



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 14, 2020 – 06:43 am BST

PDB ID : 1TH3
Title : Crystal structure of NADPH depleted bovine live catalase complexed with cyanide
Authors : Sugadev, R.; Balasundaresan, D.; Ponnuswamy, M.N.; Kumaran, D.; Swaminathan, S.; Sekar, K.
Deposited on : 2004-06-01
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

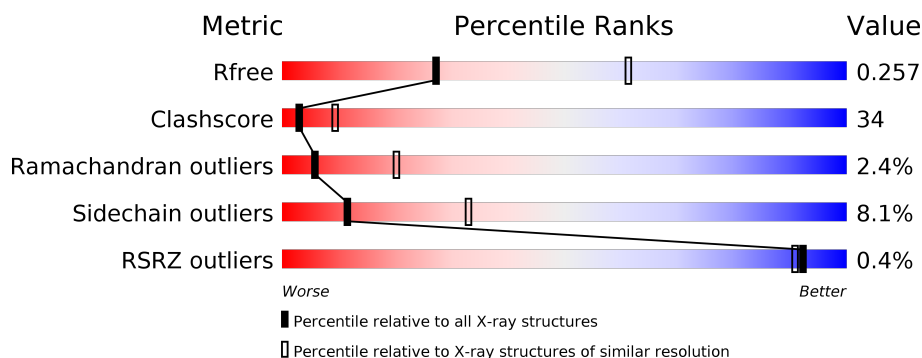
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	506	
1	B	506	
1	C	506	
1	D	506	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CYN	A	3000	-	-	X	-
3	HEM	B	2001	-	-	X	-
3	HEM	C	2002	-	-	X	-
3	HEM	D	2003	-	-	X	-

2 Entry composition [i](#)

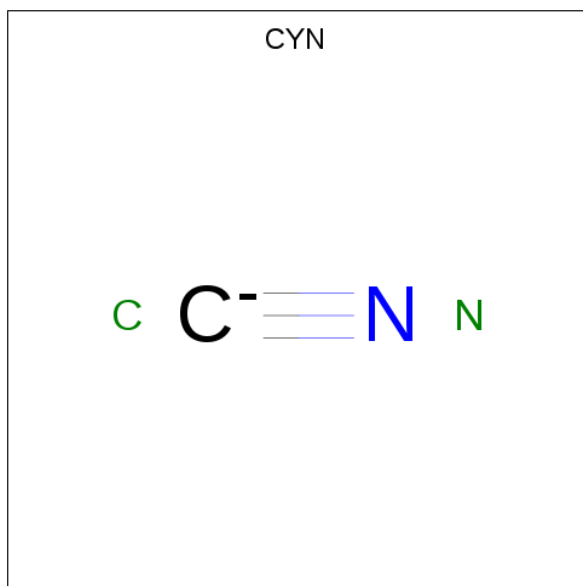
There are 4 unique types of molecules in this entry. The entry contains 16932 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

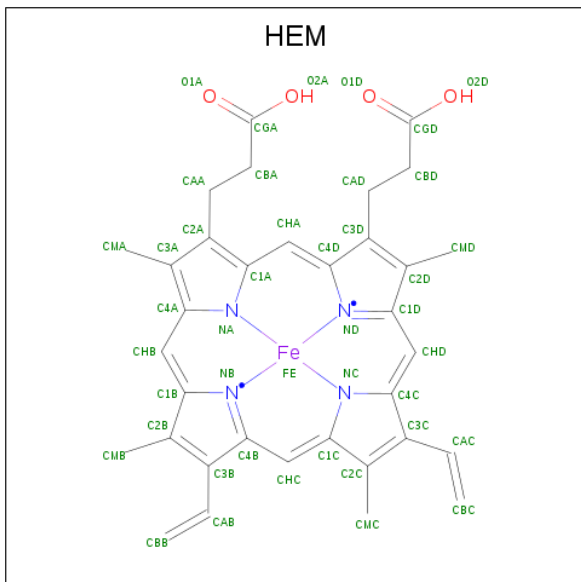
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	499	Total	C	N	O	S	0	0	0
			4017	2548	715	740	14			
1	B	499	Total	C	N	O	S	0	0	0
			4017	2548	715	740	14			
1	C	499	Total	C	N	O	S	1	0	0
			4017	2548	715	740	14			
1	D	499	Total	C	N	O	S	0	0	0
			4017	2548	715	740	14			

- Molecule 2 is CYANIDE ION (three-letter code: CYN) (formula: CN).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			2	1	1		
2	D	1	Total	C	N	0	0
			2	1	1		

