



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 09:56 PM EDT

PDB ID : 4QOQ / pdb_00004qoq
Title : Structure of Bacillus pumilus catalase with guaiacol bound
Authors : Loewen, P.C.
Deposited on : 2014-06-20
Resolution : 1.70 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 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

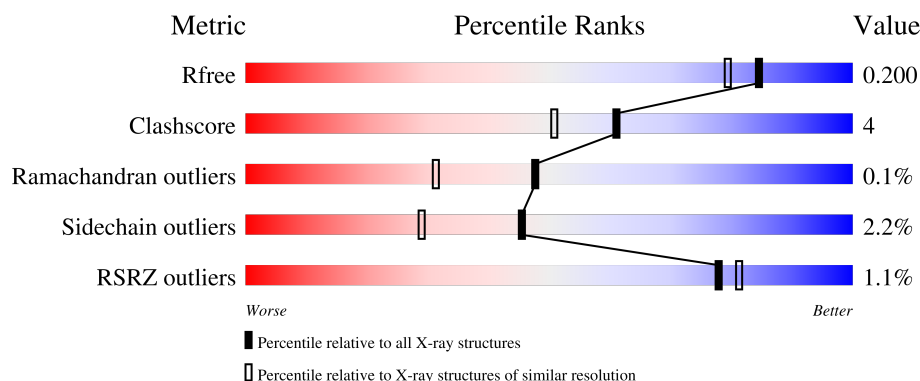
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	491	2% 90% 7% ..
1	B	491	89% 8% ..
1	C	491	% 90% 7% .
1	D	491	% 90% 8% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	JZ3	A	503	-	-	X	-
3	JZ3	B	503	-	-	X	-
3	JZ3	D	503	-	-	X	-

2 Entry composition [i](#)

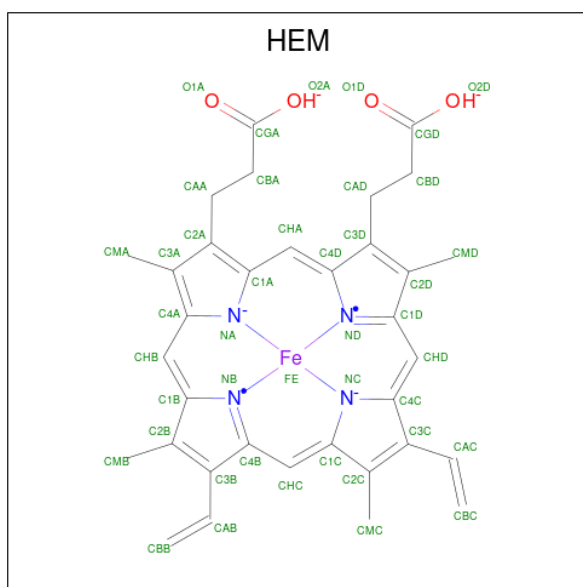
There are 6 unique types of molecules in this entry. The entry contains 17970 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Catalase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	481	Total	C	N	O	S	0	6	0
			3960	2496	693	756	15			
1	B	481	Total	C	N	O	S	0	5	0
			3959	2497	692	755	15			
1	C	481	Total	C	N	O	S	0	7	0
			3973	2506	696	756	15			
1	D	481	Total	C	N	O	S	0	6	0
			3966	2500	693	759	14			

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



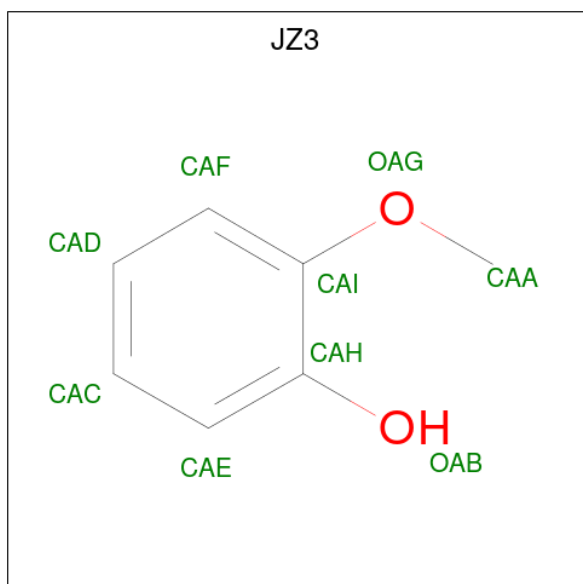
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Fe	N O	0	1
			43	34	1	4 4		
2	A	1	Total	C	Fe	N O	0	1
			43	34	1	4 4		

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

- Molecule 3 is Guaiacol (CCD ID: JZ3) (formula: C₇H₈O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O		
			9	7	2		
3	B	1	Total	C	O		
			9	7	2		
3	B	1	Total	C	O		
			9	7	2		
3	C	1	Total	C	O		
			9	7	2		
3	D	1	Total	C	O		
			9	7	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	C	O	0	0
			9	7	2		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Cl	0	0
			2	2		
4	B	1	Total	Cl	0	0
			1	1		
4	C	2	Total	Cl	0	0
			2	2		
4	D	1	Total	Cl	0	0
			1	1		

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Na	0	0
			1	1		
5	B	1	Total	Na	0	0
			1	1		

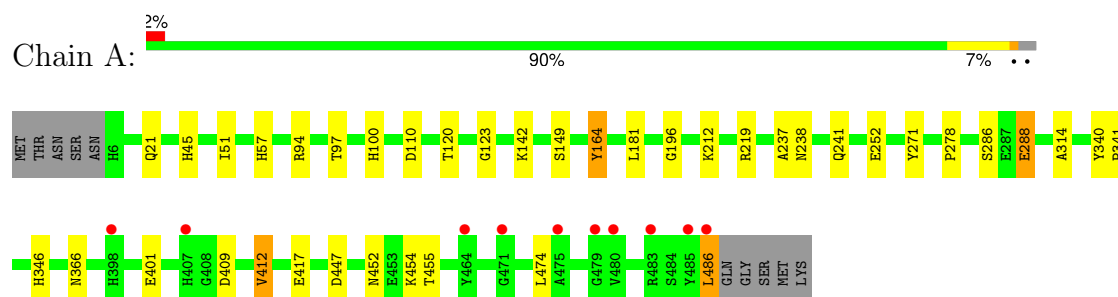
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	434	Total	O	0	0
			434	434		
6	B	429	Total	O	0	0
			429	429		
6	C	435	Total	O	0	0
			435	435		
6	D	408	Total	O	0	0
			408	408		

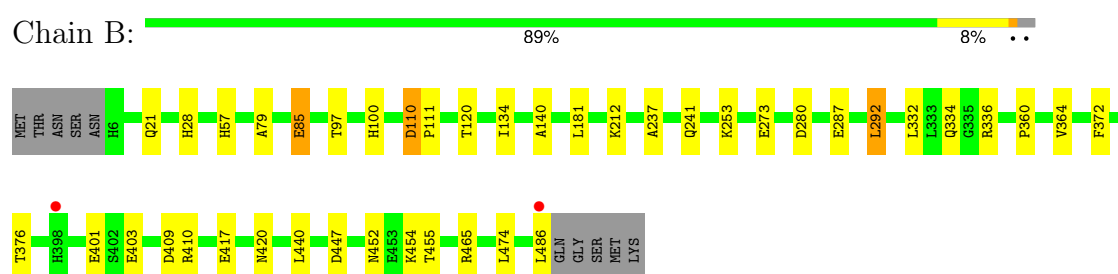
3 Residue-property plots [i](#)

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.

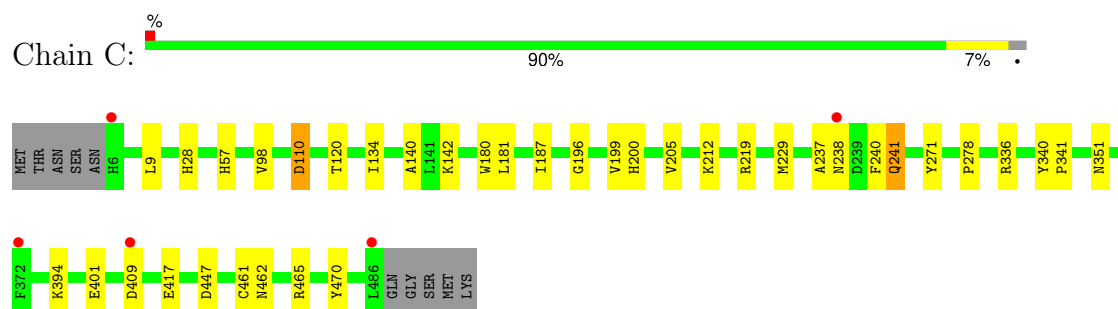
• Molecule 1: Catalase



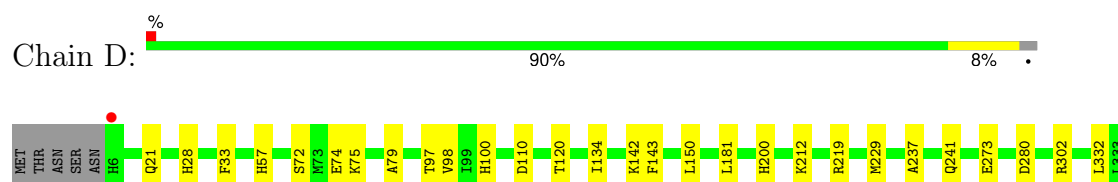
• Molecule 1: Catalase

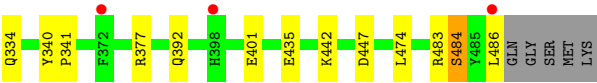


• Molecule 1: Catalase



• Molecule 1: Catalase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	91.79Å 108.11Å 103.41Å 90.00° 91.98° 90.00°	Depositor
Resolution (Å)	103.35 – 1.70 103.35 – 1.70	Depositor EDS
% Data completeness (in resolution range)	95.0 (103.35-1.70) 95.0 (103.35-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0069	Depositor
R, R_{free}	0.162 , 0.190 0.172 , 0.200	Depositor DCC
R_{free} test set	10493 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å ²)	17.6	Xtriage
Anisotropy	0.741	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 36.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.045 for -h,-l,-k 0.038 for -h,l,k 0.095 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	17970	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, JZ3, NA, 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	1.18	6/4082 (0.1%)	1.02	1/5535 (0.0%)
1	B	1.21	3/4077 (0.1%)	1.03	2/5527 (0.0%)
1	C	1.25	5/4094 (0.1%)	1.05	2/5550 (0.0%)
1	D	1.21	6/4084 (0.1%)	1.02	1/5537 (0.0%)
All	All	1.21	20/16337 (0.1%)	1.03	6/22149 (0.0%)

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	51	ILE	CA-C	6.92	1.58	1.52
1	D	280	ASP	C-N	6.87	1.39	1.33
1	D	377	ARG	N-CA	6.26	1.50	1.46
1	A	164	TYR	N-CA	-6.02	1.39	1.46
1	D	33	PHE	N-CA	-5.89	1.38	1.45
1	C	187	ILE	N-CA	5.83	1.53	1.46
1	A	314	ALA	CA-C	-5.77	1.45	1.52
1	C	470	TYR	N-CA	5.66	1.53	1.46
1	A	123	GLY	C-O	5.63	1.28	1.23
1	D	143	PHE	C-O	-5.48	1.19	1.24
1	B	280	ASP	C-N	5.42	1.38	1.33
1	C	205	VAL	N-CA	5.41	1.52	1.46
1	A	196	GLY	N-CA	5.27	1.50	1.45
1	D	79	ALA	C-O	5.23	1.30	1.23
1	A	149	SER	N-CA	5.21	1.52	1.46
1	C	394	LYS	CA-C	-5.20	1.46	1.52
1	D	200	HIS	CA-C	-5.17	1.46	1.52
1	B	336	ARG	CZ-NH2	-5.11	1.26	1.33
1	C	196	GLY	CA-C	5.10	1.56	1.51
1	B	79	ALA	C-O	5.02	1.30	1.23

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	98	VAL	N-CA-C	6.71	116.92	111.62
1	B	85	GLU	CB-CG-CD	6.05	122.88	112.60
1	A	252	GLU	CB-CG-CD	5.34	121.69	112.60
1	C	200	HIS	N-CA-C	5.27	117.93	110.50
1	B	376	THR	N-CA-C	5.25	119.32	113.02
1	C	238	ASN	CB-CA-C	-5.04	100.60	109.07

