



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 07:47 PM BST

PDB ID : 4H24
Title : Cytochrome P450BM3-CIS cyclopropanation catalyst
Authors : Coelho, P.S.; Wang, Z.J.; Ener, M.E.; Baril, S.A.; Kannan, A.; Arnold, F.H.;
Brustad, E.M.
Deposited on : 2012-09-11
Resolution : 2.50 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 : 2.13.1
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) : 2.13.1

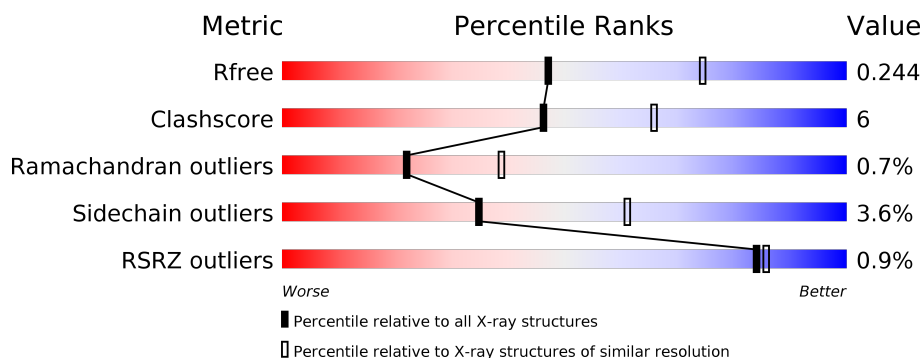
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	470	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 14%, green 81%, grey 14%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 81% 14% ... </div> </div>
1	B	470	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 14%, green 81%, grey 14%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 81% 14% ... </div> </div>
1	C	470	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, yellow 16%, green 80%, grey 16%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 80% 16% ... </div> </div>
1	D	470	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 14%, green 81%, grey 14%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 81% 14% ... </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14761 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-BM3 variant P450BM3-Cis.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	457	Total	C	N	O	S	0	2	0
			3624	2317	615	675	17			
1	B	452	Total	C	N	O	S	0	0	0
			3589	2297	613	662	17			
1	C	456	Total	C	N	O	S	0	0	0
			3605	2309	615	664	17			
1	D	455	Total	C	N	O	S	0	0	0
			3574	2284	611	662	17			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	78	ALA	VAL	ENGINEERED MUTATION	UNP P14779
A	87	VAL	PHE	ENGINEERED MUTATION	UNP P14779
A	142	SER	PRO	ENGINEERED MUTATION	UNP P14779
A	175	ILE	THR	ENGINEERED MUTATION	UNP P14779
A	184	VAL	ALA	ENGINEERED MUTATION	UNP P14779
A	226	ARG	SER	ENGINEERED MUTATION	UNP P14779
A	236	GLN	HIS	ENGINEERED MUTATION	UNP P14779
A	252	GLY	GLU	ENGINEERED MUTATION	UNP P14779
A	268	ALA	THR	ENGINEERED MUTATION	UNP P14779
A	290	VAL	ALA	ENGINEERED MUTATION	UNP P14779
A	353	VAL	LEU	ENGINEERED MUTATION	UNP P14779
A	366	VAL	ILE	ENGINEERED MUTATION	UNP P14779
A	442	LYS	GLU	ENGINEERED MUTATION	UNP P14779
A	464	HIS	-	EXPRESSION TAG	UNP P14779
A	465	HIS	-	EXPRESSION TAG	UNP P14779
A	466	HIS	-	EXPRESSION TAG	UNP P14779
A	467	HIS	-	EXPRESSION TAG	UNP P14779
A	468	HIS	-	EXPRESSION TAG	UNP P14779
A	469	HIS	-	EXPRESSION TAG	UNP P14779
B	78	ALA	VAL	ENGINEERED MUTATION	UNP P14779
B	87	VAL	PHE	ENGINEERED MUTATION	UNP P14779

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Chain	Residue	Modelled	Actual	Comment	Reference
B	142	SER	PRO	ENGINEERED MUTATION	UNP P14779
B	175	ILE	THR	ENGINEERED MUTATION	UNP P14779
B	184	VAL	ALA	ENGINEERED MUTATION	UNP P14779
B	226	ARG	SER	ENGINEERED MUTATION	UNP P14779
B	236	GLN	HIS	ENGINEERED MUTATION	UNP P14779
B	252	GLY	GLU	ENGINEERED MUTATION	UNP P14779
B	268	ALA	THR	ENGINEERED MUTATION	UNP P14779
B	290	VAL	ALA	ENGINEERED MUTATION	UNP P14779
B	353	VAL	LEU	ENGINEERED MUTATION	UNP P14779
B	366	VAL	ILE	ENGINEERED MUTATION	UNP P14779
B	442	LYS	GLU	ENGINEERED MUTATION	UNP P14779
B	464	HIS	-	EXPRESSION TAG	UNP P14779
B	465	HIS	-	EXPRESSION TAG	UNP P14779
B	466	HIS	-	EXPRESSION TAG	UNP P14779
B	467	HIS	-	EXPRESSION TAG	UNP P14779
B	468	HIS	-	EXPRESSION TAG	UNP P14779
B	469	HIS	-	EXPRESSION TAG	UNP P14779
C	78	ALA	VAL	ENGINEERED MUTATION	UNP P14779
C	87	VAL	PHE	ENGINEERED MUTATION	UNP P14779
C	142	SER	PRO	ENGINEERED MUTATION	UNP P14779
C	175	ILE	THR	ENGINEERED MUTATION	UNP P14779
C	184	VAL	ALA	ENGINEERED MUTATION	UNP P14779
C	226	ARG	SER	ENGINEERED MUTATION	UNP P14779
C	236	GLN	HIS	ENGINEERED MUTATION	UNP P14779
C	252	GLY	GLU	ENGINEERED MUTATION	UNP P14779
C	268	ALA	THR	ENGINEERED MUTATION	UNP P14779
C	290	VAL	ALA	ENGINEERED MUTATION	UNP P14779
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C	442	LYS	GLU	ENGINEERED MUTATION	UNP P14779
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C	465	HIS	-	EXPRESSION TAG	UNP P14779
C	466	HIS	-	EXPRESSION TAG	UNP P14779
C	467	HIS	-	EXPRESSION TAG	UNP P14779
C	468	HIS	-	EXPRESSION TAG	UNP P14779
C	469	HIS	-	EXPRESSION TAG	UNP P14779
D	78	ALA	VAL	ENGINEERED MUTATION	UNP P14779
D	87	VAL	PHE	ENGINEERED MUTATION	UNP P14779
D	142	SER	PRO	ENGINEERED MUTATION	UNP P14779
D	175	ILE	THR	ENGINEERED MUTATION	UNP P14779
D	184	VAL	ALA	ENGINEERED MUTATION	UNP P14779
D	226	ARG	SER	ENGINEERED MUTATION	UNP P14779

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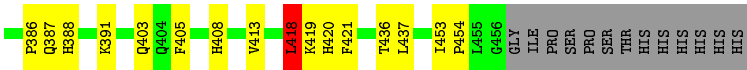
Chain	Residue	Modelled	Actual	Comment	Reference
D	236	GLN	HIS	ENGINEERED MUTATION	UNP P14779
D	252	GLY	GLU	ENGINEERED MUTATION	UNP P14779
D	268	ALA	THR	ENGINEERED MUTATION	UNP P14779
D	290	VAL	ALA	ENGINEERED MUTATION	UNP P14779
D	353	VAL	LEU	ENGINEERED MUTATION	UNP P14779
D	366	VAL	ILE	ENGINEERED MUTATION	UNP P14779
D	442	LYS	GLU	ENGINEERED MUTATION	UNP P14779
D	464	HIS	-	EXPRESSION TAG	UNP P14779
D	465	HIS	-	EXPRESSION TAG	UNP P14779
D	466	HIS	-	EXPRESSION TAG	UNP P14779
D	467	HIS	-	EXPRESSION TAG	UNP P14779
D	468	HIS	-	EXPRESSION TAG	UNP P14779
D	469	HIS	-	EXPRESSION TAG	UNP P14779

