



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:46 AM UTC

PDB ID : 7F3H / pdb_00007f3h
Title : Crystal structure of cytochrome P450DA heme domain
Authors : Wan, N.W.
Deposited on : 2021-06-16
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 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

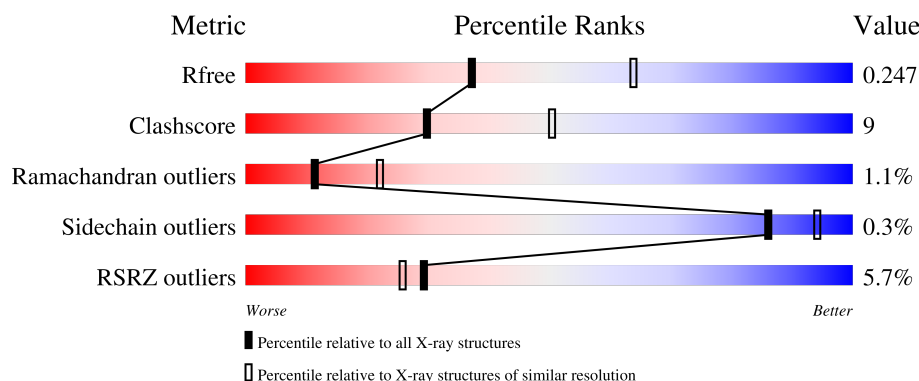
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 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	501	4% 75% 15% .. 8%
1	B	501	2% 76% 14% . 9%
1	C	501	10% 69% 19% . 10%
1	D	501	4% 72% 19% . 7%

2 Entry composition [i](#)

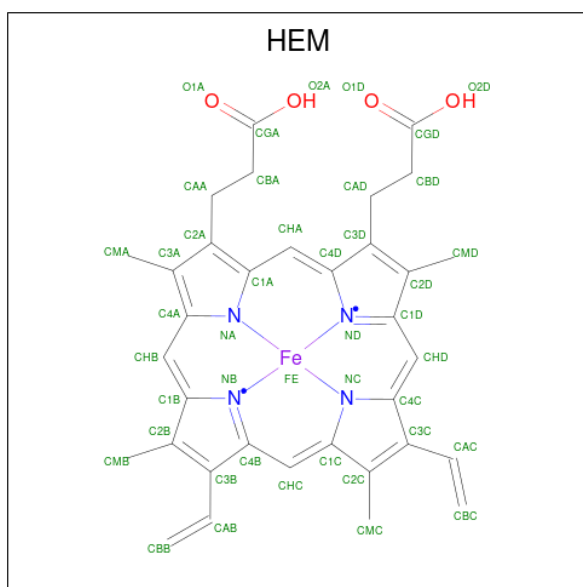
There are 5 unique types of molecules in this entry. The entry contains 15192 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Bifunctional cytochrome P450/NADPH-P450 reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	462	Total	C	N	O	S	0	1	0
			3725	2370	670	671	14			
1	B	455	Total	C	N	O	S	0	0	0
			3664	2330	659	662	13			
1	C	449	Total	C	N	O	S	0	0	0
			3611	2304	649	646	12			
1	D	464	Total	C	N	O	S	0	0	0
			3731	2375	671	672	13			

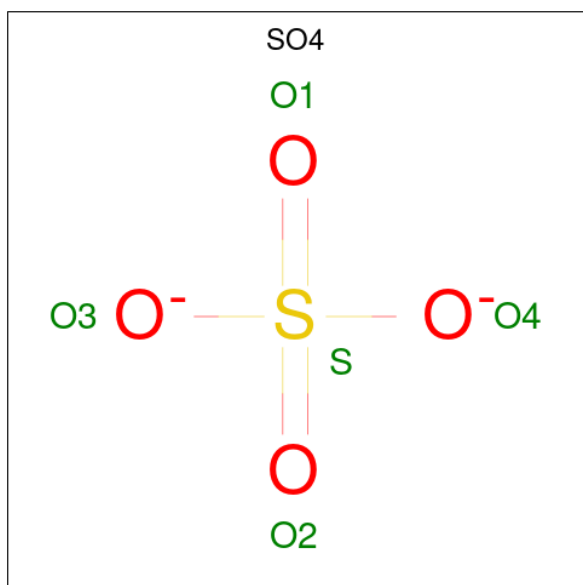
- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



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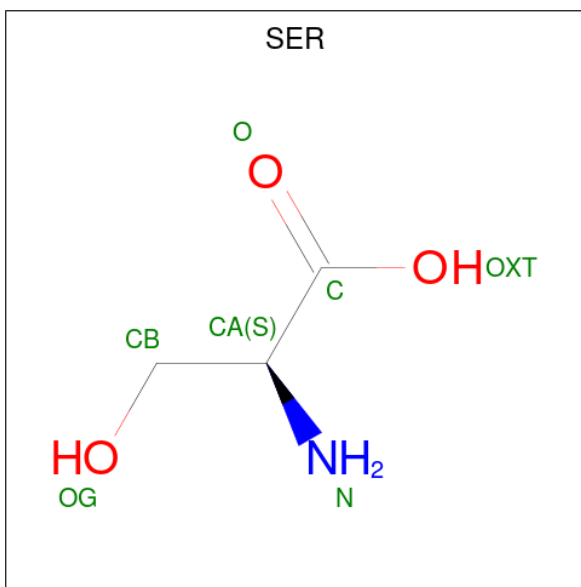
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is SERINE (CCD ID: SER) (formula: C₃H₇NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			6	3	1	2		

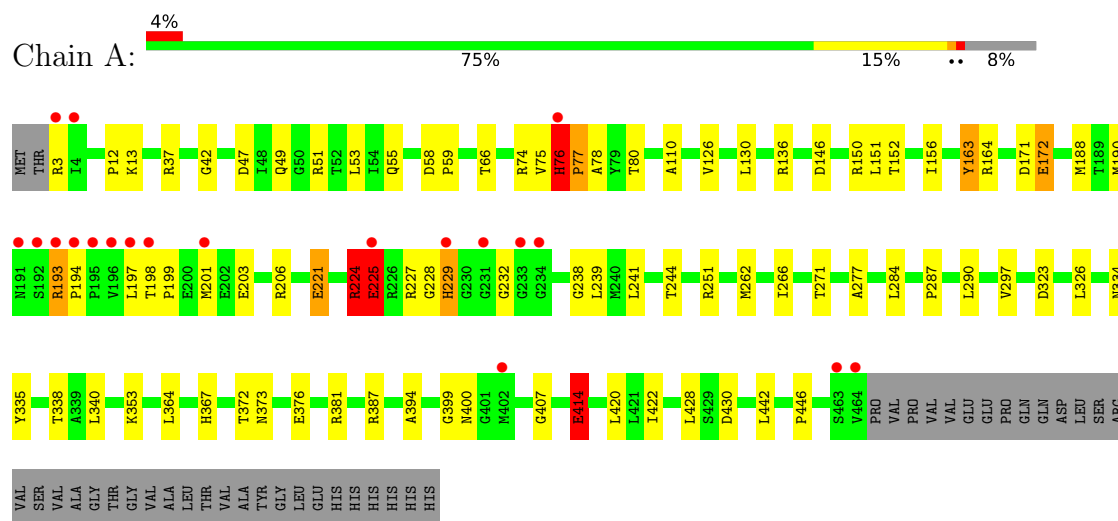
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	79	Total	O	0	0
			79	79		
5	B	69	Total	O	0	0
			69	69		
5	C	55	Total	O	0	0
			55	55		
5	D	65	Total	O	0	0
			65	65		

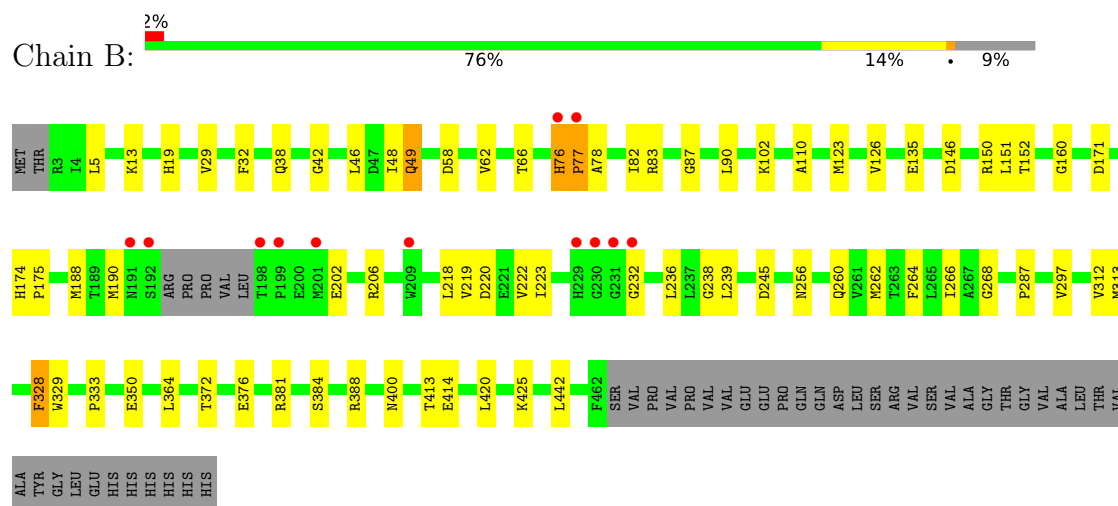
3 Residue-property plots [i](#)

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 cytochrome P450/NADPH-P450 reductase

