



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 04:53 PM EDT

PDB ID : 3NLT / pdb_00003nlt
Title : Structure of endothelial nitric oxide synthase heme domain complexed with N 1-{(3'S,4'S)-4'-[(6"-amino-4"-methylpyridin-2"-yl)methyl]pyrrolidin-3'-yl}- N 2-(3'-fluorophenethyl)ethane-1,2-diamine tetrahydrochloride
Authors : Xue, F.; Li, H.; Fang, J.; Delker, S.L.; Poulos, T.L.; Silverman, R.B.
Deposited on : 2010-06-21
Resolution : 2.74 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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

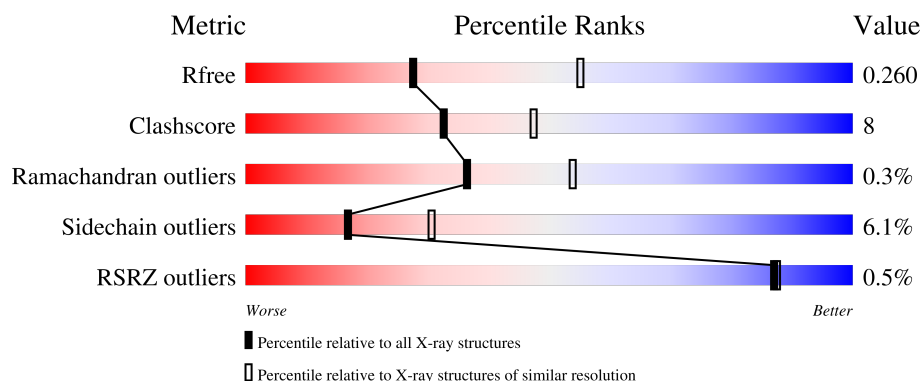
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.74 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	1819 (2.76-2.72)
Clashscore	190562	1866 (2.76-2.72)
Ramachandran outliers	187476	1830 (2.76-2.72)
Sidechain outliers	187428	1831 (2.76-2.72)
RSRZ outliers	180081	1819 (2.76-2.72)

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	444	
1	B	444	

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 6674 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.

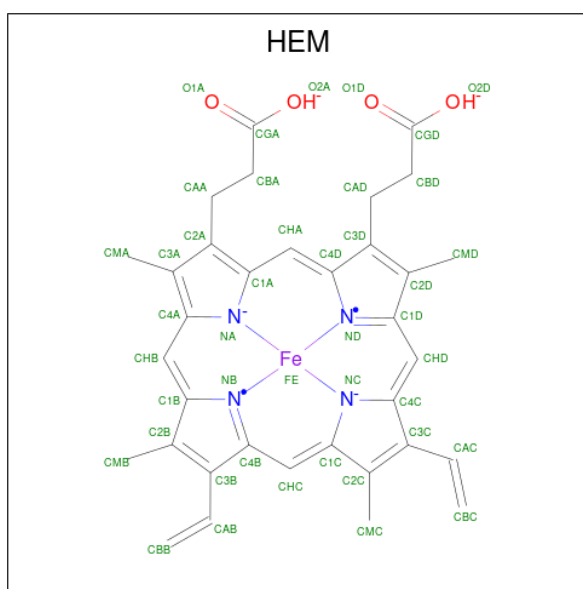
- Molecule 1 is a protein called Nitric oxide synthase, endothelial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	403	Total	C	N	O	S	0	1	0
			3210	2040	564	590	16			
1	B	403	Total	C	N	O	S	0	0	0
			3209	2040	566	587	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	ARG	CYS	SEE REMARK 999	UNP P29473
B	100	ARG	CYS	SEE REMARK 999	UNP P29473

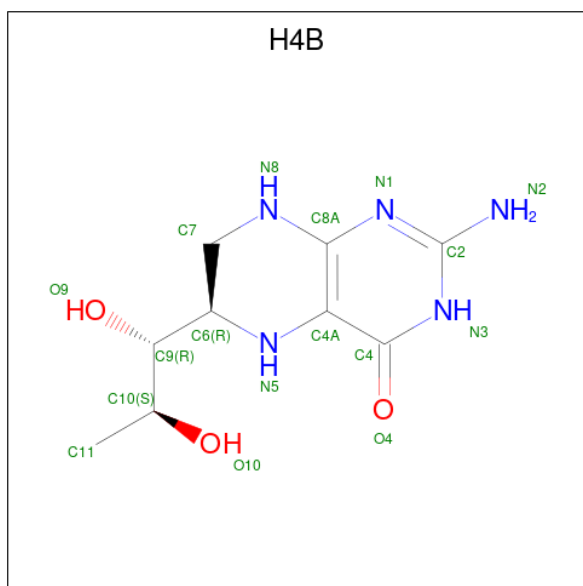
- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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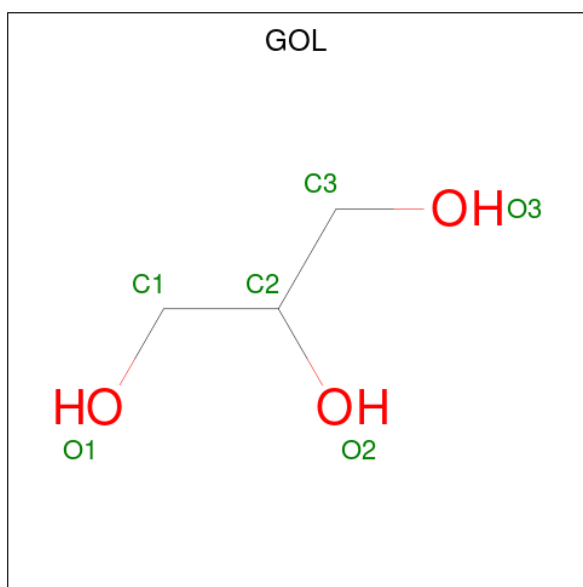
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



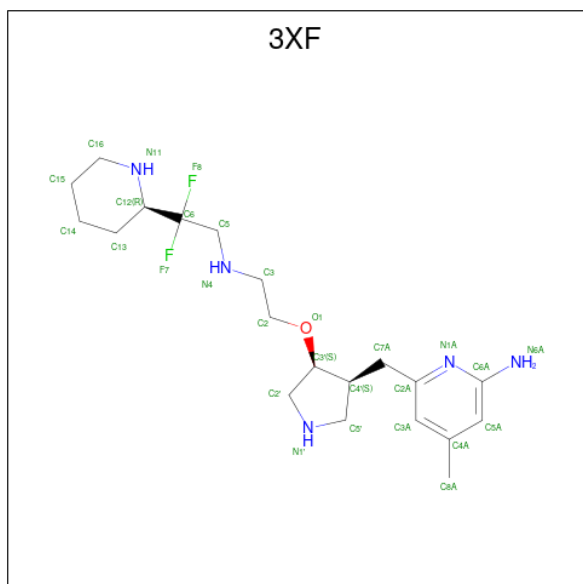
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is 6-((3S,4S)-4-[2-((2,2-difluoro-2-[(2R)-piperidin-2-yl]ethyl)amino)ethoxy]pyrrolidin-3-yl)methyl)-4-methylpyridin-2-amine (CCD ID: 3XF) (formula: C₂₀H₃₃F₂N₅O).



