Full wwPDB X-ray Structure Validation Report ⓘ

Jun 3, 2025 – 06:15 PM EDT

PDB ID	:	9C1Y / pdb_00009c1y
Title	:	Structure of human neuronal nitric oxide synthase R354A/G357D mutant heme domain in complex with 7-((3-(((4-(6-aminopyridin-2-yl)butyl)amino)methyl)phenoxy)methyl)quinolin-2-amine
Authors	:	Li, H.; Poulos, T.L.
Deposited on	:	2024-05-29
Resolution	:	2.30 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:

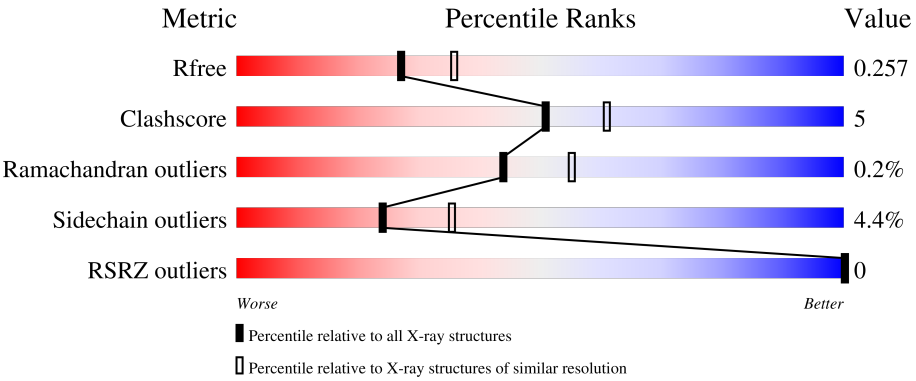
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	164625	5963 (2.30-2.30)
Clashscore	180529	6698 (2.30-2.30)
Ramachandran outliers	177936	6640 (2.30-2.30)
Sidechain outliers	177891	6640 (2.30-2.30)
RSRZ outliers	164620	5963 (2.30-2.30)

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 <=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	423	81% 16%
1	B	423	84% 12%
1	C	423	84% 13%
1	D	423	83% 14%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 14616 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.

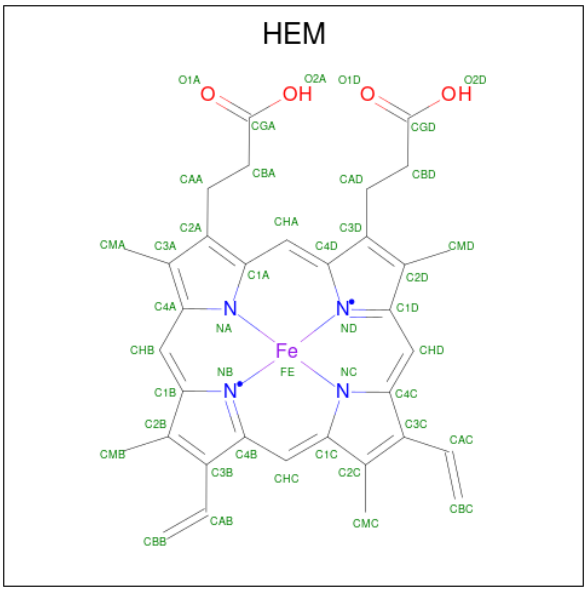
- Molecule 1 is a protein called Nitric oxide synthase, brain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	420	Total	C	N	O	S	0	5	0
			3442	2202	590	628	22			
1	B	413	Total	C	N	O	S	0	2	0
			3371	2161	574	615	21			
1	C	418	Total	C	N	O	S	0	3	0
			3417	2186	585	625	21			
1	D	411	Total	C	N	O	S	0	2	0
			3355	2150	572	612	21			

There are 16 discrepancies between the modelled and reference sequences:

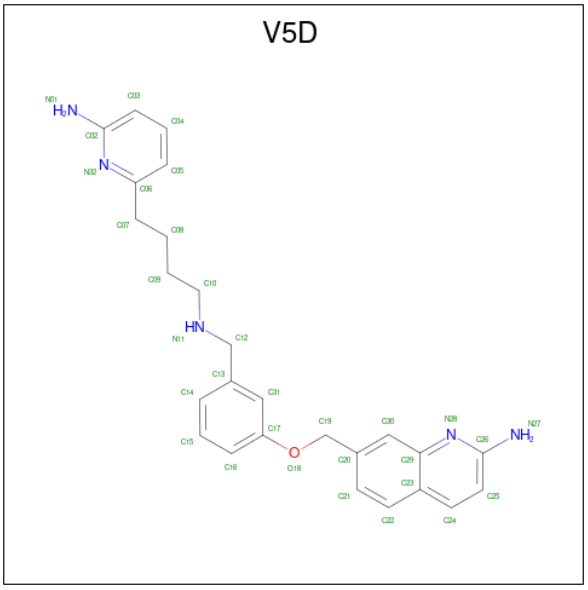
Chain	Residue	Modelled	Actual	Comment	Reference
A	354	ALA	ARG	engineered mutation	UNP P29475
A	357	ASP	GLY	engineered mutation	UNP P29475
A	723	LEU	-	expression tag	UNP P29475
A	724	VAL	-	expression tag	UNP P29475
B	354	ALA	ARG	engineered mutation	UNP P29475
B	357	ASP	GLY	engineered mutation	UNP P29475
B	723	LEU	-	expression tag	UNP P29475
B	724	VAL	-	expression tag	UNP P29475
C	354	ALA	ARG	engineered mutation	UNP P29475
C	357	ASP	GLY	engineered mutation	UNP P29475
C	723	LEU	-	expression tag	UNP P29475
C	724	VAL	-	expression tag	UNP P29475
D	354	ALA	ARG	engineered mutation	UNP P29475
D	357	ASP	GLY	engineered mutation	UNP P29475
D	723	LEU	-	expression tag	UNP P29475
D	724	VAL	-	expression tag	UNP P29475

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



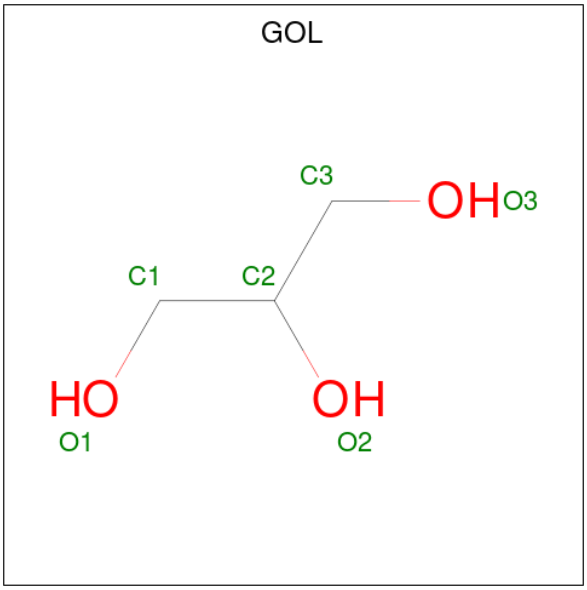
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is 7-{[3-({[4-(6-aminopyridin-2-yl)butyl]amino}methyl)phenoxy]methyl}quinolin-2-amine (CCD ID: V5D) (formula: $C_{26}H_{29}N_5O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 32 26 5 1	0	0
3	B	1	Total C N O 32 26 5 1	0	0
3	C	1	Total C N O 32 26 5 1	0	0
3	D	1	Total C N O 32 26 5 1	0	0

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



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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Zn 1 1	0	0
5	C	1	Total Zn 1 1	0	0

- Molecule 6 is water.