- # HEM

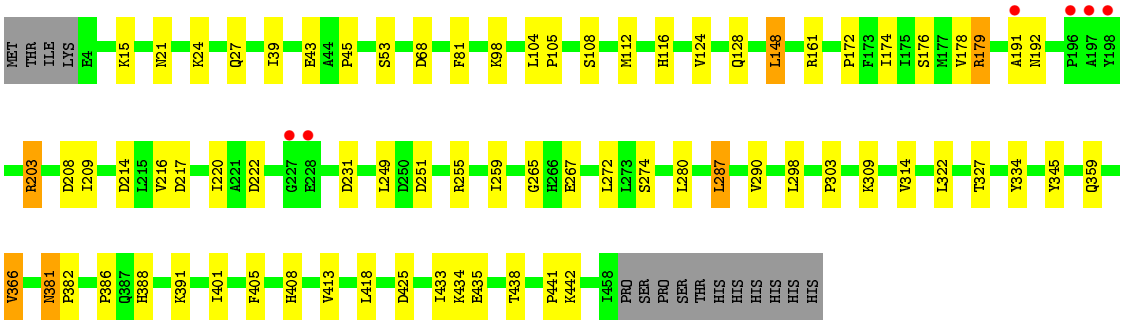
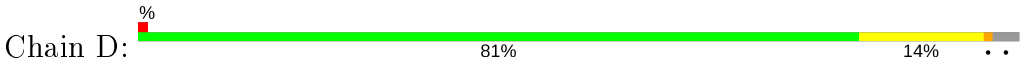
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	72	Total 72	O 72	0	0
3	B	41	Total 41	O 41	0	0
3	C	46	Total 46	O 46	0	0
3	D	38	Total 38	O 38	0	0



● Molecule 1: Cytochrome P450-BM3 variant P450BM3-Cis



4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	187.79Å 62.74Å 210.28Å 90.00° 115.75° 90.00°	Depositor
Resolution (Å)	48.58 – 2.50 48.57 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.6 (48.58-2.50) 98.6 (48.57-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.93 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.184 , 0.247 0.183 , 0.244	Depositor DCC
R_{free} test set	3821 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	47.4	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14761	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.86	2/3712 (0.1%)	0.86	4/5030 (0.1%)
1	B	0.82	1/3670 (0.0%)	0.82	3/4965 (0.1%)
1	C	0.80	3/3687 (0.1%)	0.79	2/4992 (0.0%)
1	D	0.79	0/3656	0.82	3/4955 (0.1%)
All	All	0.82	6/14725 (0.0%)	0.82	12/19942 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	143	GLU	CG-CD	7.14	1.62	1.51
1	B	247	GLU	CG-CD	6.46	1.61	1.51
1	C	35	GLU	CB-CG	6.27	1.64	1.52
1	C	35	GLU	CG-CD	6.17	1.61	1.51
1	A	156	CYS	CB-SG	-5.19	1.73	1.81
1	C	21	ASN	CB-CG	5.05	1.62	1.51

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	222	ASP	CB-CG-OD1	6.64	124.28	118.30
1	B	436	THR	C-N-CA	-6.25	106.08	121.70
1	A	425	ASP	CB-CG-OD1	6.22	123.89	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	418	LEU	CA-CB-CG	-6.05	101.39	115.30
1	B	296	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	C	418	LEU	CA-CB-CG	-5.55	102.53	115.30
1	D	161	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	B	215	LEU	CA-CB-CG	-5.33	103.03	115.30
1	C	238	LEU	CB-CG-CD1	-5.26	102.06	111.00
1	D	161	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	D	425	ASP	CB-CG-OD1	5.09	122.88	118.30
1	A	274	SER	N-CA-CB	5.03	118.05	110.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	421	PHE	Peptide

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	3624	0	3554	40	0
1	B	3589	0	3543	42	0
1	C	3605	0	3554	48	0
1	D	3574	0	3481	46	0
2	A	43	0	30	3	0
2	B	43	0	30	2	0
2	C	43	0	30	6	0
2	D	43	0	30	3	0
3	A	72	0	0	1	0
3	B	41	0	0	2	0
3	C	46	0	0	2	0
3	D	38	0	0	2	0
All	All	14761	0	14252	182	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 6.

