



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 07:55 pm BST

PDB ID : 4IMU
Title : Structure of rat neuronal nitric oxide synthase in complex with 6,6'-((5-(aminomethyl)-1,3-phenylene)bis(ethane-2,1-diyl))bis(4-methylpyridin-2-amine)
Authors : Li, H.; Poulos, T.L.
Deposited on : 2013-01-03
Resolution : 2.03 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 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

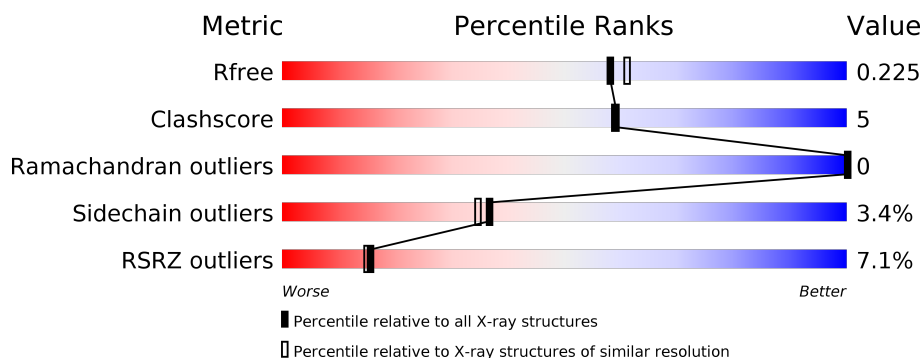
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.03 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	10434 (2.04-2.00)
Clashscore	141614	11643 (2.04-2.00)
Ramachandran outliers	138981	11493 (2.04-2.00)
Sidechain outliers	138945	11492 (2.04-2.00)
RSRZ outliers	127900	10220 (2.04-2.00)

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	422	<div> <div>10%</div> <div> <div></div> <div>82%</div> <div>12%</div> <div>• •</div> </div> </div>
1	B	422	<div> <div>4%</div> <div> <div></div> <div>87%</div> <div>9%</div> <div>• •</div> </div> </div>

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 7226 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 Nitric oxide synthase, brain.

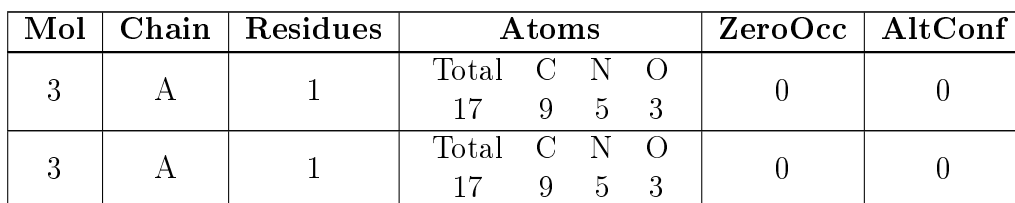
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	407	Total	C	N	O	S	0	3	0
			3327	2130	567	608	22			
1	B	411	Total	C	N	O	S	0	2	0
			3357	2148	574	614	21			

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



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

- Molecule 3 is 5,6,7,8-TETRAHYDROBIOPTERIN (three-letter code: H4B) (formula: $C_9H_{15}N_5O_3$).