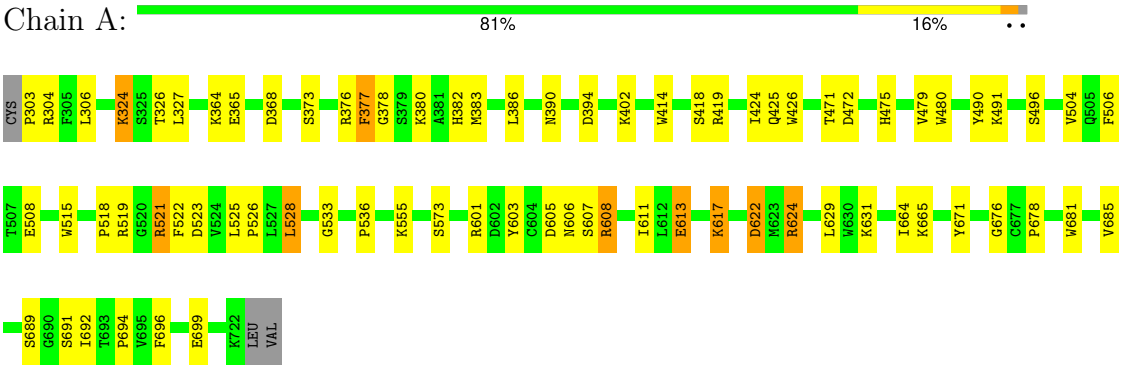
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	191	Total O 191 191	0	0
6	B	182	Total O 182 182	0	0
6	C	168	Total O 168 168	0	0
6	D	152	Total O 152 152	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

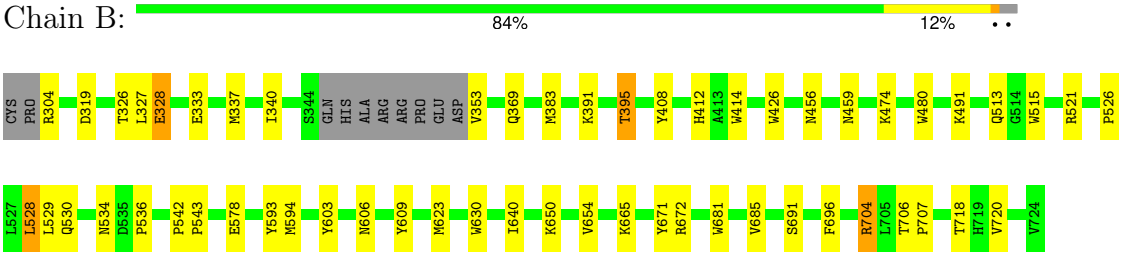
• Molecule 1: Nitric oxide synthase, brain

Chain A:



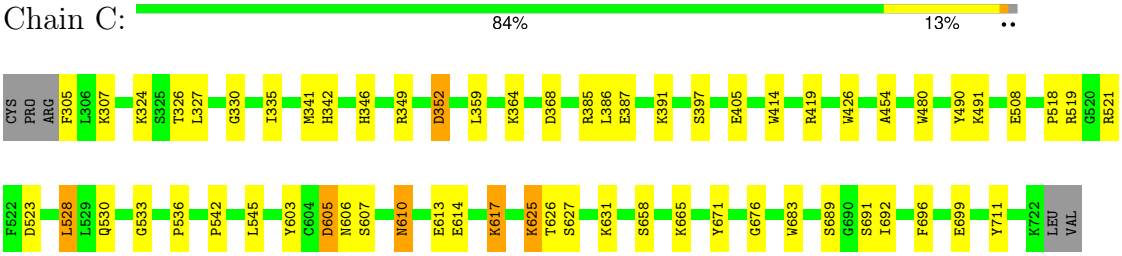
• Molecule 1: Nitric oxide synthase, brain

Chain B:



• Molecule 1: Nitric oxide synthase, brain

Chain C:



• Molecule 1: Nitric oxide synthase, brain

Chain D:


CYS PRO R304 D319 T320 L321 K324 S325 T326 L327 I340 M341 S344 GLN HIS ALA ARG ARG PRO GLU ASP V353 F360 P361 K364 S372 M383 E384 R385 T404 E405 L406 W414 R419 W426 D436 I466 W480 L484 I509 Q513 G514
W515 K516 P526 L527 L528 L529 N532 P536 Q540 I551 R552 H553 P554 K565 A571 V572 F589 M594 Y603 N606 Y609 N610 I611 L612 E613 W630 K631 K650 V654 N669 E670 Y671 R672 W683 S691 F696 T706 P707 V720
W721 K722 LEU VAL

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	51.97Å 164.13Å 118.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.68 – 2.30 49.68 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.68-2.30) 99.9 (49.68-2.30)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.26 (at 2.29Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.194 , 0.263 0.187 , 0.257	Depositor DCC
R_{free} test set	4397 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	38.7	Xtriage
Anisotropy	0.718	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 28.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.459 for h,-k,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	14616	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.24% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: ZN, HEM, V5D, GOL

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	0.31	0/3556	0.50	0/4827
1	B	0.31	0/3472	0.51	0/4710
1	C	0.32	0/3524	0.51	0/4783
1	D	0.31	0/3456	0.51	0/4689
All	All	0.31	0/14008	0.51	0/19009

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	593	TYR	Peptide

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	3442	0	3360	42	0
1	B	3371	0	3291	27	0
1	C	3417	0	3327	37	0
1	D	3355	0	3271	31	0
2	A	43	0	30	3	0
2	B	43	0	30	2	0
2	C	43	0	30	3	0
2	D	43	0	30	1	0
3	A	32	0	0	0	0
3	B	32	0	0	0	0
3	C	32	0	0	0	0
3	D	32	0	0	0	0
4	A	12	0	16	1	0
4	B	6	0	8	0	0
4	C	12	0	16	1	0
4	D	6	0	8	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
6	A	191	0	0	2	0
6	B	182	0	0	1	0
6	C	168	0	0	3	0
6	D	152	0	0	2	0
All	All	14616	0	13417	139	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 5.

