



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 02:12 am BST

PDB ID : 5IT1
Title : Streptomyces peucetius CYP105P2 complex with biphenyl compound
Authors : Lee, C.W.; Lee, J.H.
Deposited on : 2016-03-16
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The 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

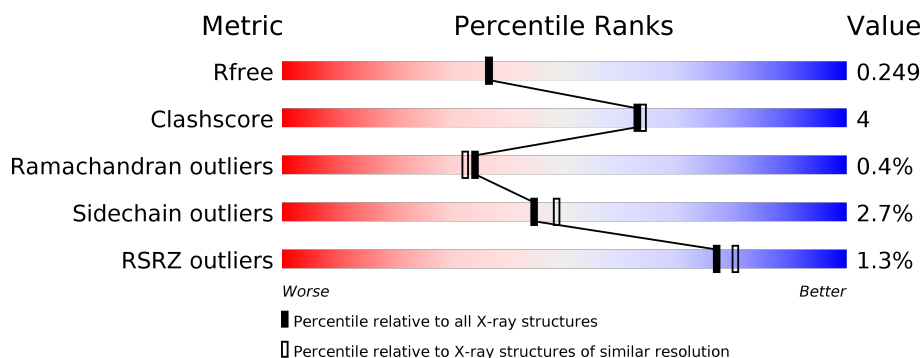
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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.



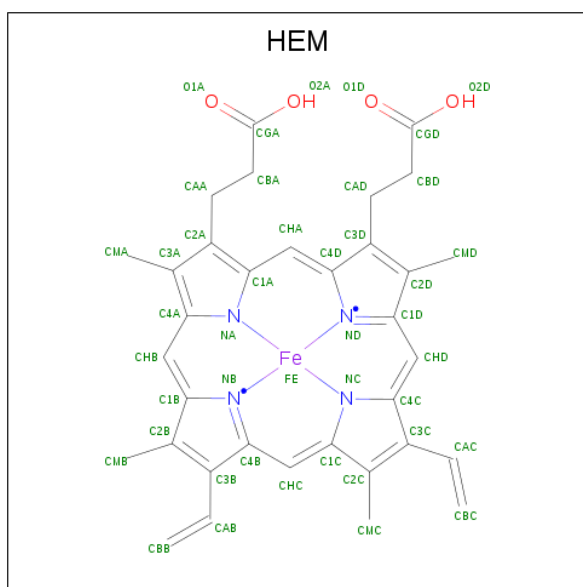
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 ≥ 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	399	<div> <div> <div>0%</div> <div>88%</div> <div>10%</div> <div>..</div> </div> </div>
1	B	399	<div> <div> <div>0%</div> <div>87%</div> <div>11%</div> <div>..</div> </div> </div>
1	C	399	<div> <div> <div>2%</div> <div>89%</div> <div>9%</div> <div>..</div> </div> </div>
1	D	399	<div> <div> <div>2%</div> <div>88%</div> <div>11%</div> <div>..</div> </div> </div>

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



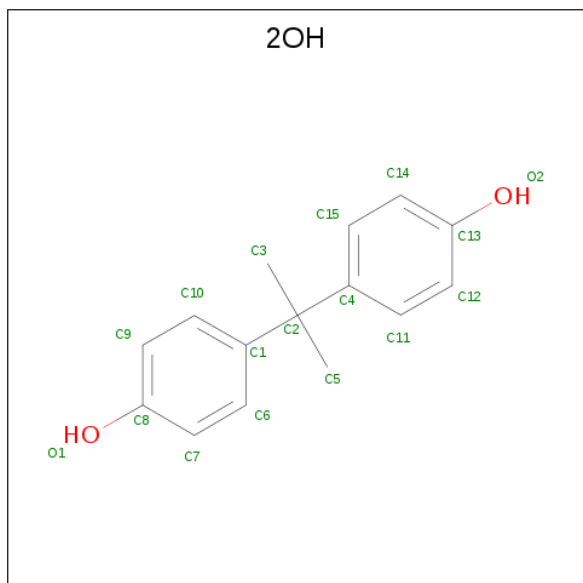
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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	

- Molecule 3 is 4,4'-PROPANE-2,2-DIYLDIPHENOL (three-letter code: 2OH) (formula: C₁₅H₁₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O		
			17	15	2		
3	B	1	Total	C	O		
			17	15	2		
3	C	1	Total	C	O		
			17	15	2		
3	D	1	Total	C	O		
			17	15	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	155	Total	O		
			155	155		
4	B	177	Total	O		
			177	177		
4	C	164	Total	O		
			164	164		

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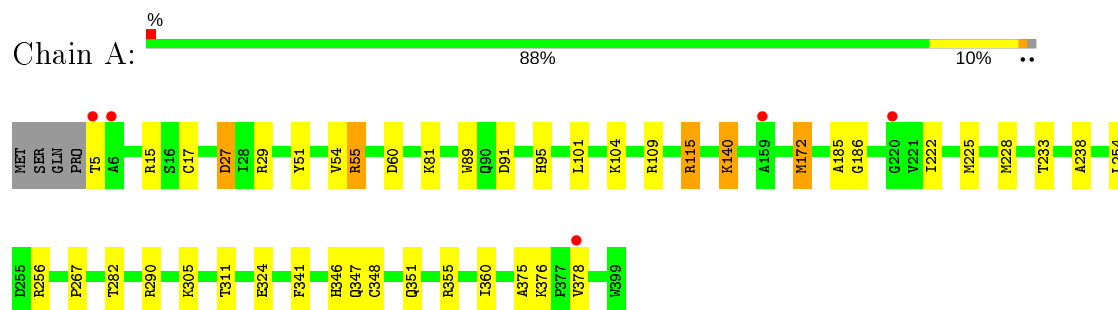
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	161	Total 161	O 161	0	0

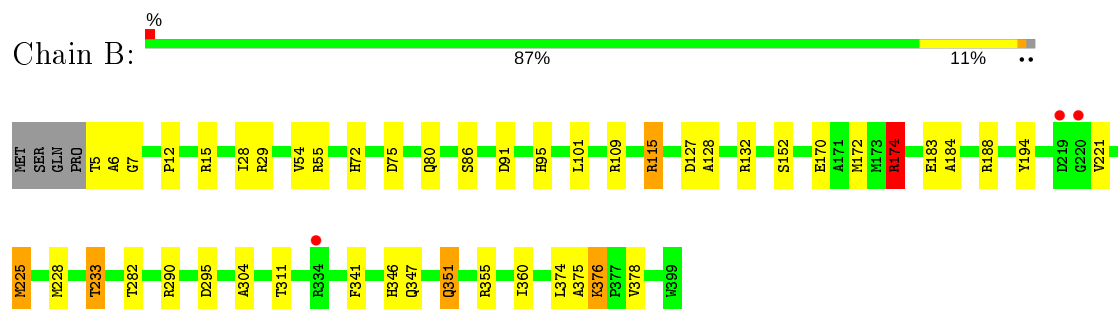
3 Residue-property plots [i](#)

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.

