



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 11:30 PM UTC

PDB ID : 4CTV / pdb_00004ctv
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

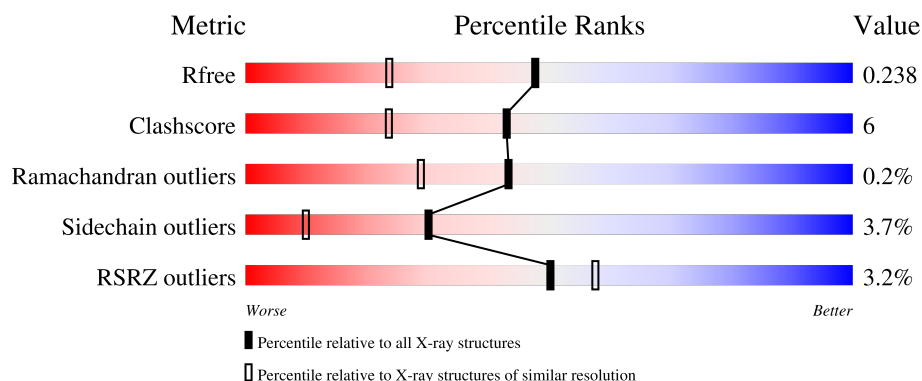
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1365 (1.78-1.78)
Clashscore	190562	1395 (1.78-1.78)
Ramachandran outliers	187476	1382 (1.78-1.78)
Sidechain outliers	187428	1382 (1.78-1.78)
RSRZ outliers	180081	1365 (1.78-1.78)

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	422	4% 79% 17% ..
1	B	422	2% 79% 16% ..

2 Entry composition [i](#)

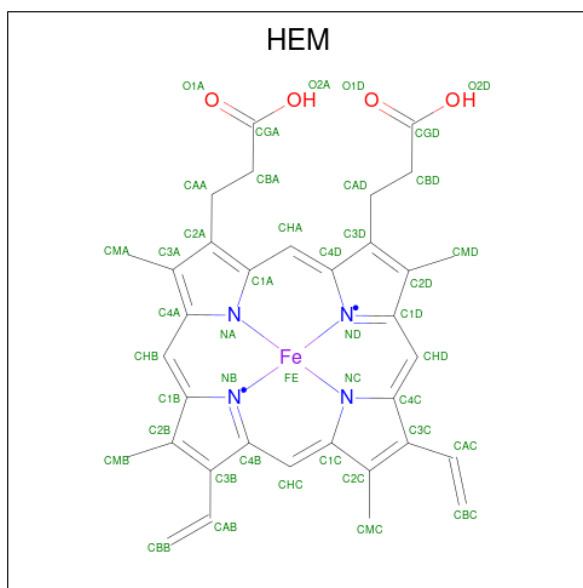
There are 7 unique types of molecules in this entry. The entry contains 7192 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

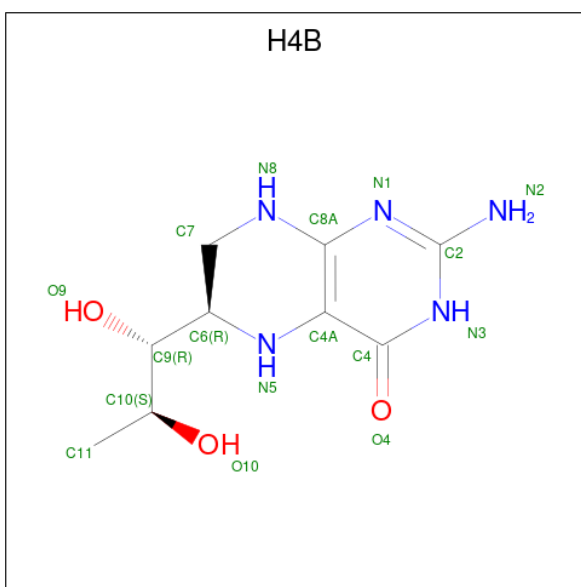
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	408	Total	C	N	O	S	0	3	1
			3326	2129	567	608	22			
1	B	411	Total	C	N	O	S	0	4	0
			3365	2156	574	613	22			

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



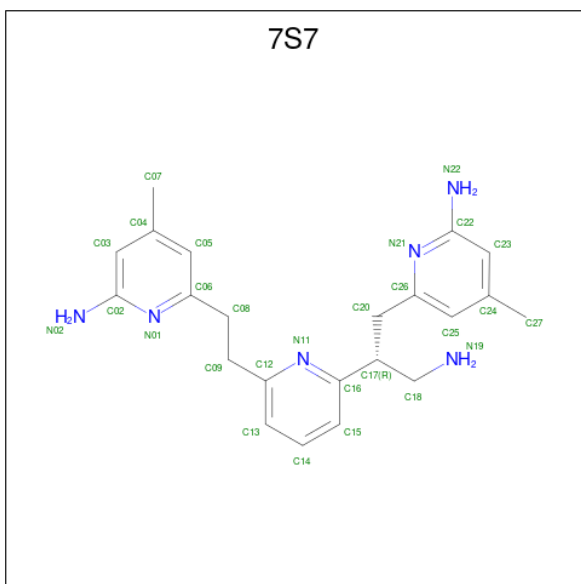
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is 5,6,7,8-TETRAHYDROBIOPTERIN (CCD ID: 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 (CCD ID: 7S7) (formula: C₂₂H₂₈N₆).



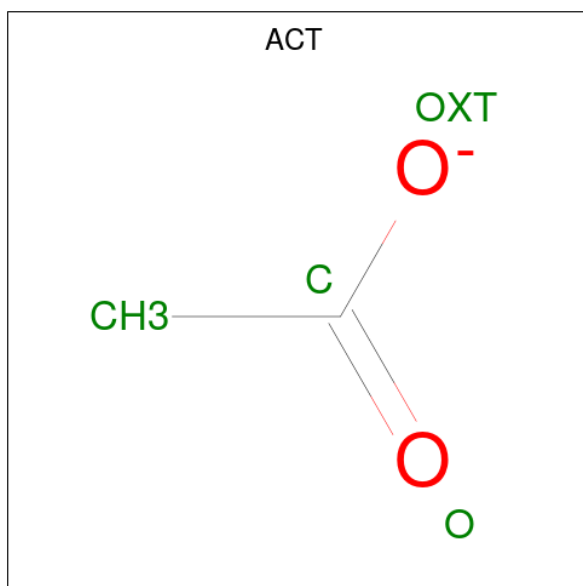
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N		0	0
			28	22	6			

Continued on next page...