All (139) 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:C:528:LEU:HD22	1:C:536:PRO:HB2	1.62	0.81
1:A:528:LEU:HD22	1:A:536:PRO:HB2	1.64	0.79
1:A:378:GLY:HA2	1:A:383:MET:HE2	1.66	0.77
1:D:528:LEU:HD22	1:D:536:PRO:HB2	1.68	0.76
1:B:528:LEU:HD22	1:B:536:PRO:HB2	1.73	0.71
1:C:349:ARG:NH2	1:C:352:ASP:O	2.26	0.67
1:C:625:LYS:HG3	1:C:627:SER:H	1.59	0.67
1:A:303:PRO:HD2	1:A:306:LEU:HD21	1.76	0.67
2:A:801:HEM:HMC2	2:A:801:HEM:HBC2	1.78	0.66
2:C:801:HEM:HBC2	2:C:801:HEM:HMC2	1.78	0.65
2:C:801:HEM:O1A	6:C:901:HOH:O	2.15	0.64
1:A:480:TRP:HB2	1:A:528:LEU:HB3	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:704:ARG:HH11	1:B:704:ARG:HB3	1.64	0.62
1:C:324:LYS:HD3	4:C:803:GOL:H12	1.80	0.61
1:D:480:TRP:HB2	1:D:528:LEU:HB3	1.83	0.60
1:A:631:LYS:NZ	6:A:904:HOH:O	2.34	0.60
2:B:802:HEM:HMC2	2:B:802:HEM:HBC2	1.84	0.60
1:B:480:TRP:HB2	1:B:528:LEU:HB3	1.84	0.59
1:D:364:LYS:NZ	6:D:905:HOH:O	2.36	0.59
2:D:801:HEM:HBC2	2:D:801:HEM:HMC2	1.85	0.59
1:A:518:PRO:HG2	1:A:523:ASP:CG	2.28	0.58
2:A:801:HEM:HBB2	2:A:801:HEM:HHC	1.84	0.58
1:C:625:LYS:HD2	1:C:627:SER:HB3	1.89	0.55
1:B:327:LEU:HG	1:B:328:GLU:H	1.71	0.54
1:D:319:ASP:HB2	1:D:671:TYR:HE2	1.73	0.54
1:C:364:LYS:NZ	1:C:368:ASP:OD2	2.40	0.53
1:D:691:SER:HA	1:D:696:PHE:CG	2.42	0.53
1:D:515:TRP:CE2	1:D:526:PRO:HD3	2.44	0.53
1:C:689:SER:HB3	1:C:692:ILE:HD11	1.91	0.52
1:B:691:SER:HA	1:B:696:PHE:CG	2.44	0.52
1:B:515:TRP:CG	1:B:526:PRO:HG3	2.45	0.52
1:C:711:TYR:OH	2:C:801:HEM:O1D	2.20	0.52
1:C:614:GLU:HA	1:C:617:LYS:HE3	1.91	0.52
1:B:414:TRP:CE3	1:B:426:TRP:HA	2.45	0.51
1:C:671:TYR:CE2	1:C:676:GLY:HA2	2.46	0.50
1:A:377:PHE:HA	1:A:382:HIS:ND1	2.26	0.50
1:D:553:HIS:CG	1:D:554:PRO:HD2	2.46	0.50
1:D:436:ASP:OD1	6:D:901:HOH:O	2.20	0.50
1:B:706:THR:HA	1:B:707:PRO:C	2.36	0.49
1:A:689:SER:HB3	1:A:692:ILE:HD11	1.94	0.49
1:C:480:TRP:HB2	1:C:528:LEU:HB3	1.94	0.49
1:A:424:ILE:HG23	1:A:425:GLN:HG2	1.93	0.49
1:A:490:TYR:CE1	1:A:519:ARG:HA	2.47	0.49
1:C:490:TYR:CE1	1:C:519:ARG:HA	2.48	0.49
1:A:376:ARG:HA	1:C:346:HIS:HE2	1.77	0.49
1:C:518:PRO:HG2	1:C:523:ASP:CG	2.37	0.49
1:C:341:MET:HG3	1:C:342:HIS:CE1	2.47	0.49
2:B:802:HEM:HHC	2:B:802:HEM:HBB2	1.94	0.48
1:C:305:PHE:HE1	1:C:307:LYS:HE2	1.78	0.48
1:A:506:PHE:HD2	1:A:525:LEU:HD13	1.79	0.48
1:A:515:TRP:CE2	1:A:526:PRO:HD3	2.49	0.48
1:D:321:LEU:HD12	1:D:324:LYS:HE2	1.97	0.47
1:A:622:ASP:OD2	1:A:624:ARG:HB2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:606:ASN:HD21	1:B:609:TYR:HB2	1.79	0.47
1:C:542:PRO:HD2	1:C:545:LEU:HD12	1.96	0.47
1:A:624:ARG:HH11	1:A:624:ARG:HB3	1.79	0.47
1:A:671:TYR:CE2	1:A:676:GLY:HA2	2.51	0.46
1:A:691:SER:HA	1:A:696:PHE:CG	2.50	0.46
1:C:610:ASN:N	1:C:613:GLU:OE1	2.34	0.46
1:B:456:ASN:HB3	1:B:459:ASN:O	2.16	0.46
1:A:699:GLU:HB3	1:B:340:ILE:HD13	1.98	0.46
1:D:706:THR:HA	1:D:707:PRO:C	2.40	0.46
1:A:515:TRP:CD1	1:A:526:PRO:HG3	2.51	0.46
1:A:664:ILE:HG13	1:A:694:PRO:HB2	1.97	0.46
1:B:623:MET:HA	1:B:630:TRP:CD1	2.51	0.45
1:C:606:ASN:CG	1:C:607:SER:H	2.23	0.45
1:A:522:PHE:N	6:A:905:HOH:O	2.34	0.45
1:C:625:LYS:HG3	1:C:627:SER:N	2.28	0.45
1:A:418[B]:SER:OG	1:A:678:PRO:HB2	2.17	0.45
1:C:631:LYS:NZ	6:C:910:HOH:O	2.50	0.45
1:B:530:GLN:HG3	1:B:534:ASN:O	2.17	0.45
1:B:480:TRP:CZ2	1:B:536:PRO:HG3	2.52	0.44
1:A:624:ARG:HB3	1:A:624:ARG:NH1	2.33	0.44
1:A:521:ARG:O	1:A:603:TYR:OH	2.32	0.44
1:A:364:LYS:NZ	1:A:368:ASP:OD2	2.41	0.44
1:C:454:ALA:HB1	6:C:903:HOH:O	2.16	0.44
1:A:613:GLU:H	1:A:613:GLU:HG2	1.68	0.44
1:D:553:HIS:CD2	1:D:554:PRO:HD2	2.53	0.44
1:C:387:GLU:O	1:C:391:LYS:HG2	2.18	0.44
1:D:360:PHE:N	1:D:361:PRO:HD2	2.33	0.44
1:A:629:LEU:HD12	1:B:640:ILE:HG13	2.00	0.43
1:D:419:ARG:HD3	1:D:683:TRP:CD2	2.53	0.43
1:A:504:VAL:O	1:A:508:GLU:HG2	2.17	0.43
1:D:326:THR:OG1	1:D:327:LEU:N	2.51	0.43
1:C:699:GLU:HB3	1:D:340:ILE:HD13	2.01	0.43
1:A:606:ASN:CG	1:A:607:SER:H	2.27	0.43
1:C:341:MET:HE2	1:C:341:MET:HB2	1.87	0.43
1:A:380:LYS:HE2	1:C:330:GLY:O	2.18	0.43
1:D:516:LYS:HD3	1:D:516:LYS:HA	1.88	0.43
1:D:611:ILE:HD13	1:D:611:ILE:HA	1.91	0.43
1:B:681:TRP:CE2	1:B:685:VAL:HG21	2.54	0.43
1:A:324:LYS:HD3	4:A:803:GOL:H12	2.01	0.43
1:A:475:HIS:HA	1:A:533:GLY:HA3	2.01	0.43
1:A:606:ASN:OD1	1:A:608:ARG:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:617:LYS:HE3	1:A:617:LYS:HB2	1.81	0.43
1:B:521:ARG:HG2	1:B:603:TYR:HE1	1.83	0.43
1:D:509:ILE:O	1:D:513:GLN:HG2	2.19	0.43
1:B:513:GLN:NE2	6:B:910:HOH:O	2.52	0.42
1:B:542:PRO:HA	1:B:543:PRO:HD3	1.97	0.42
1:C:521:ARG:C	1:C:603:TYR:HH	2.27	0.42
1:D:484:LEU:HB2	1:D:571:ALA:HB3	2.02	0.42
1:C:419:ARG:HD3	1:C:683:TRP:CD2	2.55	0.42
1:C:521:ARG:HH11	1:C:605:ASP:HB2	1.84	0.42
1:A:471:THR:OG1	1:A:472:ASP:N	2.52	0.42
1:D:385:ARG:NE	1:D:405:GLU:OE1	2.47	0.42
1:D:326:THR:HG21	1:D:706:THR:HG22	2.02	0.42
1:B:529:LEU:O	1:B:536:PRO:HA	2.20	0.42
1:C:385:ARG:NH2	1:C:405:GLU:OE2	2.47	0.42
1:C:691:SER:HA	1:C:696:PHE:CG	2.54	0.42
1:A:414:TRP:CE3	1:A:426:TRP:HA	2.55	0.42
1:B:594:MET:HA	1:B:654:VAL:O	2.19	0.42
1:D:529:LEU:O	1:D:536:PRO:HA	2.20	0.42
1:D:551:ILE:HG12	1:D:565:LYS:HA	2.02	0.42
1:D:669:ASN:OD1	1:D:672:ARG:NH1	2.53	0.42
1:A:555:LYS:HA	1:A:555:LYS:HD3	1.87	0.41
1:C:521:ARG:HB3	1:C:603:TYR:OH	2.20	0.41
1:C:617:LYS:HE3	1:C:617:LYS:HB2	1.68	0.41
1:D:610:ASN:HB2	1:D:613:GLU:OE1	2.20	0.41
1:B:391:LYS:O	1:B:395:THR:OG1	2.27	0.41
1:C:419:ARG:NH1	1:C:711:TYR:OH	2.52	0.41
1:C:530:GLN:HE21	1:C:533:GLY:HA2	1.85	0.41
1:D:572:VAL:HB	1:D:589:PHE:CE1	2.56	0.41
1:B:414:TRP:CZ3	1:B:426:TRP:HA	2.56	0.41
1:B:408:TYR:CE1	1:B:412:HIS:CE1	3.08	0.41
1:A:681:TRP:CZ2	1:A:685:VAL:HG21	2.56	0.41
1:B:319:ASP:HB2	1:B:671:TYR:HE2	1.84	0.41
1:D:406:LEU:HD11	1:D:466:ILE:HG21	2.01	0.41
1:D:414:TRP:CE3	1:D:426:TRP:HA	2.55	0.41
1:D:630:TRP:CZ3	1:D:631:LYS:HG2	2.56	0.41
1:B:515:TRP:CD1	1:B:526:PRO:HG3	2.56	0.41
1:A:521:ARG:NH2	1:A:605:ASP:OD2	2.53	0.41
1:A:496:SER:OG	1:A:607:SER:HB2	2.21	0.40
1:D:594:MET:HA	1:D:654:VAL:O	2.21	0.40
1:A:479:VAL:HG11	1:A:573:SER:HB2	2.03	0.40
1:A:419:ARG:HB2	2:A:801:HEM:HAD2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:491:LYS:HB2	1:B:491:LYS:HE3	1.90	0.40
1:C:327:LEU:HD23	1:C:327:LEU:HA	1.93	0.40
1:C:414:TRP:CE3	1:C:426:TRP:HA	2.56	0.40
1:D:606:ASN:HD21	1:D:609:TYR:HB2	1.85	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	423/423 (100%)	403 (95%)	17 (4%)	3 (1%)	19 23
1	B	411/423 (97%)	397 (97%)	14 (3%)	0	100 100
1	C	419/423 (99%)	402 (96%)	16 (4%)	1 (0%)	44 55
1	D	409/423 (97%)	396 (97%)	13 (3%)	0	100 100
All	All	1662/1692 (98%)	1598 (96%)	60 (4%)	4 (0%)	44 55

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	304	ARG
1	A	377	PHE
1	A	622	ASP
1	C	352	ASP