All (182) 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:A:162:PHE:HE1	1:A:215:LEU:HD21	1.24	0.98
1:C:405:PHE:CD1	2:C:500:HEM:HBB1	2.01	0.95
1:B:116:HIS:HD2	1:B:408:HIS:HE2	1.07	0.93
1:A:312:LYS:HG2	1:A:316:MET:HE1	1.54	0.88
1:A:162:PHE:CE1	1:A:215:LEU:HD21	2.07	0.87
1:C:9:LYS:HE3	3:C:645:HOH:O	1.75	0.86
1:D:290:VAL:CG1	1:D:418:LEU:HD13	2.09	0.83
1:D:290:VAL:HG12	1:D:418:LEU:HD13	1.63	0.81
1:C:312:LYS:HE3	1:C:316:MET:HE3	1.64	0.79
1:B:387:GLN:HG3	1:B:388:HIS:CD2	2.16	0.79
1:A:312:LYS:HG2	1:A:316:MET:CE	2.12	0.78
1:C:405:PHE:HD1	2:C:500:HEM:HBB1	1.50	0.75
1:C:330:ALA:HB1	1:C:354:MET:CE	2.17	0.75
1:D:112:MET:CE	1:D:405:PHE:HA	2.17	0.75
1:C:267:GLU:HA	1:C:267:GLU:OE2	1.85	0.74
1:A:436:THR:OG1	1:A:437:LEU:N	2.17	0.74
1:B:290:VAL:HG11	1:B:418:LEU:HD13	1.69	0.72
1:D:309:LYS:HE2	3:D:634:HOH:O	1.88	0.72
1:C:312:LYS:HE3	1:C:316:MET:CE	2.19	0.72
1:C:436:THR:OG1	1:C:437:LEU:N	2.22	0.72
1:B:116:HIS:CD2	1:B:408:HIS:HE2	2.00	0.71
1:B:290:VAL:CG1	1:B:418:LEU:HD13	2.22	0.70
1:D:251:ASP:O	1:D:255:ARG:HG3	1.94	0.68
1:B:298:LEU:HD22	1:B:303:PRO:HB3	1.76	0.68
1:A:116:HIS:HD2	1:A:408:HIS:NE2	1.92	0.67
1:B:55:GLN:NE2	1:B:387:GLN:O	2.26	0.67
1:A:388:HIS:HA	1:A:391:LYS:HD3	1.77	0.66
1:C:245:THR:O	1:C:247:GLU:N	2.23	0.66
1:B:7:GLN:HG3	1:B:41:LYS:HB3	1.78	0.65
1:A:162:PHE:HE1	1:A:215:LEU:CD2	2.05	0.65
1:D:174:ILE:O	1:D:178:VAL:HG23	1.96	0.65
1:B:420:HIS:HD2	3:B:604:HOH:O	1.79	0.64
1:A:420:HIS:HE1	3:A:662:HOH:O	1.80	0.63
1:B:377:GLU:O	1:B:380:GLU:HG2	1.99	0.63
1:B:217:ASP:OD1	1:B:255:ARG:NH1	2.32	0.63
1:D:112:MET:HE1	1:D:405:PHE:HA	1.80	0.61
1:C:116:HIS:HD2	1:C:408:HIS:NE2	1.99	0.60
1:D:381:ASN:H	1:D:381:ASN:HD22	1.48	0.60
1:D:290:VAL:CG1	1:D:418:LEU:CD1	2.79	0.60
1:D:290:VAL:HG11	1:D:418:LEU:CD1	2.32	0.60
1:B:126:LEU:HD22	1:B:148:LEU:HD13	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:500:HEM:CMB	2:C:500:HEM:HBB2	2.31	0.59
1:B:150:LEU:HD22	1:B:174:ILE:CG1	2.33	0.59
2:A:500:HEM:HMC2	2:A:500:HEM:HBC2	1.85	0.58
1:C:79:ARG:NH2	1:C:93:GLU:OE1	2.37	0.57
1:B:79:ARG:HH12	1:B:93:GLU:CD	2.07	0.57
1:C:79:ARG:HH21	1:C:89:SER:HA	1.69	0.57
1:A:312:LYS:O	1:A:316:MET:HE3	2.05	0.57
1:C:298:LEU:HD22	1:C:303:PRO:HB3	1.86	0.57
1:D:381:ASN:HD22	1:D:381:ASN:N	2.03	0.56
1:A:173:PHE:CD1	1:A:215:LEU:HD23	2.41	0.56
1:D:124:VAL:O	1:D:128:GLN:HG3	2.07	0.55
1:B:190:ARG:HH11	1:B:190:ARG:HG2	1.71	0.54
1:A:312:LYS:CG	1:A:316:MET:CE	2.85	0.54
1:C:364:LYS:C	1:C:366:VAL:H	2.10	0.54
1:D:24:LYS:HA	1:D:435:GLU:HG3	1.91	0.53
1:D:98:LYS:HD3	1:D:249:LEU:HD23	1.89	0.53
1:C:403:GLN:NE2	3:C:642:HOH:O	2.39	0.53
1:D:272:LEU:HD13	1:D:322:LEU:CD2	2.39	0.52
1:B:51:TYR:CE2	1:B:354:MET:HG2	2.44	0.52
1:D:298:LEU:HD22	1:D:303:PRO:HB3	1.89	0.52
2:B:500:HEM:HMB2	2:B:500:HEM:HBB2	1.90	0.52
1:D:265:GLY:HA2	2:D:500:HEM:CMC	2.40	0.52
1:B:20:LEU:HD21	1:B:29:LEU:HG	1.91	0.51
1:B:387:GLN:CG	1:B:388:HIS:CD2	2.93	0.51
1:C:116:HIS:HE1	1:C:303:PRO:O	1.93	0.51
1:B:267:GLU:OE1	1:B:267:GLU:HA	2.10	0.51
1:B:366:VAL:HG11	1:B:389:ALA:HB1	1.91	0.51
2:B:500:HEM:CMB	2:B:500:HEM:HBB2	2.41	0.50
1:C:59:LYS:HG3	1:C:388:HIS:HD2	1.76	0.50
1:A:148:LEU:HD21	1:A:413:VAL:HG21	1.93	0.50
1:D:366:VAL:HG22	1:D:386:PRO:HG2	1.93	0.50
1:B:366:VAL:HG11	1:B:389:ALA:CB	2.42	0.50
1:C:17:LEU:HD11	1:C:189:GLN:HA	1.93	0.49
1:A:17:LEU:HG	1:A:189:GLN:NE2	2.27	0.49
2:C:500:HEM:CBB	2:C:500:HEM:CMB	2.91	0.49
1:C:216:VAL:HG21	1:C:259:ILE:HG13	1.94	0.49
1:D:214:ASP:O	1:D:217:ASP:HB2	2.13	0.49
1:D:179:ARG:NH2	1:D:208:ASP:OD1	2.46	0.48
1:C:76:LYS:O	1:C:79:ARG:HB2	2.12	0.48
1:A:259:ILE:HG22	1:A:263:ILE:HD12	1.96	0.48
1:B:420:HIS:CD2	3:B:604:HOH:O	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:272:LEU:HD21	1:C:318:LEU:HD22	1.96	0.48
1:D:39:ILE:HG21	1:D:345:TYR:CE2	2.49	0.48
1:D:108:SER:O	1:D:112:MET:HG2	2.14	0.48
1:A:330:ALA:HB1	1:A:354:MET:CE	2.44	0.47
1:C:102:ILE:HD13	1:C:249:LEU:HG	1.95	0.47
1:D:388:HIS:HA	1:D:391:LYS:HE2	1.96	0.47
1:A:265:GLY:HA2	2:A:500:HEM:C2C	2.50	0.47
1:C:150:LEU:HD22	1:C:174:ILE:HG12	1.95	0.47
1:C:268:ALA:HB1	2:C:500:HEM:HBC2	1.95	0.47
1:C:31:LYS:O	1:C:35:GLU:HG3	2.14	0.47
1:C:140:GLU:HB3	1:C:143:GLU:OE1	2.14	0.47
1:D:214:ASP:HA	1:D:217:ASP:HB2	1.97	0.47
1:A:211:VAL:O	1:A:214:ASP:HB2	2.15	0.47
1:C:290:VAL:HG11	1:C:418:LEU:HD13	1.95	0.47
1:C:387:GLN:O	1:C:388:HIS:HB2	2.15	0.47
1:D:381:ASN:HA	1:D:382:PRO:HD3	1.78	0.47
1:B:150:LEU:HD22	1:B:174:ILE:HG13	1.96	0.46
1:C:405:PHE:CD1	2:C:500:HEM:CBB	2.88	0.46
1:D:265:GLY:HA2	2:D:500:HEM:HMC2	1.98	0.46
1:A:17:LEU:HG	1:A:189:GLN:HE22	1.81	0.46
1:A:39:ILE:HA	1:A:51:TYR:O	2.15	0.46
1:A:112:MET:HE3	1:A:112:MET:HA	1.96	0.46
1:A:229:GLN:O	1:A:230:SER:HB3	2.16	0.46
1:A:53:SER:HB3	1:A:359:GLN:HB3	1.98	0.46
1:D:112:MET:HE2	1:D:405:PHE:HA	1.95	0.46
1:D:265:GLY:HA2	2:D:500:HEM:C2C	2.50	0.46
1:D:81:PHE:HB3	1:D:209:ILE:HG12	1.97	0.46
1:A:178:VAL:O	1:A:182:ASP:HB2	2.15	0.45
1:C:177:MET:HG3	1:C:263:ILE:HG12	1.98	0.45
1:D:203:ARG:HB3	1:D:203:ARG:HE	1.48	0.45
1:B:64:GLU:OE2	1:B:397:GLN:HG2	2.16	0.45
1:B:60:GLU:OE2	1:B:342:GLY:HA2	2.16	0.45
1:D:274:SER:HB3	1:D:441:PRO:HD2	1.97	0.45
1:C:17:LEU:HB3	1:C:18:PRO:HD3	1.98	0.45
1:A:116:HIS:CD2	1:A:408:HIS:NE2	2.79	0.45
1:D:104:LEU:HB3	1:D:105:PRO:HD3	1.97	0.45
1:D:280:LEU:HB3	1:D:287:LEU:HD12	1.99	0.45
1:B:215:LEU:O	1:B:215:LEU:HG	2.16	0.45
1:C:231:ASP:OD1	1:C:235:THR:HG21	2.17	0.45
1:C:253:ASN:O	1:C:257:GLN:HG2	2.17	0.45
1:B:76:LYS:O	1:B:79:ARG:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:366:VAL:HG22	1:C:386:PRO:HG2	1.98	0.45
1:B:267:GLU:HG3	1:B:438:THR:OG1	2.17	0.44
1:B:17:LEU:HD22	1:B:45:PRO:HD2	1.99	0.44
1:B:407:LEU:HD23	1:B:407:LEU:HA	1.82	0.44
1:C:330:ALA:HB1	1:C:354:MET:HE1	1.98	0.44
1:B:218:LYS:O	1:B:219:ILE:C	2.55	0.44
1:A:317:VAL:HG13	1:A:374:PHE:HZ	1.82	0.44
1:B:104:LEU:HB3	1:B:105:PRO:HD3	1.99	0.44
1:B:280:LEU:CD2	1:B:286:VAL:HG12	2.48	0.43
1:B:81:PHE:HB3	1:B:209:ILE:HG12	2.01	0.43
1:C:419:LYS:HD3	1:C:420:HIS:CE1	2.54	0.43
1:D:15:LYS:HB3	1:D:43:GLU:O	2.19	0.43
1:D:148:LEU:HD21	1:D:413:VAL:HG21	2.00	0.43
1:C:330:ALA:HB1	1:C:354:MET:HE3	1.98	0.43
1:A:308:VAL:HG21	1:A:412:LEU:HB2	2.01	0.43
1:B:290:VAL:HG12	1:B:418:LEU:HD13	2.00	0.43
1:B:435:GLU:HG2	1:B:439:LEU:CD2	2.49	0.42
1:D:309:LYS:CE	3:D:634:HOH:O	2.56	0.42
1:C:233:LEU:HG	1:C:237:MET:CE	2.49	0.42
1:A:46:GLY:O	1:A:47:ARG:HB3	2.20	0.42
1:C:391:LYS:HD2	1:C:391:LYS:HA	1.90	0.42
1:A:366:VAL:HG11	1:A:389:ALA:HB1	2.01	0.42
1:A:158:PHE:CD1	1:A:158:PHE:N	2.87	0.42
1:A:225:ALA:O	1:A:226:ARG:CB	2.67	0.42
1:B:190:ARG:HH11	1:B:190:ARG:CG	2.33	0.42
1:B:377:GLU:O	1:B:380:GLU:CG	2.65	0.42
1:C:61:ALA:HA	1:C:67:PHE:CD2	2.55	0.42
1:D:327:THR:O	1:D:438:THR:HA	2.20	0.42
1:C:7:GLN:HG3	1:C:8:PRO:HD2	2.01	0.42
1:A:381:ASN:HA	1:A:382:PRO:HD2	1.94	0.42
1:B:39:ILE:HA	1:B:51:TYR:O	2.19	0.42
1:D:290:VAL:HG13	1:D:314:VAL:HG22	2.02	0.42
1:A:50:ARG:NH1	1:A:352:GLU:O	2.49	0.41
1:C:60:GLU:OE2	1:C:342:GLY:HA2	2.20	0.41
1:D:68:ASP:HB3	1:D:334:TYR:CE1	2.55	0.41
1:D:220:ILE:HG22	1:D:220:ILE:O	2.19	0.41
1:C:453:ILE:HA	1:C:454:PRO:HD3	1.94	0.41
1:B:275:PHE:CE2	1:B:441:PRO:HD3	2.56	0.41
1:B:129:LYS:NZ	1:B:144:ASP:OD1	2.48	0.41
1:D:116:HIS:HD2	1:D:408:HIS:NE2	2.19	0.41
1:A:169[B]:GLN:HG2	1:A:170:PRO:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:LEU:HD21	1:A:29:LEU:HG	2.02	0.41
1:A:271:GLY:HA2	1:A:440:LYS:HG3	2.03	0.41
1:C:148:LEU:HD21	1:C:413:VAL:HG21	2.03	0.41
1:D:53:SER:HB3	1:D:359:GLN:HB3	2.02	0.41
2:A:500:HEM:CMC	2:A:500:HEM:HBC2	2.50	0.41
1:D:216:VAL:HG21	1:D:259:ILE:HG13	2.02	0.41
1:C:97:LYS:HD2	1:C:97:LYS:HA	1.86	0.41
1:C:98:LYS:HE2	1:C:248:PRO:O	2.21	0.41
1:D:27:GLN:OE1	1:D:433:ILE:HB	2.21	0.40
1:D:434:LYS:HB2	1:D:442:LYS:HB2	2.01	0.40
1:B:68:ASP:OD2	1:B:336:LYS:HE2	2.21	0.40
1:C:419:LYS:HE2	1:C:453:ILE:HG21	2.02	0.40
1:C:9:LYS:HD3	1:C:11:PHE:CZ	2.57	0.40
1:D:116:HIS:HE1	1:D:303:PRO:O	2.05	0.40
1:A:214:ASP:O	1:A:217:ASP:HB2	2.22	0.40
1:A:357:ILE:HG22	1:A:361:HIS:CE1	2.56	0.40
1:A:24:LYS:HE2	1:A:433:ILE:O	2.22	0.40
1:A:280:LEU:HD12	1:A:418:LEU:HD11	2.03	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	457/470 (97%)	426 (93%)	26 (6%)	5 (1%)	14	26
1	B	448/470 (95%)	428 (96%)	19 (4%)	1 (0%)	47	68
1	C	454/470 (97%)	427 (94%)	25 (6%)	2 (0%)	34	54
1	D	453/470 (96%)	432 (95%)	17 (4%)	4 (1%)	17	31
All	All	1812/1880 (96%)	1713 (94%)	87 (5%)	12 (1%)	22	39