Continued from previous page...

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

- Molecule 5 is ACETATE ION (CCD ID: 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 (CCD ID: ZN) (formula: Zn).

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

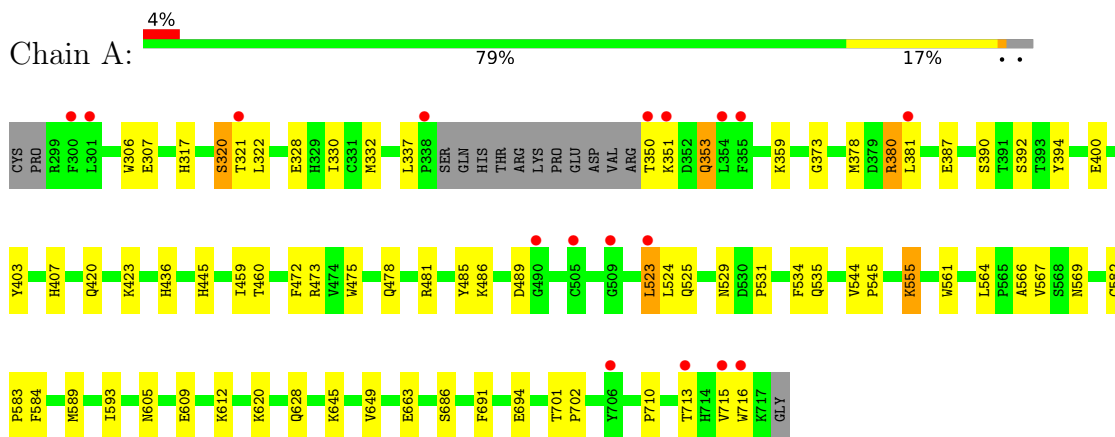
- Molecule 7 is water.

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

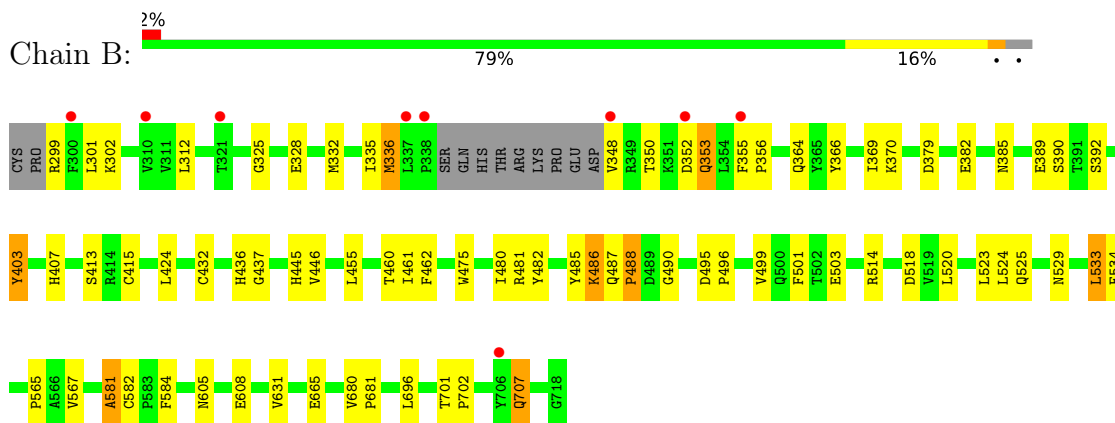
3 Residue-property plots [i](#)

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 39.04 – 1.78	Depositor EDS
% Data completeness (in resolution range)	99.3 (39.04-1.78) 99.4 (39.04-1.78)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 1.78Å)	Xtriage
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	Xtriage
Anisotropy	0.607	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 52.0	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	0.97	EDS
Total number of atoms	7192	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage'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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 7S7, HEM, ZN, H4B, 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	0.86	2/3428 (0.1%)	1.01	3/4651 (0.1%)
1	B	1.10	11/3471 (0.3%)	1.24	23/4706 (0.5%)
All	All	0.99	13/6899 (0.2%)	1.13	26/9357 (0.3%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	565	PRO	C-O	7.03	1.30	1.23
1	A	459	ILE	N-CA	6.97	1.54	1.46
1	A	716	TRP	C-N	-6.83	1.23	1.33
1	B	403	TYR	N-CA	-5.92	1.39	1.46
1	B	437	GLY	N-CA	5.91	1.53	1.45
1	B	432	CYS	N-CA	5.72	1.52	1.46
1	B	533	LEU	CA-CB	5.48	1.61	1.53
1	B	488	PRO	CA-C	5.48	1.59	1.52
1	B	499	VAL	CA-CB	5.34	1.59	1.54
1	B	366	TYR	C-O	5.22	1.30	1.24
1	B	413	SER	CA-C	5.14	1.59	1.52
1	B	369	ILE	CA-C	5.12	1.59	1.52
1	B	461	ILE	CA-CB	5.06	1.60	1.53

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	436	HIS	N-CA-C	-8.84	101.57	111.82
1	B	680	VAL	CA-C-N	8.77	126.06	119.66
1	B	680	VAL	C-N-CA	8.77	126.06	119.66
1	B	486	LYS	N-CA-C	-7.22	97.47	108.96
1	B	487	GLN	CA-C-N	7.18	126.44	118.97
1	B	487	GLN	C-N-CA	7.18	126.44	118.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	520	LEU	CA-C-N	7.05	127.01	120.03
1	B	520	LEU	C-N-CA	7.05	127.01	120.03
1	B	379	ASP	N-CA-C	-6.94	103.80	111.36
1	B	581	ALA	CA-C-O	-6.76	113.03	120.33
1	B	481	ARG	N-CA-C	-6.21	98.86	108.42
1	A	445	HIS	N-CA-C	-6.05	104.60	111.07
1	B	424	LEU	N-CA-C	-5.57	98.56	108.13
1	B	707	GLN	CA-C-N	-5.54	114.25	119.85
1	B	707	GLN	C-N-CA	-5.54	114.25	119.85
1	B	501	PHE	N-CA-C	5.32	117.08	111.28
1	B	364	GLN	CB-CA-C	-5.32	101.96	110.79
1	B	581	ALA	CB-CA-C	-5.31	102.61	110.62
1	A	564	LEU	CA-C-N	-5.29	113.23	119.84
1	A	564	LEU	C-N-CA	-5.29	113.23	119.84
1	B	681	PRO	O-C-N	5.24	123.72	121.31
1	B	446	VAL	CB-CA-C	-5.20	105.12	112.14
1	B	455	LEU	N-CA-C	5.13	117.47	110.24
1	B	665	GLU	N-CA-C	5.11	116.85	111.28
1	B	461	ILE	O-C-N	-5.10	116.44	122.66
1	B	481	ARG	CA-C-O	-5.07	115.52	121.10

