



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2024 – 09:21 PM EST

PDB ID : 3N5Q
Title : Structure of endothelial nitric oxide synthase heme domain complexed with 6,6'-((2,2'-(5-amino-1,3-phenylene)bis(ethane-2,1-diyl))bis(4-methylpyridin-2-amine))
Authors : Delker, S.L.; Li, H.; Poulos, T.L.
Deposited on : 2010-05-25
Resolution : 2.90 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

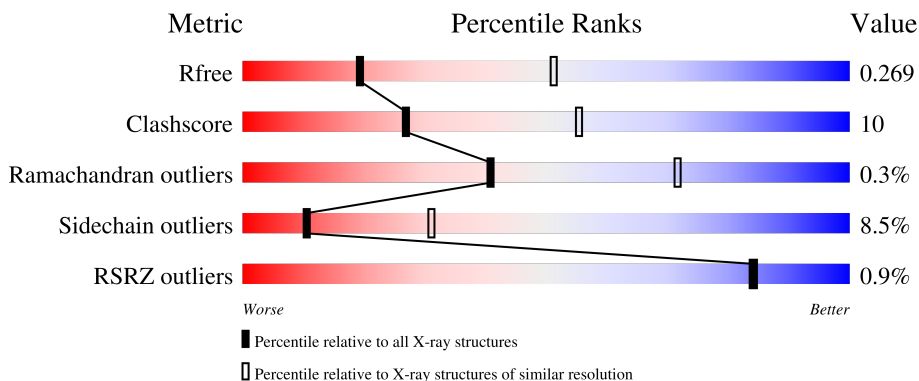
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	 73% 16% 9%
1	B	444	 66% 21% 9%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 6623 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	403	Total 3202	C 2036	N 563	O 587	S 16	0	0	0
1	B	403	Total 3211	C 2041	N 567	O 587	S 16	0	0	0

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 (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



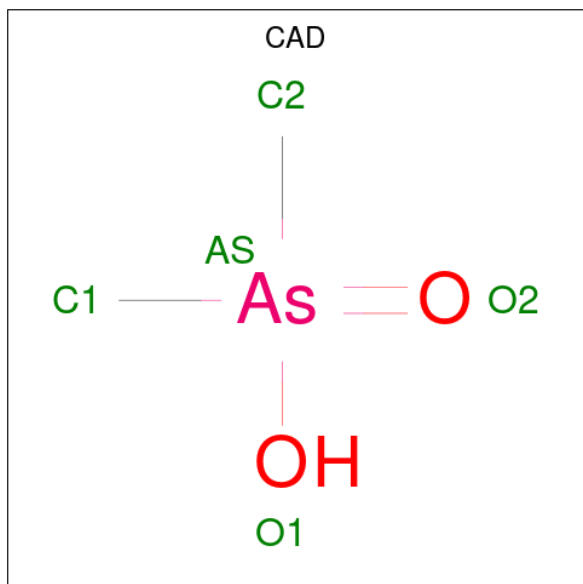
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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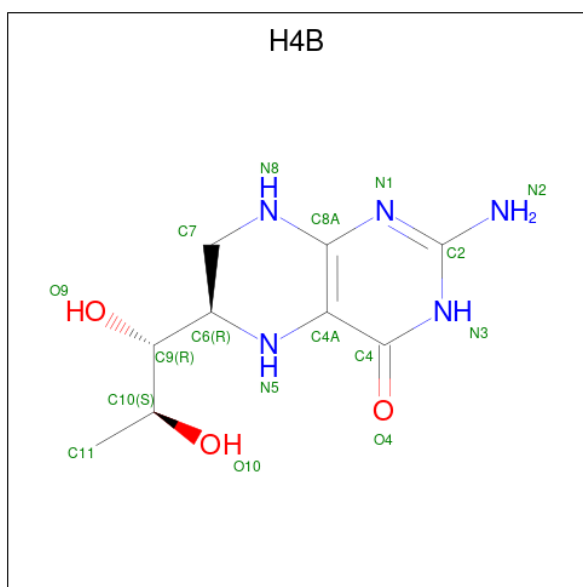
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Fe	N			O
2	B	1	43	34	1	4	4	0	0

- Molecule 3 is CACODYLIC ACID (three-letter code: CAD) (formula: $C_2H_7AsO_2$).



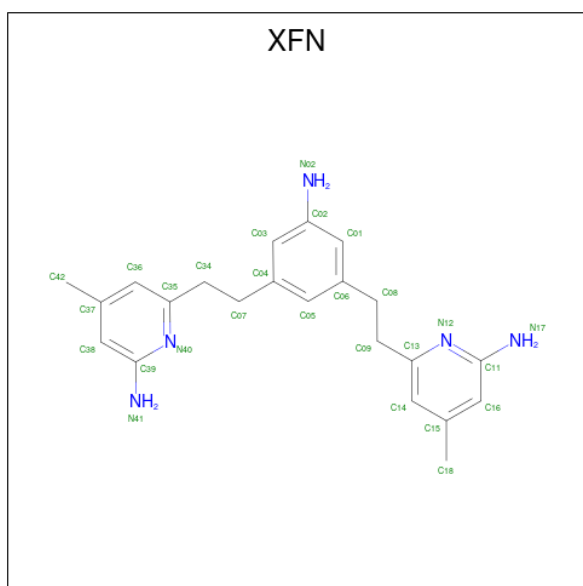
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	As	C		
3	A	1	3	1	2	0	0
3	B	1	3	1	2	0	0

- Molecule 4 is 5,6,7,8-TETRAHYDROBIOPTERIN (three-letter code: H4B) (formula: $C_9H_{15}N_5O_3$).



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

- Molecule 5 is 6,6'-[(5-aminobenzene-1,3-diyl)diethane-2,1-diyl]bis(4-methylpyridin-2-amine) (three-letter code: XFN) (formula: C₂₂H₂₇N₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N		0	0
			27	22	5			

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	N		
5	B	1	27	22	5	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

