



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:27 PM UTC

PDB ID : 6E44 / pdb_00006e44
Title : CRYSTAL STRUCTURE OF HUMAN INDOLEAMINE 2,3-DIOXYGENASE 1 (IDO1) free enzyme in the ferric state
Authors : Luo, S.; Tong, L.
Deposited on : 2018-07-16
Resolution : 1.90 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

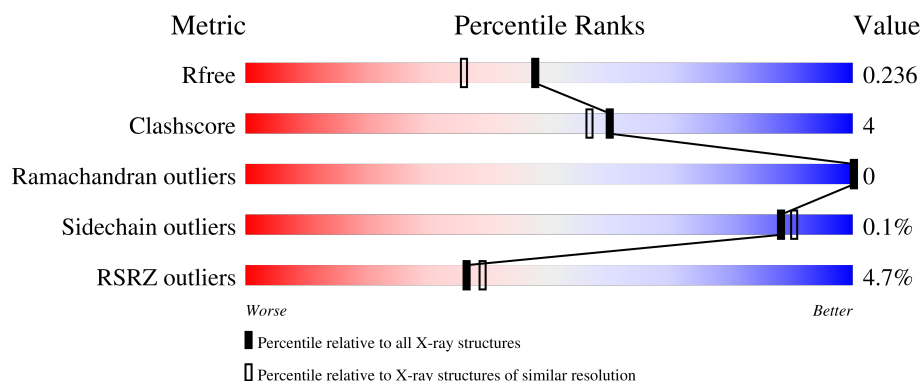
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	405	5% 77% 14% 9%
1	B	405	4% 85% 7% 7%
1	C	405	4% 80% 10% 9%
1	D	405	4% 81% 9% 9%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12847 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 Indoleamine 2,3-dioxygenase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	368	Total	C	N	O	S	0	1	0
			2917	1877	496	527	17			
1	B	375	Total	C	N	O	S	0	1	0
			2963	1905	504	537	17			
1	C	368	Total	C	N	O	S	0	2	0
			2927	1884	496	529	18			
1	D	369	Total	C	N	O	S	0	0	0
			2915	1875	497	526	17			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	UNP P14902
A	0	GLY	-	expression tag	UNP P14902
A	1	SER	-	expression tag	UNP P14902
A	2	SER	-	expression tag	UNP P14902
A	3	HIS	-	expression tag	UNP P14902
A	4	HIS	-	expression tag	UNP P14902
A	5	HIS	-	expression tag	UNP P14902
A	6	HIS	-	expression tag	UNP P14902
A	7	HIS	-	expression tag	UNP P14902
A	8	HIS	-	expression tag	UNP P14902
A	9	SER	-	expression tag	UNP P14902
A	10	SER	-	expression tag	UNP P14902
A	11	GLY	-	expression tag	UNP P14902
A	12	SER	-	expression tag	UNP P14902
A	13	ALA	-	expression tag	UNP P14902
A	14	ALA	-	expression tag	UNP P14902
A	116	ALA	LYS	engineered mutation	UNP P14902
A	117	ALA	LYS	engineered mutation	UNP P14902
B	-1	MET	-	initiating methionine	UNP P14902
B	0	GLY	-	expression tag	UNP P14902
B	1	SER	-	expression tag	UNP P14902

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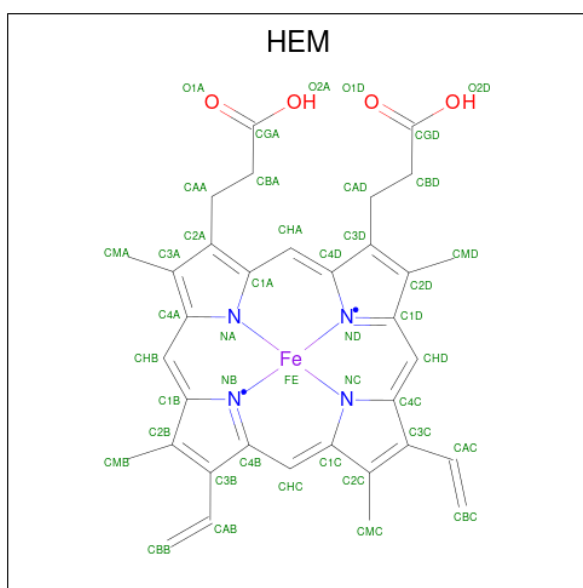
Chain	Residue	Modelled	Actual	Comment	Reference
B	2	SER	-	expression tag	UNP P14902
B	3	HIS	-	expression tag	UNP P14902
B	4	HIS	-	expression tag	UNP P14902
B	5	HIS	-	expression tag	UNP P14902
B	6	HIS	-	expression tag	UNP P14902
B	7	HIS	-	expression tag	UNP P14902
B	8	HIS	-	expression tag	UNP P14902
B	9	SER	-	expression tag	UNP P14902
B	10	SER	-	expression tag	UNP P14902
B	11	GLY	-	expression tag	UNP P14902
B	12	SER	-	expression tag	UNP P14902
B	13	ALA	-	expression tag	UNP P14902
B	14	ALA	-	expression tag	UNP P14902
B	116	ALA	LYS	engineered mutation	UNP P14902
B	117	ALA	LYS	engineered mutation	UNP P14902
C	-1	MET	-	initiating methionine	UNP P14902
C	0	GLY	-	expression tag	UNP P14902
C	1	SER	-	expression tag	UNP P14902
C	2	SER	-	expression tag	UNP P14902
C	3	HIS	-	expression tag	UNP P14902
C	4	HIS	-	expression tag	UNP P14902
C	5	HIS	-	expression tag	UNP P14902
C	6	HIS	-	expression tag	UNP P14902
C	7	HIS	-	expression tag	UNP P14902
C	8	HIS	-	expression tag	UNP P14902
C	9	SER	-	expression tag	UNP P14902
C	10	SER	-	expression tag	UNP P14902
C	11	GLY	-	expression tag	UNP P14902
C	12	SER	-	expression tag	UNP P14902
C	13	ALA	-	expression tag	UNP P14902
C	14	ALA	-	expression tag	UNP P14902
C	116	ALA	LYS	engineered mutation	UNP P14902
C	117	ALA	LYS	engineered mutation	UNP P14902
D	-1	MET	-	initiating methionine	UNP P14902
D	0	GLY	-	expression tag	UNP P14902
D	1	SER	-	expression tag	UNP P14902
D	2	SER	-	expression tag	UNP P14902
D	3	HIS	-	expression tag	UNP P14902
D	4	HIS	-	expression tag	UNP P14902
D	5	HIS	-	expression tag	UNP P14902
D	6	HIS	-	expression tag	UNP P14902
D	7	HIS	-	expression tag	UNP P14902

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Chain	Residue	Modelled	Actual	Comment	Reference
D	8	HIS	-	expression tag	UNP P14902
D	9	SER	-	expression tag	UNP P14902
D	10	SER	-	expression tag	UNP P14902
D	11	GLY	-	expression tag	UNP P14902
D	12	SER	-	expression tag	UNP P14902
D	13	ALA	-	expression tag	UNP P14902
D	14	ALA	-	expression tag	UNP P14902
D	116	ALA	LYS	engineered mutation	UNP P14902
D	117	ALA	LYS	engineered mutation	UNP P14902

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



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 PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).