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	3326	0	3237	44	0
1	B	3365	0	3284	38	0
2	A	43	0	30	4	0
2	B	43	0	30	6	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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	84	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 (84) 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:332:MET:HE1	1:B:301:LEU:HD22	1.61	0.81
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:A:373:GLY:HA2	1:A:378:MET:HE3	1.78	0.65
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:B:462:PHE:HB2	1:B:581:ALA:HB3	1.81	0.61
1:A:306:TRP:CD2	1:B:336:MET:HE3	2.36	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:436:HIS:CD2	1:A:534:PHE:HE2	2.34	0.46
1:A:478:GLN:HB2	1:A:481:ARG:HG3	1.96	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:701:THR:HA	1:A:702:PRO:C	2.42	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:B:701:THR:HA	1:B:702:PRO:C	2.42	0.44
1:A:473:ARG:NH2	1:A:710:PRO:HD3	2.32	0.44
1:A:306:TRP:CE2	1:B:336:MET:HE3	2.53	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:NZ	1:A:555:LYS:HB3	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
1:B:475:TRP:HB2	1:B:523:LEU:HB3	2.00	0.42
1:B:328:GLU:H	1:B:328:GLU:CD	2.27	0.42
1:A:584:PHE:CD1	2:A:1717:HEM:CAC	3.03	0.42
1:A:475:TRP:CE2	1:A:710:PRO:HB2	2.54	0.42
2:A:1717:HEM:HBA1	4:A:1719:7S7:H17	2.02	0.42
1:B:482:TYR:HA	1:B:518:ASP:O	2.20	0.42
1:B:488:PRO:C	1:B:490:GLY:H	2.28	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:582:CYS:O	1:A:583:PRO:C	2.63	0.41
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:A:328:GLU:H	1:A:328:GLU:CD	2.29	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: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
1:A:544:VAL:HA	1:A:545:PRO:HD2	1.95	0.40
1:B:299:ARG:NH1	1:B:299:ARG:HB3	2.36	0.40
1:B:415:CYS:HB2	2:B:1719:HEM:ND	2.37	0.40
1:B:445:HIS:CD2	1:B:445:HIS:C	3.00	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%)	43	29
1	B	411/422 (97%)	400 (97%)	10 (2%)	1 (0%)	43	29
All	All	818/844 (97%)	794 (97%)	22 (3%)	2 (0%)	43	29

All (2) Ramachandran outliers are listed below:

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

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	366/377 (97%)	348 (95%)	18 (5%)	22	5
1	B	370/377 (98%)	360 (97%)	10 (3%)	39	19
All	All	736/754 (98%)	708 (96%)	28 (4%)	30	9

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	307[A]	GLU
1	A	307[B]	GLU
1	A	320	SER
1	A	353	GLN
1	A	380	ARG
1	A	390	SER
1	A	485	TYR
1	A	486	LYS
1	A	523	LEU
1	A	535	GLN
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	336	MET
1	B	348	VAL
1	B	353	GLN
1	B	389	GLU
1	B	390	SER
1	B	392	SER
1	B	480	ILE
1	B	486	LYS
1	B	503	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	707	GLN

Sometimes 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	364	GLN
1	A	385	ASN
1	A	407	HIS
1	A	436	HIS
1	A	454	ASN
1	A	500	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	407	HIS
1	B	454	ASN
1	B	478	GLN
1	B	507	GLN
1	B	605	ASN
1	B	697	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry

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$
4	7S7	A	1719	-	29,30,30	1.27	3 (10%)	35,41,41	2.58	12 (34%)
2	HEM	A	1717	1	50,50,50	1.57	8 (16%)	67,82,82	1.49	14 (20%)
3	H4B	A	1718	-	17,18,18	2.13	3 (17%)	14,26,26	2.57	6 (42%)
4	7S7	B	1721	-	29,30,30	1.07	1 (3%)	35,41,41	2.33	12 (34%)
2	HEM	B	1719	1	50,50,50	1.59	8 (16%)	67,82,82	1.60	13 (19%)
3	H4B	B	1720	-	17,18,18	1.67	4 (23%)	14,26,26	2.25	6 (42%)
5	ACT	A	1720	-	3,3,3	0.90	0	3,3,3	0.72	0
5	ACT	B	1722	-	3,3,3	0.60	0	3,3,3	1.36	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	7S7	A	1719	-	-	7/15/15/15	0/3/3/3
2	HEM	A	1717	1	-	4/14/54/54	-
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	-	2/14/54/54	-
3	H4B	B	1720	-	-	1/8/17/17	0/2/2/2

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1718	H4B	C7-N8	7.22	1.53	1.46
2	A	1717	HEM	FE-NB	4.99	2.10	1.94
3	B	1720	H4B	C7-N8	4.08	1.50	1.46
2	B	1719	HEM	FE-NB	3.96	2.07	1.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1717	HEM	C3B-C4B	3.91	1.52	1.44
2	B	1719	HEM	C1C-C2C	-3.76	1.37	1.45
4	A	1719	7S7	C16-N11	3.59	1.39	1.34
2	B	1719	HEM	C1B-NB	-3.57	1.34	1.40
2	B	1719	HEM	C3B-C4B	3.32	1.51	1.44
2	B	1719	HEM	FE-NC	3.30	2.06	1.95
2	A	1717	HEM	FE-NC	3.30	2.06	1.95
2	B	1719	HEM	C4C-NC	-3.15	1.33	1.39
2	A	1717	HEM	C4B-NB	-3.15	1.32	1.38
3	A	1718	H4B	C2-N2	2.89	1.40	1.34
2	A	1717	HEM	C1B-NB	-2.86	1.35	1.40
4	A	1719	7S7	C23-C24	2.61	1.43	1.39
3	B	1720	H4B	O4-C4	2.49	1.28	1.23
3	B	1720	H4B	C8A-N1	2.48	1.40	1.36
2	A	1717	HEM	C1C-C2C	-2.41	1.40	1.45
2	A	1717	HEM	C4D-ND	-2.40	1.36	1.40
2	B	1719	HEM	C3C-C4C	-2.38	1.41	1.46
3	B	1720	H4B	C2-N1	2.31	1.38	1.33
4	A	1719	7S7	C20-C17	-2.29	1.49	1.54
2	B	1719	HEM	C4D-C3D	2.23	1.48	1.45
4	B	1721	7S7	C25-C24	2.18	1.42	1.39
3	A	1718	H4B	O4-C4	2.14	1.27	1.23
2	A	1717	HEM	C4D-C3D	2.04	1.48	1.45

