



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:33 PM UTC

PDB ID : 6FWF / pdb_00006fwf
Title : Low resolution structure of Neisseria meningitidis qNOR
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Deposited on : 2018-03-06
Resolution : 4.20 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

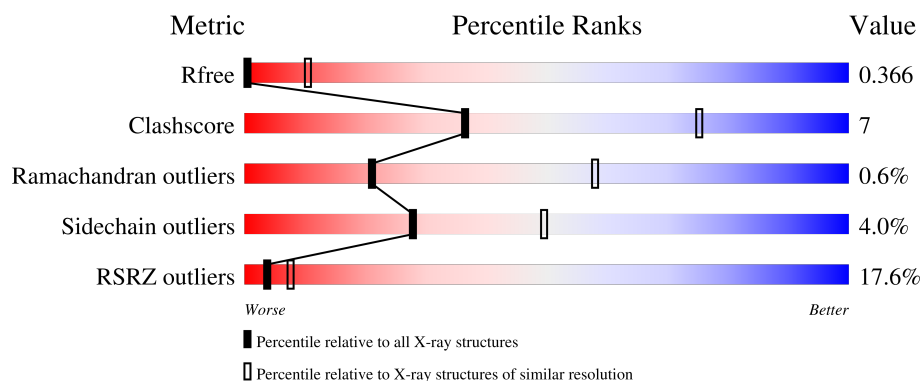
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.20 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	1004 (4.52-3.88)
Clashscore	190562	1019 (4.50-3.90)
Ramachandran outliers	187476	1020 (4.56-3.84)
Sidechain outliers	187428	1006 (4.56-3.84)
RSRZ outliers	180081	1001 (4.52-3.88)

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	751	17% 78% 16% • 5%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5761 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 reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	712	Total	C	N	O	S	0	0	0
			5673	3772	897	980	24			

- 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	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		

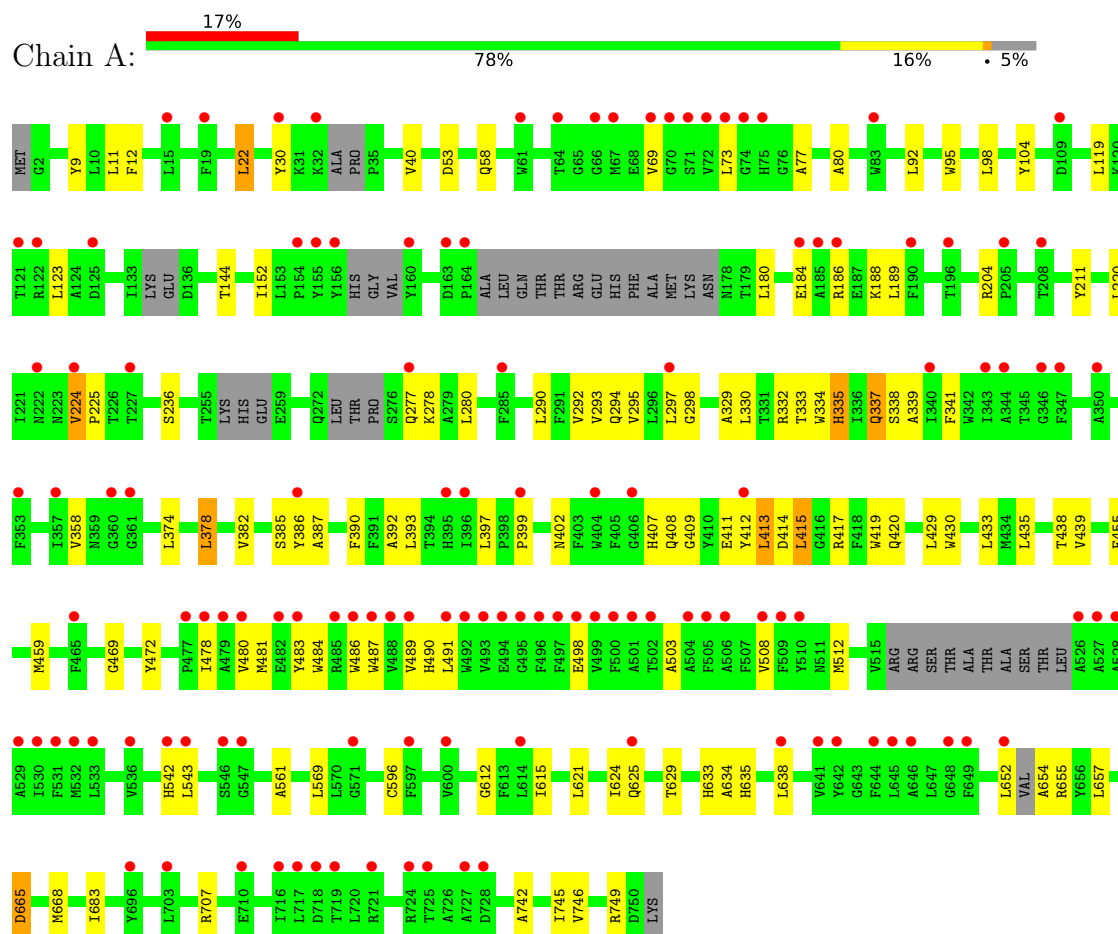
- Molecule 4 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Fe	0	0
			1	1		