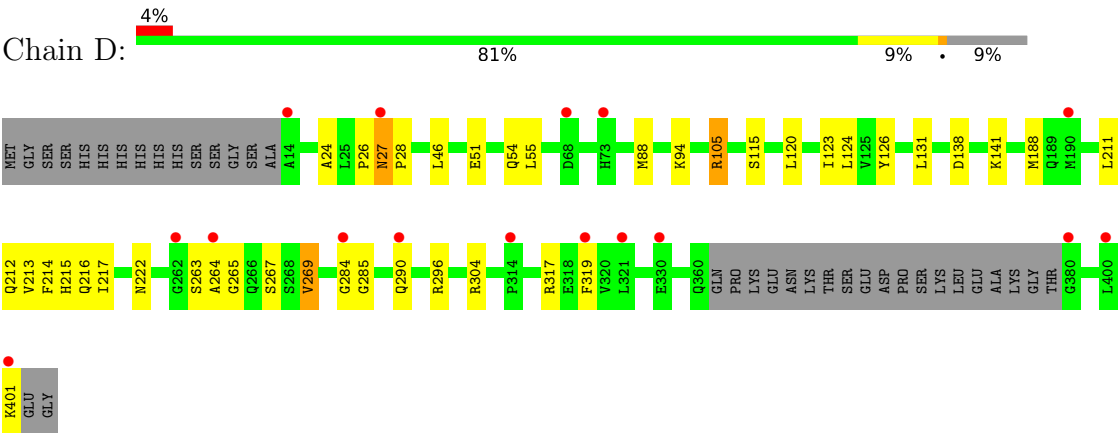


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	215	Total	O	0	0
			215	215		
4	B	249	Total	O	0	0
			249	249		
4	C	228	Total	O	0	0
			228	228		
4	D	246	Total	O	0	0
			246	246		

● Molecule 1: Indoleamine 2,3-dioxygenase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	80.08Å 197.00Å 116.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.04 – 1.90 47.04 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.2 (47.04-1.90) 99.2 (47.04-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 1.91Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.194 , 0.235 0.196 , 0.236	Depositor DCC
R_{free} test set	2157 reflections (1.26%)	wwPDB-VP
Wilson B-factor (Å ²)	32.0	Xtriage
Anisotropy	0.219	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 37.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	12847	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.87 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.4342e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, PO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.65	15/2988 (0.5%)	0.56	3/4045 (0.1%)
1	B	0.31	0/3034	0.49	0/4106
1	C	0.62	14/3000 (0.5%)	0.58	2/4059 (0.0%)
1	D	0.62	10/2983 (0.3%)	0.54	0/4038
All	All	0.56	39/12005 (0.3%)	0.54	5/16248 (0.0%)

