



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 12:38 PM UTC

PDB ID : 5DYP / pdb_00005dyp
Title : Crystal structure of Asp251Gly/Gln307His mutant of cytochrome P450 BM3
Authors : Di Nardo, G.; Dell'Angelo, V.; Gilardi, G.
Deposited on : 2015-09-25
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

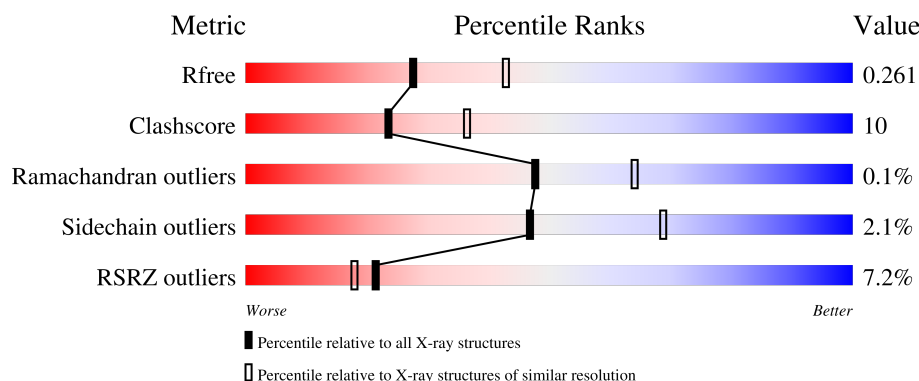
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

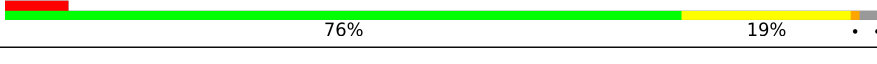
The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	
1	C	470	

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.

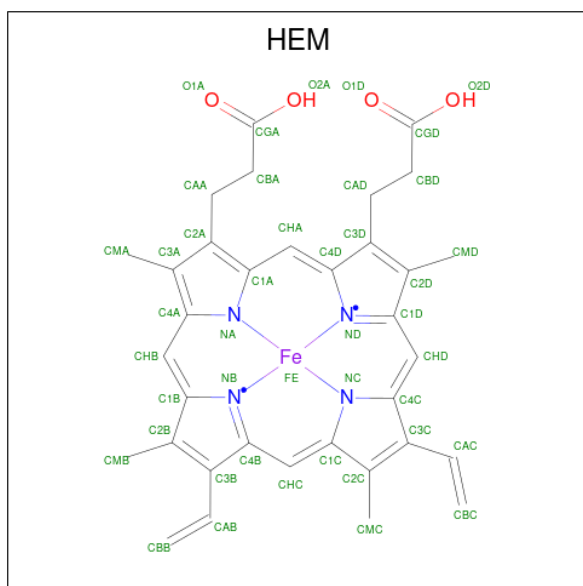
- Molecule 1 is a protein called Bifunctional P-450/NADPH-P450 reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	440	Total	C	N	O	S	0	0	0
			3550	2276	604	653	17			
1	C	450	Total	C	N	O	S	0	0	0
			3627	2321	615	674	17			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	251	GLY	ASP	engineered mutation	UNP P14779
A	307	HIS	GLN	engineered mutation	UNP P14779
C	251	GLY	ASP	engineered mutation	UNP P14779
C	307	HIS	GLN	engineered mutation	UNP P14779

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 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

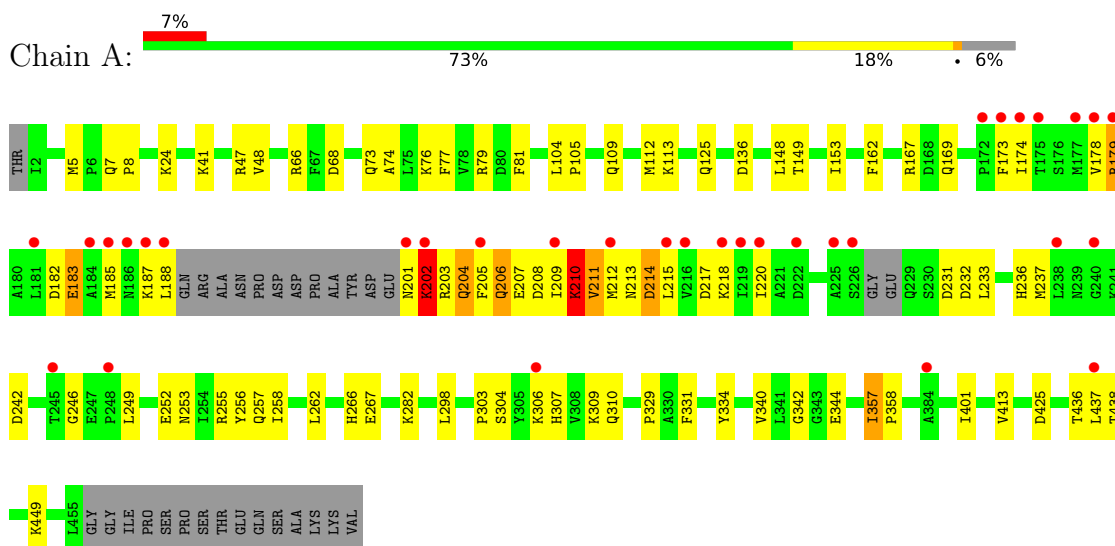
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	98	Total 98	O 98	0	0
3	C	50	Total 50	O 50	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Bifunctional P-450/NADPH-P450 reductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	61.13Å 118.45Å 146.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.00 – 2.40 47.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.3 (47.00-2.40) 98.2 (47.00-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.220 , 0.257 0.226 , 0.261	Depositor DCC
R_{free} test set	2071 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	49.4	Xtriage
Anisotropy	0.312	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 46.1	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	0.94	EDS
Total number of atoms	7411	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% 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	0.41	0/3631	0.92	13/4903 (0.3%)
1	C	0.40	0/3710	0.95	20/5012 (0.4%)
All	All	0.41	0/7341	0.94	33/9915 (0.3%)