3 Residue-property plots

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 reductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	93.68Å 123.10Å 130.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	53.64 – 4.20 53.64 – 4.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (53.64-4.20) 99.8 (53.64-4.20)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 4.14Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.333 , 0.373 0.336 , 0.366	Depositor DCC
R_{free} test set	509 reflections (4.41%)	wwPDB-VP
Wilson B-factor (Å ²)	194.8	Xtriage
Anisotropy	0.396	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 479.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	5761	wwPDB-VP
Average B, all atoms (Å ²)	293.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.38% 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: FE, CA, 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	0.71	0/5851	0.90	1/7965 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	665	ASP	N-CA-C	5.41	117.37	110.61

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	5673	0	5560	79	0
2	A	86	0	60	14	0
3	A	1	0	0	0	0
4	A	1	0	0	0	0
All	All	5761	0	5620	82	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 7.

All (82) 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:294:GLN:HE21	1:A:339:ALA:HB2	1.35	0.91
1:A:335:HIS:CE1	2:A:1002:HEM:C1D	2.70	0.80
1:A:335:HIS:HE1	2:A:1002:HEM:C1D	2.03	0.77
1:A:298:GLY:HA2	1:A:335:HIS:HD2	1.54	0.73
1:A:224:VAL:HG22	1:A:225:PRO:HD2	1.79	0.63
1:A:334:TRP:CD1	1:A:386:TYR:HB2	2.34	0.62
1:A:378:LEU:O	1:A:382:VAL:HG23	2.01	0.61
2:A:1002:HEM:HBB2	2:A:1002:HEM:HMB2	1.83	0.61
1:A:508:VAL:HG12	1:A:512:MET:HE2	1.84	0.60
1:A:358:VAL:HG11	1:A:438:THR:HG22	1.83	0.59
1:A:98:LEU:HD22	1:A:144:THR:HG23	1.83	0.59
1:A:624:ILE:HG23	1:A:629:THR:OG1	2.03	0.58
1:A:385:SER:HA	1:A:419:TRP:CD1	2.40	0.57
1:A:58:GLN:HE21	1:A:481:MET:HE1	1.70	0.56
1:A:341:PHE:CG	1:A:382:VAL:HG22	2.41	0.55
1:A:420:GLN:HE22	1:A:469:GLY:C	2.15	0.54
1:A:407:HIS:CE1	1:A:409:GLY:HA2	2.42	0.54
1:A:335:HIS:C	1:A:335:HIS:HD1	2.16	0.54
1:A:341:PHE:CD1	1:A:382:VAL:HG22	2.44	0.53
1:A:417:ARG:NH1	1:A:420:GLN:OE1	2.42	0.52
1:A:615:ILE:HG22	1:A:621:LEU:HD13	1.90	0.52
1:A:335:HIS:C	1:A:335:HIS:ND1	2.67	0.52
1:A:412:TYR:CD2	1:A:489:VAL:HG21	2.46	0.51
1:A:411:GLU:OE2	2:A:1002:HEM:O2D	2.27	0.51
1:A:484:TRP:HA	1:A:487:TRP:HB2	1.93	0.50
1:A:298:GLY:CA	1:A:335:HIS:HD2	2.20	0.50
1:A:9:TYR:HA	1:A:12:PHE:HB3	1.94	0.50
1:A:80:ALA:O	1:A:707:ARG:NH2	2.43	0.50
1:A:742:ALA:O	1:A:745:ILE:HG22	2.11	0.50
1:A:337:GLN:HE21	1:A:414:ASP:HB2	1.77	0.49
1:A:236:SER:HB2	1:A:561:ALA:HB2	1.94	0.49