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	27	ASN	C-O	-11.12	1.18	1.23
1	A	27	ASN	C-O	-10.99	1.18	1.23
1	A	30[A]	GLU	CA-C	8.54	1.64	1.52
1	A	30[B]	GLU	CA-C	8.54	1.64	1.52
1	C	55	LEU	C-O	-8.39	1.14	1.24
1	D	212	GLN	C-O	-8.03	1.14	1.24
1	A	46	LEU	C-O	-8.02	1.17	1.24
1	D	215	HIS	C-O	-7.80	1.14	1.24
1	C	26	PRO	C-O	-7.68	1.15	1.23
1	D	211	LEU	C-O	-7.47	1.15	1.24
1	A	25	LEU	C-O	-7.33	1.15	1.24
1	D	26	PRO	C-O	-7.24	1.15	1.23
1	D	28	PRO	C-O	-7.22	1.15	1.23
1	C	30[A]	GLU	CA-C	7.13	1.62	1.52
1	C	30[B]	GLU	CA-C	7.13	1.62	1.52
1	D	214	PHE	C-O	-7.12	1.15	1.24
1	C	29	GLN	C-O	-7.08	1.15	1.23
1	D	213	VAL	C-O	-6.95	1.16	1.24
1	A	23	PHE	C-O	-6.89	1.15	1.24
1	C	25	LEU	C-O	-6.77	1.15	1.24
1	C	46	LEU	C-O	-6.70	1.18	1.24
1	A	26	PRO	C-O	-6.57	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	28	PRO	C-O	-6.56	1.16	1.23
1	C	28	PRO	C-O	-6.54	1.16	1.23
1	A	22	GLY	C-O	-6.45	1.14	1.24
1	C	346	HIS	C-O	-6.23	1.16	1.24
1	C	24	ALA	C-O	-6.17	1.15	1.23
1	A	31	ASN	C-O	-6.08	1.16	1.23
1	A	24	ALA	C-O	-6.03	1.16	1.23
1	A	30[A]	GLU	C-O	-6.01	1.16	1.24
1	A	30[B]	GLU	C-O	-6.01	1.16	1.24
1	D	105	ARG	C-O	-5.87	1.16	1.24
1	D	216	GLN	C-O	-5.71	1.16	1.24
1	C	30[A]	GLU	C-O	-5.62	1.16	1.24
1	C	30[B]	GLU	C-O	-5.62	1.16	1.24
1	A	356	ILE	CA-CB	-5.60	1.51	1.54
1	C	27	ASN	C-O	-5.41	1.17	1.24
1	C	31	ASN	C-O	-5.20	1.17	1.24
1	A	29	GLN	C-O	-5.15	1.17	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	30[A]	GLU	N-CA-C	8.51	124.05	112.90
1	C	30[B]	GLU	N-CA-C	8.51	124.05	112.90
1	A	21	VAL	N-CA-C	6.07	117.93	112.17
1	A	30[A]	GLU	N-CA-C	5.62	120.26	112.90
1	A	30[B]	GLU	N-CA-C	5.62	120.26	112.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2917	0	2927	33	0
1	B	2963	0	2975	21	0
1	C	2927	0	2938	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2915	0	2924	26	0
2	A	43	0	30	3	0
2	B	43	0	30	2	0
2	C	43	0	30	1	0
2	D	43	0	30	3	0
3	B	5	0	0	0	0
3	D	10	0	0	0	0
4	A	215	0	0	6	0
4	B	249	0	0	6	0
4	C	228	0	0	2	0
4	D	246	0	0	4	0
All	All	12847	0	11884	102	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 (102) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:PHE:HE1	1:A:295:MET:HE3	1.28	0.94
1:A:295:MET:HE1	2:A:501:HEM:HAD2	1.58	0.84
1:A:291:PHE:CE1	1:A:295:MET:HE3	2.12	0.82
1:B:56:ARG:NH2	1:B:98:ASP:O	2.14	0.78
1:A:352:LYS:NZ	4:A:602:HOH:O	2.19	0.75
1:B:377:LYS:NZ	4:B:601:HOH:O	2.15	0.74
1:C:295[B]:MET:HE1	2:C:501:HEM:HAD2	1.70	0.73
1:C:295[A]:MET:SD	4:C:659:HOH:O	2.47	0.73
1:C:291:PHE:CE1	1:C:295[B]:MET:HE3	2.25	0.72
1:C:146:GLU:HG2	1:D:222:ASN:HB2	1.73	0.70
1:B:212:GLN:NE2	4:B:602:HOH:O	2.25	0.70
1:C:146:GLU:HG2	1:D:222:ASN:CB	2.21	0.70
1:B:294:ASP:OD1	1:B:297:ARG:NH2	2.30	0.64
1:B:88:MET:HE1	1:B:123:ILE:HG13	1.80	0.63
1:A:294:ASP:OD1	1:A:297:ARG:NH2	2.30	0.63
1:A:386:ASN:O	1:A:390:THR:HG23	1.99	0.62
2:A:501:HEM:HBB2	2:A:501:HEM:HMB2	1.81	0.61
2:D:501:HEM:HBB2	2:D:501:HEM:HMB2	1.83	0.61
1:A:71:THR:HB	1:D:54:GLN:HG2	1.83	0.61
1:A:355:LEU:HD11	1:A:385:MET:CG	2.30	0.60
1:C:188:MET:HE3	1:C:319:PHE:HB2	1.83	0.60
1:D:105:ARG:HD2	4:D:763:HOH:O	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:317:ARG:NH1	4:D:603:HOH:O	2.35	0.59
1:D:88:MET:HE3	1:D:124:LEU:H	1.67	0.59
1:B:237:TRP:HZ2	1:B:249:TYR:HH	1.52	0.57
1:C:356:ILE:O	1:C:360:GLN:HG3	2.05	0.57
1:A:355:LEU:HD11	1:A:385:MET:HG3	1.87	0.57
1:B:88:MET:HE3	1:B:124:LEU:H	1.70	0.56
1:D:188:MET:HE3	1:D:319:PHE:HB2	1.88	0.56
1:A:329:ARG:HE	1:A:401:LYS:HE2	1.72	0.55
1:A:188:MET:HE3	1:A:319:PHE:HB2	1.90	0.54
1:A:275:VAL:HG13	1:A:311:GLU:HG3	1.90	0.54
2:B:501:HEM:HMB2	2:B:501:HEM:HBB2	1.90	0.53
1:A:51:GLU:O	1:A:94:LYS:NZ	2.42	0.53
1:C:274:ASP:OD2	1:C:281:GLN:HG3	2.09	0.52
1:B:209:LYS:NZ	4:B:605:HOH:O	2.32	0.52
1:A:220:HIS:HE1	4:A:765:HOH:O	1.92	0.52
1:B:58:ARG:HH22	1:C:139:PRO:HD2	1.75	0.52
1:A:68:ASP:OD1	4:A:601:HOH:O	2.19	0.51
1:B:30[B]:GLU:HG3	4:B:672:HOH:O	2.10	0.51
1:C:54:GLN:OE1	1:C:58:ARG:NH1	2.43	0.51
1:B:254:GLU:HG2	4:B:659:HOH:O	2.11	0.51
1:C:355:LEU:HD11	1:C:385:MET:HE3	1.92	0.50
1:A:337:LYS:HG3	1:A:399:LEU:HD21	1.91	0.50
1:A:295:MET:CE	2:A:501:HEM:HAD2	2.35	0.50
1:A:115:SER:HB3	1:A:120:LEU:O	2.12	0.49
1:B:115:SER:HB3	1:B:120:LEU:O	2.13	0.49
1:C:205:SER:O	1:C:209:LYS:HG3	2.13	0.49
1:D:284:GLY:O	4:D:601:HOH:O	2.20	0.49
1:D:263:SER:OG	1:D:265:GLY:N	2.33	0.48
1:A:166:VAL:HG11	1:A:217:ILE:HG12	1.95	0.48
1:C:190:MET:HA	1:C:190:MET:HE2	1.96	0.48
1:C:337:LYS:HG3	1:C:399:LEU:HD21	1.96	0.48
1:B:146:GLU:H	1:B:146:GLU:CD	2.21	0.48
1:D:88:MET:HE1	1:D:123:ILE:HG13	1.95	0.48
1:D:265:GLY:HA2	2:D:501:HEM:C3D	2.49	0.47
1:C:68:ASP:OD2	4:C:601:HOH:O	2.20	0.47
1:C:146:GLU:HG2	1:D:222:ASN:HB3	1.97	0.47
1:C:189:GLN:OE1	1:C:190:MET:HE3	2.15	0.47
1:D:126:TYR:CD1	1:D:264:ALA:HA	2.50	0.47
1:D:296:ARG:O	1:D:304:ARG:HD3	2.15	0.47
1:A:329:ARG:HE	1:A:401:LYS:CE	2.28	0.47
1:C:296:ARG:O	1:C:304:ARG:HD3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:24:ALA:HA	1:D:131:LEU:HD22	1.97	0.47
1:C:295[A]:MET:HA	1:C:295[A]:MET:HE2	1.96	0.46
1:D:27:ASN:ND2	4:D:611:HOH:O	2.48	0.46
1:A:209:LYS:NZ	4:A:612:HOH:O	2.48	0.45
1:A:265:GLY:O	1:A:295:MET:HE2	2.17	0.45
1:A:290:GLN:NE2	1:A:290:GLN:HA	2.31	0.44
1:C:291:PHE:HD1	1:C:387:PHE:CZ	2.35	0.44
1:D:285:GLY:O	1:D:290:GLN:NE2	2.50	0.44
1:A:125:VAL:HG13	1:A:127:ALA:H	1.82	0.44
1:A:189:GLN:NE2	4:A:615:HOH:O	2.51	0.44
1:A:284:GLY:O	4:A:603:HOH:O	2.21	0.43
1:D:115:SER:HB3	1:D:120:LEU:O	2.18	0.43
1:D:401:LYS:HA	1:D:401:LYS:HD3	1.88	0.43
1:C:115:SER:HB3	1:C:120:LEU:O	2.18	0.43
1:B:135:LYS:NZ	4:B:611:HOH:O	2.51	0.43
1:B:321:LEU:HD21	1:B:400:LEU:HD22	2.01	0.43
1:A:125:VAL:CG2	1:A:298:TYR:HB3	2.49	0.43
1:A:54:GLN:O	1:A:58:ARG:HG2	2.19	0.42
1:A:319:PHE:O	1:A:323:LYS:HG2	2.19	0.42
1:B:296:ARG:O	1:B:304:ARG:HD3	2.19	0.42
1:D:217:ILE:HD13	2:D:501:HEM:HAB	2.01	0.42
1:B:197:LEU:HD22	1:B:331:ALA:HB2	2.01	0.42
1:D:188:MET:HE3	1:D:319:PHE:CB	2.50	0.42
1:C:84:GLY:O	1:C:88:MET:HG2	2.19	0.42
1:C:350:VAL:HG12	1:C:385:MET:HE1	2.00	0.42
1:D:267:SER:OG	1:D:269:VAL:HG13	2.20	0.42
1:D:51:GLU:O	1:D:94:LYS:NZ	2.32	0.42
1:A:121:PRO:HG2	1:A:298:TYR:CD2	2.55	0.41
1:A:299:MET:O	1:A:304:ARG:NH1	2.53	0.41
1:B:275:VAL:HG13	1:B:311:GLU:HG3	2.01	0.41
1:B:237:TRP:HZ2	1:B:249:TYR:OH	2.02	0.41
1:A:55:LEU:O	1:A:55:LEU:HG	2.06	0.41
1:A:296:ARG:O	1:A:304:ARG:HD3	2.19	0.41
1:B:384:LEU:HD11	2:B:501:HEM:HMA3	2.03	0.41
1:D:55:LEU:O	1:D:55:LEU:HG	2.07	0.41
1:C:226:PHE:HE2	1:C:354:ILE:HD11	1.85	0.41
1:B:121:PRO:HG2	1:B:298:TYR:CD2	2.56	0.41
1:D:138:ASP:OD2	1:D:141:LYS:HE2	2.20	0.40
1:D:46:LEU:HD12	1:D:46:LEU:HA	1.95	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	365/405 (90%)	355 (97%)	10 (3%)	0	100	100
1	B	372/405 (92%)	365 (98%)	7 (2%)	0	100	100
1	C	364/405 (90%)	354 (97%)	10 (3%)	0	100	100
1	D	365/405 (90%)	358 (98%)	7 (2%)	0	100	100
All	All	1466/1620 (90%)	1432 (98%)	34 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	317/346 (92%)	317 (100%)	0	100	100
1	B	321/346 (93%)	321 (100%)	0	100	100
1	C	319/346 (92%)	319 (100%)	0	100	100
1	D	316/346 (91%)	315 (100%)	1 (0%)	86	88
All	All	1273/1384 (92%)	1272 (100%)	1 (0%)	88	90