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

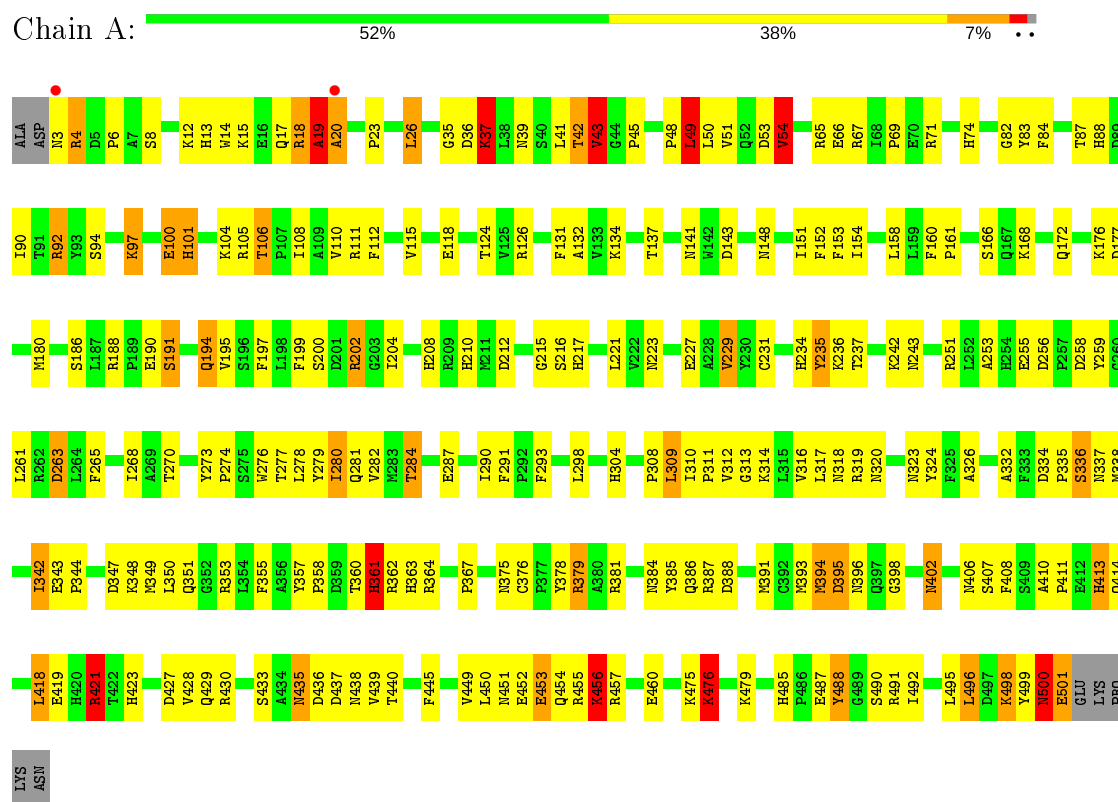
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	201	Total	O	0	0
			201	201		
4	B	195	Total	O	0	0
			195	195		
4	C	138	Total	O	0	0
			138	138		
4	D	154	Total	O	0	0
			154	154		

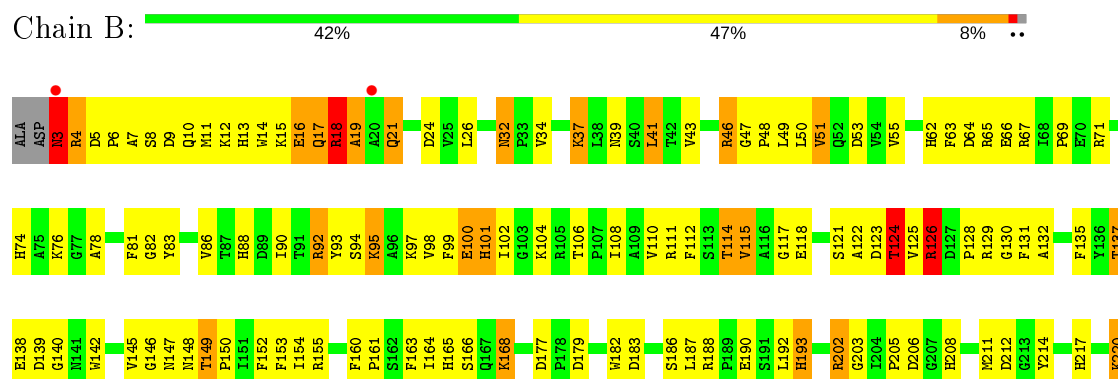
3 Residue-property plots

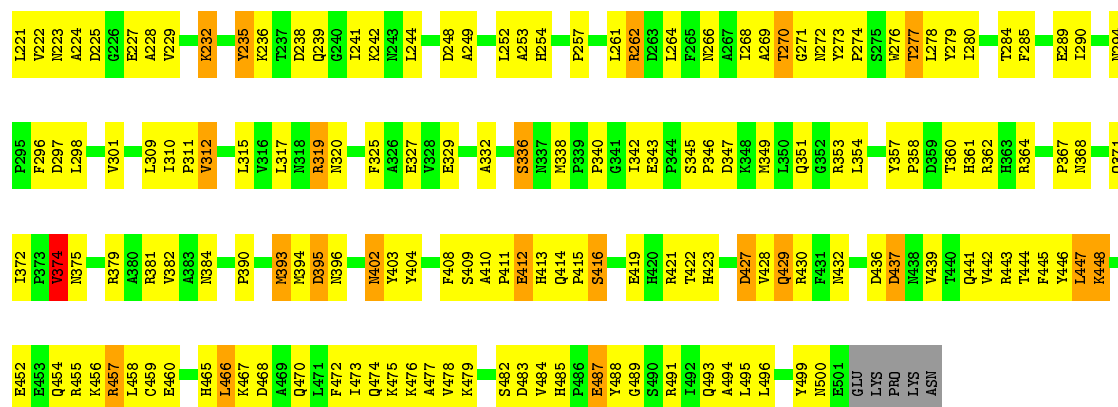
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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