1:A:612:GLY:HA3	2:A:1001:HEM:C3C	2.47	0.49
1:A:438:THR:OG1	1:A:459:MET:HE1	2.12	0.49
1:A:413:LEU:HD23	1:A:413:LEU:N	2.28	0.48
1:A:746:VAL:HG12	1:A:749:ARG:NH2	2.29	0.48
1:A:624:ILE:HG23	1:A:629:THR:HG1	1.78	0.48
1:A:387:ALA:O	1:A:390:PHE:HB3	2.13	0.48
1:A:333:THR:HG21	1:A:393:LEU:HD11	1.96	0.47
1:A:483:TYR:HA	1:A:543:LEU:HD21	1.96	0.47
1:A:392:ALA:HB3	1:A:407:HIS:H	1.80	0.47
1:A:277:GLN:HA	1:A:280:LEU:HD23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:HIS:HE1	2:A:1002:HEM:CHD	2.28	0.47
1:A:397:LEU:HD23	1:A:402:ASN:HD22	1.80	0.47
1:A:634:ALA:HB1	2:A:1002:HEM:HMD3	1.97	0.47
1:A:455:PHE:HB2	1:A:503:ALA:HB1	1.98	0.46
2:A:1002:HEM:HBC2	2:A:1002:HEM:HMC1	1.97	0.46
1:A:635:HIS:CD2	2:A:1002:HEM:NC	2.83	0.46
1:A:277:GLN:HE22	1:A:657:LEU:HD21	1.81	0.46
1:A:330:LEU:HD23	1:A:393:LEU:HD12	1.98	0.46
1:A:337:GLN:OE1	1:A:415:LEU:HD23	2.16	0.46
1:A:408:GLN:NE2	1:A:413:LEU:O	2.50	0.45
1:A:633:HIS:CD2	2:A:1001:HEM:NA	2.83	0.45
1:A:22:LEU:HD11	1:A:491:LEU:HD11	1.99	0.45
1:A:92:LEU:HD12	1:A:95:TRP:CE3	2.52	0.45
1:A:104:TYR:CE1	1:A:119:LEU:HD13	2.51	0.45
1:A:486:TRP:HA	1:A:489:VAL:HG12	1.98	0.45
1:A:95:TRP:HB3	1:A:123:LEU:HD22	2.00	0.44
1:A:654:ALA:HB1	1:A:745:ILE:HD12	2.00	0.44
1:A:290:LEU:HA	1:A:293:VAL:HG22	1.99	0.44
1:A:633:HIS:CD2	2:A:1001:HEM:C1A	3.05	0.44
1:A:186:ARG:O	1:A:189:LEU:HB3	2.18	0.44
1:A:665:ASP:HA	1:A:668:MET:HG2	2.00	0.44
1:A:615:ILE:CG2	1:A:621:LEU:HD13	2.47	0.43
1:A:615:ILE:HG12	1:A:624:ILE:HG21	1.99	0.43
1:A:417:ARG:NH2	1:A:472:TYR:HB3	2.33	0.43
1:A:294:GLN:HB2	1:A:338:SER:HB3	2.00	0.43
1:A:490:HIS:CG	1:A:542:HIS:HE1	2.37	0.42
1:A:330:LEU:HD23	1:A:393:LEU:CD1	2.50	0.42
1:A:615:ILE:HG22	2:A:1001:HEM:CMD	2.50	0.42
1:A:98:LEU:CD2	1:A:144:THR:HG23	2.50	0.42
1:A:53:ASP:O	1:A:188:LYS:HB3	2.20	0.41
1:A:329:ALA:HB1	1:A:393:LEU:HD22	2.02	0.41
1:A:429:LEU:HD23	1:A:433:LEU:HG	2.01	0.41
1:A:77:ALA:HB2	1:A:332:ARG:HE	1.86	0.41
1:A:435:LEU:O	1:A:439:VAL:HG23	2.21	0.41
1:A:30:TYR:HA	1:A:480:VAL:HG22	2.03	0.41
2:A:1001:HEM:HMC2	2:A:1001:HEM:HBC2	2.03	0.41
1:A:204:ARG:NH2	1:A:211:TYR:O	2.54	0.41
1:A:374:LEU:HD11	1:A:430:TRP:HB2	2.03	0.41
1:A:292:VAL:O	1:A:295:VAL:HG22	2.20	0.41
1:A:615:ILE:HG22	2:A:1001:HEM:HMD3	2.03	0.41
1:A:330:LEU:HD21	1:A:390:PHE:HA	2.04	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	694/751 (92%)	624 (90%)	66 (10%)	4 (1%)	21 58

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	69	VAL
1	A	625	GLN
1	A	180	LEU
1	A	399	PRO

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	582/615 (95%)	559 (96%)	23 (4%)	28 49

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	22	LEU
1	A	40	VAL
1	A	73	LEU