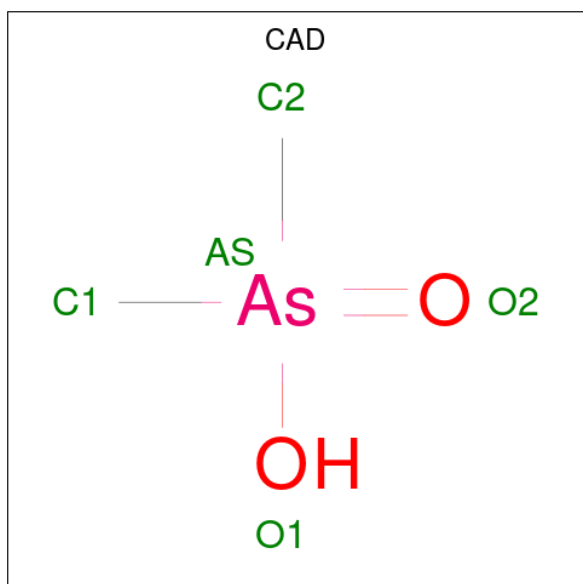
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	F	N	O	0	0
			28	20	2	5	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	F	N	O	0	0
			28	20	2	5	1		

- Molecule 6 is CACODYLIC ACID (CCD ID: CAD) (formula: $C_2H_7AsO_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	As	C	0	0
			3	1	2		
6	B	1	Total	As	C	0	0
			3	1	2		

- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 8 is water.

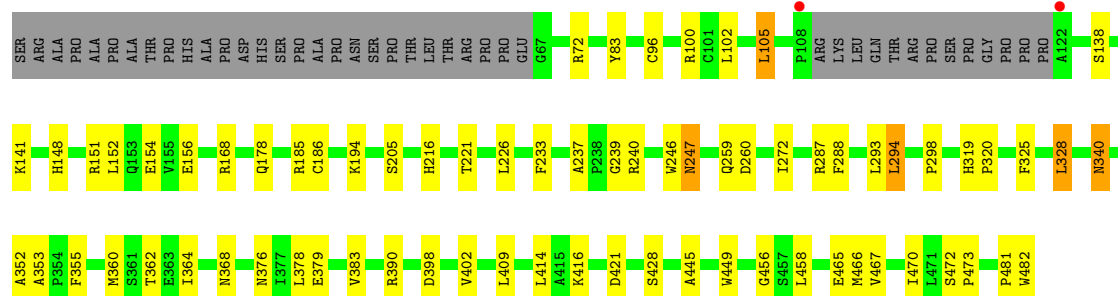
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	32	Total	O	0	0
			32	32		
8	B	28	Total	O	0	0
			28	28		

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.

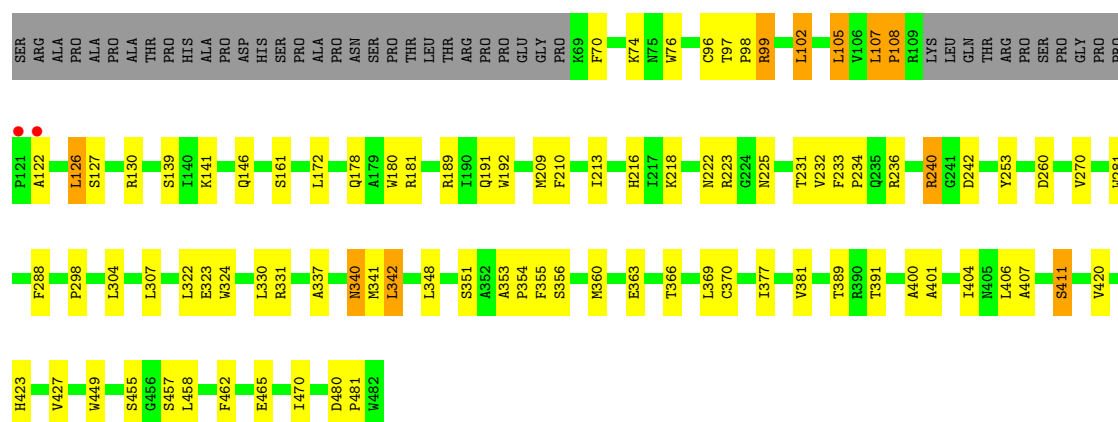
- Molecule 1: Nitric oxide synthase, endothelial

Chain A: 



- Molecule 1: Nitric oxide synthase, endothelial

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.91Å 106.91Å 157.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.85 – 2.74 36.85 – 2.74	Depositor EDS
% Data completeness (in resolution range)	97.3 (36.85-2.74) 97.3 (36.85-2.74)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 2.72Å)	Xtriage
Refinement program	REFMAC 5.5.0102, CNS	Depositor
R, R_{free}	0.186 , 0.262 0.184 , 0.260	Depositor DCC
R_{free} test set	1241 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	46.7	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 32.0	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	0.95	EDS
Total number of atoms	6674	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, GOL, 3XF, H4B, ZN, CAD

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	0.80	0/3299	0.98	3/4494 (0.1%)
1	B	0.79	0/3298	1.02	7/4491 (0.2%)
All	All	0.80	0/6597	1.00	10/8985 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	107	LEU	CA-C-N	12.89	135.95	119.84
1	B	107	LEU	C-N-CA	12.89	135.95	119.84
1	B	70	PHE	CA-C-N	6.56	126.47	119.85
1	B	70	PHE	C-N-CA	6.56	126.47	119.85
1	B	348	LEU	N-CA-C	-6.05	101.04	110.42
1	B	240	ARG	N-CA-C	5.63	117.34	108.96
1	A	100	ARG	N-CA-C	5.60	117.62	108.55
1	A	353	ALA	CA-C-N	5.50	125.42	119.76
1	A	353	ALA	C-N-CA	5.50	125.42	119.76
1	B	108	PRO	N-CA-C	5.05	122.88	112.47

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	3210	0	3110	46	0
1	B	3209	0	3117	48	0
2	A	43	0	30	8	0
2	B	43	0	30	8	0
3	A	17	0	15	2	0
3	B	17	0	15	1	0
4	A	6	0	8	0	0
4	B	6	0	8	0	0
5	A	28	0	33	0	0
5	B	28	0	33	4	0
6	A	3	0	0	0	0
6	B	3	0	0	1	0
7	A	1	0	0	0	0
8	A	32	0	0	6	0
8	B	28	0	0	0	0
All	All	6674	0	6399	102	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 8.