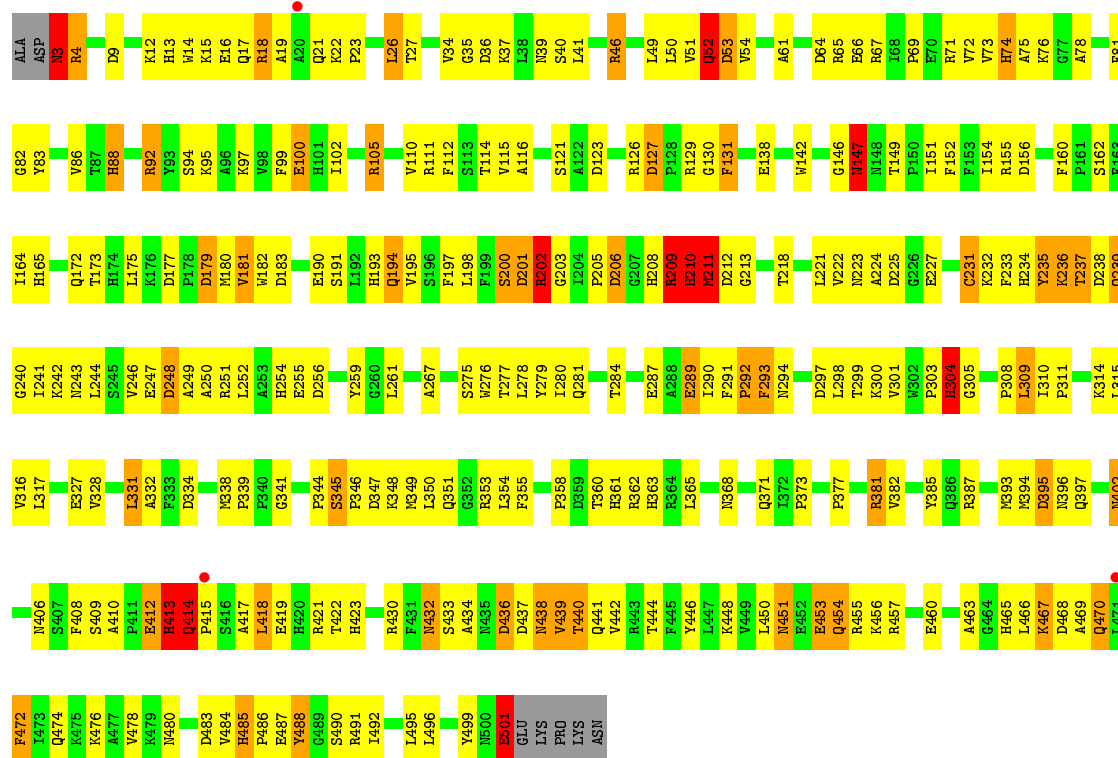


• Molecule 1: Catalase

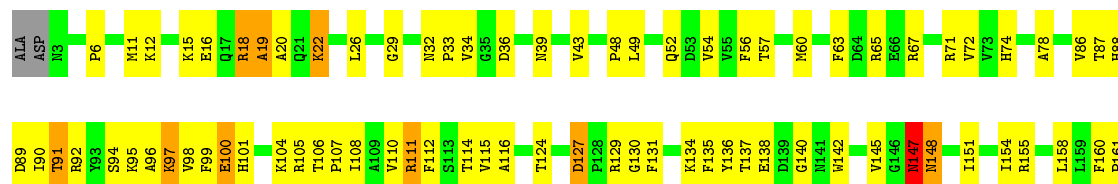




• Molecule 1: Catalase



• Molecule 1: Catalase



E501	S407	E329	Q239	L164
GLU	F408	E332	K242	H165
LYS	S409	A332	V246	K168
PRO	A410	F333	E247	R169
LYS	P411	D334	L261	N170
ASN	E412	P335	R262	F171
	H413	S336	D263	Q172
	L418	N337	N266	T173
	E419	P338	T270	H174
	H420	P339	G271	D177
	R421	I342	N271	F178
	T422	E343	N272	D179
	H423	P346	Y273	M180
	Q429	D347	P274	V181
	R430	K348	S275	M182
	F431	N349	W276	D183
	D437	R353	T277	L187
	N438	Y357	L278	R188
	V439	P358	Y279	P189
	T440	H361	I280	E190
	Q441	R362	Q281	S191
	V442	R362	T284	L192
	F445	N368	F285	H193
	V449	K371	S286	Q194
	L450	I372	E287	V195
	N451	P373	A288	D206
	E452	N375	E289	G207
	Q454	G376	L290	H208
	R455	P377	F291	R209
	E460	Y378	P292	D212
	L466	R379	F293	S216
	R467	A380	N294	H217
	L471	R381	P295	T218
	V478	V382	F296	T219
	K479	A383	D297	F219
	N480	N384	L298	K220
	V484	D388	T299	L221
	H485	G389	K300	V222
	P486	F390	V301	N223
	E487	M391	W302	A224
	Y488	C392	P303	D225
	I492	M393	H304	G226
	Q493	M394	D306	E227
	A494	N397	Y307	A228
	L495	Q397	P308	V229
	Y499	N402	L309	Y230
	N500	Y403	I310	C231
		P405	P311	K232
			V312	F233
			L317	H234
			V322	Y235
			N323	K236
				T237
				D238

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.06Å 140.11Å 226.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.21 – 2.80 42.27 – 2.80	Depositor EDS
% Data completeness (in resolution range)	76.4 (39.21-2.80) 76.5 (42.27-2.80)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.07 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.198 , 0.261 0.199 , 0.257	Depositor DCC
R_{free} test set	1553 reflections (2.98%)	wwPDB-VP
Wilson B-factor (Å ²)	34.6	Xtriage
Anisotropy	0.578	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 53.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	16932	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% 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, CYN

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	0.71	8/4137 (0.2%)	1.63	67/5619 (1.2%)
1	B	0.98	5/4137 (0.1%)	1.47	29/5619 (0.5%)
1	C	0.70	12/4137 (0.3%)	1.63	50/5619 (0.9%)
1	D	0.60	1/4137 (0.0%)	0.83	8/5619 (0.1%)
All	All	0.76	26/16548 (0.2%)	1.43	154/22476 (0.7%)

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	2	6
1	B	0	4
1	C	3	4
All	All	5	14

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	319	ARG	CD-NE	48.75	2.29	1.46
1	D	413	HIS	CA-CB	-20.31	1.09	1.53
1	A	43	VAL	C-O	18.23	1.57	1.23
1	C	202	ARG	NE-CZ	16.64	1.54	1.33
1	B	319	ARG	NE-CZ	15.74	1.53	1.33