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- Chemical structure of 1ET (1-ethyl-3-(4-aminophenyl)-5-(4-aminophenyl)-1H-pyrazole) is shown. The structure features a central pyrazole ring (N1, N2) connected to two 4-aminophenyl groups (C11-C16 and C23-C28) and an ethyl group (C17-C18). The atoms are labeled as follows: N1, N2, C11, C12, C13, C14, C15, C16, C17, C18, C23, C24, C25, C26, C27, C28, C29, C30, C31, C32, C33, C34, C35, C36, C37, C38, C39, C40, C41, C42, C43, C44, C45, C46, C47, C48, C49, C50, C51, C52, C53, C54, C55, C56, C57, C58, C59, C60, C61, C62, C63, C64, C65, C66, C67, C68, C69, C70, C71, C72, C73, C74, C75, C76, C77, C78, C79, C80, C81, C82, C83, C84, C85, C86, C87, C88, C89, C90, C91, C92, C93, C94, C95, C96, C97, C98, C99, C100, C101, C102, C103, C104, C105, C106, C107, C108, C109, C110, C111, C112, C113, C114, C115, C116, C117, C118, C119, C120, C121, C122, C123, C124, C125, C126, C127, C128, C129, C130, C131, C132, C133, C134, C135, C136, C137, C138, C139, C140, C141, C142, C143, C144, C145, C146, C147, C148, C149, C150, C151, C152, C153, C154, C155, C156, C157, C158, C159, C160, C161, C162, C163, C164, C165, C166, C167, C168, C169, C170, C171, C172, C173, C174, C175, C176, C177, C178, C179, C180, C181, C182, C183, C184, C185, C186, C187, C188, C189, C190, C191, C192, C193, C194, C195, C196, C197, C198, C199, C200, C201, C202, C203, C204, C205, C206, C207, C208, C209, C210, C211, C212, C213, C214, C215, C216, C217, C218, C219, C220, C221, C222, C223, C224, C225, C226, C227, C228, C229, C230, C231, C232, C233, C234, C235, C236, C237, C238, C239, C240, C241, C242, C243, C244, C245, C246, C247, C248, C249, C250, C251, C252, C253, C254, C255, C256, C257, C258, C259, C260, C261, C262, C263, C264, C265, C266, C267, C268, C269, C270, C271, C272, C273, C274, C275, C276, C277, C278, C279, C280, C281, C282, C283, C284, C285, C286, C287, C288, C289, C290, C291, C292, C293, C294, C295, C296, C297, C298, C299, C300, C301, C302, C303, C304, C305, C306, C307, C308, C309, C310, C311, C312, C313, C314, C315, C316, C317, C318, C319, C320, C321, C322, C323, C324, C325, C326, C327, C328, C329, C330, C331, C332, C333, C334, C335, C336, C337, C338, C339, C340, C341, C342, C343, C344, C345, C346, C347, C348, C349, C350, C351, C352, C353, C354, C355, C356, C357, C358, C359, C360, C361, C362, C363, C364, C365, C366, C367, C368, C369, C370, C371, C372, C373, C374, C375, C376, C377, C378, C379, C380, C381, C382, C383, C384, C385, C386, C387, C388, C389, C390, C391, C392, C393, C394, C395, C396, C397, C398, C399, C400, C401, C402, C403, C404, C405, C406, C407, C408, C409, C410, C411, C412, C413, C414, C415, C416, C417, C418, C419, C420, C421, C422, C423, C424, C425, C426, C427, C428, C429, C430, C431, C432, C433, C434, C435, C436, C437, C438, C439, C440, C441, C442, C443, C444, C445, C446, C447, C448, C449, C450, C451, C452, C453, C454, C455, C456, C457, C458, C459, C460, C461, C462, C463, C464, C465, C466, C467, C468, C469, C470, C471, C472, C473, C474, C475, C476, C477, C478, C479, C480, C481, C482, C483, C484, C485, C486, C487, C488, C489, C490, C491, C492, C493, C494, C495, C496, C497, C498, C499, C500, C501, C502, C503, C504, C505, C506, C507, C508, C509, C510, C511, C512, C513, C514, C515, C516, C517, C518, C519, C520, C521, C522, C523, C524, C525, C526, C527, C528, C529, C530, C531, C532, C533, C534, C535, C536, C537, C538, C539, C540, C541, C542, C543, C544, C545, C546, C547, C548, C549, C550, C551, C552, C553, C554, C555, C556, C557, C558, C559, C560, C561, C562, C563, C564, C565, C566, C567, C568, C569, C570, C571, C572, C573, C574, C575, C576, C577, C578, C579, C580, C581, C582, C583, C584, C585, C586, C587, C588, C589, C590, C591, C592, C593, C594, C595, C596, C597, C598, C599, C600, C601, C602, C603, C604, C605, C606, C607, C608, C609, C610, C611, C612, C613, C614, C615, C616, C617, C618, C619, C620, C621, C622, C623, C624, C625, C626, C627, C628, C629, C630, C631, C632, C633, C634, C635, C636, C637, C638, C639, C640, C641, C642, C643, C644, C645, C646, C647, C648, C649, C650, C651, C652, C653, C654, C655, C656, C657, C658, C659, C660, C661, C662, C663, C664, C665, C666, C667, C668, C669, C670, C671, C672, C673, C674, C675, C676, C677, C678, C679, C680, C681, C682, C683, C684, C685, C686, C687, C688, C689, C690, C691, C692, C693, C694, C695, C696, C697, C698, C699, C700, C701, C702, C703, C704, C705, C706, C707, C708, C709, C710, C711, C712, C713, C714, C715, C716, C717, C718, C719, C720, C721, C722, C723, C724, C725, C726, C727, C728, C729, C730, C731, C732, C733, C734, C735, C736, C737, C738, C739, C740, C741, C742, C743, C744, C745, C746, C747, C748, C749, C750, C751, C752, C753, C754, C755, C756, C757, C758, C759, C760, C761, C762, C763, C764, C765, C766, C767, C768, C769, C770, C771, C772, C773, C774, C775, C776, C777, C778, C779, C780, C781, C782, C783, C784, C785, C786, C787, C788, C789, C790, C791, C792, C793, C794, C795, C796, C797, C798, C799, C800, C801, C802, C803, C804, C805, C806, C807, C808, C809, C810, C811, C812, C813, C814, C815, C816, C817, C818, C819, C

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			28	23	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	N	0	0
			28	23	5		

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Zn	0	0
			1	1		
6	A	2	Total	Zn	0	0
			2	2		

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	2	Total	Cl	0	0
			2	2		
7	A	2	Total	Cl	0	0
			2	2		

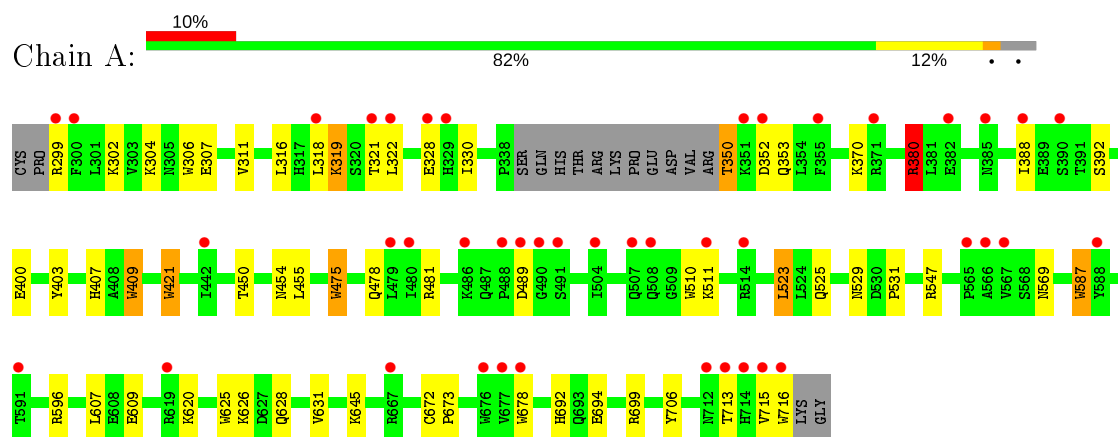
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	147	Total 147	O 147	0	0
8	B	204	Total 204	O 204	0	0

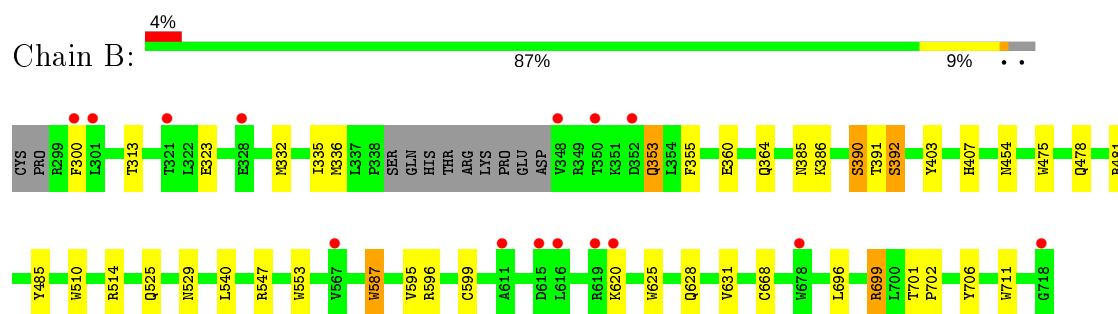
3 Residue-property plots [i](#)