All (102) 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:260[B]:ASP:O	1:A:260[B]:ASP:OD1	1.70	1.09
2:B:500:HEM:HBB2	2:B:500:HEM:HHC	1.49	0.95
1:B:423:HIS:O	1:B:427:VAL:HG23	1.68	0.93
2:B:500:HEM:HMC1	2:B:500:HEM:HBC2	1.48	0.92
1:A:260[B]:ASP:OD1	1:A:260[B]:ASP:C	2.15	0.89
2:B:500:HEM:HBC2	2:B:500:HEM:CMC	2.13	0.79
1:B:281:TRP:HB2	1:B:304:LEU:HD21	1.65	0.78
1:B:337:ALA:HB2	1:B:356:SER:HB3	1.69	0.74
2:A:500:HEM:HBB2	2:A:500:HEM:HHC	1.73	0.71
1:A:364:ILE:HA	1:A:368:ASN:HD22	1.57	0.69
1:B:340:ASN:HD22	1:B:340:ASN:C	2.00	0.69
2:B:500:HEM:HHC	2:B:500:HEM:CBB	2.22	0.68
2:B:500:HEM:HBB2	2:B:500:HEM:CHC	2.20	0.66
1:B:363:GLU:OE1	5:B:800:3XF:H5'A	1.96	0.66
1:B:342:LEU:C	1:B:342:LEU:HD23	2.23	0.64
1:B:178:GLN:HE22	1:B:181:ARG:HH11	1.46	0.63
1:B:377:ILE:O	1:B:381:VAL:HG23	1.98	0.63
1:B:369:LEU:O	1:B:377:ILE:HG12	1.99	0.62
1:A:465:GLU:HB3	1:B:105:LEU:HD22	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:337:ALA:CB	1:B:356:SER:HB3	2.29	0.62
1:A:360:MET:HE3	1:A:362:THR:OG1	2.00	0.61
1:A:205:SER:HB3	8:A:1031:HOH:O	2.01	0.61
1:A:355:PHE:CD1	2:A:500:HEM:HAC	2.36	0.61
1:A:378:LEU:HB2	8:A:1022:HOH:O	2.00	0.61
1:B:236:ARG:HD3	1:B:351:SER:HB3	1.83	0.60
1:B:210:PHE:HE1	1:B:307:LEU:HD23	1.66	0.60
1:A:178:GLN:HB3	1:A:473:PRO:HG2	1.84	0.60
1:A:325:PHE:HA	1:A:328:LEU:HD22	1.84	0.59
1:A:481:PRO:HD2	1:A:482:TRP:CE3	2.37	0.59
1:B:122:ALA:O	1:B:126:LEU:HB2	2.02	0.59
1:A:239:GLY:C	8:A:1001:HOH:O	2.45	0.59
1:A:105:LEU:HD23	1:A:105:LEU:N	2.18	0.58
1:A:186:CYS:HB2	2:A:500:HEM:ND	2.17	0.58
1:A:240:ARG:HD3	1:A:298:PRO:HB3	1.85	0.58
2:B:500:HEM:HMC1	2:B:500:HEM:CBC	2.30	0.58
2:A:500:HEM:HHC	2:A:500:HEM:CBB	2.35	0.56
1:A:246:TRP:HB2	1:A:294:LEU:HB3	1.87	0.56
1:B:400:ALA:O	1:B:404:ILE:HG13	2.06	0.56
1:A:216:HIS:CD2	1:A:216:HIS:C	2.86	0.53
1:B:366:THR:O	1:B:370:CYS:HB2	2.09	0.53
1:A:472:SER:HA	1:A:473:PRO:C	2.34	0.52
1:A:398:ASP:O	1:A:402:VAL:HG23	2.10	0.52
1:A:186:CYS:HB2	2:A:500:HEM:C4D	2.45	0.51
1:B:457:SER:HA	1:B:462:PHE:CG	2.45	0.51
1:A:246:TRP:CD1	1:A:481:PRO:HG2	2.45	0.51
1:A:237:ALA:HB3	1:A:240:ARG:HB3	1.93	0.50
1:A:72:ARG:HB2	1:A:83:TYR:CE2	2.46	0.50
1:B:449:TRP:HA	3:B:600:H4B:N1	2.26	0.50
1:B:231:THR:O	1:B:354:PRO:HD2	2.12	0.50
1:B:172:LEU:HD11	1:B:232:VAL:HG11	1.94	0.50
1:B:231:THR:O	1:B:353:ALA:HA	2.12	0.50
1:B:360:MET:HA	1:B:420:VAL:O	2.12	0.49
5:B:800:3XF:H5'A	5:B:800:3XF:N1A	2.28	0.49
1:A:185:ARG:HD3	1:A:449:TRP:CD2	2.49	0.48
2:B:500:HEM:C1C	5:B:800:3XF:H8AB	2.48	0.48
1:B:455:SER:O	1:B:458:LEU:HB2	2.14	0.48
1:A:233:PHE:HB2	1:A:352:ALA:O	2.13	0.47
1:B:407:ALA:O	1:B:411:SER:OG	2.24	0.47
1:A:355:PHE:CD1	2:A:500:HEM:CAC	2.96	0.47
1:B:180:TRP:CE3	1:B:192:TRP:HA	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:500:HEM:HBB2	2:A:500:HEM:CHC	2.40	0.47
1:A:364:ILE:HA	1:A:368:ASN:ND2	2.28	0.47
2:B:500:HEM:HBA1	5:B:800:3XF:H7AA	1.97	0.46
1:A:105:LEU:HD22	1:B:465:GLU:HB3	1.98	0.46
1:B:324:TRP:HB2	6:B:950:CAD:C1	2.45	0.46
1:B:130:ARG:HB3	1:B:130:ARG:CZ	2.46	0.46
1:B:99:ARG:HB2	1:B:99:ARG:HH11	1.81	0.46
1:A:148:HIS:CD2	1:A:148:HIS:C	2.95	0.45
1:B:74:LYS:HD3	1:B:76:TRP:CE2	2.52	0.45
1:A:221:THR:O	1:A:226:LEU:HD12	2.15	0.45
1:B:340:ASN:HD22	1:B:341:MET:N	2.14	0.44
1:A:287:ARG:HB2	1:A:288:PHE:CD2	2.53	0.44
1:A:141:LYS:HA	1:A:141:LYS:HD3	1.79	0.44
1:B:233:PHE:HB3	1:B:234:PRO:CD	2.48	0.44
1:A:247:ASN:OD1	1:A:247:ASN:N	2.51	0.44
1:A:152:LEU:O	1:A:156:GLU:HG2	2.17	0.44
1:A:445:ALA:HB3	1:A:466:MET:HB3	1.99	0.44
1:B:209:MET:O	1:B:213:ILE:HG13	2.19	0.43
1:B:236:ARG:HD2	1:B:242:ASP:CG	2.44	0.43
1:B:189:ARG:C	1:B:191:GLN:H	2.27	0.43
1:B:337:ALA:HA	1:B:355:PHE:O	2.19	0.43
1:A:239:GLY:HA2	8:A:1001:HOH:O	2.19	0.42
1:B:189:ARG:C	1:B:191:GLN:N	2.77	0.42
1:B:240:ARG:HD2	1:B:298:PRO:HB3	2.01	0.42
1:A:151:ARG:HD3	1:A:168:ARG:HH21	1.85	0.42
1:B:406:LEU:HD12	1:B:406:LEU:HA	1.95	0.41
1:B:480:ASP:HA	1:B:481:PRO:HD3	1.94	0.41
1:A:376:ASN:ND2	8:A:1022:HOH:O	2.34	0.41
1:B:216:HIS:CD2	1:B:216:HIS:C	2.98	0.41
1:A:319:HIS:CG	1:A:320:PRO:HD2	2.55	0.41
1:A:409:LEU:HD21	1:A:421:ASP:HB3	2.02	0.41
1:B:253:TYR:CE2	1:B:288:PHE:HD1	2.38	0.41
1:B:340:ASN:C	1:B:340:ASN:ND2	2.71	0.41
1:A:470:ILE:HA	8:A:1023:HOH:O	2.21	0.41
1:A:458:LEU:HD21	1:B:401:ALA:CB	2.51	0.41
1:A:96:CYS:HB3	1:B:96:CYS:HB3	2.03	0.40
1:A:467:VAL:HG13	1:B:102:LEU:HD13	2.03	0.40
1:B:222:ASN:HB3	1:B:225:ASN:O	2.21	0.40
1:A:449:TRP:HA	3:A:600:H4B:N1	2.36	0.40
1:B:97:THR:HB	1:B:98:PRO:HD2	2.03	0.40
1:A:340:ASN:H	1:A:340:ASN:HD22	1.70	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:500:HEM:HAA2	3:A:600:H4B:HN22	1.86	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	400/444 (90%)	379 (95%)	20 (5%)	1 (0%)	36	54
1	B	399/444 (90%)	372 (93%)	26 (6%)	1 (0%)	36	54
All	All	799/888 (90%)	751 (94%)	46 (6%)	2 (0%)	36	54

