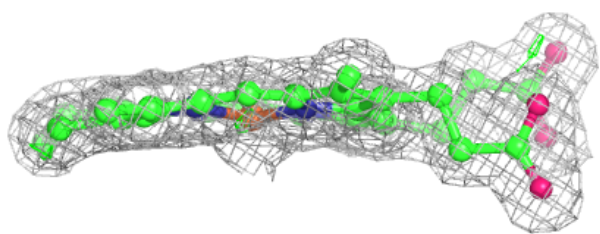
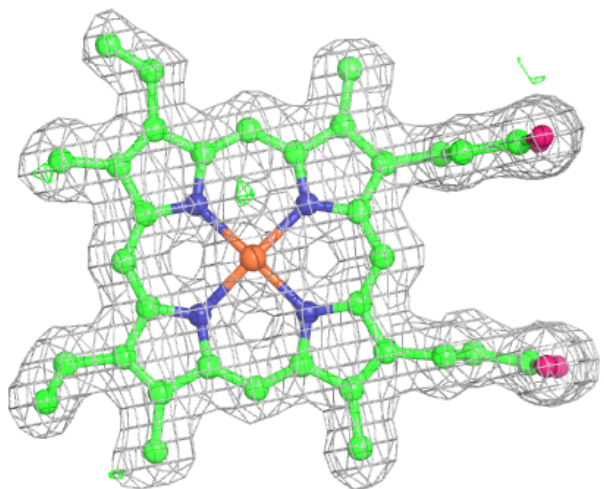
**Electron density around HEM B 462:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEM F 462:**

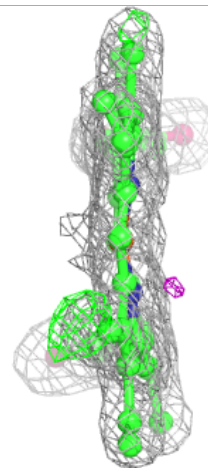
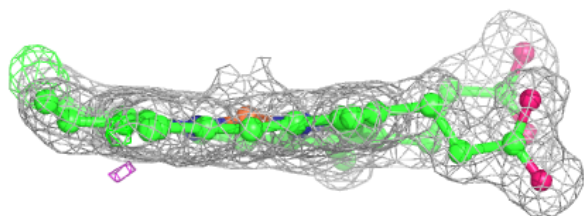
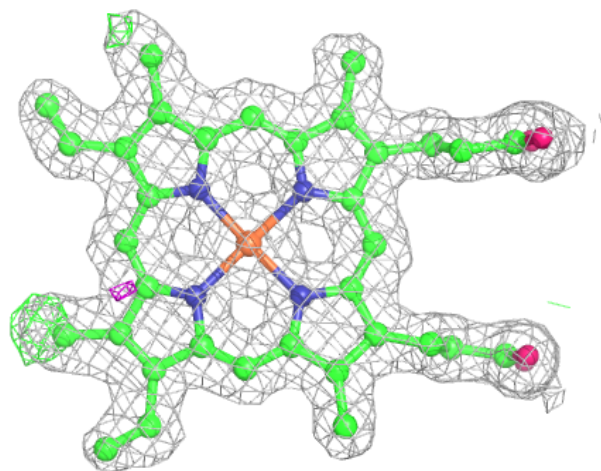
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





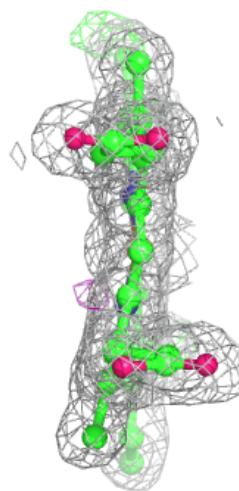
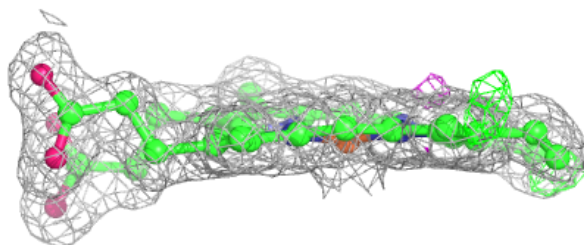
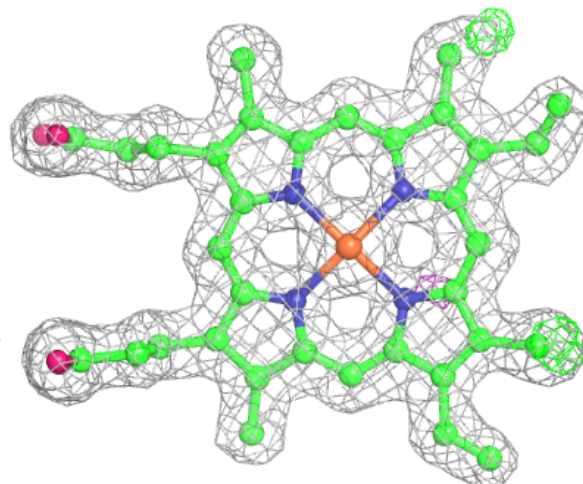
**Electron density around HEM C 462:**