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	3960	0	3764	30	0
1	B	3959	0	3767	35	0
1	C	3973	0	3787	29	0
1	D	3966	0	3769	26	0
2	A	86	0	60	9	0
2	B	86	0	60	9	0
2	C	86	0	60	12	0
2	D	86	0	60	3	0
3	A	9	0	8	4	0
3	B	18	0	16	5	0
3	C	9	0	8	3	0
3	D	18	0	15	4	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
4	C	2	0	0	0	0
4	D	1	0	0	0	0
5	A	1	0	0	1	0
5	B	1	0	0	0	0
6	A	434	0	0	10	0
6	B	429	0	0	5	0
6	C	435	0	0	12	0
6	D	408	0	0	9	0
All	All	17970	0	15374	134	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 (134) 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:212:LYS:HE2	6:C:905:HOH:O	1.24	1.31
1:D:72[B]:SER:OG	1:D:74:GLU:OE1	1.60	1.17
1:B:372[A]:PHE:CE2	6:D:904:HOH:O	2.06	1.05
1:D:212:LYS:HE2	6:D:714:HOH:O	1.63	0.96
1:A:212:LYS:HE2	6:A:699:HOH:O	1.67	0.95
1:D:181:LEU:HD21	3:D:503:JZ3:HAF	1.48	0.94
2:B:501[A]:HEM:CMC	2:B:501[A]:HEM:HBC2	2.00	0.89
2:C:501[A]:HEM:HBB2	2:C:501[A]:HEM:HMB2	1.57	0.87
1:A:181:LEU:HD21	3:A:503:JZ3:HAF	1.58	0.86
2:C:501[A]:HEM:HBB2	2:C:501[A]:HEM:CMB	2.08	0.83
2:B:501[A]:HEM:HBC2	2:B:501[A]:HEM:HMC2	1.58	0.83
1:C:181:LEU:HD21	3:C:503:JZ3:HAF	1.60	0.81
1:B:287:GLU:HG2	1:B:292:LEU:HD21	1.61	0.80
5:A:506:NA:NA	6:A:843:HOH:O	1.56	0.78
2:C:502[B]:HEM:HBC2	2:C:502[B]:HEM:HMC2	1.67	0.75
2:A:501[A]:HEM:CMC	2:A:501[A]:HEM:HBC2	2.15	0.74
1:B:287:GLU:CG	1:B:292:LEU:HD21	2.17	0.73
1:A:452:ASN:HD22	1:A:455:THR:H	1.38	0.70
1:B:452:ASN:HD22	1:B:455:THR:H	1.39	0.70
1:C:212:LYS:NZ	6:C:906:HOH:O	2.26	0.68
2:C:501[A]:HEM:HMB2	2:C:501[A]:HEM:CBB	2.24	0.68
1:A:45:HIS:HE1	1:C:351:ASN:OD1	1.76	0.68
1:B:292:LEU:HD23	6:B:999:HOH:O	1.94	0.67
2:B:501[A]:HEM:HMC2	2:B:501[A]:HEM:CBC	2.27	0.65
2:B:501[A]:HEM:CMB	2:B:501[A]:HEM:HBB2	2.26	0.64
1:C:219:ARG:HD2	6:C:1001:HOH:O	1.97	0.64
1:B:110:ASP:OD1	3:B:503:JZ3:OAG	2.16	0.64
1:A:412[A]:VAL:HG13	1:B:403:GLU:OE2	1.98	0.63
1:B:465:ARG:CZ	6:B:926:HOH:O	2.45	0.63
2:C:502[B]:HEM:CMB	2:C:502[B]:HEM:HBB2	2.29	0.62
1:B:292:LEU:N	1:B:292:LEU:CD2	2.63	0.61
1:C:465:ARG:NE	6:C:1032:HOH:O	2.33	0.61
1:D:483:ARG:O	1:D:484:SER:CB	2.47	0.61
1:D:181:LEU:CD2	3:D:503:JZ3:HAF	2.29	0.61
2:A:501[A]:HEM:HBC2	2:A:501[A]:HEM:HMC2	1.84	0.60
6:A:803:HOH:O	1:D:100:HIS:HE1	1.85	0.60
1:B:372[A]:PHE:CD2	6:D:904:HOH:O	2.39	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:LYS:NZ	6:B:898:HOH:O	2.35	0.59
1:D:332:LEU:HD12	2:D:501[A]:HEM:HBB1	1.85	0.59
1:A:100:HIS:HE1	6:A:673:HOH:O	1.85	0.59
2:C:501[A]:HEM:HBC2	2:C:501[A]:HEM:CMC	2.32	0.58
1:C:240:PHE:C	1:C:241:GLN:HG3	2.28	0.58
1:A:346:HIS:HE1	6:D:904:HOH:O	1.87	0.58
1:B:181:LEU:HD21	3:B:503:JZ3:CAF	2.33	0.57
1:A:417:GLU:HG2	1:D:28:HIS:CD2	2.39	0.57
1:B:452:ASN:HD21	1:B:454:LYS:HB3	1.68	0.57
1:B:465:ARG:NH2	6:B:926:HOH:O	2.37	0.57
1:D:181:LEU:HD21	3:D:503:JZ3:CAF	2.28	0.56
2:D:502[B]:HEM:HMC2	2:D:502[B]:HEM:HBC2	1.88	0.56
1:A:238:ASN:HB2	6:A:781:HOH:O	2.06	0.54
1:A:452:ASN:HD21	1:A:454:LYS:HB3	1.71	0.54
2:B:501[A]:HEM:HBB2	2:B:501[A]:HEM:HMB2	1.87	0.54
1:C:219:ARG:HD2	6:C:727:HOH:O	2.07	0.54
1:D:219:ARG:HD3	6:D:855:HOH:O	2.07	0.53
1:B:292:LEU:N	1:B:292:LEU:HD22	2.24	0.53
2:A:501[A]:HEM:CMB	2:A:501[A]:HEM:HBB2	2.38	0.52
1:D:219:ARG:CG	6:D:855:HOH:O	2.58	0.52
3:C:503:JZ3:HAC	6:C:940:HOH:O	2.09	0.51
2:C:501[A]:HEM:HBC2	2:C:501[A]:HEM:HMC2	1.91	0.51
2:C:502[B]:HEM:HBB2	2:C:502[B]:HEM:HMB1	1.92	0.51
1:A:181:LEU:CD2	3:A:503:JZ3:HAF	2.36	0.51
1:C:465:ARG:CD	6:C:1032:HOH:O	2.58	0.51
1:A:271:TYR:CD1	1:A:278:PRO:HD2	2.45	0.51
1:B:237:ALA:HB2	1:C:237:ALA:HB2	1.93	0.51
1:C:461[B]:CYS:SG	1:C:465:ARG:CZ	3.00	0.50
1:A:271:TYR:HD1	1:A:278:PRO:HD2	1.75	0.50
1:B:292:LEU:CD2	1:B:292:LEU:H	2.24	0.50
1:D:435:GLU:HG3	6:D:897:HOH:O	2.12	0.50
1:B:181:LEU:HD21	3:B:503:JZ3:HAF	1.93	0.50
2:A:501[A]:HEM:HMC2	2:A:501[A]:HEM:CBC	2.41	0.49
1:A:219:ARG:HD2	6:A:836:HOH:O	2.13	0.49
2:B:501[A]:HEM:HMB2	2:B:501[A]:HEM:CBB	2.43	0.49
1:A:45:HIS:HD2	6:A:688:HOH:O	1.96	0.48
1:A:181:LEU:HD21	3:A:503:JZ3:CAF	2.38	0.48
1:B:134[B]:ILE:HD13	1:B:134[B]:ILE:H	1.78	0.47
1:C:134[B]:ILE:HD11	1:C:180:TRP:CD1	2.48	0.47
1:B:332:LEU:HD12	2:B:501[A]:HEM:HBB1	1.96	0.47
1:C:140:ALA:HA	2:C:501[A]:HEM:HBB1	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:271:TYR:HD1	1:C:278:PRO:HD2	1.79	0.47
1:A:164:TYR:OH	3:A:503:JZ3:HAC	2.15	0.46
1:C:336:ARG:HG2	2:C:502[B]:HEM:C2C	2.50	0.46
1:B:181:LEU:HD21	3:B:503:JZ3:CAD	2.45	0.46
1:B:420:ASN:ND2	6:B:729:HOH:O	2.43	0.46
1:C:229:MET:HE1	6:C:976:HOH:O	2.15	0.45
1:B:334:GLN:HG3	6:C:704:HOH:O	2.16	0.45
1:B:100:HIS:HE1	6:C:703:HOH:O	1.99	0.45
1:D:57:HIS:HA	1:D:97:THR:O	2.17	0.45
1:A:417:GLU:H	1:D:28:HIS:CD2	2.35	0.45
1:C:219:ARG:CD	6:C:727:HOH:O	2.65	0.45
1:A:21:GLN:HA	1:D:142:LYS:HD3	1.99	0.44
2:A:502[B]:HEM:HBC2	2:A:502[B]:HEM:CMC	2.47	0.44
1:B:28:HIS:CE1	1:C:417:GLU:CG	3.01	0.44
1:C:461[B]:CYS:SG	1:C:465:ARG:NH2	2.91	0.44
6:A:984:HOH:O	1:D:334:GLN:HG3	2.16	0.44
1:A:286:SER:OG	1:A:288:GLU:HG2	2.17	0.44
2:A:502[B]:HEM:CMB	2:A:502[B]:HEM:HBB2	2.48	0.44
1:A:366:ASN:HA	1:C:9[B]:LEU:CD2	2.48	0.43
1:A:452:ASN:ND2	1:A:455:THR:H	2.11	0.43
6:A:667:HOH:O	1:B:410:ARG:HD2	2.17	0.43
1:C:110:ASP:OD1	3:C:503:JZ3:OAG	2.36	0.43
1:D:302:ARG:HD2	6:D:823:HOH:O	2.18	0.43
1:D:332:LEU:CD1	2:D:501[A]:HEM:HBB1	2.48	0.43
2:C:502[B]:HEM:HMB1	2:C:502[B]:HEM:CBB	2.48	0.43
1:D:483:ARG:O	1:D:484:SER:HB3	2.18	0.43
2:B:502[B]:HEM:CMC	2:B:502[B]:HEM:HBC2	2.48	0.43
1:B:287:GLU:HG2	1:B:292:LEU:CD2	2.40	0.43
1:D:392:GLN:NE2	6:D:892:HOH:O	2.44	0.43
1:C:199:VAL:HG11	2:C:502[B]:HEM:HBB1	2.01	0.43
1:D:134[B]:ILE:H	1:D:134[B]:ILE:HD13	1.83	0.43
1:A:57:HIS:HA	1:A:97:THR:O	2.19	0.42
1:A:486:LEU:HD12	1:A:486:LEU:HA	1.84	0.42
1:C:340:TYR:HB2	1:C:341:PRO:HD3	2.01	0.42
1:B:57:HIS:HA	1:B:97:THR:O	2.19	0.42
1:A:57:HIS:CD2	2:A:501[A]:HEM:C4D	3.08	0.42
1:B:140:ALA:HA	2:B:501[A]:HEM:HBB1	2.02	0.42
1:B:287:GLU:CD	1:B:292:LEU:HD21	2.45	0.42
1:B:111:PRO:HD3	3:B:503:JZ3:HAAB	2.02	0.41
2:A:501[A]:HEM:CMB	2:A:501[A]:HEM:CBB	2.98	0.41
1:B:292:LEU:HD23	1:B:292:LEU:H	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:271:TYR:CD1	1:C:278:PRO:HD2	2.54	0.41
1:A:142:LYS:HD3	1:D:21:GLN:HA	2.02	0.41
1:A:237:ALA:HB2	1:D:237:ALA:HB2	2.03	0.41
1:A:340:TYR:HB2	1:A:341:PRO:HD3	2.02	0.41
1:C:57:HIS:CE1	1:C:98:VAL:HG22	2.55	0.41
1:B:360:PRO:HG2	1:B:364:VAL:CG2	2.51	0.41
1:A:219:ARG:HG2	6:A:1015:HOH:O	2.21	0.41
1:D:340:TYR:HB2	1:D:341:PRO:HD3	2.03	0.40
1:B:417:GLU:HG3	1:C:28:HIS:CE1	2.56	0.40
1:C:465:ARG:CZ	6:C:1032:HOH:O	2.69	0.40
1:D:229:MET:HE3	1:D:442:LYS:NZ	2.37	0.40
1:A:94:ARG:HD3	2:A:501[A]:HEM:O1D	2.21	0.40
1:B:21:GLN:HA	1:C:142:LYS:HD3	2.03	0.40
1:C:462:ASN:OD1	1:C:465:ARG:NH1	2.54	0.40
1:D:150:LEU:HD13	3:D:503:JZ3:HAAA	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	485/491 (99%)	475 (98%)	10 (2%)	0	100	100
1	B	484/491 (99%)	472 (98%)	12 (2%)	0	100	100
1	C	486/491 (99%)	474 (98%)	12 (2%)	0	100	100
1	D	485/491 (99%)	469 (97%)	15 (3%)	1 (0%)	43	28
All	All	1940/1964 (99%)	1890 (97%)	49 (2%)	1 (0%)	48	31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	484	SER