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1719	7S7	C02-N01-C06	8.66	124.55	118.07
4	B	1721	7S7	C02-N01-C06	7.06	123.35	118.07
3	A	1718	H4B	C2-N1-C8A	5.58	123.20	113.36
4	A	1719	7S7	C27-C24-C23	5.30	128.10	120.92
4	B	1721	7S7	C16-N11-C12	5.15	123.42	118.55
4	A	1719	7S7	C27-C24-C25	-5.09	114.02	120.92
3	B	1720	H4B	C2-N1-C8A	4.43	121.17	113.36
3	A	1718	H4B	C11-C10-C9	-4.17	107.01	112.11
4	A	1719	7S7	C09-C12-N11	3.87	121.92	116.06
3	A	1718	H4B	C2-N3-C4	-3.78	118.25	125.11
2	A	1717	HEM	CHA-C4D-ND	3.50	128.69	124.37
4	B	1721	7S7	C27-C24-C23	3.48	125.63	120.92
4	A	1719	7S7	C05-C06-N01	-3.47	118.77	122.73
4	B	1721	7S7	C15-C16-N11	-3.43	118.84	122.39
2	B	1719	HEM	O2D-CGD-CBD	3.38	124.68	114.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1719	HEM	C2D-C1D-ND	3.37	113.80	109.90
2	A	1717	HEM	CBA-CAA-C2A	-3.32	103.34	112.53
4	B	1721	7S7	C20-C26-N21	3.31	120.62	116.57
4	A	1719	7S7	C20-C26-N21	3.29	120.60	116.57
2	A	1717	HEM	CHA-C4D-C3D	-3.26	119.21	125.23
3	B	1720	H4B	C4A-C4-N3	3.25	121.06	112.13
4	B	1721	7S7	C22-N21-C26	3.25	120.50	118.07
3	B	1720	H4B	O4-C4-C4A	-3.23	119.47	127.26
2	B	1719	HEM	C4A-NA-C1A	-3.23	100.55	105.82
4	B	1721	7S7	C27-C24-C25	-3.23	116.55	120.92
3	A	1718	H4B	C4A-C4-N3	2.99	120.33	112.13
3	A	1718	H4B	O4-C4-C4A	-2.96	120.12	127.26
4	A	1719	7S7	C16-N11-C12	2.95	121.34	118.55
2	A	1717	HEM	C4C-CHD-C1D	-2.95	119.75	126.02
4	B	1721	7S7	C09-C12-N11	2.86	120.40	116.06
2	B	1719	HEM	C4B-C3B-C2B	-2.85	104.66	107.28
2	A	1717	HEM	C1B-NB-C4B	2.82	108.55	105.21
2	B	1719	HEM	C4A-CHB-C1B	-2.81	119.63	126.25
4	A	1719	7S7	N22-C22-N21	-2.75	112.16	116.59
2	A	1717	HEM	C4B-C3B-C2B	-2.74	104.76	107.28
3	B	1720	H4B	C2-N3-C4	-2.73	120.17	125.11
2	B	1719	HEM	CBA-CAA-C2A	-2.64	105.22	112.53
4	A	1719	7S7	C20-C26-C25	-2.64	115.64	121.06
4	B	1721	7S7	C05-C06-N01	-2.59	119.78	122.73
2	B	1719	HEM	C3A-C4A-NA	2.57	114.26	110.14
4	A	1719	7S7	C13-C12-N11	-2.56	119.16	122.40
2	A	1717	HEM	CHD-C1D-ND	2.56	127.17	124.42
2	B	1719	HEM	CHD-C1D-C2D	-2.52	121.05	125.03
2	B	1719	HEM	C1D-C2D-C3D	-2.52	104.33	106.98
3	B	1720	H4B	O9-C9-C6	-2.51	103.25	109.28
4	B	1721	7S7	C13-C12-N11	-2.49	119.25	122.40
3	B	1720	H4B	N2-C2-N1	2.41	124.38	119.67
4	A	1719	7S7	C23-C22-N22	2.41	127.01	121.81
2	A	1717	HEM	O1D-CGD-CBD	-2.40	115.49	123.09
2	B	1719	HEM	C1B-NB-C4B	2.35	107.99	105.21
4	B	1721	7S7	C05-C04-C03	2.30	120.67	118.11
2	A	1717	HEM	CAD-CBD-CGD	-2.24	107.72	113.67
2	A	1717	HEM	CBD-CAD-C3D	-2.23	106.36	112.53
2	B	1719	HEM	O1D-CGD-CBD	-2.21	116.07	123.09
4	B	1721	7S7	C20-C17-C16	-2.21	106.48	111.16
2	A	1717	HEM	CMB-C2B-C1B	2.21	128.49	125.03
2	B	1719	HEM	O2A-CGA-CBA	2.18	120.90	114.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1718	H4B	O9-C9-C6	-2.18	104.04	109.28
2	A	1717	HEM	O2D-CGD-CBD	2.15	120.79	114.00
2	B	1719	HEM	C4A-C3A-C2A	-2.15	104.36	106.82
2	A	1717	HEM	CMC-C2C-C1C	2.08	128.40	124.73
2	A	1717	HEM	C4A-NA-C1A	-2.06	102.47	105.82
4	A	1719	7S7	C03-C02-N01	-2.03	117.70	121.76

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1719	7S7	C18-C17-C20-C26
4	A	1719	7S7	C16-C17-C20-C26
4	A	1719	7S7	C20-C17-C18-N19
4	A	1719	7S7	N11-C16-C17-C18
4	B	1721	7S7	C18-C17-C20-C26
4	B	1721	7S7	C16-C17-C20-C26
4	B	1721	7S7	C06-C08-C09-C12
4	A	1719	7S7	C06-C08-C09-C12
2	A	1717	HEM	C4D-C3D-CAD-CBD
2	A	1717	HEM	C2D-C3D-CAD-CBD
4	A	1719	7S7	C15-C16-C17-C18
4	B	1721	7S7	N11-C16-C17-C18
4	A	1719	7S7	C16-C17-C18-N19
2	B	1719	HEM	CAA-CBA-CGA-O1A
2	A	1717	HEM	CAD-CBD-CGD-O1D
2	B	1719	HEM	CAA-CBA-CGA-O2A
3	B	1720	H4B	O10-C10-C9-O9
2	A	1717	HEM	CAD-CBD-CGD-O2D