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	47	ARG
1	A	226	ARG
1	C	246	GLY
1	D	191	ALA
1	D	222	ASP
1	A	196	PRO
1	A	229	GLN
1	A	230	SER
1	C	267	GLU
1	D	45	PRO
1	D	172	PRO
1	B	193	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	384/411 (93%)	372 (97%)	12 (3%)	40	67
1	B	381/411 (93%)	365 (96%)	16 (4%)	30	54
1	C	381/411 (93%)	366 (96%)	15 (4%)	32	57
1	D	374/411 (91%)	362 (97%)	12 (3%)	39	65
All	All	1520/1644 (92%)	1465 (96%)	55 (4%)	35	61

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	GLU
1	A	17	LEU
1	A	21	ASN
1	A	148	LEU
1	A	182	ASP
1	A	185	MET
1	A	187	LYS
1	A	266	HIS
1	A	353	VAL
1	A	369	ASP

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Mol	Chain	Res	Type
1	A	418	LEU
1	A	422	ASP
1	B	21	ASN
1	B	22	THR
1	B	34	ASP
1	B	41	LYS
1	B	47	ARG
1	B	68	ASP
1	B	93	GLU
1	B	210	LYS
1	B	218	LYS
1	B	266	HIS
1	B	267	GLU
1	B	333	LEU
1	B	353	VAL
1	B	381	ASN
1	B	418	LEU
1	B	442	LYS
1	C	5	MET
1	C	22	THR
1	C	47	ARG
1	C	136	ASP
1	C	148	LEU
1	C	193	PRO
1	C	215	LEU
1	C	230	SER
1	C	231	ASP
1	C	235	THR
1	C	250	ASP
1	C	267	GLU
1	C	353	VAL
1	C	366	VAL
1	C	418	LEU
1	D	21	ASN
1	D	148	LEU
1	D	176	SER
1	D	179	ARG
1	D	192	ASN
1	D	203	ARG
1	D	231	ASP
1	D	267	GLU
1	D	287	LEU

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Mol	Chain	Res	Type
1	D	366	VAL
1	D	381	ASN
1	D	401	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	116	HIS
1	A	128	GLN
1	A	201	ASN
1	A	420	HIS
1	B	21	ASN
1	B	116	HIS
1	B	403	GLN
1	B	420	HIS
1	C	116	HIS
1	C	128	GLN
1	C	201	ASN
1	C	310	GLN
1	C	388	HIS
1	C	403	GLN
1	C	404	GLN
1	D	21	ASN
1	D	116	HIS
1	D	192	ASN
1	D	204	GLN
1	D	381	ASN
1	D	403	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	HEM	B	500	1	27,50,50	2.03	8 (29%)	17,82,82	2.02	6 (35%)
2	HEM	A	500	1,3	27,50,50	2.04	7 (25%)	17,82,82	1.81	6 (35%)
2	HEM	D	500	1	27,50,50	2.12	8 (29%)	17,82,82	2.10	5 (29%)
2	HEM	C	500	1,3	27,50,50	2.36	8 (29%)	17,82,82	2.22	5 (29%)

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	500	1	-	0/6/54/54	-
2	HEM	A	500	1,3	-	0/6/54/54	-
2	HEM	D	500	1	-	0/6/54/54	-
2	HEM	C	500	1,3	-	0/6/54/54	-