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: Nitric oxide synthase, brain



- Molecule 1: Nitric oxide synthase, brain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	51.91Å 110.22Å 163.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.03 40.74 – 2.03	Depositor EDS
% Data completeness (in resolution range)	98.7 (50.00-2.03) 98.8 (40.74-2.03)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.38 (at 2.03Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.184 , 0.225 0.183 , 0.225	Depositor DCC
R_{free} test set	3007 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	32.6	Xtriage
Anisotropy	0.804	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 42.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7226	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.93% 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: ZN, H4B, CL, 1ET, ACT, HEM

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.69	9/3429 (0.3%)	0.69	2/4652 (0.0%)
1	B	0.71	6/3456 (0.2%)	0.70	0/4685
All	All	0.70	15/6885 (0.2%)	0.69	2/9337 (0.0%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	409	TRP	CD2-CE2	6.32	1.49	1.41
1	A	716	TRP	CD2-CE2	5.66	1.48	1.41
1	A	510	TRP	CD2-CE2	5.59	1.48	1.41
1	B	587	TRP	CD2-CE2	5.58	1.48	1.41
1	B	625	TRP	CD2-CE2	5.52	1.48	1.41
1	A	421	TRP	CD2-CE2	5.47	1.48	1.41
1	B	553	TRP	CD2-CE2	5.45	1.47	1.41
1	B	510	TRP	CD2-CE2	5.35	1.47	1.41
1	A	587	TRP	CD2-CE2	5.30	1.47	1.41
1	A	678	TRP	CD2-CE2	5.28	1.47	1.41
1	A	475	TRP	CD2-CE2	5.23	1.47	1.41
1	A	625	TRP	CD2-CE2	5.18	1.47	1.41
1	A	306	TRP	CD2-CE2	5.13	1.47	1.41
1	B	711	TRP	CD2-CE2	5.03	1.47	1.41
1	B	475	TRP	CD2-CE2	5.00	1.47	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	380	ARG	NE-CZ-NH1	6.29	123.45	120.30
1	A	380	ARG	NE-CZ-NH2	-6.05	117.27	120.30

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	3327	0	3238	31	0
1	B	3357	0	3271	24	0
2	A	43	0	30	9	0
2	B	43	0	30	8	0
3	A	34	0	30	2	0
4	A	28	0	29	3	0
4	B	28	0	29	6	0
5	A	4	0	3	1	0
5	B	4	0	3	0	0
6	A	2	0	0	0	0
6	B	1	0	0	0	0
7	A	2	0	0	0	0
7	B	2	0	0	0	0
8	A	147	0	0	2	0
8	B	204	0	0	3	0
All	All	7226	0	6663	64	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 5.

All (64) 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:299:ARG:HA	1:A:318:LEU:HD21	1.54	0.87
1:A:523:LEU:HD22	1:A:531:PRO:HB2	1.60	0.83
2:A:801:HEM:O1D	4:A:803:1ET:H11	1.77	0.83
2:A:801:HEM:HMC2	2:A:801:HEM:HBC2	1.64	0.79
1:B:668:CYS:HB3	8:B:929:HOH:O	1.82	0.78
2:B:801:HEM:HBC2	2:B:801:HEM:HMC2	1.64	0.77
1:B:699:ARG:HH11	1:B:699:ARG:HB2	1.51	0.75
1:A:307[B]:GLU:HG2	1:A:692:HIS:CG	2.23	0.73
1:A:489:ASP:HB2	8:A:1019:HOH:O	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:809:H4B:HN22	2:B:801:HEM:CGA	2.06	0.69
1:A:380:ARG:HD3	1:A:400:GLU:OE1	1.95	0.66
2:A:801:HEM:CGA	3:A:802:H4B:HN22	2.13	0.62
1:A:631:VAL:HG11	1:B:628:GLN:HG3	1.84	0.58
1:A:628:GLN:HG3	1:B:631:VAL:HG11	1.83	0.58
1:B:478:GLN:HB2	1:B:481:ARG:HG3	1.86	0.58
1:A:609:GLU:HG3	8:A:983:HOH:O	2.03	0.58
1:A:350:THR:N	1:A:353:GLN:HE21	2.02	0.57
2:A:801:HEM:CMC	2:A:801:HEM:HBC2	2.35	0.56
1:B:364:GLN:NE2	8:B:1088:HOH:O	2.37	0.56
1:A:475:TRP:HB2	1:A:523:LEU:HB3	1.88	0.55
1:A:403:TYR:CE1	1:A:407:HIS:CE1	2.95	0.55
1:A:322:LEU:HB2	1:A:699:ARG:HE	1.72	0.54
1:A:478:GLN:HB2	1:A:481:ARG:HG3	1.89	0.53
1:A:304:LYS:O	1:A:694:GLU:HG3	2.09	0.53
1:B:485:TYR:CE1	1:B:514:ARG:HA	2.43	0.53
4:B:802:1ET:H12	4:B:802:1ET:H7	1.91	0.52
1:B:596:ARG:HE	4:B:802:1ET:H15	1.59	0.50
1:B:525:GLN:HG3	1:B:529:ASN:O	2.12	0.49
2:A:801:HEM:C1C	4:A:803:1ET:H30	2.47	0.49
1:B:485:TYR:CZ	1:B:514:ARG:HA	2.49	0.48
1:A:607:LEU:HD13	1:A:626:LYS:HG2	1.95	0.48
1:A:330:ILE:HD11	1:B:696:LEU:HD22	1.95	0.48
1:A:370:LYS:HE3	1:A:370:LYS:HB2	1.60	0.48
1:B:701:THR:HA	1:B:702:PRO:C	2.34	0.48
1:B:699:ARG:HH11	1:B:699:ARG:CB	2.23	0.47
1:B:595:VAL:O	1:B:599:CYS:HB2	2.15	0.47
1:A:321:THR:HG23	1:A:322:LEU:HG	1.97	0.47
1:B:386:LYS:O	1:B:390:SER:HB3	2.15	0.47
1:B:587:TRP:H	2:B:801:HEM:HAB	1.80	0.47
2:A:801:HEM:HMB3	5:A:804:ACT:H2	1.97	0.46
1:B:391:THR:O	1:B:392:SER:HB2	2.15	0.45
1:B:454:ASN:ND2	8:B:926:HOH:O	2.49	0.45
1:A:525:GLN:HG3	1:A:529:ASN:O	2.16	0.45
1:A:321:THR:HG23	1:A:322:LEU:H	1.82	0.44
1:B:300:PHE:HB3	1:B:313:THR:CG2	2.47	0.44
1:A:409:TRP:CE3	1:A:421:TRP:HA	2.52	0.44
1:B:403:TYR:CE1	1:B:407:HIS:CE1	3.06	0.44
1:A:388:ILE:O	1:A:392:SER:HA	2.18	0.43
1:A:302:LYS:HE3	1:A:311:VAL:HG11	2.01	0.43
2:B:801:HEM:C1C	4:B:802:1ET:H30	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:587:TRP:H	2:A:801:HEM:HAB	1.84	0.42
2:B:801:HEM:O1D	4:B:802:1ET:H8	2.19	0.42
2:B:801:HEM:O1D	4:B:802:1ET:H11	2.20	0.42
2:B:801:HEM:CBA	4:B:802:1ET:H22	2.49	0.42
1:A:596:ARG:NH1	2:A:801:HEM:O2A	2.53	0.41
1:A:481:ARG:NH2	4:A:803:1ET:H13	2.36	0.41
1:B:353:GLN:HB3	1:B:353:GLN:HE21	1.70	0.41
1:A:694:GLU:HB3	1:B:335:ILE:HD13	2.03	0.41
1:B:355:PHE:CE1	1:B:385:ASN:HB2	2.56	0.40
1:B:706:TYR:OH	2:B:801:HEM:O2D	2.20	0.40
1:A:672:CYS:HA	1:A:673:PRO:HD2	1.96	0.40
1:A:316:LEU:HD12	1:A:319:LYS:HD3	2.03	0.40
1:A:450:THR:HA	1:A:455:LEU:HD22	2.04	0.40
1:A:706:TYR:OH	2:A:801:HEM:O2D	2.34	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	406/422 (96%)	392 (97%)	14 (3%)	0	100	100
1	B	409/422 (97%)	402 (98%)	7 (2%)	0	100	100
All	All	815/844 (97%)	794 (97%)	21 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	366/377 (97%)	352 (96%)	14 (4%)	33	30
1	B	368/377 (98%)	357 (97%)	11 (3%)	41	40
All	All	734/754 (97%)	709 (97%)	25 (3%)	37	35