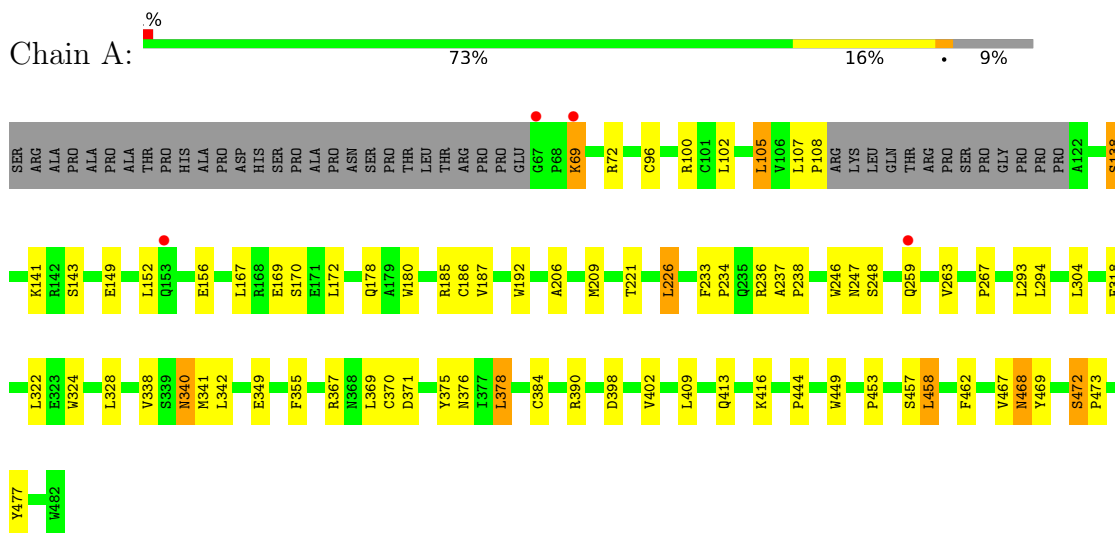
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	14	14	14	0	0
7	B	15	15	15	0	0

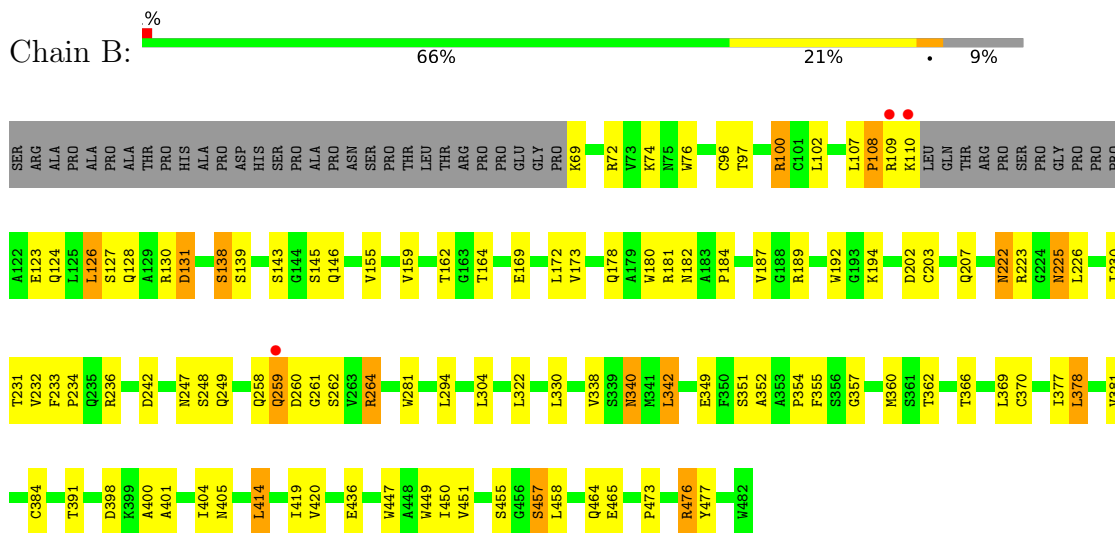
3 Residue-property plots [i](#)

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



- Molecule 1: Nitric oxide synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.85Å 107.09Å 157.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.73 – 2.90 42.73 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.9 (42.73-2.90) 97.9 (42.73-2.90)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 2.90Å)	Xtrriage
Refinement program	REFMAC 5.5.0109, CNS	Depositor
R, R_{free}	0.192 , 0.269 0.189 , 0.269	Depositor DCC
R_{free} test set	1097 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	48.3	Xtrriage
Anisotropy	0.302	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 36.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6623	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.76% 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: H4B, HEM, CAD, ZN, XFN

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	0.62	0/3291	0.69	0/4483
1	B	0.61	1/3299 (0.0%)	0.72	1/4491 (0.0%)
All	All	0.62	1/6590 (0.0%)	0.70	1/8974 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	203	CYS	CB-SG	-5.42	1.73	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	414	LEU	CA-CB-CG	6.11	129.35	115.30

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	3202	0	3107	44	0
1	B	3211	0	3123	69	0
2	A	43	0	30	11	0
2	B	43	0	30	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	3	0	0	1	0
3	B	3	0	0	2	0
4	A	17	0	15	1	0
4	B	17	0	15	4	0
5	A	27	0	27	8	0
5	B	27	0	27	4	0
6	A	1	0	0	0	0
7	A	14	0	0	0	0
7	B	15	0	0	1	0
All	All	6623	0	6374	132	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 10.