The worst 5 of 154 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	202	ARG	NE-CZ-NH2	-52.37	94.12	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	319	ARG	NE-CZ-NH1	-46.12	97.24	120.30
1	C	202	ARG	NE-CZ-NH1	43.99	142.29	120.30
1	B	319	ARG	CG-CD-NE	-41.07	25.55	111.80
1	A	19	ALA	O-C-N	-36.47	64.35	122.70

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	43	VAL	CA
1	A	395	ASP	CA
1	C	147	ASN	CA
1	C	453	GLU	CA
1	C	501	GLU	CA

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	19	ALA	Mainchain,Peptide
1	A	42	THR	Peptide
1	A	421	ARG	Sidechain
1	A	43	VAL	Mainchain,Peptide
1	B	3	ASN	Mainchain

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	4017	0	3837	240	0
1	B	4017	0	3840	343	0
1	C	4017	0	3839	327	0
1	D	4017	0	3839	270	0
2	A	2	0	0	6	0
2	D	2	0	0	0	0
3	A	43	0	30	16	0
3	B	43	0	30	25	0
3	C	43	0	30	26	0
3	D	43	0	30	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	201	0	0	33	0
4	B	195	0	0	33	0
4	C	138	0	0	16	0
4	D	154	0	0	20	0
All	All	16932	0	15475	1083	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 34.

The worst 5 of 1083 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:92:ARG:CD	1:A:92:ARG:CG	1.87	1.49
1:C:147:ASN:CG	3:C:2002:HEM:HAC	1.16	1.45
1:C:147:ASN:OD1	3:C:2002:HEM:CAC	1.63	1.42
1:C:147:ASN:ND2	3:C:2002:HEM:HAC	1.26	1.40
1:B:111:ARG:CD	3:B:2001:HEM:O1D	1.70	1.38

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	497/506 (98%)	450 (90%)	39 (8%)	8 (2%)	9	31
1	B	497/506 (98%)	425 (86%)	58 (12%)	14 (3%)	5	17
1	C	497/506 (98%)	427 (86%)	54 (11%)	16 (3%)	4	13
1	D	497/506 (98%)	438 (88%)	50 (10%)	9 (2%)	8	28
All	All	1988/2024 (98%)	1740 (88%)	201 (10%)	47 (2%)	6	20

5 of 47 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	VAL
1	A	100	GLU
1	B	4	ARG
1	B	100	GLU
1	B	124	THR

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	431/437 (99%)	400 (93%)	31 (7%)	14	38
1	B	431/437 (99%)	392 (91%)	39 (9%)	9	28
1	C	431/437 (99%)	388 (90%)	43 (10%)	7	22
1	D	431/437 (99%)	404 (94%)	27 (6%)	18	46
All	All	1724/1748 (99%)	1584 (92%)	140 (8%)	11	33

5 of 140 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	402	ASN
1	C	92	ARG
1	D	301	VAL
1	B	416	SER
1	C	4	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 53 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	435	ASN
1	C	239	GLN
1	D	337	ASN
1	B	461	ASN
1	C	52	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

6 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	$\# Z > 2$
3	HEM	B	2001	1	27,50,50	12.24	9 (33%)	17,82,82	14.50	6 (35%)
2	CYN	D	3001	3	0,1,1	0.00	-	-		
3	HEM	A	2000	1	27,50,50	11.72	7 (25%)	17,82,82	12.89	2 (11%)
2	CYN	A	3000	-	0,1,1	0.00	-	-		
3	HEM	D	2003	1,2	27,50,50	1.79	6 (22%)	17,82,82	11.21	6 (35%)
3	HEM	C	2002	1	27,50,50	1.70	5 (18%)	17,82,82	2.84	2 (11%)

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	HEM	B	2001	1	-	3/6/54/54	-
3	HEM	A	2000	1	-	0/6/54/54	-
3	HEM	D	2003	1,2	-	3/6/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEM	C	2002	1	-	0/6/54/54	-

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2000	HEM	CMC-C2C	46.72	2.62	1.51
3	B	2001	HEM	CMC-C2C	46.53	2.62	1.51
3	B	2001	HEM	C3C-CAC	42.28	2.34	1.47
3	A	2000	HEM	C3C-CAC	38.07	2.25	1.47
3	B	2001	HEM	C3B-CAB	-4.51	1.38	1.47

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2000	HEM	CMC-C2C-C3C	-53.03	25.47	124.68
3	B	2001	HEM	CMC-C2C-C3C	-52.48	26.48	124.68
3	D	2003	HEM	CAA-CBA-CGA	34.43	170.43	112.67
3	D	2003	HEM	CBA-CAA-C2A	24.00	156.75	112.49
3	B	2001	HEM	CBD-CAD-C3D	16.51	142.90	112.48

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	2001	HEM	C2D-C3D-CAD-CBD
3	B	2001	HEM	C4D-C3D-CAD-CBD
3	D	2003	HEM	C2A-CAA-CBA-CGA
3	D	2003	HEM	C2D-C3D-CAD-CBD
3	D	2003	HEM	C4D-C3D-CAD-CBD