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	380/378 (100%)	361 (95%)	19 (5%)	20	30
1	B	371/378 (98%)	353 (95%)	18 (5%)	21	31
1	C	376/378 (100%)	360 (96%)	16 (4%)	25	36
1	D	369/378 (98%)	355 (96%)	14 (4%)	28	42
All	All	1496/1512 (99%)	1429 (96%)	67 (4%)	24	34

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	324	LYS
1	A	326	THR
1	A	327	LEU
1	A	365	GLU
1	A	373	SER
1	A	386	LEU
1	A	390	ASN
1	A	394	ASP
1	A	402	LYS
1	A	491	LYS
1	A	521	ARG
1	A	528	LEU
1	A	601	ARG
1	A	608	ARG
1	A	611	ILE
1	A	613	GLU
1	A	617	LYS
1	A	624	ARG
1	A	665	LYS
1	B	304	ARG
1	B	326	THR
1	B	328	GLU
1	B	333	GLU
1	B	337	MET
1	B	353	VAL
1	B	369	GLN
1	B	383	MET
1	B	395	THR
1	B	474	LYS
1	B	528	LEU

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Mol	Chain	Res	Type
1	B	578	GLU
1	B	650	LYS
1	B	665	LYS
1	B	672	ARG
1	B	704	ARG
1	B	718	THR
1	B	720	VAL
1	C	326	THR
1	C	335	ILE
1	C	359	LEU
1	C	386	LEU
1	C	397	SER
1	C	491	LYS
1	C	508	GLU
1	C	528	LEU
1	C	605	ASP
1	C	610	ASN
1	C	617	LYS
1	C	625	LYS
1	C	626	THR
1	C	658[A]	SER
1	C	658[B]	SER
1	C	665	LYS
1	D	304	ARG
1	D	327	LEU
1	D	341	MET
1	D	353	VAL
1	D	372	SER
1	D	383	MET
1	D	404	THR
1	D	528	LEU
1	D	532	ASN
1	D	540	GLN
1	D	603	TYR
1	D	610	ASN
1	D	650	LYS
1	D	720	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	412	HIS

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Mol	Chain	Res	Type
1	A	469	GLN
1	B	412	HIS
1	B	610	ASN
1	C	342	HIS
1	C	345	GLN
1	C	475	HIS
1	C	610	ASN
1	D	532	ASN
1	D	610	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 16 ligands modelled in this entry, 2 are monoatomic - leaving 14 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	D	803	-	5,5,5	0.42	0	5,5,5	0.35	0
4	GOL	B	804	-	5,5,5	0.38	0	5,5,5	0.21	0
4	GOL	C	803	-	5,5,5	0.40	0	5,5,5	0.27	0
4	GOL	C	804	-	5,5,5	0.23	0	5,5,5	0.67	0
3	V5D	D	802	-	35,35,35	1.46	2 (5%)	45,46,46	1.31	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	HEM	A	801	1	42,50,50	1.58	8 (19%)	46,82,82	1.83	10 (21%)
3	V5D	A	802	-	35,35,35	1.45	2 (5%)	45,46,46	1.47	5 (11%)
3	V5D	B	803	-	35,35,35	1.42	2 (5%)	45,46,46	1.36	5 (11%)
3	V5D	C	802	-	35,35,35	1.41	2 (5%)	45,46,46	1.33	4 (8%)
2	HEM	C	801	1	42,50,50	1.51	7 (16%)	46,82,82	1.90	10 (21%)
2	HEM	B	802	1	42,50,50	1.53	6 (14%)	46,82,82	1.71	10 (21%)
2	HEM	D	801	1	42,50,50	1.51	7 (16%)	46,82,82	1.56	8 (17%)
4	GOL	A	803	-	5,5,5	0.38	0	5,5,5	0.37	0
4	GOL	A	804	-	5,5,5	0.30	0	5,5,5	0.40	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	GOL	D	803	-	-	2/4/4/4	-
4	GOL	B	804	-	-	4/4/4/4	-
4	GOL	C	803	-	-	2/4/4/4	-
4	GOL	C	804	-	-	2/4/4/4	-
3	V5D	D	802	-	-	1/14/14/14	0/4/4/4
2	HEM	A	801	1	-	2/12/54/54	-
3	V5D	A	802	-	-	2/14/14/14	0/4/4/4
3	V5D	B	803	-	-	4/14/14/14	0/4/4/4
3	V5D	C	802	-	-	1/14/14/14	0/4/4/4
2	HEM	C	801	1	-	0/12/54/54	-
2	HEM	B	802	1	-	1/12/54/54	-
2	HEM	D	801	1	-	1/12/54/54	-
4	GOL	A	803	-	-	4/4/4/4	-
4	GOL	A	804	-	-	4/4/4/4	-

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	802	V5D	O18-C17	6.52	1.52	1.37
3	A	802	V5D	O18-C17	6.35	1.52	1.37
3	B	803	V5D	O18-C17	6.32	1.52	1.37
3	C	802	V5D	O18-C17	6.21	1.51	1.37
2	A	801	HEM	C3C-C2C	-4.61	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	802	HEM	C3C-C2C	-3.93	1.35	1.40
2	D	801	HEM	C3C-C2C	-3.80	1.35	1.40
2	C	801	HEM	C3C-C2C	-3.68	1.35	1.40
2	B	802	HEM	C3C-C4C	3.58	1.46	1.41
2	C	801	HEM	C3C-CAC	3.46	1.55	1.47
2	B	802	HEM	C3C-CAC	3.34	1.55	1.47
2	D	801	HEM	C3C-CAC	3.34	1.55	1.47
2	A	801	HEM	C3C-CAC	3.29	1.55	1.47
3	D	802	V5D	O18-C19	3.20	1.53	1.43
2	B	802	HEM	CAB-C3B	3.14	1.55	1.47
3	C	802	V5D	O18-C19	3.12	1.53	1.43
3	A	802	V5D	O18-C19	3.11	1.53	1.43
2	D	801	HEM	CAB-C3B	3.10	1.55	1.47
3	B	803	V5D	O18-C19	3.08	1.53	1.43
2	C	801	HEM	CAB-C3B	3.08	1.55	1.47
2	A	801	HEM	CAB-C3B	2.96	1.55	1.47
2	D	801	HEM	C3C-C4C	2.86	1.45	1.41
2	C	801	HEM	C3C-C4C	2.77	1.45	1.41
2	A	801	HEM	C3C-C4C	2.73	1.45	1.41
2	A	801	HEM	CMB-C2B	2.45	1.55	1.50
2	D	801	HEM	CMB-C2B	2.40	1.55	1.50
2	B	802	HEM	CMD-C2D	2.36	1.55	1.50
2	D	801	HEM	CMD-C2D	2.29	1.55	1.50
2	A	801	HEM	C2C-C1C	2.28	1.47	1.42
2	A	801	HEM	CHA-C4D	2.23	1.40	1.34
2	C	801	HEM	CMB-C2B	2.21	1.55	1.50
2	B	802	HEM	CMB-C2B	2.21	1.55	1.50
2	C	801	HEM	CMA-C3A	2.16	1.55	1.51
2	C	801	HEM	CMC-C2C	2.08	1.56	1.51
2	A	801	HEM	CMD-C2D	2.07	1.55	1.50
2	D	801	HEM	CHB-C1B	2.06	1.39	1.34