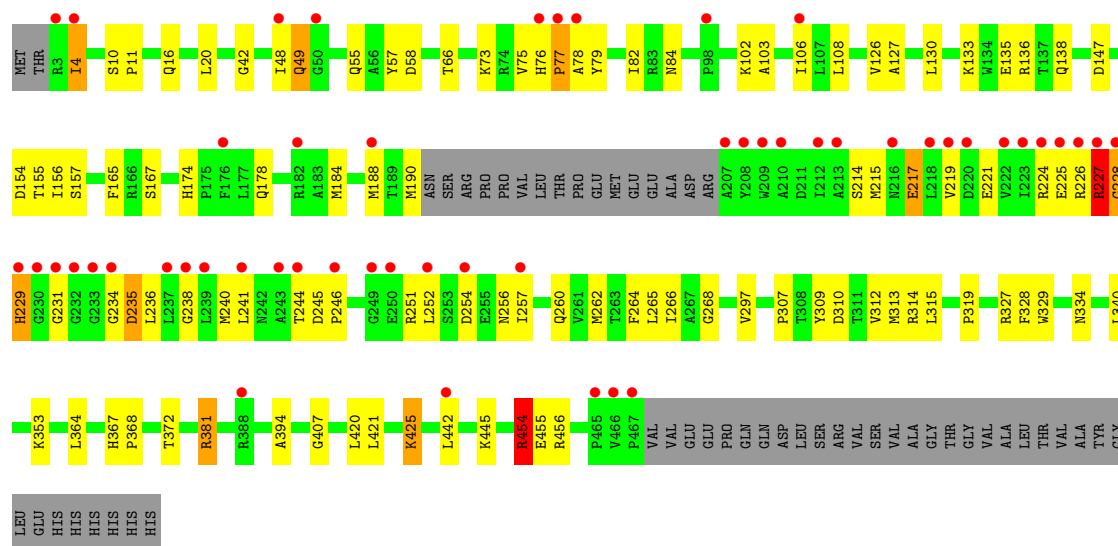


- Molecule 1: Bifunctional cytochrome P450/NADPH-P450 reductase

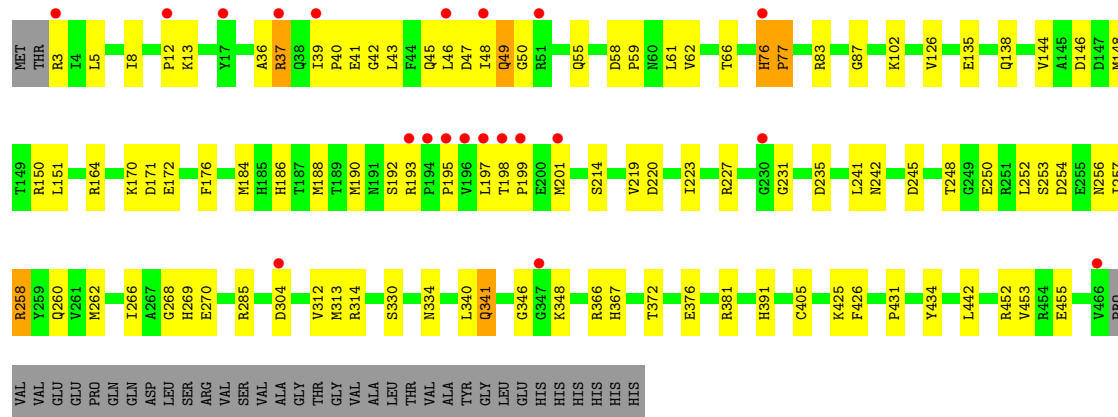


- Molecule 1: Bifunctional cytochrome P450/NADPH-P450 reductase





● Molecule 1: Bifunctional cytochrome P450/NADPH-P450 reductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	426.30Å 62.80Å 95.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.00 – 2.50 29.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	89.2 (29.00-2.50) 89.1 (29.00-2.50)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.45 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.18.1_3865	Depositor
R, R_{free}	0.200 , 0.246 0.201 , 0.247	Depositor DCC
R_{free} test set	1929 reflections (2.15%)	wwPDB-VP
Wilson B-factor (Å ²)	33.9	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 34.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	15192	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% 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, SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.61	3/3820 (0.1%)	1.05	31/5185 (0.6%)
1	B	0.48	0/3756	0.72	2/5095 (0.0%)
1	C	0.50	1/3704 (0.0%)	0.90	16/5028 (0.3%)
1	D	0.57	1/3827 (0.0%)	0.91	13/5197 (0.3%)
All	All	0.54	5/15107 (0.0%)	0.90	62/20505 (0.3%)

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	A	0	9
1	B	0	1
1	C	0	2
1	D	0	2
All	All	0	14

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	76	HIS	C-N	9.09	1.55	1.33
1	C	425	LYS	CB-CG	-6.33	1.33	1.52
1	A	225	GLU	C-O	6.29	1.32	1.24
1	A	373	ASN	C-O	6.27	1.26	1.23
1	D	341	GLN	CD-NE2	5.79	1.45	1.33

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	76	HIS	N-CA-C	-16.83	72.62	109.81
1	D	36	ALA	CA-C-N	-14.66	100.44	122.86
1	D	36	ALA	C-N-CA	-14.66	100.44	122.86
1	C	227	ARG	CB-CG-CD	14.42	144.46	111.30
1	C	227	ARG	CA-CB-CG	-14.31	85.47	114.10
1	A	76	HIS	N-CA-CB	13.44	134.29	110.37
1	A	221	GLU	CA-CB-CG	13.04	140.18	114.10
1	A	51	ARG	CB-CG-CD	-12.17	83.32	111.30
1	A	76	HIS	CB-CA-C	-11.40	87.72	110.17
1	C	227	ARG	NE-CZ-NH2	11.22	129.30	119.20
1	C	454	ARG	NE-CZ-NH2	10.77	128.90	119.20
1	C	454	ARG	NE-CZ-NH1	-10.75	110.75	121.50
1	A	172	GLU	CG-CD-OE1	10.41	142.35	118.40
1	A	172	GLU	OE1-CD-OE2	-9.78	99.44	122.90
1	A	221	GLU	N-CA-CB	-8.60	97.55	110.01
1	A	229	HIS	CB-CA-C	-8.27	93.97	110.42
1	A	225	GLU	CA-C-N	8.16	134.56	120.68
1	A	225	GLU	C-N-CA	8.16	134.56	120.68
1	A	225	GLU	CB-CA-C	8.16	124.18	109.99
1	C	454	ARG	CD-NE-CZ	7.95	135.53	124.40
1	D	340	LEU	CA-C-N	7.89	134.98	122.59
1	D	340	LEU	C-N-CA	7.89	134.98	122.59
1	A	225	GLU	CG-CD-OE2	-7.82	100.43	118.40
1	A	225	GLU	N-CA-CB	-7.77	99.23	110.80
1	D	268	GLY	CA-C-N	-7.62	105.34	121.80
1	D	268	GLY	C-N-CA	-7.62	105.34	121.80
1	D	37	ARG	NE-CZ-NH1	-7.62	113.88	121.50
1	D	47	ASP	N-CA-C	-7.16	95.55	110.80
1	C	454	ARG	CB-CA-C	7.14	123.82	109.68
1	C	445	LYS	CD-CE-NZ	-7.13	89.08	111.90
1	A	172	GLU	CG-CD-OE2	-6.95	102.42	118.40
1	A	76	HIS	CB-CG-ND1	-6.92	112.32	122.70
1	C	4	ILE	CG1-CB-CG2	-6.86	90.11	110.70
1	C	425	LYS	CA-CB-CG	6.62	127.35	114.10
1	A	225	GLU	CA-CB-CG	6.55	127.20	114.10
1	A	3	ARG	NE-CZ-NH1	-6.47	115.03	121.50
1	A	225	GLU	N-CA-C	-6.44	103.95	113.61
1	D	37	ARG	NE-CZ-NH2	6.32	124.89	119.20
1	D	37	ARG	CD-NE-CZ	-6.24	115.66	124.40
1	C	227	ARG	NE-CZ-NH1	-6.15	115.35	121.50
1	C	268	GLY	CA-C-N	-6.07	108.69	121.80
1	C	268	GLY	C-N-CA	-6.07	108.69	121.80
1	A	221	GLU	CB-CA-C	6.05	120.38	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	47	ASP	N-CA-CB	6.04	120.34	110.37
1	A	172	GLU	N-CA-C	-5.96	99.94	109.96
1	A	224	ARG	CD-NE-CZ	5.72	132.42	124.40
1	A	224	ARG	CB-CG-CD	-5.71	98.17	111.30
1	A	51	ARG	N-CA-C	5.68	117.40	110.41
1	D	47	ASP	CB-CA-C	5.65	121.67	110.42
1	C	425	LYS	CG-CD-CE	-5.53	98.59	111.30
1	A	224	ARG	N-CA-C	-5.51	105.66	112.38
1	D	47	ASP	N-CA-CB	-5.47	101.25	110.49
1	A	51	ARG	CA-CB-CG	5.42	124.94	114.10
1	A	229	HIS	N-CA-CB	5.39	119.60	110.49
1	D	258	ARG	CA-CB-CG	5.34	124.78	114.10
1	C	381	ARG	CG-CD-NE	-5.29	100.37	112.00
1	C	217	GLU	CA-CB-CG	5.26	124.62	114.10
1	B	268	GLY	CA-C-N	-5.24	112.22	121.81
1	B	268	GLY	C-N-CA	-5.24	112.22	121.81
1	A	224	ARG	CA-CB-CG	5.20	124.50	114.10
1	A	3	ARG	CG-CD-NE	-5.10	100.78	112.00
1	A	414	GLU	CB-CA-C	-5.03	102.98	110.88

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	163	TYR	Sidechain
1	A	172	GLU	Sidechain
1	A	224	ARG	Peptide
1	A	225	GLU	Peptide,Sidechain
1	A	228	GLY	Peptide
1	A	414	GLU	Sidechain
1	A	75	VAL	Peptide
1	A	76	HIS	Sidechain
1	B	328	PHE	Sidechain
1	C	228	GLY	Peptide
1	C	454	ARG	Sidechain
1	D	341	GLN	Sidechain
1	D	46	LEU	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	3725	0	3680	63	0
1	B	3664	0	3610	44	0
1	C	3611	0	3573	73	0
1	D	3731	0	3688	68	0
2	A	43	0	30	6	0
2	B	43	0	30	0	0
2	C	43	0	30	5	0
2	D	43	0	30	4	0
3	A	10	0	0	0	0
3	D	5	0	0	0	0
4	B	6	0	4	0	0
5	A	79	0	0	4	0
5	B	69	0	0	0	0
5	C	55	0	0	1	0
5	D	65	0	0	3	0
All	All	15192	0	14675	252	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 9.