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	500	HEM	C3C-C2C	-5.95	1.32	1.40
2	C	500	HEM	C3D-C2D	5.62	1.54	1.37
2	D	500	HEM	C3D-C2D	5.59	1.54	1.37
2	A	500	HEM	C3D-C2D	5.49	1.53	1.37
2	D	500	HEM	C3C-C2C	-4.78	1.33	1.40
2	B	500	HEM	C3D-C2D	4.75	1.51	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	HEM	C3C-C2C	-4.28	1.34	1.40
2	B	500	HEM	C3C-C2C	-4.13	1.34	1.40
2	C	500	HEM	C3B-C2B	-3.66	1.35	1.40
2	B	500	HEM	C3B-CAB	3.20	1.54	1.47
2	C	500	HEM	C3C-CAC	3.20	1.54	1.47
2	D	500	HEM	C3C-CAC	3.19	1.54	1.47
2	A	500	HEM	C3B-C2B	-3.11	1.36	1.40
2	A	500	HEM	CMB-C2B	2.91	1.58	1.51
2	B	500	HEM	C3C-CAC	2.91	1.53	1.47
2	B	500	HEM	C3B-C2B	-2.89	1.36	1.40
2	D	500	HEM	C3B-CAB	2.84	1.53	1.47
2	C	500	HEM	C3B-CAB	2.82	1.53	1.47
2	D	500	HEM	C3B-C2B	-2.81	1.36	1.40
2	A	500	HEM	C3B-CAB	2.73	1.53	1.47
2	C	500	HEM	C1D-ND	2.70	1.41	1.36
2	D	500	HEM	CAA-C2A	2.65	1.55	1.52
2	A	500	HEM	C3C-CAC	2.57	1.53	1.47
2	C	500	HEM	CAA-C2A	2.43	1.55	1.52
2	B	500	HEM	C4B-NB	2.40	1.41	1.36
2	B	500	HEM	CMC-C2C	2.40	1.57	1.51
2	D	500	HEM	CMB-C2B	2.39	1.57	1.51
2	A	500	HEM	CAD-C3D	2.20	1.56	1.52
2	C	500	HEM	C4D-C3D	2.06	1.47	1.42
2	D	500	HEM	CMC-C2C	2.06	1.56	1.51
2	B	500	HEM	CMB-C2B	2.01	1.56	1.51

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	500	HEM	C1D-C2D-C3D	-4.74	103.70	107.00
2	B	500	HEM	CBD-CAD-C3D	-4.67	103.88	112.48
2	D	500	HEM	CBD-CAD-C3D	-4.63	103.95	112.48
2	C	500	HEM	CBA-CAA-C2A	-4.60	104.00	112.49
2	C	500	HEM	C4C-C3C-C2C	4.08	109.75	106.90
2	C	500	HEM	C1D-C2D-C3D	-3.73	104.40	107.00
2	C	500	HEM	CBD-CAD-C3D	-3.46	106.10	112.48
2	B	500	HEM	C4C-C3C-C2C	3.09	109.05	106.90
2	A	500	HEM	CMA-C3A-C4A	-3.03	123.81	128.46
2	A	500	HEM	CMA-C3A-C2A	2.84	130.30	124.94
2	A	500	HEM	CMB-C2B-C3B	2.73	129.79	124.68
2	D	500	HEM	C4C-C3C-C2C	2.69	108.77	106.90
2	B	500	HEM	C1D-C2D-C3D	-2.65	105.15	107.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	500	HEM	CMA-C3A-C4A	-2.62	124.43	128.46
2	B	500	HEM	CMA-C3A-C4A	-2.60	124.47	128.46
2	D	500	HEM	CMA-C3A-C4A	-2.31	124.91	128.46
2	A	500	HEM	CBA-CAA-C2A	-2.31	108.23	112.49
2	A	500	HEM	C4C-C3C-C2C	2.29	108.50	106.90
2	B	500	HEM	CAD-CBD-CGD	2.26	116.46	112.67
2	D	500	HEM	CBA-CAA-C2A	-2.19	108.45	112.49
2	A	500	HEM	CMC-C2C-C3C	2.15	128.71	124.68
2	B	500	HEM	CBA-CAA-C2A	2.03	116.22	112.49

There are no chirality outliers.

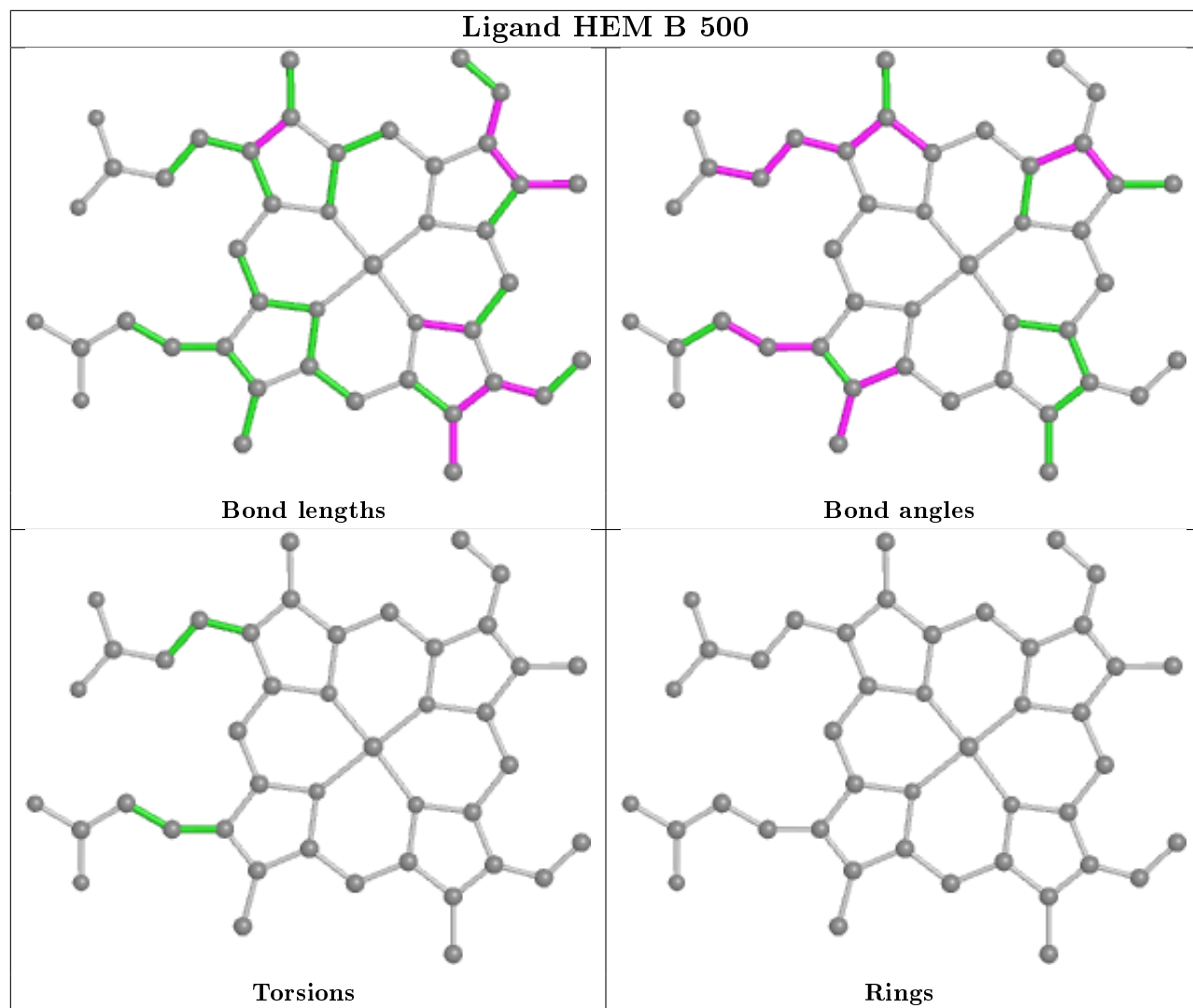
There are no torsion outliers.