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	319	LYS
1	A	328	GLU
1	A	350	THR
1	A	352	ASP
1	A	380	ARG
1	A	454	ASN
1	A	511	LYS
1	A	523	LEU
1	A	547	ARG
1	A	569	ASN
1	A	620	LYS
1	A	645	LYS
1	A	713	THR
1	A	715	VAL
1	B	323	GLU
1	B	332	MET
1	B	336	MET
1	B	353	GLN
1	B	360	GLU
1	B	390	SER
1	B	392	SER
1	B	540	LEU
1	B	547	ARG
1	B	620	LYS
1	B	699	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	353	GLN
1	A	425	GLN

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Mol	Chain	Res	Type
1	A	454	ASN
1	A	487	GLN
1	A	527	ASN
1	A	569	ASN
1	A	605	ASN
1	A	642	GLN
1	A	697	ASN
1	B	364	GLN
1	B	385	ASN
1	B	425	GLN
1	B	454	ASN
1	B	507	GLN
1	B	527	ASN
1	B	601	ASN
1	B	605	ASN
1	B	692	HIS
1	B	697	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 7 are monoatomic - leaving 8 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
4	1ET	B	802	-	30,30,30	0.67	0	41,41,41	1.80	8 (19%)
2	HEM	B	801	1	27,50,50	2.28	8 (29%)	17,82,82	3.49	10 (58%)
3	H4B	A	802	-	16,18,18	0.91	0	11,26,26	2.87	7 (63%)
3	H4B	A	809	-	16,18,18	1.13	0	11,26,26	2.70	7 (63%)
5	ACT	B	803	-	1,3,3	1.46	0	0,3,3	0.00	-
4	1ET	A	803	-	30,30,30	0.70	0	41,41,41	1.60	7 (17%)
2	HEM	A	801	1	27,50,50	2.22	10 (37%)	17,82,82	3.39	9 (52%)
5	ACT	A	804	-	1,3,3	1.64	0	0,3,3	0.00	-

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
4	1ET	B	802	-	-	5/12/12/12	0/3/3/3
2	HEM	B	801	1	-	1/6/54/54	-
3	H4B	A	802	-	-	0/8/17/17	0/2/2/2
3	H4B	A	809	-	-	0/8/17/17	0/2/2/2
4	1ET	A	803	-	-	3/12/12/12	0/3/3/3
2	HEM	A	801	1	-	1/6/54/54	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	HEM	C3C-C2C	5.75	1.48	1.40
2	B	801	HEM	C4A-NA	5.13	1.46	1.36
2	B	801	HEM	C3C-C2C	4.86	1.47	1.40
2	A	801	HEM	C4A-NA	4.37	1.45	1.36
2	B	801	HEM	C1A-NA	4.27	1.45	1.36
2	B	801	HEM	C3B-C2B	4.09	1.46	1.40
2	A	801	HEM	C1A-NA	4.08	1.44	1.36
2	A	801	HEM	C2A-C3A	3.51	1.48	1.37
2	B	801	HEM	C2A-C3A	3.39	1.47	1.37
2	A	801	HEM	C3B-C2B	3.31	1.45	1.40
2	B	801	HEM	C3D-C2D	2.86	1.46	1.37
2	A	801	HEM	C3D-C2D	2.82	1.46	1.37
2	B	801	HEM	C1C-C2C	2.68	1.48	1.42
2	B	801	HEM	C4D-C3D	2.63	1.48	1.42
2	A	801	HEM	C1C-C2C	2.57	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	HEM	C4D-C3D	2.25	1.47	1.42
2	A	801	HEM	C1B-C2B	2.25	1.47	1.42
2	A	801	HEM	C4B-CHC	2.12	1.46	1.41