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	802	V5D	C02-N32-C06	5.36	122.08	118.07
3	B	803	V5D	C02-N32-C06	5.34	122.07	118.07
3	A	802	V5D	C02-N32-C06	5.24	121.99	118.07
2	B	802	HEM	C4B-CHC-C1C	4.99	129.14	122.56
2	A	801	HEM	C4B-CHC-C1C	4.94	129.08	122.56
2	D	801	HEM	C4B-CHC-C1C	4.91	129.03	122.56
2	C	801	HEM	CBA-CAA-C2A	-4.68	104.68	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	801	HEM	C4B-CHC-C1C	4.67	128.73	122.56
3	D	802	V5D	C02-N32-C06	4.44	121.39	118.07
3	D	802	V5D	C07-C06-N32	3.86	121.90	116.06
2	A	801	HEM	C3B-C4B-NB	-3.84	106.71	109.47
2	A	801	HEM	C3D-C4D-ND	-3.77	106.04	110.17
3	A	802	V5D	C07-C06-N32	3.67	121.61	116.06
2	C	801	HEM	C3B-C4B-NB	-3.63	106.86	109.47
2	A	801	HEM	CHD-C1D-ND	3.26	127.94	124.44
2	C	801	HEM	CBD-CAD-C3D	-3.25	103.56	112.53
3	B	803	V5D	C07-C06-N32	3.15	120.83	116.06
2	D	801	HEM	C3B-C2B-C1B	3.09	108.73	106.41
2	C	801	HEM	C1B-NB-C4B	3.06	108.83	105.21
2	C	801	HEM	CMA-C3A-C4A	-3.00	124.06	128.46
2	B	802	HEM	CMA-C3A-C4A	-2.98	124.08	128.46
2	A	801	HEM	CBD-CAD-C3D	-2.91	104.48	112.53
2	B	802	HEM	C3B-C2B-C1B	2.89	108.58	106.41
3	C	802	V5D	C19-O18-C17	-2.87	110.79	117.62
3	B	803	V5D	C19-O18-C17	-2.86	110.81	117.62
3	A	802	V5D	N01-C02-N32	2.84	121.16	116.59
2	A	801	HEM	CMA-C3A-C4A	-2.84	124.30	128.46
3	A	802	V5D	C03-C02-N32	-2.73	118.54	121.83
2	C	801	HEM	C3B-C2B-C1B	2.68	108.42	106.41
2	A	801	HEM	C1B-NB-C4B	2.67	108.36	105.21
2	C	801	HEM	C3D-C4D-ND	-2.63	107.28	110.17
2	A	801	HEM	C4D-ND-C1D	2.60	108.29	105.21
2	A	801	HEM	CAD-C3D-C2D	-2.60	123.00	127.87
2	C	801	HEM	C4D-ND-C1D	2.59	108.28	105.21
2	D	801	HEM	C1B-NB-C4B	2.59	108.28	105.21
3	A	802	V5D	C19-O18-C17	-2.59	111.45	117.62
2	B	802	HEM	C3D-C4D-ND	-2.57	107.35	110.17
3	D	802	V5D	N01-C02-N32	2.54	120.67	116.59
2	B	802	HEM	CHD-C1D-ND	2.50	127.13	124.44
3	C	802	V5D	C07-C06-N32	2.49	119.83	116.06
2	B	802	HEM	CMC-C2C-C3C	2.46	129.59	124.68
2	D	801	HEM	CMC-C2C-C3C	2.43	129.53	124.68
2	A	801	HEM	CHC-C4B-C3B	2.41	128.25	124.57
2	B	802	HEM	CHA-C4D-ND	2.39	127.34	124.37
2	D	801	HEM	CBA-CAA-C2A	-2.37	108.56	112.54
2	B	802	HEM	C3B-C4B-NB	-2.29	107.82	109.47
2	D	801	HEM	C3B-C4B-NB	-2.27	107.83	109.47
2	D	801	HEM	C2B-C1B-NB	-2.24	107.26	109.84
3	D	802	V5D	C19-O18-C17	-2.21	112.35	117.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	801	HEM	C2B-C1B-NB	-2.20	107.31	109.84
3	C	802	V5D	C05-C06-N32	-2.19	119.64	122.40
2	B	802	HEM	CAB-C3B-C2B	-2.18	121.34	128.43
3	B	803	V5D	N01-C02-N32	2.17	120.08	116.59
3	B	803	V5D	C05-C06-N32	-2.15	119.69	122.40
2	B	802	HEM	C1B-NB-C4B	2.07	107.66	105.21
2	D	801	HEM	C3D-C4D-ND	-2.03	107.95	110.17

There are no chirality outliers.

All (30) torsion outliers are listed below:

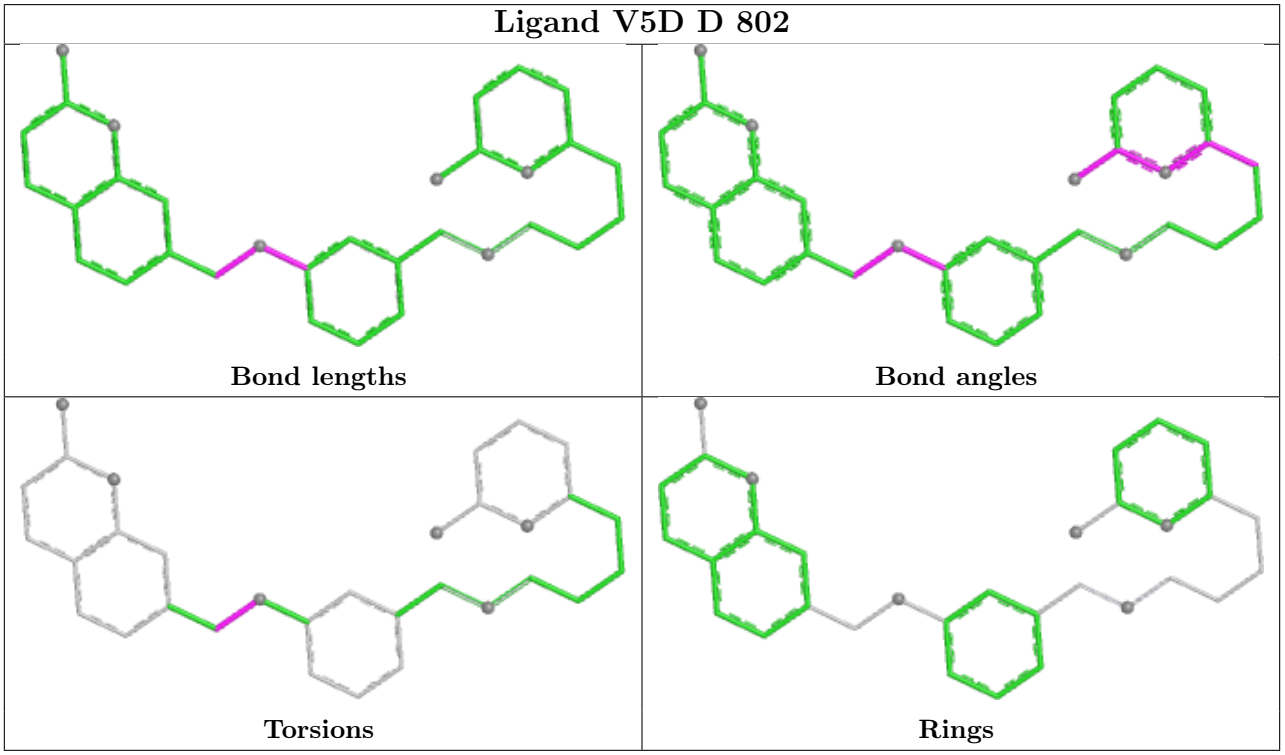
Mol	Chain	Res	Type	Atoms
2	A	801	HEM	C2A-CAA-CBA-CGA
4	A	803	GOL	O1-C1-C2-C3
4	A	803	GOL	C1-C2-C3-O3
4	A	804	GOL	C1-C2-C3-O3
4	B	804	GOL	O1-C1-C2-C3
4	C	804	GOL	O1-C1-C2-O2
4	D	803	GOL	O1-C1-C2-C3
2	B	802	HEM	C2A-CAA-CBA-CGA
4	A	804	GOL	O1-C1-C2-C3
4	C	803	GOL	C1-C2-C3-O3
4	C	804	GOL	O1-C1-C2-C3
4	A	803	GOL	O2-C2-C3-O3
4	A	804	GOL	O1-C1-C2-O2
4	A	804	GOL	O2-C2-C3-O3
4	C	803	GOL	O2-C2-C3-O3
4	D	803	GOL	O1-C1-C2-O2
4	A	803	GOL	O1-C1-C2-O2
4	B	804	GOL	O1-C1-C2-O2
4	B	804	GOL	O2-C2-C3-O3
2	D	801	HEM	C2A-CAA-CBA-CGA
3	B	803	V5D	C13-C12-N11-C10
3	B	803	V5D	C20-C19-O18-C17
3	C	802	V5D	C20-C19-O18-C17
3	B	803	V5D	C31-C17-O18-C19
3	B	803	V5D	C16-C17-O18-C19
3	A	802	V5D	C20-C19-O18-C17
3	D	802	V5D	C20-C19-O18-C17
4	B	804	GOL	C1-C2-C3-O3
2	A	801	HEM	C4B-C3B-CAB-CBB
3	A	802	V5D	C09-C10-N11-C12

There are no ring outliers.