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	242	ASP	CA-C-N	-11.56	105.39	119.84
1	C	242	ASP	C-N-CA	-11.56	105.39	119.84
1	C	244	GLU	N-CA-C	-9.15	100.43	111.69
1	C	199	ASP	N-CA-C	-8.96	100.09	111.02
1	A	214	ASP	N-CA-C	-8.86	101.31	110.97
1	C	375	ARG	CA-C-N	8.48	128.60	119.28
1	C	375	ARG	C-N-CA	8.48	128.60	119.28
1	C	196	PRO	N-CA-C	8.01	124.67	113.53
1	C	309	LYS	N-CA-C	6.75	120.61	112.38
1	C	199	ASP	N-CA-CB	6.56	119.79	109.82
1	A	182	ASP	N-CA-C	-6.38	104.75	112.54
1	A	210	LYS	CA-CB-CG	6.36	126.82	114.10
1	C	114	GLY	N-CA-C	-5.93	105.18	112.77
1	A	214	ASP	N-CA-CB	5.88	118.49	109.91
1	A	206	GLN	N-CA-C	-5.69	105.17	111.71
1	A	249	LEU	N-CA-C	-5.58	101.38	109.59
1	A	357	ILE	CB-CA-C	-5.41	108.61	114.35
1	C	7	GLN	CA-C-N	-5.38	114.38	119.76
1	C	7	GLN	C-N-CA	-5.38	114.38	119.76
1	C	381	ASN	CA-C-N	5.37	125.70	119.47
1	C	381	ASN	C-N-CA	5.37	125.70	119.47
1	A	204	GLN	N-CA-C	-5.34	106.61	113.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	304	SER	CA-C-N	5.26	127.60	120.65
1	C	304	SER	C-N-CA	5.26	127.60	120.65
1	A	210	LYS	CB-CG-CD	5.24	123.36	111.30
1	C	357	ILE	CB-CA-C	-5.23	108.81	114.35
1	A	202	LYS	CA-C-O	5.22	127.98	120.51
1	A	210	LYS	N-CA-CB	5.22	117.73	109.94
1	C	10	THR	N-CA-C	5.06	117.21	110.53
1	A	24	LYS	CA-C-N	5.01	124.61	119.05
1	A	24	LYS	C-N-CA	5.01	124.61	119.05
1	C	283	ASN	CA-C-N	5.00	125.03	119.32
1	C	283	ASN	C-N-CA	5.00	125.03	119.32

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	3550	0	3544	74	0
1	C	3627	0	3604	71	0
2	A	43	0	30	1	0
2	C	43	0	30	3	0
3	A	98	0	0	3	0
3	C	50	0	0	14	0
All	All	7411	0	7208	147	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 10.