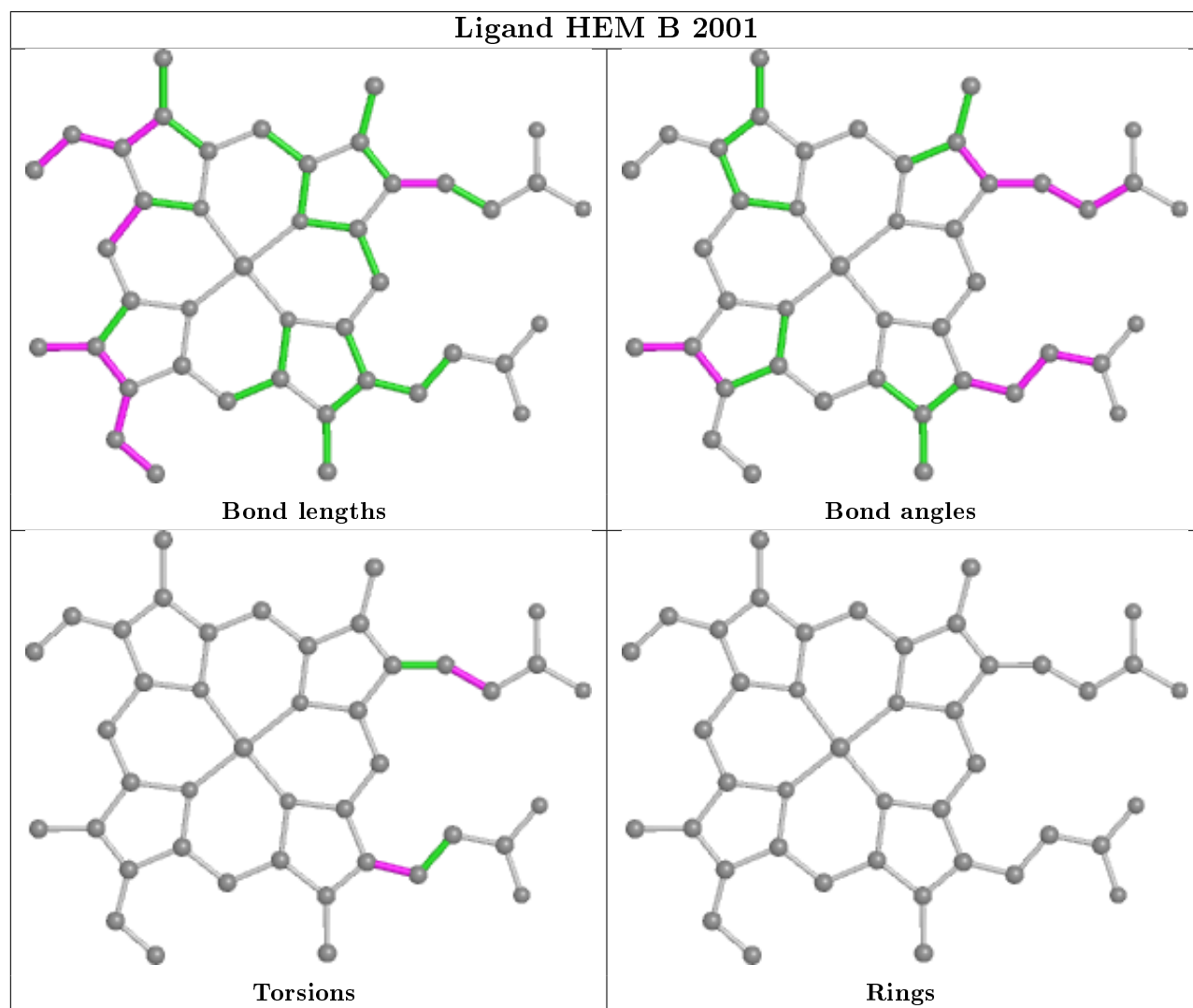
There are no ring outliers.

5 monomers are involved in 88 short contacts:

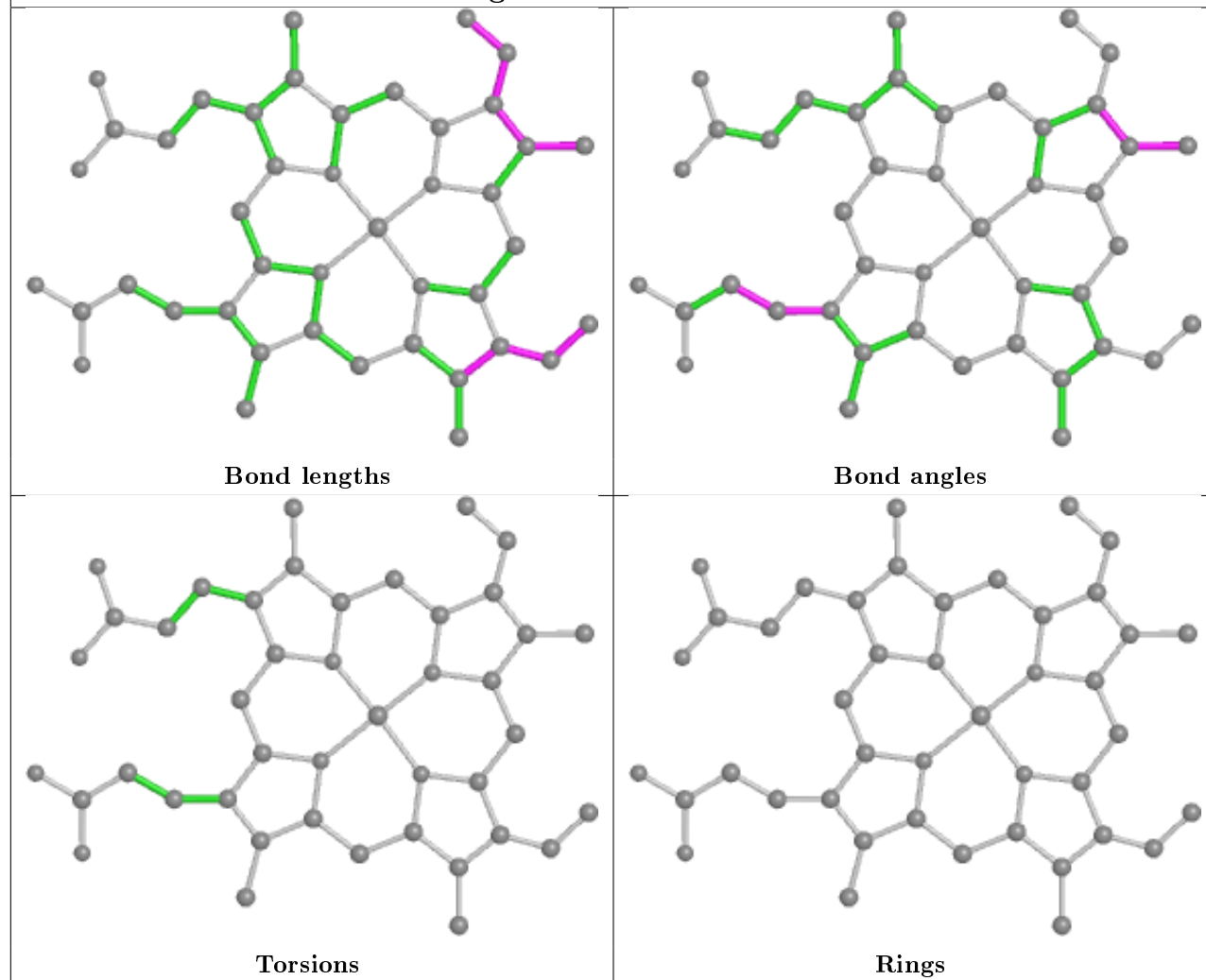
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2001	HEM	25	0
3	A	2000	HEM	16	0
2	A	3000	CYN	6	0
3	D	2003	HEM	21	0
3	C	2002	HEM	26	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

