



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 10:08 PM BST

PDB ID : 4CTV
Title : Structure of rat neuronal nitric oxide synthase heme domain in complex with 6-(3-amino-2-(6-(2-(6-amino-4-methylpyridin-2-yl)ethyl) pyridin-2-yl)propyl)-4-methylpyridin-2-amine
Authors : Li, H.; Poulos, T.L.
Deposited on : 2014-03-15
Resolution : 1.78 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 : 2.13.1
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) : 2.13.1

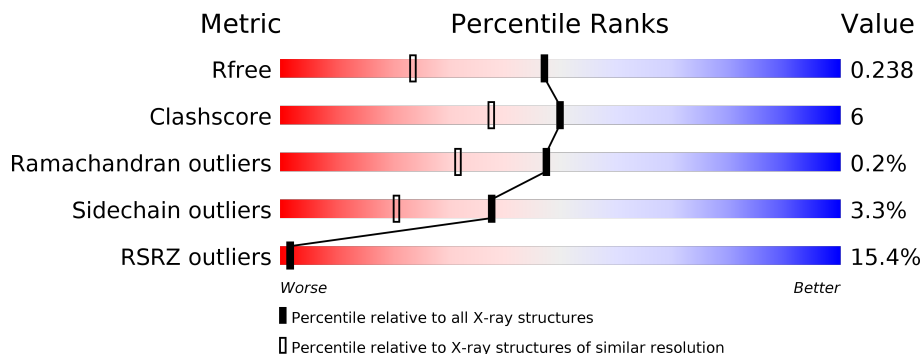
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.78 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	9185 (1.80-1.76)
Clashscore	141614	10184 (1.80-1.76)
Ramachandran outliers	138981	10051 (1.80-1.76)
Sidechain outliers	138945	10050 (1.80-1.76)
RSRZ outliers	127900	9032 (1.80-1.76)

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	
1	B	422	

2 Entry composition i

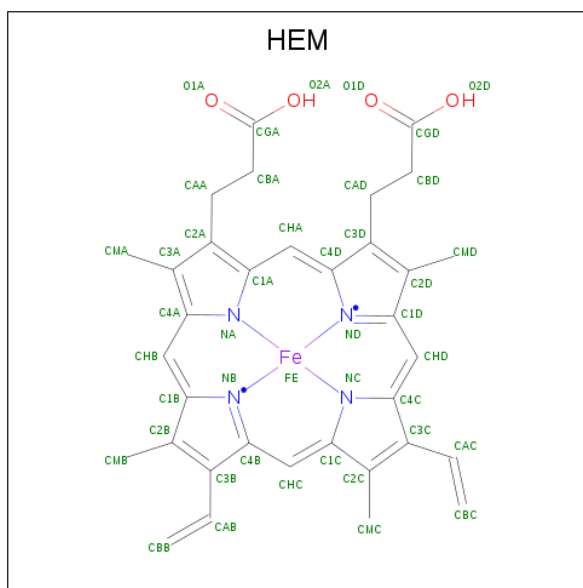
There are 7 unique types of molecules in this entry. The entry contains 7192 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	A	408	Total	C	N	O	S	0	3	1
			3326	2129	567	608	22			
1	B	411	Total	C	N	O	S	0	4	0
			3365	2156	574	613	22			

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



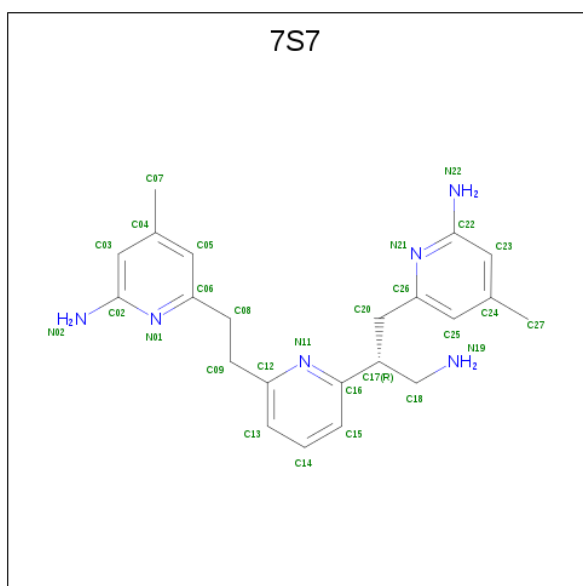
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 4 is 6-(3-amino-2-(6-(2-(6-amino-4-methylpyridin-2-yl)ethyl)pyridin-2-yl)propyl)-4-methylpyridin-2-amine (three-letter code: 7S7) (formula: C₂₂H₂₈N₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
4	A	1	Total	C	N		0	0
			28	22	6			

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	N		
4	B	1	28	22	6	0	0

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



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

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

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

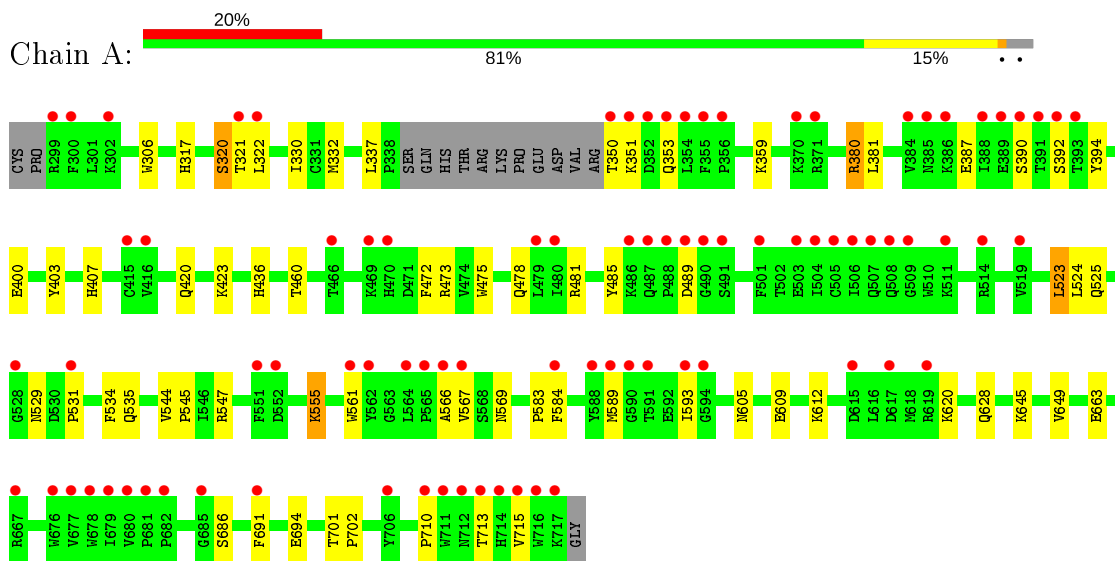
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	140	140	140	0	0
7	B	176	176	176	0	0