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	HEM	C1D-C2D-C3D	-9.68	100.26	107.00
2	B	801	HEM	C1D-C2D-C3D	-8.36	101.18	107.00
4	B	802	1ET	C02-N01-C06	5.69	122.41	118.10
2	B	801	HEM	CBA-CAA-C2A	-5.53	102.29	112.49
3	A	809	H4B	C4-C4A-C8A	5.15	119.15	114.57
3	A	802	H4B	C4-C4A-N5	5.00	123.31	119.12
2	A	801	HEM	C3B-C4B-NB	4.95	115.60	109.21
2	B	801	HEM	CMB-C2B-C3B	4.87	133.79	124.68
2	B	801	HEM	C4A-C3A-C2A	-4.37	103.96	107.00
4	A	803	1ET	C05-C06-N01	-4.32	118.32	122.90
2	A	801	HEM	CAD-CBD-CGD	-4.31	105.43	112.67
2	B	801	HEM	C3B-C4B-NB	4.21	114.66	109.21
2	A	801	HEM	CMB-C2B-C3B	4.04	132.24	124.68
3	A	802	H4B	C4-C4A-C8A	3.99	118.11	114.57
4	B	802	1ET	C05-C06-N01	-3.98	118.68	122.90
4	A	803	1ET	C22-N21-C26	3.95	121.09	118.10
4	A	803	1ET	C02-N01-C06	3.83	121.00	118.10
4	B	802	1ET	C08-C06-N01	3.81	121.62	115.95
3	A	802	H4B	C4-N3-C2	3.76	121.91	115.93
3	A	809	H4B	C4-N3-C2	3.76	121.90	115.93
2	B	801	HEM	CMD-C2D-C3D	3.65	131.82	124.94
3	A	802	H4B	N3-C2-N1	-3.45	120.00	125.42
3	A	809	H4B	N3-C2-N1	-3.43	120.04	125.42
2	B	801	HEM	CAA-CBA-CGA	-3.20	107.31	112.67
4	A	803	1ET	C08-C06-N01	3.07	120.52	115.95
3	A	802	H4B	N2-C2-N3	3.02	121.95	117.25
3	A	809	H4B	N2-C2-N3	2.93	121.81	117.25
4	B	802	1ET	C29-C28-C26	-2.88	106.53	112.99
2	A	801	HEM	CBA-CAA-C2A	-2.78	107.35	112.49
4	A	803	1ET	C25-C26-N21	-2.78	119.95	122.90
4	B	802	1ET	C28-C26-N21	2.76	120.07	115.95
2	A	801	HEM	CMC-C2C-C3C	2.72	129.77	124.68
3	A	809	H4B	C4-C4A-N5	2.55	121.26	119.12
2	B	801	HEM	CAD-CBD-CGD	-2.50	108.48	112.67
2	A	801	HEM	C4A-C3A-C2A	-2.45	105.29	107.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	802	1ET	N22-C22-N21	2.43	120.32	116.49
3	A	802	H4B	C2-N1-C8A	2.42	119.97	114.54
2	A	801	HEM	CMD-C2D-C1D	2.42	132.19	128.46
2	A	801	HEM	CBD-CAD-C3D	-2.39	108.07	112.48
2	B	801	HEM	CBD-CAD-C3D	-2.30	108.24	112.48
2	B	801	HEM	CMC-C2C-C3C	2.21	128.82	124.68
3	A	809	H4B	C2-N1-C8A	2.17	119.40	114.54
4	B	802	1ET	C07-C04-C05	-2.16	117.73	120.94
4	A	803	1ET	C09-C08-C06	-2.12	108.23	112.99
4	A	803	1ET	C28-C26-N21	2.08	119.05	115.95
3	A	809	H4B	C4A-C4-N3	-2.07	118.12	124.01
3	A	802	H4B	C4A-N5-C6	-2.03	115.64	121.16
4	B	802	1ET	C22-N21-C26	2.01	119.62	118.10

There are no chirality outliers.

All (10) torsion outliers are listed below:

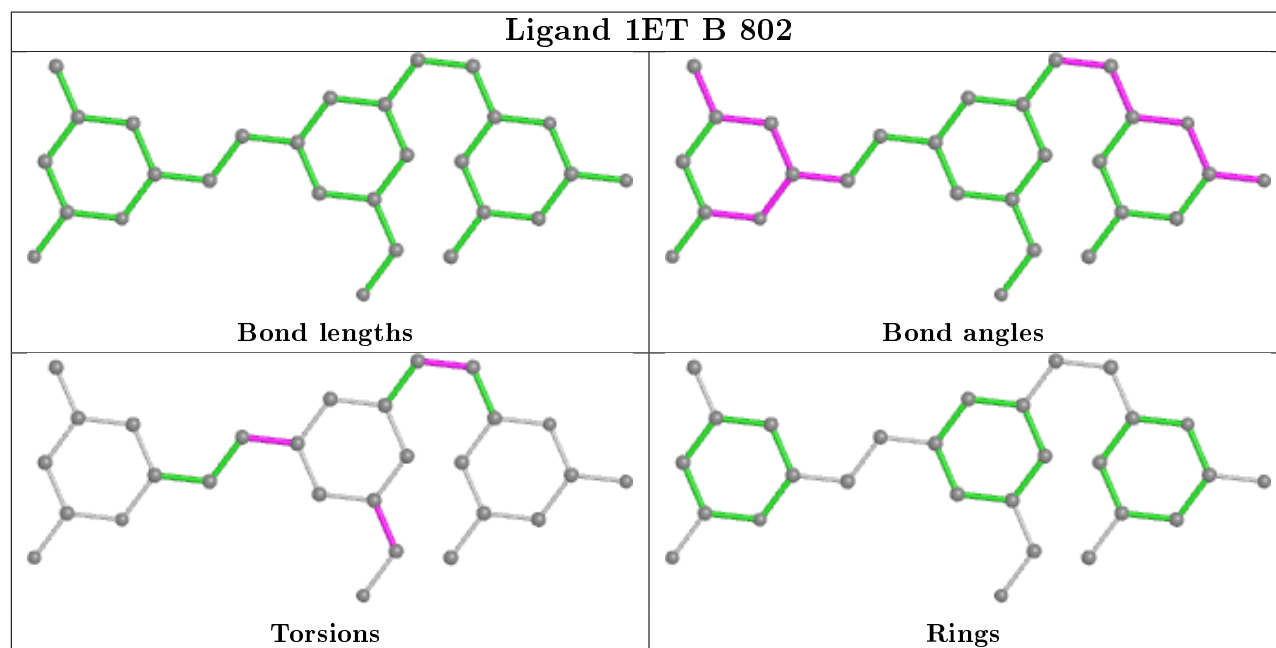
Mol	Chain	Res	Type	Atoms
4	B	802	1ET	C26-C28-C29-C15
4	A	803	1ET	C26-C28-C29-C15
2	A	801	HEM	C2A-CAA-CBA-CGA
4	B	802	1ET	C14-C13-C17-N18
4	B	802	1ET	C08-C09-C11-C16
4	B	802	1ET	C08-C09-C11-C12
4	A	803	1ET	C08-C09-C11-C12
4	B	802	1ET	C12-C13-C17-N18
4	A	803	1ET	C08-C09-C11-C16
2	B	801	HEM	C2A-CAA-CBA-CGA