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	108	PRO
1	A	456	GLY

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	343/377 (91%)	325 (95%)	18 (5%)	21	38
1	B	343/377 (91%)	319 (93%)	24 (7%)	14	26
All	All	686/754 (91%)	644 (94%)	42 (6%)	17	30

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	102	LEU
1	A	105	LEU
1	A	138	SER
1	A	154	GLU
1	A	194	LYS
1	A	247	ASN
1	A	259	GLN
1	A	272	ILE
1	A	293	LEU
1	A	294	LEU
1	A	328	LEU
1	A	340	ASN
1	A	379	GLU
1	A	383	VAL
1	A	390	ARG
1	A	414	LEU
1	A	416	LYS
1	A	428	SER
1	B	99	ARG
1	B	102	LEU
1	B	105	LEU
1	B	107	LEU
1	B	126	LEU
1	B	127	SER
1	B	139	SER
1	B	141	LYS
1	B	146	GLN
1	B	161	SER
1	B	218	LYS
1	B	223	ARG
1	B	260	ASP
1	B	270	VAL
1	B	322	LEU
1	B	323	GLU
1	B	330	LEU
1	B	331	ARG
1	B	340	ASN
1	B	342	LEU
1	B	389	THR
1	B	391	THR
1	B	411	SER
1	B	470	ILE

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

Mol	Chain	Res	Type
1	A	153	GLN
1	A	166	HIS
1	A	191	GLN
1	A	340	ASN
1	A	368	ASN
1	A	468	ASN
1	B	178	GLN
1	B	191	GLN
1	B	215	ASN
1	B	222	ASN
1	B	225	ASN
1	B	296	GLN
1	B	340	ASN
1	B	376	ASN
1	B	405	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 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	GOL	B	880	-	5,5,5	0.40	0	5,5,5	0.68	0
6	CAD	B	950	1	0,2,4	-	-	0,1,6	-	-
5	3XF	A	800	-	28,30,30	0.69	0	26,41,41	2.33	6 (23%)
2	HEM	A	500	1	50,50,50	1.73	8 (16%)	67,82,82	1.31	8 (11%)
3	H4B	A	600	-	17,18,18	1.34	2 (11%)	14,26,26	2.64	8 (57%)
6	CAD	A	950	1	0,2,4	-	-	0,1,6	-	-
4	GOL	A	880	-	5,5,5	0.32	0	5,5,5	0.81	0
3	H4B	B	600	-	17,18,18	0.85	0	14,26,26	2.00	6 (42%)
5	3XF	B	800	-	28,30,30	0.66	0	26,41,41	2.46	8 (30%)
2	HEM	B	500	1	50,50,50	1.79	10 (20%)	67,82,82	1.27	8 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	B	880	-	-	0/4/4/4	-
5	3XF	A	800	-	-	8/16/37/37	0/3/3/3
2	HEM	A	500	1	-	4/14/54/54	-
3	H4B	A	600	-	-	0/8/17/17	0/2/2/2
4	GOL	A	880	-	-	2/4/4/4	-
3	H4B	B	600	-	-	0/8/17/17	0/2/2/2
5	3XF	B	800	-	-	9/16/37/37	0/3/3/3
2	HEM	B	500	1	-	1/14/54/54	-

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	HEM	C3D-C2D	7.23	1.52	1.36
2	A	500	HEM	C3D-C2D	6.55	1.50	1.36
2	A	500	HEM	FE-NA	4.39	2.09	1.95
2	B	500	HEM	FE-NA	3.35	2.06	1.95
3	A	600	H4B	C7-C6	3.29	1.55	1.52
2	B	500	HEM	FE-ND	3.20	2.04	1.94
2	A	500	HEM	FE-ND	2.98	2.04	1.94
2	B	500	HEM	CAB-C3B	2.94	1.55	1.47
2	A	500	HEM	CAC-C3C	2.82	1.54	1.47
3	A	600	H4B	C7-N8	2.77	1.49	1.46
2	B	500	HEM	CAC-C3C	2.65	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	HEM	CAB-C3B	2.55	1.54	1.47
2	B	500	HEM	CMC-C2C	2.47	1.55	1.50
2	B	500	HEM	O1D-CGD	2.47	1.30	1.22
2	B	500	HEM	FE-NB	2.36	2.02	1.94
2	A	500	HEM	CHC-C1C	-2.31	1.33	1.38
2	B	500	HEM	FE-NC	2.28	2.02	1.95
2	A	500	HEM	CMB-C2B	2.14	1.55	1.50
2	A	500	HEM	CMC-C2C	2.05	1.55	1.50
2	B	500	HEM	C4C-NC	-2.02	1.35	1.39