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	428/432 (99%)	417 (97%)	11 (3%)	40	23
1	B	427/432 (99%)	414 (97%)	13 (3%)	36	19
1	C	429/432 (99%)	423 (99%)	6 (1%)	59	46
1	D	428/432 (99%)	419 (98%)	9 (2%)	47	30
All	All	1712/1728 (99%)	1673 (98%)	39 (2%)	45	27

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	110	ASP
1	A	120	THR
1	A	241	GLN
1	A	288	GLU
1	A	401	GLU
1	A	409	ASP
1	A	412[A]	VAL
1	A	412[B]	VAL
1	A	447	ASP
1	A	474	LEU
1	A	486	LEU
1	B	85	GLU
1	B	110	ASP
1	B	120	THR
1	B	241	GLN
1	B	253	LYS
1	B	273	GLU
1	B	292	LEU
1	B	401	GLU
1	B	409	ASP
1	B	440	LEU

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Mol	Chain	Res	Type
1	B	447	ASP
1	B	474	LEU
1	B	486	LEU
1	C	110	ASP
1	C	120	THR
1	C	241	GLN
1	C	401	GLU
1	C	409	ASP
1	C	447	ASP
1	D	75	LYS
1	D	110	ASP
1	D	120	THR
1	D	241	GLN
1	D	273	GLU
1	D	401	GLU
1	D	447	ASP
1	D	474	LEU
1	D	486	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	HIS
1	A	76	HIS
1	A	100	HIS
1	A	157	ASN
1	A	236	GLN
1	A	346	HIS
1	A	367	ASN
1	A	452	ASN
1	A	472	GLN
1	B	6	HIS
1	B	100	HIS
1	B	157	ASN
1	B	236	GLN
1	B	365	HIS
1	B	367	ASN
1	B	392	GLN
1	B	398	HIS
1	B	452	ASN
1	B	472	GLN
1	C	71	ASN

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Mol	Chain	Res	Type
1	C	157	ASN
1	C	226	ASN
1	C	236	GLN
1	C	238	ASN
1	C	365	HIS
1	C	367	ASN
1	C	398	HIS
1	C	472	GLN
1	D	28	HIS
1	D	88	GLN
1	D	100	HIS
1	D	157	ASN
1	D	236	GLN
1	D	346	HIS
1	D	365	HIS
1	D	367	ASN
1	D	392	GLN
1	D	398	HIS
1	D	472	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](#)

Of 22 ligands modelled in this entry, 8 are monoatomic - leaving 14 for Mogul analysis.

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$
3	JZ3	C	503	-	9,9,9	1.76	1 (11%)	11,11,11	3.22	6 (54%)
2	HEM	D	502[B]	1	50,50,50	1.56	7 (14%)	67,82,82	1.66	12 (17%)
2	HEM	D	501[A]	1	50,50,50	1.42	6 (12%)	67,82,82	1.89	15 (22%)
2	HEM	A	501[A]	1	50,50,50	1.68	11 (22%)	67,82,82	1.93	18 (26%)
3	JZ3	D	504	-	9,9,9	1.69	1 (11%)	11,11,11	2.11	3 (27%)
3	JZ3	B	504	-	9,9,9	1.51	1 (11%)	11,11,11	0.93	0
3	JZ3	D	503	-	9,9,9	2.13	2 (22%)	11,11,11	3.74	5 (45%)
3	JZ3	A	503	-	9,9,9	1.89	1 (11%)	11,11,11	3.29	4 (36%)
2	HEM	A	502[B]	1	50,50,50	1.54	8 (16%)	67,82,82	2.09	15 (22%)
3	JZ3	B	503	-	9,9,9	2.35	1 (11%)	11,11,11	3.62	5 (45%)
2	HEM	B	501[A]	1,6	50,50,50	1.61	11 (22%)	67,82,82	1.92	18 (26%)
2	HEM	C	502[B]	1	50,50,50	1.62	10 (20%)	67,82,82	1.94	16 (23%)
2	HEM	C	501[A]	1	50,50,50	1.64	11 (22%)	67,82,82	2.09	18 (26%)
2	HEM	B	502[B]	1,6	50,50,50	1.56	9 (18%)	67,82,82	1.78	14 (20%)

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
3	JZ3	C	503	-	-	2/2/2/2	0/1/1/1
2	HEM	D	502[B]	1	-	3/14/54/54	-
2	HEM	D	501[A]	1	-	4/14/54/54	-
2	HEM	A	501[A]	1	-	3/14/54/54	-
3	JZ3	D	504	-	-	0/2/2/2	0/1/1/1
3	JZ3	B	504	-	-	0/2/2/2	0/1/1/1
3	JZ3	D	503	-	-	2/2/2/2	0/1/1/1
3	JZ3	A	503	-	-	2/2/2/2	0/1/1/1
2	HEM	A	502[B]	1	-	2/14/54/54	-
3	JZ3	B	503	-	-	0/2/2/2	0/1/1/1
2	HEM	B	501[A]	1,6	-	2/14/54/54	-
2	HEM	C	502[B]	1	-	2/14/54/54	-
2	HEM	C	501[A]	1	-	2/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	B	502[B]	1,6	-	2/14/54/54	-

All (80) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	503	JZ3	CAH-CAI	6.35	1.51	1.40
3	D	503	JZ3	CAH-CAI	5.73	1.50	1.40
3	A	503	JZ3	CAH-CAI	5.27	1.49	1.40
3	C	503	JZ3	CAH-CAI	4.93	1.49	1.40
2	A	501[A]	HEM	FE-NB	4.83	2.09	1.94
3	D	504	JZ3	CAH-CAI	4.83	1.48	1.40
2	B	502[B]	HEM	FE-NB	4.74	2.09	1.94
2	B	501[A]	HEM	FE-NB	4.72	2.09	1.94
2	B	502[B]	HEM	FE-NC	4.55	2.10	1.95
2	A	502[B]	HEM	FE-NB	4.38	2.08	1.94
2	D	502[B]	HEM	FE-NC	4.30	2.09	1.95
2	A	501[A]	HEM	FE-NC	4.24	2.09	1.95
2	D	501[A]	HEM	C1B-NB	-4.08	1.33	1.40
2	B	501[A]	HEM	FE-NC	4.05	2.08	1.95
2	C	501[A]	HEM	C4D-C3D	3.98	1.51	1.45
2	C	502[B]	HEM	FE-NC	3.93	2.08	1.95
2	C	502[B]	HEM	FE-NB	3.90	2.06	1.94
2	D	501[A]	HEM	FE-NB	3.90	2.06	1.94
2	A	502[B]	HEM	C4B-NB	-3.82	1.31	1.38
2	C	501[A]	HEM	FE-NB	3.80	2.06	1.94
2	C	501[A]	HEM	C3C-C4C	-3.77	1.39	1.46
3	B	504	JZ3	CAH-CAI	3.77	1.46	1.40
2	C	502[B]	HEM	C1B-NB	-3.72	1.33	1.40
2	D	502[B]	HEM	C4D-C3D	3.66	1.51	1.45
2	C	501[A]	HEM	FE-NC	3.50	2.06	1.95
2	C	501[A]	HEM	C1B-NB	-3.49	1.34	1.40
2	D	502[B]	HEM	FE-NB	3.43	2.05	1.94
2	D	501[A]	HEM	FE-NC	3.39	2.06	1.95
2	C	502[B]	HEM	C4D-C3D	3.33	1.50	1.45
2	A	501[A]	HEM	C1C-NC	-3.27	1.33	1.39
2	A	502[B]	HEM	FE-NC	3.26	2.05	1.95
2	B	502[B]	HEM	C1B-NB	-3.15	1.34	1.40
2	B	502[B]	HEM	C4B-NB	-3.11	1.32	1.38
2	D	502[B]	HEM	FE-NA	3.07	2.05	1.95
2	C	502[B]	HEM	FE-NA	3.06	2.05	1.95
2	D	502[B]	HEM	C1B-NB	-3.04	1.35	1.40
2	A	501[A]	HEM	C3C-C4C	-3.04	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	502[B]	HEM	C1B-NB	-3.01	1.35	1.40
2	A	502[B]	HEM	C1C-C2C	-2.99	1.39	1.45
2	B	501[A]	HEM	C4D-C3D	2.95	1.50	1.45
2	A	501[A]	HEM	FE-NA	2.93	2.04	1.95
2	D	501[A]	HEM	FE-NA	2.91	2.04	1.95
2	C	502[B]	HEM	CHB-C1B	2.83	1.44	1.38
2	C	502[B]	HEM	C3C-C4C	-2.82	1.41	1.46
2	C	501[A]	HEM	C4C-NC	-2.76	1.34	1.39
2	A	502[B]	HEM	C4D-C3D	2.72	1.49	1.45
2	C	502[B]	HEM	C1C-C2C	-2.71	1.40	1.45
2	A	501[A]	HEM	C1C-C2C	-2.71	1.40	1.45
2	C	501[A]	HEM	C1C-C2C	-2.66	1.40	1.45
2	C	502[B]	HEM	C4D-ND	-2.64	1.35	1.40
2	B	501[A]	HEM	C3B-C4B	2.61	1.50	1.44
2	B	501[A]	HEM	C1B-NB	-2.59	1.35	1.40
2	C	501[A]	HEM	FE-NA	2.55	2.03	1.95
2	C	502[B]	HEM	O1D-CGD	2.53	1.30	1.22
2	B	502[B]	HEM	C4D-C3D	2.46	1.49	1.45
2	A	502[B]	HEM	C4D-ND	-2.39	1.36	1.40
2	A	501[A]	HEM	C4B-NB	-2.37	1.34	1.38
3	D	503	JZ3	OAG-CAI	2.36	1.41	1.37
2	D	501[A]	HEM	C1C-C2C	-2.36	1.40	1.45
2	A	501[A]	HEM	C4D-ND	-2.34	1.36	1.40
2	D	502[B]	HEM	CHB-C1B	2.32	1.43	1.38
2	B	501[A]	HEM	O1D-CGD	2.31	1.29	1.22
2	B	501[A]	HEM	C3C-C4C	-2.29	1.42	1.46
2	B	502[B]	HEM	O2A-CGA	-2.28	1.23	1.30
2	B	502[B]	HEM	C2A-C3A	-2.27	1.33	1.38
2	C	501[A]	HEM	CHB-C1B	2.26	1.43	1.38
2	A	501[A]	HEM	C3B-C4B	2.22	1.49	1.44
2	A	501[A]	HEM	C4D-C3D	2.21	1.48	1.45
2	C	501[A]	HEM	C1D-ND	-2.20	1.34	1.38
2	D	501[A]	HEM	C4D-C3D	2.18	1.48	1.45
2	B	501[A]	HEM	C1D-C2D	2.17	1.48	1.44
2	D	502[B]	HEM	C1C-C2C	-2.15	1.41	1.45
2	C	501[A]	HEM	O1A-CGA	2.13	1.29	1.22
2	B	501[A]	HEM	C4D-ND	-2.10	1.36	1.40
2	B	501[A]	HEM	C1C-NC	-2.09	1.35	1.39
2	A	501[A]	HEM	C1B-NB	-2.09	1.36	1.40
2	B	502[B]	HEM	C4D-ND	-2.07	1.36	1.40
2	B	502[B]	HEM	O1D-CGD	2.07	1.28	1.22
2	B	501[A]	HEM	FE-NA	2.04	2.01	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	502[B]	HEM	O2D-CGD	-2.03	1.24	1.30