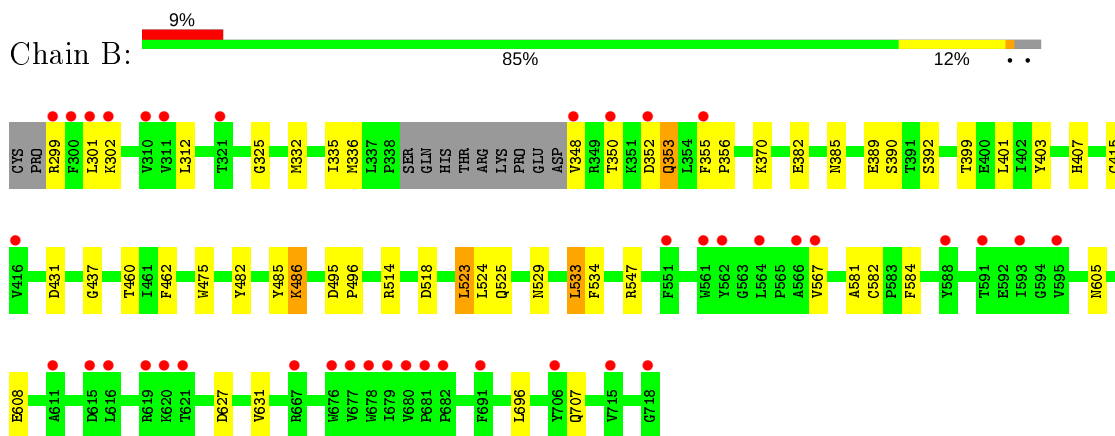
3 Residue-property plots [i](#)

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: 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	51.92Å 111.06Å 164.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.04 – 1.78 39.01 – 1.78	Depositor EDS
% Data completeness (in resolution range)	99.3 (39.04-1.78) 99.4 (39.01-1.78)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 1.78Å)	Xtrriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.200 , 0.239 0.200 , 0.238	Depositor DCC
R_{free} test set	4551 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	31.2	Xtrriage
Anisotropy	0.607	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 48.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7192	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.81% 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: HEM, ZN, H4B, 7S7, ACT

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	0.67	0/3428	0.76	0/4651
1	B	0.82	1/3471 (0.0%)	0.94	8/4706 (0.2%)
All	All	0.75	1/6899 (0.0%)	0.85	8/9357 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	437	GLY	N-CA	5.26	1.53	1.46

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	533	LEU	CB-CG-CD2	7.42	123.61	111.00
1	B	533	LEU	CB-CG-CD1	-6.92	99.23	111.00
1	B	401	LEU	CB-CG-CD2	-5.95	100.88	111.00
1	B	399	THR	CA-CB-CG2	-5.85	104.21	112.40
1	B	401	LEU	CB-CG-CD1	-5.42	101.79	111.00
1	B	431	ASP	CB-CG-OD1	5.34	123.11	118.30
1	B	523	LEU	CA-CB-CG	5.11	127.05	115.30
1	B	486	LYS	N-CA-C	-5.01	97.47	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3326	0	3237	42	0
1	B	3365	0	3284	35	0
2	A	43	0	30	4	0
2	B	43	0	30	7	0
3	A	17	0	15	0	0
3	B	17	0	15	0	0
4	A	28	0	28	6	0
4	B	28	0	28	6	0
5	A	4	0	3	0	0
5	B	4	0	3	0	0
6	A	1	0	0	0	0
7	A	140	0	0	3	0
7	B	176	0	0	4	0
All	All	7192	0	6673	79	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 6.

All (79) 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)
2:B:1719:HEM:HBD1	4:B:1721:7S7:C14	2.16	0.76
1:A:523:LEU:HD22	1:A:531:PRO:HB2	1.69	0.73
1:B:382:GLU:HG3	7:B:2020:HOH:O	1.89	0.72
1:A:420:GLN:OE1	1:A:423:LYS:HE2	1.94	0.68
1:B:608:GLU:HG3	7:B:2146:HOH:O	1.96	0.65
2:A:1717:HEM:HBD1	4:A:1719:7S7:H14	1.80	0.64
1:A:567:VAL:HG21	4:A:1719:7S7:C14	2.27	0.64
2:B:1719:HEM:HBA2	4:B:1721:7S7:H17	1.80	0.64
2:B:1719:HEM:O2D	7:B:2174:HOH:O	2.15	0.63
1:A:306:TRP:CD2	1:B:336:MET:HE3	2.35	0.62
1:B:462:PHE:HB2	1:B:581:ALA:HB3	1.81	0.61
1:B:325:GLY:O	1:B:332:MET:HG3	2.01	0.60
1:B:485:TYR:CZ	1:B:514:ARG:HA	2.38	0.58
1:B:355[B]:PHE:HB2	1:B:356:PRO:CD	2.33	0.58
1:A:380:ARG:HD3	1:A:400:GLU:OE2	2.06	0.56
1:B:605:ASN:ND2	7:B:2144:HOH:O	2.37	0.56
1:A:350:THR:N	1:A:353:GLN:NE2	2.53	0.55
1:A:628:GLN:HG2	1:B:631:VAL:HG11	1.89	0.54
1:A:686:SER:HA	1:A:691:PHE:CG	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:ILE:HD11	1:B:696:LEU:HB3	1.91	0.53
1:A:525:GLN:HG3	1:A:529:ASN:O	2.09	0.53
1:B:370:LYS:N	1:B:370:LYS:HD3	2.24	0.53
1:B:524:LEU:HD12	1:B:534:PHE:CD2	2.46	0.51
1:B:355[A]:PHE:CE1	1:B:385:ASN:HB2	2.46	0.51
2:B:1719:HEM:HBD1	4:B:1721:7S7:C13	2.40	0.50
1:A:351:LYS:HE2	1:A:392:SER:HB3	1.92	0.50
1:B:350:THR:O	1:B:353:GLN:HG2	2.12	0.50
1:A:694:GLU:HB3	1:B:335:ILE:HD13	1.94	0.50
1:A:460:THR:O	1:A:583:PRO:HD2	2.11	0.49
1:B:567:VAL:HG21	4:B:1721:7S7:C14	2.42	0.49
1:A:609:GLU:HG3	7:A:2108:HOH:O	2.12	0.49
1:A:306:TRP:CE2	1:B:336:MET:HE3	2.48	0.49
1:A:420:GLN:OE1	1:A:423:LYS:CE	2.61	0.48
1:B:403:TYR:CE2	1:B:407:HIS:CE1	3.01	0.48
2:A:1717:HEM:HBD1	4:A:1719:7S7:C14	2.44	0.47
1:A:605:ASN:ND2	7:A:2105:HOH:O	2.41	0.47
1:B:460:THR:O	1:B:582:CYS:HA	2.15	0.47
1:A:472:PHE:HA	1:A:525:GLN:O	2.15	0.47
1:A:359:LYS:HE2	1:A:381:LEU:HD21	1.96	0.47
1:A:567:VAL:HG23	4:A:1719:7S7:H25	1.96	0.47
1:A:524:LEU:O	1:A:531:PRO:HA	2.15	0.46
1:B:302:LYS:HA	1:B:312:LEU:O	2.15	0.46
1:A:387:GLU:OE2	1:A:394:TYR:HA	2.16	0.46
1:A:478:GLN:HB2	1:A:481:ARG:HG3	1.96	0.46
1:A:436:HIS:CD2	1:A:534:PHE:HE2	2.34	0.46
1:A:403:TYR:CE2	1:A:407:HIS:CE1	3.04	0.45
1:B:485:TYR:CE1	1:B:514:ARG:HA	2.51	0.45
1:A:317:HIS:O	1:A:320:SER:HB3	2.16	0.45
1:A:321:THR:HG22	7:A:2005:HOH:O	2.16	0.45
1:B:567:VAL:HG23	4:B:1721:7S7:H25	1.99	0.45
1:A:332:MET:CE	1:B:301:LEU:HD22	2.47	0.45
1:A:473:ARG:NH2	1:A:710:PRO:HD3	2.32	0.44
1:B:302:LYS:HE3	1:B:302:LYS:HB2	1.70	0.44
1:B:523:LEU:HD13	1:B:533:LEU:HG	1.99	0.44
1:A:321:THR:HG23	1:A:322:LEU:HG	2.00	0.44
1:A:555:LYS:HB3	1:A:555:LYS:NZ	2.32	0.43
2:B:1719:HEM:HBD1	4:B:1721:7S7:H14	1.97	0.43
1:B:350:THR:OG1	1:B:353:GLN:NE2	2.51	0.43
1:A:475:TRP:CZ2	1:A:531:PRO:HG3	2.53	0.43
1:A:561:TRP:CD1	1:A:593:ILE:HG12	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:475:TRP:HB2	1:B:523:LEU:HB3	2.00	0.42
1:A:584:PHE:CD1	2:A:1717:HEM:CAC	3.03	0.42
2:A:1717:HEM:HBA1	4:A:1719:7S7:H17	2.02	0.42
1:A:475:TRP:CE2	1:A:710:PRO:HB2	2.54	0.42
1:B:482:TYR:HA	1:B:518:ASP:O	2.20	0.42
1:B:567:VAL:N	1:B:584:PHE:O	2.53	0.41
1:A:589:MET:HA	1:A:649:VAL:O	2.20	0.41
1:A:337:LEU:HD21	4:A:1719:7S7:H03	2.02	0.41
1:B:355[B]:PHE:HB2	1:B:356:PRO:HD3	2.03	0.41
1:B:495:ASP:HA	1:B:496:PRO:HD3	1.87	0.41
1:B:525:GLN:HG3	1:B:529:ASN:O	2.21	0.41
1:A:701:THR:HA	1:A:702:PRO:C	2.42	0.41
1:A:478:GLN:HA	1:A:566:ALA:O	2.20	0.40
1:A:473:ARG:HD2	1:A:473:ARG:HA	1.93	0.40
2:B:1719:HEM:HBA1	2:B:1719:HEM:HMA2	2.02	0.40
1:A:332:MET:HE3	1:B:301:LEU:HD22	2.04	0.40
1:A:544:VAL:HA	1:A:545:PRO:HD2	1.95	0.40
1:B:299:ARG:HB3	1:B:299:ARG:NH1	2.36	0.40
1:B:415:CYS:HB2	2:B:1719:HEM:ND	2.37	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	407/422 (96%)	394 (97%)	12 (3%)	1 (0%)	47	32
1	B	411/422 (97%)	400 (97%)	10 (2%)	1 (0%)	47	32
All	All	818/844 (97%)	794 (97%)	22 (3%)	2 (0%)	47	32