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	800	3XF	C6A-N1A-C2A	7.05	123.34	118.07
5	A	800	3XF	C16-N11-C12	6.85	123.07	111.97
5	B	800	3XF	C16-N11-C12	6.58	122.63	111.97
5	A	800	3XF	C6A-N1A-C2A	5.78	122.40	118.07
5	A	800	3XF	C3-N4-C5	5.15	123.77	113.35
3	A	600	H4B	C2-N1-C8A	4.90	122.00	113.36
2	B	500	HEM	C4D-ND-C1D	4.74	110.82	105.21
3	A	600	H4B	C11-C10-C9	-4.50	106.61	112.11
2	A	500	HEM	C4D-ND-C1D	4.44	110.46	105.21
3	B	600	H4B	C2-N1-C8A	3.47	119.48	113.36
3	A	600	H4B	C4A-C4-N3	3.25	121.07	112.13
5	B	800	3XF	F8-C6-F7	3.10	110.04	106.04
3	B	600	H4B	O4-C4-C4A	-3.10	119.79	127.26
5	B	800	3XF	C5'-N1'-C2'	3.06	113.07	105.45
5	B	800	3XF	C3-N4-C5	3.05	119.53	113.35
3	A	600	H4B	O4-C4-C4A	-3.03	119.96	127.26
2	B	500	HEM	CBA-CAA-C2A	-2.99	104.25	112.53
3	A	600	H4B	C2-N3-C4	-2.92	119.82	125.11
2	A	500	HEM	CAD-CBD-CGD	-2.91	105.94	113.67
3	B	600	H4B	C11-C10-C9	-2.89	108.58	112.11
5	B	800	3XF	C3A-C2A-N1A	-2.87	119.46	122.73
5	A	800	3XF	C5'-N1'-C2'	2.83	112.49	105.45
3	B	600	H4B	C4A-C4-N3	2.83	119.90	112.13
2	A	500	HEM	CHA-C4D-ND	2.73	127.74	124.37
2	A	500	HEM	CHC-C4B-NB	2.70	127.33	124.42
5	B	800	3XF	C15-C14-C13	2.69	116.94	111.42
3	A	600	H4B	O9-C9-C10	-2.61	104.17	109.14
5	A	800	3XF	C3A-C2A-N1A	-2.54	119.84	122.73
5	A	800	3XF	F8-C6-F7	2.52	109.30	106.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	HEM	CMB-C2B-C1B	2.46	128.88	125.03
2	B	500	HEM	CAD-CBD-CGD	-2.37	107.38	113.67
3	B	600	H4B	O9-C9-C6	2.27	114.72	109.28
3	A	600	H4B	O10-C10-C9	2.26	113.52	109.77
2	B	500	HEM	CAD-C3D-C4D	2.25	128.61	124.70
2	A	500	HEM	CAD-C3D-C4D	2.22	128.57	124.70
2	B	500	HEM	CHC-C4B-NB	2.22	126.81	124.42
3	B	600	H4B	C2-N3-C4	-2.21	121.11	125.11
5	B	800	3XF	C14-C13-C12	2.16	114.41	111.14
2	B	500	HEM	CAA-CBA-CGA	2.15	119.37	113.67
2	B	500	HEM	C1D-C2D-C3D	-2.13	104.74	106.98
2	A	500	HEM	CBA-CAA-C2A	-2.13	106.64	112.53
3	A	600	H4B	O9-C9-C6	2.04	114.17	109.28
2	B	500	HEM	CMD-C2D-C1D	2.04	128.22	125.03
2	A	500	HEM	CMD-C2D-C1D	2.02	128.19	125.03

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	880	GOL	C1-C2-C3-O3
4	A	880	GOL	O2-C2-C3-O3
5	A	800	3XF	C2'-C3'-O1-C2
5	A	800	3XF	C4'-C3'-O1-C2
5	A	800	3XF	N4-C5-C6-F7
5	A	800	3XF	N4-C5-C6-F8
5	A	800	3XF	C13-C12-C6-F7
5	A	800	3XF	C13-C12-C6-F8
5	B	800	3XF	C4'-C3'-O1-C2
5	B	800	3XF	N4-C5-C6-F7
5	B	800	3XF	N4-C5-C6-F8
5	B	800	3XF	N11-C12-C6-F7
5	B	800	3XF	C13-C12-C6-F7
5	B	800	3XF	N11-C12-C6-F8
5	B	800	3XF	C13-C12-C6-F8
5	A	800	3XF	C2-C3-N4-C5
5	B	800	3XF	C2'-C3'-O1-C2
5	B	800	3XF	C2-C3-N4-C5
5	A	800	3XF	C6-C5-N4-C3
2	B	500	HEM	C2A-CAA-CBA-CGA
2	A	500	HEM	CAA-CBA-CGA-O2A
2	A	500	HEM	CAA-CBA-CGA-O1A

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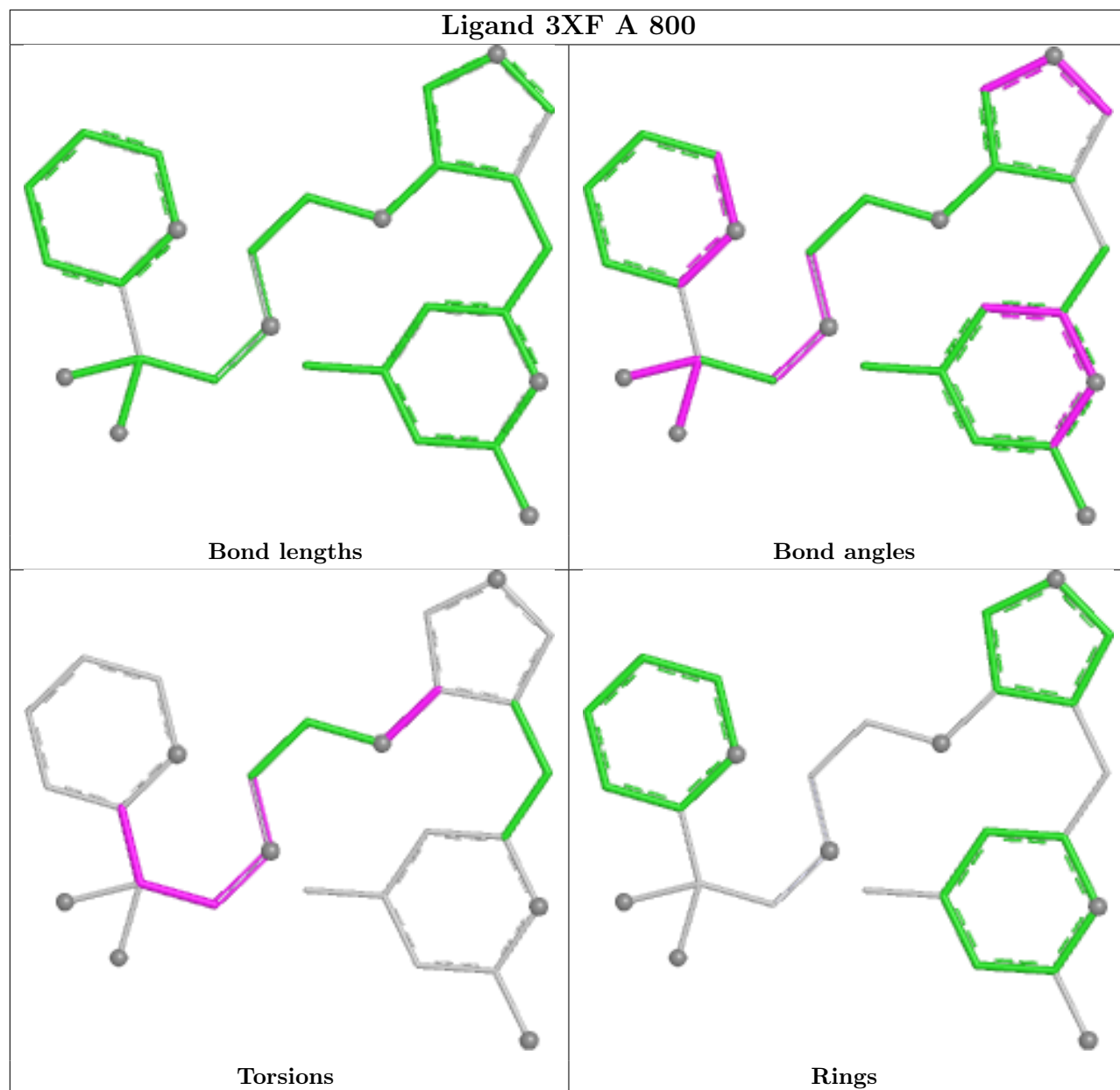
Mol	Chain	Res	Type	Atoms
2	A	500	HEM	C4C-C3C-CAC-CBC
2	A	500	HEM	C2C-C3C-CAC-CBC