All (252) 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:C:227:ARG:NH2	1:C:254:ASP:OD1	1.90	1.04
1:A:224:ARG:HG2	1:A:225:GLU:HB2	1.50	0.91
1:D:227:ARG:NH1	1:D:254:ASP:OD1	2.07	0.88
1:A:76:HIS:HB2	1:A:77:PRO:HD3	1.57	0.86
1:A:55:GLN:HE22	1:A:334:ASN:HD21	1.23	0.85
1:D:197:LEU:HD23	1:D:201:MET:HE2	1.60	0.84
1:A:76:HIS:HB2	1:A:77:PRO:CD	2.08	0.82
1:D:76:HIS:HB3	1:D:77:PRO:HD3	1.63	0.80
1:D:42:GLY:HA3	1:D:58:ASP:HB2	1.65	0.78
1:C:55:GLN:HE22	1:C:334:ASN:HD21	1.31	0.77
1:A:372:THR:O	1:A:381:ARG:NH2	2.18	0.77
1:B:219:VAL:HG21	1:B:262:MET:HE3	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:ARG:NH2	1:B:171:ASP:O	2.20	0.74
1:D:146:ASP:OD2	1:D:150:ARG:NH1	2.21	0.74
1:C:231:GLY:HA3	1:C:238:GLY:HA2	1.69	0.73
1:B:135:GLU:OE1	1:B:425:LYS:NZ	2.21	0.72
1:C:135:GLU:OE2	1:C:425:LYS:HE3	1.91	0.71
1:C:156:ILE:HG23	1:C:265:LEU:HD22	1.74	0.70
1:C:227:ARG:HE	1:C:241:LEU:HD22	1.56	0.70
1:B:188:MET:HE3	1:B:442:LEU:HB2	1.74	0.70
1:D:372:THR:O	1:D:381:ARG:NH2	2.26	0.69
1:A:197:LEU:HG	1:A:201:MET:HE2	1.74	0.69
1:C:226:ARG:NH2	1:C:235:ASP:OD2	2.25	0.68
1:D:102:LYS:HE2	1:D:252:LEU:HD23	1.73	0.68
1:D:43:LEU:HD23	1:D:61:LEU:HD13	1.74	0.68
1:D:188:MET:HE3	1:D:442:LEU:HB2	1.76	0.68
1:C:309:TYR:CE1	1:C:313:MET:HE3	2.27	0.68
1:A:146:ASP:OD2	1:A:150:ARG:NH1	2.26	0.68
1:A:290:LEU:HD23	1:B:287:PRO:HB2	1.73	0.68
2:D:601:HEM:HBB2	2:D:601:HEM:HMB1	1.75	0.68
1:B:372:THR:O	1:B:381:ARG:NH2	2.28	0.67
1:D:262:MET:O	1:D:266:ILE:HG12	1.94	0.67
1:C:372:THR:O	1:C:381:ARG:NH2	2.28	0.66
1:C:188:MET:HE3	1:C:442:LEU:HB2	1.76	0.65
1:C:227:ARG:NE	1:C:241:LEU:HD22	2.11	0.65
1:C:84:ASN:HD22	1:C:190:MET:HE1	1.60	0.65
1:D:184:MET:HE1	1:D:266:ILE:HG23	1.79	0.65
1:A:42:GLY:HA3	1:A:58:ASP:HB2	1.79	0.65
1:D:245:ASP:OD2	1:D:248:THR:HG22	1.96	0.64
1:D:431:PRO:HG3	1:D:452:ARG:HG3	1.78	0.64
1:B:202:GLU:O	1:B:206:ARG:HG3	1.98	0.63
1:A:297:VAL:HG22	1:A:420:LEU:HD12	1.80	0.63
1:A:364:LEU:HD11	1:A:394:ALA:HA	1.80	0.62
1:D:8:ILE:HG12	1:D:43:LEU:HD11	1.80	0.62
1:D:220:ASP:OD1	1:D:258:ARG:HG3	1.98	0.62
1:D:76:HIS:CB	1:D:77:PRO:HD3	2.29	0.62
1:C:244:THR:O	1:C:246:PRO:HD3	1.99	0.61
1:D:176:PHE:HZ	1:D:262:MET:HE1	1.64	0.61
2:A:601:HEM:HMC1	2:A:601:HEM:HBC2	1.81	0.61
1:A:74:ARG:HB3	1:A:76:HIS:CD2	2.36	0.61
1:C:340:LEU:O	1:C:353:LYS:HG3	2.01	0.60
1:A:66:THR:HG23	1:A:400:ASN:OD1	2.00	0.60
1:A:221:GLU:O	1:A:225:GLU:HB3	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:MET:HE1	1:B:413:THR:HG22	1.84	0.60
1:A:76:HIS:CB	1:A:77:PRO:HD3	2.26	0.60
1:A:221:GLU:O	1:A:225:GLU:CB	2.49	0.60
1:D:176:PHE:CZ	1:D:262:MET:HE1	2.36	0.60
1:A:76:HIS:H	1:A:77:PRO:CD	2.12	0.60
1:C:240:MET:HE2	1:C:257:ILE:HG23	1.84	0.60
1:C:106:ILE:HD12	1:C:252:LEU:HG	1.84	0.59
1:A:136:ARG:NH1	5:A:705:HOH:O	2.35	0.59
2:C:601:HEM:HMC2	2:C:601:HEM:HBC2	1.85	0.59
1:D:219:VAL:HG21	1:D:262:MET:HE3	1.83	0.58
1:C:454:ARG:HH11	1:D:376:GLU:HG2	1.67	0.58
1:B:110:ALA:HB2	1:B:239:LEU:HD13	1.85	0.58
1:C:135:GLU:OE2	1:C:425:LYS:CE	2.51	0.58
1:C:225:GLU:O	1:C:229:HIS:ND1	2.36	0.58
1:D:48:ILE:O	1:D:50:GLY:N	2.37	0.58
1:D:55:GLN:HE22	1:D:334:ASN:HD21	1.49	0.58
1:D:269:HIS:CE1	1:D:270:GLU:HG3	2.37	0.58
1:B:146:ASP:OD2	1:B:150:ARG:NH1	2.36	0.57
2:C:601:HEM:HBB2	2:C:601:HEM:HMB2	1.86	0.57
1:C:136:ARG:NH1	5:C:702:HOH:O	2.36	0.57
1:A:37:ARG:NH1	5:A:706:HOH:O	2.35	0.57
1:D:186:HIS:O	1:D:190:MET:HG3	2.05	0.57
1:C:82:ILE:HD11	1:C:266:ILE:HG21	1.85	0.57
1:D:62:VAL:O	1:D:66:THR:OG1	2.16	0.57
1:D:198:THR:HB	1:D:199:PRO:HD2	1.85	0.57
1:D:170:LYS:HE2	1:D:172:GLU:HB2	1.87	0.57
1:C:174:HIS:O	1:C:178:GLN:HG3	2.05	0.57
1:C:20:LEU:HD11	1:C:49:GLN:HG3	1.87	0.56
1:A:152:THR:HG22	1:A:414:GLU:OE1	2.05	0.56
1:A:232:GLY:HA2	1:A:238:GLY:HA3	1.87	0.56
1:A:66:THR:HG21	5:A:768:HOH:O	2.04	0.56
1:B:174:HIS:ND1	1:B:175:PRO:HD2	2.21	0.56
1:D:312:VAL:HG12	1:D:313:MET:HE2	1.88	0.56
1:A:190:MET:HG2	1:A:193:ARG:NH2	2.21	0.56
1:A:198:THR:HB	1:A:199:PRO:HD2	1.88	0.55
1:C:157:SER:HB3	1:C:165:PHE:HE2	1.72	0.55
1:D:126:VAL:HG12	1:D:151:LEU:HD12	1.87	0.55
1:C:217:GLU:O	1:C:221:GLU:HG3	2.05	0.55
1:D:135:GLU:OE2	1:D:425:LYS:NZ	2.39	0.55
1:D:253:SER:O	1:D:257:ILE:HG13	2.07	0.55
1:C:214:SER:O	1:C:217:GLU:HB3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:297:VAL:HG22	1:C:420:LEU:HD12	1.90	0.54
1:C:48:ILE:O	1:C:49:GLN:C	2.51	0.54
1:D:3:ARG:HH22	1:D:5:LEU:HD12	1.73	0.54
1:A:323:ASP:OD2	1:A:387:ARG:NH2	2.41	0.54
1:C:126:VAL:HG21	1:C:155:THR:HA	1.90	0.53
2:D:601:HEM:HBC2	2:D:601:HEM:HMC2	1.90	0.53
1:C:138:GLN:NE2	1:C:455:GLU:HG3	2.24	0.53
1:C:234:GLY:O	1:C:235:ASP:HB2	2.09	0.52
1:D:39:ILE:HG22	1:D:41:GLU:OE1	2.10	0.52
1:D:192:SER:O	1:D:193:ARG:HG2	2.10	0.52
1:A:271:THR:HB	2:A:601:HEM:C2C	2.46	0.51
1:C:262:MET:HA	1:C:262:MET:HE2	1.93	0.51
1:B:102:LYS:HG2	1:B:245:ASP:OD2	2.10	0.51
1:B:297:VAL:HG22	1:B:420:LEU:HD12	1.92	0.51
1:C:73:LYS:HE3	1:C:79:TYR:CZ	2.47	0.50
1:B:218:LEU:O	1:B:222:VAL:HG23	2.12	0.50
1:D:256:ASN:O	1:D:260:GLN:HG2	2.10	0.50
1:C:228:GLY:C	1:C:229:HIS:CG	2.89	0.50
1:C:188:MET:CE	1:C:442:LEU:HB2	2.41	0.50
1:A:188:MET:HE3	1:A:442:LEU:HB2	1.94	0.50
1:C:244:THR:HG22	1:C:251:ARG:HG3	1.94	0.50
1:D:346:GLY:O	1:D:348:LYS:HG3	2.11	0.50
1:A:163:TYR:HD1	1:A:164:ARG:N	2.10	0.49
1:C:184:MET:SD	1:C:266:ILE:HD12	2.52	0.49
1:A:12:PRO:O	1:A:13:LYS:HB3	2.13	0.49
1:B:76:HIS:O	1:B:77:PRO:C	2.55	0.49
1:B:42:GLY:HA3	1:B:58:ASP:HB2	1.93	0.49
1:B:328:PHE:HB3	1:B:329:TRP:CD1	2.46	0.49
1:C:262:MET:O	1:C:266:ILE:HG12	2.13	0.49
1:D:8:ILE:CG2	1:D:45:GLN:HG2	2.41	0.49
1:D:248:THR:HG23	1:D:250:GLU:CG	2.41	0.49
1:C:407:GLY:HA3	2:C:601:HEM:C2B	2.47	0.49
1:B:29:VAL:HG21	1:B:333:PRO:HB2	1.94	0.49
1:C:312:VAL:HG12	1:C:313:MET:HE2	1.95	0.49
1:D:138:GLN:HE22	1:D:455:GLU:HG3	1.78	0.49