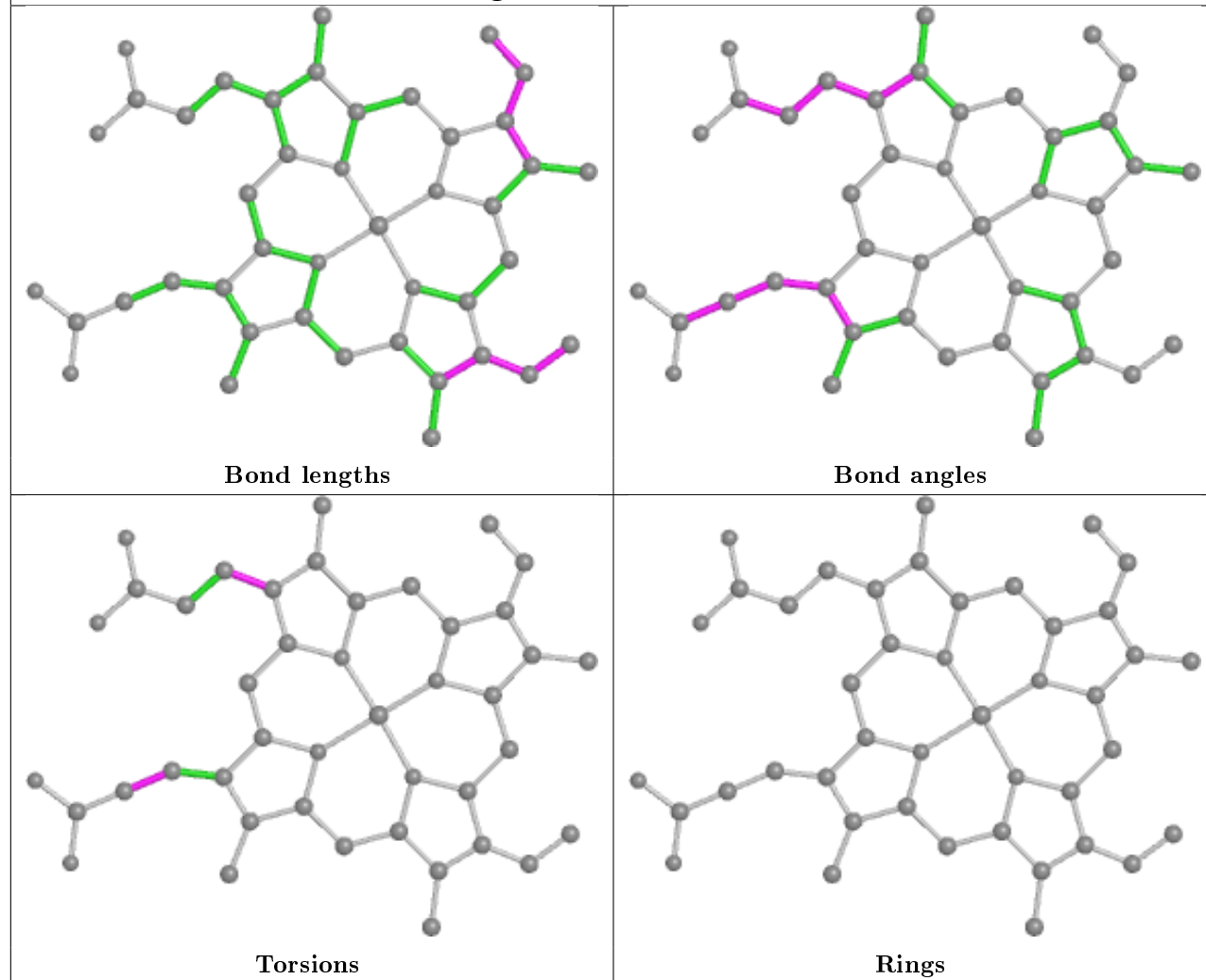
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.