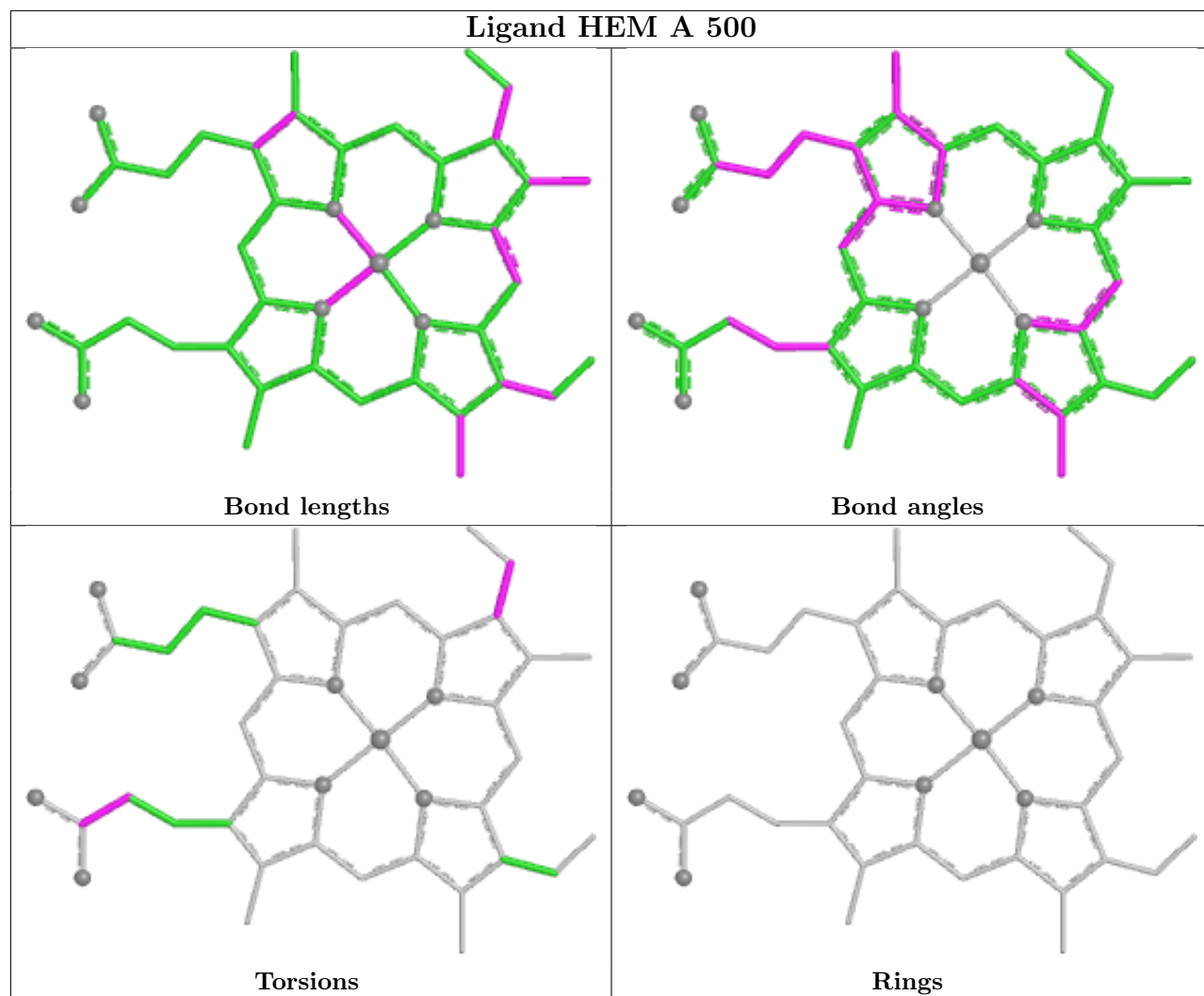
There are no ring outliers.

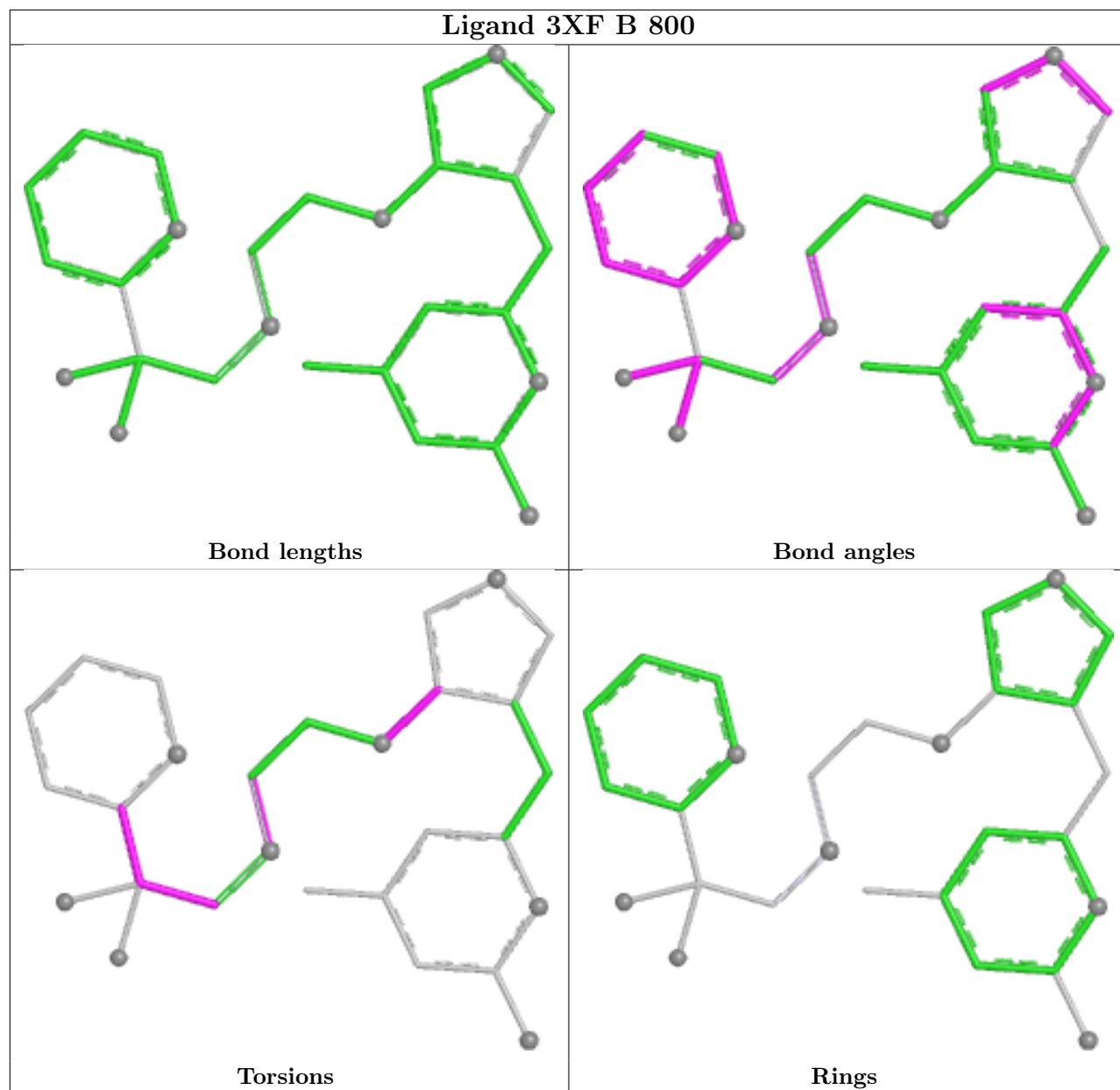
6 monomers are involved in 21 short contacts:

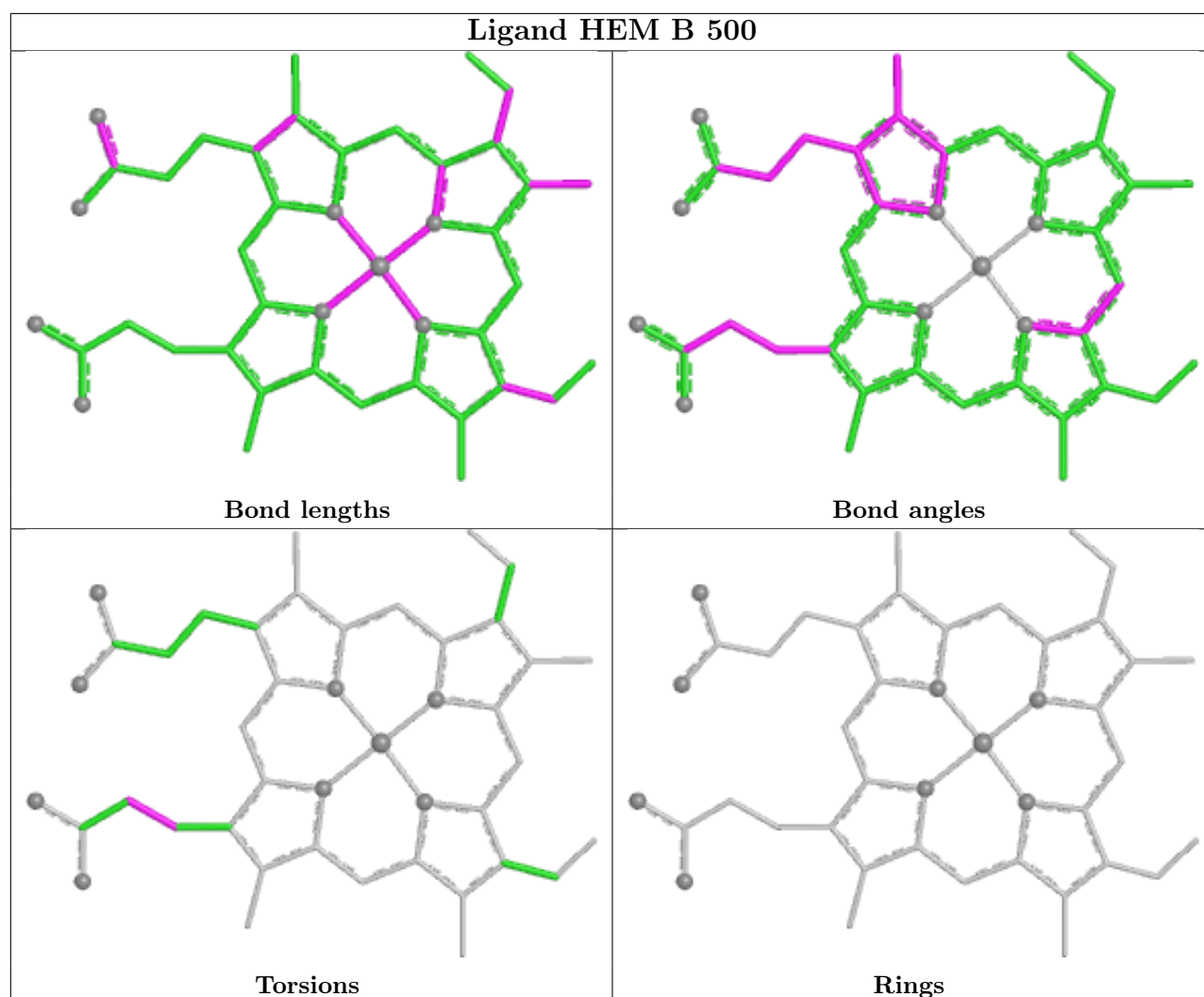
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	950	CAD	1	0
2	A	500	HEM	8	0
3	A	600	H4B	2	0
3	B	600	H4B	1	0
5	B	800	3XF	4	0
2	B	500	HEM	8	0

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	403/444 (90%)	-0.52	2 (0%) 87 87	25, 40, 64, 81	1 (0%)
1	B	403/444 (90%)	-0.43	2 (0%) 87 87	26, 43, 68, 86	0
All	All	806/888 (90%)	-0.48	4 (0%) 87 87	25, 41, 66, 86	1 (0%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	108	PRO	3.1
1	B	121	PRO	2.6
1	B	122	ALA	2.1
1	A	122	ALA	2.1

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(Å ²)	Q<0.9
4	GOL	A	880	6/6	0.89	0.14	55,57,57,58	0

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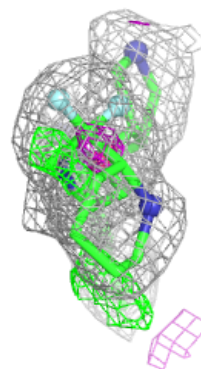
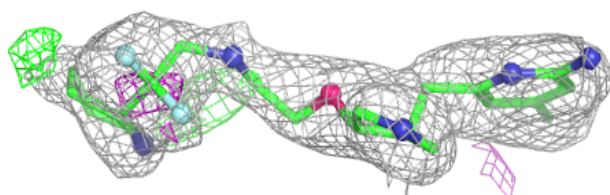
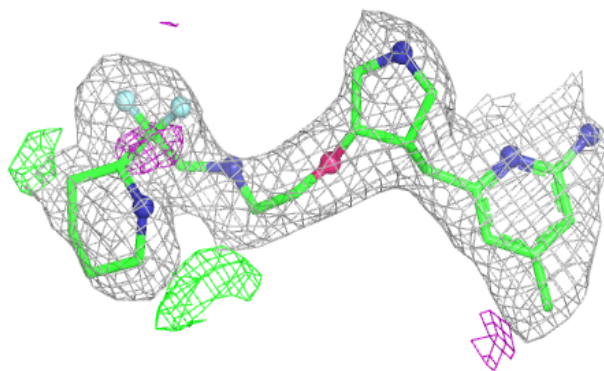
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	3XF	A	800	28/28	0.90	0.14	27,46,77,77	0
5	3XF	B	800	28/28	0.90	0.14	45,58,83,84	0
4	GOL	B	880	6/6	0.92	0.16	55,56,56,57	0
3	H4B	B	600	17/17	0.96	0.06	34,37,40,40	0
6	CAD	A	950	3/5	0.96	0.11	69,69,70,72	0
3	H4B	A	600	17/17	0.97	0.05	20,28,33,37	0
2	HEM	B	500	43/43	0.98	0.06	26,30,38,41	0
2	HEM	A	500	43/43	0.98	0.07	21,27,43,46	0
6	CAD	B	950	3/5	0.99	0.06	63,63,64,64	0
7	ZN	A	900	1/1	1.00	0.01	35,35,35,35	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.