1:C:154:ASP:OD1	1:C:167:SER:OG	2.29	0.48
1:A:262:MET:O	1:A:266:ILE:HG12	2.12	0.48
1:C:215:MET:O	1:C:219:VAL:HG23	2.13	0.48
1:B:188:MET:CE	1:B:442:LEU:HB2	2.43	0.48
1:C:364:LEU:HD11	1:C:394:ALA:HA	1.95	0.48
2:D:601:HEM:HBB2	2:D:601:HEM:CMB	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:405:CYS:HB2	2:D:601:HEM:NA	2.28	0.48
1:A:130:LEU:HD21	1:A:422:ILE:HD11	1.96	0.48
1:B:123:MET:HE1	1:B:413:THR:CG2	2.43	0.47
1:D:248:THR:HG23	1:D:250:GLU:HG2	1.96	0.47
1:C:76:HIS:O	1:C:77:PRO:C	2.57	0.47
1:D:41:GLU:OE1	1:D:41:GLU:N	2.46	0.47
1:A:76:HIS:CE1	1:A:338:THR:HG21	2.49	0.47
1:B:13:LYS:HD3	1:B:19:HIS:NE2	2.29	0.47
1:A:53:LEU:HD12	5:A:755:HOH:O	2.15	0.47
1:A:77:PRO:HD2	1:A:78:ALA:H	1.80	0.47
1:A:221:GLU:O	1:A:225:GLU:HB2	2.15	0.47
1:B:160:GLY:HA2	1:B:236:LEU:HB2	1.96	0.47
1:C:127:ALA:O	1:C:130:LEU:HB3	2.15	0.46
1:D:12:PRO:O	1:D:13:LYS:HB2	2.15	0.46
1:D:76:HIS:HB3	1:D:77:PRO:CD	2.39	0.46
1:D:144:VAL:O	1:D:148:MET:HG2	2.15	0.46
1:B:256:ASN:O	1:B:260:GLN:HG2	2.15	0.46
1:D:37:ARG:HH11	1:D:37:ARG:HD2	1.48	0.46
1:A:227:ARG:CZ	1:A:241:LEU:HD22	2.45	0.46
1:C:156:ILE:CG2	1:C:265:LEU:HD22	2.45	0.46
1:B:384:SER:O	1:B:388:ARG:HG3	2.16	0.46
1:C:307:PRO:HG3	1:C:421:LEU:HD21	1.97	0.46
1:C:256:ASN:O	1:C:260:GLN:HG2	2.16	0.46
1:C:103:ALA:HB1	1:C:260:GLN:NE2	2.31	0.46
1:B:66:THR:HG23	1:B:400:ASN:OD1	2.16	0.46
1:C:102:LYS:HG3	1:C:245:ASP:OD1	2.16	0.46
1:A:335:TYR:CZ	1:A:399:GLY:HA2	2.51	0.45
1:A:340:LEU:O	1:A:353:LYS:HG3	2.16	0.45
1:B:126:VAL:HG12	1:B:151:LEU:HD12	1.98	0.45
1:B:190:MET:HE2	1:B:190:MET:HB3	1.81	0.45
1:C:310:ASP:OD2	1:C:314:ARG:NH2	2.39	0.45
1:D:48:ILE:O	1:D:49:GLN:C	2.59	0.45
1:A:193:ARG:HB2	1:A:194:PRO:CD	2.46	0.45
1:A:193:ARG:HD2	1:A:201:MET:HE3	1.97	0.45
1:A:326:LEU:HD22	2:A:601:HEM:HBC1	1.97	0.45
1:B:38:GLN:OE1	1:D:214:SER:HB3	2.16	0.45
1:D:8:ILE:HG22	1:D:45:GLN:HG2	1.98	0.45
1:C:42:GLY:HA3	1:C:58:ASP:HB2	1.99	0.45
1:C:106:ILE:CD1	1:C:252:LEU:HG	2.45	0.45
1:C:127:ALA:HB1	1:C:421:LEU:HD12	1.97	0.45
1:D:188:MET:HE1	1:D:442:LEU:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:PRO:HD3	1:A:367:HIS:CD2	2.52	0.45
1:B:83:ARG:HG3	1:B:87:GLY:O	2.16	0.45
1:D:366:ARG:NH2	5:D:714:HOH:O	2.49	0.45
1:A:76:HIS:N	1:A:77:PRO:CD	2.69	0.45
1:A:376:GLU:O	1:A:381:ARG:NH1	2.50	0.45
1:C:425:LYS:O	1:C:456:ARG:HG3	2.16	0.45
1:D:59:PRO:HB2	1:D:391:HIS:CD2	2.52	0.45
1:A:126:VAL:HG12	1:A:151:LEU:HD12	1.99	0.45
1:D:83:ARG:HG3	1:D:87:GLY:O	2.16	0.45
1:B:312:VAL:HG12	1:B:313:MET:HE2	1.99	0.44
2:A:601:HEM:HMB2	2:A:601:HEM:HBB2	1.99	0.44
1:D:164:ARG:HA	5:D:736:HOH:O	2.15	0.44
1:C:103:ALA:CB	1:C:260:GLN:NE2	2.80	0.44
1:C:240:MET:HE1	1:C:260:GLN:HB2	1.98	0.44
1:C:226:ARG:HG2	1:C:231:GLY:HA2	1.99	0.44
1:A:287:PRO:HB3	1:B:287:PRO:HB3	1.99	0.44
1:A:244:THR:HG22	1:A:251:ARG:HG3	2.00	0.44
1:C:75:VAL:HG13	1:C:79:TYR:HB2	2.01	0.43
1:B:110:ALA:HB2	1:B:239:LEU:CD1	2.48	0.43
1:B:232:GLY:HA3	1:B:238:GLY:HA2	2.00	0.43
1:C:221:GLU:HG2	1:C:224:ARG:NH2	2.33	0.43
1:D:43:LEU:HD23	1:D:61:LEU:CD1	2.47	0.43
2:A:601:HEM:HBC2	2:A:601:HEM:CMC	2.47	0.43
1:C:236:LEU:HD13	1:C:264:PHE:CE2	2.54	0.43
1:C:133:LYS:NZ	1:C:147:ASP:OD1	2.45	0.43
1:B:220:ASP:HA	1:B:223:ILE:HD12	2.01	0.43
1:A:193:ARG:HB2	1:A:194:PRO:HD2	2.00	0.43
1:D:150:ARG:NH2	1:D:171:ASP:O	2.50	0.43
1:B:376:GLU:O	1:B:381:ARG:NH1	2.51	0.43
1:D:3:ARG:NH2	1:D:5:LEU:HD12	2.34	0.43
1:C:231:GLY:HA3	1:C:238:GLY:CA	2.43	0.42
1:B:48:ILE:O	1:B:49:GLN:C	2.61	0.42
1:C:327:ARG:NH2	1:C:381:ARG:NH1	2.67	0.42
1:A:221:GLU:HA	1:A:224:ARG:HE	1.85	0.42
2:C:601:HEM:HBC2	2:C:601:HEM:CMC	2.49	0.42
1:A:232:GLY:HA2	1:A:238:GLY:CA	2.48	0.42
1:A:277:ALA:HB1	1:A:446:PRO:HG2	2.02	0.42
1:C:315:LEU:HB3	1:C:319:PRO:HD3	2.02	0.42
1:D:37:ARG:NH2	1:D:367:HIS:HA	2.34	0.42
1:A:188:MET:HE1	1:A:442:LEU:HD13	2.02	0.42
1:D:348:LYS:HB3	1:D:348:LYS:HE2	1.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:138:GLN:NE2	1:D:455:GLU:HG3	2.35	0.42
1:D:285:ARG:NH2	1:D:434:TYR:O	2.50	0.42
1:A:221:GLU:CA	1:A:224:ARG:HH21	2.32	0.42
1:D:223:ILE:HG23	1:D:241:LEU:HD21	2.02	0.42
1:D:426:PHE:HB3	1:D:453:VAL:HB	2.01	0.42
1:B:236:LEU:HD13	1:B:264:PHE:CE2	2.55	0.41
1:C:157:SER:CB	1:C:165:PHE:HE2	2.33	0.41
1:A:203:GLU:HG2	1:A:206:ARG:HH12	1.86	0.41
1:A:80:THR:HG21	1:C:16:GLN:HE22	1.85	0.41
1:A:224:ARG:CG	1:A:225:GLU:HB2	2.36	0.41
1:C:227:ARG:HE	1:C:241:LEU:CD2	2.30	0.41
1:C:367:HIS:HA	1:C:368:PRO:HD3	1.97	0.41
1:A:110:ALA:HB2	1:A:239:LEU:HD13	2.03	0.41
1:B:62:VAL:HG21	1:B:364:LEU:HD13	2.02	0.41
1:C:328:PHE:HB3	1:C:329:TRP:CD1	2.55	0.41
1:D:231:GLY:O	1:D:242:ASN:ND2	2.53	0.41
1:B:152:THR:HA	1:B:414:GLU:OE2	2.19	0.41
1:D:188:MET:CE	1:D:442:LEU:HB2	2.47	0.41
1:A:150:ARG:NH2	1:A:171:ASP:O	2.54	0.41
1:B:32:PHE:CE1	1:B:46:LEU:HD11	2.55	0.41
1:C:42:GLY:HA2	1:C:57:TYR:CE1	2.56	0.41
1:D:227:ARG:CZ	1:D:241:LEU:HD22	2.51	0.41
1:A:221:GLU:HA	1:A:224:ARG:HH21	1.86	0.41
1:A:284:LEU:HD13	1:A:430:ASP:HB2	2.02	0.41
1:B:82:ILE:HD11	1:B:266:ILE:HG21	2.03	0.41
1:C:10:SER:HA	1:C:11:PRO:HD3	1.90	0.41
1:A:428:LEU:O	1:B:287:PRO:HD2	2.21	0.40
1:D:330:SER:HB3	5:D:724:HOH:O	2.20	0.40
1:D:314:ARG:H	1:D:314:ARG:HG2	1.76	0.40
1:B:5:LEU:HD13	1:B:350:GLU:HB2	2.03	0.40
1:B:90:LEU:HA	1:B:90:LEU:HD23	1.82	0.40
2:C:601:HEM:HBB2	2:C:601:HEM:CMB	2.51	0.40
1:A:156:ILE:HD12	1:A:156:ILE:HA	1.85	0.40
1:A:407:GLY:HA3	2:A:601:HEM:C2B	2.56	0.40
1:C:108:LEU:HD23	1:C:108: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	461/501 (92%)	440 (95%)	17 (4%)	4 (1%)	14	27
1	B	451/501 (90%)	432 (96%)	15 (3%)	4 (1%)	14	27
1	C	445/501 (89%)	421 (95%)	18 (4%)	6 (1%)	9	18
1	D	462/501 (92%)	435 (94%)	21 (4%)	6 (1%)	9	18
All	All	1819/2004 (91%)	1728 (95%)	71 (4%)	20 (1%)	11	22