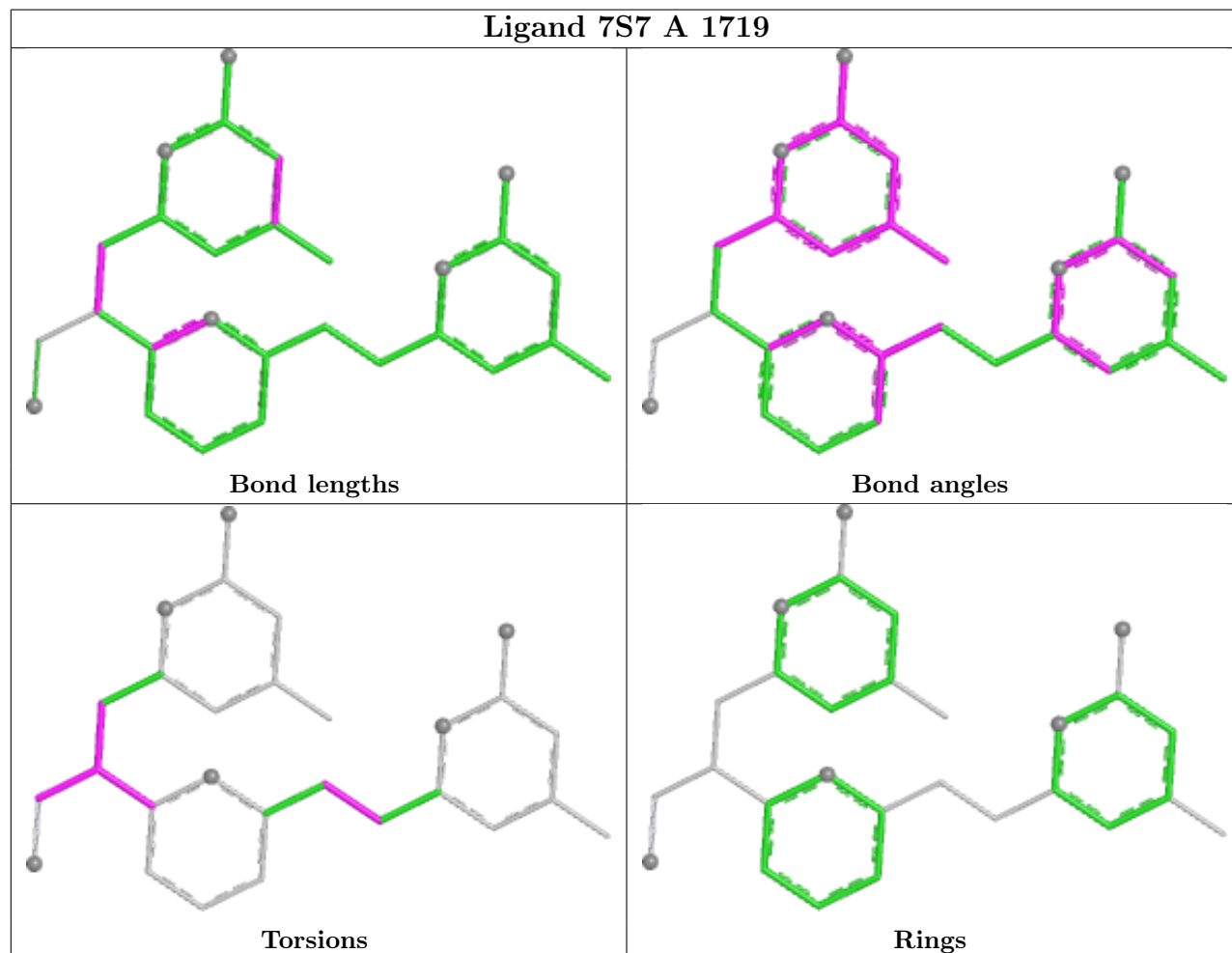
There are no ring outliers.

4 monomers are involved in 15 short contacts:

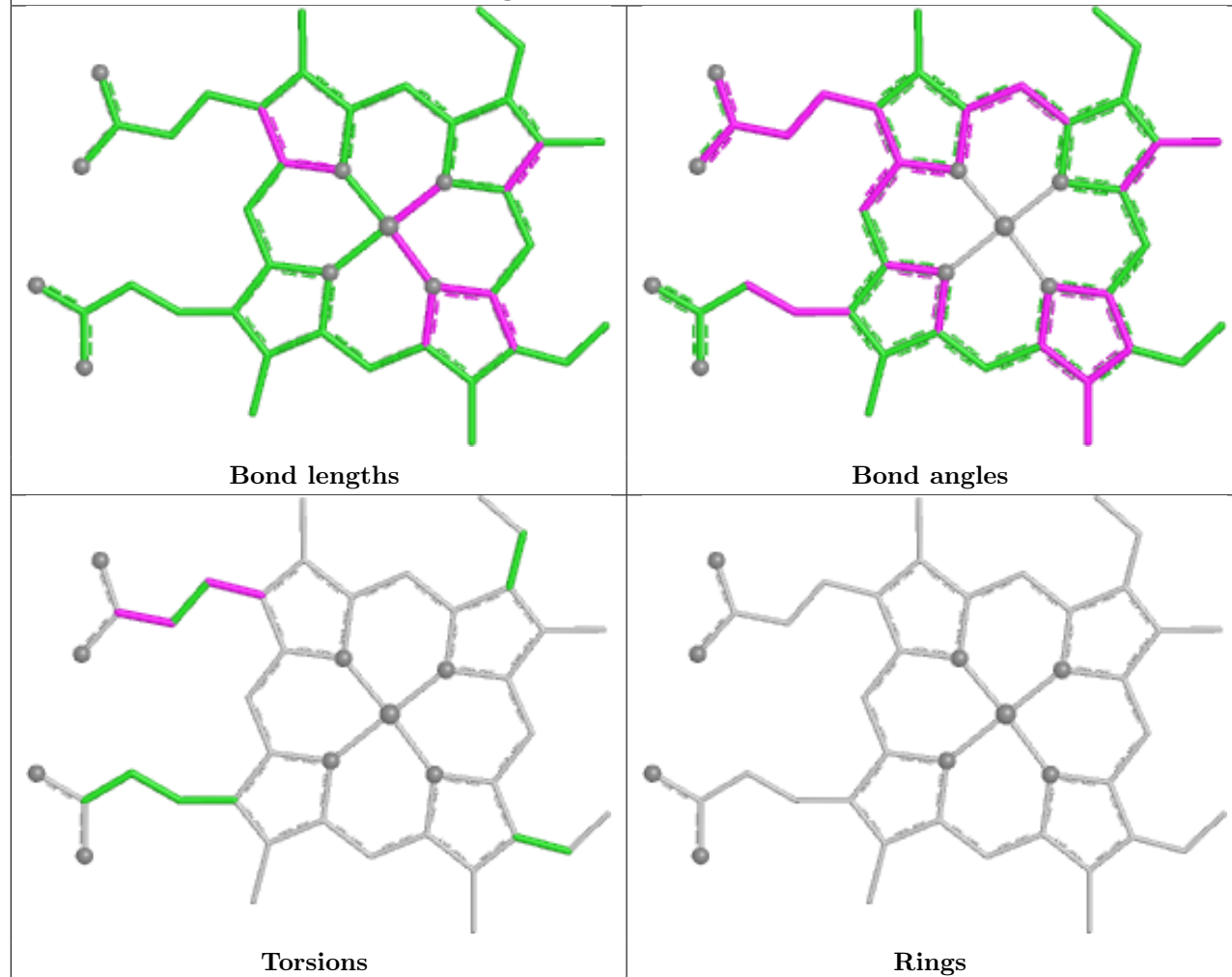
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1719	7S7	6	0
2	A	1717	HEM	4	0
4	B	1721	7S7	6	0
2	B	1719	HEM	6	0