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	352	ASP
1	A	489	ASP

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%)	351 (96%)	15 (4%)	30	14
1	B	370/377 (98%)	361 (98%)	9 (2%)	49	33
All	All	736/754 (98%)	712 (97%)	24 (3%)	38	21

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	320	SER
1	A	380	ARG
1	A	390	SER
1	A	485	TYR
1	A	523	LEU
1	A	535	GLN
1	A	547	ARG
1	A	555	LYS
1	A	569	ASN
1	A	612	LYS
1	A	620	LYS
1	A	645	LYS
1	A	663	GLU
1	A	713	THR
1	A	715	VAL
1	B	348	VAL
1	B	353	GLN
1	B	389	GLU
1	B	390	SER
1	B	392	SER
1	B	486	LYS
1	B	547	ARG

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Mol	Chain	Res	Type
1	B	627	ASP
1	B	707	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	353	GLN
1	A	436	HIS
1	A	454	ASN
1	A	507	GLN
1	A	527	ASN
1	A	569	ASN
1	A	642	GLN
1	A	697	ASN
1	B	353	GLN
1	B	364	GLN
1	B	454	ASN
1	B	507	GLN
1	B	601	ASN
1	B	605	ASN
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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 1 is 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
3	H4B	A	1718	-	16,18,18	1.86	2 (12%)	11,26,26	3.29	5 (45%)
4	7S7	B	1721	-	29,30,30	1.21	3 (10%)	37,41,41	2.23	13 (35%)
2	HEM	B	1719	1	27,50,50	1.18	4 (14%)	17,82,82	2.12	6 (35%)
2	HEM	A	1717	1	27,50,50	1.14	3 (11%)	17,82,82	1.89	3 (17%)
5	ACT	B	1722	-	1,3,3	1.28	0	0,3,3	0.00	-
5	ACT	A	1720	-	1,3,3	2.22	1 (100%)	0,3,3	0.00	-
4	7S7	A	1719	-	29,30,30	1.42	3 (10%)	37,41,41	2.42	12 (32%)
3	H4B	B	1720	-	16,18,18	1.66	2 (12%)	11,26,26	2.97	7 (63%)

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	H4B	A	1718	-	-	0/8/17/17	0/2/2/2
4	7S7	B	1721	-	-	4/15/15/15	0/3/3/3
2	HEM	B	1719	1	-	0/6/54/54	-
2	HEM	A	1717	1	-	2/6/54/54	-
4	7S7	A	1719	-	-	7/15/15/15	0/3/3/3
3	H4B	B	1720	-	-	1/8/17/17	0/2/2/2

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1718	H4B	C7-N8	5.28	1.53	1.44
4	A	1719	7S7	C20-C17	-4.03	1.49	1.54
4	A	1719	7S7	C16-N11	3.85	1.39	1.34
3	A	1718	H4B	C2-N2	3.52	1.40	1.33
3	B	1720	H4B	C7-N8	3.42	1.50	1.44
4	B	1721	7S7	C20-C17	-3.33	1.50	1.54
3	B	1720	H4B	C8A-N1	2.88	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1719	HEM	C4D-C3D	2.76	1.48	1.42
2	A	1717	HEM	C4D-C3D	2.62	1.48	1.42
4	B	1721	7S7	C22-N21	2.53	1.39	1.35
2	A	1717	HEM	C1A-NA	2.52	1.41	1.36
4	A	1719	7S7	C23-C24	2.44	1.43	1.39
5	A	1720	ACT	CH3-C	2.22	1.51	1.48
2	B	1719	HEM	C1A-NA	2.22	1.40	1.36
2	B	1719	HEM	C3C-C2C	-2.18	1.37	1.40
2	A	1717	HEM	C3B-C2B	-2.15	1.37	1.40
2	B	1719	HEM	C1C-C2C	-2.06	1.37	1.42
4	B	1721	7S7	C25-C24	2.05	1.42	1.39