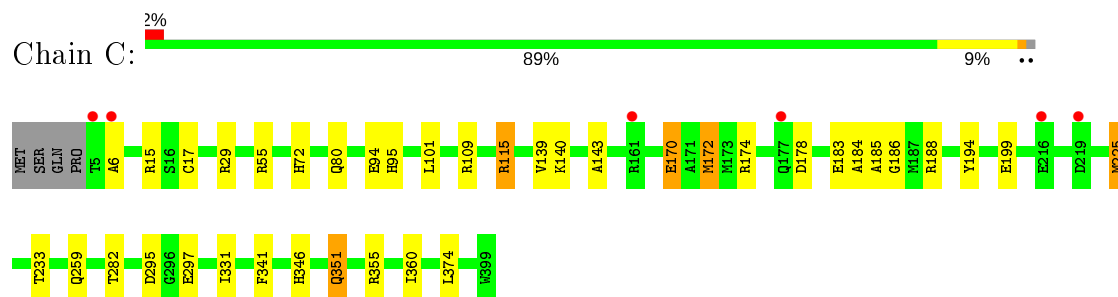
• Molecule 1: Putative cytochrome P450



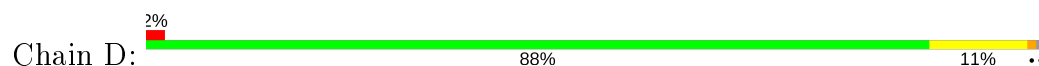
• Molecule 1: Putative cytochrome P450

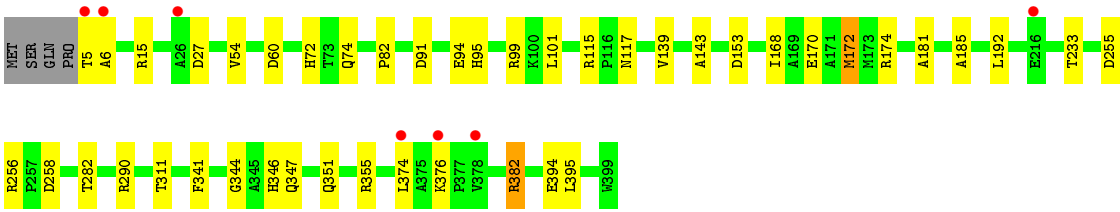


• Molecule 1: Putative cytochrome P450



• Molecule 1: Putative cytochrome P450





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	123.02Å 122.94Å 193.29Å 90.00° 90.03° 90.00°	Depositor
Resolution (Å)	50.00 – 2.10 38.01 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.9 (50.00-2.10) 98.9 (38.01-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.45 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.200 , 0.243 0.208 , 0.249	Depositor DCC
R_{free} test set	8315 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	41.8	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 34.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.428 for k,h,-l 0.437 for -k,-h,-l 0.460 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13065	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² 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: 2OH, HEM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.93	0/3106	1.04	12/4224 (0.3%)
1	B	0.93	2/3106 (0.1%)	1.00	15/4224 (0.4%)
1	C	0.94	1/3106 (0.0%)	1.00	10/4224 (0.2%)
1	D	0.92	0/3106	0.99	12/4224 (0.3%)
All	All	0.93	3/12424 (0.0%)	1.01	49/16896 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	351	GLN	CB-CG	-5.15	1.38	1.52
1	C	199	GLU	CG-CD	5.05	1.59	1.51
1	B	233	THR	CB-CG2	-5.04	1.35	1.52

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	29	ARG	NE-CZ-NH1	12.03	126.32	120.30
1	A	55	ARG	NE-CZ-NH2	-10.46	115.07	120.30
1	A	29	ARG	NE-CZ-NH2	-9.85	115.38	120.30
1	C	29	ARG	NE-CZ-NH1	9.71	125.16	120.30
1	D	172	MET	CG-SD-CE	-8.30	86.92	100.20
1	C	29	ARG	NE-CZ-NH2	-8.01	116.29	120.30
1	A	15	ARG	NE-CZ-NH1	7.83	124.22	120.30
1	C	225	MET	CG-SD-CE	-7.26	88.58	100.20
1	A	91	ASP	CB-CG-OD1	7.13	124.72	118.30
1	B	174	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	C	15	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	D	15	ARG	NE-CZ-NH1	6.85	123.72	120.30
1	B	75	ASP	CB-CG-OD1	6.75	124.38	118.30
1	B	29	ARG	NE-CZ-NH1	6.73	123.66	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	172	MET	CG-SD-CE	6.73	110.97	100.20
1	A	172	MET	CG-SD-CE	-6.72	89.45	100.20
1	A	55	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	C	172	MET	CG-SD-CE	-6.66	89.54	100.20
1	B	233	THR	N-CA-CB	6.41	122.47	110.30
1	A	290	ARG	NE-CZ-NH1	6.33	123.47	120.30
1	C	295	ASP	CB-CG-OD1	6.19	123.87	118.30
1	D	91	ASP	CB-CG-OD1	6.18	123.86	118.30
1	B	75	ASP	CB-CG-OD2	-6.12	112.79	118.30
1	B	101	LEU	CA-CB-CG	6.11	129.36	115.30
1	A	347	GLN	CB-CA-C	-6.10	98.20	110.40
1	A	101	LEU	CA-CB-CG	5.94	128.97	115.30
1	B	15	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	D	290	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	B	29	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	D	258	ASP	N-CA-CB	-5.62	100.48	110.60
1	B	225	MET	CG-SD-CE	-5.54	91.33	100.20
1	B	295	ASP	CB-CG-OD1	5.53	123.27	118.30
1	D	99	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	D	174	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	A	60	ASP	CB-CG-OD1	5.47	123.22	118.30
1	D	60	ASP	CB-CG-OD1	5.41	123.17	118.30
1	C	101	LEU	CA-CB-CG	5.38	127.67	115.30
1	B	290	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	B	91	ASP	CB-CG-OD1	5.37	123.13	118.30
1	B	55	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	C	55	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	B	127	ASP	CB-CG-OD1	5.26	123.03	118.30
1	C	351	GLN	CB-CA-C	-5.19	100.03	110.40
1	D	101	LEU	CA-CB-CG	5.17	127.20	115.30
1	A	256	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	D	374	LEU	CA-CB-CG	5.13	127.11	115.30
1	D	290	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	D	382	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	C	178	ASP	CB-CG-OD2	5.04	122.84	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	3042	0	3032	21	0
1	B	3042	0	3032	42	0
1	C	3042	0	3032	40	0
1	D	3042	0	3032	22	0
2	A	43	0	30	5	0
2	B	43	0	30	2	0
2	C	43	0	30	3	0
2	D	43	0	30	4	0
3	A	17	0	15	0	0
3	B	17	0	15	3	0
3	C	17	0	15	0	0
3	D	17	0	15	0	0
4	A	155	0	0	2	0
4	B	177	0	0	2	0
4	C	164	0	0	5	0
4	D	161	0	0	3	0
All	All	13065	0	12308	107	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 4.