All (149) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	503	JZ3	CAA-OAG-CAI	9.61	131.60	117.51
3	B	503	JZ3	CAA-OAG-CAI	8.73	130.32	117.51
3	A	503	JZ3	CAA-OAG-CAI	8.51	129.99	117.51
2	C	501[A]	HEM	CHC-C4B-NB	8.10	133.14	124.42
3	C	503	JZ3	CAA-OAG-CAI	7.89	129.08	117.51
2	A	502[B]	HEM	CHC-C4B-NB	6.81	131.75	124.42
2	C	501[A]	HEM	C3B-C4B-NB	-6.20	105.01	109.47
2	A	502[B]	HEM	C1B-NB-C4B	6.19	112.53	105.21
2	A	502[B]	HEM	C3B-C4B-NB	-6.14	105.06	109.47
3	B	503	JZ3	OAG-CAI-CAH	6.10	123.70	114.55
2	B	501[A]	HEM	CHC-C4B-NB	5.94	130.82	124.42
2	D	501[A]	HEM	CHC-C4B-NB	5.90	130.78	124.42
2	B	502[B]	HEM	C1B-NB-C4B	5.78	112.05	105.21
2	B	502[B]	HEM	CHC-C4B-NB	5.52	130.37	124.42
3	D	503	JZ3	OAG-CAI-CAH	5.45	122.73	114.55
2	C	502[B]	HEM	CHC-C4B-NB	5.42	130.26	124.42
3	C	503	JZ3	OAG-CAI-CAH	5.08	122.16	114.55
3	A	503	JZ3	OAG-CAI-CAH	5.03	122.10	114.55
2	C	502[B]	HEM	CHD-C1D-ND	5.03	129.83	124.42
2	C	501[A]	HEM	C1B-NB-C4B	5.01	111.14	105.21
2	C	502[B]	HEM	C1B-NB-C4B	4.95	111.07	105.21
2	A	501[A]	HEM	CHC-C4B-NB	4.92	129.72	124.42
2	A	502[B]	HEM	CHD-C4C-NC	4.77	129.65	124.45
2	D	501[A]	HEM	CHD-C1D-ND	4.73	129.51	124.42
2	D	501[A]	HEM	C1B-NB-C4B	4.71	110.79	105.21
2	B	501[A]	HEM	C3B-C4B-NB	-4.67	106.11	109.47
2	B	501[A]	HEM	C1B-NB-C4B	4.67	110.74	105.21
2	A	501[A]	HEM	C1B-NB-C4B	4.58	110.63	105.21
2	C	502[B]	HEM	CHD-C1D-C2D	-4.47	117.96	125.03
3	D	504	JZ3	CAA-OAG-CAI	4.45	124.05	117.51
2	D	502[B]	HEM	CHD-C1D-ND	4.34	129.09	124.42
3	D	504	JZ3	OAG-CAI-CAH	4.30	121.00	114.55
2	D	502[B]	HEM	C1B-NB-C4B	4.15	110.12	105.21
2	D	501[A]	HEM	C3B-C4B-NB	-4.02	106.58	109.47
2	A	501[A]	HEM	CHB-C1B-NB	4.01	129.33	124.37
2	A	501[A]	HEM	CHD-C4C-NC	3.99	128.80	124.45
2	A	501[A]	HEM	CHA-C4D-ND	3.99	129.30	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	502[B]	HEM	CHB-C1B-NB	3.99	129.30	124.37
2	B	501[A]	HEM	CAD-C3D-C4D	3.98	131.64	124.70
2	A	502[B]	HEM	CHB-C1B-NB	3.97	129.27	124.37
2	B	501[A]	HEM	CHD-C4C-NC	3.91	128.71	124.45
2	B	502[B]	HEM	CHD-C1D-ND	3.82	128.53	124.42
2	D	501[A]	HEM	CHA-C4D-ND	3.80	129.06	124.37
2	C	502[B]	HEM	CMD-C2D-C1D	-3.80	119.10	125.03
2	D	502[B]	HEM	CHD-C1D-C2D	-3.74	119.13	125.03
2	C	501[A]	HEM	C4C-C3C-C2C	3.71	110.03	106.81
2	D	501[A]	HEM	CHD-C1D-C2D	-3.68	119.21	125.03
2	A	501[A]	HEM	CHD-C1D-ND	3.48	128.16	124.42
2	C	501[A]	HEM	CHD-C4C-NC	3.46	128.22	124.45
2	C	501[A]	HEM	CHD-C1D-C2D	-3.45	119.58	125.03
2	A	501[A]	HEM	C4C-NC-C1C	3.40	111.37	105.82
2	B	502[B]	HEM	CHD-C1D-C2D	-3.34	119.75	125.03
2	C	502[B]	HEM	C2A-C1A-NA	-3.32	106.47	110.15
3	D	503	JZ3	CAF-CAI-CAH	-3.30	115.97	119.87
2	A	502[B]	HEM	C2D-C1D-ND	3.30	113.71	109.90
2	D	502[B]	HEM	CHA-C1A-NA	3.28	129.80	123.86
2	B	501[A]	HEM	CHD-C1D-ND	3.26	127.93	124.42
2	B	501[A]	HEM	CMD-C2D-C1D	3.22	130.06	125.03
2	B	502[B]	HEM	C3B-C4B-NB	-3.12	107.23	109.47
2	B	502[B]	HEM	O2D-CGD-CBD	3.09	123.77	114.00
2	D	502[B]	HEM	CHC-C4B-NB	3.08	127.74	124.42
2	C	501[A]	HEM	CMB-C2B-C1B	3.08	129.85	125.03
2	C	501[A]	HEM	CHA-C4D-ND	3.07	128.16	124.37
2	A	502[B]	HEM	CAA-CBA-CGA	-3.05	105.57	113.67
2	D	501[A]	HEM	O2D-CGD-CBD	3.02	123.53	114.00
2	A	501[A]	HEM	CHD-C1D-C2D	-3.01	120.27	125.03
2	A	501[A]	HEM	C3B-C4B-NB	-2.96	107.34	109.47
2	D	501[A]	HEM	CHA-C4D-C3D	-2.93	119.82	125.23
2	C	502[B]	HEM	C3B-C4B-NB	-2.89	107.39	109.47
2	B	502[B]	HEM	CHB-C1B-NB	2.89	127.94	124.37
3	B	503	JZ3	CAF-CAI-CAH	-2.87	116.47	119.87
2	A	502[B]	HEM	CHD-C1D-C2D	-2.83	120.56	125.03
2	D	502[B]	HEM	CMA-C3A-C4A	2.80	129.69	125.42
2	C	501[A]	HEM	C2D-C1D-ND	2.77	113.11	109.90
2	C	501[A]	HEM	C3C-C2C-C1C	-2.75	104.44	107.05
2	C	502[B]	HEM	CMD-C2D-C3D	2.74	133.55	126.15
2	B	501[A]	HEM	CAD-C3D-C2D	-2.72	122.77	127.87
2	A	501[A]	HEM	CHC-C1C-NC	2.68	127.37	124.45
2	D	501[A]	HEM	O2A-CGA-CBA	2.68	122.47	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	503	JZ3	OAG-CAI-CAF	-2.66	119.81	124.30
2	D	501[A]	HEM	C1A-CHA-C4D	-2.66	119.99	126.25
2	C	502[B]	HEM	CHC-C1C-NC	2.66	127.34	124.45
2	A	502[B]	HEM	C4C-NC-C1C	2.65	110.14	105.82
2	B	502[B]	HEM	CHA-C4D-ND	2.62	127.61	124.37
2	D	501[A]	HEM	O1D-CGD-CBD	-2.61	114.81	123.09
2	B	501[A]	HEM	CHA-C4D-ND	2.59	127.57	124.37
2	D	501[A]	HEM	C3B-C2B-C1B	2.59	108.36	106.41
3	D	503	JZ3	CAD-CAF-CAI	2.58	124.29	119.60
2	B	502[B]	HEM	O2D-CGD-O1D	-2.58	116.71	123.33
2	C	501[A]	HEM	CHD-C1D-ND	2.57	127.19	124.42
2	D	502[B]	HEM	C2A-C1A-NA	-2.57	107.30	110.15
2	C	502[B]	HEM	C3C-C2C-C1C	2.56	109.47	107.05
2	C	502[B]	HEM	CMB-C2B-C1B	2.54	129.00	125.03
2	A	501[A]	HEM	CMA-C3A-C4A	-2.53	121.57	125.42
2	A	501[A]	HEM	CAD-C3D-C4D	2.53	129.10	124.70
3	C	503	JZ3	CAE-CAH-CAI	-2.52	116.69	119.55
2	B	501[A]	HEM	O2A-CGA-CBA	2.52	121.95	114.00
2	A	501[A]	HEM	CMA-C3A-C2A	2.52	130.96	125.62
3	B	503	JZ3	OAB-CAH-CAI	2.51	126.02	120.13
2	B	501[A]	HEM	CHD-C1D-C2D	-2.45	121.16	125.03
3	A	503	JZ3	OAG-CAI-CAF	-2.45	120.17	124.30
2	C	502[B]	HEM	C3B-C2B-C1B	2.43	108.23	106.41
2	A	502[B]	HEM	CAA-C2A-C1A	2.39	129.61	124.94
2	B	501[A]	HEM	CHB-C1B-NB	2.37	127.30	124.37
2	D	501[A]	HEM	CHB-C1B-NB	2.37	127.30	124.37
2	D	502[B]	HEM	CAA-CBA-CGA	-2.36	107.41	113.67
2	B	501[A]	HEM	C4C-NC-C1C	2.36	109.67	105.82
2	C	501[A]	HEM	O2D-CGD-CBD	2.35	121.43	114.00
2	B	502[B]	HEM	CHA-C4D-C3D	-2.35	120.89	125.23
2	A	502[B]	HEM	CAA-C2A-C3A	-2.34	121.81	127.07
3	C	503	JZ3	OAG-CAI-CAF	-2.34	120.35	124.30
2	C	502[B]	HEM	CMB-C2B-C3B	-2.34	122.77	128.43
2	B	501[A]	HEM	C1A-CHA-C4D	-2.34	120.75	126.25
2	A	501[A]	HEM	C1A-CHA-C4D	-2.31	120.81	126.25
2	C	501[A]	HEM	C1C-CHC-C4B	-2.30	121.12	126.02
3	D	503	JZ3	CAC-CAE-CAH	2.29	122.87	120.05
2	C	502[B]	HEM	C3D-C4D-ND	2.29	112.68	110.17
2	C	501[A]	HEM	CAC-C3C-C4C	-2.28	119.37	124.82
2	B	501[A]	HEM	CHA-C1A-NA	2.27	127.97	123.86
2	C	501[A]	HEM	CMB-C2B-C3B	-2.26	122.95	128.43
2	D	501[A]	HEM	C4C-CHD-C1D	-2.25	121.24	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501[A]	HEM	O2D-CGD-CBD	2.24	121.07	114.00
2	D	502[B]	HEM	C1A-CHA-C4D	-2.23	121.01	126.25
2	B	501[A]	HEM	CBC-CAC-C3C	-2.22	116.42	127.53
2	C	502[B]	HEM	CBD-CAD-C3D	-2.21	106.42	112.53
2	A	501[A]	HEM	CAD-C3D-C2D	-2.21	123.73	127.87
2	A	501[A]	HEM	CHA-C4D-C3D	-2.20	121.16	125.23
2	A	502[B]	HEM	C2A-C1A-NA	-2.20	107.71	110.15
2	A	502[B]	HEM	CHA-C4D-C3D	-2.20	121.17	125.23
2	B	501[A]	HEM	CHA-C4D-C3D	-2.19	121.18	125.23
2	B	502[B]	HEM	O2A-CGA-O1A	-2.19	117.70	123.33
2	A	501[A]	HEM	CBC-CAC-C3C	-2.17	116.70	127.53
2	D	502[B]	HEM	C3B-C4B-NB	-2.16	107.92	109.47
3	A	503	JZ3	CAE-CAH-CAI	-2.15	117.11	119.55
2	B	502[B]	HEM	C1A-CHA-C4D	-2.13	121.23	126.25
2	B	502[B]	HEM	CBC-CAC-C3C	-2.13	116.90	127.53
2	A	502[B]	HEM	C4C-CHD-C1D	-2.13	121.50	126.02
3	C	503	JZ3	CAD-CAF-CAI	2.12	123.44	119.60
2	D	501[A]	HEM	CHD-C4C-NC	2.10	126.74	124.45
2	B	502[B]	HEM	C4A-C3A-C2A	2.09	109.22	106.82
2	C	502[B]	HEM	CHA-C1A-NA	2.09	127.65	123.86
2	C	501[A]	HEM	O1D-CGD-CBD	-2.07	116.52	123.09
2	A	502[B]	HEM	O1A-CGA-CBA	-2.06	116.57	123.09
2	C	501[A]	HEM	CBC-CAC-C3C	-2.05	117.28	127.53
3	C	503	JZ3	CAF-CAI-CAH	-2.04	117.45	119.87
2	C	501[A]	HEM	C4C-CHD-C1D	-2.04	121.68	126.02
3	D	504	JZ3	OAG-CAI-CAF	-2.03	120.87	124.30
2	D	502[B]	HEM	CMA-C3A-C2A	-2.02	121.34	125.62
2	B	501[A]	HEM	O1D-CGD-CBD	-2.01	116.73	123.09