All (147) 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:113:LYS:O	3:A:601:HOH:O	1.81	0.99
1:C:84:ASP:O	3:C:601:HOH:O	1.81	0.95
1:A:125:GLN:OE1	3:A:602:HOH:O	1.87	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:ILE:O	3:A:603:HOH:O	1.90	0.88
1:C:349:LYS:O	3:C:602:HOH:O	1.96	0.81
1:C:241:LYS:HZ3	1:C:247:GLU:N	1.82	0.77
1:C:196:PRO:O	1:C:199:ASP:N	2.20	0.73
1:A:304:SER:OG	1:A:307:HIS:ND1	2.22	0.70
1:C:348:GLU:OE2	3:C:604:HOH:O	2.10	0.69
1:A:252:GLU:HG2	1:A:256:TYR:CE2	2.27	0.69
1:C:219:ILE:O	3:C:603:HOH:O	2.10	0.68
1:C:7:GLN:OE1	1:C:41:LYS:NZ	2.26	0.68
1:C:84:ASP:OD2	3:C:606:HOH:O	2.12	0.67
1:C:2:ILE:O	1:C:3:LYS:HD3	1.96	0.65
1:C:389:ALA:O	3:C:607:HOH:O	2.15	0.64
1:A:179:ARG:HH21	1:A:204:GLN:HG3	1.62	0.64
1:C:195:ASP:O	1:C:198:TYR:HB2	1.97	0.64
1:C:343:GLY:N	3:C:610:HOH:O	2.26	0.63
1:C:112:MET:HB3	1:C:305:TYR:OH	1.99	0.62
1:C:280:LEU:HB3	1:C:287:LEU:HD13	1.82	0.62
1:A:74:ALA:HB1	1:A:437:LEU:HD21	1.82	0.62
1:C:2:ILE:C	1:C:3:LYS:HD3	2.25	0.62
2:C:501:HEM:HBB2	2:C:501:HEM:HMB1	1.83	0.61
1:A:211:VAL:HA	1:A:214:ASP:CG	2.25	0.60
1:A:217:ASP:OD1	1:A:255:ARG:NH2	2.34	0.60
1:C:388:HIS:HA	1:C:391:LYS:HE2	1.84	0.60
1:C:3:LYS:HG2	1:C:344:GLU:HB3	1.84	0.60
1:C:148:LEU:HD21	1:C:413:VAL:HG21	1.84	0.59
1:A:206:GLN:O	1:A:210:LYS:HD3	2.01	0.59
1:A:282:LYS:NZ	1:A:425:ASP:OD2	2.26	0.59
1:A:233:LEU:HG	1:A:237:MET:HE3	1.86	0.58
1:C:253:ASN:O	1:C:257:GLN:HG2	2.04	0.57
1:A:231:ASP:OD1	1:A:236:HIS:NE2	2.37	0.57
1:A:214:ASP:HB3	1:A:218:LYS:NZ	2.20	0.57
1:A:436:THR:C	1:A:438:THR:H	2.13	0.56
1:C:436:THR:C	1:C:438:THR:H	2.13	0.56
1:C:8:PRO:O	1:C:16:ASN:ND2	2.33	0.56
1:A:253:ASN:HA	1:A:256:TYR:HD2	1.70	0.55
1:C:217:ASP:OD1	1:C:255:ARG:NH2	2.36	0.55
1:A:252:GLU:HG2	1:A:256:TYR:HE2	1.71	0.55
1:A:253:ASN:O	1:A:257:GLN:HG2	2.07	0.55
1:C:162:PHE:CE1	1:C:215:LEU:HD21	2.43	0.54
1:A:220:ILE:HD11	1:A:255:ARG:HG2	1.89	0.54
1:C:5:MET:SD	1:C:50:ARG:HG2	2.47	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:ARG:HB3	1:A:206:GLN:HB3	1.90	0.54
1:A:202:LYS:C	1:A:203:ARG:HD3	2.33	0.54
2:A:501:HEM:HMC2	2:A:501:HEM:HBC2	1.89	0.54
1:C:98:LYS:NZ	3:C:617:HOH:O	2.39	0.54
1:C:161:ARG:HA	3:C:630:HOH:O	2.07	0.53
1:A:207:GLU:HA	1:A:210:LYS:HG2	1.90	0.53
1:C:232:ASP:O	1:C:236:HIS:ND1	2.33	0.53
1:A:204:GLN:HA	1:A:207:GLU:HB3	1.91	0.53
1:A:242:ASP:O	1:A:246:GLY:N	2.38	0.52
1:A:162:PHE:HE1	1:A:215:LEU:HD11	1.75	0.52
1:A:179:ARG:HH21	1:A:204:GLN:CG	2.22	0.52
1:C:116:HIS:HB2	1:C:305:TYR:CD2	2.44	0.52
1:C:1:THR:O	1:C:344:GLU:HA	2.11	0.51
1:A:255:ARG:HA	1:A:258:ILE:HD12	1.93	0.51
1:C:298:LEU:HB2	1:C:419:LYS:HD2	1.93	0.51
1:C:234:LEU:HA	1:C:237:MET:HE3	1.93	0.50
2:C:501:HEM:HBC2	2:C:501:HEM:HMC2	1.94	0.49
1:A:204:GLN:O	1:A:207:GLU:HB3	2.11	0.49
1:A:207:GLU:HA	1:A:210:LYS:CD	2.42	0.49
1:A:167:ARG:HB3	1:A:169:GLN:NE2	2.27	0.49
1:A:148:LEU:HD21	1:A:413:VAL:HG21	1.95	0.49
1:A:169:GLN:N	1:A:169:GLN:OE1	2.47	0.48
1:C:7:GLN:HG2	1:C:8:PRO:O	2.13	0.48
1:C:196:PRO:C	1:C:198:TYR:N	2.69	0.48
1:C:241:LYS:HZ3	1:C:246:GLY:C	2.21	0.48
1:A:206:GLN:O	1:A:209:ILE:HB	2.14	0.48
1:C:243:PRO:HA	1:C:246:GLY:H	1.78	0.48
1:A:109:GLN:HA	1:A:112:MET:HB2	1.95	0.47
1:A:173:PHE:CE1	1:A:212:MET:HG2	2.48	0.47
1:A:68:ASP:HB3	1:A:334:TYR:CE1	2.49	0.47
1:A:208:ASP:HA	1:A:211:VAL:HG13	1.96	0.47
1:C:118:MET:SD	3:C:648:HOH:O	2.61	0.47