All (107) 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:225:MET:HE1	1:C:184:ALA:HA	1.40	1.02
1:B:351:GLN:HE21	1:B:355:ARG:HH12	1.19	0.90
1:D:351:GLN:HE21	1:D:355:ARG:HH12	1.21	0.87
1:C:351:GLN:HE21	1:C:355:ARG:HH12	1.19	0.86
1:A:172:MET:HE1	1:A:185:ALA:C	1.99	0.83
1:A:17:CYS:HB3	4:A:636:HOH:O	1.79	0.81
1:A:351:GLN:HE21	1:A:355:ARG:HH12	1.29	0.81
1:B:225:MET:CE	1:C:184:ALA:HA	2.11	0.81
1:B:184:ALA:N	1:C:225:MET:HE1	1.97	0.79
1:B:184:ALA:HA	1:C:225:MET:HE1	1.64	0.79
1:B:233:THR:HG22	3:B:402:2OH:O2	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:17:CYS:HB3	4:C:645:HOH:O	1.83	0.78
1:B:225:MET:HE1	1:C:184:ALA:CA	2.13	0.77
1:B:184:ALA:CA	1:C:225:MET:HE1	2.16	0.75
1:C:95:HIS:HD2	4:C:567:HOH:O	1.68	0.75
1:C:172:MET:HE1	1:C:185:ALA:C	2.08	0.74
1:B:225:MET:CE	1:C:184:ALA:CA	2.67	0.72
1:B:183:GLU:C	1:C:225:MET:HE1	2.11	0.71
1:B:95:HIS:HD2	4:B:545:HOH:O	1.75	0.69
1:B:225:MET:CE	1:C:184:ALA:N	2.54	0.69
1:B:86:SER:O	1:B:233:THR:HG21	1.92	0.68
1:A:95:HIS:HD2	4:A:569:HOH:O	1.76	0.66
1:D:95:HIS:HD2	4:D:532:HOH:O	1.77	0.66
1:B:184:ALA:N	1:C:225:MET:CE	2.59	0.65
1:C:297:GLU:HG2	4:C:509:HOH:O	1.98	0.63
1:C:72:HIS:HD2	4:C:513:HOH:O	1.80	0.63
1:D:255:ASP:OD2	1:D:256:ARG:NH1	2.34	0.61
1:D:172:MET:HE1	1:D:185:ALA:C	2.22	0.60
1:C:115:ARG:HG2	1:C:360:ILE:HD11	1.82	0.60
1:C:351:GLN:HE21	1:C:355:ARG:NH1	1.96	0.58
1:C:170:GLU:OE2	1:C:174:ARG:NH2	2.37	0.58
1:A:346:HIS:HD2	2:A:401:HEM:O2A	1.87	0.57
1:B:225:MET:HE3	1:C:184:ALA:N	2.17	0.57
1:D:72:HIS:HD2	4:D:509:HOH:O	1.87	0.57
1:B:72:HIS:HD2	4:B:512:HOH:O	1.87	0.56
1:A:172:MET:HE1	1:A:186:GLY:N	2.21	0.55
1:B:184:ALA:CA	1:C:225:MET:CE	2.84	0.55
1:C:346:HIS:HD2	2:C:401:HEM:O1A	1.91	0.54
1:D:192:LEU:C	1:D:192:LEU:HD23	2.29	0.53
1:C:172:MET:HE1	1:C:185:ALA:O	2.07	0.53
2:C:401:HEM:HMC1	2:C:401:HEM:HBC2	1.89	0.53
1:B:225:MET:CE	1:C:183:GLU:C	2.77	0.53
1:B:184:ALA:HA	1:C:225:MET:CE	2.36	0.52
1:D:382:ARG:HH12	1:D:394:GLU:HG2	1.74	0.52
1:D:54:VAL:HG13	1:D:311:THR:HB	1.92	0.52
1:B:80:GLN:HG2	1:C:80:GLN:NE2	2.24	0.52
1:B:115:ARG:HG2	1:B:360:ILE:HD11	1.91	0.52
1:D:382:ARG:NH1	1:D:394:GLU:HG2	2.26	0.51
1:B:346:HIS:HD2	2:B:401:HEM:O1D	1.94	0.51
1:B:5:THR:O	1:B:6:ALA:HB3	2.11	0.51
1:C:341:PHE:CG	1:C:351:GLN:HG2	2.46	0.51
1:A:225:MET:HA	1:A:228:MET:HE3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:259:GLN:NE2	1:C:331:ILE:H	2.09	0.49
1:D:82:PRO:HD3	1:D:181:ALA:HB2	1.94	0.49
1:B:225:MET:HE3	1:C:183:GLU:C	2.32	0.49
1:A:375:ALA:O	1:A:376:LYS:HG3	2.12	0.49
1:B:233:THR:HG22	3:B:402:2OH:HO2	1.77	0.49
1:A:267:PRO:HB2	1:B:304:ALA:HB1	1.93	0.49
1:C:351:GLN:NE2	1:C:355:ARG:HH12	1.99	0.49
1:B:12:PRO:HG2	1:B:28:ILE:HD12	1.95	0.48
1:B:174:ARG:CG	1:B:174:ARG:HH11	2.26	0.48
1:B:194:TYR:CE1	1:C:188:ARG:HD2	2.48	0.48
1:A:95:HIS:HE1	2:A:401:HEM:O1A	1.96	0.48
1:D:346:HIS:HD2	2:D:401:HEM:O1D	1.96	0.48
1:A:115:ARG:HG2	1:A:360:ILE:HD11	1.95	0.48
2:D:401:HEM:HMC2	2:D:401:HEM:HBC2	1.95	0.48
1:D:168:ILE:HD12	1:D:192:LEU:HD12	1.95	0.47
1:D:172:MET:HE1	1:D:185:ALA:O	2.14	0.47
1:A:172:MET:HE2	1:A:172:MET:HA	1.97	0.47
1:D:95:HIS:HE1	2:D:401:HEM:O2D	1.96	0.46
1:A:140:LYS:HA	1:A:140:LYS:HE3	1.97	0.46
1:B:225:MET:HE1	1:C:184:ALA:N	2.27	0.46
1:D:344:GLY:O	1:D:347:GLN:HB2	2.16	0.46
1:B:225:MET:HA	1:B:228:MET:HE3	1.98	0.46
1:B:128:ALA:O	1:B:132:ARG:HG2	2.17	0.45
1:B:95:HIS:HE1	2:B:401:HEM:O2D	1.99	0.45
1:B:54:VAL:HG13	1:B:311:THR:HB	1.98	0.45
1:C:94:GLU:HG3	4:C:551:HOH:O	2.17	0.45
1:D:172:MET:HB2	1:D:172:MET:HE3	1.72	0.45
1:B:188:ARG:HD2	1:C:194:TYR:CE1	2.52	0.44
1:C:139:VAL:HA	1:C:143:ALA:HB3	2.00	0.44
1:B:341:PHE:CD2	1:B:351:GLN:HG2	2.52	0.44
1:A:341:PHE:CG	1:A:351:GLN:HG2	2.52	0.44
1:D:5:THR:OG1	1:D:6:ALA:HA	2.17	0.44
1:B:174:ARG:CG	1:B:174:ARG:NH1	2.81	0.44
1:B:225:MET:HE1	1:C:183:GLU:C	2.38	0.44
1:D:94:GLU:HG3	4:D:578:HOH:O	2.17	0.43
1:A:172:MET:HE1	1:A:185:ALA:O	2.17	0.43
1:C:95:HIS:HE1	2:C:401:HEM:O2A	2.01	0.43
2:A:401:HEM:HBC2	2:A:401:HEM:HMC1	2.00	0.42
1:A:81:LYS:HD2	1:A:89:TRP:CD2	2.54	0.42
1:B:233:THR:HG23	3:B:402:2OH:H12	2.01	0.42
2:D:401:HEM:CMB	2:D:401:HEM:HBB2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:ASP:OD1	1:A:27:ASP:N	2.38	0.42
1:A:54:VAL:HG13	1:A:311:THR:HB	2.01	0.42
1:A:348:CYS:HB2	2:A:401:HEM:ND	2.34	0.42
1:A:238:ALA:HB2	2:A:401:HEM:HMB1	2.00	0.42
1:B:375:ALA:O	1:B:376:LYS:HG2	2.20	0.42
1:A:51:TYR:CE1	1:A:55:ARG:HD2	2.55	0.42
1:D:117:ASN:HD22	1:D:117:ASN:H	1.69	0.41
1:D:341:PHE:CD2	1:D:351:GLN:HG2	2.55	0.41
1:D:395:LEU:HA	1:D:395:LEU:HD12	1.93	0.41
1:B:5:THR:HG23	1:B:7:GLY:H	1.84	0.41
1:C:172:MET:HE1	1:C:186:GLY:N	2.36	0.41
1:B:183:GLU:C	1:C:225:MET:CE	2.87	0.40
1:C:172:MET:HE2	1:C:185:ALA:HB1	2.04	0.40
1:D:139:VAL:HA	1:D:143:ALA:HB3	2.04	0.40