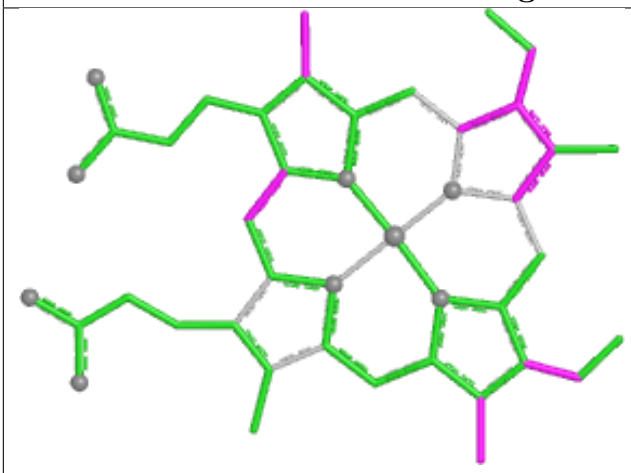
6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	803	GOL	1	0
2	A	801	HEM	3	0
2	C	801	HEM	3	0
2	B	802	HEM	2	0
2	D	801	HEM	1	0
4	A	803	GOL	1	0

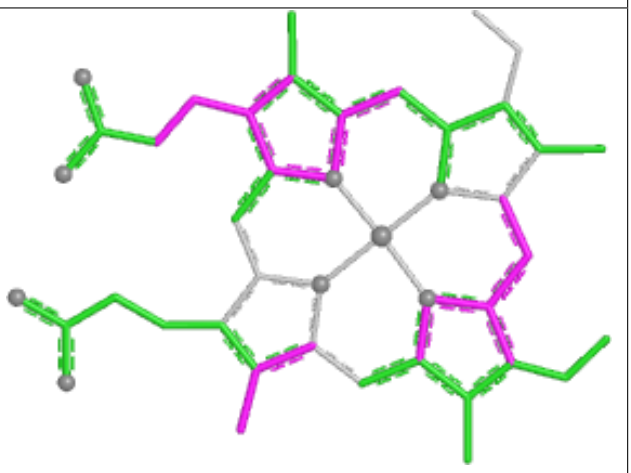
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.