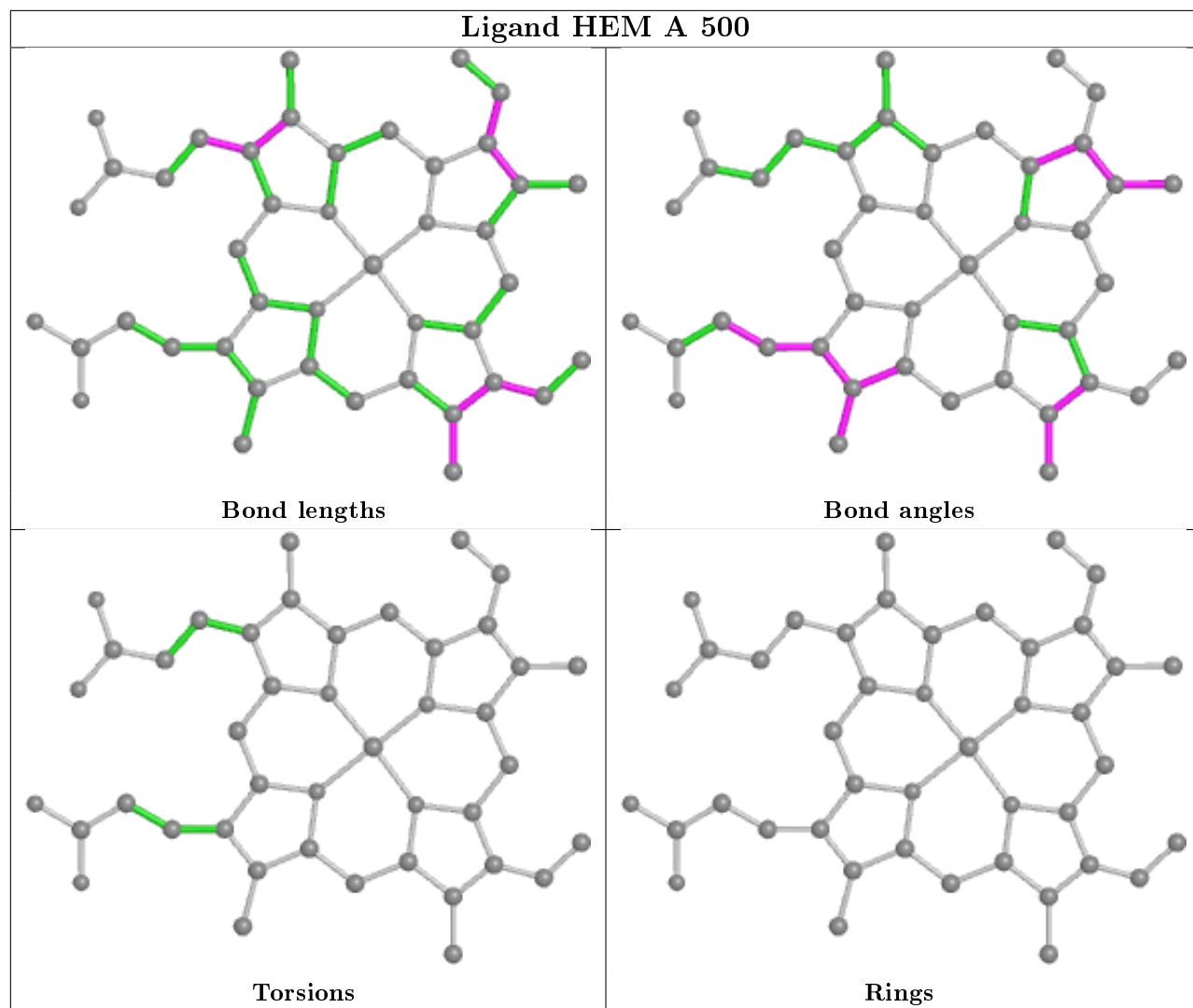
There are no ring outliers.

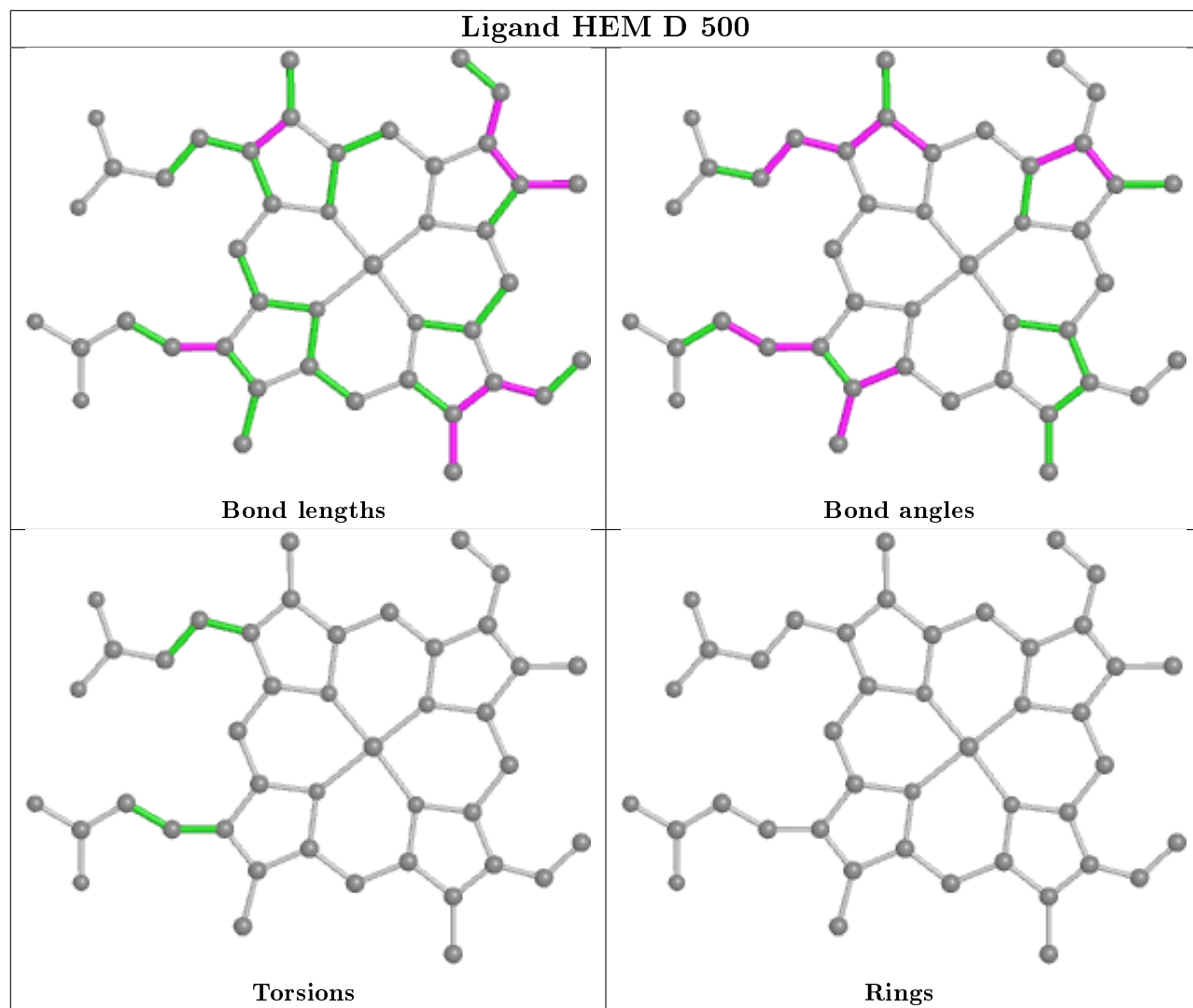
4 monomers are involved in 14 short contacts:

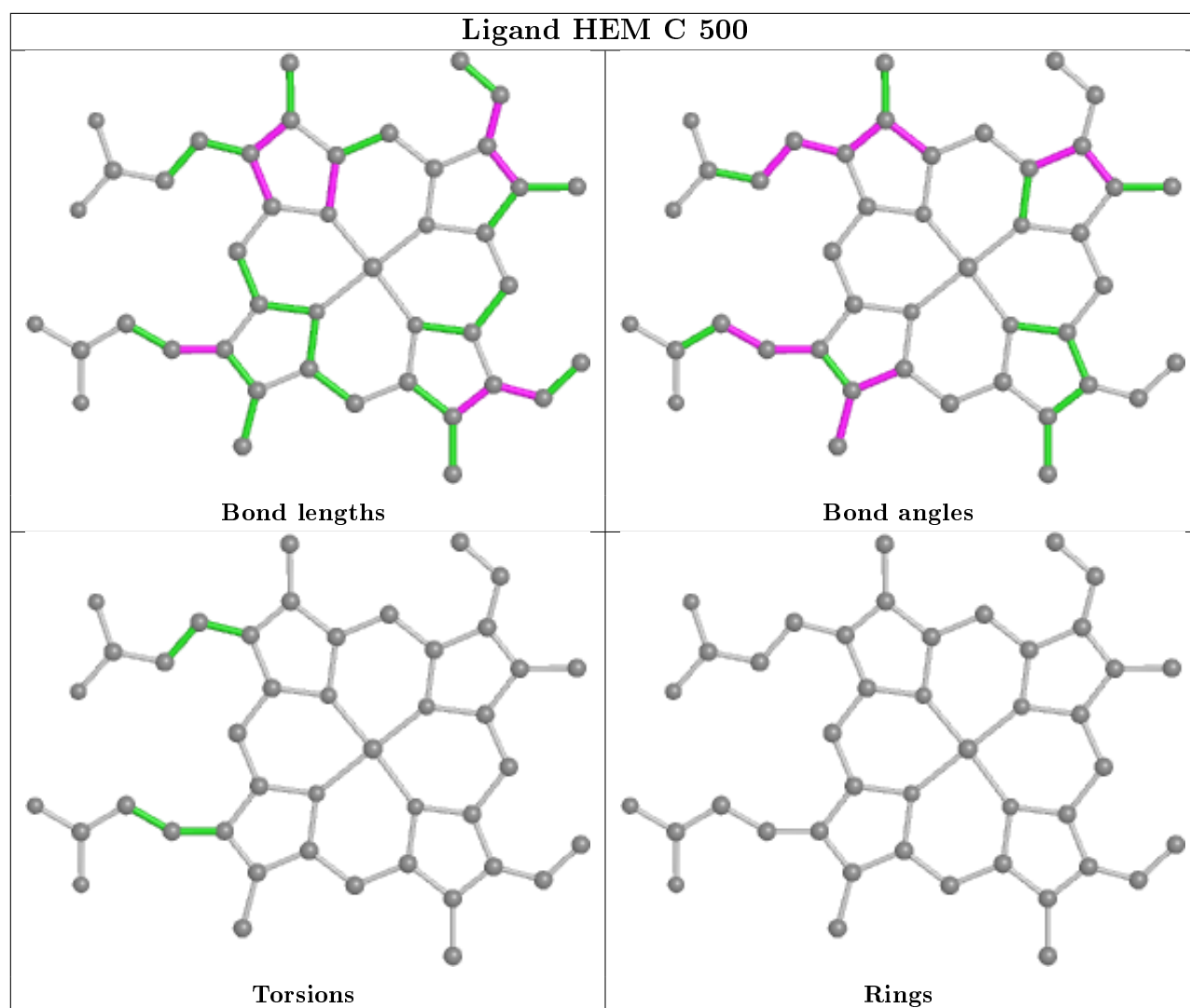
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	500	HEM	2	0
2	A	500	HEM	3	0
2	D	500	HEM	3	0
2	C	500	HEM	6	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	457/470 (97%)	-0.30	3 (0%) 87 89	27, 42, 72, 108	0
1	B	452/470 (96%)	-0.25	5 (1%) 80 82	28, 47, 78, 97	0
1	C	456/470 (97%)	-0.36	2 (0%) 92 93	29, 47, 70, 95	0
1	D	455/470 (96%)	-0.35	6 (1%) 77 79	31, 45, 71, 94	0
All	All	1820/1880 (96%)	-0.31	16 (0%) 84 86	27, 45, 74, 108	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	229	GLN	3.8
1	C	227	GLY	3.7
1	D	227	GLY	3.7
1	D	196	PRO	3.5
1	A	191	ALA	3.5
1	B	1	THR	3.5
1	B	343	GLY	2.8
1	D	228	GLU	2.8
1	B	366	VAL	2.8
1	A	196	PRO	2.6
1	D	197	ALA	2.6
1	B	383	SER	2.5
1	D	191	ALA	2.5
1	A	456	GLY	2.4
1	D	198	TYR	2.2
1	B	382	PRO	2.2

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](#)

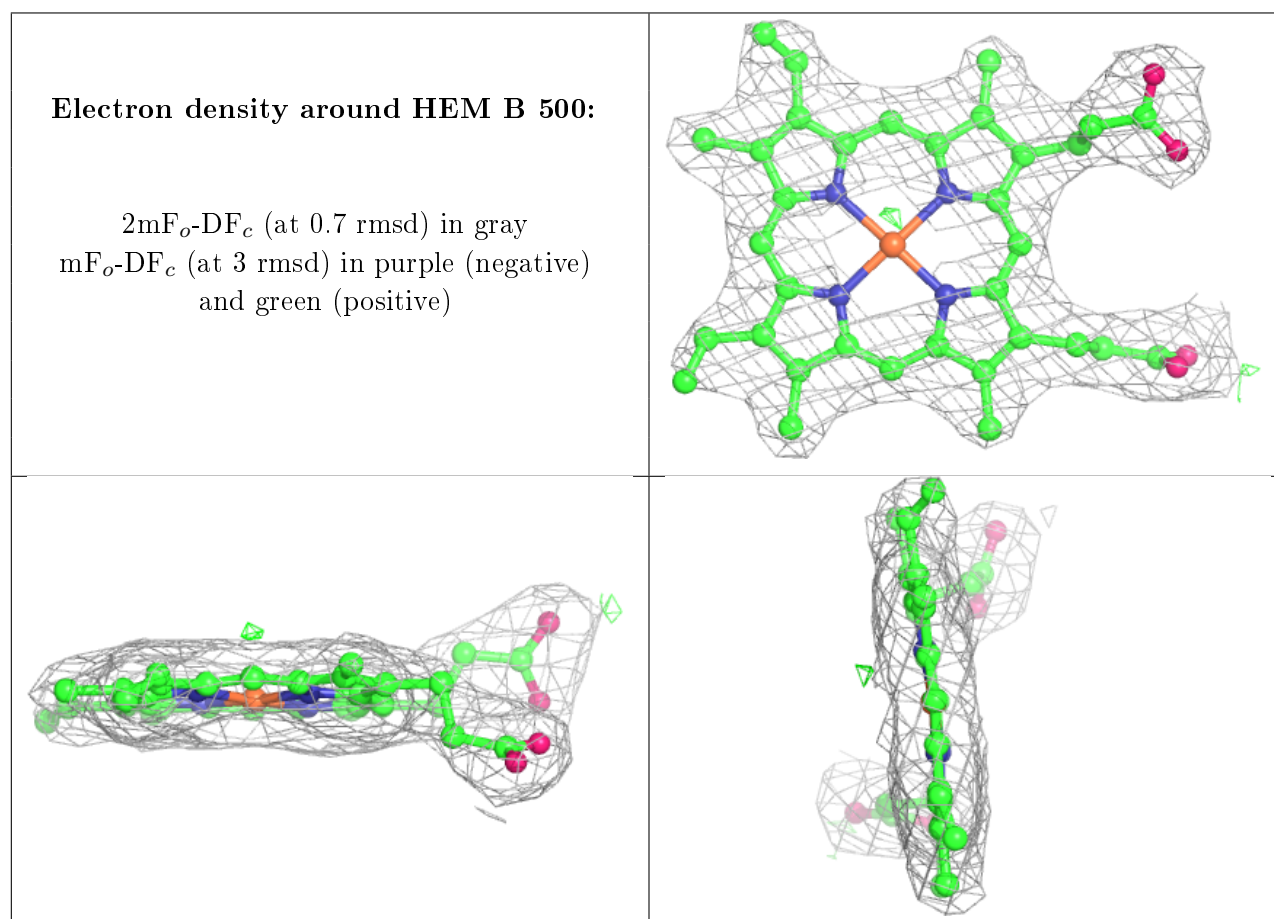
There are no monosaccharides in this entry.