There are no symmetry-related clashes.

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	393/399 (98%)	383 (98%)	9 (2%)	1 (0%)	41	41
1	B	393/399 (98%)	380 (97%)	11 (3%)	2 (0%)	29	26
1	C	393/399 (98%)	381 (97%)	10 (2%)	2 (0%)	29	26
1	D	393/399 (98%)	381 (97%)	11 (3%)	1 (0%)	41	41
All	All	1572/1596 (98%)	1525 (97%)	41 (3%)	6 (0%)	34	32

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	282	THR

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Mol	Chain	Res	Type
1	B	282	THR
1	C	6	ALA
1	C	282	THR
1	D	282	THR
1	B	347	GLN

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	316/320 (99%)	304 (96%)	12 (4%)	33	34
1	B	316/320 (99%)	307 (97%)	9 (3%)	43	47
1	C	316/320 (99%)	310 (98%)	6 (2%)	57	63
1	D	316/320 (99%)	309 (98%)	7 (2%)	52	57
All	All	1264/1280 (99%)	1230 (97%)	34 (3%)	44	48

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	27	ASP
1	A	104	LYS
1	A	109	ARG
1	A	115	ARG
1	A	140	LYS
1	A	222	ILE
1	A	233	THR
1	A	254	LEU
1	A	305	LYS
1	A	324	GLU
1	A	378	VAL
1	B	109	ARG
1	B	115	ARG
1	B	152	SER
1	B	170	GLU

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Mol	Chain	Res	Type
1	B	174	ARG
1	B	221	VAL
1	B	374	LEU
1	B	376	LYS
1	B	378	VAL
1	C	109	ARG
1	C	115	ARG
1	C	140	LYS
1	C	170	GLU
1	C	233	THR
1	C	374	LEU
1	D	27	ASP
1	D	74	GLN
1	D	115	ARG
1	D	153	ASP
1	D	170	GLU
1	D	233	THR
1	D	376	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	HIS
1	A	80	GLN
1	A	95	HIS
1	A	117	ASN
1	A	346	HIS
1	A	347	GLN
1	A	351	GLN
1	B	72	HIS
1	B	95	HIS
1	B	112	GLN
1	B	117	ASN
1	B	346	HIS
1	B	347	GLN
1	B	351	GLN
1	C	72	HIS
1	C	95	HIS
1	C	112	GLN
1	C	117	ASN
1	C	259	GLN
1	C	264	GLN

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Mol	Chain	Res	Type
1	C	346	HIS
1	C	347	GLN
1	C	351	GLN
1	D	72	HIS
1	D	95	HIS
1	D	112	GLN
1	D	117	ASN
1	D	346	HIS
1	D	351	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	HEM	D	401	1	27,50,50	0.87	1 (3%)	17,82,82	1.19	2 (11%)
3	2OH	D	402	-	18,18,18	1.00	1 (5%)	26,26,26	0.73	0
3	2OH	B	402	-	18,18,18	1.03	1 (5%)	26,26,26	0.98	1 (3%)
3	2OH	C	402	-	18,18,18	0.86	0	26,26,26	1.11	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	2OH	A	402	-	18,18,18	1.00	1 (5%)	26,26,26	1.13	0
2	HEM	A	401	1	27,50,50	1.34	2 (7%)	17,82,82	1.87	6 (35%)
2	HEM	C	401	1	27,50,50	1.17	1 (3%)	17,82,82	2.06	6 (35%)
2	HEM	B	401	1	27,50,50	1.00	2 (7%)	17,82,82	1.29	2 (11%)