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

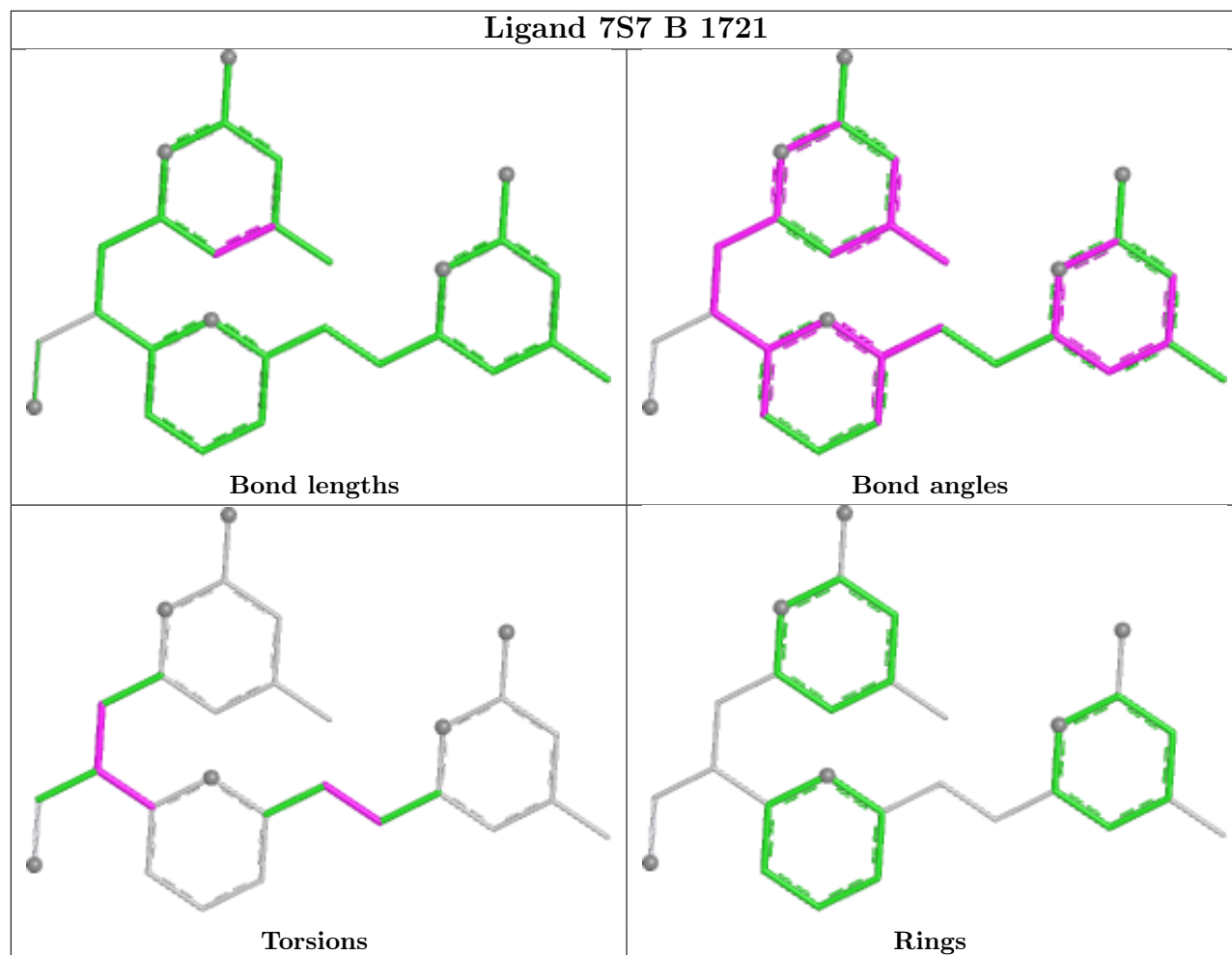
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.