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	503	JZ3	CAH-CAI-OAG-CAA
3	A	503	JZ3	CAH-CAI-OAG-CAA
3	C	503	JZ3	CAH-CAI-OAG-CAA
3	C	503	JZ3	CAF-CAI-OAG-CAA
3	D	503	JZ3	CAF-CAI-OAG-CAA
3	A	503	JZ3	CAF-CAI-OAG-CAA
2	C	502[B]	HEM	CAA-CBA-CGA-O2A
2	D	502[B]	HEM	CAA-CBA-CGA-O2A
2	B	501[A]	HEM	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
2	B	502[B]	HEM	CAA-CBA-CGA-O1A
2	A	502[B]	HEM	CAA-CBA-CGA-O1A
2	B	501[A]	HEM	CAD-CBD-CGD-O2D
2	B	502[B]	HEM	CAA-CBA-CGA-O2A
2	A	501[A]	HEM	CAD-CBD-CGD-O2D
2	A	501[A]	HEM	CAD-CBD-CGD-O1D
2	D	502[B]	HEM	CAA-CBA-CGA-O1A
2	A	502[B]	HEM	CAA-CBA-CGA-O2A
2	C	502[B]	HEM	CAA-CBA-CGA-O1A
2	D	501[A]	HEM	CAD-CBD-CGD-O2D
2	D	501[A]	HEM	CAA-CBA-CGA-O2A
2	C	501[A]	HEM	CAD-CBD-CGD-O2D
2	D	501[A]	HEM	CAA-CBA-CGA-O1A
2	D	501[A]	HEM	CAD-CBD-CGD-O1D
2	C	501[A]	HEM	CAD-CBD-CGD-O1D
2	D	502[B]	HEM	CAD-CBD-CGD-O2D
2	A	501[A]	HEM	CAA-CBA-CGA-O2A

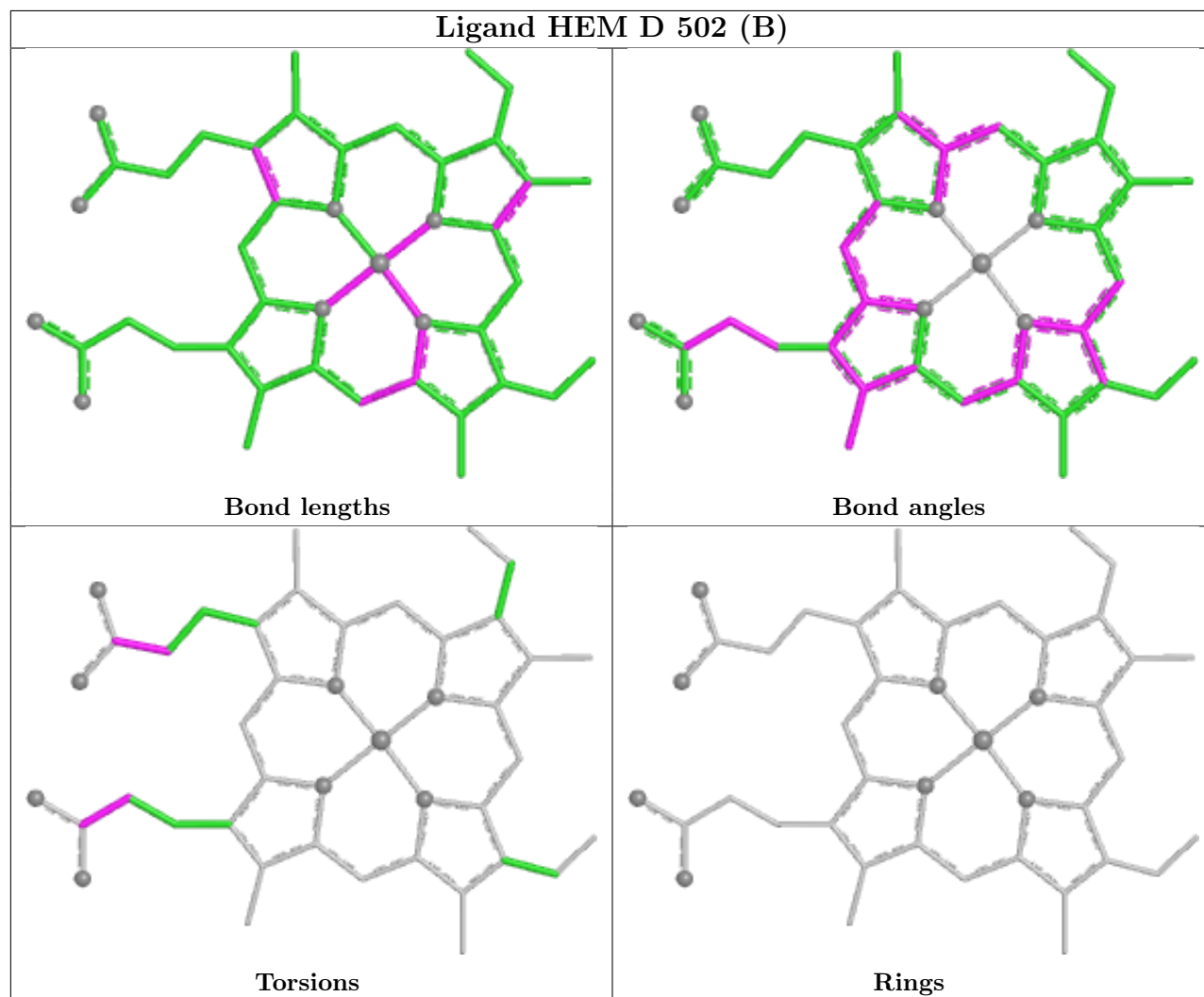
There are no ring outliers.

12 monomers are involved in 49 short contacts:

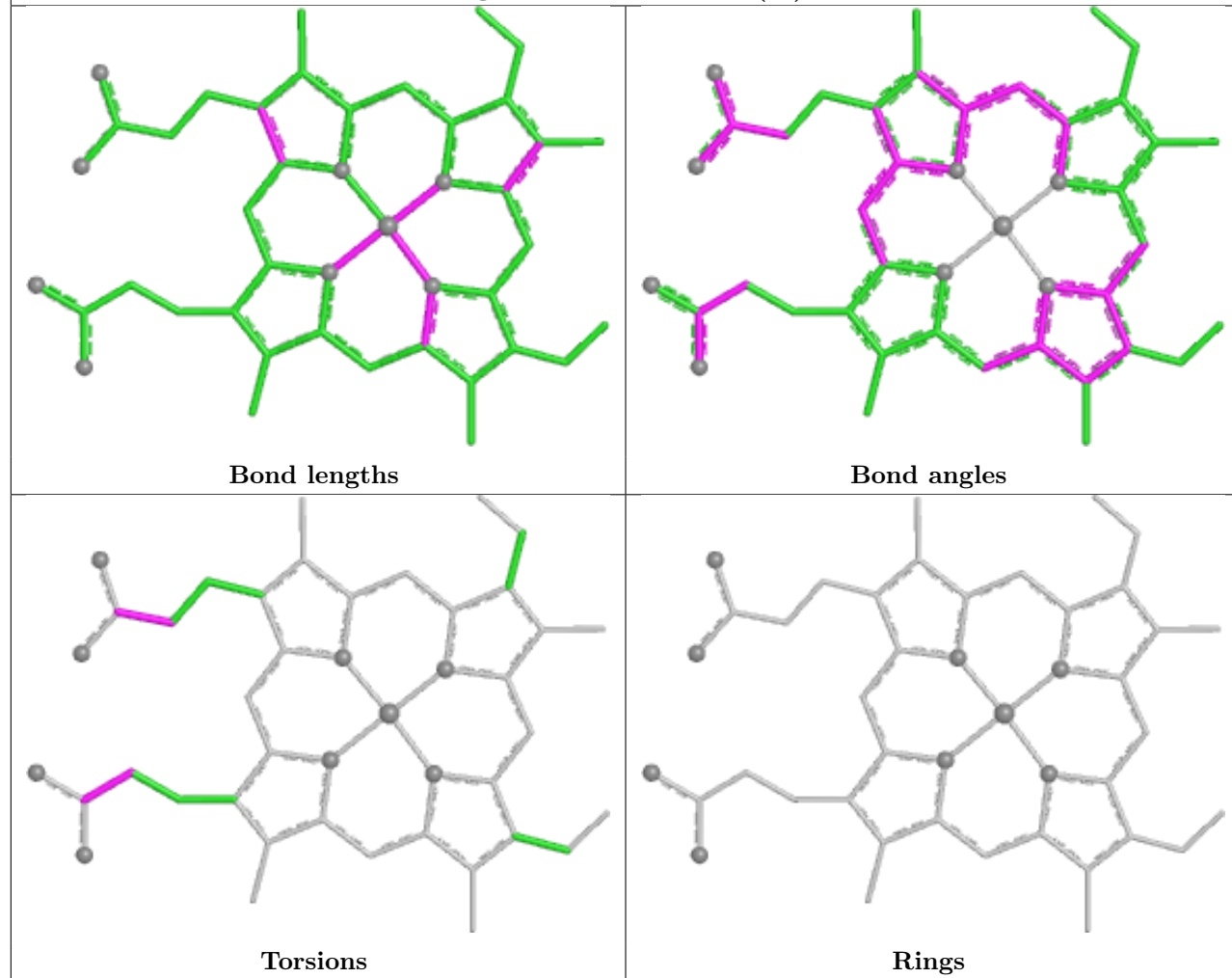
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	503	JZ3	3	0
2	D	502[B]	HEM	1	0
2	D	501[A]	HEM	2	0
2	A	501[A]	HEM	7	0
3	D	503	JZ3	4	0
3	A	503	JZ3	4	0
2	A	502[B]	HEM	2	0
3	B	503	JZ3	5	0
2	B	501[A]	HEM	8	0
2	C	502[B]	HEM	6	0
2	C	501[A]	HEM	6	0
2	B	502[B]	HEM	1	0

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

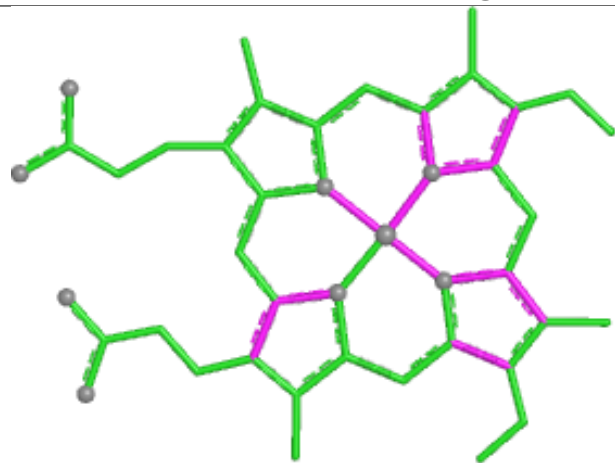
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



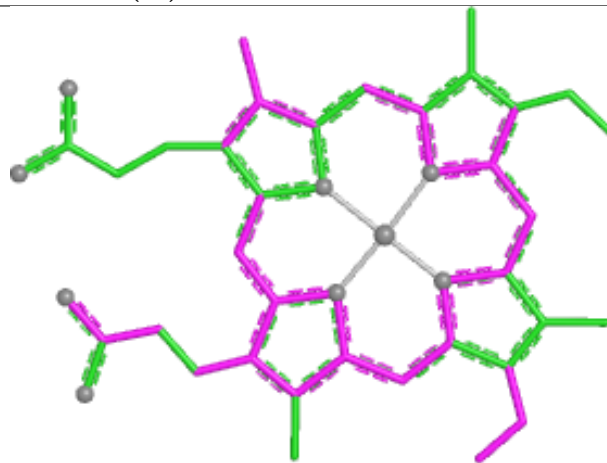
Ligand HEM D 501 (A)



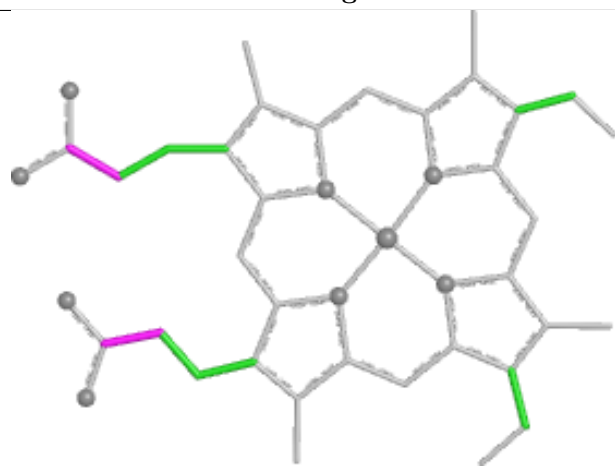
Ligand HEM A 501 (A)