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Mol	Chain	Res	Type
1	A	152	ILE
1	A	184	GLU
1	A	220	LEU
1	A	224	VAL
1	A	278	LYS
1	A	297	LEU
1	A	335	HIS
1	A	337	GLN
1	A	378	LEU
1	A	413	LEU
1	A	415	LEU
1	A	478	ILE
1	A	498	GLU
1	A	569	LEU
1	A	596	CYS
1	A	638	LEU
1	A	652	LEU
1	A	655	ARG
1	A	683	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	HIS
1	A	101	GLN
1	A	129	ASN
1	A	213	ASN
1	A	214	ASN
1	A	408	GLN
1	A	490	HIS
1	A	581	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\# Z > 2$
2	HEM	A	1002	1,3	50,50,50	1.65	7 (14%)	67,82,82	1.55	13 (19%)
2	HEM	A	1001	1,3	50,50,50	1.65	8 (16%)	67,82,82	1.59	13 (19%)

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
2	HEM	A	1002	1,3	-	5/14/54/54	-
2	HEM	A	1001	1,3	-	3/14/54/54	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1002	HEM	FE-NB	5.78	2.12	1.94
2	A	1001	HEM	FE-NB	5.15	2.10	1.94
2	A	1002	HEM	FE-NC	4.95	2.11	1.95
2	A	1001	HEM	FE-NC	4.94	2.11	1.95
2	A	1002	HEM	C1B-NB	-3.76	1.33	1.40
2	A	1001	HEM	C1B-NB	-3.58	1.34	1.40
2	A	1001	HEM	C4D-ND	-3.17	1.34	1.40
2	A	1002	HEM	C4D-ND	-2.53	1.35	1.40
2	A	1001	HEM	FE-ND	-2.44	1.87	1.94
2	A	1002	HEM	C4B-NB	-2.44	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	HEM	C4B-NB	-2.38	1.34	1.38
2	A	1001	HEM	C1D-ND	-2.15	1.34	1.38
2	A	1002	HEM	C3B-C4B	2.14	1.49	1.44
2	A	1002	HEM	C1C-C2C	-2.09	1.41	1.45
2	A	1001	HEM	C4D-C3D	2.03	1.48	1.45

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	HEM	CHC-C4B-NB	4.87	129.67	124.42
2	A	1001	HEM	CHD-C1D-ND	4.57	129.35	124.42
2	A	1002	HEM	CHD-C1D-ND	4.40	129.16	124.42
2	A	1002	HEM	CHC-C4B-NB	3.90	128.62	124.42
2	A	1001	HEM	C1B-NB-C4B	3.48	109.32	105.21
2	A	1002	HEM	C4D-ND-C1D	3.35	109.18	105.21
2	A	1001	HEM	C4B-C3B-C2B	-3.34	104.21	107.28
2	A	1002	HEM	CHA-C4D-ND	3.13	128.24	124.37
2	A	1001	HEM	CHD-C1D-C2D	-2.92	120.42	125.03
2	A	1001	HEM	O2A-CGA-CBA	2.90	123.17	114.00
2	A	1001	HEM	CHA-C4D-ND	2.89	127.94	124.37
2	A	1002	HEM	CAD-CBD-CGD	-2.86	106.08	113.67
2	A	1001	HEM	O2A-CGA-O1A	-2.74	116.30	123.33
2	A	1002	HEM	CHB-C1B-NB	2.73	127.74	124.37
2	A	1001	HEM	CHB-C1B-NB	2.71	127.72	124.37
2	A	1002	HEM	CAA-C2A-C1A	2.60	130.01	124.94
2	A	1001	HEM	O2D-CGD-CBD	2.48	121.83	114.00
2	A	1002	HEM	C4B-C3B-C2B	-2.45	105.03	107.28
2	A	1001	HEM	C3B-C2B-C1B	2.26	108.11	106.41
2	A	1002	HEM	CHB-C1B-C2B	-2.23	120.61	126.95
2	A	1002	HEM	CBD-CAD-C3D	2.23	118.69	112.53
2	A	1001	HEM	O2D-CGD-O1D	-2.21	117.66	123.33
2	A	1002	HEM	CAA-C2A-C3A	-2.18	122.19	127.07
2	A	1002	HEM	CAA-CBA-CGA	-2.05	108.23	113.67
2	A	1002	HEM	C1B-NB-C4B	2.02	107.60	105.21
2	A	1001	HEM	C4D-ND-C1D	2.02	107.60	105.21

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	HEM	C2D-C3D-CAD-CBD
2	A	1001	HEM	C3D-CAD-CBD-CGD