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1718	H4B	C4-C4A-C8A	8.55	122.16	114.57
4	A	1719	7S7	C02-N01-C06	8.50	124.55	118.10
4	B	1721	7S7	C02-N01-C06	6.93	123.35	118.10
3	B	1720	H4B	C4-C4A-C8A	5.76	119.69	114.57
2	A	1717	HEM	CBA-CAA-C2A	-4.96	103.34	112.49
4	A	1719	7S7	C27-C24-C23	4.84	128.10	120.94
4	A	1719	7S7	C27-C24-C25	-4.67	114.02	120.94
3	B	1720	H4B	N2-C2-N1	4.58	124.38	117.25
4	B	1721	7S7	C16-N11-C12	4.37	123.42	118.61
4	A	1719	7S7	C09-C12-N11	4.01	121.92	115.95
2	B	1719	HEM	CBA-CAA-C2A	-3.94	105.22	112.49
4	A	1719	7S7	C05-C06-N01	-3.89	118.77	122.90
3	A	1718	H4B	C2-N1-C8A	3.86	123.20	114.54
2	B	1719	HEM	C1D-C2D-C3D	-3.83	104.33	107.00
2	B	1719	HEM	C4A-C3A-C2A	-3.79	104.36	107.00
3	B	1720	H4B	N3-C2-N1	-3.60	119.78	125.42
4	B	1721	7S7	C15-C16-N11	-3.48	118.84	122.45
2	A	1717	HEM	CBD-CAD-C3D	-3.32	106.36	112.48
3	A	1718	H4B	C4A-N5-C6	-3.21	112.42	121.16
4	B	1721	7S7	C27-C24-C23	3.17	125.63	120.94
4	B	1721	7S7	C22-N21-C26	3.16	120.50	118.10
4	B	1721	7S7	C09-C12-N11	2.99	120.40	115.95
4	B	1721	7S7	C27-C24-C25	-2.96	116.55	120.94
3	B	1720	H4B	C2-N1-C8A	2.96	121.17	114.54
2	A	1717	HEM	CAD-CBD-CGD	-2.95	107.72	112.67
4	B	1721	7S7	C05-C06-N01	-2.94	119.78	122.90
4	B	1721	7S7	C04-C05-C06	-2.76	118.51	120.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1719	HEM	CAD-CBD-CGD	2.76	117.30	112.67
4	A	1719	7S7	N22-C22-N21	-2.74	112.16	116.49
3	B	1720	H4B	C4-N3-C2	2.67	120.17	115.93
4	B	1721	7S7	C18-C17-C16	2.65	115.59	111.00
4	A	1719	7S7	C13-C12-N11	-2.56	119.16	122.41
4	A	1719	7S7	C20-C26-C25	-2.54	115.64	121.04
3	A	1718	H4B	N3-C2-N1	-2.53	121.45	125.42
4	B	1721	7S7	C13-C12-N11	-2.49	119.25	122.41
4	A	1719	7S7	C16-N11-C12	2.48	121.34	118.61
3	B	1720	H4B	O9-C9-C6	-2.40	103.25	108.98
2	B	1719	HEM	CMB-C2B-C3B	2.36	129.09	124.68
2	B	1719	HEM	CMA-C3A-C2A	2.36	129.39	124.94
3	B	1720	H4B	C4-C4A-N5	2.32	121.07	119.12
4	A	1719	7S7	C23-C22-N22	2.27	127.01	121.82
4	A	1719	7S7	C04-C05-C06	-2.20	118.88	120.32
4	B	1721	7S7	C20-C17-C16	-2.19	106.48	111.14
4	B	1721	7S7	C05-C04-C03	2.16	120.67	118.09
3	A	1718	H4B	O9-C9-C6	-2.06	104.04	108.98
4	A	1719	7S7	N02-C02-N01	2.02	119.69	116.49

There are no chirality outliers.

All (14) torsion outliers are listed below:

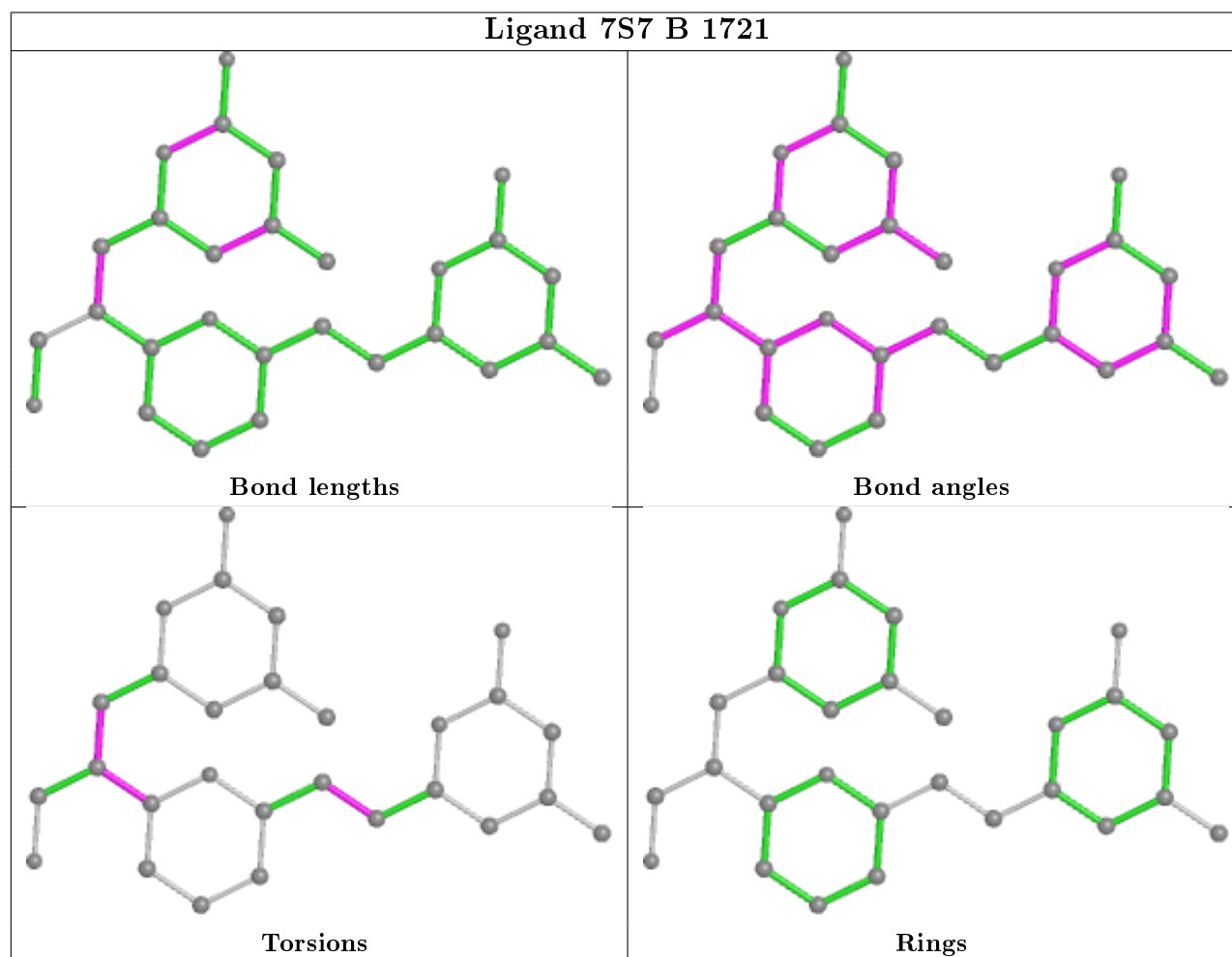
Mol	Chain	Res	Type	Atoms
4	B	1721	7S7	C16-C17-C20-C26
4	B	1721	7S7	C06-C08-C09-C12
4	A	1719	7S7	C16-C17-C20-C26
4	A	1719	7S7	C20-C17-C18-N19
4	A	1719	7S7	C16-C17-C18-N19
4	A	1719	7S7	N11-C16-C17-C18
4	B	1721	7S7	C15-C16-C17-C18
4	A	1719	7S7	C15-C16-C17-C18
4	A	1719	7S7	C06-C08-C09-C12
2	A	1717	HEM	C2D-C3D-CAD-CBD
2	A	1717	HEM	C4D-C3D-CAD-CBD
3	B	1720	H4B	O10-C10-C9-O9
4	B	1721	7S7	C18-C17-C20-C26
4	A	1719	7S7	C18-C17-C20-C26