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	D	401	1	-	0/6/54/54	-
3	2OH	D	402	-	-	0/12/12/12	0/2/2/2
3	2OH	B	402	-	-	0/12/12/12	0/2/2/2
3	2OH	C	402	-	-	0/12/12/12	0/2/2/2
3	2OH	A	402	-	-	0/12/12/12	0/2/2/2
2	HEM	A	401	1	-	0/6/54/54	-
2	HEM	C	401	1	-	0/6/54/54	-
2	HEM	B	401	1	-	0/6/54/54	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	HEM	C3B-C2B	-3.38	1.35	1.40
3	B	402	2OH	C5-C2	-2.89	1.49	1.54
3	D	402	2OH	C3-C2	-2.86	1.49	1.54
2	C	401	HEM	C3B-C2B	-2.47	1.36	1.40
2	A	401	HEM	C4B-NB	-2.27	1.31	1.36
2	B	401	HEM	C3B-C2B	-2.26	1.37	1.40
2	D	401	HEM	C3B-C2B	-2.22	1.37	1.40
3	A	402	2OH	C5-C2	-2.12	1.51	1.54
2	B	401	HEM	CAA-C2A	2.05	1.55	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	HEM	CAA-CBA-CGA	4.36	119.98	112.67
2	C	401	HEM	C4C-C3C-C2C	3.98	109.68	106.90
2	C	401	HEM	CAA-CBA-CGA	3.68	118.84	112.67
2	C	401	HEM	CAD-CBD-CGD	-3.60	106.63	112.67
2	B	401	HEM	CAA-CBA-CGA	-3.25	107.23	112.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	HEM	C4C-C3C-C2C	3.05	109.03	106.90
2	A	401	HEM	CAD-CBD-CGD	-2.99	107.65	112.67
3	B	402	2OH	C5-C2-C3	-2.76	104.17	107.58
2	C	401	HEM	CBD-CAD-C3D	2.67	117.39	112.48
2	A	401	HEM	CBD-CAD-C3D	2.62	117.31	112.48
2	D	401	HEM	CMC-C2C-C3C	2.60	129.55	124.68
2	B	401	HEM	CMC-C2C-C3C	2.42	129.21	124.68
2	A	401	HEM	CBA-CAA-C2A	-2.35	108.16	112.49
2	C	401	HEM	C3C-C4C-NC	-2.33	106.54	110.94
2	C	401	HEM	C1D-C2D-C3D	-2.28	105.41	107.00
2	D	401	HEM	CAA-CBA-CGA	-2.18	109.01	112.67
3	C	402	2OH	C3-C2-C4	2.09	115.30	109.84
2	A	401	HEM	C3C-C4C-NC	-2.08	107.01	110.94

There are no chirality outliers.

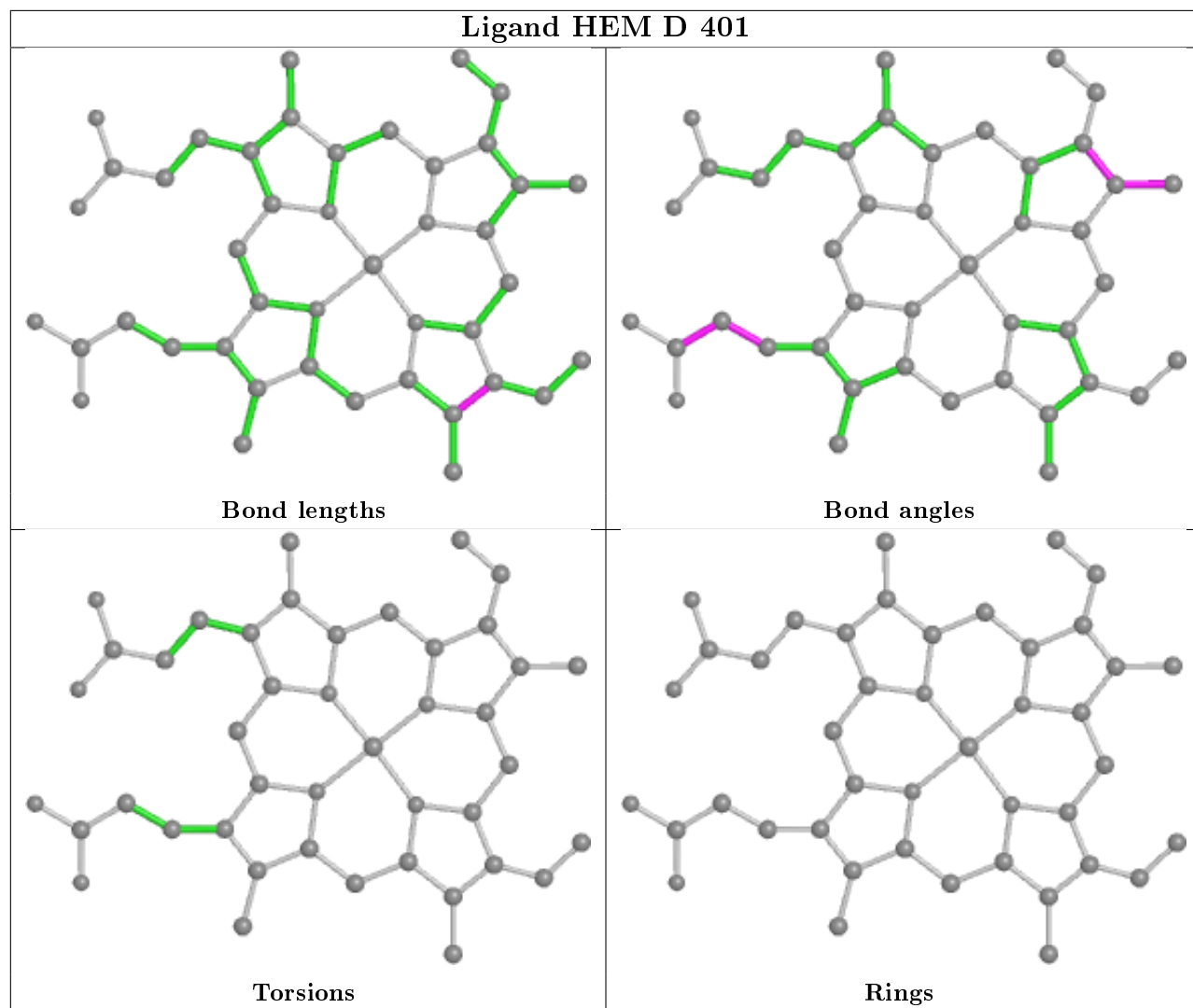
There are no torsion outliers.