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Mol	Chain	Res	Type	Atoms
2	A	1002	HEM	CAA-CBA-CGA-O1A
2	A	1002	HEM	CAA-CBA-CGA-O2A
2	A	1002	HEM	C4D-C3D-CAD-CBD
2	A	1002	HEM	CAD-CBD-CGD-O2D
2	A	1002	HEM	CAD-CBD-CGD-O1D
2	A	1001	HEM	C4D-C3D-CAD-CBD

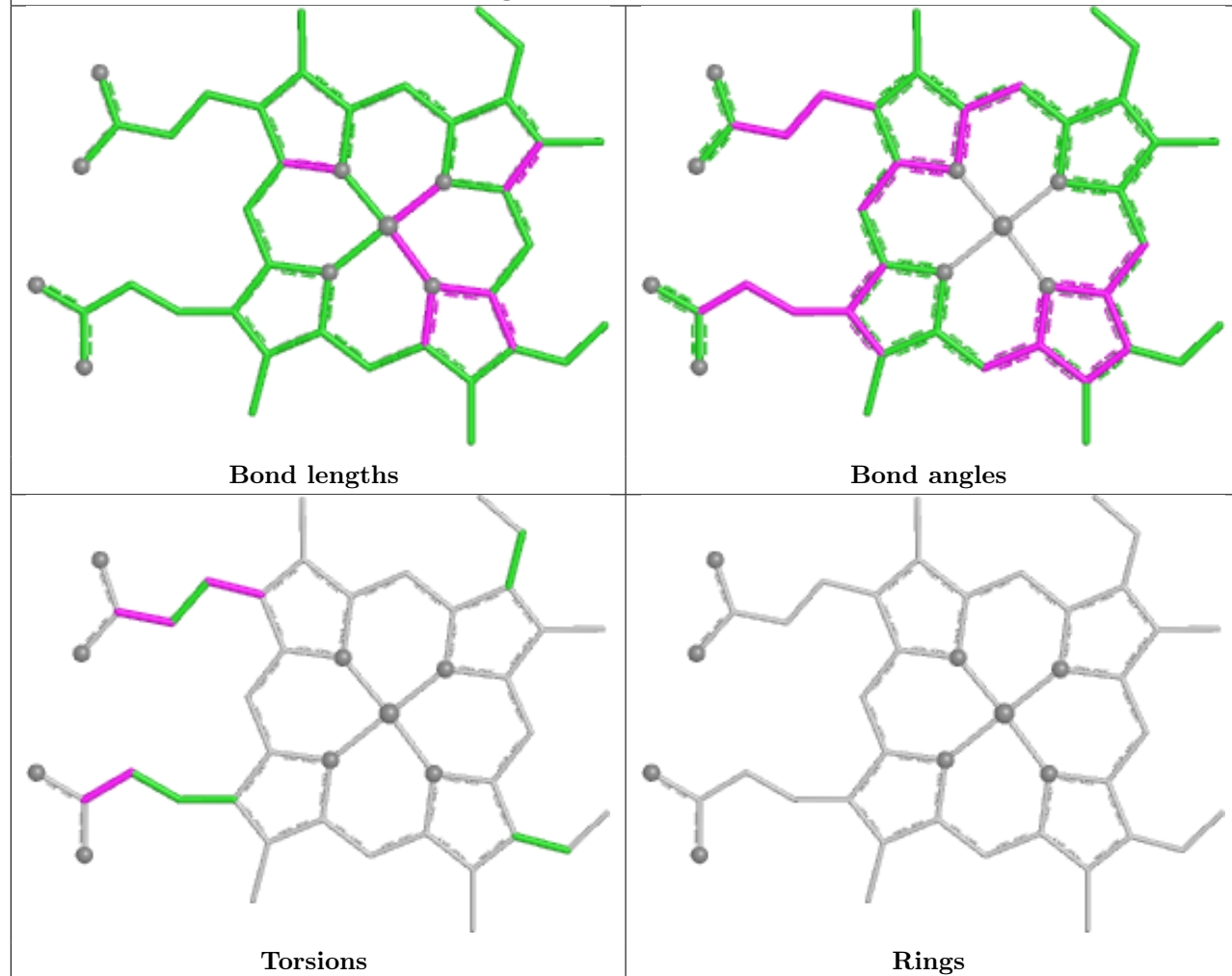
There are no ring outliers.