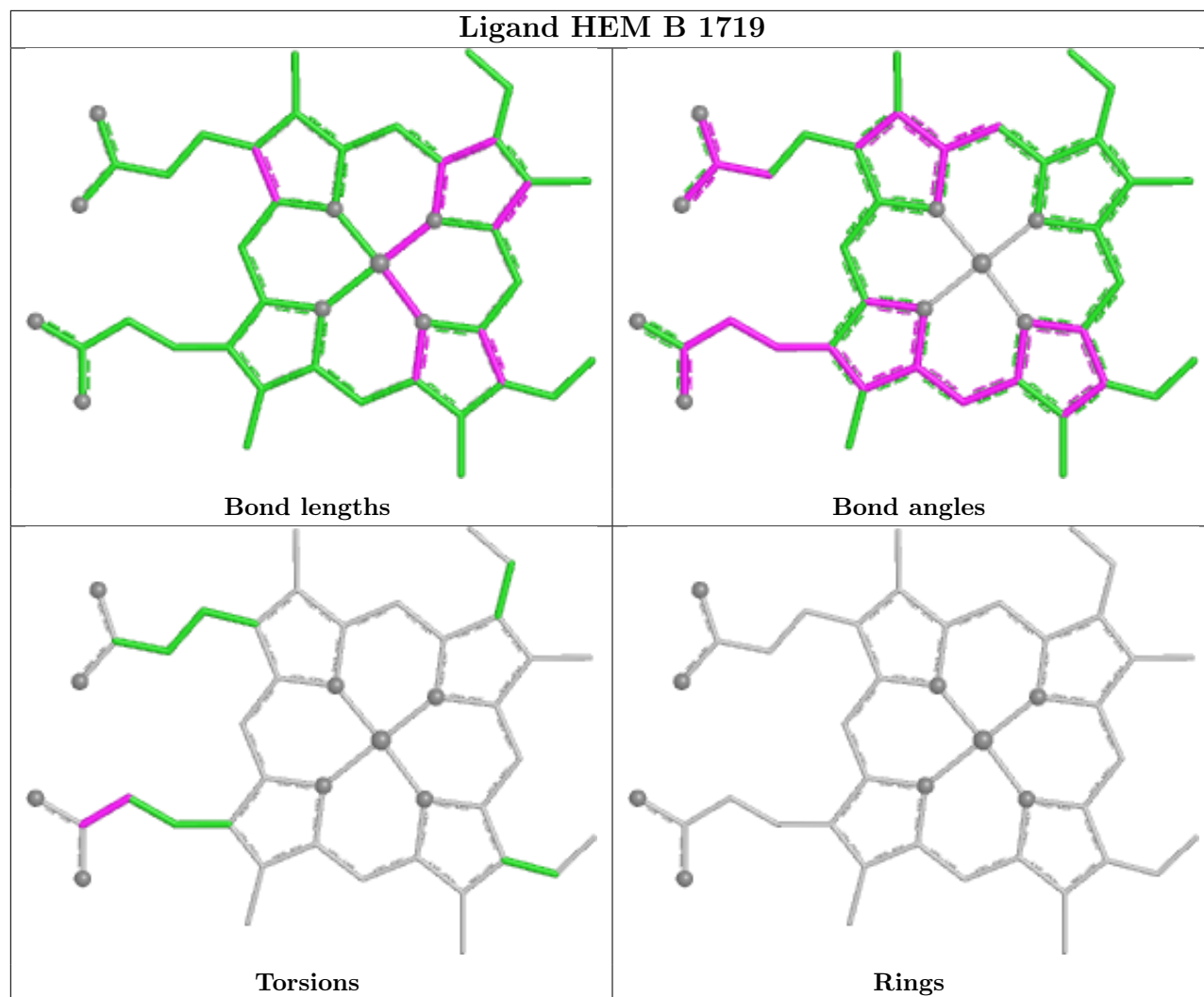


Ligand HEM A 1717



Ligand 7S7 B 1721





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	408/422 (96%)	0.46	17 (4%)	40 47	22, 48, 85, 104	3 (0%)
1	B	411/422 (97%)	0.16	9 (2%)	62 70	21, 38, 66, 88	4 (0%)
All	All	819/844 (97%)	0.31	26 (3%)	50 57	21, 43, 80, 104	7 (0%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	355[A]	PHE	5.4
1	B	348	VAL	5.3
1	A	355	PHE	5.1
1	A	706	TYR	4.8
1	B	706	TYR	4.2
1	A	300	PHE	4.2
1	B	300	PHE	3.5
1	A	350	THR	3.0
1	A	338	PRO	2.7
1	A	715	VAL	2.5
1	A	509	GLY	2.5
1	A	351	LYS	2.4
1	B	338	PRO	2.3
1	A	490	GLY	2.3
1	A	321	THR	2.3
1	A	523	LEU	2.3
1	B	337	LEU	2.2
1	A	381	LEU	2.2
1	B	352	ASP	2.2
1	B	310	VAL	2.1
1	A	505	CYS	2.1
1	A	354	LEU	2.1
1	A	301	LEU	2.1
1	B	321	THR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	716	TRP	2.1
1	A	713	THR	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](#)

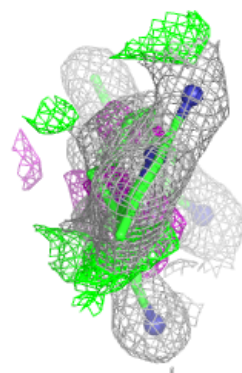
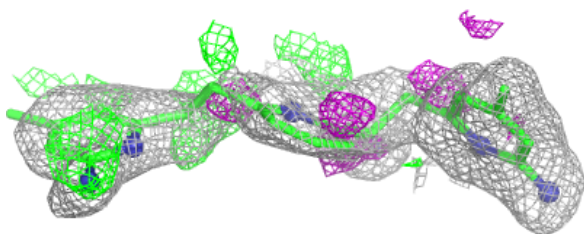
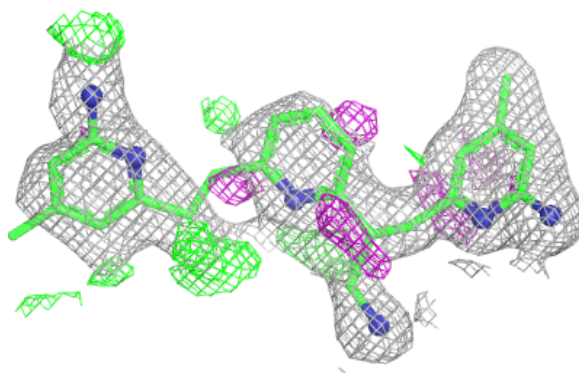
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
5	ACT	A	1720	4/4	0.84	0.18	65,69,72,74	0
4	7S7	B	1721	28/28	0.85	0.15	26,51,63,64	0
4	7S7	A	1719	28/28	0.86	0.15	16,43,50,52	0
5	ACT	B	1722	4/4	0.89	0.14	57,62,63,63	0
3	H4B	A	1718	17/17	0.95	0.06	25,28,31,33	0
3	H4B	B	1720	17/17	0.95	0.07	29,32,36,38	0
2	HEM	A	1717	43/43	0.97	0.08	28,32,39,45	0
2	HEM	B	1719	43/43	0.97	0.08	21,29,47,57	0
6	ZN	A	1721	1/1	1.00	0.01	39,39,39,39	0