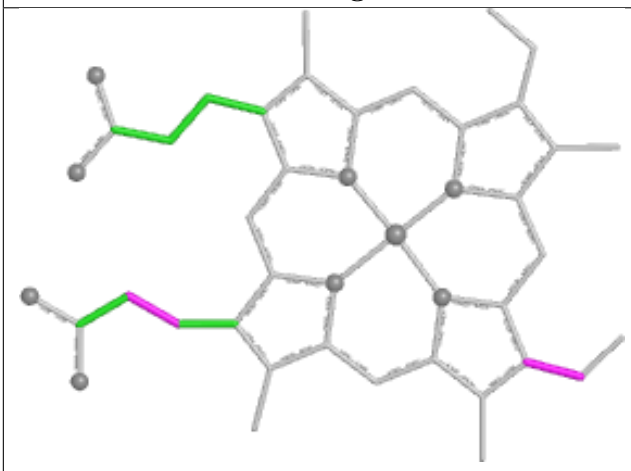
Ligand HEM A 801



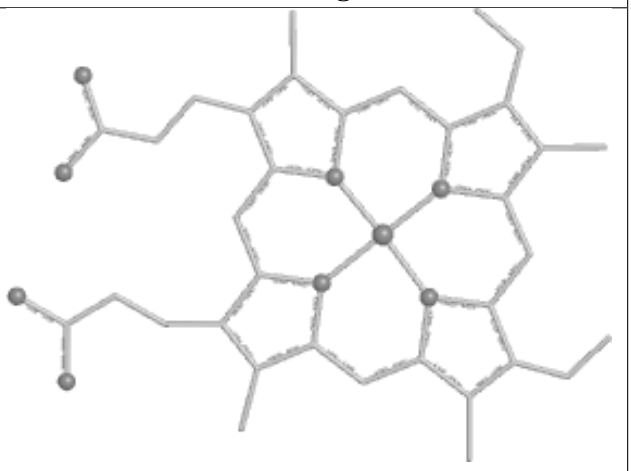
Bond lengths



Bond angles

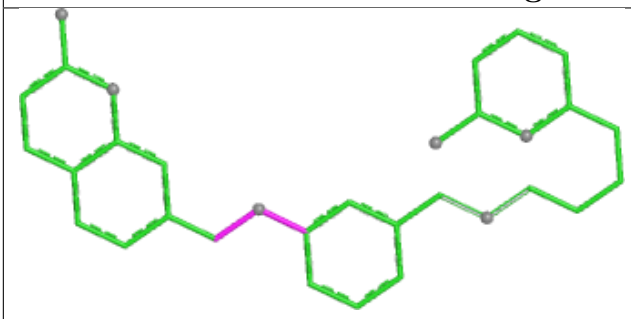


Torsions

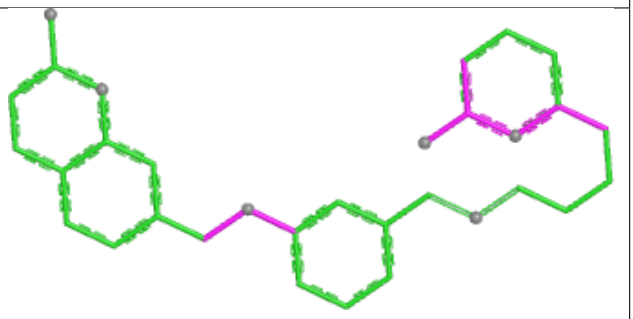


Rings

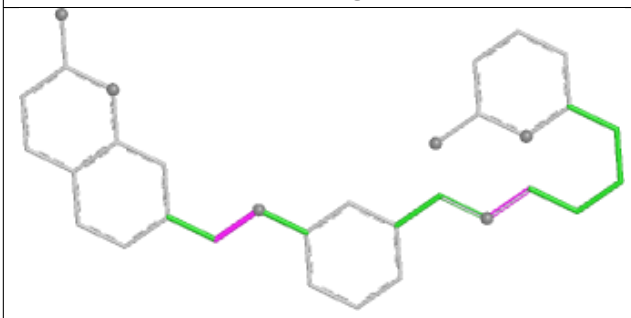
Ligand V5D A 802



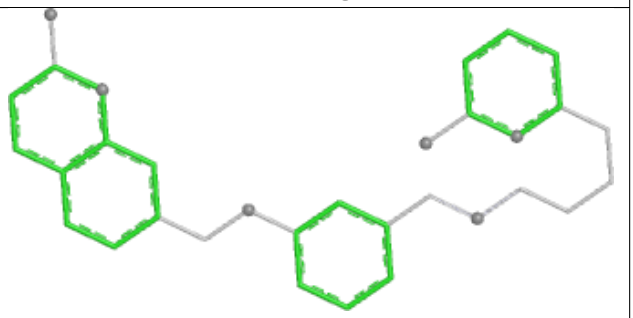
Bond lengths



Bond angles

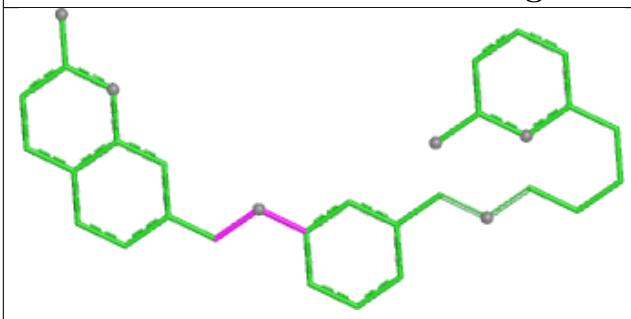


Torsions

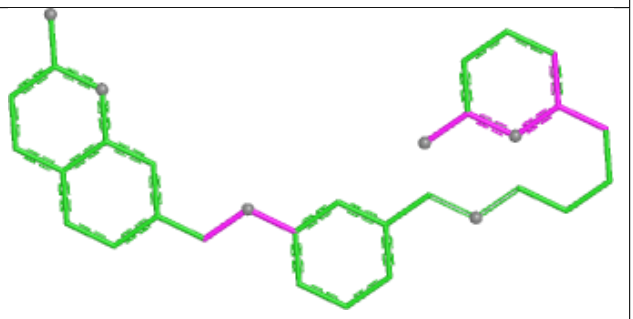


Rings

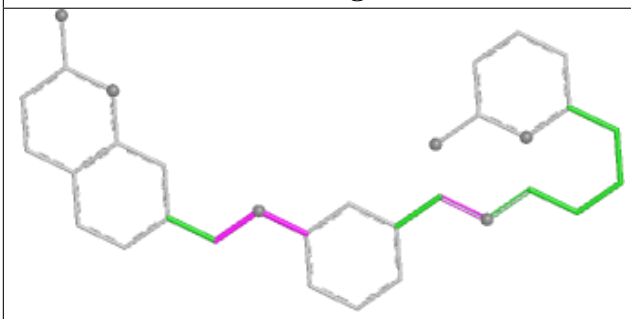
Ligand V5D B 803



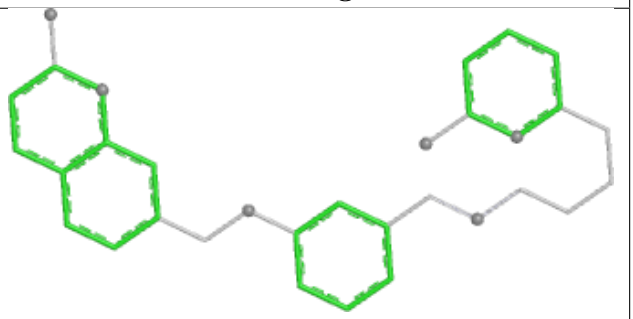
Bond lengths



Bond angles

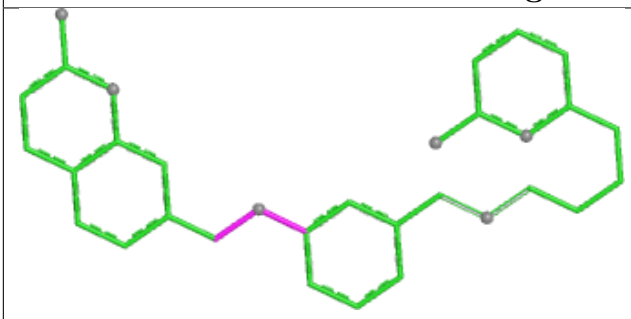


Torsions

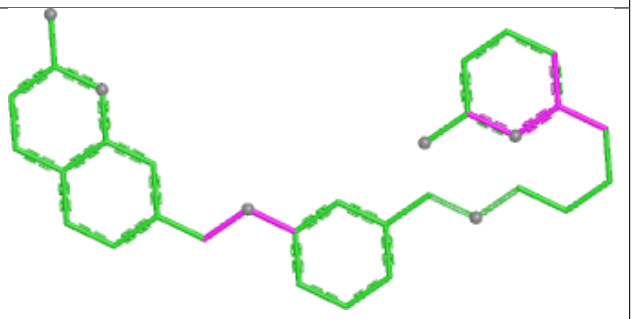


Rings

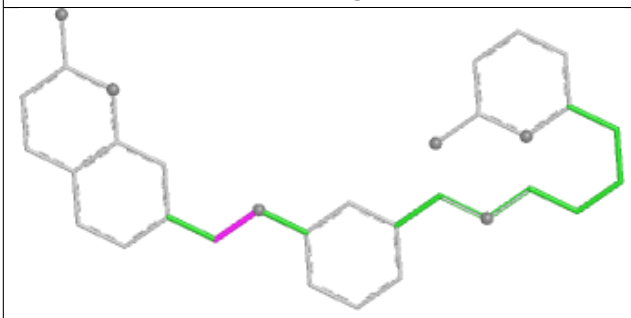
Ligand V5D C 802



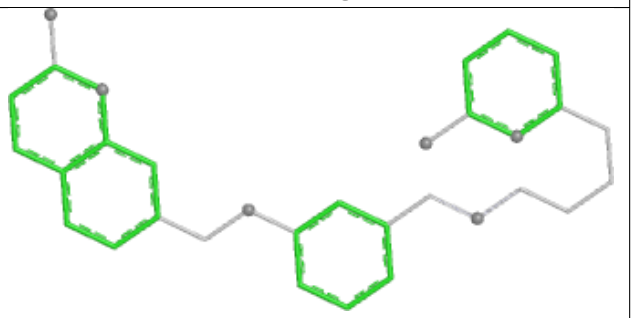
Bond lengths



Bond angles

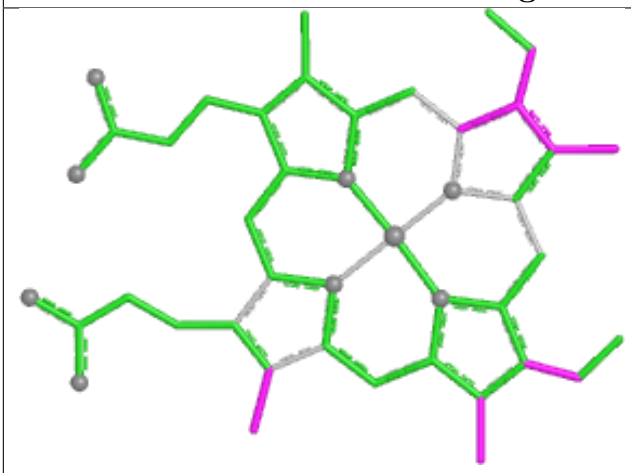


Torsions

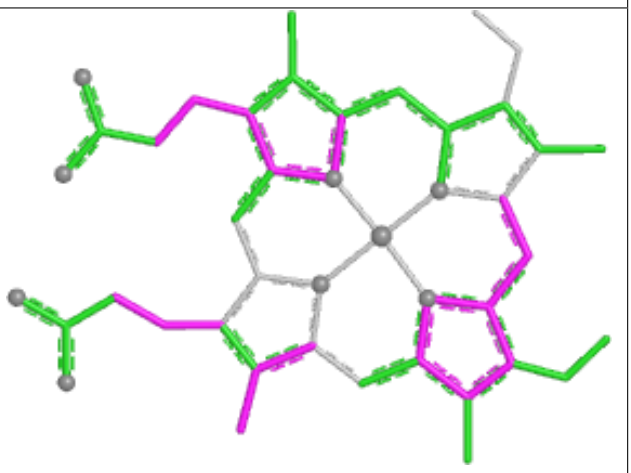


Rings

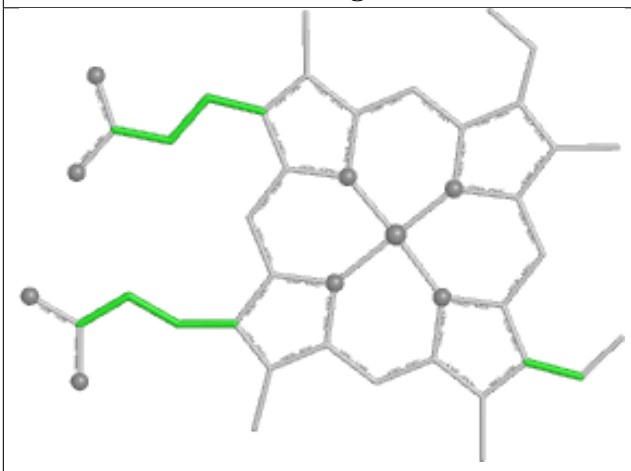
Ligand HEM C 801



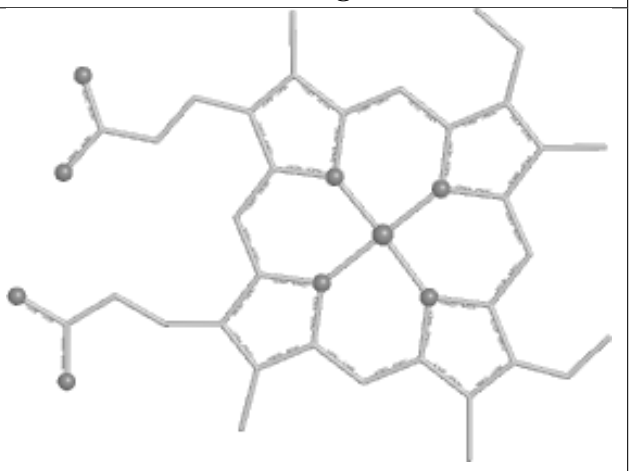
Bond lengths



Bond angles

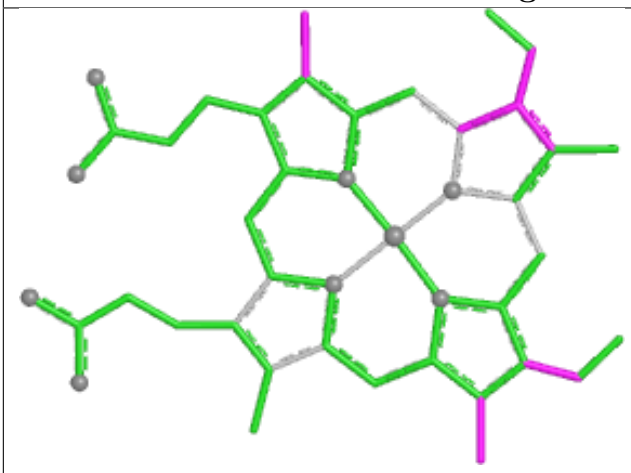


Torsions

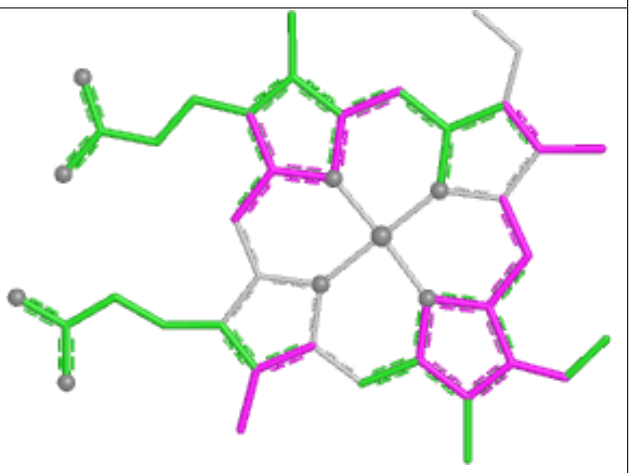


Rings

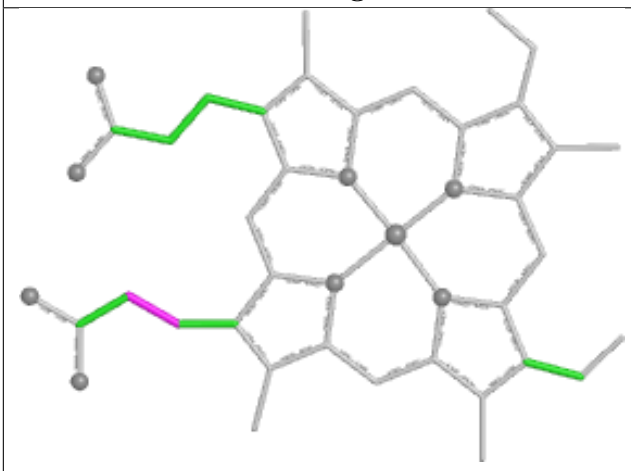
Ligand HEM B 802



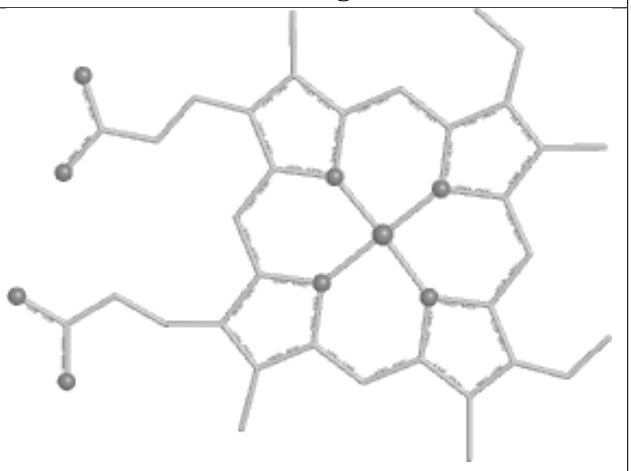