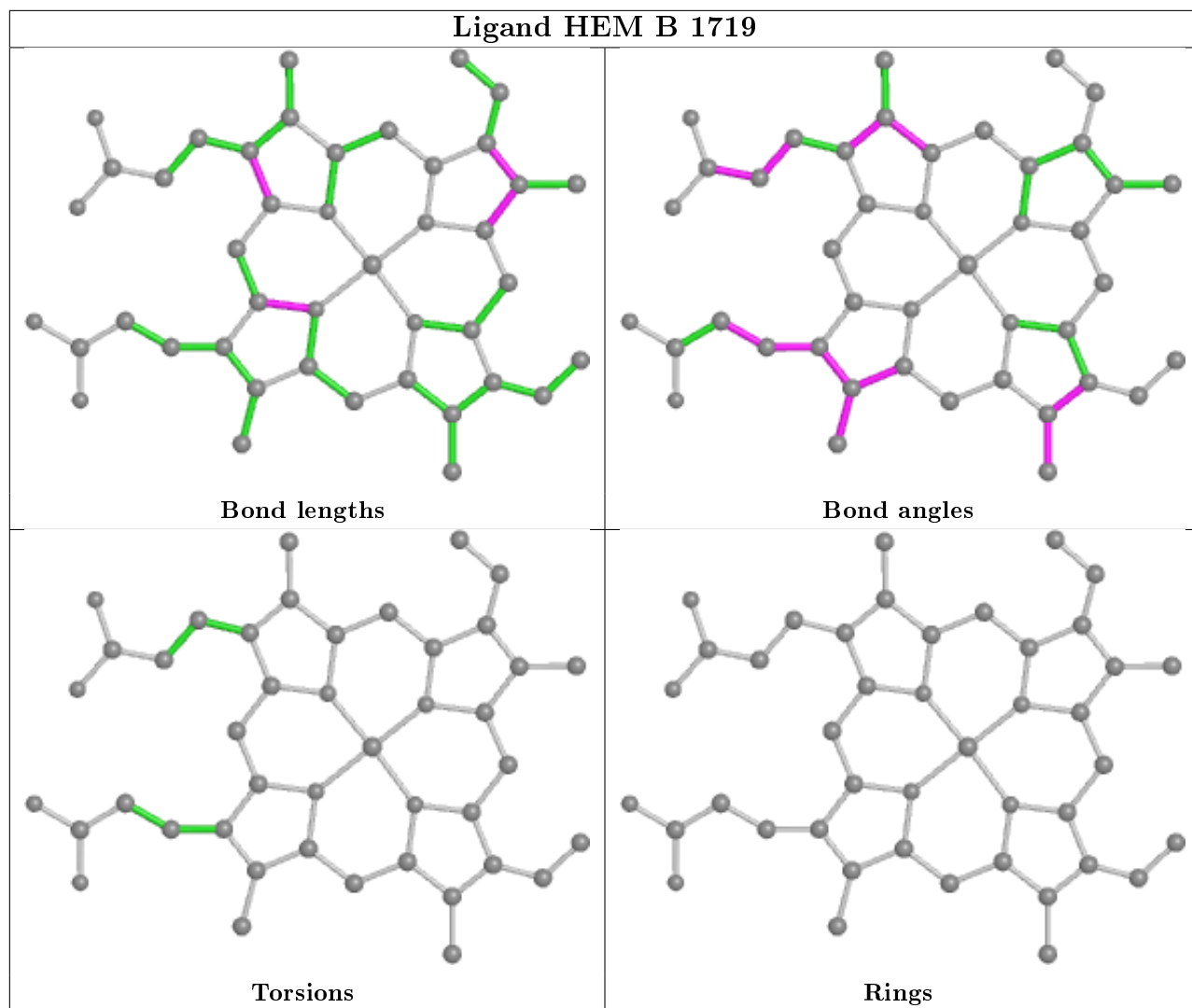
There are no ring outliers.

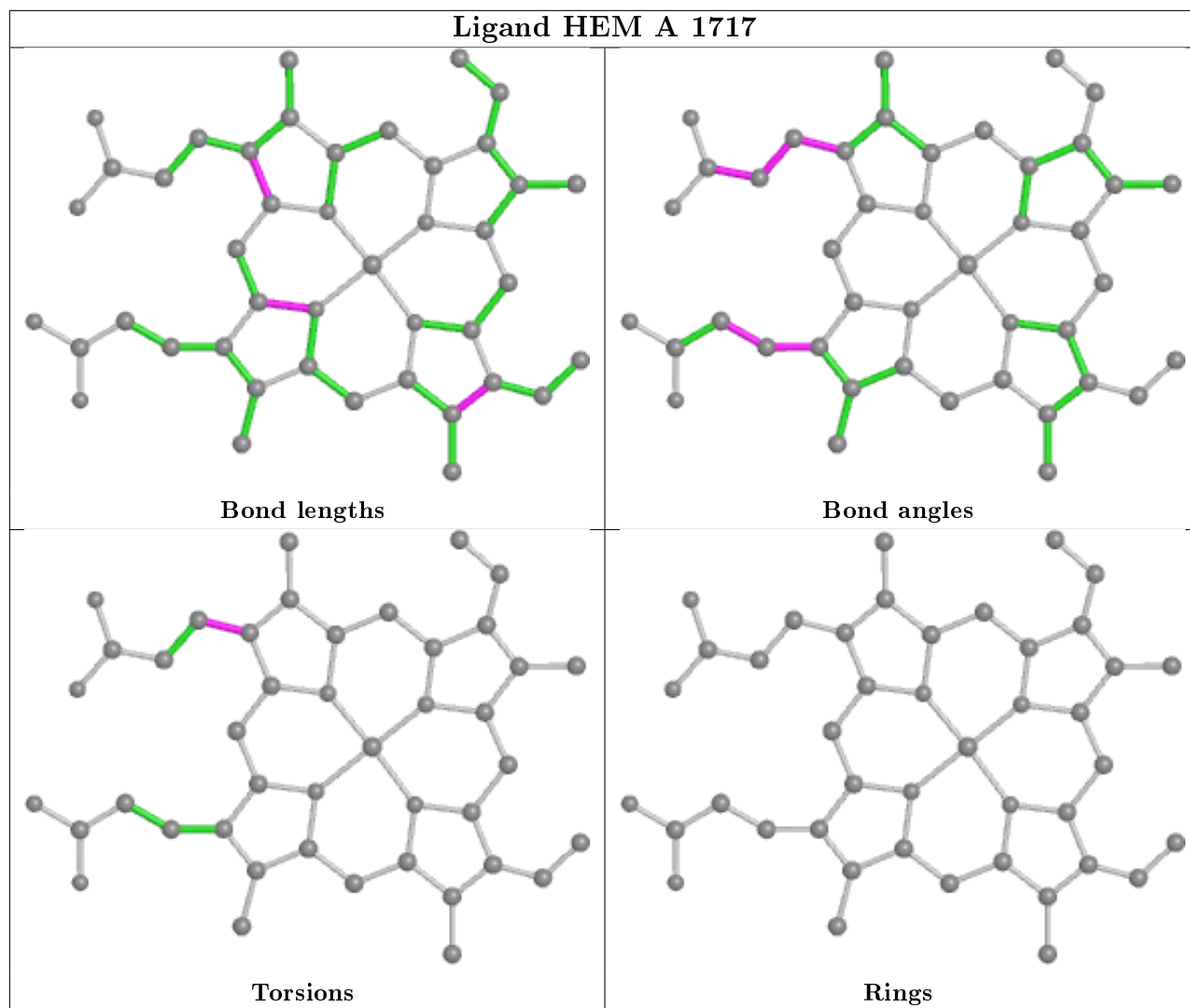
4 monomers are involved in 16 short contacts:

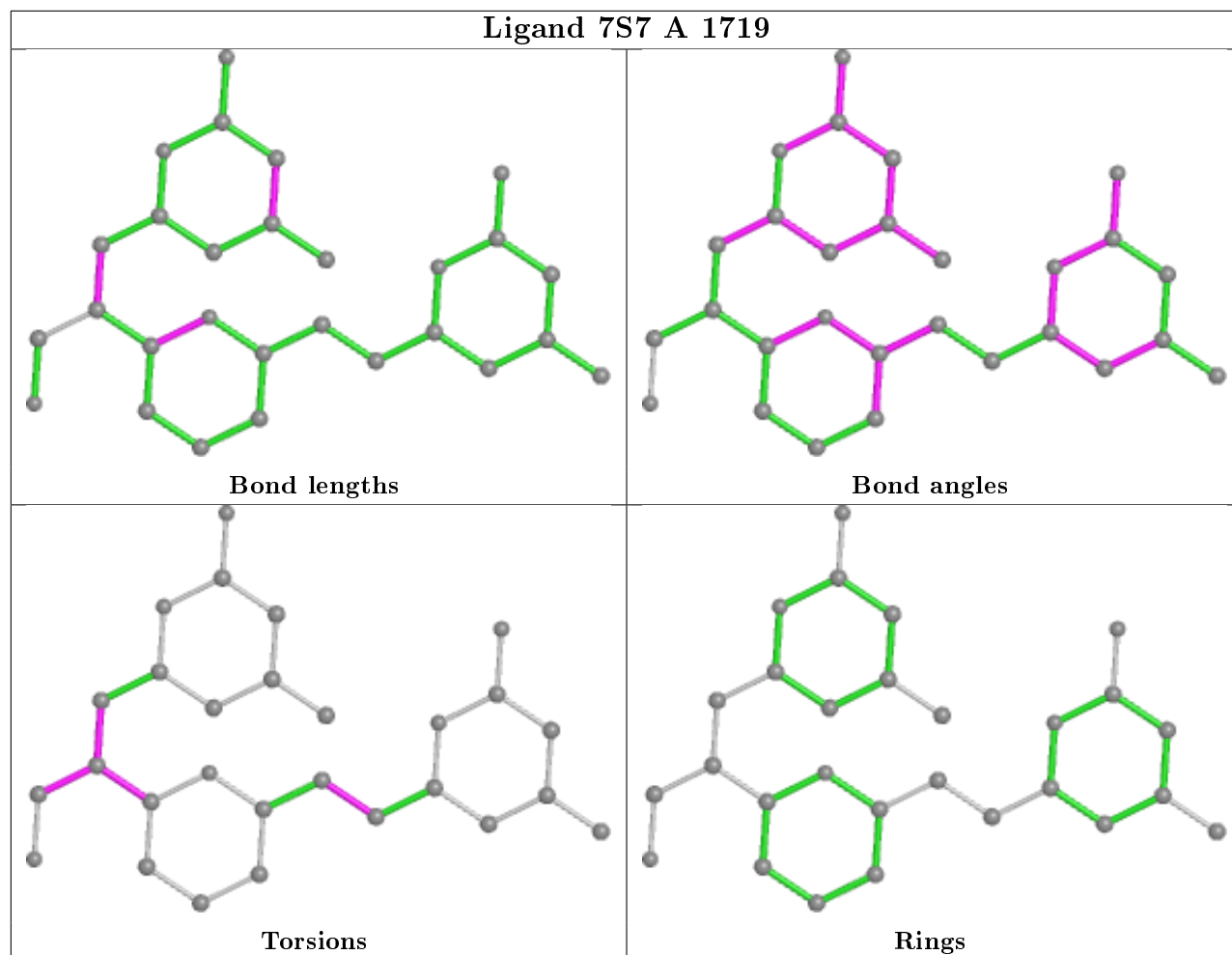
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1721	7S7	6	0
2	B	1719	HEM	7	0
2	A	1717	HEM	4	0
4	A	1719	7S7	6	0

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 [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	408/422 (96%)	1.11	86 (21%) 1 0	25, 49, 85, 104	0
1	B	411/422 (97%)	0.58	40 (9%) 7 7	21, 38, 66, 88	0
All	All	819/844 (97%)	0.84	126 (15%) 2 2	21, 43, 80, 104	0

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	716	TRP	9.5
1	A	488	PRO	8.5
1	B	300	PHE	8.5
1	A	715	VAL	7.9
1	B	348	VAL	7.8
1	A	355	PHE	7.4
1	A	713	THR	5.7
1	A	300	PHE	5.4
1	A	352	ASP	5.1
1	A	717	LYS	4.8
1	B	619	ARG	4.7
1	A	507	GLN	4.6
1	B	350	THR	4.5
1	B	616	LEU	4.5
1	B	677	VAL	4.5
1	A	551	PHE	4.4
1	A	619	ARG	4.4
1	A	486	LYS	4.4
1	B	718	GLY	4.4
1	A	390	SER	4.4
1	A	506	ILE	4.4
1	A	491	SER	4.3
1	B	680	VAL	4.2
1	A	676	TRP	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	706	TYR	4.1
1	A	351	LYS	4.1
1	A	392	SER	4.1
1	A	469	LYS	4.1
1	B	355[A]	PHE	4.0
1	A	389	GLU	3.9
1	A	480	ILE	3.9
1	A	353	GLN	3.8
1	A	386	LYS	3.8
1	A	503	GLU	3.8
1	B	615	ASP	3.8
1	A	588	TYR	3.7
1	A	714	HIS	3.6
1	A	388	ILE	3.6
1	A	712	ASN	3.6
1	B	299	ARG	3.5
1	B	706	TYR	3.5
1	A	711	TRP	3.5
1	A	489	ASP	3.5
1	A	677	VAL	3.5
1	A	593	ILE	3.5
1	A	678	TRP	3.4
1	B	678	TRP	3.4
1	A	321	THR	3.4
1	A	680	VAL	3.4
1	B	561	TRP	3.4
1	A	391	THR	3.3
1	A	511	LYS	3.3
1	A	385	ASN	3.3
1	A	528	GLY	3.2
1	B	310	VAL	3.2
1	A	350	THR	3.2
1	A	504	ILE	3.2
1	A	508	GLN	3.2
1	A	490	GLY	3.1
1	B	676	TRP	3.1
1	B	591	THR	3.1
1	A	561	TRP	3.1
1	A	591	THR	3.1
1	B	321	THR	3.0
1	A	679	ILE	3.0
1	A	509	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	620	LYS	3.0
1	B	562	TYR	3.0
1	B	691	PHE	3.0
1	B	679	ILE	2.9
1	A	487	GLN	2.9
1	A	617	ASP	2.9
1	B	301	LEU	2.9
1	A	567	VAL	2.8
1	B	595	VAL	2.8
1	B	302	LYS	2.8
1	B	588	TYR	2.8
1	A	384	VAL	2.8
1	A	479	LEU	2.8
1	A	691	PHE	2.7
1	A	505	CYS	2.7
1	B	682	PRO	2.7
1	B	567	VAL	2.7
1	A	370	LYS	2.7
1	A	393	THR	2.7
1	A	710	PRO	2.7
1	A	514	ARG	2.6
1	A	416	VAL	2.6
1	A	299	ARG	2.6
1	B	352	ASP	2.6
1	B	667	ARG	2.5
1	A	302	LYS	2.5
1	A	466	THR	2.5
1	A	552	ASP	2.5
1	A	501	PHE	2.5
1	B	311	VAL	2.5
1	A	681	PRO	2.5
1	A	682	PRO	2.5
1	B	611	ALA	2.5
1	A	564	LEU	2.5
1	A	685	GLY	2.5
1	A	562	TYR	2.4
1	A	565	PRO	2.4
1	A	322	LEU	2.4
1	A	470	HIS	2.4
1	A	519	VAL	2.4
1	B	564	LEU	2.4
1	A	584	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	354	LEU	2.3
1	B	416	VAL	2.3
1	B	593	ILE	2.3
1	A	594	GLY	2.2
1	A	667	ARG	2.2
1	A	356	PRO	2.2
1	A	531	PRO	2.2
1	B	681	PRO	2.2
1	A	615	ASP	2.2
1	B	566	ALA	2.2
1	A	371	ARG	2.1
1	B	715	VAL	2.1
1	A	415	CYS	2.1
1	A	566	ALA	2.1
1	A	589	MET	2.0
1	B	551	PHE	2.0
1	B	621	THR	2.0
1	A	590	GLY	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 monosaccharides 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.