All (132) 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:B:384:CYS:SG	3:B:950:CAD:AS	2.50	1.29
1:A:384:CYS:SG	3:A:950:CAD:AS	2.55	1.25
2:B:500:HEM:HBB2	2:B:500:HEM:HHC	1.26	1.08
1:B:476:ARG:HG3	1:B:476:ARG:HH11	1.27	0.99
2:A:500:HEM:HBC2	2:A:500:HEM:HMC1	1.45	0.95
2:B:500:HEM:HHC	2:B:500:HEM:CBB	2.07	0.84
1:B:476:ARG:HG3	1:B:476:ARG:NH1	1.91	0.83
1:B:236:ARG:HD2	1:B:242:ASP:OD1	1.79	0.83
1:B:476:ARG:HH11	1:B:476:ARG:CG	1.92	0.82
2:A:500:HEM:HBC2	2:A:500:HEM:CMC	2.13	0.78
2:B:500:HEM:HBB2	2:B:500:HEM:CHC	2.07	0.78
1:A:246:TRP:HB2	1:A:294:LEU:HB3	1.67	0.77
1:A:105:LEU:HD23	1:A:105:LEU:N	2.00	0.77
1:B:370:CYS:HB3	1:B:378:LEU:HD22	1.67	0.75
1:B:258:GLN:HE21	1:B:264:ARG:HB3	1.51	0.73
1:A:186:CYS:HB2	2:A:500:HEM:ND	2.05	0.72
1:B:178:GLN:HB3	1:B:473:PRO:HG2	1.72	0.72
1:B:182:ASN:O	1:B:184:PRO:HD3	1.90	0.72
1:B:340:ASN:HD22	1:B:340:ASN:C	1.95	0.70
1:B:178:GLN:HE22	1:B:181:ARG:HH11	1.42	0.67
2:B:500:HEM:HMC1	2:B:500:HEM:HBC2	1.76	0.67
1:B:258:GLN:NE2	1:B:264:ARG:HB3	2.09	0.67
2:B:500:HEM:HBA1	5:B:800:XFN:H34	1.79	0.65
1:A:338:VAL:HG22	5:A:800:XFN:H03	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:400:ALA:O	1:B:404:ILE:HG13	1.96	0.64
2:B:500:HEM:HBC2	2:B:500:HEM:CMC	2.29	0.62
2:A:500:HEM:O2A	5:A:800:XFN:H08A	1.99	0.62
1:B:222:ASN:HB3	1:B:225:ASN:O	2.00	0.61
1:B:230:ILE:HG13	1:B:355:PHE:HB3	1.83	0.61
2:B:500:HEM:CGA	4:B:600:H4B:HN3	2.14	0.60
1:A:178:GLN:HB3	1:A:473:PRO:HG2	1.82	0.59
1:A:409:LEU:O	1:A:413:GLN:HG3	2.02	0.59
1:B:247:ASN:ND2	7:B:1024:HOH:O	2.35	0.59
5:A:800:XFN:H01	5:A:800:XFN:C13	2.33	0.59
1:A:468:ASN:HD22	1:A:469:TYR:N	2.02	0.58
1:A:96:CYS:HB3	1:B:96:CYS:HB3	1.86	0.58
1:B:126:LEU:O	1:B:130:ARG:HG3	2.04	0.57
1:B:377:ILE:O	1:B:381:VAL:HG23	2.05	0.57
1:A:167:LEU:HD12	1:A:172:LEU:HD12	1.88	0.56
1:A:187:VAL:HG22	1:A:187:VAL:O	2.06	0.55
1:A:221:THR:O	1:A:226:LEU:HD12	2.06	0.55
5:A:800:XFN:H01	5:A:800:XFN:C14	2.37	0.55
1:A:477:TYR:CE1	5:A:800:XFN:N17	2.75	0.54
1:A:105:LEU:N	1:A:105:LEU:CD2	2.69	0.54
1:B:342:LEU:C	1:B:342:LEU:HD23	2.28	0.54
1:B:248:SER:HA	1:B:340:ASN:HB3	1.89	0.54
1:B:233:PHE:HB3	1:B:234:PRO:HD2	1.90	0.53
1:A:370:CYS:HB3	1:A:378:LEU:HD22	1.91	0.53
1:B:369:LEU:HB3	1:B:377:ILE:HD11	1.90	0.53
1:B:72:ARG:NH2	1:B:74:LYS:HD2	2.24	0.53
1:A:369:LEU:HA	1:A:375:TYR:HB2	1.91	0.52
1:B:178:GLN:O	1:B:182:ASN:ND2	2.42	0.52
2:A:500:HEM:HMC1	2:A:500:HEM:CBC	2.31	0.52
1:A:180:TRP:CE3	1:A:192:TRP:HA	2.44	0.52
1:B:447:TRP:CZ2	1:B:451:VAL:HG21	2.45	0.52
1:B:130:ARG:HB3	1:B:130:ARG:NH1	2.25	0.51
1:B:138:SER:HA	1:B:143:SER:HB2	1.91	0.51
1:B:381:VAL:HG21	1:B:404:ILE:HD11	1.93	0.51
1:A:138:SER:O	1:A:141:LYS:HD3	2.11	0.51
1:B:360:MET:HA	1:B:420:VAL:O	2.11	0.51
1:B:74:LYS:HD3	1:B:76:TRP:CE2	2.45	0.51
2:A:500:HEM:HBA1	5:A:800:XFN:H34	1.93	0.51
1:B:384:CYS:CB	3:B:950:CAD:AS	3.19	0.50
1:A:180:TRP:CZ3	1:A:192:TRP:HA	2.46	0.50
5:B:800:XFN:H01	5:B:800:XFN:C14	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:CYS:HB2	2:A:500:HEM:C4D	2.46	0.50
1:A:453:PRO:HB2	1:B:457:SER:HB3	1.93	0.49
1:B:464:GLN:HG3	1:B:465:GLU:O	2.11	0.49
1:B:72:ARG:HH22	1:B:74:LYS:HD2	1.77	0.49
1:B:155:VAL:O	1:B:159:VAL:HG23	2.13	0.49
1:A:468:ASN:HD22	1:A:468:ASN:C	2.16	0.49
1:B:338:VAL:O	1:B:354:PRO:HA	2.13	0.49
1:A:105:LEU:HD22	1:B:465:GLU:HB3	1.94	0.48
1:B:181:ARG:NE	1:B:436:GLU:OE2	2.42	0.48
1:B:247:ASN:HB3	1:B:249:GLN:O	2.14	0.48
1:A:367:ARG:NH2	1:A:371:ASP:OD2	2.38	0.47
1:B:236:ARG:HD3	1:B:351:SER:HB3	1.95	0.47
1:B:180:TRP:CE3	1:B:192:TRP:HA	2.50	0.47
1:B:189:ARG:O	1:B:192:TRP:HD1	1.98	0.47
1:A:248:SER:HA	1:A:340:ASN:HB3	1.96	0.47
1:A:206:ALA:O	1:A:209:MET:HB2	2.16	0.46
1:A:322:LEU:HD13	1:A:324:TRP:CZ2	2.50	0.46
1:B:162:THR:OG1	1:B:164:THR:O	2.33	0.46
1:A:233:PHE:HB3	1:A:234:PRO:CD	2.46	0.46
1:B:233:PHE:HB2	1:B:352:ALA:HB3	1.98	0.46
1:A:338:VAL:HB	1:A:355:PHE:CZ	2.51	0.46
1:B:108:PRO:HB2	1:B:110:LYS:HG3	1.97	0.46
1:A:398:ASP:O	1:A:402:VAL:HG23	2.15	0.45
1:B:340:ASN:C	1:B:340:ASN:ND2	2.67	0.45
1:A:263:VAL:HG11	1:A:267:PRO:HA	1.98	0.45
1:B:124:GLN:O	1:B:128:GLN:HG3	2.17	0.45
1:A:444:PRO:HA	1:A:467:VAL:O	2.17	0.45
1:B:230:ILE:HG13	1:B:354:PRO:O	2.17	0.44
2:B:500:HEM:HMC1	2:B:500:HEM:CBC	2.46	0.44
1:A:237:ALA:HB1	1:A:238:PRO:HD2	2.00	0.44
1:A:338:VAL:HG11	1:A:341:MET:HG3	1.99	0.43
1:B:281:TRP:HB2	1:B:304:LEU:HD21	2.00	0.43
1:A:458:LEU:HD21	1:B:401:ALA:HB2	2.01	0.43
2:A:500:HEM:O2A	5:A:800:XFN:H05	2.18	0.43
1:B:172:LEU:HD11	1:B:232:VAL:HG11	2.01	0.43
1:A:185:ARG:HD3	1:A:449:TRP:CD2	2.54	0.43
2:B:500:HEM:HAA2	4:B:600:H4B:HN22	1.84	0.43
1:B:231:THR:O	1:B:354:PRO:HD2	2.19	0.43
1:B:362:THR:HA	1:B:405:ASN:HD21	1.83	0.43
1:B:455:SER:HB3	1:B:458:LEU:HD22	2.01	0.43
1:B:342:LEU:HD11	1:B:349:GLU:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:LEU:HD23	1:A:152:LEU:HA	1.92	0.42
2:A:500:HEM:CGA	4:A:600:H4B:HN22	2.32	0.42
5:B:800:XFN:H01	5:B:800:XFN:C13	2.50	0.42
2:A:500:HEM:HBB2	2:A:500:HEM:HHC	2.01	0.42
1:A:96:CYS:HB3	1:B:96:CYS:CB	2.48	0.42
1:B:169:GLU:O	1:B:173:VAL:HG23	2.20	0.42
1:B:366:THR:O	1:B:370:CYS:HB2	2.20	0.42
1:B:226:LEU:HD23	1:B:357:GLY:O	2.20	0.41
5:A:800:XFN:C13	5:A:800:XFN:C01	2.99	0.41
1:B:260:ASP:HB2	1:B:262:SER:HB2	2.02	0.41
1:B:127:SER:O	1:B:131:ASP:HB3	2.20	0.41
1:B:259:GLN:C	1:B:261:GLY:H	2.23	0.41
1:B:110:LYS:H	1:B:110:LYS:HG2	1.69	0.41
1:A:107:LEU:HA	1:A:108:PRO:HD3	1.92	0.41
1:B:97:THR:HG23	1:B:100:ARG:NH1	2.36	0.41
2:B:500:HEM:CAA	4:B:600:H4B:HN22	2.33	0.41
1:A:69:LYS:NZ	1:A:69:LYS:HA	2.36	0.41
1:A:342:LEU:HD21	1:A:349:GLU:HG2	2.03	0.41
1:B:338:VAL:HB	1:B:355:PHE:CZ	2.57	0.40
2:A:500:HEM:CMC	2:A:500:HEM:CBC	2.91	0.40
1:A:457:SER:HA	1:A:462:PHE:CG	2.56	0.40
1:B:449:TRP:HA	4:B:600:H4B:N1	2.36	0.40
1:B:477:TYR:CE1	5:B:800:XFN:N17	2.89	0.40
1:A:338:VAL:HB	1:A:355:PHE:CE1	2.56	0.40
1:A:472:SER:HA	1:A:473:PRO:C	2.42	0.40
1:B:187:VAL:HG23	1:B:450:ILE:HG23	2.03	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	399/444 (90%)	366 (92%)	33 (8%)	0	100	100
1	B	399/444 (90%)	370 (93%)	27 (7%)	2 (0%)	29	61
All	All	798/888 (90%)	736 (92%)	60 (8%)	2 (0%)	41	71