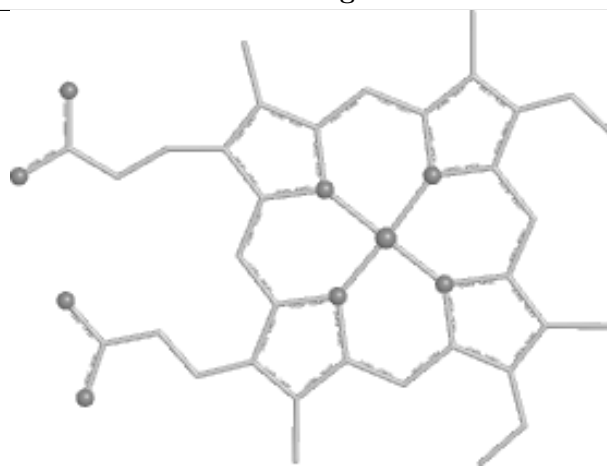
Bond lengths



Bond angles

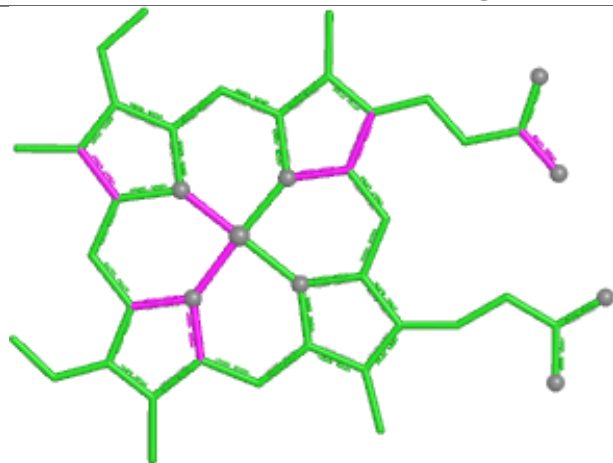


Torsions

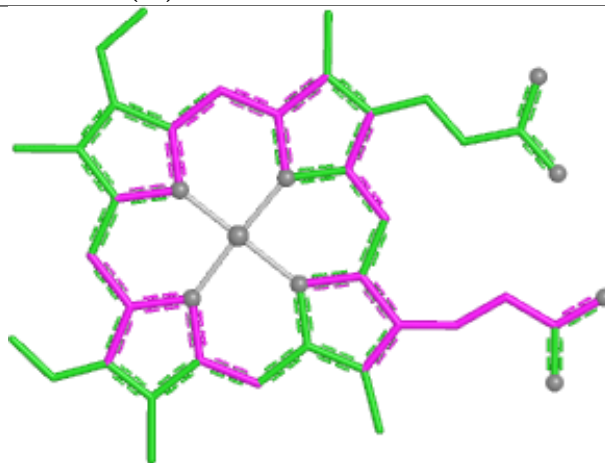


Rings

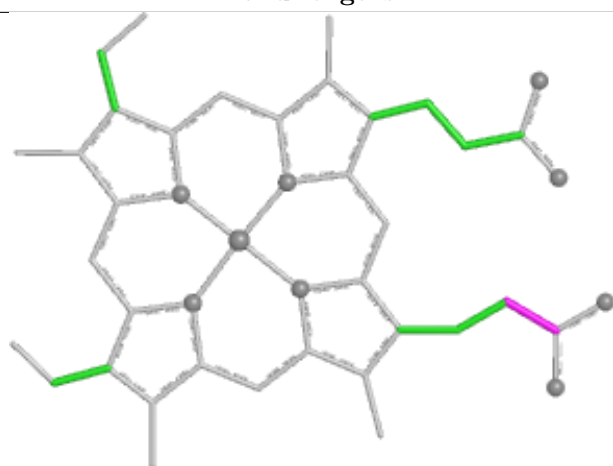
Ligand HEM A 502 (B)



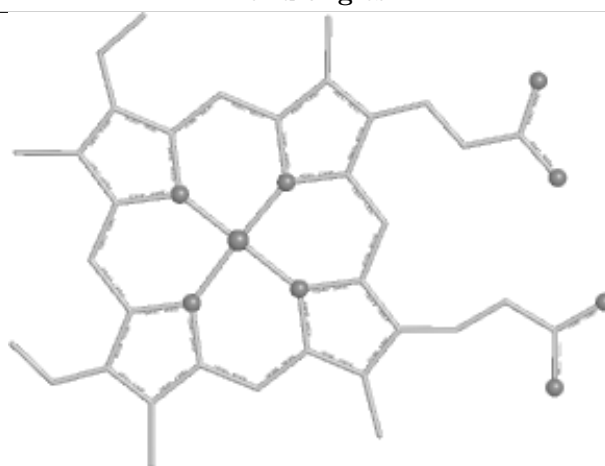
Bond lengths



Bond angles

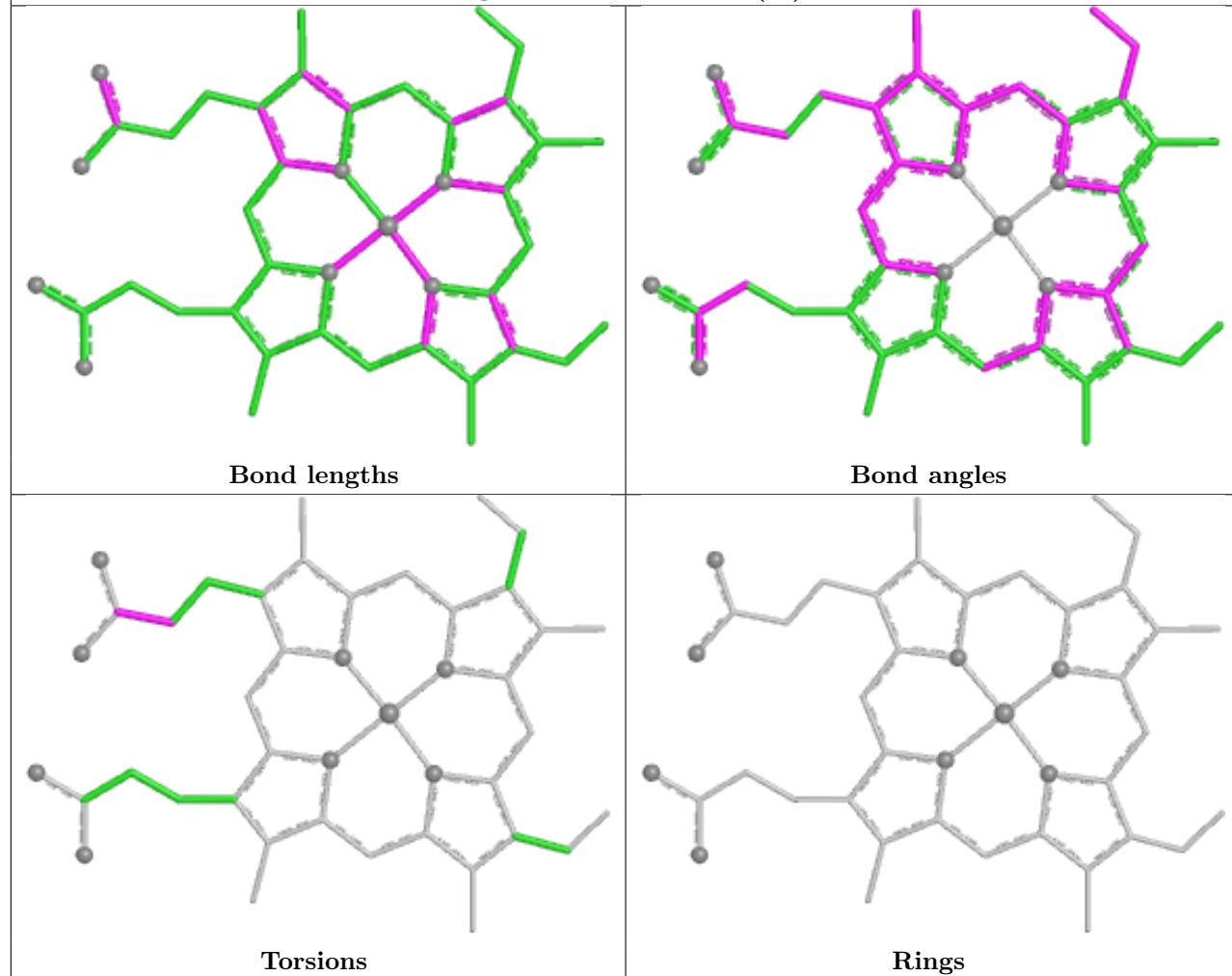


Torsions

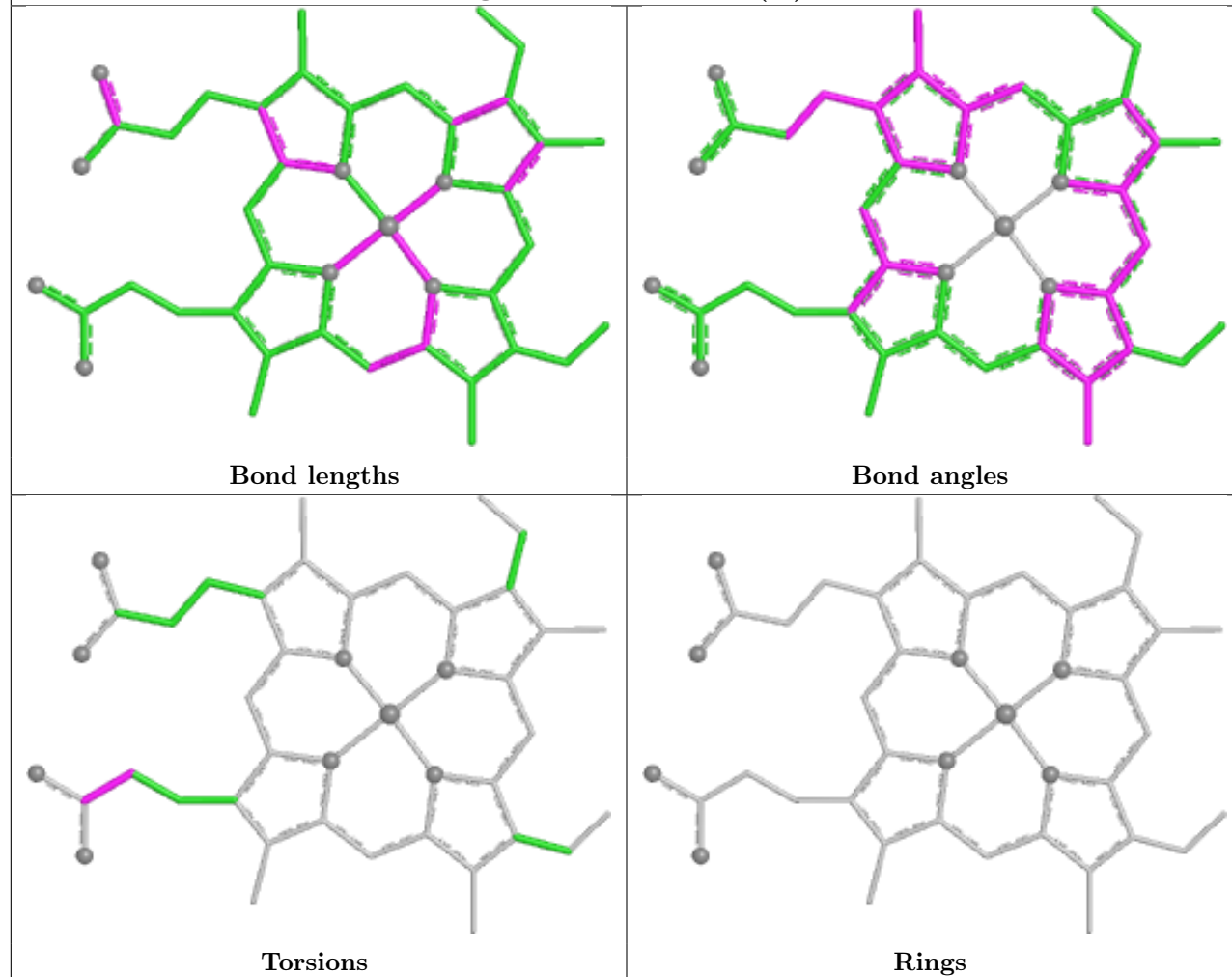


Rings

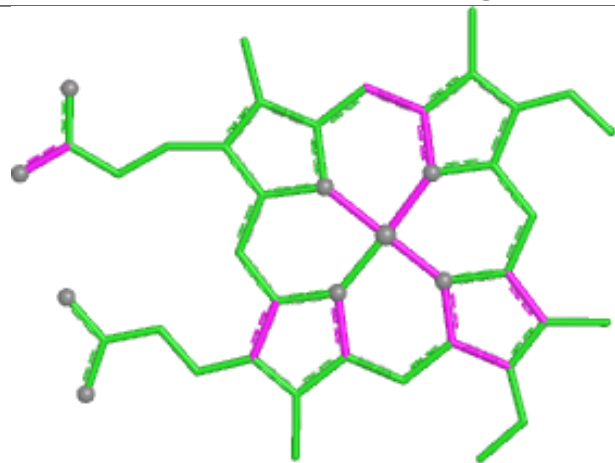
Ligand HEM B 501 (A)