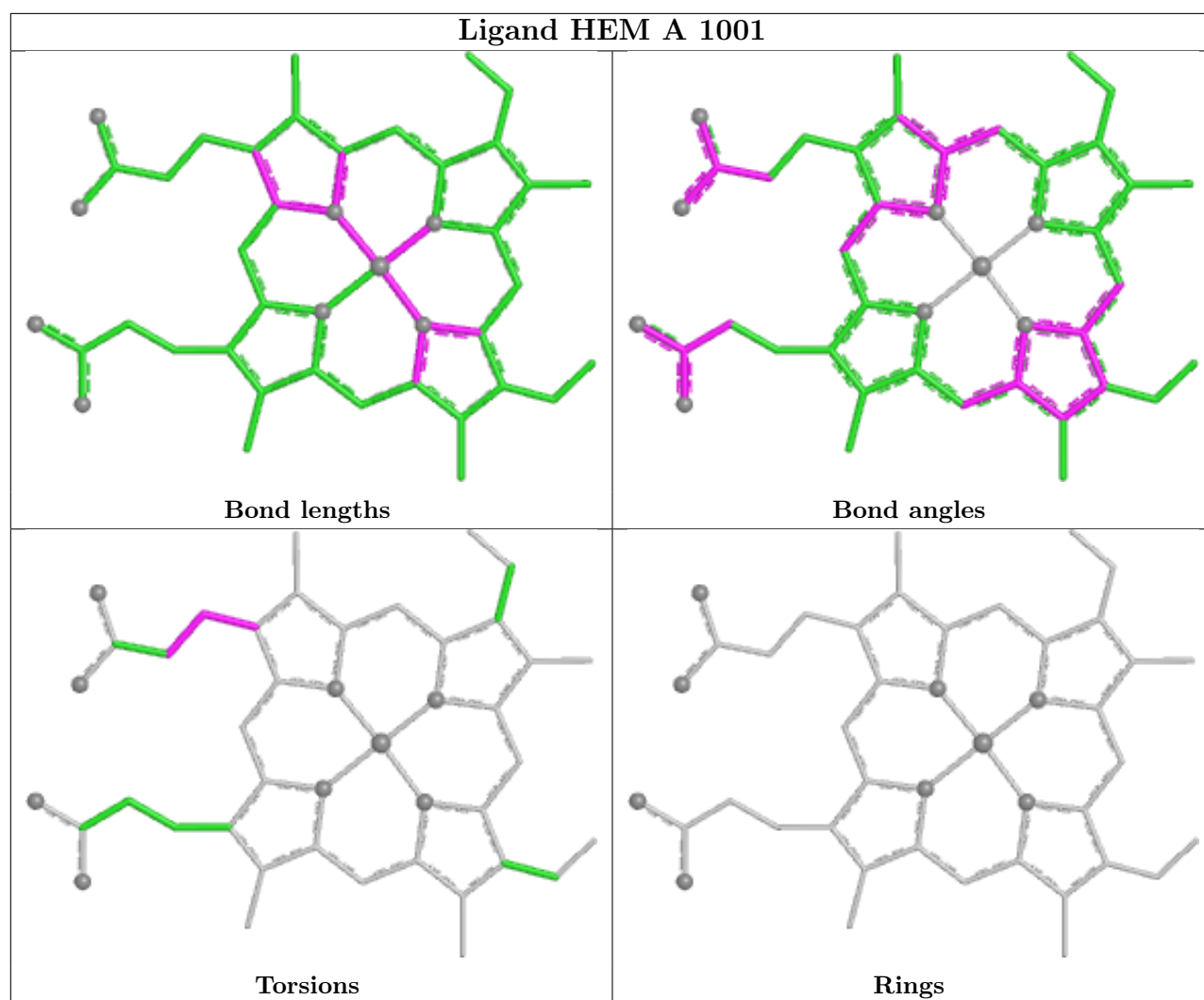
2 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1002	HEM	8	0
2	A	1001	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 1002





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	712/751 (94%)	1.10	125 (17%) 4 7	121, 290, 427, 584	0

All (125) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	546	SER	16.8
1	A	75	HIS	16.1
1	A	497	PHE	15.4
1	A	498	GLU	15.0
1	A	505	PHE	14.5
1	A	496	PHE	13.9
1	A	642	TYR	13.6
1	A	649	PHE	12.9
1	A	479	ALA	12.2
1	A	502	THR	11.7
1	A	477	PRO	11.5
1	A	493	VAL	11.3
1	A	489	VAL	11.1
1	A	482	GLU	10.8
1	A	73	LEU	10.7
1	A	532	MET	10.4
1	A	501	ALA	10.3
1	A	72	VAL	9.9
1	A	494	GLU	8.9
1	A	645	LEU	8.8
1	A	74	GLY	8.5
1	A	347	PHE	8.1
1	A	486	TRP	7.6
1	A	164	PRO	7.4
1	A	492	TRP	7.3
1	A	15	LEU	7.2
1	A	526	ALA	7.1