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	229	HIS
1	B	76	HIS
1	B	77	PRO
1	C	77	PRO
1	C	235	ASP
1	D	49	GLN
1	D	76	HIS
1	A	49	GLN
1	A	77	PRO
1	B	49	GLN
1	C	78	ALA
1	C	49	GLN
1	C	227	ARG
1	C	229	HIS
1	D	77	PRO
1	D	195	PRO
1	D	235	ASP
1	B	78	ALA
1	D	40	PRO
1	A	193	ARG

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	391/423 (92%)	390 (100%)	1 (0%)	86	94
1	B	383/423 (90%)	383 (100%)	0	100	100
1	C	378/423 (89%)	376 (100%)	2 (0%)	81	92
1	D	392/423 (93%)	391 (100%)	1 (0%)	86	94
All	All	1544/1692 (91%)	1540 (100%)	4 (0%)	86	94

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	HIS
1	C	4	ILE
1	C	66	THR
1	D	304	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	HIS
1	A	113	GLN
1	A	186	HIS
1	A	242	ASN
1	A	286	HIS
1	A	334	ASN
1	A	341	GLN
1	A	356	GLN
1	B	16	GLN
1	B	76	HIS
1	B	186	HIS
1	B	242	ASN
1	B	356	GLN
1	C	16	GLN
1	C	38	GLN

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Mol	Chain	Res	Type
1	C	84	ASN
1	C	104	HIS
1	C	186	HIS
1	C	334	ASN
1	D	76	HIS
1	D	113	GLN
1	D	186	HIS
1	D	334	ASN
1	D	356	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](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	HEM	D	601	1	50,50,50	1.52	9 (18%)	67,82,82	1.52	15 (22%)
3	SO4	D	602	-	4,4,4	0.41	0	6,6,6	0.27	0
4	SER	B	601	-	4,5,6	0.69	0	1,5,7	0.65	0
2	HEM	A	601	1	50,50,50	1.47	7 (14%)	67,82,82	1.43	13 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEM	B	602	1	50,50,50	1.47	8 (16%)	67,82,82	1.28	9 (13%)
2	HEM	C	601	1	50,50,50	1.66	9 (18%)	67,82,82	1.48	11 (16%)
3	SO4	A	602	-	4,4,4	0.42	0	6,6,6	0.14	0
3	SO4	A	603	-	4,4,4	0.50	0	6,6,6	0.24	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	601	1	-	2/14/54/54	-
4	SER	B	601	-	-	1/2/4/6	-
2	HEM	A	601	1	-	2/14/54/54	-
2	HEM	B	602	1	-	2/14/54/54	-
2	HEM	C	601	1	-	2/14/54/54	-

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	HEM	FE-NB	4.90	2.10	1.94
2	C	601	HEM	FE-NB	4.73	2.09	1.94
2	D	601	HEM	FE-NA	4.61	2.10	1.95
2	C	601	HEM	FE-NC	4.22	2.09	1.95
2	C	601	HEM	FE-NA	4.01	2.08	1.95
2	B	602	HEM	FE-NA	3.94	2.08	1.95
2	B	602	HEM	FE-NB	3.87	2.06	1.94
2	C	601	HEM	FE-ND	3.60	2.06	1.94
2	B	602	HEM	FE-ND	3.44	2.05	1.94
2	D	601	HEM	FE-NB	3.41	2.05	1.94
2	A	601	HEM	FE-NC	3.26	2.05	1.95
2	C	601	HEM	CMC-C2C	3.08	1.57	1.50
2	A	601	HEM	FE-NA	3.06	2.05	1.95
2	D	601	HEM	CMC-C2C	3.01	1.56	1.50
2	C	601	HEM	CAB-C3B	3.01	1.55	1.47
2	D	601	HEM	CAC-C3C	2.87	1.55	1.47
2	D	601	HEM	FE-ND	2.83	2.03	1.94
2	A	601	HEM	CAB-C3B	2.82	1.54	1.47
2	B	602	HEM	CAC-C3C	2.81	1.54	1.47
2	B	602	HEM	CAB-C3B	2.76	1.54	1.47
2	A	601	HEM	CMC-C2C	2.63	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	HEM	CMB-C2B	2.62	1.56	1.50
2	C	601	HEM	CMB-C2B	2.60	1.56	1.50
2	B	602	HEM	CMC-C2C	2.59	1.56	1.50
2	D	601	HEM	CMA-C3A	2.41	1.55	1.50
2	A	601	HEM	CMD-C2D	2.38	1.55	1.50
2	B	602	HEM	FE-NC	2.36	2.02	1.95
2	D	601	HEM	CAB-C3B	2.32	1.53	1.47
2	A	601	HEM	CMA-C3A	2.29	1.55	1.50
2	C	601	HEM	CMA-C3A	2.19	1.55	1.50
2	D	601	HEM	CMD-C2D	2.04	1.54	1.50
2	C	601	HEM	CAC-C3C	2.02	1.52	1.47
2	B	602	HEM	CMA-C3A	2.02	1.54	1.50

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	HEM	C4C-C3C-C2C	3.40	109.76	106.81
2	B	602	HEM	CHD-C4C-NC	3.33	128.07	124.45
2	D	601	HEM	C2A-C1A-NA	-3.30	106.49	110.15
2	A	601	HEM	CBD-CAD-C3D	-3.28	103.46	112.53
2	A	601	HEM	CHD-C4C-NC	3.12	127.85	124.45
2	C	601	HEM	C3B-C4B-NB	-3.07	107.26	109.47
2	C	601	HEM	CBD-CAD-C3D	-3.02	104.18	112.53
2	C	601	HEM	CAC-C3C-C4C	-3.00	117.66	124.82
2	A	601	HEM	C4C-C3C-C2C	2.98	109.40	106.81
2	C	601	HEM	CHD-C4C-NC	2.94	127.65	124.45
2	C	601	HEM	C1B-NB-C4B	2.88	108.62	105.21
2	D	601	HEM	O1D-CGD-CBD	-2.87	113.98	123.09
2	A	601	HEM	O2A-CGA-CBA	2.87	123.07	114.00
2	C	601	HEM	C2A-C1A-NA	-2.85	106.99	110.15
2	D	601	HEM	CHC-C4B-NB	2.83	127.47	124.42
2	D	601	HEM	C3D-C4D-ND	-2.83	107.07	110.17
2	D	601	HEM	CAD-CBD-CGD	-2.69	106.53	113.67
2	D	601	HEM	C4D-ND-C1D	2.64	108.33	105.21
2	A	601	HEM	O1D-CGD-CBD	-2.62	114.78	123.09
2	B	602	HEM	C4D-ND-C1D	2.58	108.26	105.21
2	D	601	HEM	C3B-C4B-NB	-2.56	107.63	109.47
2	A	601	HEM	CAC-C3C-C4C	-2.55	118.73	124.82
2	D	601	HEM	C4B-C3B-C2B	2.54	109.62	107.28
2	A	601	HEM	C3D-C4D-ND	-2.52	107.41	110.17
2	D	601	HEM	C4C-C3C-C2C	2.46	108.95	106.81
2	A	601	HEM	C2A-C1A-NA	-2.45	107.43	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	602	HEM	C4C-C3C-C2C	2.40	108.89	106.81
2	D	601	HEM	CAC-C3C-C4C	-2.38	119.13	124.82
2	D	601	HEM	C1B-NB-C4B	2.35	107.99	105.21
2	B	602	HEM	C1B-NB-C4B	2.33	107.97	105.21
2	B	602	HEM	CBA-CAA-C2A	-2.31	106.15	112.53
2	C	601	HEM	CHC-C4B-NB	2.28	126.88	124.42
2	A	601	HEM	C4D-ND-C1D	2.28	107.91	105.21
2	D	601	HEM	O2A-CGA-CBA	2.23	121.03	114.00
2	B	602	HEM	CAC-C3C-C4C	-2.21	119.54	124.82
2	D	601	HEM	CHD-C1D-ND	2.21	126.80	124.42
2	B	602	HEM	CHC-C4B-NB	2.14	126.72	124.42
2	A	601	HEM	O1A-CGA-CBA	-2.13	116.32	123.09
2	C	601	HEM	C4D-ND-C1D	2.11	107.71	105.21
2	B	602	HEM	C3D-C4D-ND	-2.11	107.86	110.17
2	C	601	HEM	C3A-C4A-NA	-2.11	106.77	110.14
2	D	601	HEM	C3C-C2C-C1C	-2.10	105.06	107.05
2	C	601	HEM	C4A-NA-C1A	2.09	109.23	105.82
2	A	601	HEM	C1B-NB-C4B	2.09	107.68	105.21
2	A	601	HEM	CHC-C4B-NB	2.09	126.67	124.42
2	B	602	HEM	C2A-C1A-NA	-2.05	107.88	110.15
2	D	601	HEM	O1A-CGA-CBA	-2.04	116.61	123.09
2	A	601	HEM	O2D-CGD-CBD	2.01	120.34	114.00

There are no chirality outliers.