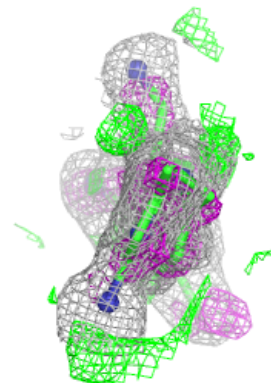
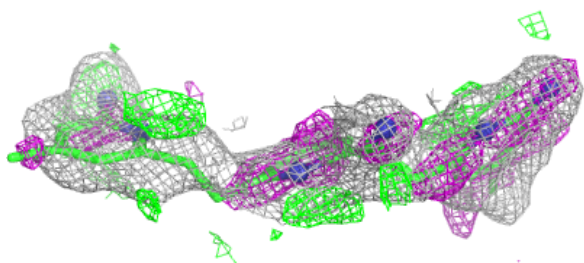
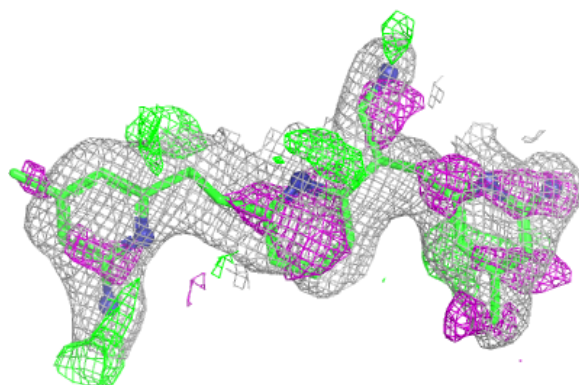
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 7S7 B 1721:

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

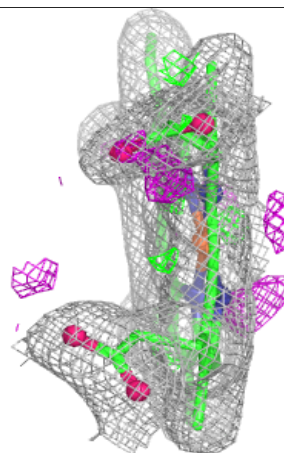
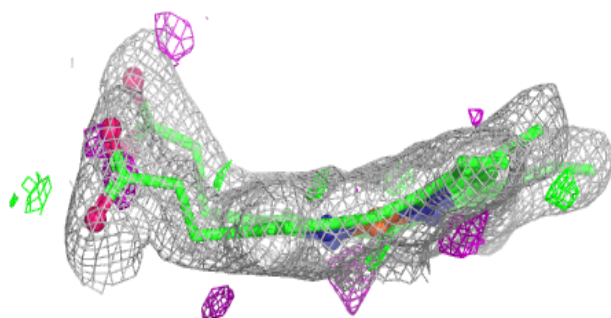
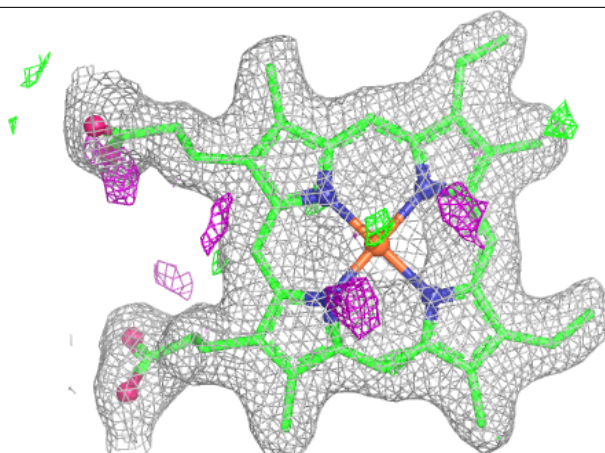
**Electron density around 7S7 A 1719:**

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



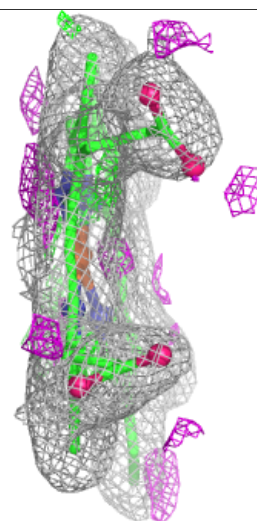
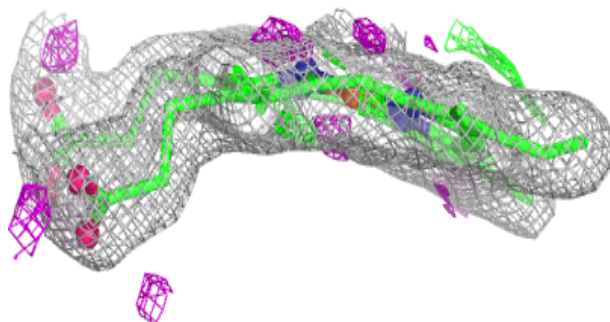
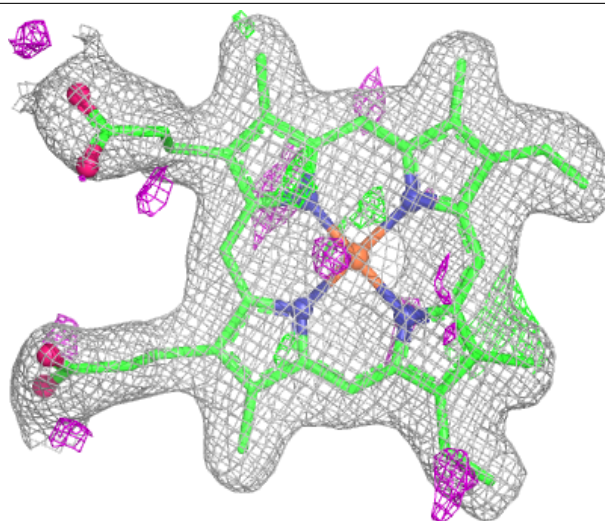
Electron density around HEM A 1717:

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



Electron density around HEM B 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.