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	269	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	A	76	GLN
1	A	212	GLN
1	A	220	HIS
1	A	290	GLN
1	A	293	GLN
1	B	16	HIS
1	B	73	HIS
1	B	96	HIS
1	B	222	ASN
1	B	290	GLN
1	B	293	GLN
1	C	27	ASN
1	C	242	GLN
1	D	73	HIS
1	D	216	GLN
1	D	290	GLN
1	D	360	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

7 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	501	1	50,50,50	1.37	4 (8%)	67,82,82	1.08	3 (4%)
3	PO4	D	503	-	4,4,4	0.86	0	6,6,6	0.53	0
2	HEM	C	501	1	50,50,50	1.36	8 (16%)	67,82,82	1.25	8 (11%)
2	HEM	A	501	1	50,50,50	1.44	7 (14%)	67,82,82	1.25	6 (8%)
3	PO4	D	502	-	4,4,4	0.88	0	6,6,6	0.84	0
3	PO4	B	502	-	4,4,4	0.80	0	6,6,6	0.47	0
2	HEM	D	501	1	50,50,50	1.29	4 (8%)	67,82,82	1.05	0

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	501	1	-	0/14/54/54	-
2	HEM	C	501	1	-	3/14/54/54	-
2	HEM	B	501	1	-	2/14/54/54	-
2	HEM	A	501	1	-	2/14/54/54	-

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	HEM	FE-ND	4.36	2.08	1.94
2	A	501	HEM	FE-ND	3.86	2.06	1.94
2	A	501	HEM	FE-NB	3.80	2.06	1.94
2	C	501	HEM	FE-ND	3.48	2.05	1.94
2	A	501	HEM	FE-NC	3.20	2.05	1.95
2	C	501	HEM	CAB-C3B	3.06	1.55	1.47
2	B	501	HEM	CAC-C3C	3.05	1.55	1.47
2	D	501	HEM	CAC-C3C	2.99	1.55	1.47
2	A	501	HEM	CAB-C3B	2.97	1.55	1.47
2	B	501	HEM	FE-NC	2.97	2.04	1.95
2	B	501	HEM	CAB-C3B	2.92	1.55	1.47
2	D	501	HEM	FE-NC	2.92	2.04	1.95
2	C	501	HEM	CAC-C3C	2.92	1.55	1.47
2	D	501	HEM	CAB-C3B	2.91	1.55	1.47
2	A	501	HEM	CAC-C3C	2.85	1.55	1.47
2	C	501	HEM	FE-NB	2.63	2.03	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	HEM	FE-ND	2.62	2.03	1.94
2	A	501	HEM	CMB-C2B	2.22	1.55	1.50
2	C	501	HEM	CMA-C3A	2.20	1.55	1.50
2	C	501	HEM	FE-NC	2.12	2.02	1.95
2	A	501	HEM	CMD-C2D	2.09	1.55	1.50
2	C	501	HEM	CMC-C2C	2.04	1.55	1.50
2	C	501	HEM	CMD-C2D	2.02	1.54	1.50

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	HEM	CHD-C4C-NC	3.42	128.18	124.45
2	A	501	HEM	CHD-C4C-NC	3.20	127.94	124.45
2	C	501	HEM	C3B-C2B-C1B	3.13	108.76	106.41
2	A	501	HEM	C1B-NB-C4B	2.83	108.56	105.21
2	B	501	HEM	CHD-C4C-NC	2.53	127.21	124.45
2	A	501	HEM	C2A-C1A-NA	-2.32	107.58	110.15
2	A	501	HEM	C4D-ND-C1D	2.32	107.95	105.21
2	C	501	HEM	CMB-C2B-C1B	-2.26	121.50	125.03
2	C	501	HEM	CAA-CBA-CGA	-2.16	107.94	113.67
2	C	501	HEM	C1B-NB-C4B	2.13	107.72	105.21
2	A	501	HEM	C3D-C4D-ND	-2.10	107.86	110.17
2	B	501	HEM	CHB-C1B-NB	2.09	126.95	124.37
2	A	501	HEM	C3B-C2B-C1B	2.04	107.94	106.41
2	B	501	HEM	CMB-C2B-C1B	-2.04	121.85	125.03
2	C	501	HEM	C3D-C4D-ND	-2.03	107.94	110.17
2	C	501	HEM	C4D-ND-C1D	2.03	107.61	105.21
2	C	501	HEM	CHB-C1B-NB	2.00	126.84	124.37

There are no chirality outliers.

All (7) torsion outliers are listed below:

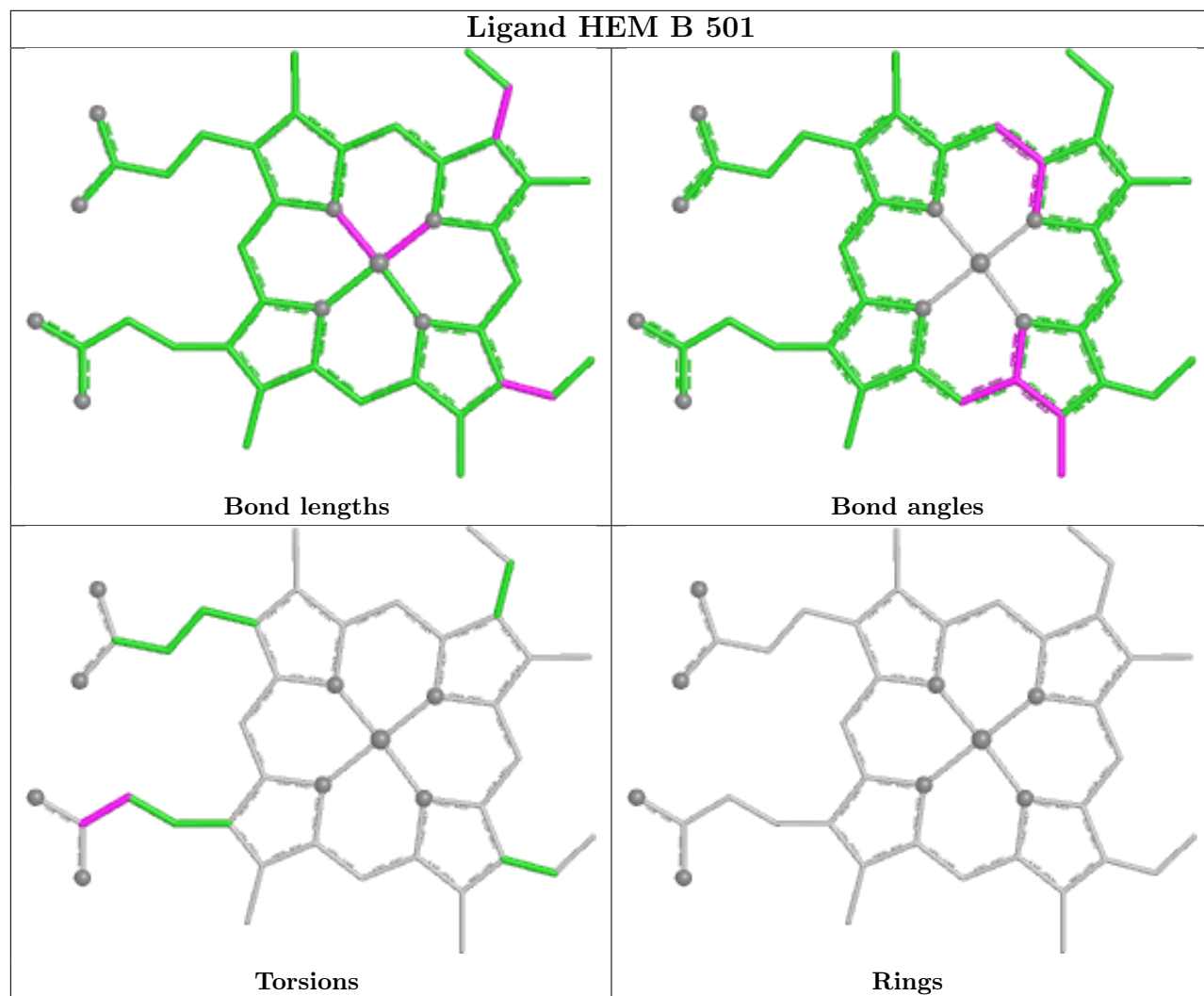
Mol	Chain	Res	Type	Atoms
2	C	501	HEM	C3D-CAD-CBD-CGD
2	C	501	HEM	CAA-CBA-CGA-O2A
2	B	501	HEM	CAA-CBA-CGA-O2A
2	A	501	HEM	CAA-CBA-CGA-O2A
2	C	501	HEM	CAA-CBA-CGA-O1A
2	A	501	HEM	CAA-CBA-CGA-O1A
2	B	501	HEM	CAA-CBA-CGA-O1A

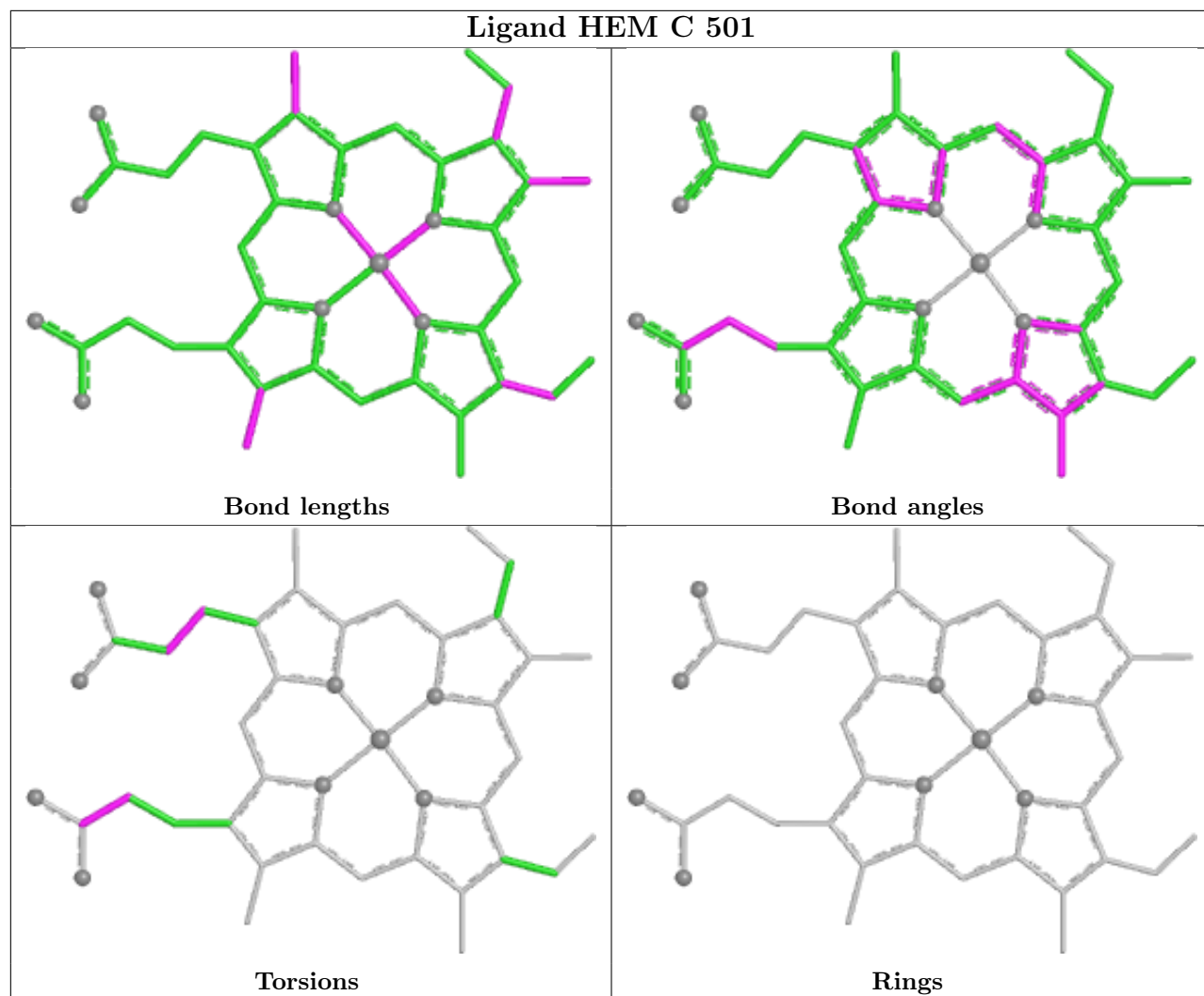
There are no ring outliers.