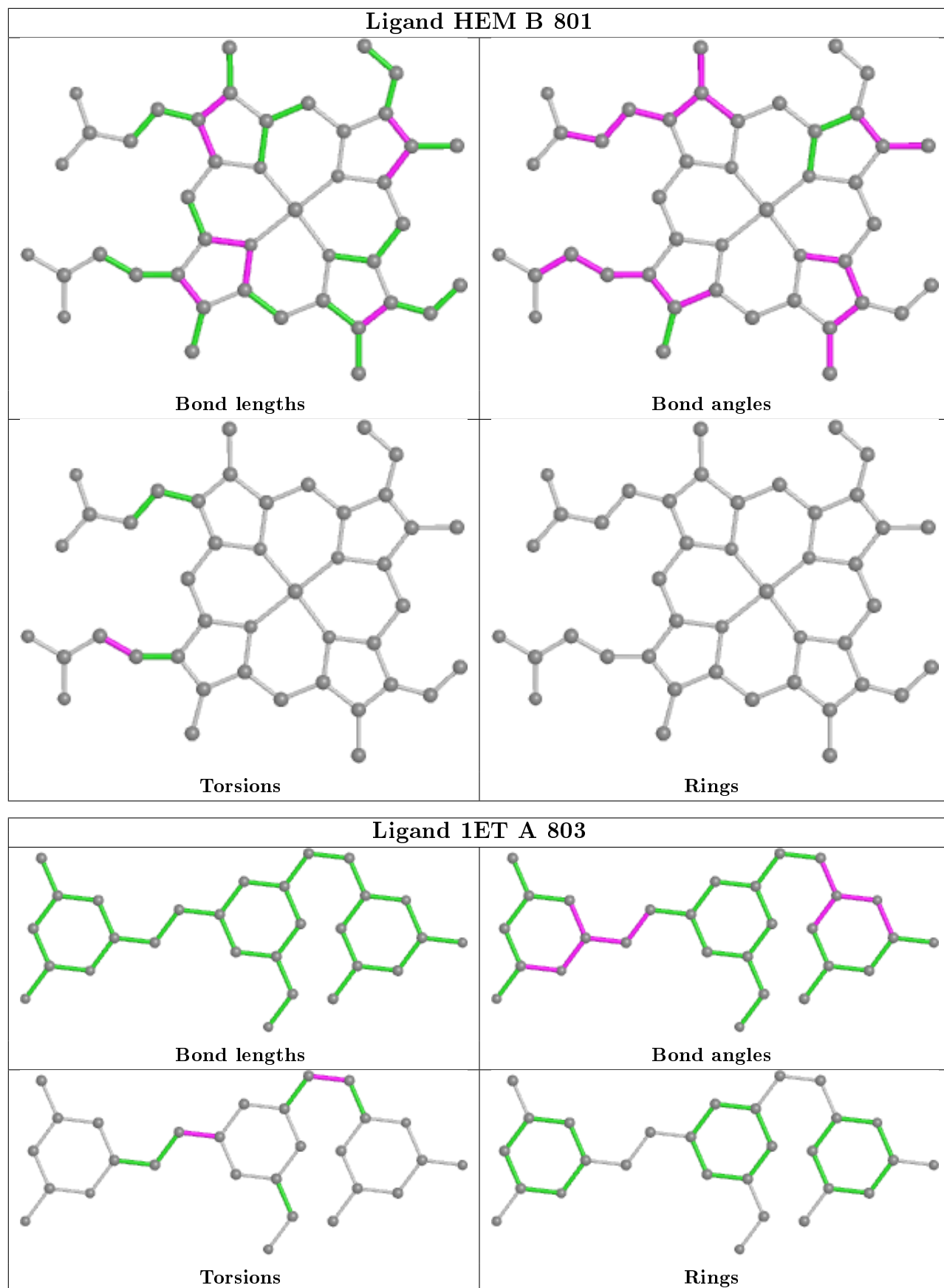
There are no ring outliers.