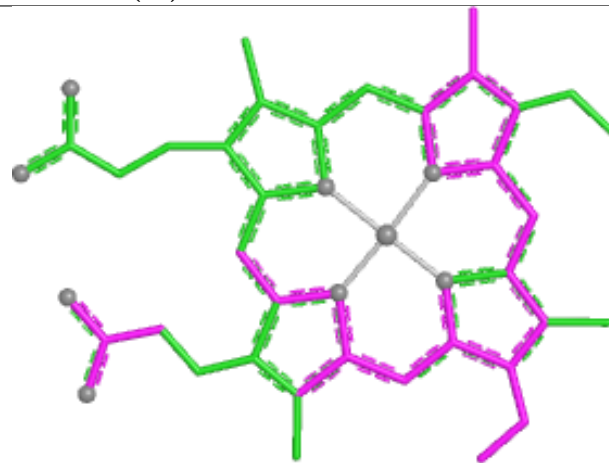
Ligand HEM C 502 (B)



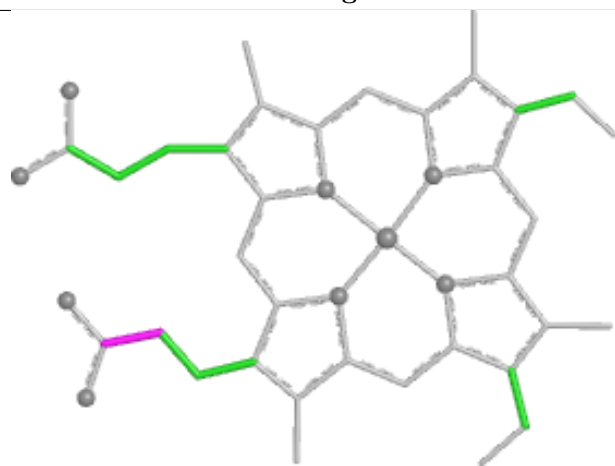
Ligand HEM C 501 (A)



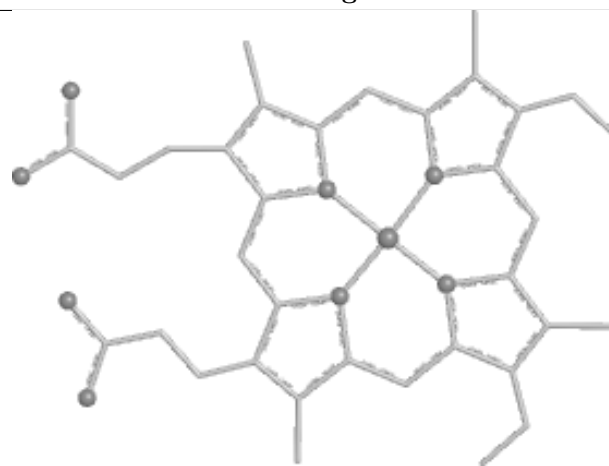
Bond lengths



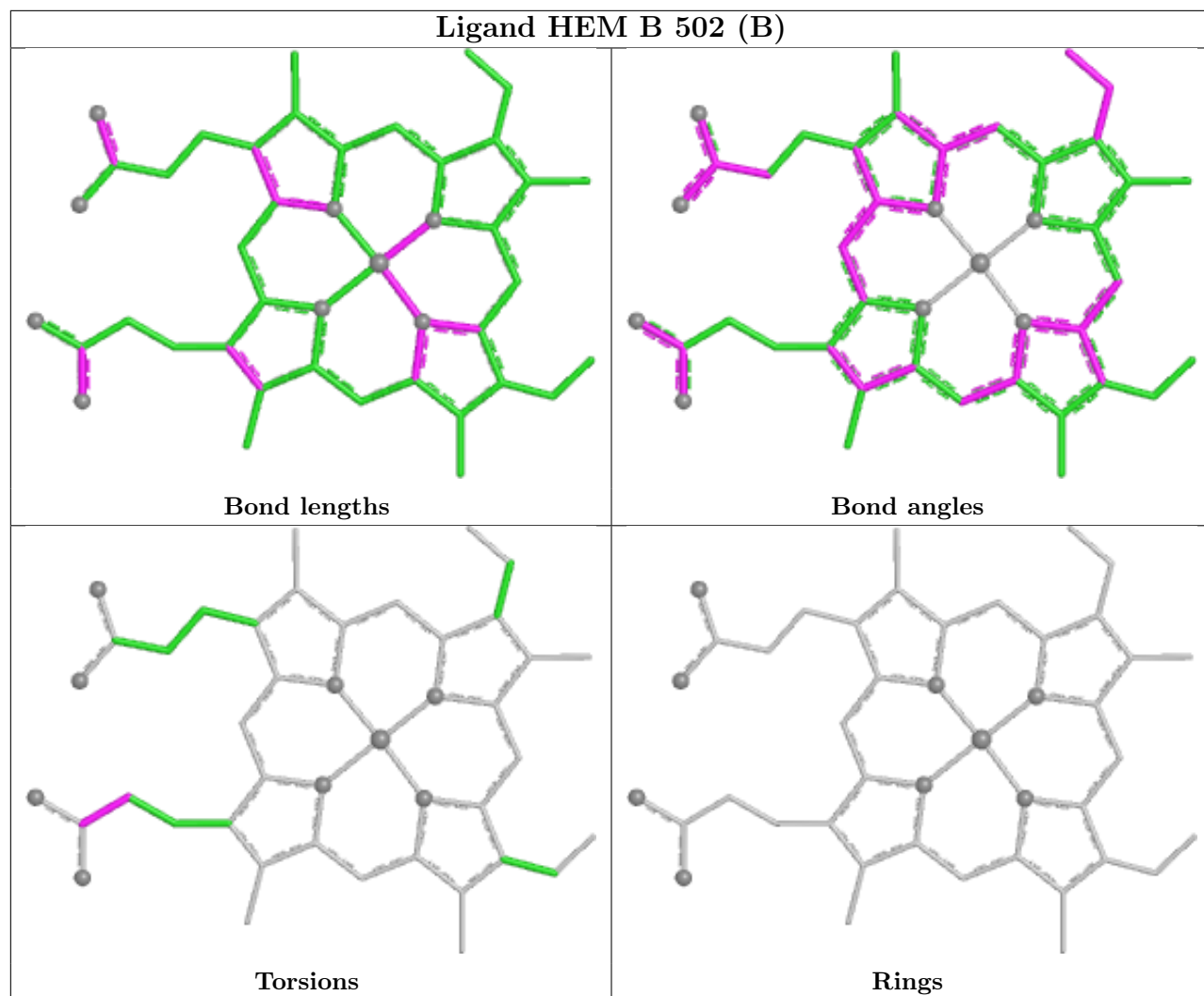
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	481/491 (97%)	-0.01	10 (2%) 63 68	7, 21, 36, 63	6 (1%)
1	B	481/491 (97%)	-0.16	2 (0%) 88 90	8, 19, 33, 55	5 (1%)
1	C	481/491 (97%)	-0.16	5 (1%) 79 82	8, 18, 32, 71	7 (1%)
1	D	481/491 (97%)	-0.08	4 (0%) 82 85	8, 21, 36, 60	6 (1%)
All	All	1924/1964 (97%)	-0.10	21 (1%) 78 81	7, 19, 35, 71	24 (1%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	486	LEU	4.4
1	B	486	LEU	3.9
1	D	486	LEU	2.9
1	A	485	TYR	2.8
1	A	471	GLY	2.6
1	A	486	LEU	2.6
1	B	398	HIS	2.6
1	A	475	ALA	2.4
1	C	372[A]	PHE	2.4
1	A	479	GLY	2.4
1	A	480	VAL	2.4
1	D	398	HIS	2.3
1	C	238	ASN	2.2
1	A	398	HIS	2.2
1	A	407	HIS	2.2
1	C	409	ASP	2.2
1	C	6	HIS	2.2
1	A	483	ARG	2.2
1	D	6	HIS	2.1
1	A	464	TYR	2.1
1	D	372[A]	PHE	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](#)

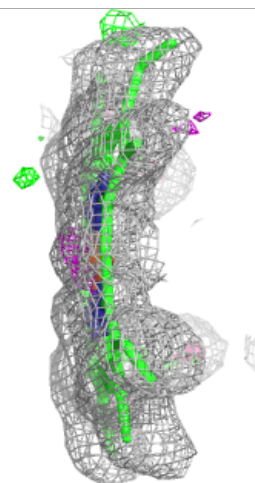
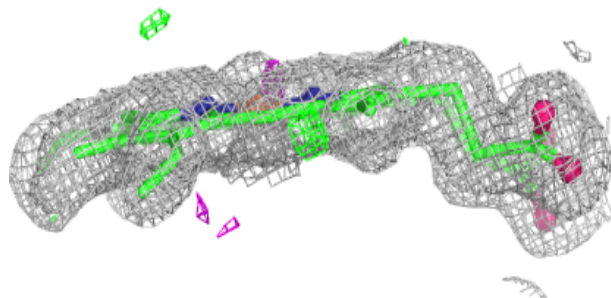
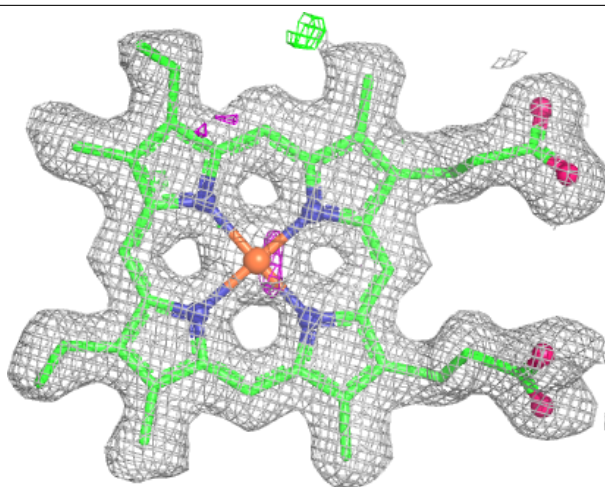
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	JZ3	A	503	9/9	0.74	0.20	54,57,64,66	0
3	JZ3	B	503	9/9	0.77	0.22	45,53,59,60	0
3	JZ3	D	503	9/9	0.77	0.19	49,56,62,64	0
3	JZ3	C	503	9/9	0.80	0.18	42,45,52,52	0
3	JZ3	D	504	9/9	0.84	0.12	40,43,50,51	0
3	JZ3	B	504	9/9	0.91	0.11	34,38,40,45	0
2	HEM	D	501[A]	43/43	0.95	0.07	14,16,17,24	43
2	HEM	B	501[A]	43/43	0.96	0.07	11,15,16,23	43
2	HEM	C	501[A]	43/43	0.97	0.06	10,13,15,19	43
2	HEM	C	502[B]	43/43	0.97	0.06	10,11,13,13	43
2	HEM	A	501[A]	43/43	0.97	0.06	12,15,16,20	43
2	HEM	B	502[B]	43/43	0.98	0.05	8,10,11,11	43
2	HEM	A	502[B]	43/43	0.98	0.06	11,13,14,15	43
2	HEM	D	502[B]	43/43	0.98	0.06	10,12,13,14	43
4	CL	B	505	1/1	0.98	0.04	18,18,18,18	0
5	NA	B	506	1/1	0.98	0.05	19,19,19,19	0
4	CL	C	504	1/1	0.99	0.04	23,23,23,23	0
4	CL	D	505	1/1	0.99	0.05	18,18,18,18	0
4	CL	A	504	1/1	0.99	0.08	25,25,25,25	0
4	CL	A	505	1/1	1.00	0.01	18,18,18,18	0
5	NA	A	506	1/1	1.00	0.04	6,6,6,6	0
4	CL	C	505	1/1	1.00	0.02	20,20,20,20	0

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

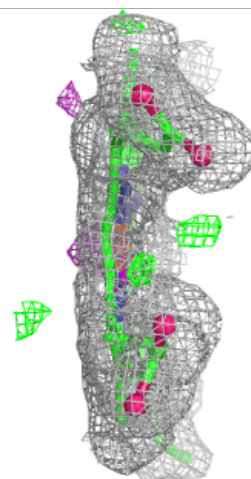
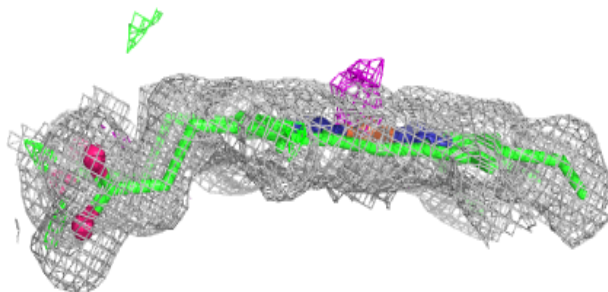
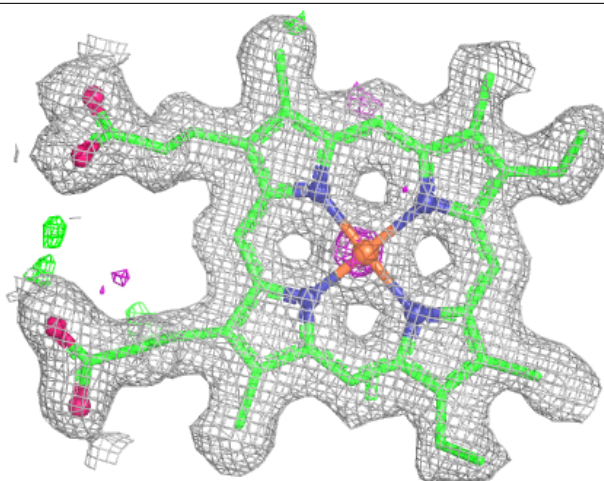
Electron density around HEM D 501 (A):