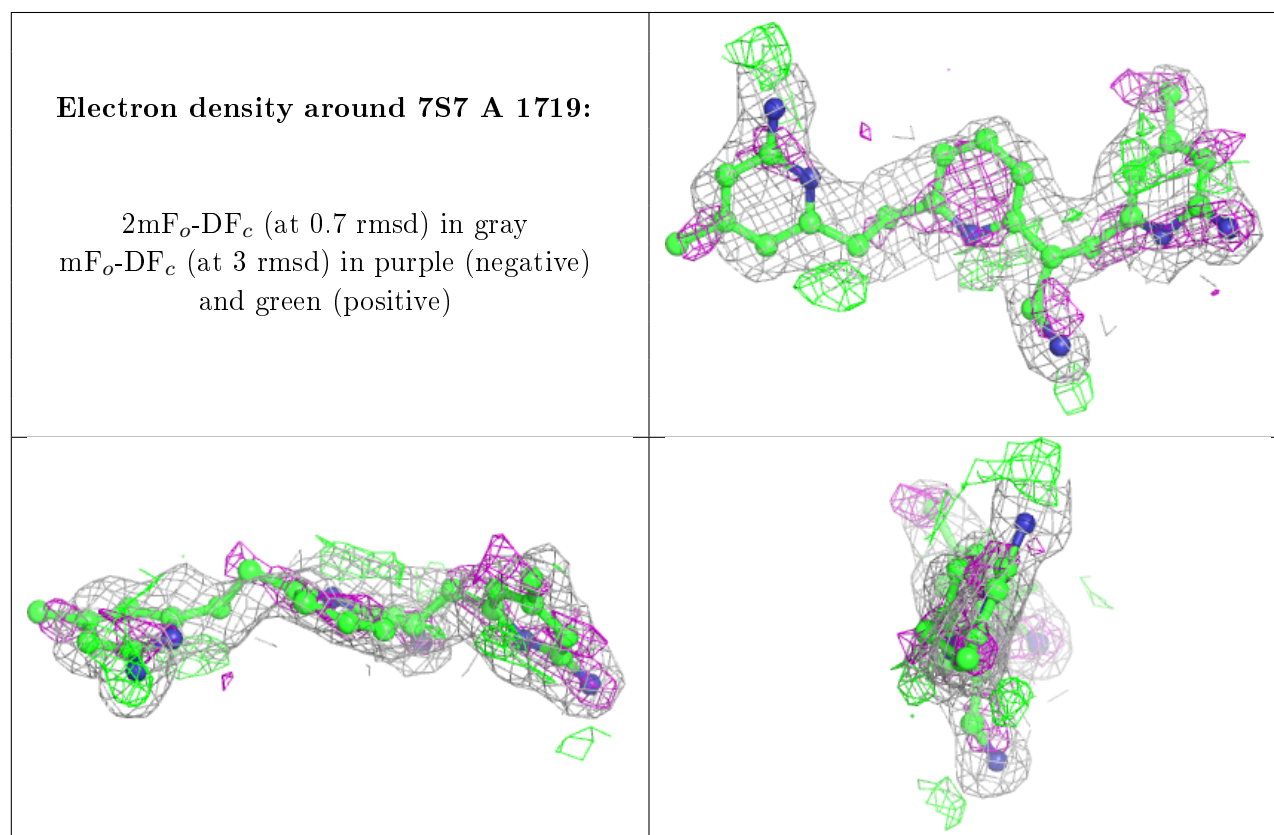
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	7S7	A	1719	28/28	0.87	0.17	16,43,50,52	0
4	7S7	B	1721	28/28	0.90	0.19	26,51,63,64	0
5	ACT	A	1720	4/4	0.91	0.22	65,69,72,74	0
5	ACT	B	1722	4/4	0.94	0.12	57,62,63,63	0
3	H4B	B	1720	17/17	0.95	0.17	29,32,36,38	0

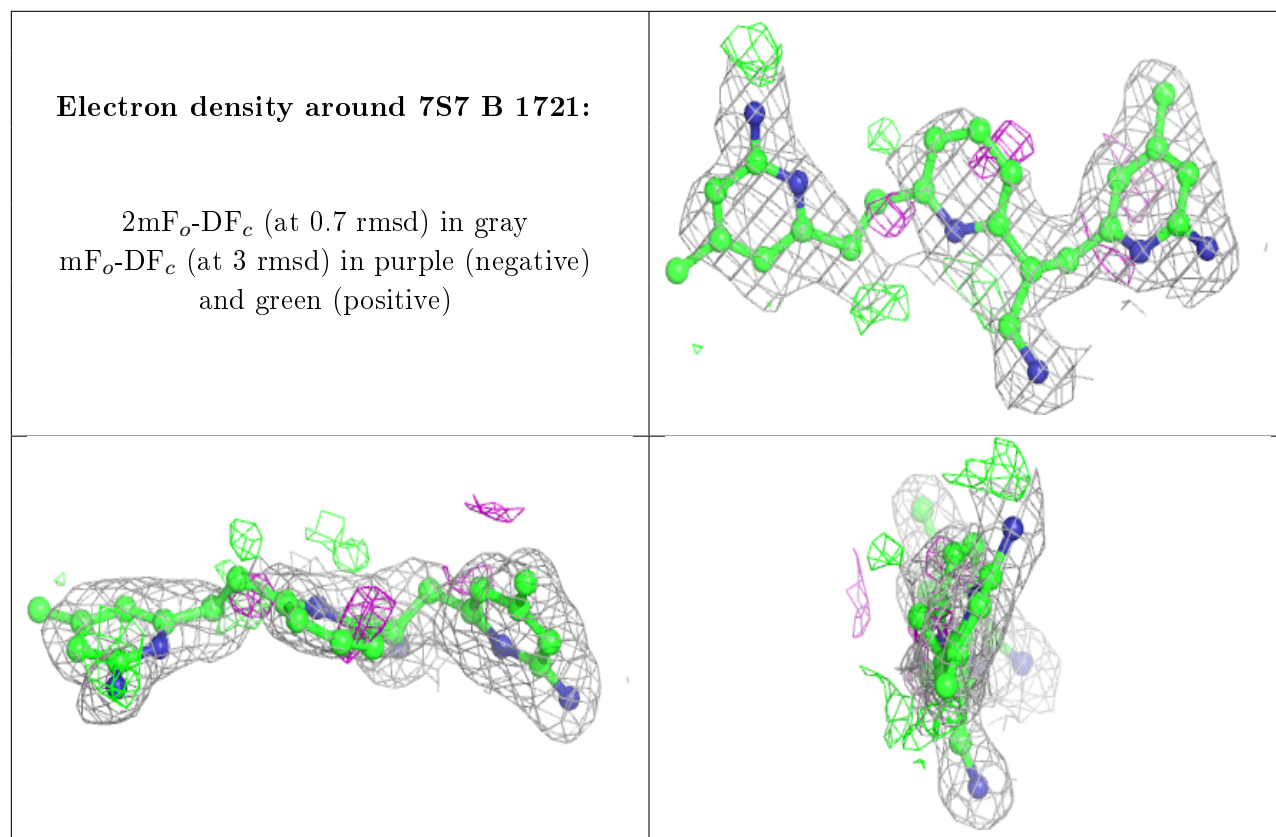
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	HEM	B	1719	43/43	0.97	0.16	21,29,47,57	0
2	HEM	A	1717	43/43	0.97	0.18	28,32,39,45	0
3	H4B	A	1718	17/17	0.97	0.12	25,28,31,33	0
6	ZN	A	1721	1/1	1.00	0.09	39,39,39,39	0