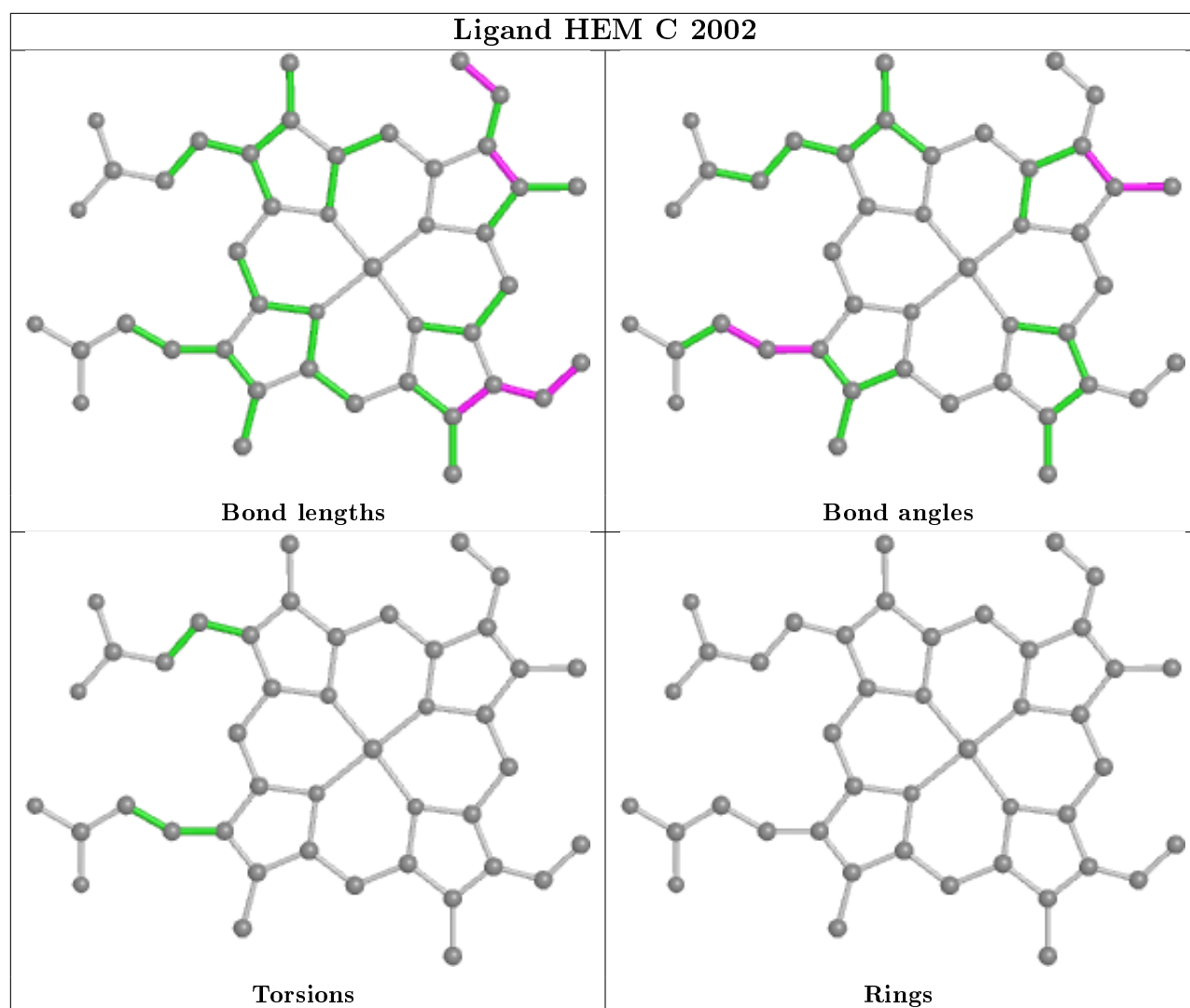


Ligand HEM A 2000



Ligand HEM D 2003





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	499/506 (98%)	-0.62	2 (0%) 92 91	9, 29, 55, 85	0
1	B	499/506 (98%)	-0.50	2 (0%) 92 91	12, 37, 64, 97	0
1	C	499/506 (98%)	-0.49	3 (0%) 89 86	12, 33, 65, 90	1 (0%)
1	D	499/506 (98%)	-0.49	0 100 100	10, 35, 69, 89	0
All	All	1996/2024 (98%)	-0.52	7 (0%) 92 91	9, 34, 64, 97	1 (0%)

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	3	ASN	2.8
1	A	3	ASN	2.6
1	C	20	ALA	2.6
1	A	20	ALA	2.4
1	C	471	LEU	2.3

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 carbohydrates in this entry.

6.4 Ligands [i](#)

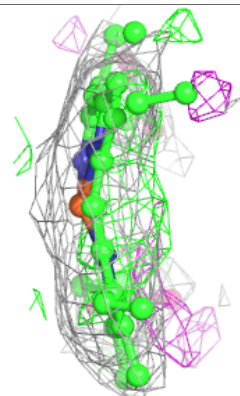
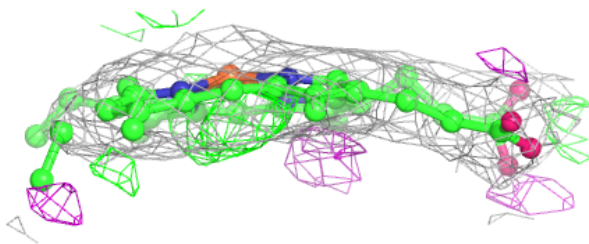
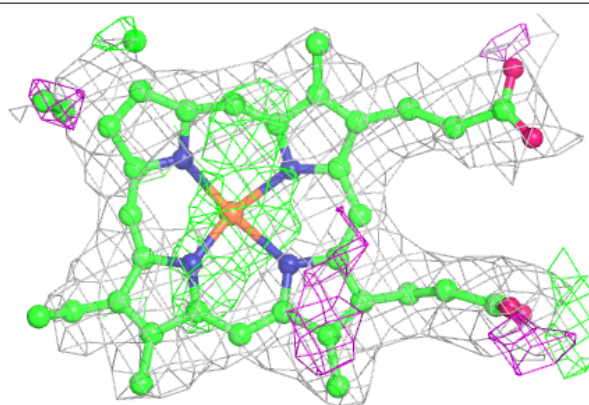
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	HEM	B	2001	43/43	0.92	0.25	20,37,58,100	0
3	HEM	D	2003	43/43	0.93	0.27	21,48,68,78	0
3	HEM	C	2002	43/43	0.94	0.21	22,37,54,101	0
3	HEM	A	2000	43/43	0.97	0.18	7,26,38,101	0
2	CYN	D	3001	2/2	0.99	0.12	57,57,57,63	0
2	CYN	A	3000	2/2	1.00	0.17	41,41,41,48	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.