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	145	SER
1	B	108	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	342/377 (91%)	315 (92%)	27 (8%)	12	34
1	B	343/377 (91%)	312 (91%)	31 (9%)	9	29
All	All	685/754 (91%)	627 (92%)	58 (8%)	10	31

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	LYS
1	A	72	ARG
1	A	100	ARG
1	A	102	LEU
1	A	105	LEU
1	A	138	SER
1	A	143	SER
1	A	149	GLU
1	A	156	GLU
1	A	169	GLU
1	A	170	SER
1	A	226	LEU
1	A	236	ARG
1	A	247	ASN

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Mol	Chain	Res	Type
1	A	259	GLN
1	A	293	LEU
1	A	304	LEU
1	A	318	GLU
1	A	328	LEU
1	A	340	ASN
1	A	376	ASN
1	A	378	LEU
1	A	390	ARG
1	A	416	LYS
1	A	458	LEU
1	A	468	ASN
1	A	472	SER
1	B	69	LYS
1	B	100	ARG
1	B	102	LEU
1	B	107	LEU
1	B	109	ARG
1	B	123	GLU
1	B	126	LEU
1	B	131	ASP
1	B	138	SER
1	B	139	SER
1	B	146	GLN
1	B	194	LYS
1	B	202	ASP
1	B	207	GLN
1	B	222	ASN
1	B	223	ARG
1	B	225	ASN
1	B	259	GLN
1	B	264	ARG
1	B	294	LEU
1	B	322	LEU
1	B	330	LEU
1	B	340	ASN
1	B	342	LEU
1	B	378	LEU
1	B	391	THR
1	B	398	ASP
1	B	414	LEU
1	B	419	ILE

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Mol	Chain	Res	Type
1	B	457	SER
1	B	476	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	191	GLN
1	A	340	ASN
1	A	376	ASN
1	A	468	ASN
1	B	146	GLN
1	B	178	GLN
1	B	191	GLN
1	B	222	ASN
1	B	225	ASN
1	B	258	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 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
2	HEM	B	500	1	41,50,50	1.96	5 (12%)	45,82,82	1.69	9 (20%)
3	CAD	B	950	-	0,2,4	-	-	0,1,6	-	-
4	H4B	B	600	-	16,18,18	1.12	1 (6%)	11,26,26	2.65	5 (45%)
4	H4B	A	600	-	16,18,18	0.99	1 (6%)	11,26,26	2.62	6 (54%)
5	XFN	B	800	-	29,29,29	0.56	0	38,40,40	1.68	8 (21%)
3	CAD	A	950	-	0,2,4	-	-	0,1,6	-	-
2	HEM	A	500	1	41,50,50	1.87	7 (17%)	45,82,82	1.57	8 (17%)
5	XFN	A	800	-	29,29,29	0.72	0	38,40,40	1.71	6 (15%)

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	B	500	1	-	2/12/54/54	-
4	H4B	B	600	-	-	0/8/17/17	0/2/2/2
4	H4B	A	600	-	-	0/8/17/17	0/2/2/2
5	XFN	B	800	-	-	1/10/10/10	0/3/3/3
2	HEM	A	500	1	-	2/12/54/54	-
5	XFN	A	800	-	-	0/10/10/10	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	HEM	C3D-C2D	7.76	1.53	1.36
2	A	500	HEM	C3D-C2D	7.08	1.51	1.36
2	B	500	HEM	C3C-C2C	-4.94	1.33	1.40
2	A	500	HEM	C3C-C2C	-4.44	1.34	1.40
2	B	500	HEM	C3C-CAC	3.30	1.54	1.47
2	A	500	HEM	CAB-C3B	3.12	1.55	1.47
2	A	500	HEM	C3C-CAC	2.93	1.53	1.47
2	B	500	HEM	CAB-C3B	2.67	1.54	1.47
4	A	600	H4B	C4-N3	2.59	1.37	1.33
2	B	500	HEM	CAA-C2A	2.56	1.55	1.52
4	B	600	H4B	C4A-C4	-2.27	1.38	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	HEM	CAA-C2A	2.17	1.55	1.52
2	A	500	HEM	C3B-C2B	-2.08	1.33	1.37
2	A	500	HEM	CMA-C3A	2.04	1.55	1.51