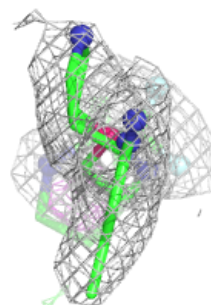
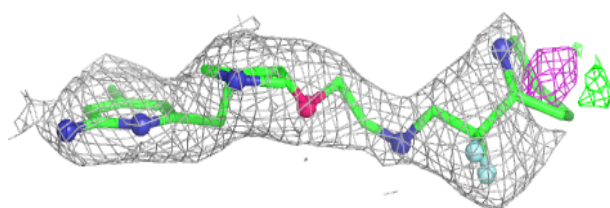
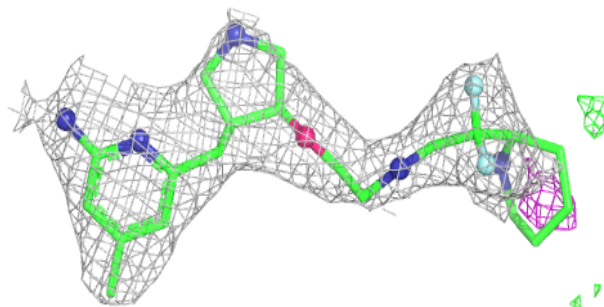
Electron density around 3XF A 800:

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



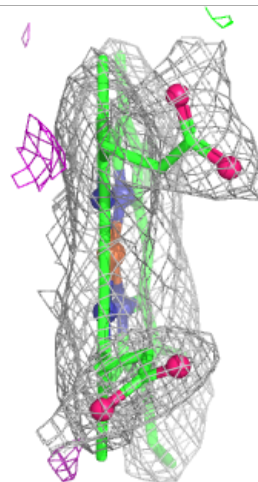
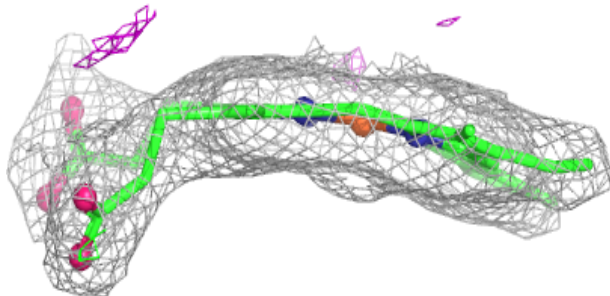
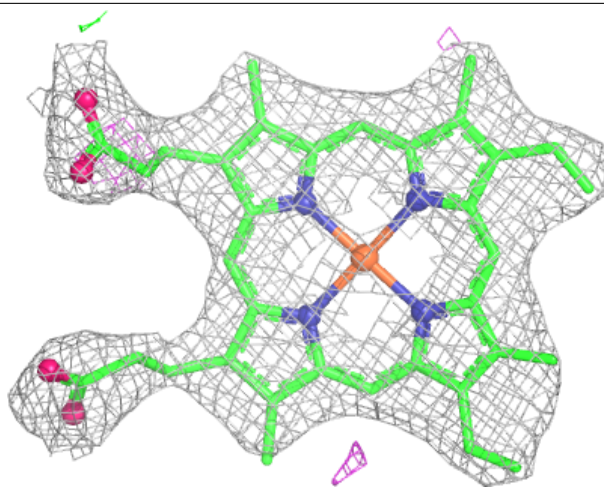
Electron density around 3XF B 800:

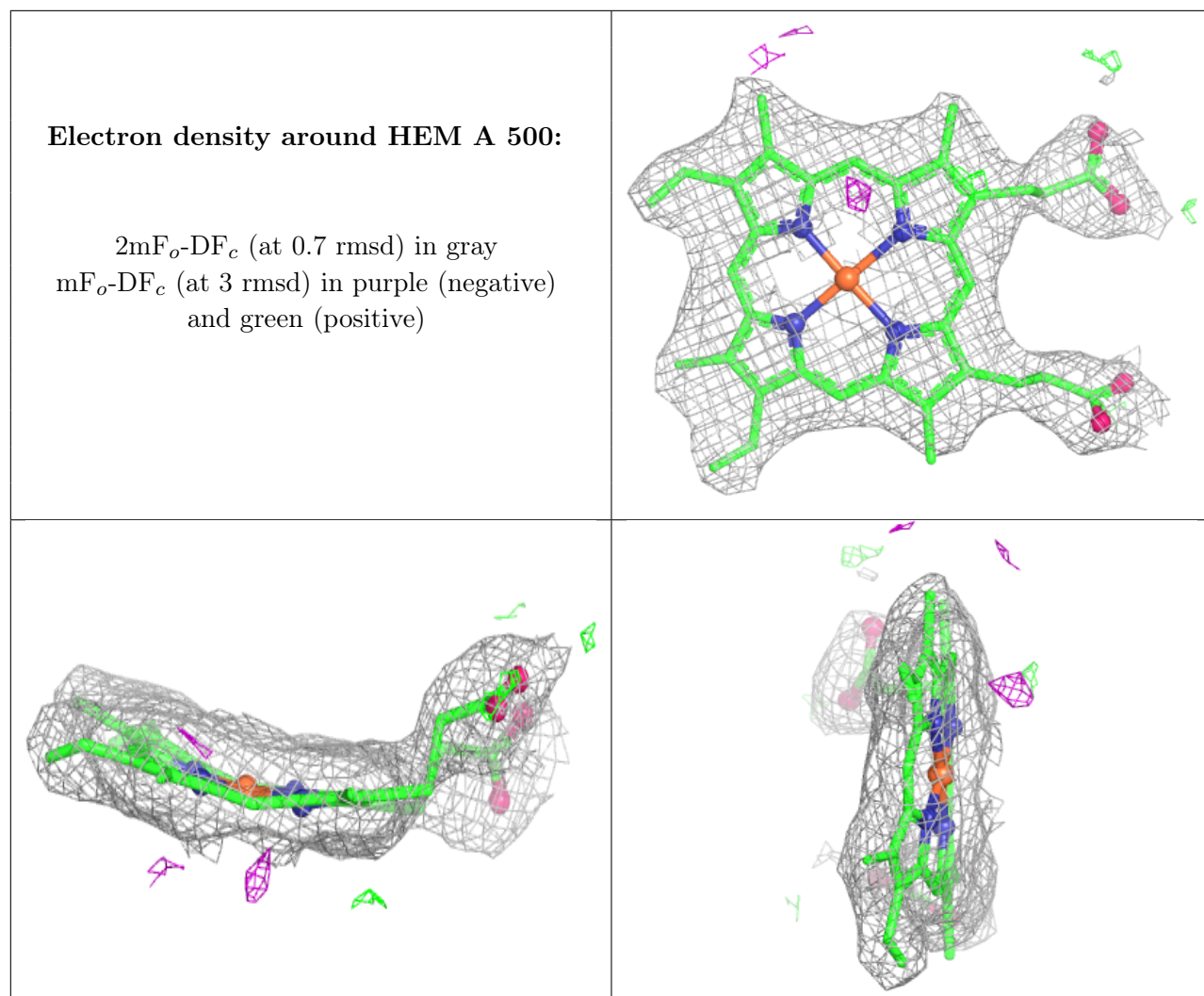
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM B 500:

$2mF_o-DF_c$ (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.