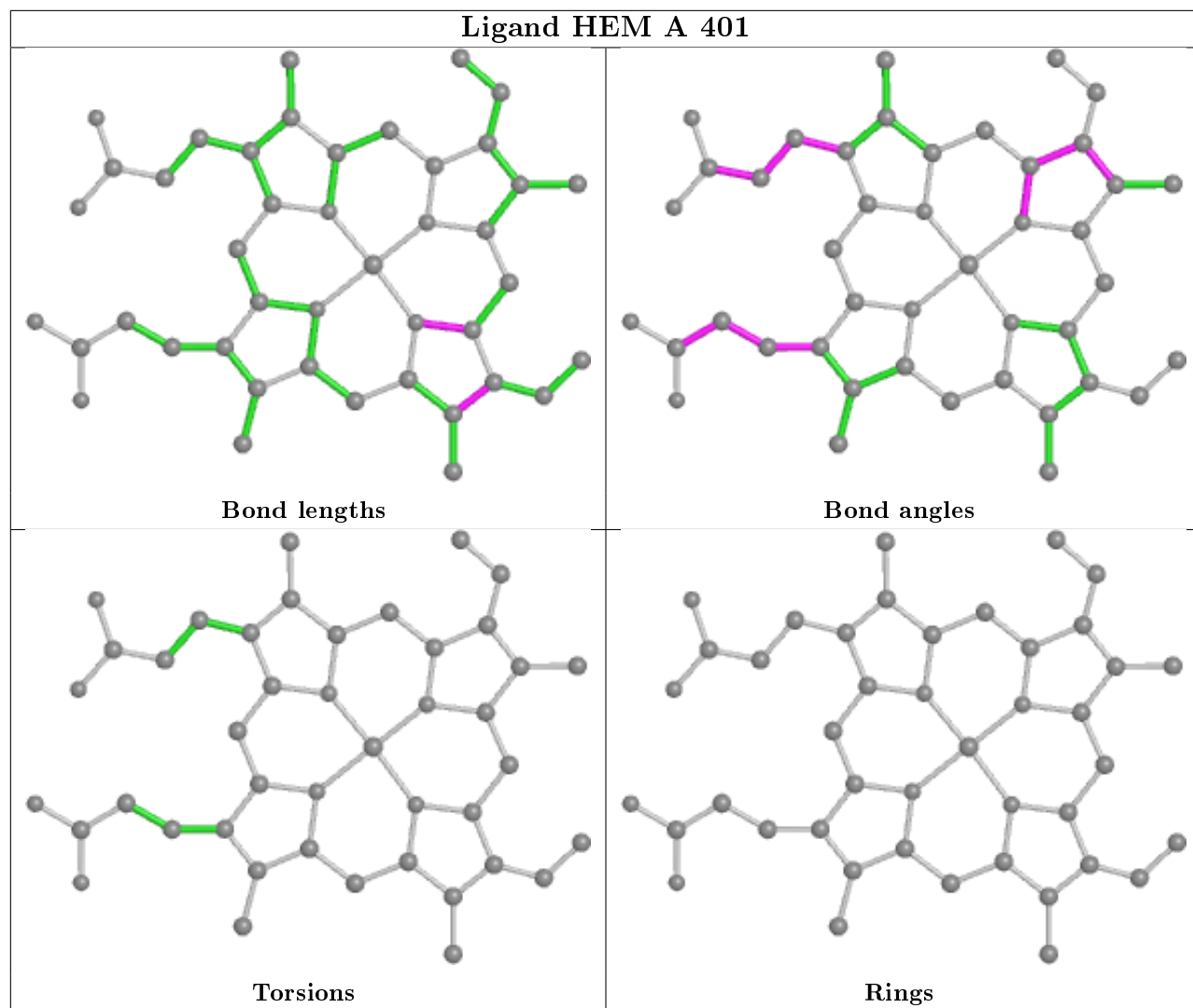
There are no ring outliers.

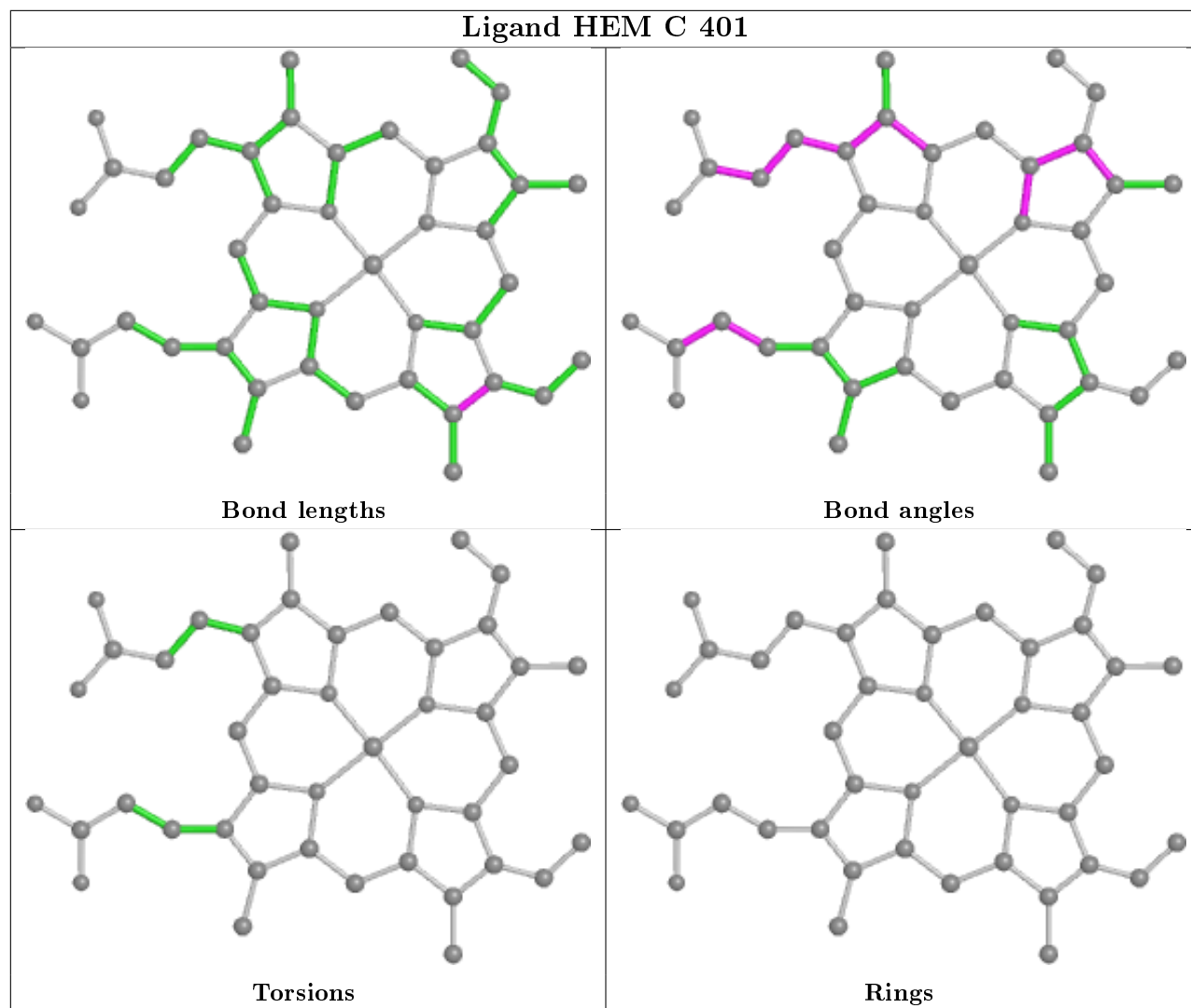
5 monomers are involved in 17 short contacts:

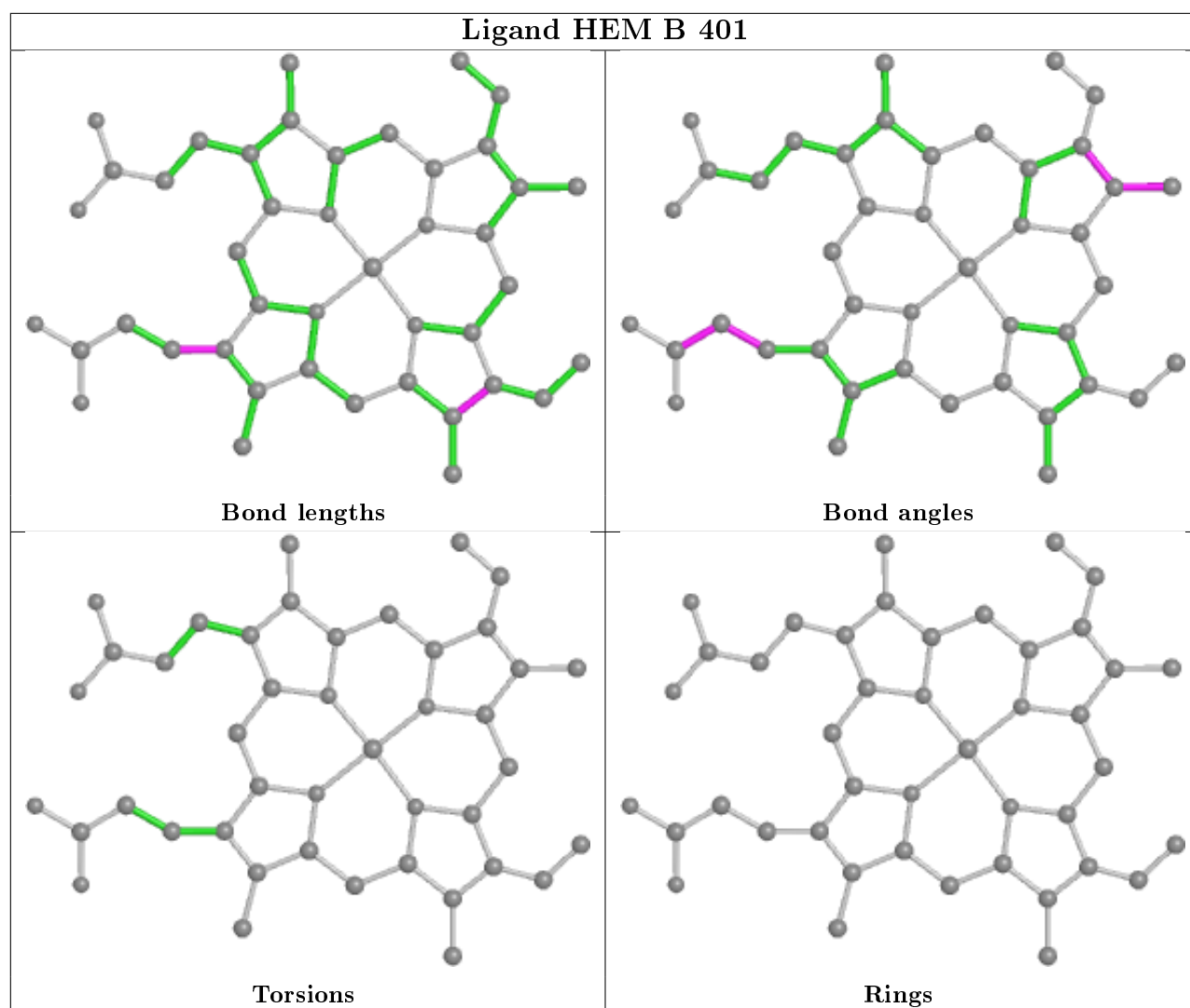
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	401	HEM	4	0
3	B	402	2OH	3	0
2	A	401	HEM	5	0
2	C	401	HEM	3	0
2	B	401	HEM	2	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	395/399 (98%)	0.22	5 (1%) 77 80	33, 45, 69, 103	0
1	B	395/399 (98%)	0.12	3 (0%) 86 88	34, 45, 69, 102	0
1	C	395/399 (98%)	0.16	6 (1%) 73 77	33, 45, 70, 103	0
1	D	395/399 (98%)	0.22	7 (1%) 68 72	33, 45, 69, 103	0
All	All	1580/1596 (98%)	0.18	21 (1%) 77 80	33, 45, 70, 103	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	5	THR	6.8
1	C	6	ALA	5.2
1	C	5	THR	4.8
1	D	5	THR	4.8
1	A	220	GLY	3.2
1	D	376	LYS	3.2
1	C	219	ASP	2.7
1	D	6	ALA	2.6
1	C	177	GLN	2.6
1	B	334	ARG	2.5
1	D	378	VAL	2.4
1	B	220	GLY	2.3
1	A	6	ALA	2.3
1	C	216	GLU	2.2
1	A	378	VAL	2.2
1	B	219	ASP	2.2
1	A	159	ALA	2.2
1	C	161	ARG	2.1
1	D	374	LEU	2.1
1	D	26	ALA	2.1
1	D	216	GLU	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](#)