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Mol	Chain	Res	Type	RSRZ
1	A	527	ALA	7.1
1	A	528	ALA	7.1
1	A	64	THR	6.5
1	A	186	ARG	6.2
1	A	412	TYR	6.2
1	A	395	HIS	6.0
1	A	485	ARG	6.0
1	A	495	GLY	5.9
1	A	641	VAL	5.9
1	A	491	LEU	5.9
1	A	543	LEU	5.8
1	A	478	ILE	5.7
1	A	222	ASN	5.7
1	A	83	TRP	5.7
1	A	509	PHE	5.7
1	A	504	ALA	5.6
1	A	625	GLN	5.5
1	A	499	VAL	5.5
1	A	208	THR	5.4
1	A	480	VAL	5.2
1	A	614	LEU	5.2
1	A	155	TYR	4.9
1	A	156	TYR	4.9
1	A	500	PHE	4.7
1	A	646	ALA	4.7
1	A	648	GLY	4.5
1	A	285	PHE	4.4
1	A	19	PHE	4.3
1	A	350	ALA	4.2
1	A	710	GLU	4.2
1	A	340	ILE	4.1
1	A	227	THR	4.0
1	A	353	PHE	4.0
1	A	30	TYR	3.9
1	A	277	GLN	3.9
1	A	185	ALA	3.9
1	A	70	GLY	3.8
1	A	344	ALA	3.8
1	A	652	LEU	3.7
1	A	638	LEU	3.7
1	A	121	THR	3.7
1	A	488	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	510	TYR	3.5
1	A	66	GLY	3.4
1	A	721	ARG	3.4
1	A	718	ASP	3.3
1	A	703	LEU	3.3
1	A	508	VAL	3.3
1	A	696	TYR	3.2
1	A	224	VAL	3.2
1	A	531	PHE	3.2
1	A	644	PHE	3.2
1	A	346	GLY	3.2
1	A	71	SER	3.2
1	A	536	VAL	3.1
1	A	719	THR	3.1
1	A	109	ASP	3.1
1	A	717	LEU	3.1
1	A	61	TRP	3.0
1	A	724	ARG	2.9
1	A	160	TYR	2.9
1	A	597	PHE	2.9
1	A	465	PHE	2.8
1	A	184	GLU	2.8
1	A	125	ASP	2.8
1	A	163	ASP	2.7
1	A	600	VAL	2.6
1	A	727	ALA	2.6
1	A	154	PRO	2.6
1	A	547	GLY	2.5
1	A	360	GLY	2.5
1	A	506	ALA	2.5
1	A	396	ILE	2.5
1	A	122	ARG	2.5
1	A	205	PRO	2.4
1	A	32	LYS	2.4
1	A	196	THR	2.4
1	A	343	ILE	2.4
1	A	386	TYR	2.4
1	A	529	ALA	2.3
1	A	67	MET	2.3
1	A	361	GLY	2.3
1	A	725	THR	2.3
1	A	716	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	571	GLY	2.3
1	A	404	TRP	2.2
1	A	542	HIS	2.2
1	A	399	PRO	2.2
1	A	530	ILE	2.2
1	A	297	LEU	2.2
1	A	69	VAL	2.1
1	A	190	PHE	2.1
1	A	357	ILE	2.1
1	A	487	TRP	2.1
1	A	483	TYR	2.1
1	A	533	LEU	2.0
1	A	406	GLY	2.0
1	A	728	ASP	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](#)

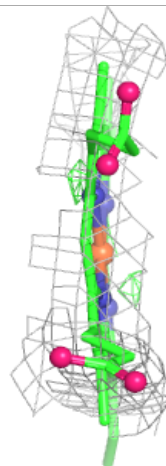
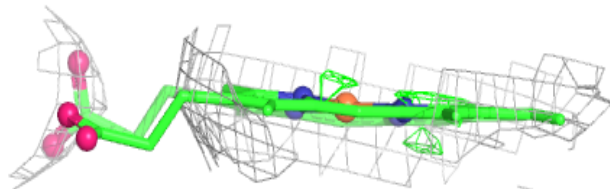
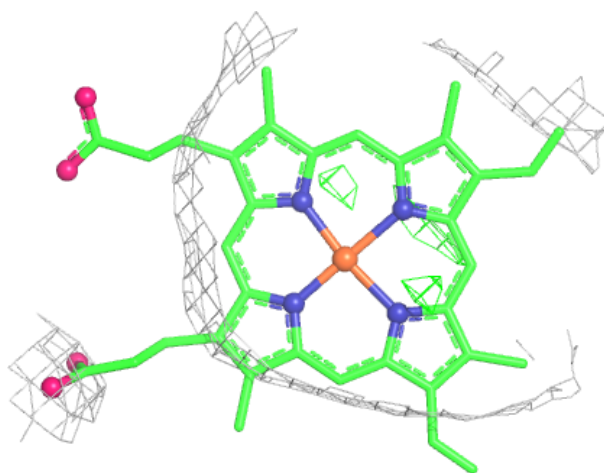
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