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	600	H4B	C8A-C4A-C4	6.10	119.99	114.57
4	A	600	H4B	C8A-C4A-C4	6.09	119.98	114.57
2	A	500	HEM	C4D-ND-C1D	5.64	110.90	105.07
5	B	800	XFN	C39-N40-C35	5.55	122.30	118.10
2	B	500	HEM	C4D-ND-C1D	5.51	110.77	105.07
5	A	800	XFN	C39-N40-C35	5.07	121.94	118.10
5	A	800	XFN	C14-C13-N12	-3.92	118.75	122.90
5	A	800	XFN	C11-N12-C13	3.85	121.02	118.10
2	B	500	HEM	C4A-C3A-C2A	3.83	109.66	107.00
5	B	800	XFN	C11-N12-C13	3.74	120.93	118.10
5	B	800	XFN	C36-C35-N40	-3.66	119.02	122.90
4	B	600	H4B	C2-N3-C4	3.38	121.30	115.93
5	A	800	XFN	C36-C35-N40	-3.37	119.33	122.90
5	A	800	XFN	C07-C34-C35	3.22	120.22	112.99
2	B	500	HEM	CMA-C3A-C4A	-3.13	123.65	128.46
4	A	600	H4B	C2-N3-C4	3.11	120.87	115.93
4	B	600	H4B	N1-C2-N3	-2.87	120.92	125.42
2	A	500	HEM	CBD-CAD-C3D	-2.84	104.75	112.63
5	B	800	XFN	C07-C34-C35	2.83	119.33	112.99
2	A	500	HEM	CAD-C3D-C4D	2.69	129.36	124.66
2	B	500	HEM	C1D-C2D-C3D	-2.67	104.15	106.96
4	A	600	H4B	N1-C2-N3	-2.65	121.27	125.42
5	B	800	XFN	C14-C13-N12	-2.56	120.18	122.90
2	A	500	HEM	C4B-CHC-C1C	2.56	125.94	122.56
2	B	500	HEM	CHC-C4B-NB	2.55	127.20	124.43
5	B	800	XFN	C09-C13-N12	2.48	119.65	115.95
5	A	800	XFN	C09-C13-N12	2.41	119.55	115.95
4	B	600	H4B	C4-C4A-N5	2.37	121.11	119.12
4	A	600	H4B	C2-N1-C8A	2.31	119.72	114.54
5	B	800	XFN	C34-C07-C04	-2.28	105.26	113.28
4	A	600	H4B	C4-C4A-N5	2.22	120.98	119.12
2	B	500	HEM	C3B-C2B-C1B	2.16	108.09	106.49
2	B	500	HEM	C4C-CHD-C1D	2.15	125.39	122.56
2	A	500	HEM	C3B-C2B-C1B	2.12	108.06	106.49
4	A	600	H4B	C4A-C4-N3	-2.10	118.03	124.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	HEM	C4B-CHC-C1C	2.09	125.32	122.56
2	B	500	HEM	CBD-CAD-C3D	-2.07	106.86	112.63
2	A	500	HEM	O2A-CGA-CBA	2.04	120.60	114.03
2	A	500	HEM	CMD-C2D-C1D	2.03	128.13	125.04
2	A	500	HEM	C2C-C3C-C4C	2.03	108.31	106.90
5	B	800	XFN	C34-C35-N40	2.02	118.96	115.95
4	B	600	H4B	N2-C2-N1	2.01	120.39	117.25

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	800	XFN	C04-C07-C34-C35
2	B	500	HEM	C2A-CAA-CBA-CGA
2	B	500	HEM	C4B-C3B-CAB-CBB
2	A	500	HEM	CAD-CBD-CGD-O2D
2	A	500	HEM	CAD-CBD-CGD-O1D

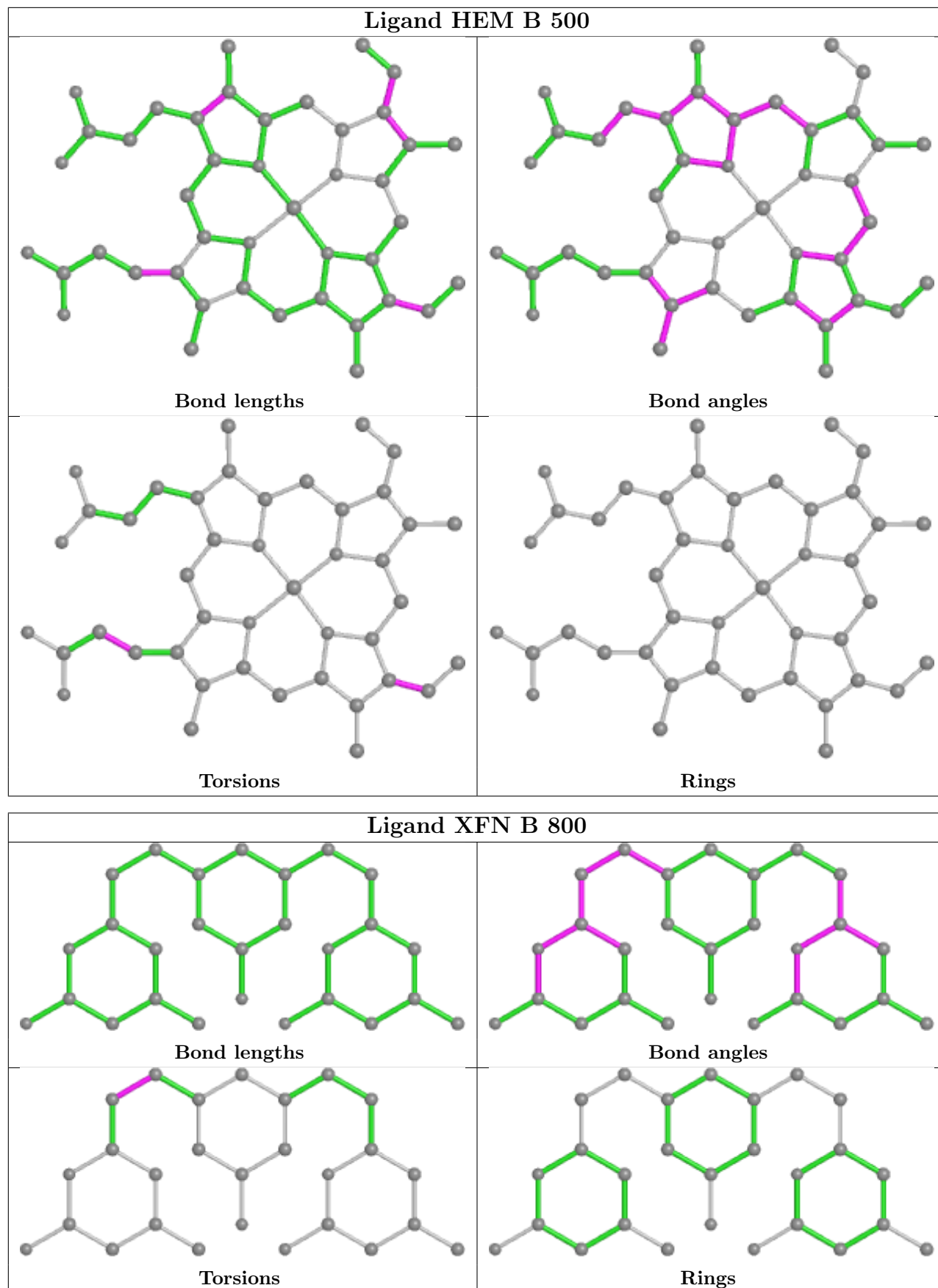
There are no ring outliers.