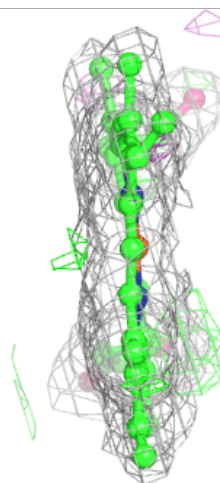
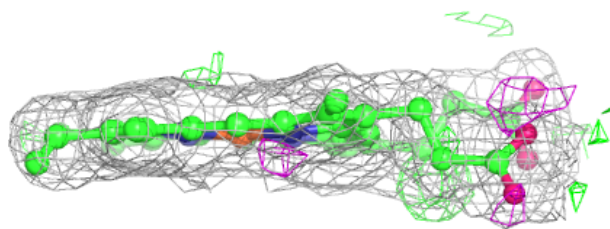
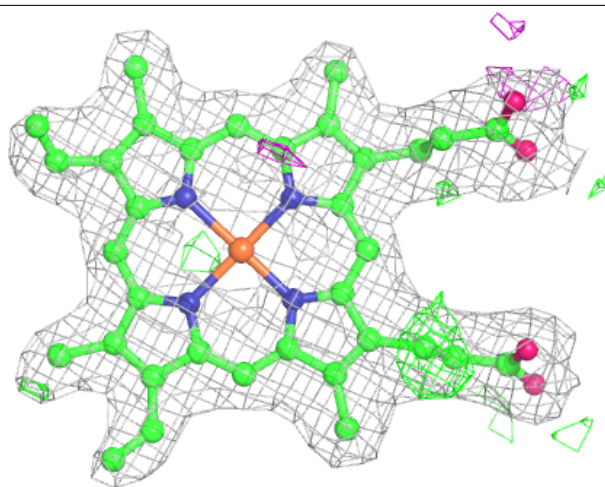
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	2OH	D	402	17/17	0.89	0.15	36,43,53,62	0
3	2OH	B	402	17/17	0.90	0.13	36,42,51,64	0
3	2OH	C	402	17/17	0.90	0.18	39,46,52,59	0
3	2OH	A	402	17/17	0.95	0.12	36,43,52,60	0
2	HEM	C	401	43/43	0.95	0.12	30,37,42,55	0
2	HEM	A	401	43/43	0.96	0.11	34,37,43,53	0
2	HEM	D	401	43/43	0.96	0.13	31,36,41,43	0
2	HEM	B	401	43/43	0.96	0.14	28,36,42,48	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.

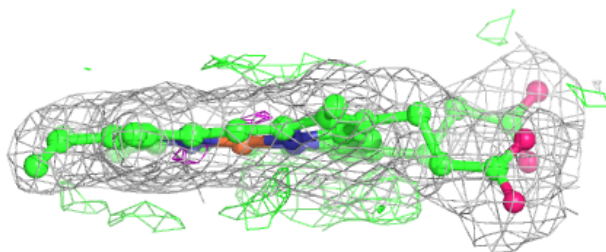
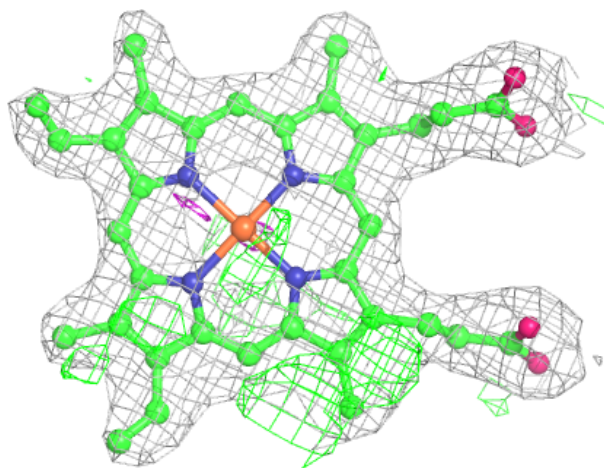
Electron density around HEM C 401:

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



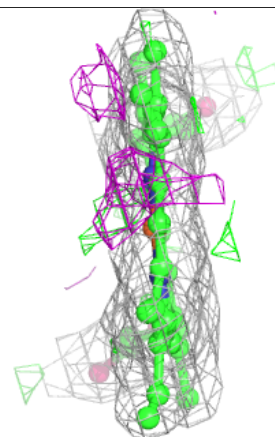
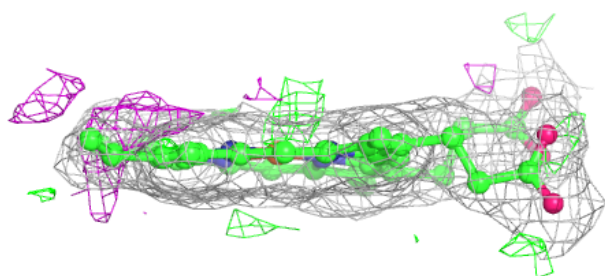
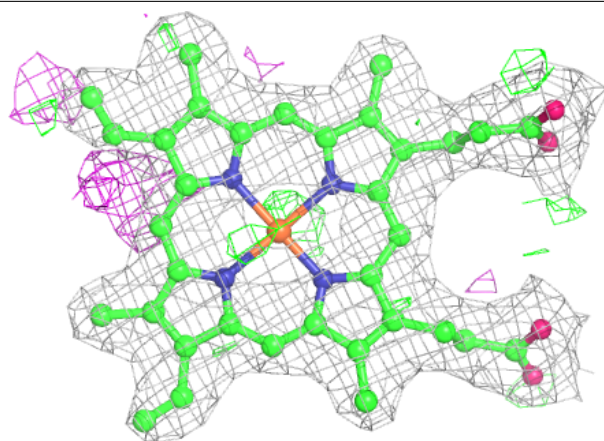
Electron density around HEM A 401:

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



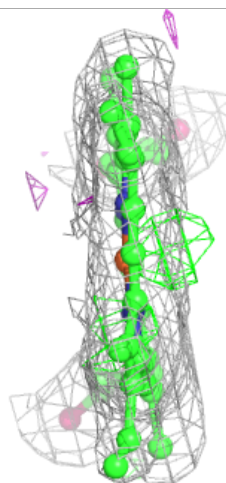
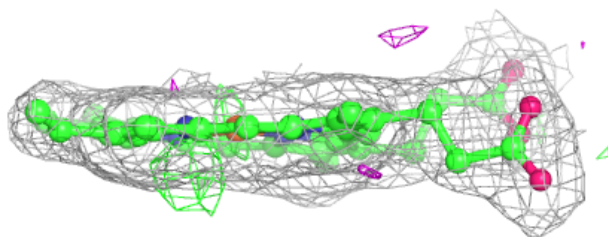
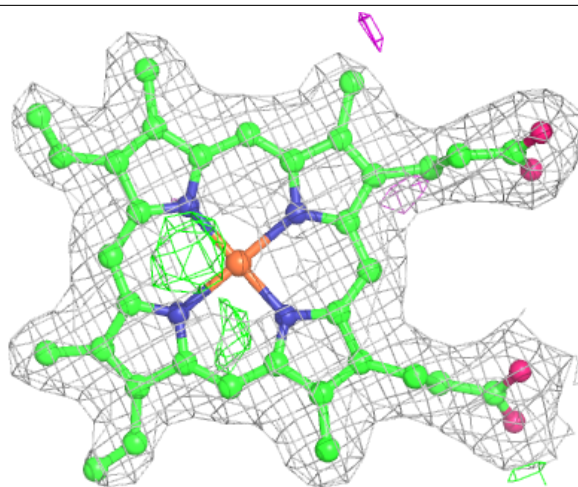
Electron density around HEM D 401:

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



Electron density around HEM 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.