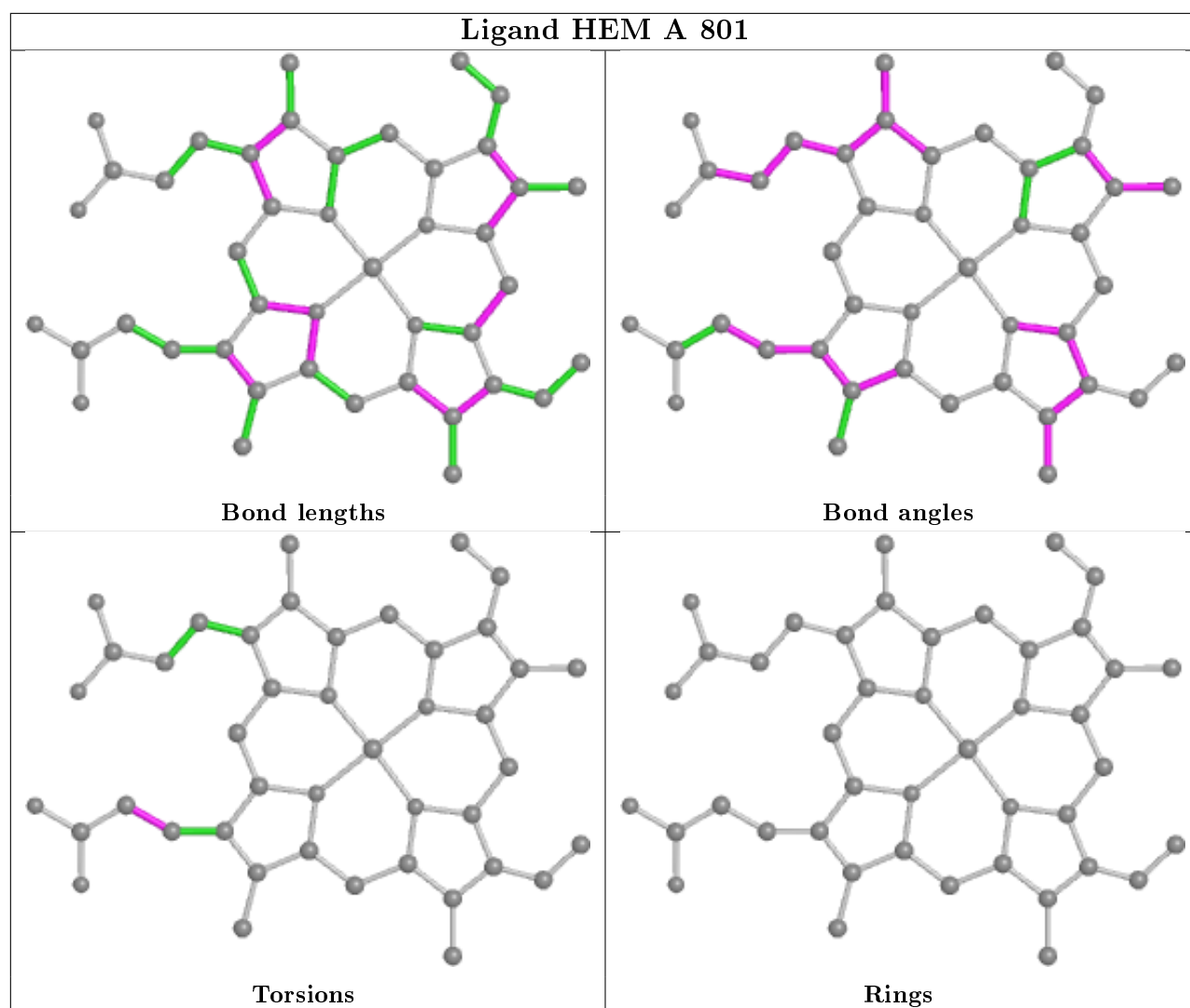
7 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	802	1ET	6	0
2	B	801	HEM	8	0
3	A	802	H4B	1	0
3	A	809	H4B	1	0
4	A	803	1ET	3	0
2	A	801	HEM	9	0
5	A	804	ACT	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	407/422 (96%)	0.50	43 (10%) 6 5	28, 44, 76, 99	0
1	B	411/422 (97%)	0.10	15 (3%) 42 42	26, 38, 62, 83	0
All	All	818/844 (96%)	0.30	58 (7%) 16 15	26, 41, 71, 99	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	300	PHE	6.8
1	A	716	TRP	5.8
1	A	715	VAL	5.1
1	A	300	PHE	5.0
1	A	488	PRO	4.5
1	A	486	LYS	4.3
1	A	299	ARG	4.3
1	A	355	PHE	4.1
1	A	507	GLN	4.1
1	B	718	GLY	4.0
1	A	713	THR	3.8
1	B	619	ARG	3.7
1	B	350	THR	3.5
1	B	616	LEU	3.3
1	A	352	ASP	3.3
1	A	567	VAL	3.3
1	A	678	TRP	3.2
1	A	318	LEU	3.1
1	B	352	ASP	3.0
1	A	390	SER	2.7
1	B	348	VAL	2.7
1	A	712	ASN	2.6
1	A	677	VAL	2.5
1	A	491	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	588	TYR	2.5
1	A	490	GLY	2.5
1	A	371	ARG	2.5
1	B	567	VAL	2.5
1	A	479	LEU	2.4
1	A	480	ILE	2.4
1	A	508	GLN	2.4
1	A	322	LEU	2.4
1	A	328	GLU	2.4
1	B	301	LEU	2.4
1	B	611	ALA	2.3
1	A	714	HIS	2.3
1	B	321	THR	2.3
1	A	504	ILE	2.3
1	A	382	GLU	2.3
1	A	489	ASP	2.3
1	B	615	ASP	2.2
1	A	514	ARG	2.2
1	A	566	ALA	2.2
1	A	321	THR	2.2
1	A	591	THR	2.2
1	A	385	ASN	2.2
1	A	676	TRP	2.2
1	A	511	LYS	2.2
1	B	328	GLU	2.2
1	A	619	ARG	2.1
1	B	620	LYS	2.1
1	A	329	HIS	2.1
1	A	388	ILE	2.1
1	A	442	ILE	2.1
1	A	667	ARG	2.0
1	A	565	PRO	2.0
1	B	678	TRP	2.0
1	A	351	LYS	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 carbohydrates in this entry.

6.4 Ligands ⓘ

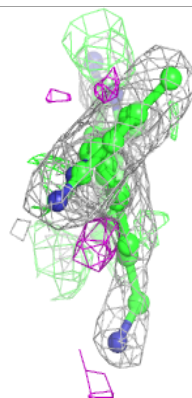
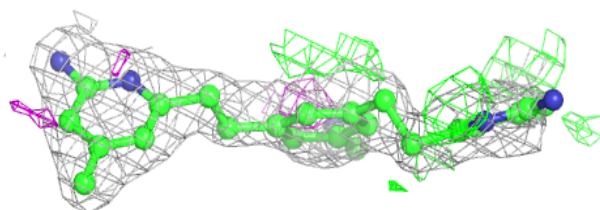
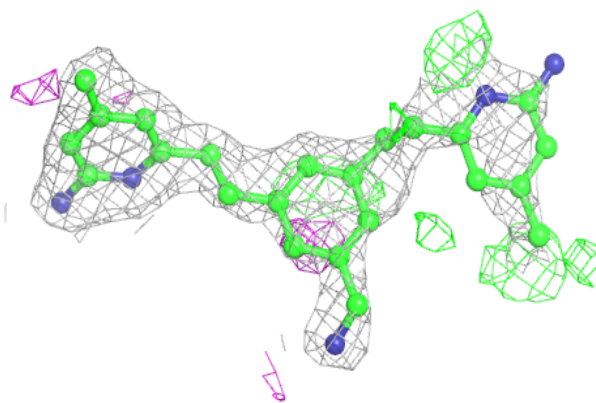
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	H4B	A	802	17/17	0.87	0.21	51,55,61,63	0
3	H4B	A	809	17/17	0.87	0.21	50,55,59,60	0
4	1ET	B	802	28/28	0.90	0.28	33,63,90,92	0
4	1ET	A	803	28/28	0.91	0.33	33,70,110,111	0
7	CL	A	808	1/1	0.95	0.18	58,58,58,58	0
7	CL	B	806	1/1	0.97	0.14	51,51,51,51	0
6	ZN	A	806	1/1	0.98	0.12	40,40,40,40	1
7	CL	A	807	1/1	0.98	0.11	50,50,50,50	0
5	ACT	B	803	4/4	0.98	0.11	48,50,50,51	0
2	HEM	B	801	43/43	0.98	0.18	28,31,51,61	0
2	HEM	A	801	43/43	0.98	0.21	29,32,57,68	0
5	ACT	A	804	4/4	0.98	0.16	53,55,58,61	0
7	CL	B	805	1/1	0.99	0.11	51,51,51,51	0
6	ZN	B	804	1/1	0.99	0.08	42,42,42,42	1
6	ZN	A	805	1/1	0.99	0.06	39,39,39,39	0