All (9) torsion outliers are listed below:

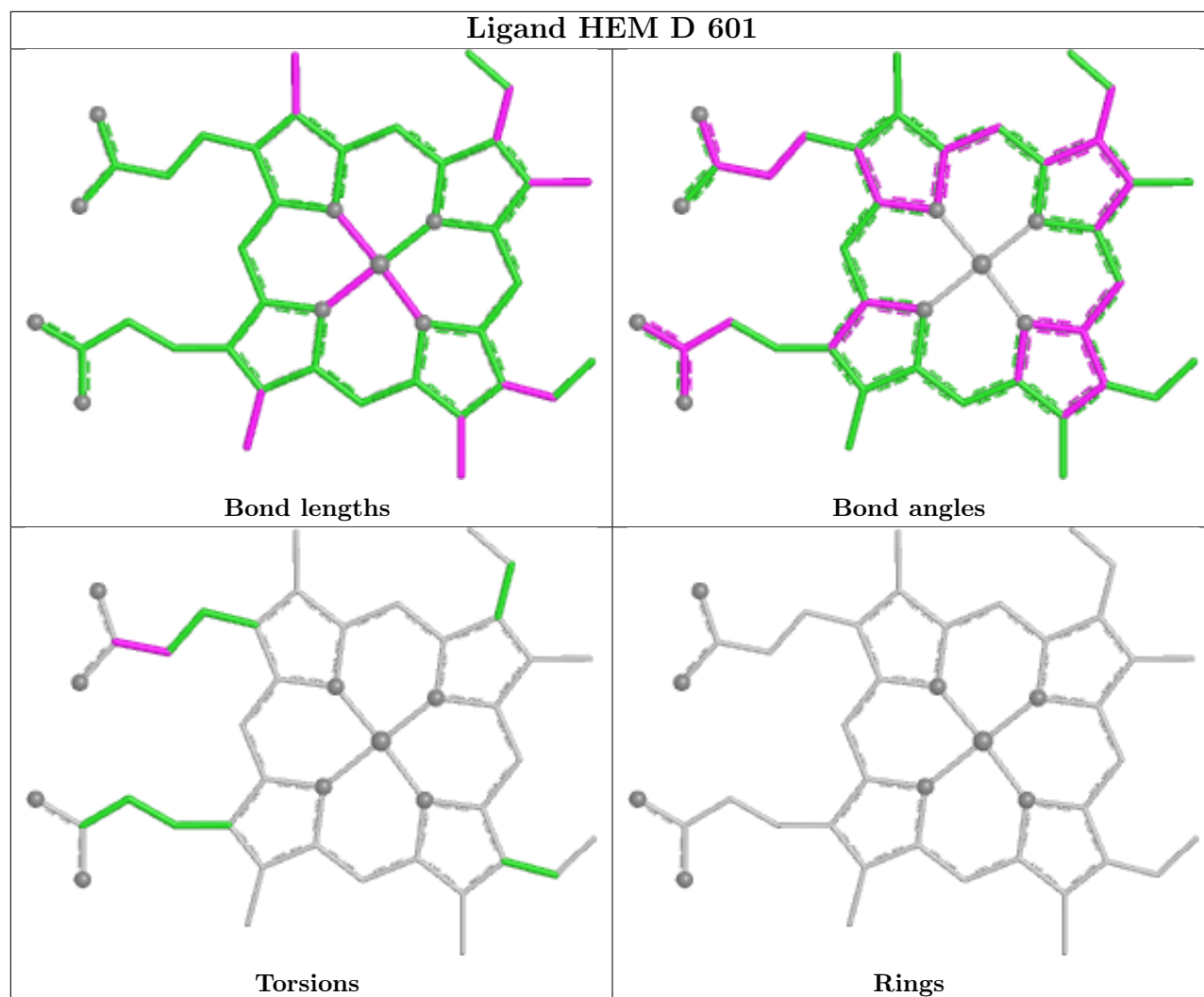
Mol	Chain	Res	Type	Atoms
4	B	601	SER	C-CA-CB-OG
2	C	601	HEM	CAA-CBA-CGA-O1A
2	A	601	HEM	CAA-CBA-CGA-O1A
2	D	601	HEM	CAD-CBD-CGD-O2D
2	C	601	HEM	CAA-CBA-CGA-O2A
2	B	602	HEM	CAD-CBD-CGD-O2D
2	B	602	HEM	CAD-CBD-CGD-O1D
2	D	601	HEM	CAD-CBD-CGD-O1D
2	A	601	HEM	CAA-CBA-CGA-O2A

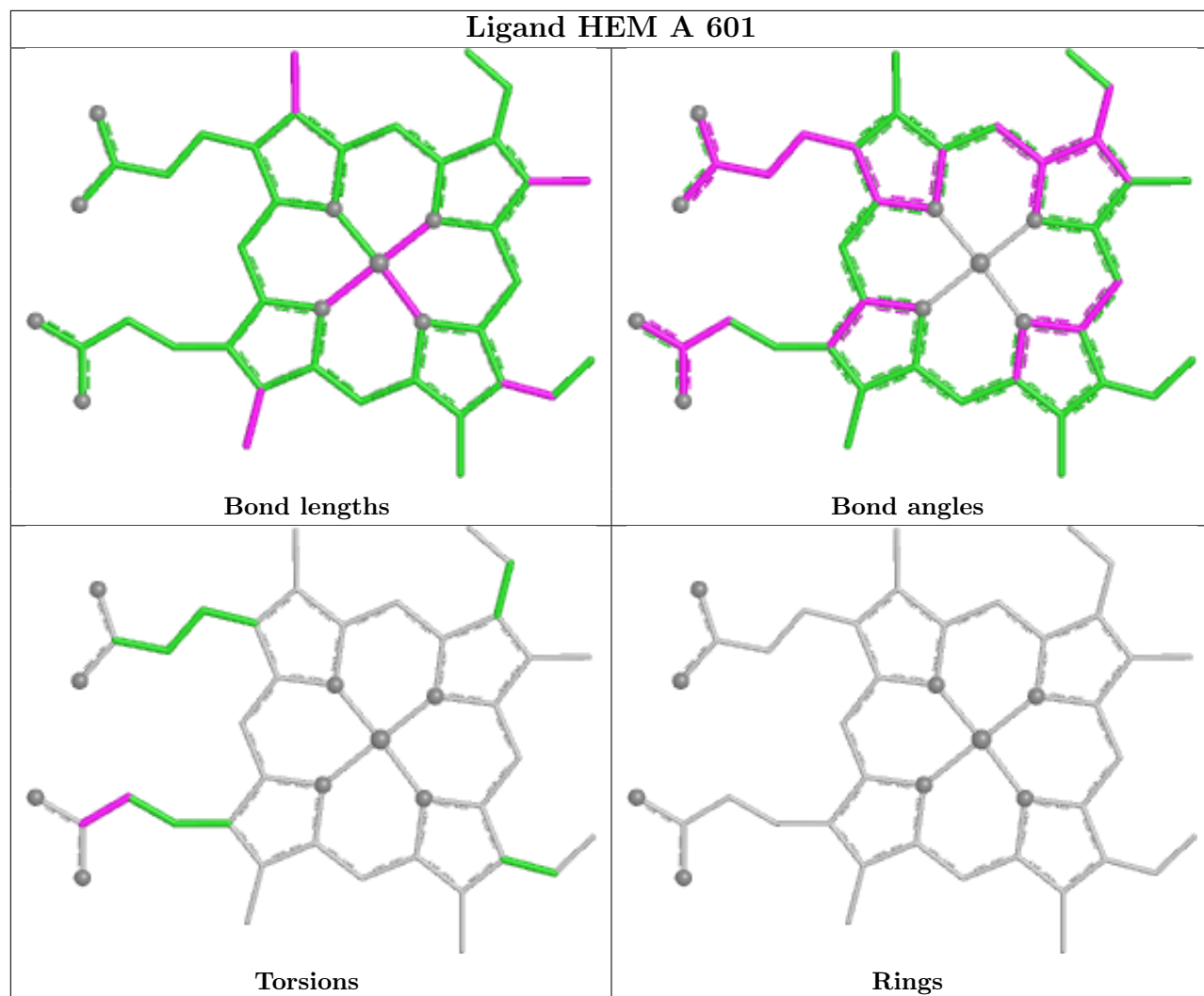
There are no ring outliers.