1:A:203:ARG:HA	1:A:206:GLN:H	1.80	0.46
1:A:204:GLN:HA	1:A:207:GLU:CB	2.45	0.46
1:A:306:LYS:O	1:A:310:GLN:HG3	2.15	0.46
1:C:50:ARG:HB2	1:C:353:LEU:HD23	1.98	0.46
1:A:331:PHE:HD1	1:A:357:ILE:HD11	1.81	0.46
1:C:151:ASP:OD1	1:C:162:PHE:HB2	2.16	0.46
1:A:185:MET:O	1:A:188:LEU:HG	2.16	0.45
1:C:183:GLU:O	1:C:187:LYS:HG3	2.16	0.45
1:C:399:ALA:O	3:C:608:HOH:O	2.21	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:GLN:NE2	1:C:168:ASP:OD1	2.45	0.45
1:A:211:VAL:HA	1:A:214:ASP:OD2	2.16	0.45
1:C:79:ARG:HG3	1:C:83:GLY:O	2.16	0.45
1:A:149:THR:O	1:A:153:ILE:HG22	2.17	0.45
1:A:173:PHE:HE1	1:A:212:MET:HG2	1.81	0.45
1:A:214:ASP:HB3	1:A:218:LYS:HZ2	1.80	0.45
1:C:201:ASN:OD1	1:C:202:LYS:N	2.50	0.45
1:A:47:ARG:NH2	1:A:73:GLN:HB2	2.32	0.45
1:A:266:HIS:CG	1:A:267:GLU:N	2.85	0.44
1:A:73:GLN:HG3	1:A:77:PHE:CE2	2.52	0.44
1:C:196:PRO:C	1:C:199:ASP:H	2.22	0.44
1:C:5:MET:HE3	1:C:5:MET:HB2	1.79	0.44
1:C:196:PRO:O	1:C:197:ALA:C	2.61	0.44
1:A:7:GLN:HG3	1:A:41:LYS:O	2.18	0.44
1:A:207:GLU:HA	1:A:210:LYS:CG	2.48	0.44
1:C:113:LYS:HE3	1:C:306:LYS:HE3	2.00	0.43
1:C:199:ASP:O	1:C:202:LYS:HB3	2.19	0.43
1:A:81:PHE:HB3	1:A:209:ILE:HG12	1.99	0.43
1:A:173:PHE:CD1	1:A:215:LEU:HD22	2.53	0.43
1:A:183:GLU:O	1:A:187:LYS:HG3	2.18	0.43
1:C:104:LEU:HA	1:C:401:ILE:HD11	2.00	0.43
1:A:201:ASN:OD1	1:A:204:GLN:HB3	2.18	0.43
1:C:215:LEU:HD12	1:C:215:LEU:HA	1.77	0.43
1:C:112:MET:HE1	1:C:405:PHE:HA	2.00	0.43
1:C:241:LYS:HE3	1:C:241:LYS:HB3	1.46	0.43
1:C:158:PHE:HE1	1:C:237:MET:HE1	1.83	0.43
1:C:440:LYS:NZ	3:C:605:HOH:O	2.11	0.43
1:A:174:ILE:O	1:A:178:VAL:HG23	2.19	0.43
1:C:31:LYS:HB2	1:C:31:LYS:HE2	1.57	0.43
1:C:241:LYS:HZ2	1:C:242:ASP:N	2.17	0.43
1:A:449:LYS:HE2	1:A:449:LYS:HB3	1.76	0.42
1:A:183:GLU:OE1	1:A:205:PHE:HB2	2.20	0.42
1:C:304:SER:OG	1:C:307:HIS:CE1	2.73	0.42
1:A:76:LYS:O	1:A:79:ARG:HB3	2.18	0.42
1:A:262:LEU:HD23	1:A:262:LEU:HA	1.81	0.42
1:C:116:HIS:HB2	1:C:305:TYR:HD2	1.83	0.42
1:C:304:SER:HG	1:C:307:HIS:CE1	2.38	0.42
1:A:68:ASP:HB3	1:A:334:TYR:CZ	2.54	0.42
1:A:232:ASP:O	1:A:236:HIS:HD2	2.01	0.42
1:C:202:LYS:HD2	1:C:206:GLN:HG2	2.00	0.42
1:C:257:GLN:O	1:C:261:PHE:HD2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:GLU:HA	1:A:210:LYS:HE2	2.01	0.42
1:C:400:CYS:HB2	2:C:501:HEM:NA	2.34	0.42
1:C:169:GLN:HG2	1:C:170:PRO:O	2.19	0.42
1:C:435:GLU:HB3	3:C:634:HOH:O	2.20	0.42
1:A:203:ARG:HA	1:A:206:GLN:HB3	2.03	0.41
1:A:331:PHE:CD1	1:A:357:ILE:HD11	2.55	0.41
1:A:329:PRO:O	1:A:358:PRO:HD3	2.21	0.41
1:A:342:GLY:O	1:A:344:GLU:HG3	2.20	0.41
1:C:198:TYR:N	1:C:198:TYR:CD1	2.86	0.41
1:C:250:ASP:O	1:C:254:ILE:HG13	2.21	0.41
1:A:66:ARG:NH2	1:A:340:VAL:O	2.53	0.41
1:C:113:LYS:HD3	1:C:305:TYR:CG	2.56	0.41
1:A:7:GLN:HA	1:A:8:PRO:HD3	1.95	0.41
1:A:104:LEU:N	1:A:105:PRO:HD2	2.36	0.41
1:C:378:ARG:N	3:C:622:HOH:O	2.53	0.41
1:A:47:ARG:HE	1:A:47:ARG:HB2	1.67	0.40
1:C:241:LYS:HZ1	1:C:242:ASP:C	2.29	0.40
1:A:5:MET:HE3	1:A:5:MET:HB2	1.99	0.40
1:C:7:GLN:HG3	1:C:41:LYS:O	2.21	0.40
1:C:414:LEU:O	1:C:418:LEU:HG	2.21	0.40
1:A:298:LEU:HD22	1:A:303:PRO:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	434/470 (92%)	422 (97%)	11 (2%)	1 (0%)	43	58
1	C	444/470 (94%)	430 (97%)	14 (3%)	0	100	100
All	All	878/940 (93%)	852 (97%)	25 (3%)	1 (0%)	48	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	202	LYS