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



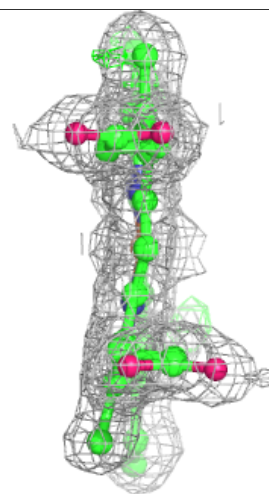
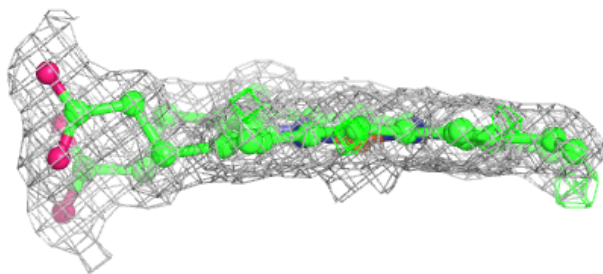
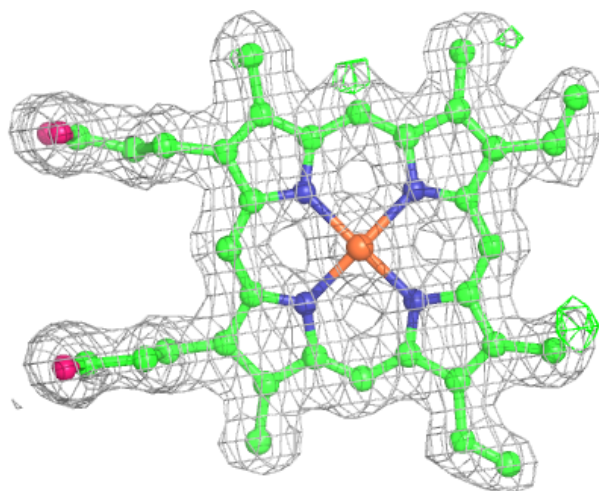
**Electron density around HEM D 462:**

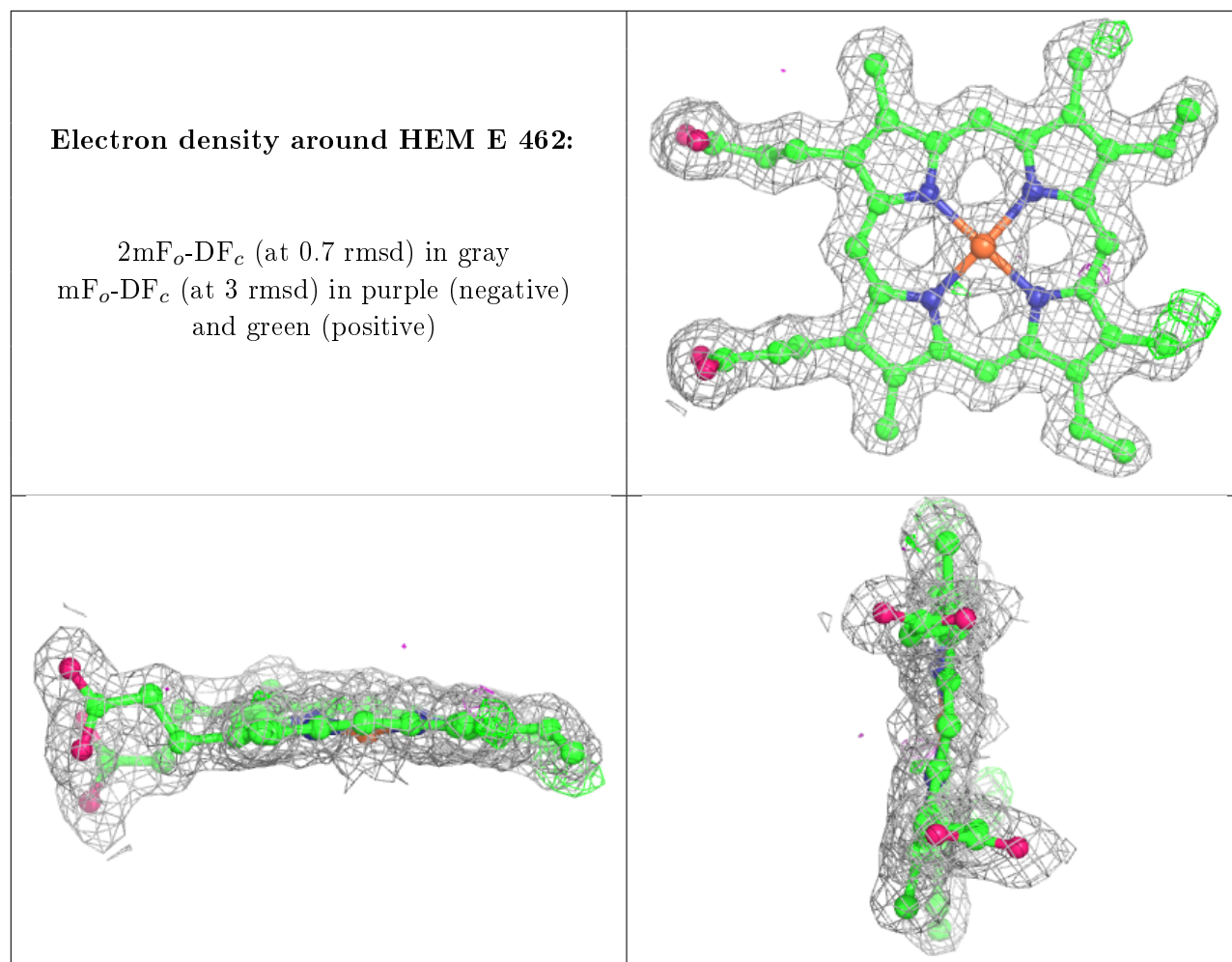
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEM A 462:**

$2mF_o-DF_c$  (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.