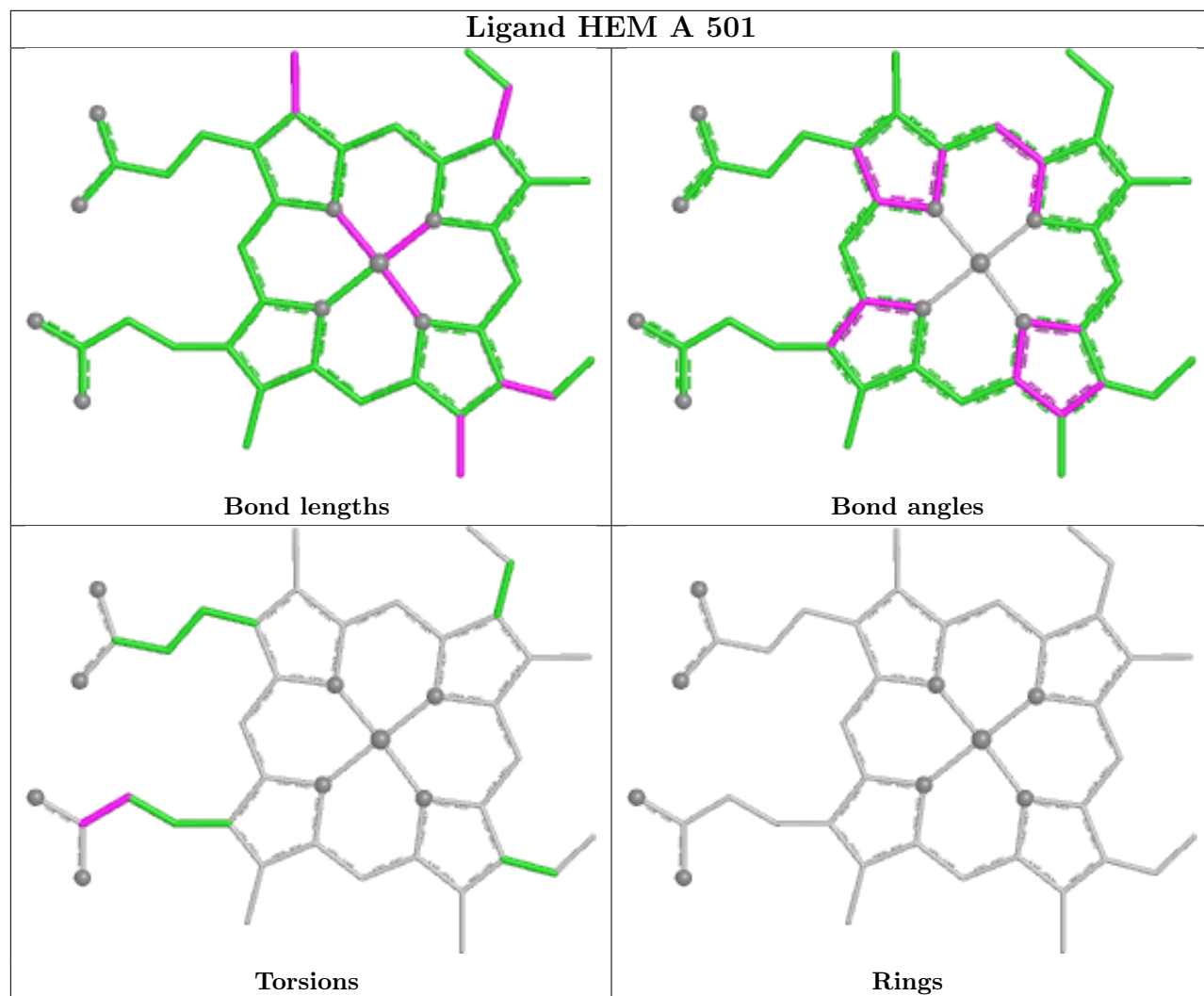
4 monomers are involved in 9 short contacts:

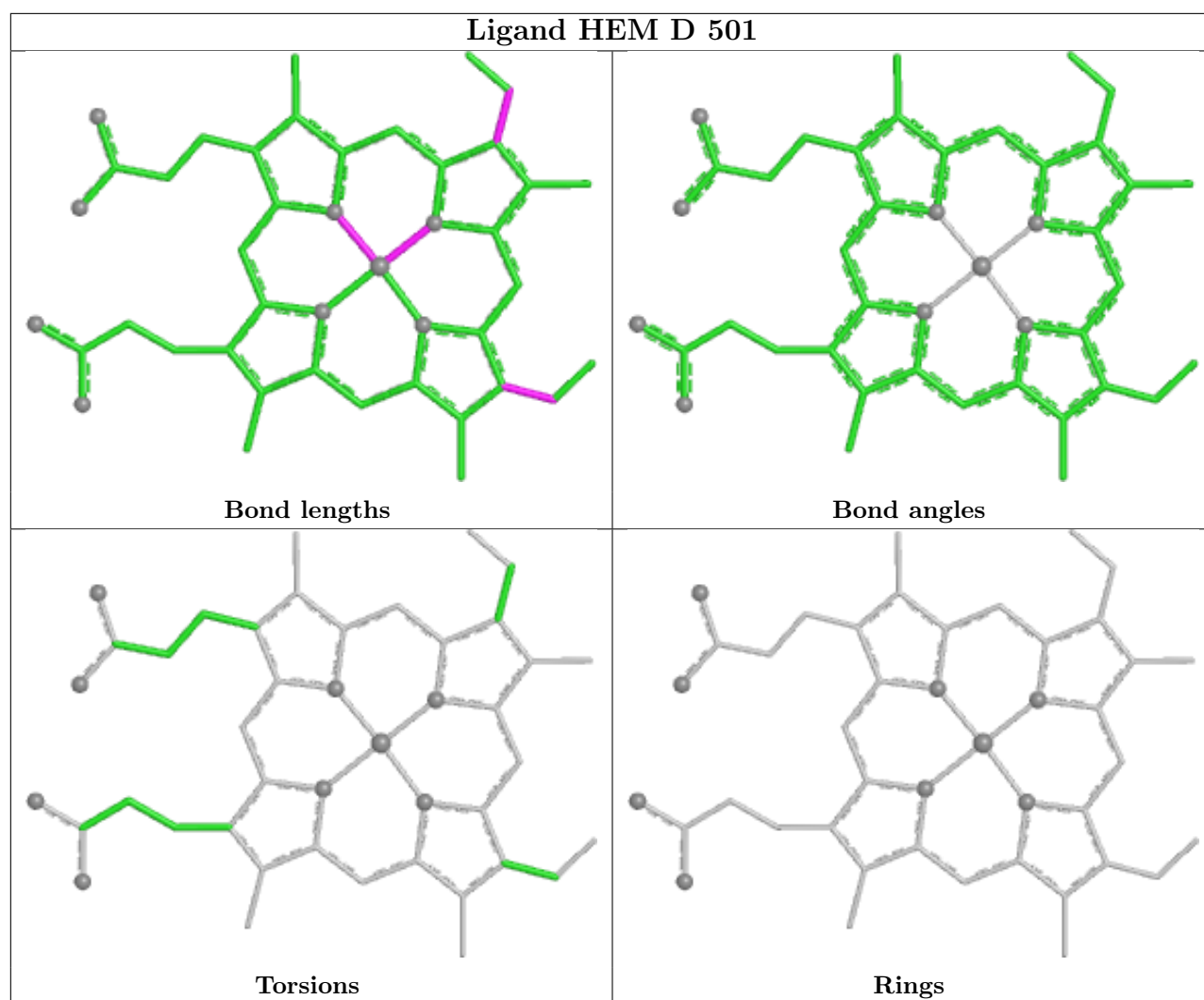
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	HEM	2	0
2	C	501	HEM	1	0
2	A	501	HEM	3	0
2	D	501	HEM	3	0