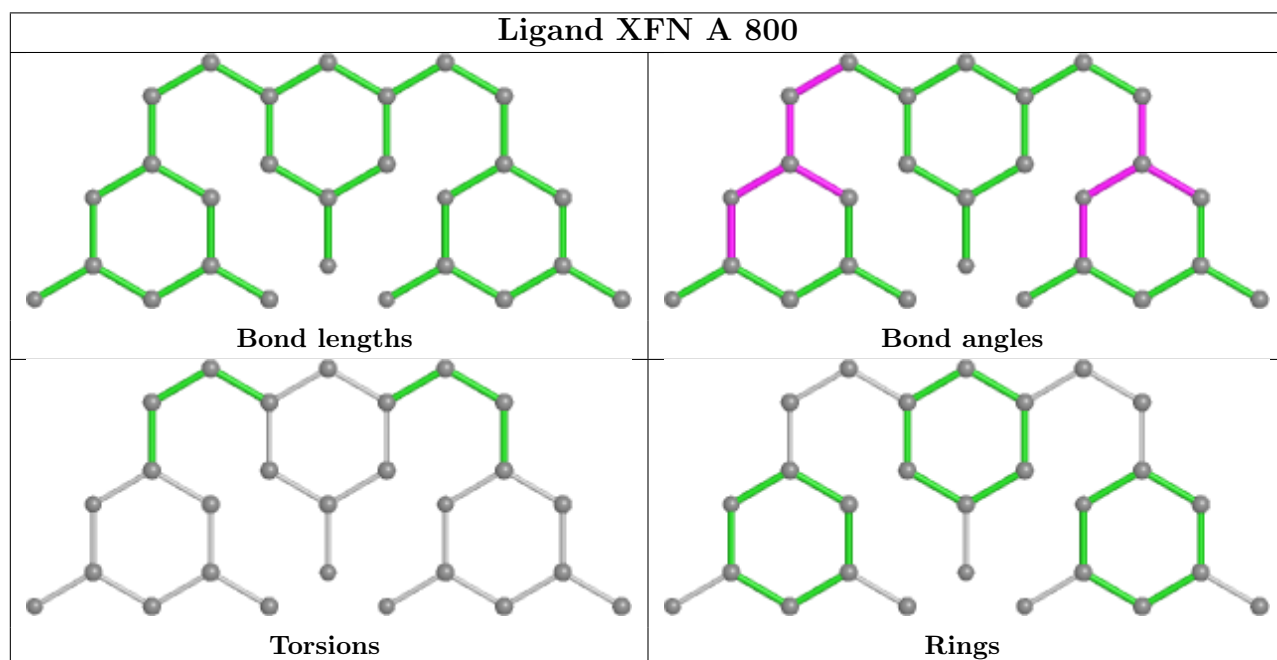
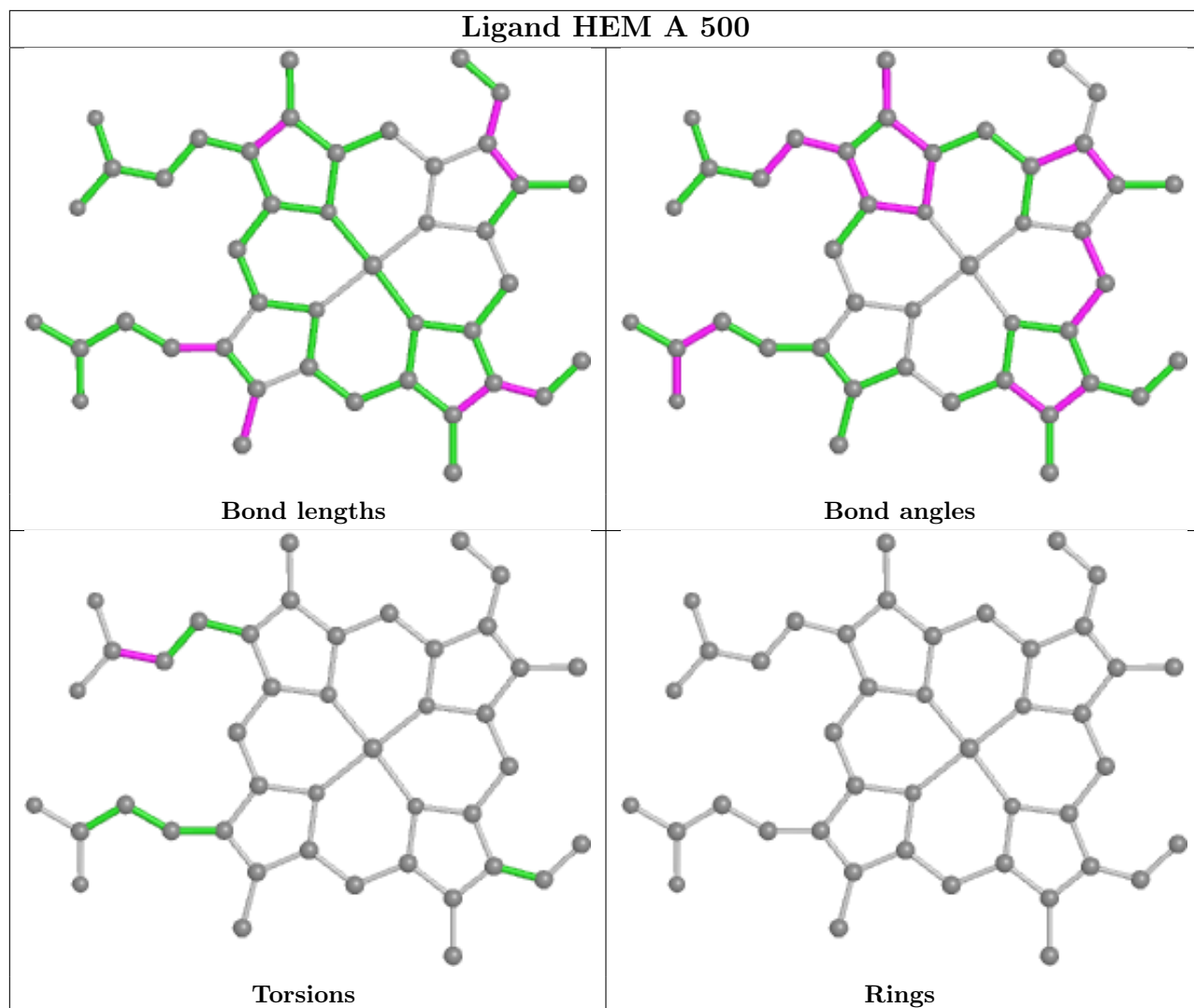
8 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	500	HEM	10	0
3	B	950	CAD	2	0
4	B	600	H4B	4	0
4	A	600	H4B	1	0
5	B	800	XFN	4	0
3	A	950	CAD	1	0
2	A	500	HEM	11	0
5	A	800	XFN	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%)	-0.40	4 (0%) 82 82	27, 44, 68, 81	0
1	B	403/444 (90%)	-0.43	3 (0%) 87 87	27, 47, 68, 95	0
All	All	806/888 (90%)	-0.41	7 (0%) 84 84	27, 45, 68, 95	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	259	GLN	2.6
1	A	67	GLY	2.4
1	A	69	LYS	2.4
1	A	153	GLN	2.3
1	B	109	ARG	2.2
1	A	259	GLN	2.1
1	B	110	LYS	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](#)