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	386/410 (94%)	378 (98%)	8 (2%)	47	69
1	C	394/410 (96%)	386 (98%)	8 (2%)	48	70
All	All	780/820 (95%)	764 (98%)	16 (2%)	47	69

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	VAL
1	A	136	ASP
1	A	179	ARG
1	A	183	GLU
1	A	210	LYS
1	A	211	VAL
1	A	213	ASN
1	A	309	LYS
1	C	13	GLU
1	C	31	LYS
1	C	48	VAL
1	C	136	ASP
1	C	196	PRO
1	C	241	LYS
1	C	247	GLU
1	C	387	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	100	HIS
1	A	186	ASN
1	A	239	ASN
1	A	397	GLN
1	C	206	GLN
1	C	283	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	C	501	1	50,50,50	1.86	10 (20%)	67,82,82	1.19	2 (2%)
2	HEM	A	501	1	50,50,50	1.87	10 (20%)	67,82,82	1.20	2 (2%)

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	C	501	1	-	2/14/54/54	-
2	HEM	A	501	1	-	4/14/54/54	-

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	HEM	C3D-C2D	7.97	1.54	1.36
2	A	501	HEM	C3D-C2D	7.70	1.53	1.36
2	A	501	HEM	FE-ND	4.93	2.10	1.94
2	C	501	HEM	FE-ND	4.27	2.08	1.94
2	C	501	HEM	FE-NA	3.70	2.07	1.95
2	A	501	HEM	FE-NA	3.49	2.06	1.95
2	C	501	HEM	FE-NB	3.45	2.05	1.94
2	A	501	HEM	FE-NB	3.27	2.05	1.94
2	C	501	HEM	CAB-C3B	3.07	1.55	1.47
2	C	501	HEM	CAC-C3C	3.06	1.55	1.47
2	A	501	HEM	CAC-C3C	3.05	1.55	1.47
2	A	501	HEM	CAB-C3B	3.01	1.55	1.47
2	A	501	HEM	FE-NC	2.84	2.04	1.95
2	C	501	HEM	FE-NC	2.46	2.03	1.95
2	A	501	HEM	CMB-C2B	2.33	1.55	1.50
2	C	501	HEM	CMB-C2B	2.30	1.55	1.50
2	C	501	HEM	CMC-C2C	2.15	1.55	1.50
2	A	501	HEM	CMA-C3A	2.07	1.55	1.50
2	C	501	HEM	CMD-C2D	2.05	1.55	1.50
2	A	501	HEM	CMC-C2C	2.03	1.54	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	HEM	C4D-ND-C1D	5.23	111.41	105.21
2	C	501	HEM	C4D-ND-C1D	5.18	111.34	105.21
2	A	501	HEM	CBD-CAD-C3D	-2.36	106.00	112.53
2	C	501	HEM	C2A-C1A-NA	-2.08	107.85	110.15

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	501	HEM	C2D-C3D-CAD-CBD
2	A	501	HEM	CAD-CBD-CGD-O2D
2	A	501	HEM	CAD-CBD-CGD-O1D