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	368/405 (90%)	0.44	20 (5%) 31 33	19, 36, 55, 72	1 (0%)
1	B	375/405 (92%)	0.27	18 (4%) 35 38	17, 33, 53, 65	1 (0%)
1	C	368/405 (90%)	0.25	15 (4%) 41 44	19, 33, 50, 72	2 (0%)
1	D	369/405 (91%)	0.28	16 (4%) 40 42	20, 33, 51, 67	0
All	All	1480/1620 (91%)	0.31	69 (4%) 36 39	17, 33, 53, 72	4 (0%)

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	376	ALA	6.2
1	B	262	GLY	5.3
1	D	14	ALA	4.9
1	D	262	GLY	4.8
1	C	14	ALA	4.7
1	A	14	ALA	4.6
1	B	14	ALA	4.5
1	D	380	GLY	4.4
1	A	381	GLY	4.1
1	C	283	ALA	4.1
1	C	291	PHE	3.9
1	C	380	GLY	3.8
1	D	264	ALA	3.7
1	B	374	LEU	3.4
1	D	401	LYS	3.2
1	C	382	THR	3.2
1	B	379	THR	3.1
1	B	264	ALA	2.9
1	A	295	MET	2.9
1	A	283	ALA	2.8
1	C	286	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	237	TRP	2.8
1	C	95	GLY	2.7
1	D	321	LEU	2.7
1	C	287	HIS	2.7
1	B	254	GLU	2.7
1	B	318	GLU	2.7
1	D	314	PRO	2.6
1	A	291	PHE	2.5
1	C	68	ASP	2.5
1	D	400	LEU	2.5
1	A	287	HIS	2.5
1	B	56	ARG	2.5
1	C	359	SER	2.5
1	C	381	GLY	2.4
1	D	27	ASN	2.4
1	B	190	MET	2.4
1	A	284	GLY	2.4
1	A	382	THR	2.3
1	D	190	MET	2.3
1	A	355	LEU	2.3
1	A	285	GLY	2.3
1	D	68	ASP	2.3
1	A	96	HIS	2.3
1	A	390	THR	2.3
1	B	375	GLU	2.2
1	A	359	SER	2.2
1	C	282	THR	2.2
1	C	96	HIS	2.2
1	A	400	LEU	2.2
1	B	285	GLY	2.2
1	D	284	GLY	2.2
1	D	330	GLU	2.1
1	A	401	LYS	2.1
1	A	358	ALA	2.1
1	D	319	PHE	2.1
1	A	48	ASP	2.1
1	C	309	SER	2.1
1	B	287	HIS	2.1
1	A	330	GLU	2.1
1	A	140	ASN	2.1
1	D	290	GLN	2.1
1	A	286	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	73	HIS	2.0
1	B	380	GLY	2.0
1	B	243	LEU	2.0
1	C	355	LEU	2.0
1	D	73	HIS	2.0
1	B	58	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

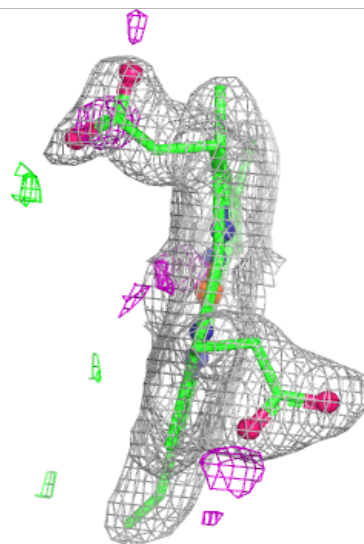
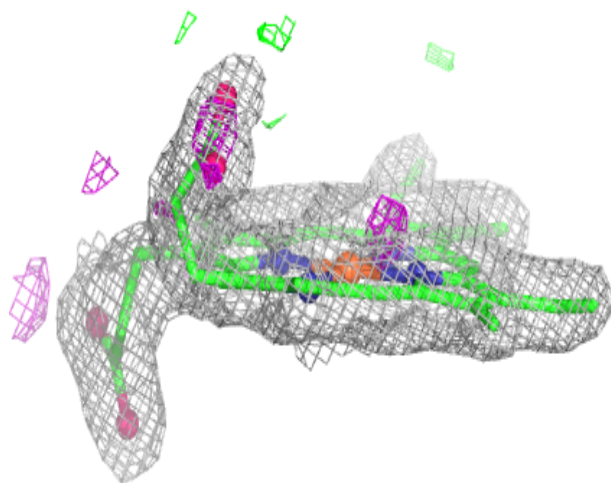
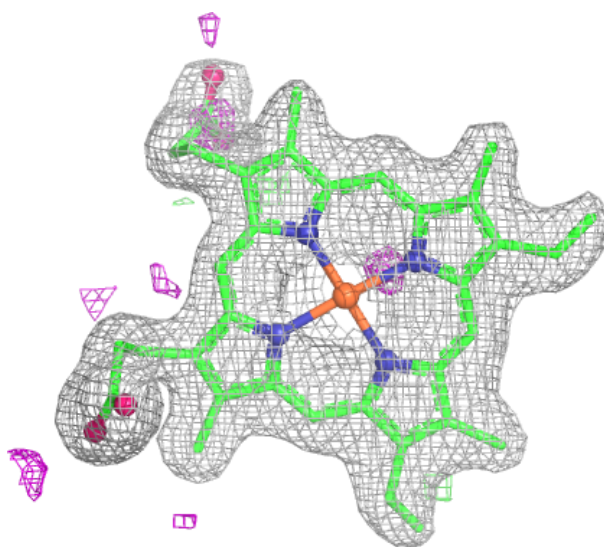
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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
3	PO4	D	502	5/5	0.81	0.12	42,45,51,55	0
3	PO4	B	502	5/5	0.88	0.10	40,44,46,52	0
3	PO4	D	503	5/5	0.96	0.09	40,40,45,46	0
2	HEM	A	501	43/43	0.97	0.08	32,37,44,55	0
2	HEM	B	501	43/43	0.97	0.08	30,35,47,55	0
2	HEM	C	501	43/43	0.97	0.07	27,31,40,47	0
2	HEM	D	501	43/43	0.98	0.07	31,34,46,55	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.