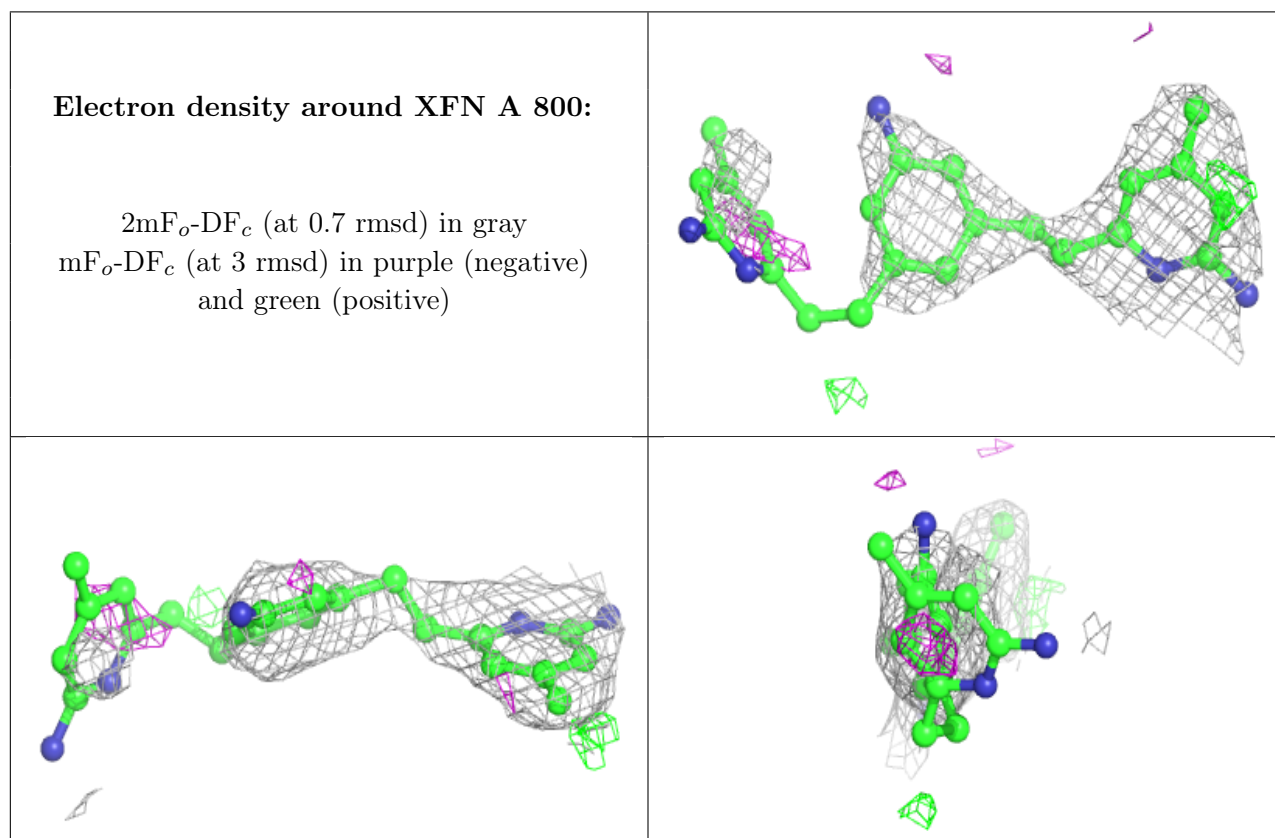
There are no monosaccharides in this entry.

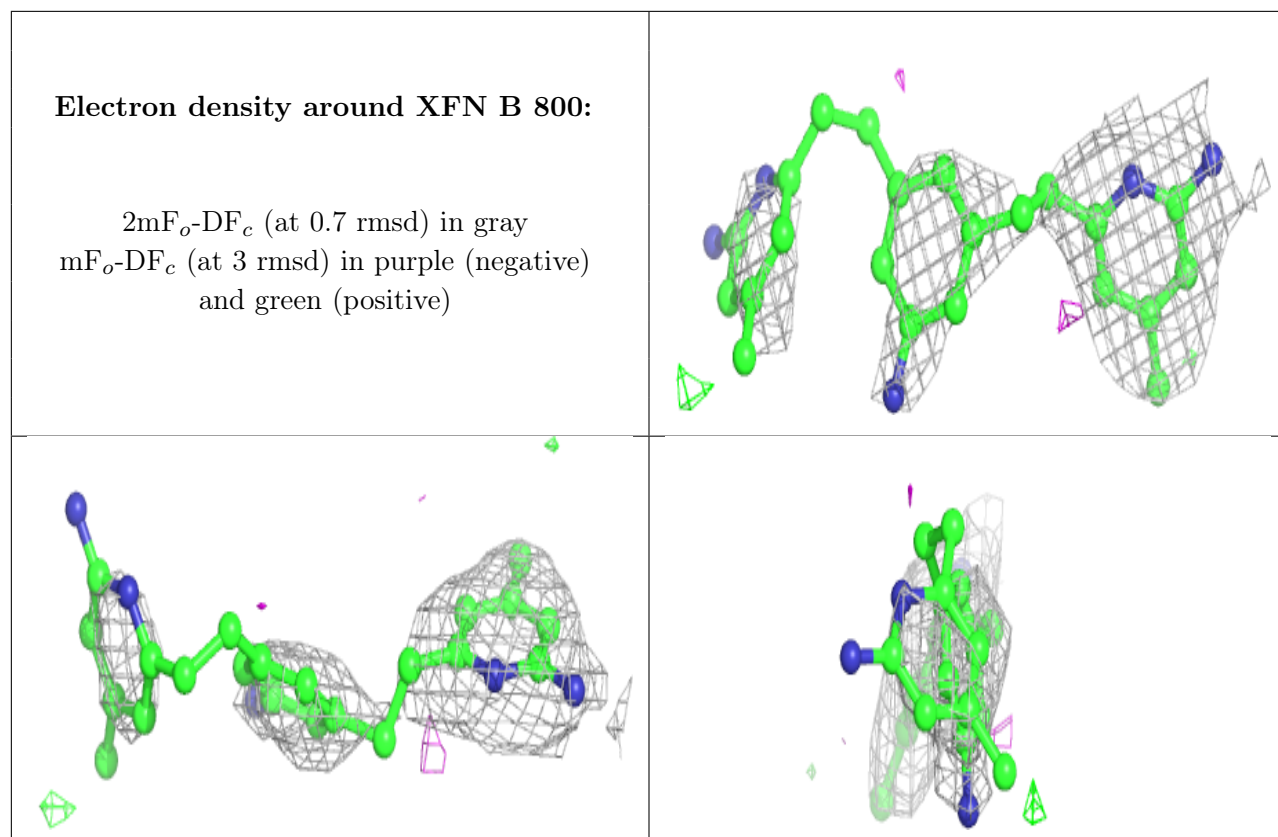
6.4 Ligands [i](#)