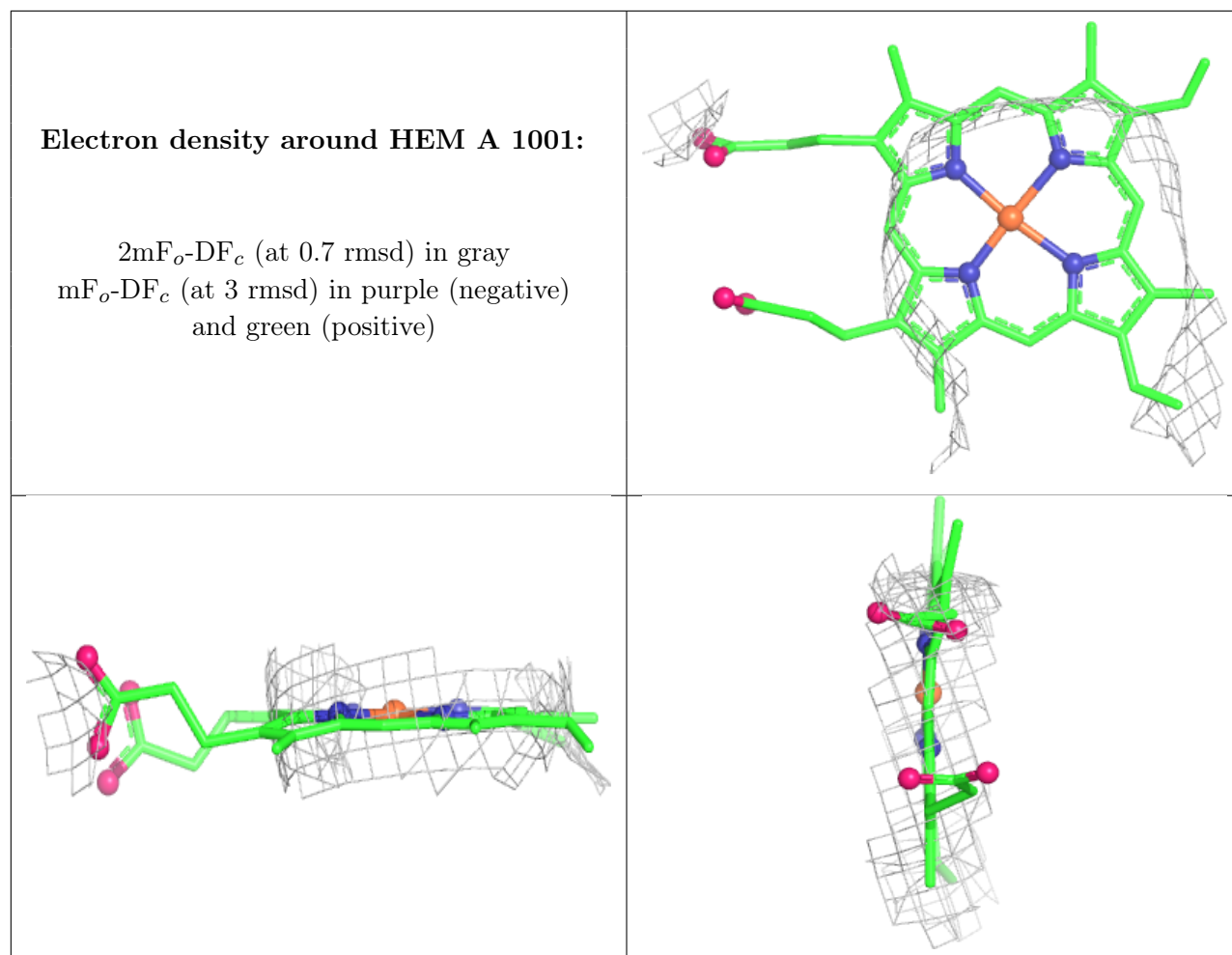
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	HEM	A	1002	43/43	0.94	0.22	143,215,252,295	0
2	HEM	A	1001	43/43	0.95	0.17	232,284,309,325	0
4	FE	A	1004	1/1	0.95	0.06	256,256,256,256	0
3	CA	A	1003	1/1	0.98	0.09	219,219,219,219	0

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 A 1002:

$2mF_o-DF_c$ (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.