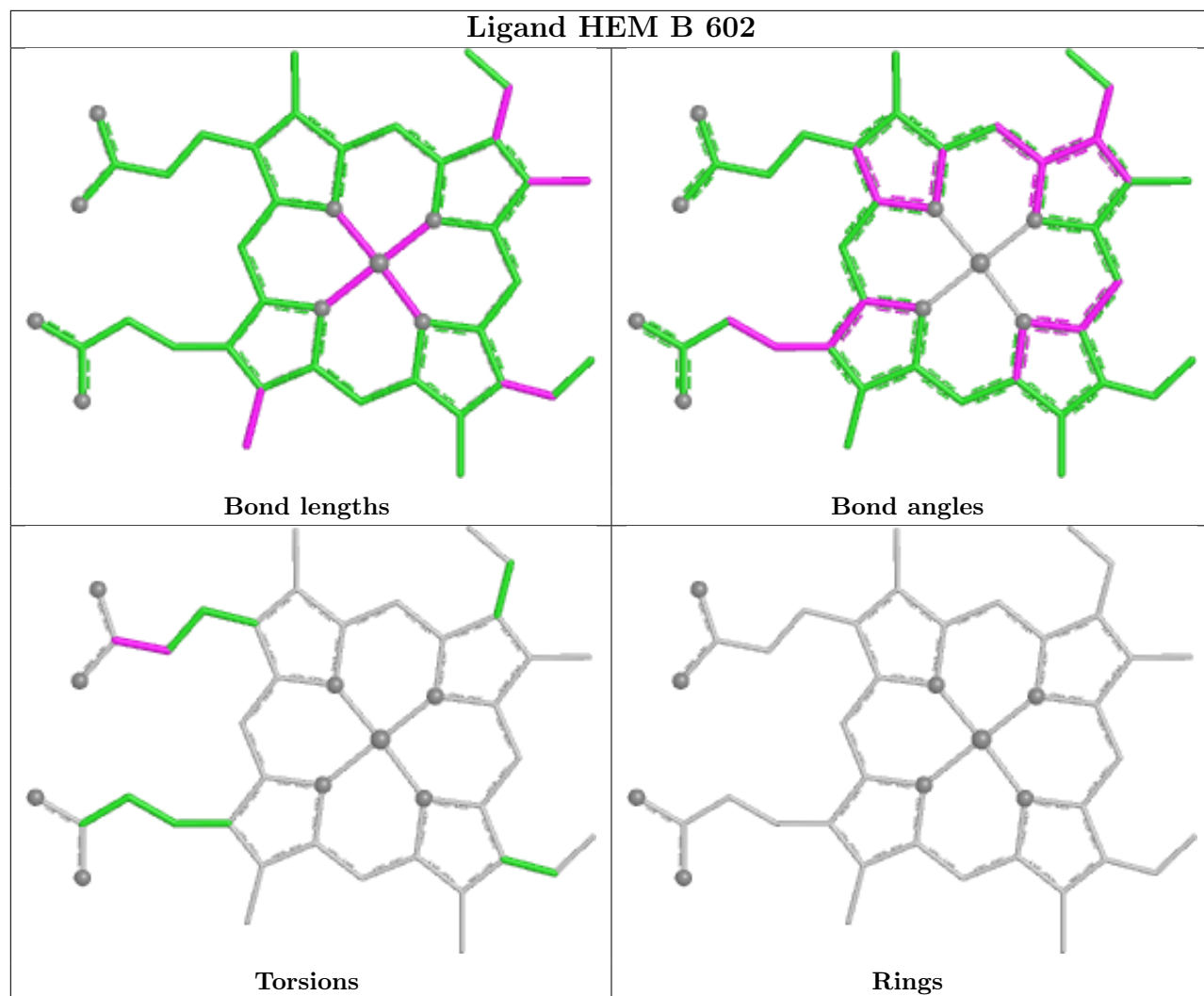
3 monomers are involved in 15 short contacts:

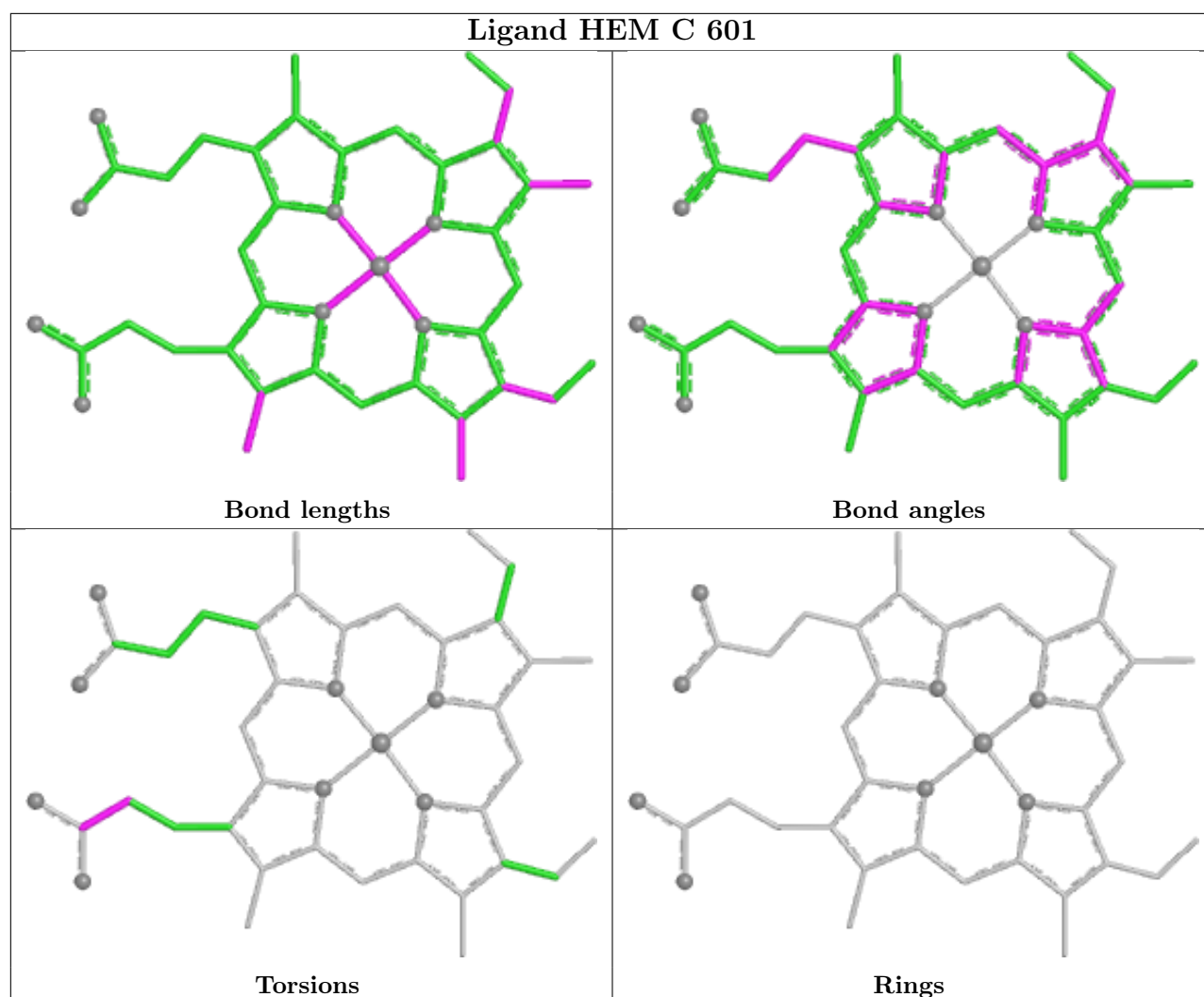
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	601	HEM	4	0
2	A	601	HEM	6	0
2	C	601	HEM	5	0

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	462/501 (92%)	-0.22	20 (4%)	40	35	21, 33, 69, 126	1 (0%)
1	B	455/501 (90%)	-0.12	12 (2%)	57	52	22, 36, 67, 109	0
1	C	449/501 (89%)	0.29	52 (11%)	9	8	22, 39, 84, 118	0
1	D	464/501 (92%)	-0.04	21 (4%)	38	33	20, 34, 77, 115	0
All	All	1830/2004 (91%)	-0.02	105 (5%)	29	26	20, 35, 79, 126	1 (0%)

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	77	PRO	6.9
1	B	77	PRO	6.7
1	C	76	HIS	6.5
1	B	76	HIS	6.1
1	D	196	VAL	5.3
1	B	192	SER	5.3
1	C	223	ILE	5.2
1	A	464	VAL	4.9
1	A	196	VAL	4.8
1	C	467	PRO	4.8
1	D	39	ILE	4.5
1	D	197	LEU	4.4
1	A	76	HIS	4.4
1	C	230	GLY	4.3
1	C	4	ILE	4.1
1	C	207	ALA	4.1
1	C	229	HIS	4.0
1	A	194	PRO	4.0
1	D	76	HIS	3.8
1	A	195	PRO	3.7
1	B	198	THR	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	48	ILE	3.5
1	C	225	GLU	3.4
1	A	197	LEU	3.4
1	B	231	GLY	3.3
1	C	465	PRO	3.3
1	C	232	GLY	3.3
1	D	37	ARG	3.1
1	C	227	ARG	3.1
1	C	243	ALA	3.1
1	B	201	MET	3.1
1	A	3	ARG	3.1
1	C	228	GLY	3.1
1	A	231	GLY	3.0
1	C	78	ALA	2.9
1	A	193	ARG	2.9
1	C	233	GLY	2.9
1	D	195	PRO	2.9
1	C	209	TRP	2.9
1	C	254	ASP	2.9
1	C	252	LEU	2.9
1	C	50	GLY	2.9
1	B	230	GLY	2.8
1	A	463	SER	2.8
1	B	199	PRO	2.7
1	C	213	ALA	2.7
1	C	208	TYR	2.7
1	C	222	VAL	2.7
1	D	201	MET	2.7
1	A	229	HIS	2.7
1	C	234	GLY	2.7
1	C	212	ILE	2.7
1	D	199	PRO	2.6
1	A	201	MET	2.6
1	A	402[A]	MET	2.6
1	B	229	HIS	2.6
1	C	231	GLY	2.6
1	C	188	MET	2.6
1	C	218	LEU	2.6
1	C	220	ASP	2.6
1	C	466	VAL	2.6
1	C	237	LEU	2.5
1	D	12	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	234	GLY	2.5
1	D	193	ARG	2.5
1	D	194	PRO	2.4
1	C	3	ARG	2.4
1	D	466	VAL	2.4
1	A	192	SER	2.4
1	C	246	PRO	2.4
1	B	232	GLY	2.4
1	D	17	TYR	2.4
1	A	191	ASN	2.4
1	A	4	ILE	2.3
1	B	191	ASN	2.3
1	C	238	GLY	2.3
1	C	442	LEU	2.3
1	B	209	TRP	2.3
1	C	257	ILE	2.3
1	C	98	PRO	2.3
1	D	347	GLY	2.3
1	C	48	ILE	2.3
1	C	241	LEU	2.3
1	C	216	ASN	2.2
1	A	198	THR	2.2
1	C	226	ARG	2.2
1	C	210	ALA	2.2
1	D	198	THR	2.2
1	A	225	GLU	2.2
1	C	244	THR	2.2
1	C	239	LEU	2.2
1	C	106	ILE	2.2
1	D	304	ASP	2.2
1	C	219	VAL	2.1
1	A	233	GLY	2.1
1	C	176	PHE	2.1
1	C	182	ARG	2.1
1	D	3	ARG	2.1
1	C	388	ARG	2.1
1	C	250	GLU	2.1
1	D	51	ARG	2.0
1	C	224	ARG	2.0
1	D	46	LEU	2.0
1	C	249	GLY	2.0
1	D	230	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