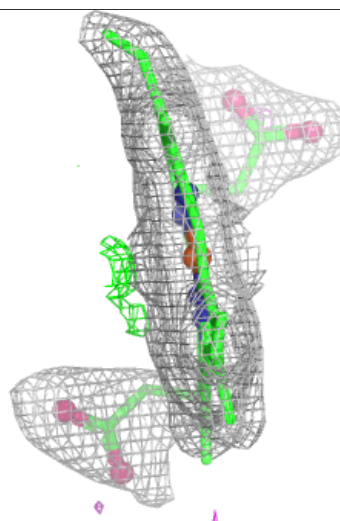
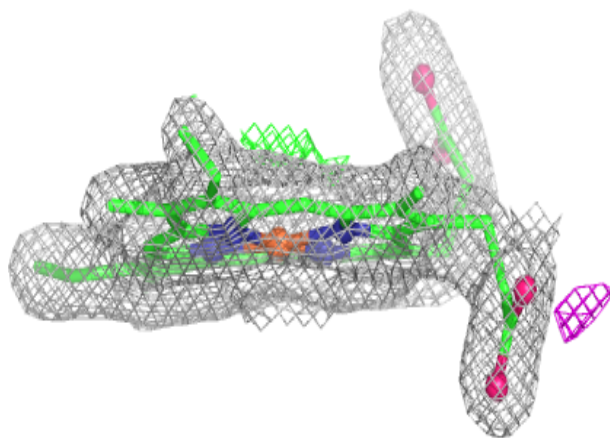
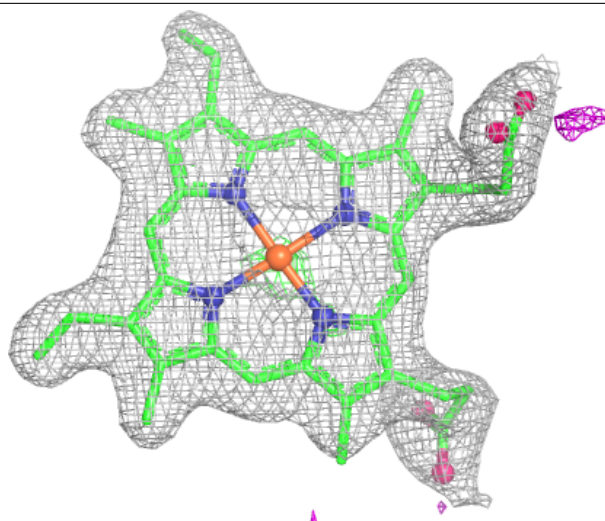
Electron density around HEM A 501:

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



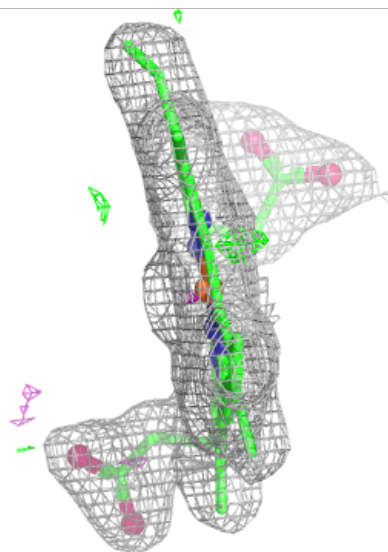
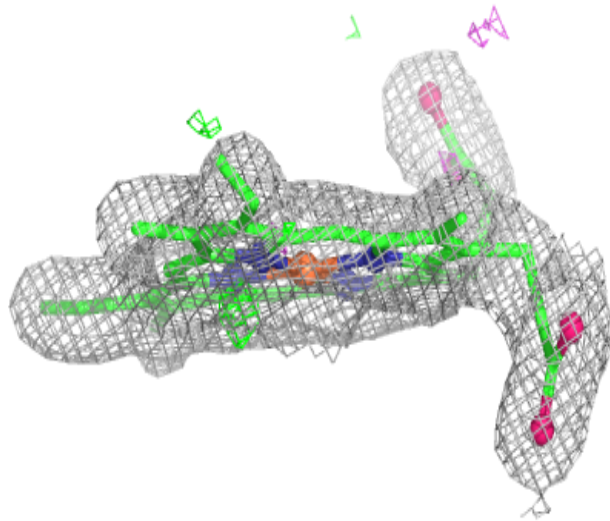
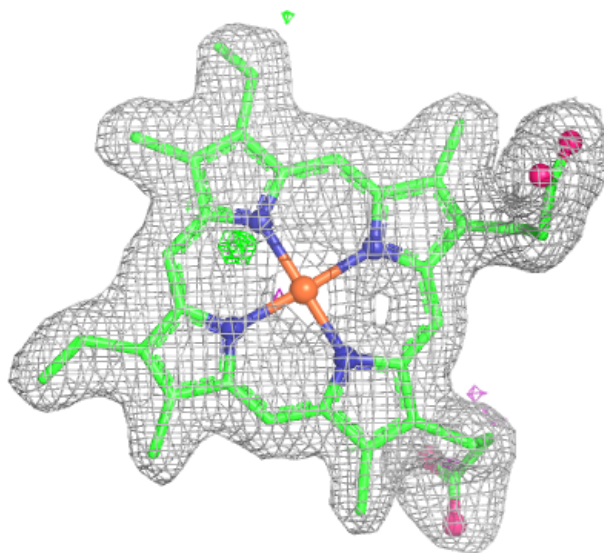
Electron density around HEM B 501:

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



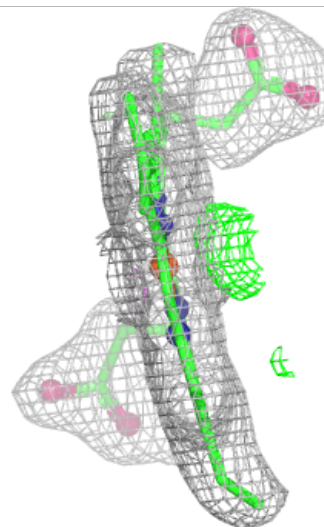
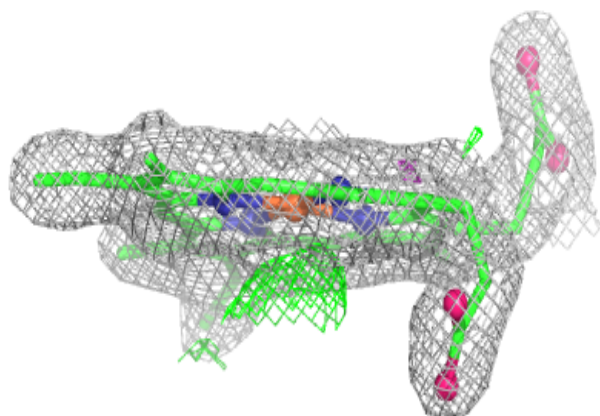
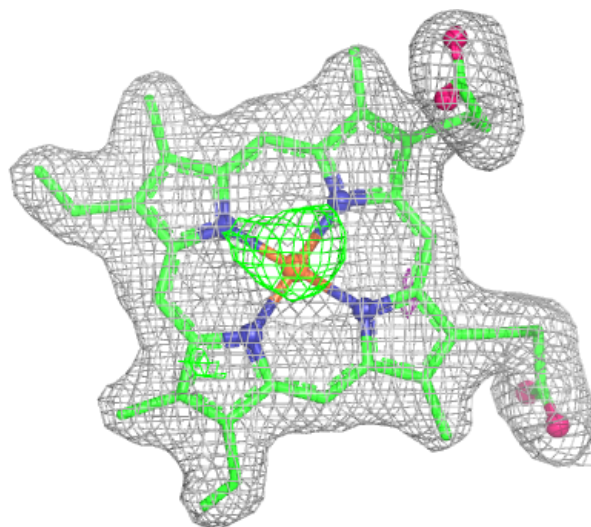
Electron density around HEM C 501:

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



Electron density around HEM D 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 ⓘ

There are no such residues in this entry.