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
5	XFN	A	800	27/27	0.84	0.33	55,76,102,103	0
5	XFN	B	800	27/27	0.91	0.26	46,68,86,87	0
4	H4B	A	600	17/17	0.94	0.16	41,46,48,49	0
4	H4B	B	600	17/17	0.95	0.17	50,51,53,54	0
2	HEM	A	500	43/43	0.97	0.17	31,36,45,50	0
2	HEM	B	500	43/43	0.97	0.17	26,34,51,53	0
3	CAD	B	950	3/5	0.98	0.11	72,72,73,74	0
3	CAD	A	950	3/5	0.99	0.09	68,68,69,70	0
6	ZN	A	900	1/1	0.99	0.08	46,46,46,46	0

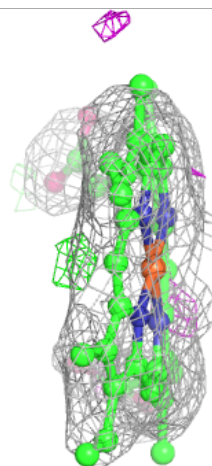
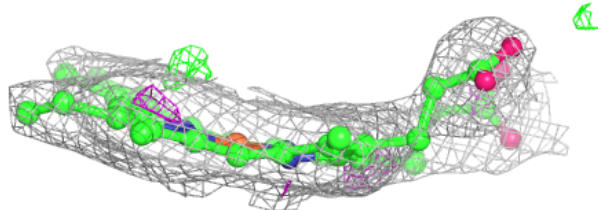
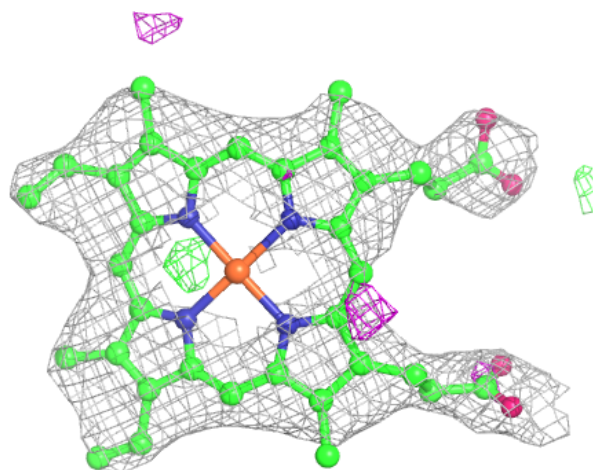
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

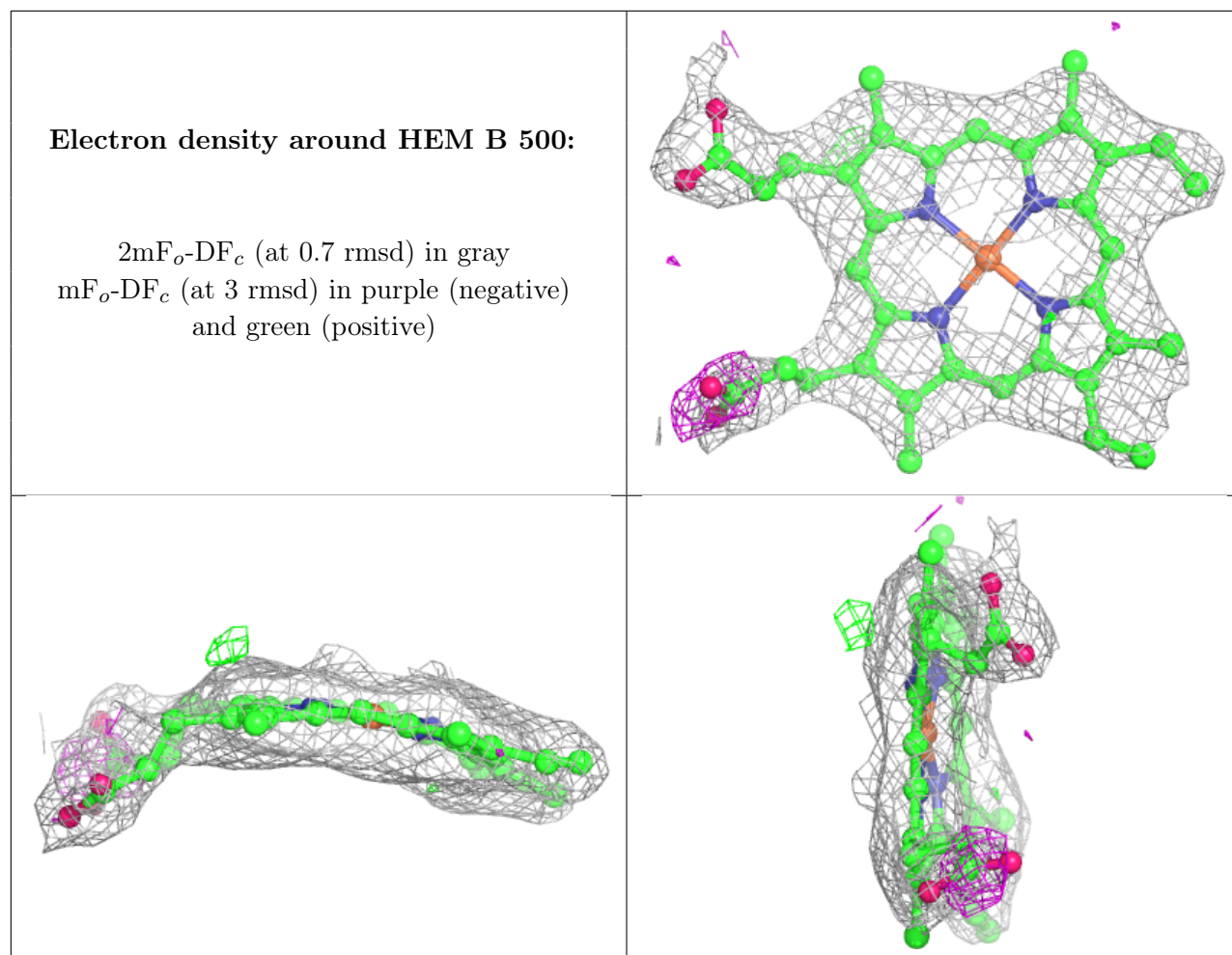




Electron density around HEM A 500:

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





6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.