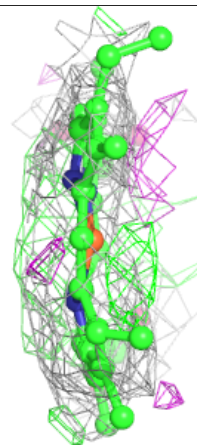
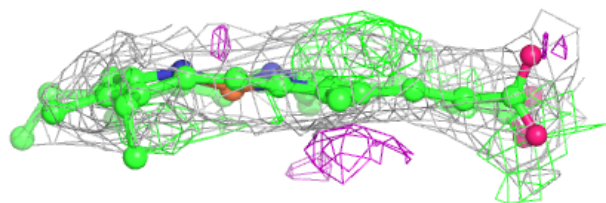
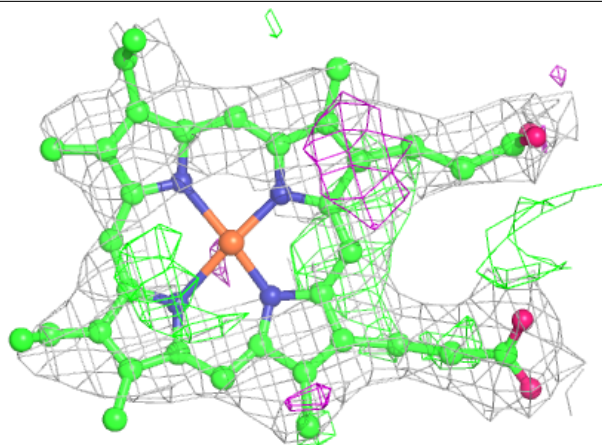
Electron density around HEM B 2001:

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



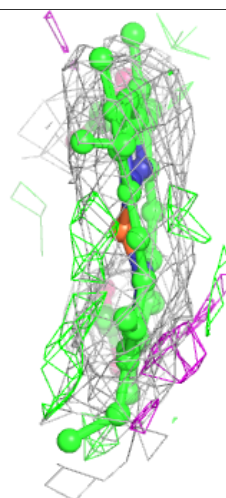
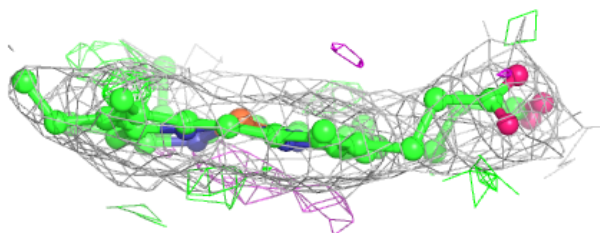
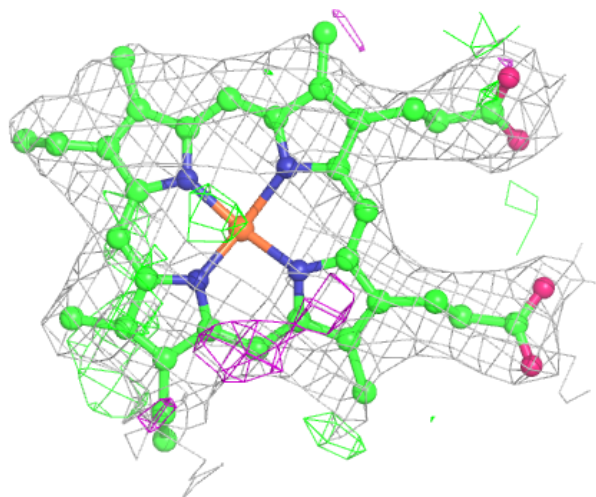
Electron density around HEM D 2003:

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



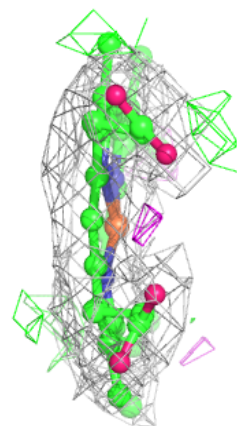
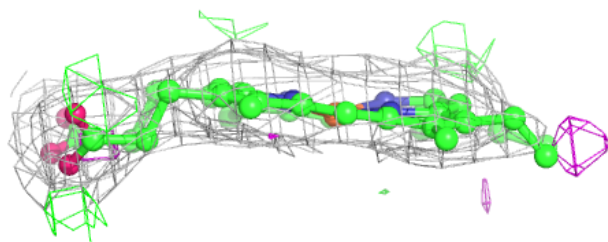
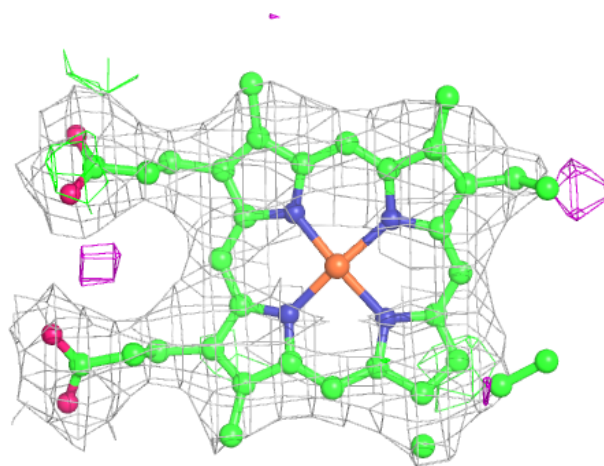
Electron density around HEM C 2002:

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



Electron density around HEM A 2000:

$2mF_o-DF_c$ (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.