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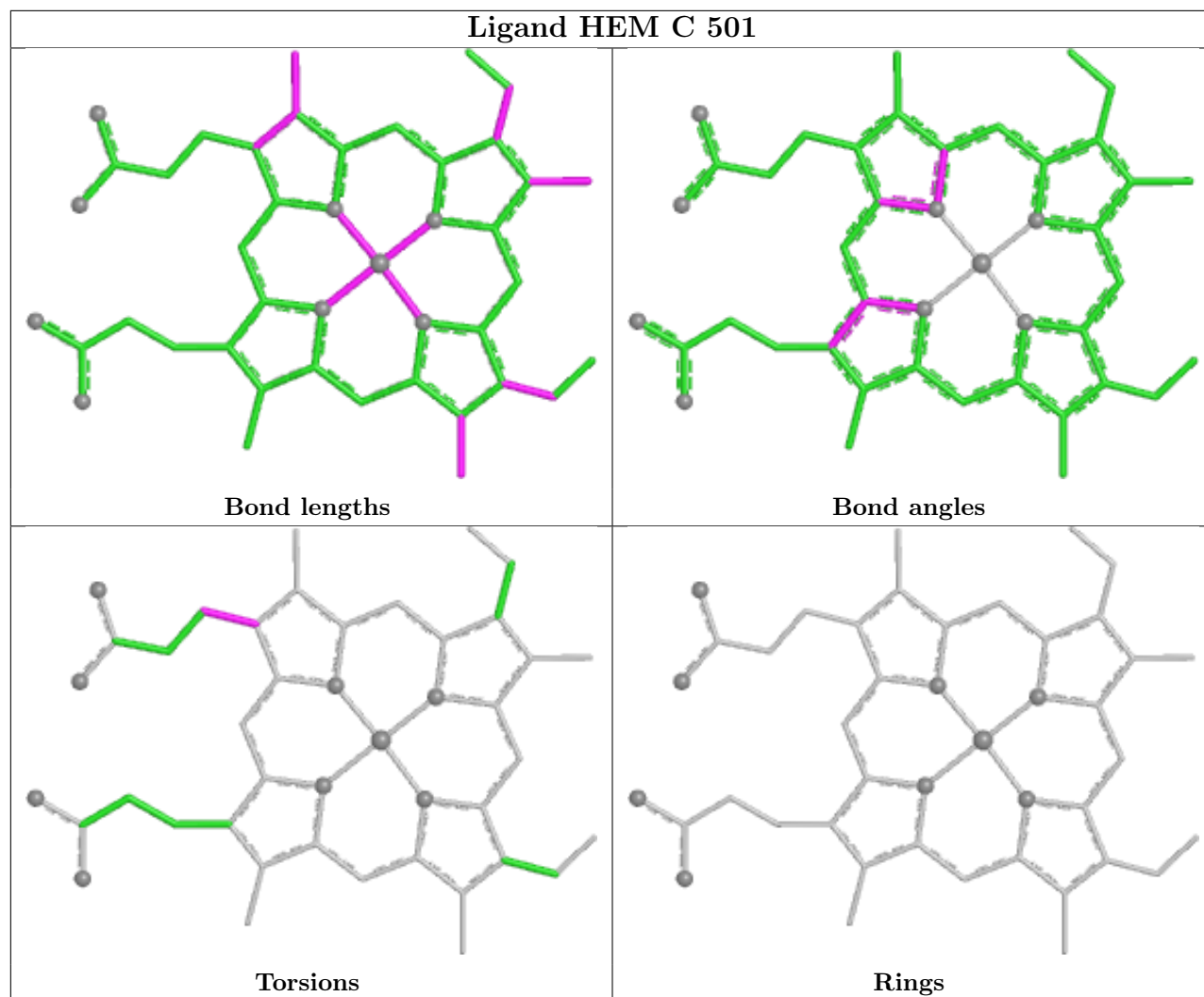
Mol	Chain	Res	Type	Atoms
2	A	501	HEM	CAA-CBA-CGA-O2A
2	C	501	HEM	C4D-C3D-CAD-CBD
2	A	501	HEM	CAA-CBA-CGA-O1A