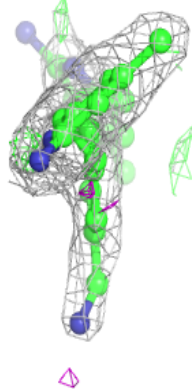
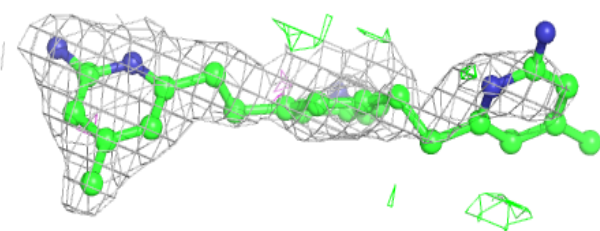
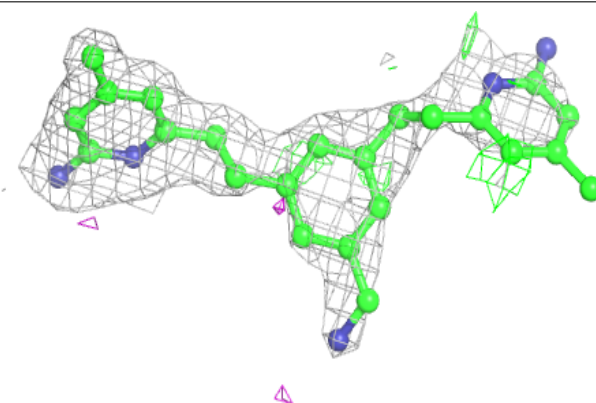
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 1ET B 802:

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

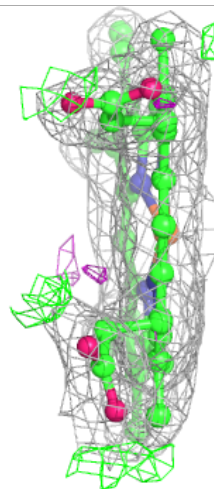
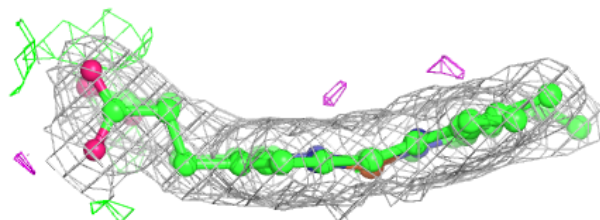
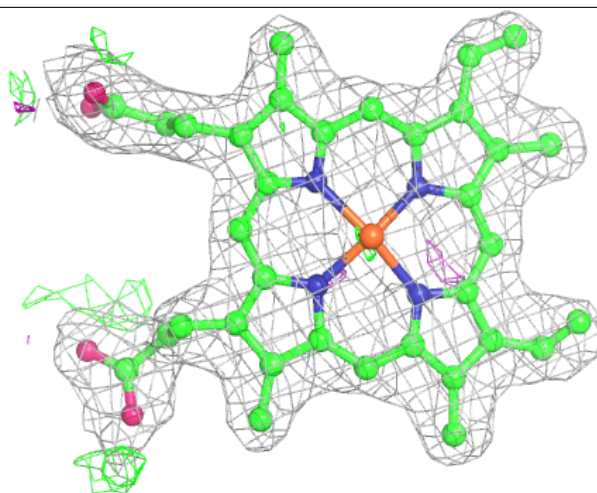
**Electron density around 1ET A 803:**

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



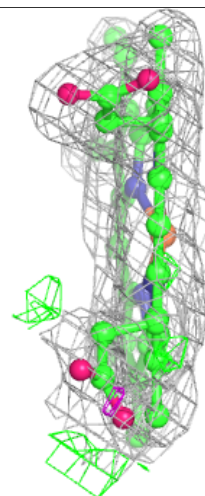
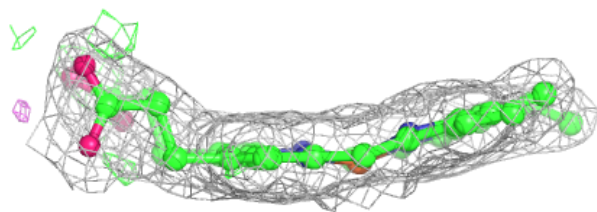
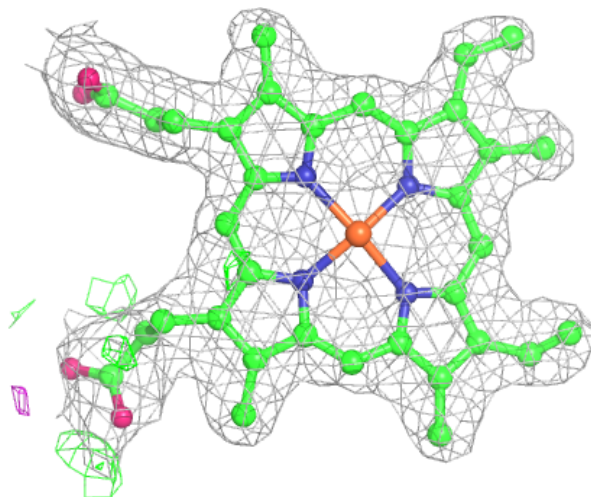
Electron density around HEM B 801:

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



Electron density around HEM A 801:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.