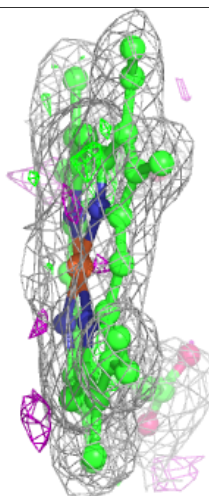
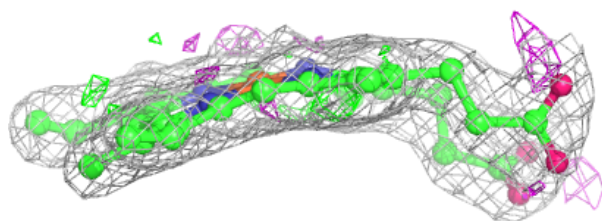
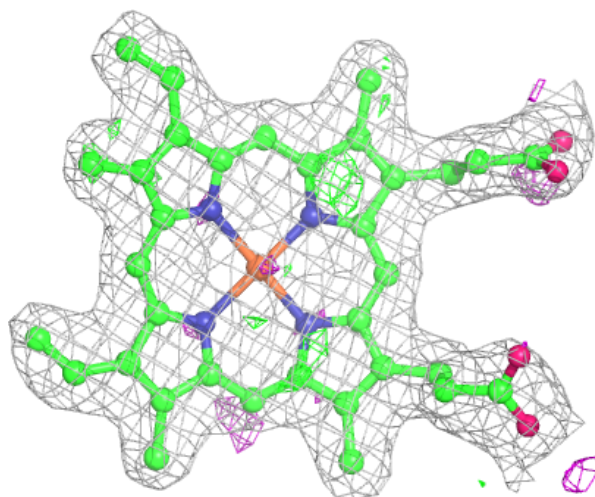
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

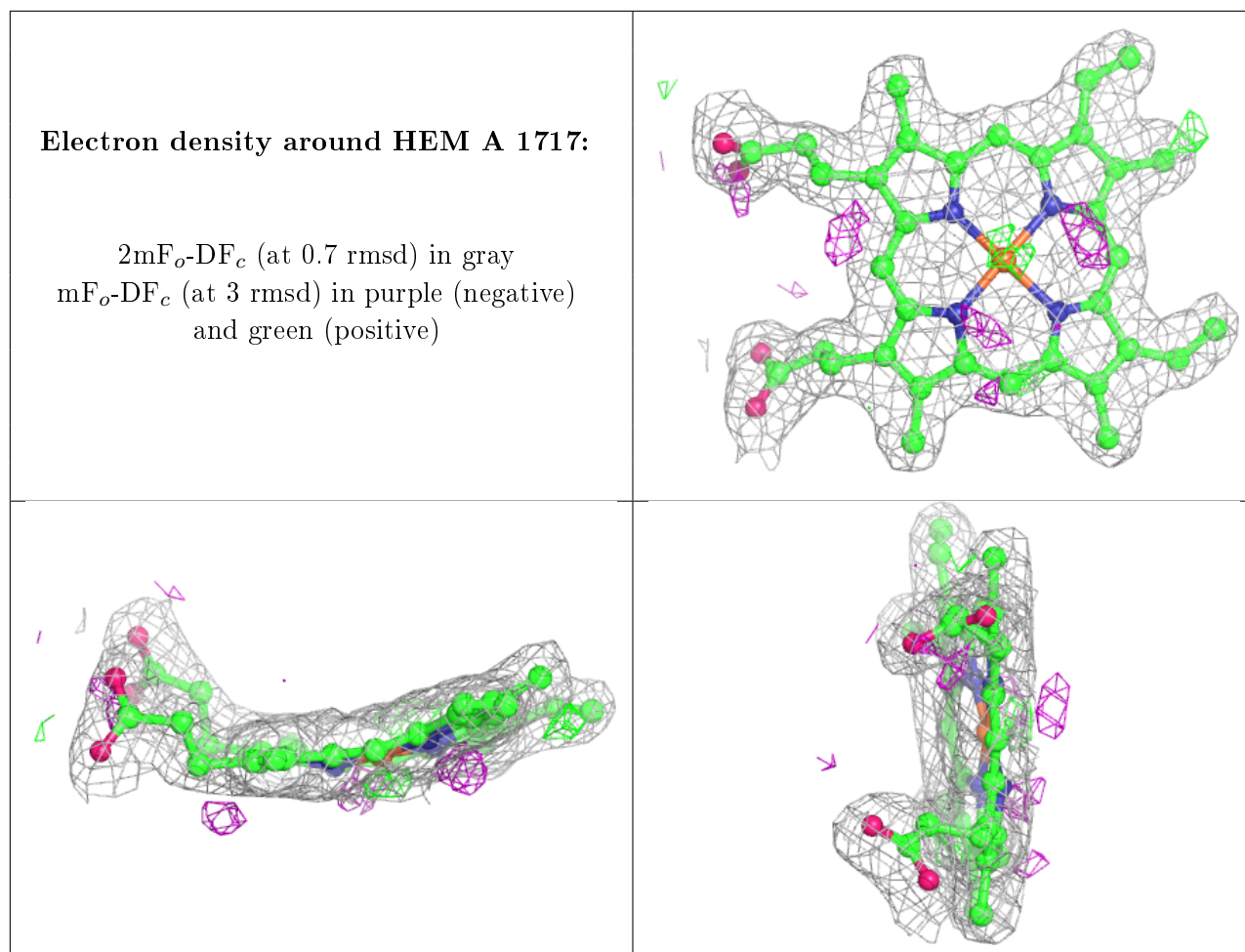




Electron density around HEM B 1719:

$2mF_o-DF_c$ (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.