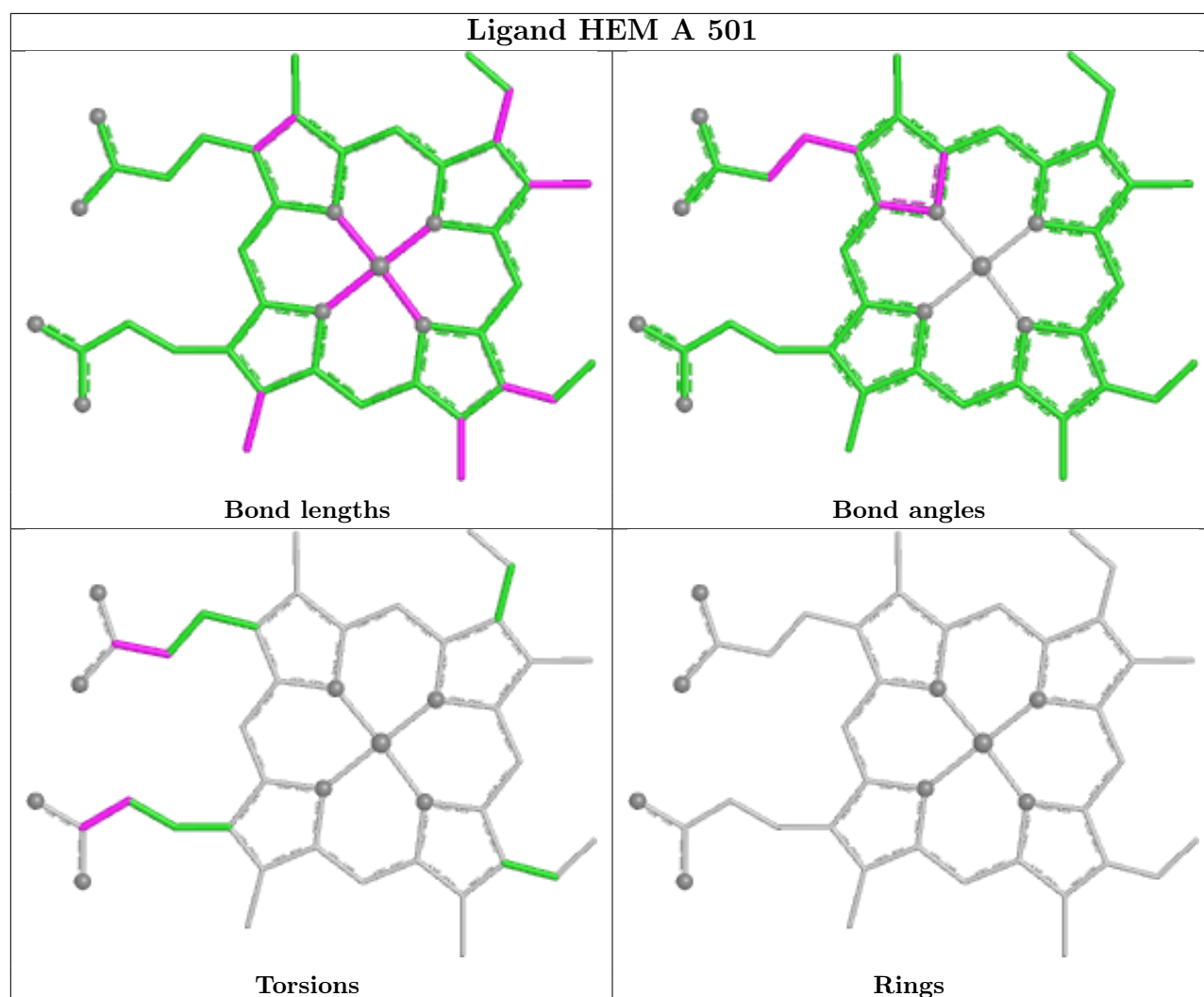
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	HEM	3	0
2	A	501	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, 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	440/470 (93%)	0.33	33 (7%)	20 17	36, 62, 125, 191	0
1	C	450/470 (95%)	0.64	31 (6%)	23 19	48, 76, 118, 150	0
All	All	890/940 (94%)	0.49	64 (7%)	21 18	36, 70, 120, 191	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	305	TYR	5.9
1	C	243	PRO	5.1
1	A	181	LEU	4.2
1	A	188	LEU	4.1
1	C	196	PRO	4.1
1	C	456	GLY	4.1
1	A	437	LEU	3.7
1	A	212	MET	3.7
1	C	294	ALA	3.5
1	C	110	GLN	3.4
1	A	216	VAL	3.4
1	A	172	PRO	3.4
1	A	178	VAL	3.3
1	A	173	PHE	3.2
1	A	175	THR	3.2
1	A	238	LEU	3.1
1	A	185	MET	3.0
1	A	184	ALA	3.0
1	A	215	LEU	3.0
1	C	23	ASP	3.0
1	A	209	ILE	2.9
1	C	9	LYS	2.9
1	C	310	GLN	2.9
1	C	287	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	248	PRO	2.8
1	C	136	ASP	2.8
1	A	222	ASP	2.8
1	A	202	LYS	2.7
1	A	177	MET	2.7
1	C	244	GLU	2.6
1	A	205	PHE	2.5
1	C	11	PHE	2.5
1	C	221	ALA	2.5
1	A	174	ILE	2.5
1	A	220	ILE	2.4
1	A	186	ASN	2.4
1	A	226	SER	2.4
1	C	226	SER	2.4
1	C	229	GLN	2.4
1	A	218	LYS	2.4
1	C	68	ASP	2.4
1	C	111	ALA	2.3
1	A	219	ILE	2.3
1	C	242	ASP	2.3
1	C	17	LEU	2.2
1	C	194	ASP	2.2
1	C	335	ALA	2.2
1	A	240	GLY	2.2
1	C	214	ASP	2.2
1	C	2	ILE	2.2
1	A	187	LYS	2.2
1	A	225	ALA	2.2
1	A	306	LYS	2.2
1	C	189	GLN	2.1
1	A	245	THR	2.1
1	C	8	PRO	2.1
1	C	188	LEU	2.1
1	A	179	ARG	2.1
1	C	246	GLY	2.1
1	C	307	HIS	2.1
1	A	384	ALA	2.1
1	A	201	ASN	2.1
1	C	112	MET	2.1
1	C	306	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

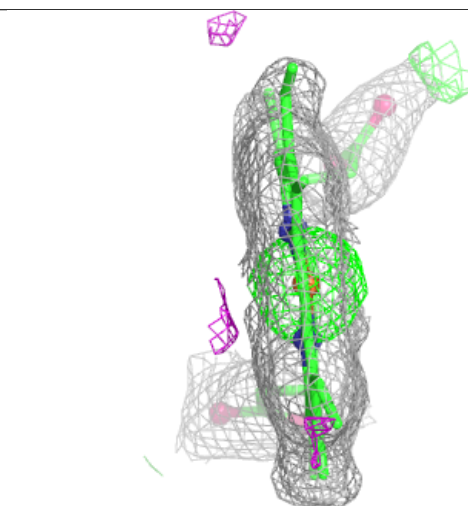
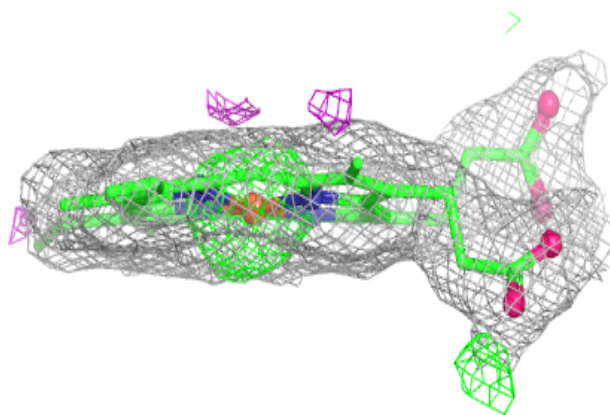
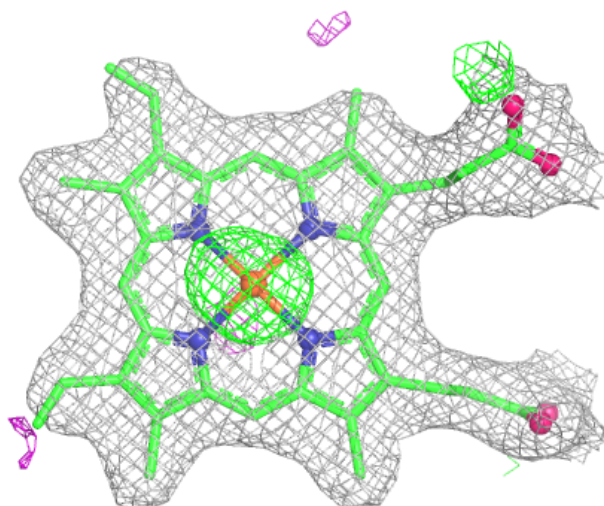
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