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.

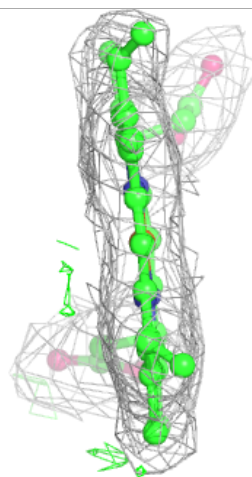
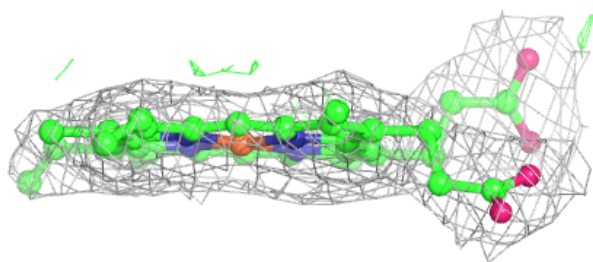
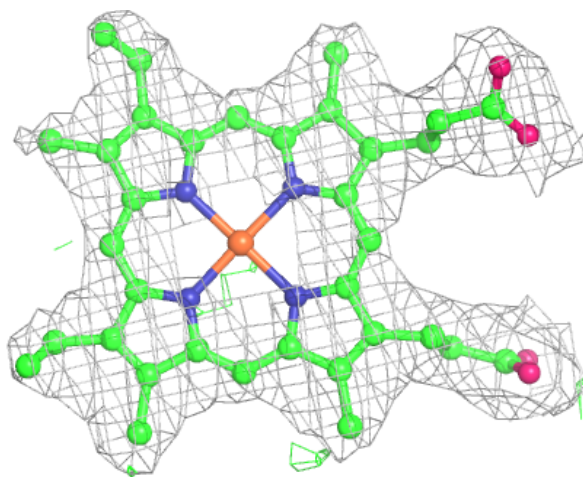
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	HEM	B	500	43/43	0.98	0.15	29,33,38,42	0
2	HEM	D	500	43/43	0.98	0.12	28,33,37,40	0
2	HEM	C	500	43/43	0.98	0.13	28,37,41,44	0
2	HEM	A	500	43/43	0.99	0.14	20,26,32,39	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



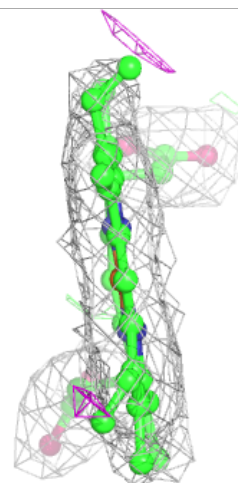
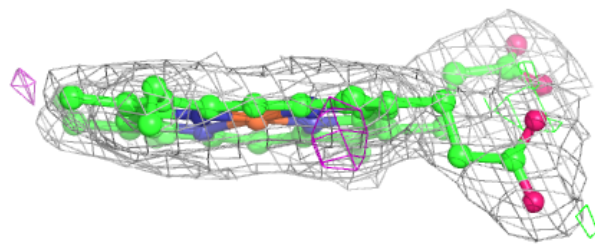
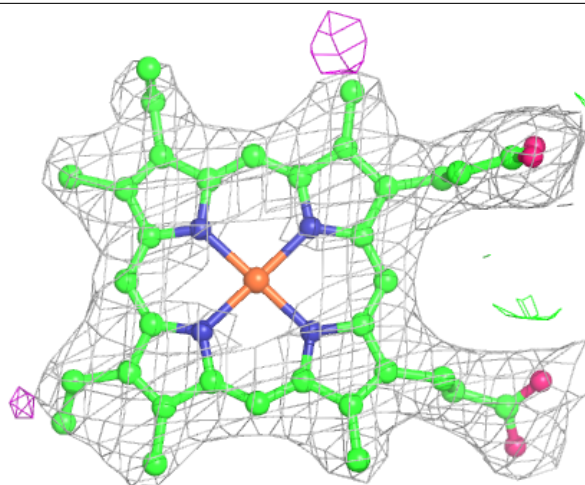
Electron density around HEM D 500:

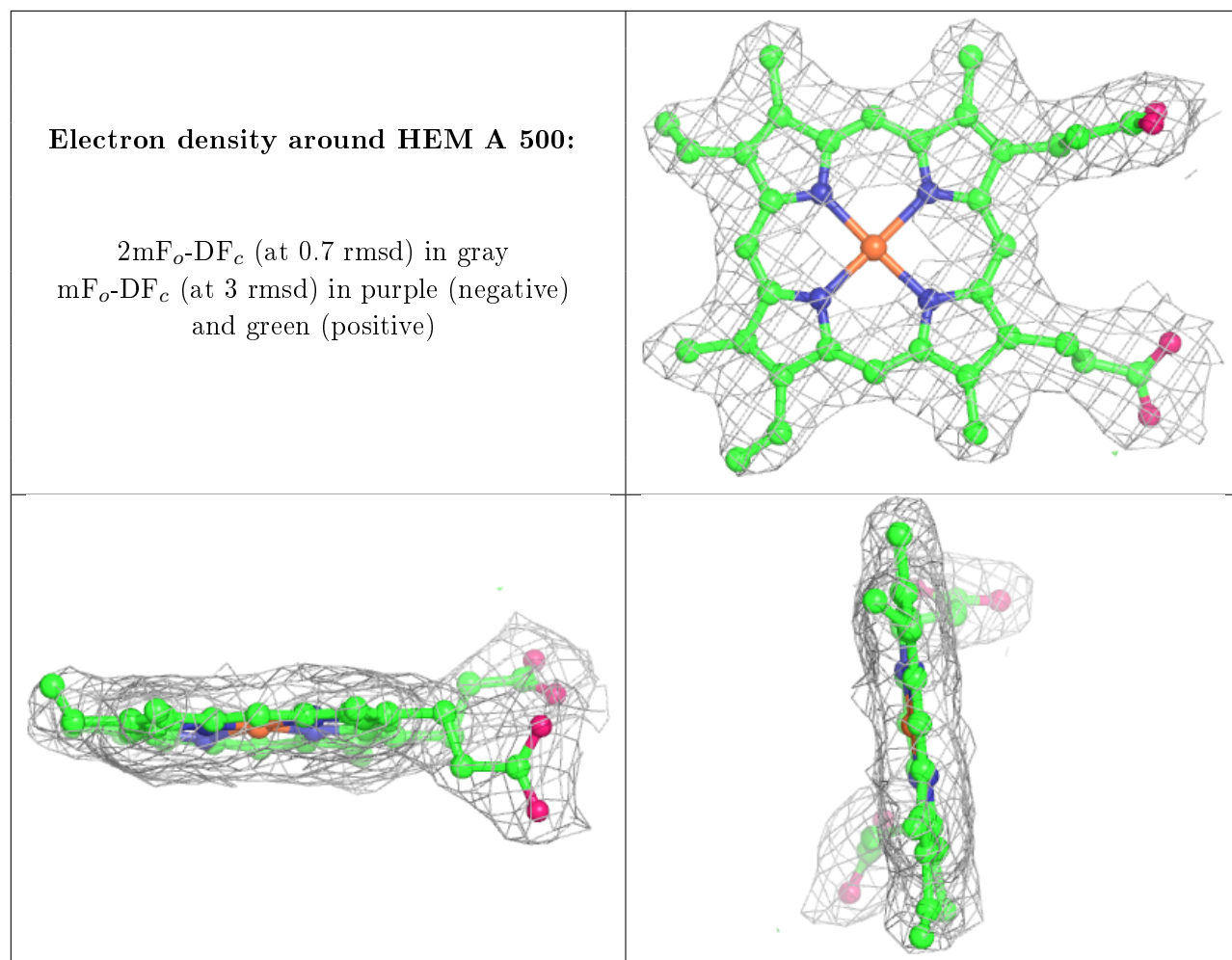
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM C 500:

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.