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



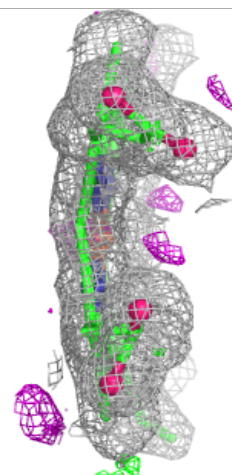
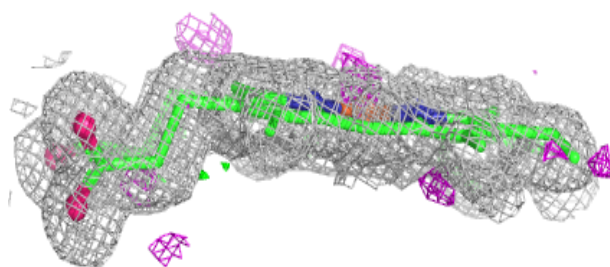
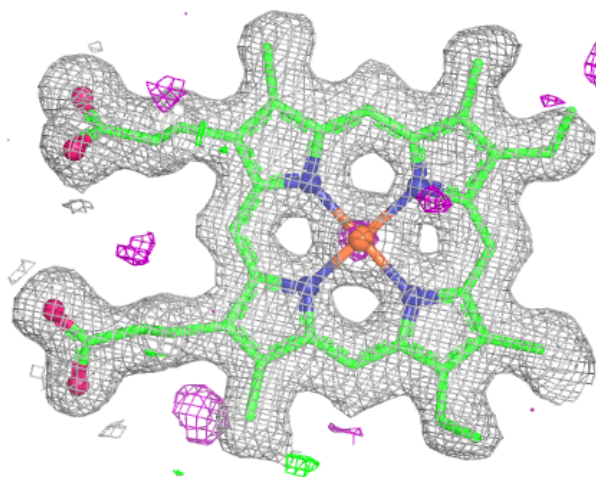
Electron density around HEM B 501 (A):

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



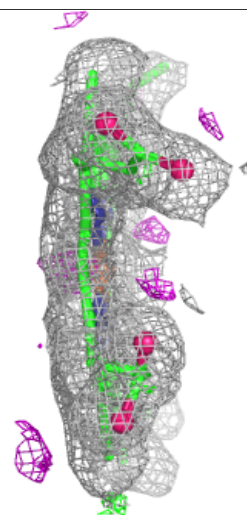
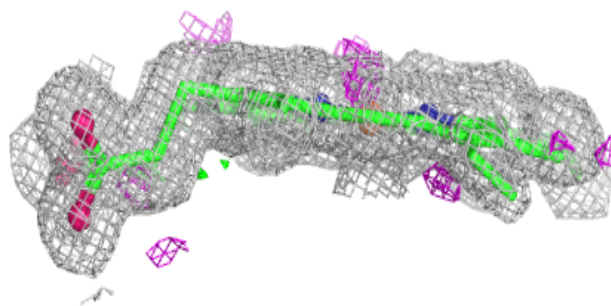
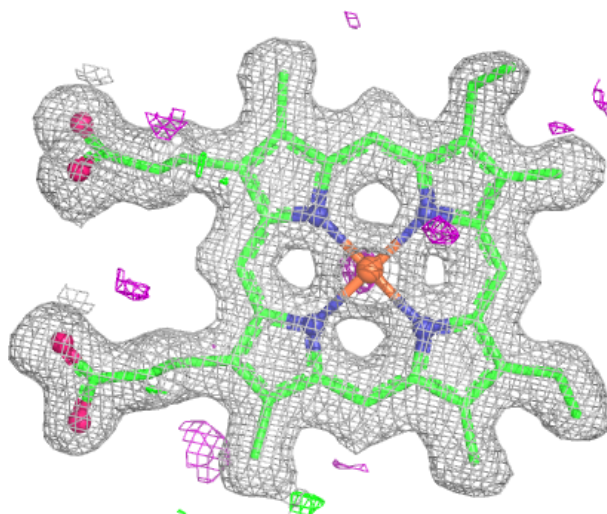
Electron density around HEM C 501 (A):

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



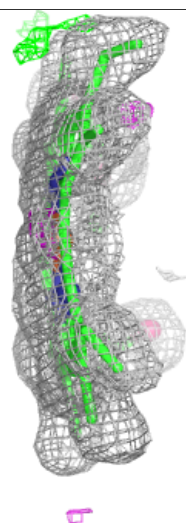
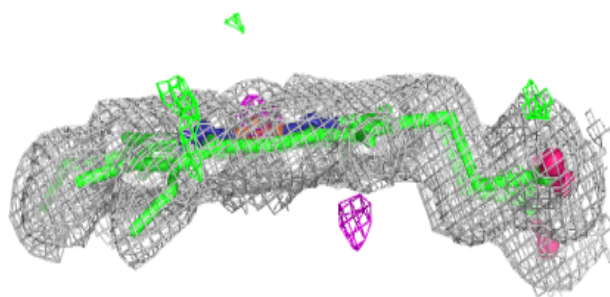
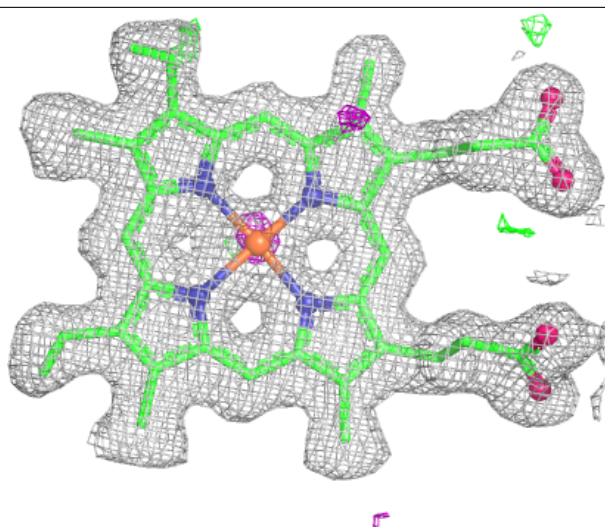
Electron density around HEM C 502 (B):

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



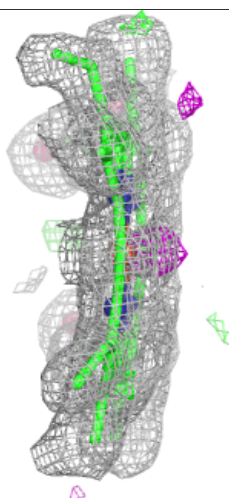
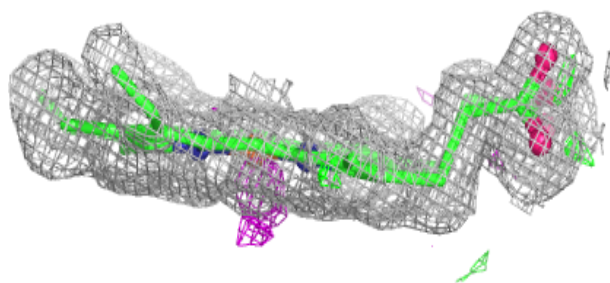
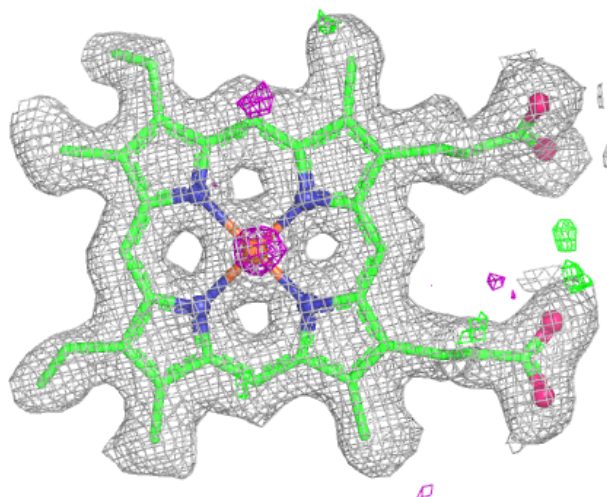
Electron density around HEM A 501 (A):

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



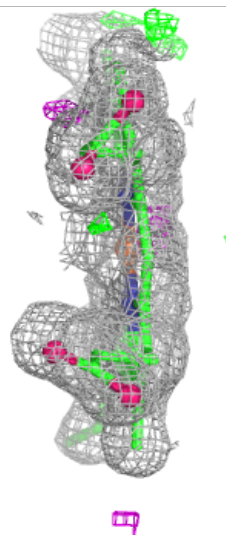
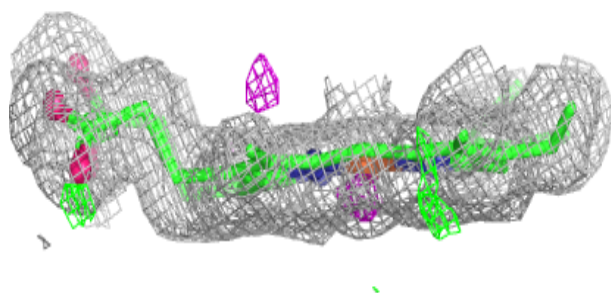
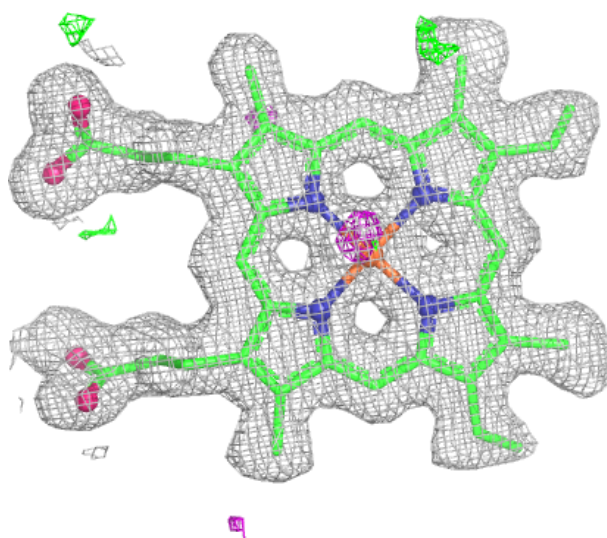
Electron density around HEM B 502 (B):

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



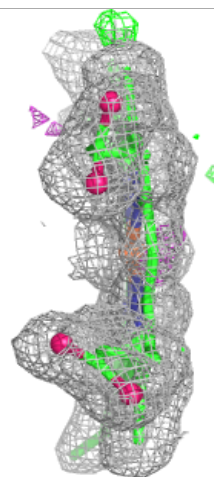
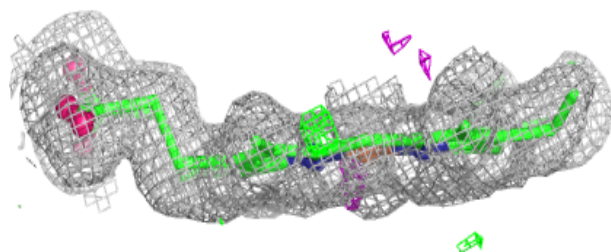
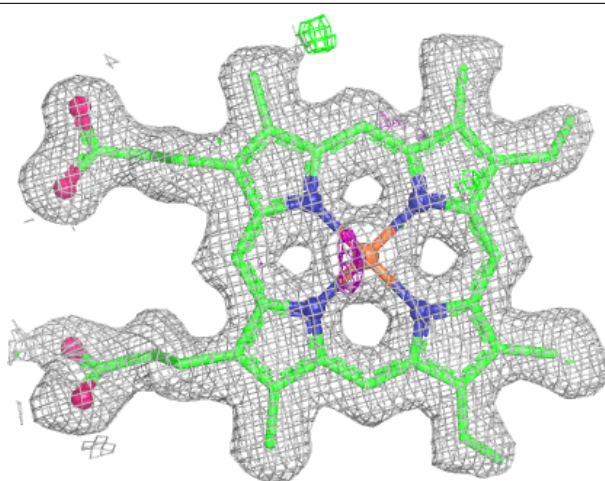
Electron density around HEM A 502 (B):

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



Electron density around HEM D 502 (B):

$2mF_o-DF_c$ (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.