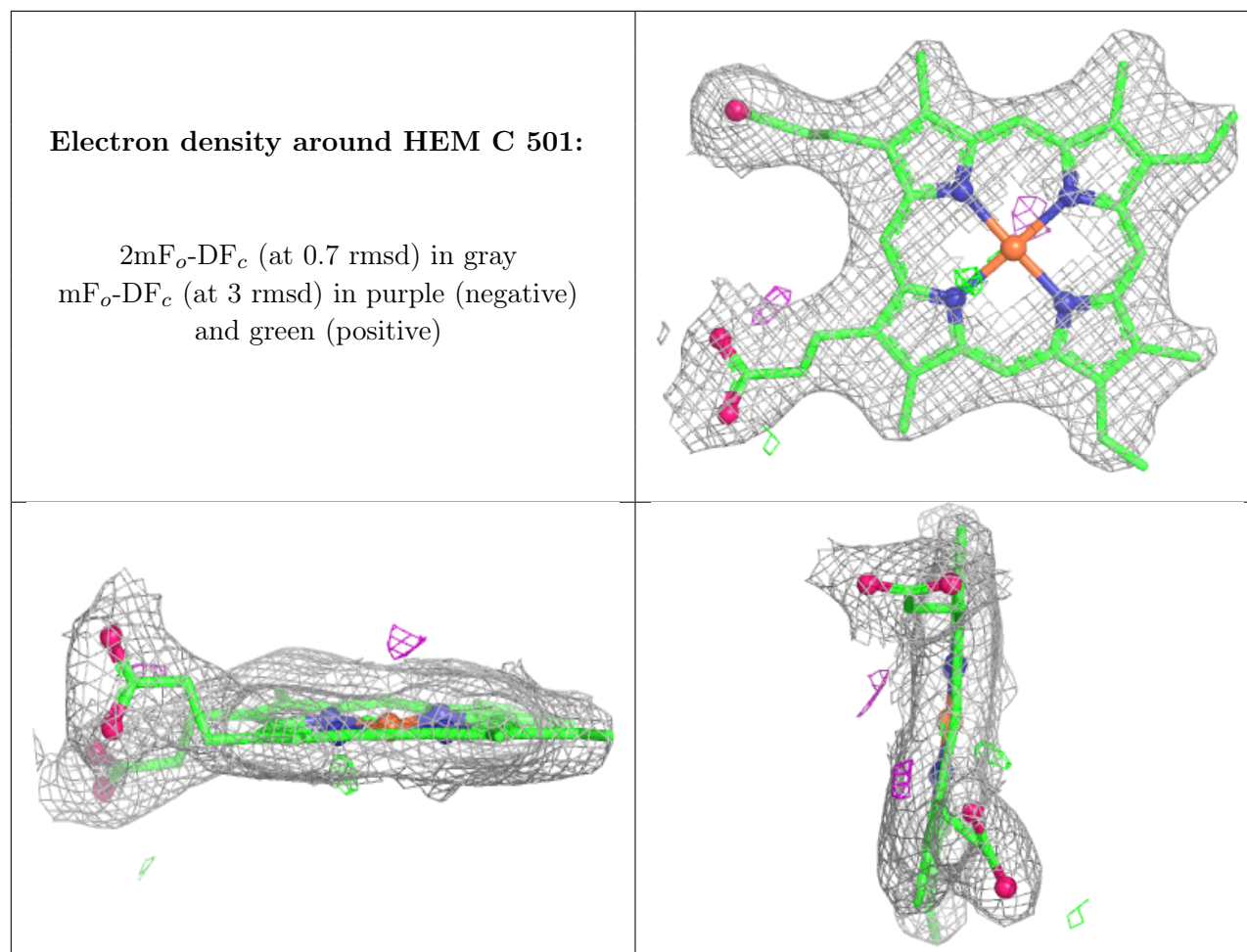
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	HEM	A	501	43/43	0.92	0.09	20,41,52,88	0
2	HEM	C	501	43/43	0.97	0.09	27,49,64,67	0

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 A 501:

$2mF_o-DF_c$ (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.