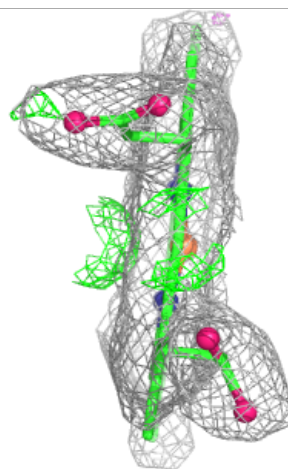
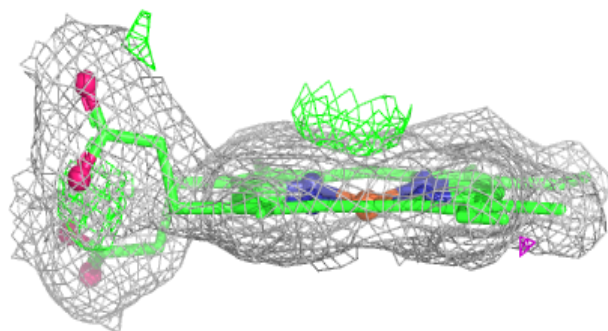
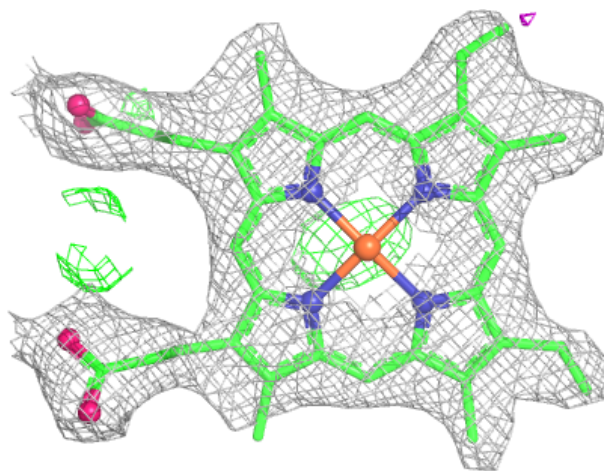
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SER	B	601	6/7	0.78	0.15	68,71,74,77	0
3	SO4	A	603	5/5	0.87	0.21	54,55,73,88	0
3	SO4	D	602	5/5	0.92	0.21	51,54,67,73	0
3	SO4	A	602	5/5	0.92	0.26	50,61,68,74	0
2	HEM	C	601	43/43	0.97	0.08	24,37,45,49	0
2	HEM	A	601	43/43	0.98	0.07	17,24,30,35	0
2	HEM	D	601	43/43	0.98	0.07	19,25,29,33	0
2	HEM	B	602	43/43	0.98	0.06	19,29,35,43	0

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

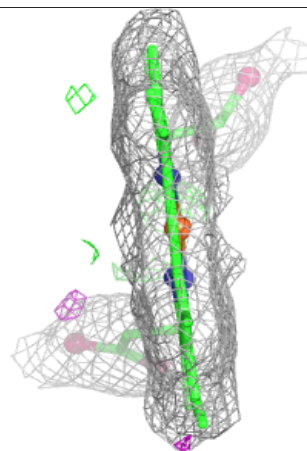
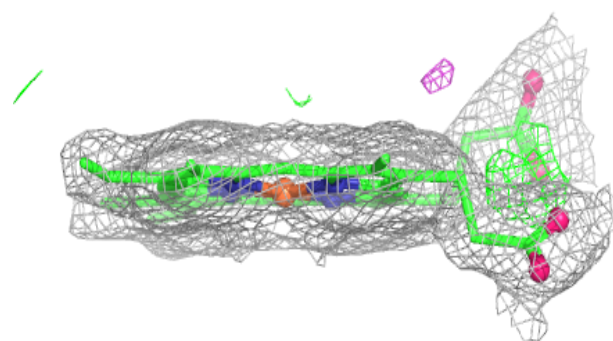
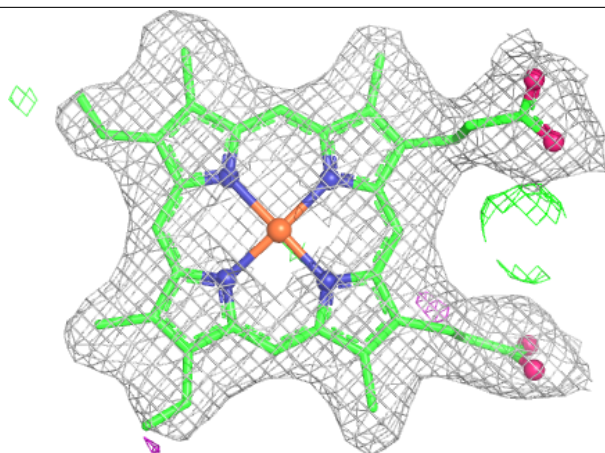
Electron density around HEM C 601:

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



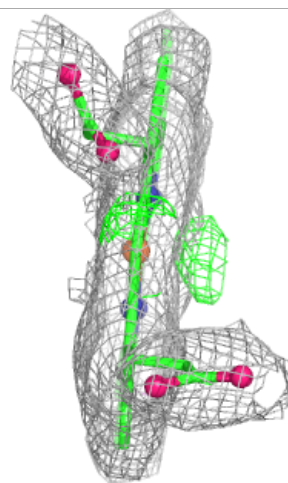
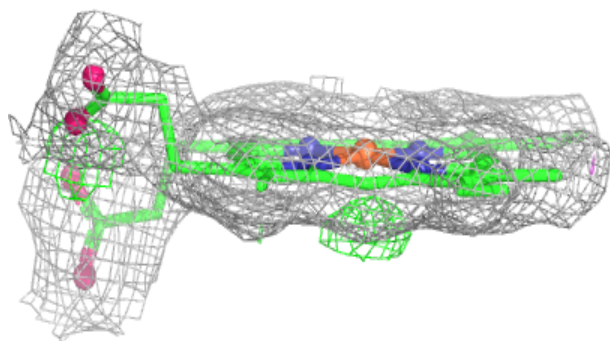
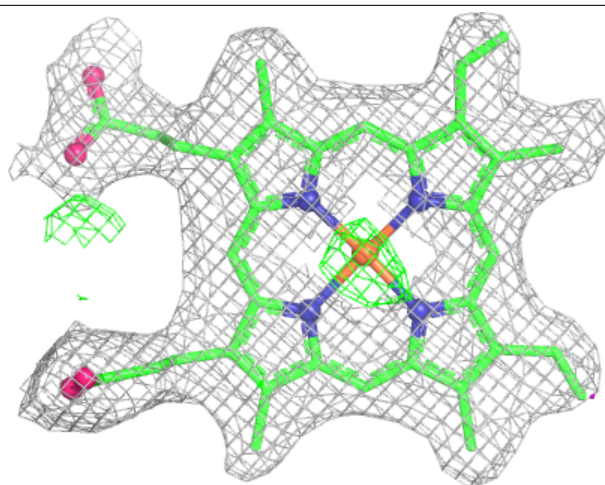
Electron density around HEM A 601:

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



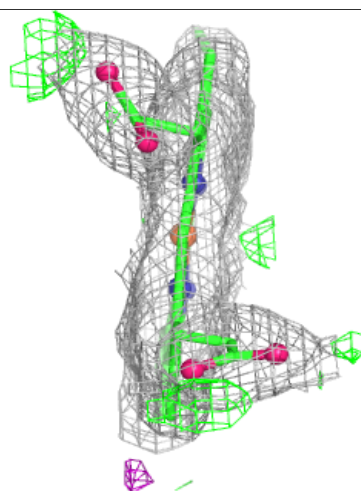
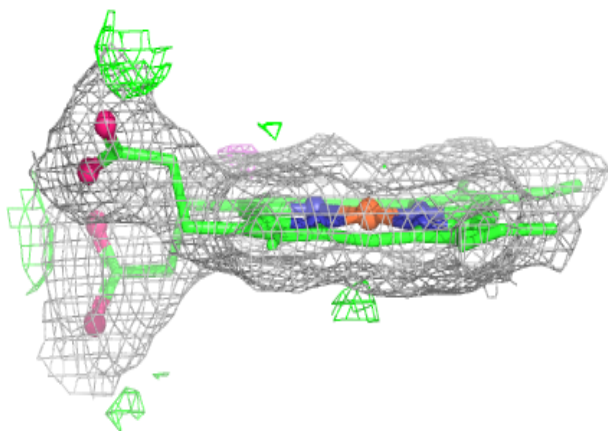
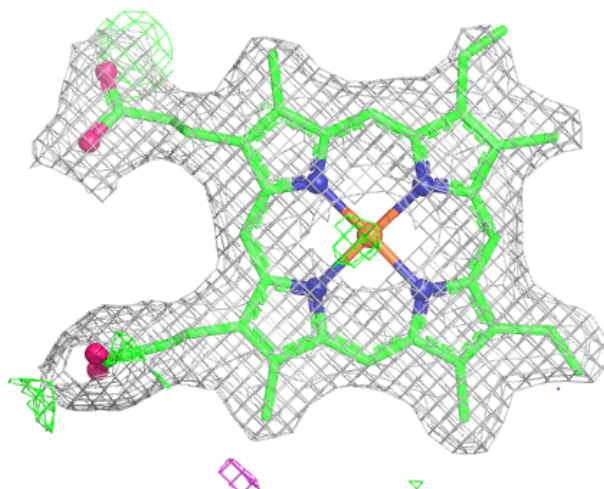
Electron density around HEM D 601:

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



Electron density around HEM B 602:

$2mF_o-DF_c$ (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.