Bond lengths



Bond angles

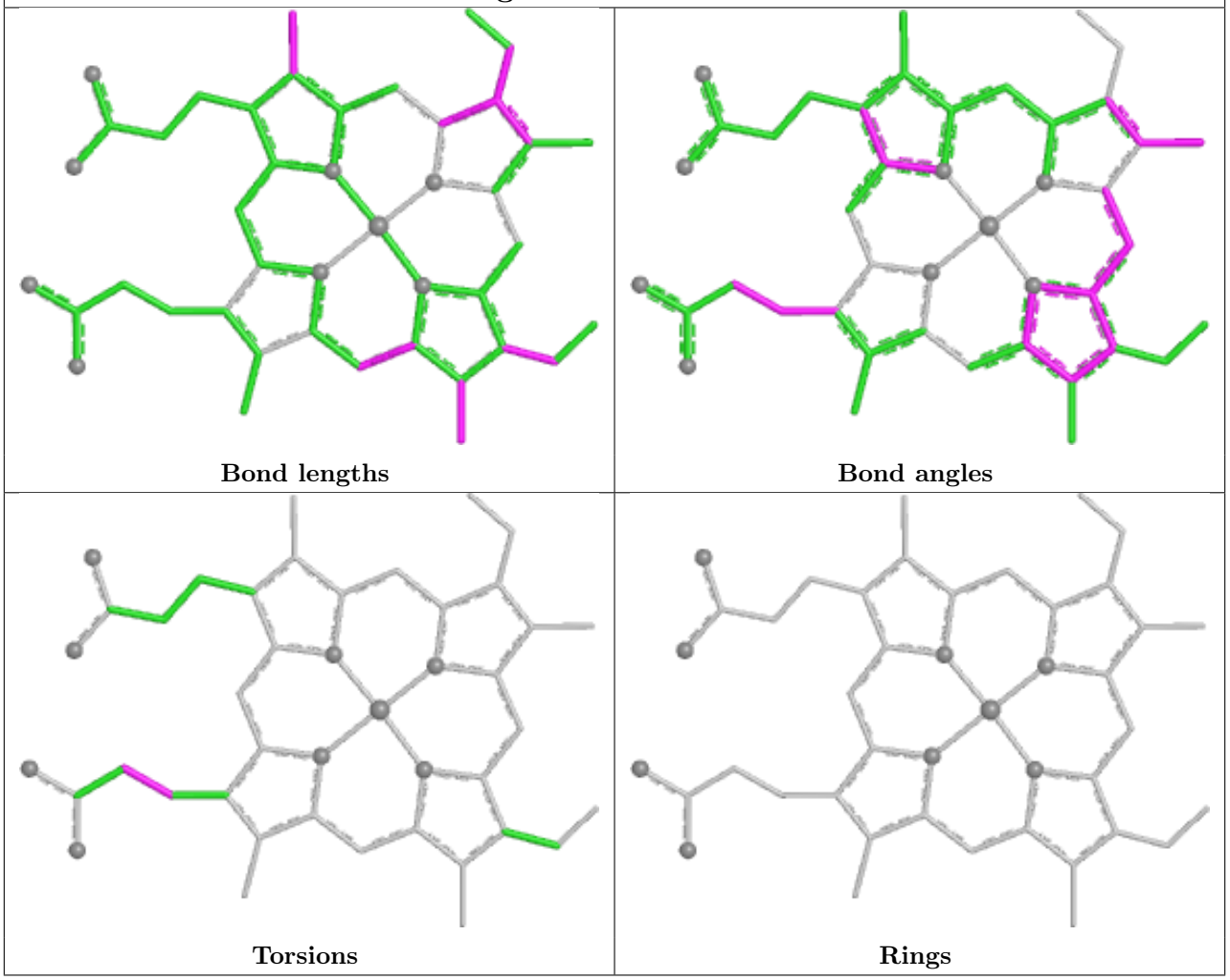


Torsions



Rings

Ligand HEM D 801



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	420/423 (99%)	-1.55	0	100	100	20, 48, 91, 137	5 (1%)
1	B	413/423 (97%)	-1.54	0	100	100	24, 45, 86, 169	2 (0%)
1	C	418/423 (98%)	-1.55	0	100	100	24, 49, 90, 153	3 (0%)
1	D	411/423 (97%)	-1.56	0	100	100	23, 46, 84, 181	2 (0%)
All	All	1662/1692 (98%)	-1.55	0	100	100	20, 47, 89, 181	12 (0%)

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

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, 95^{th} 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	804	6/6	0.98	0.05	64,69,74,84	0
3	V5D	B	803	32/32	0.99	0.04	26,55,94,94	0
3	V5D	C	802	32/32	0.99	0.04	26,61,92,93	0
3	V5D	D	802	32/32	0.99	0.05	31,57,87,88	0

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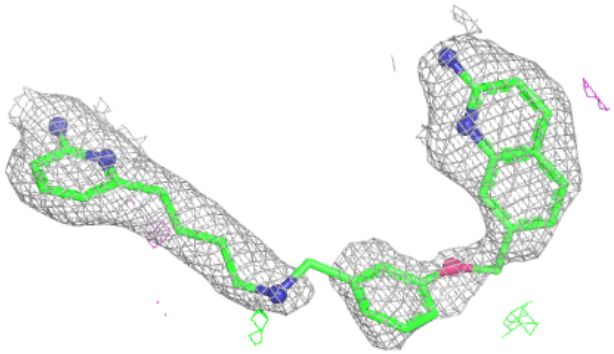
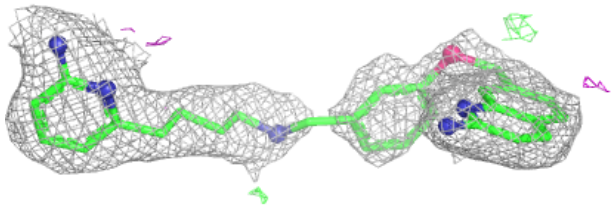
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GOL	A	803	6/6	0.99	0.04	75,85,90,91	0
3	V5D	A	802	32/32	0.99	0.04	29,54,86,88	0
4	GOL	B	804	6/6	0.99	0.04	41,73,76,80	0
4	GOL	C	803	6/6	0.99	0.05	76,80,81,82	0
4	GOL	C	804	6/6	0.99	0.05	49,55,63,65	0
4	GOL	D	803	6/6	0.99	0.05	57,66,69,70	0
2	HEM	C	801	43/43	1.00	0.03	17,42,60,66	0
2	HEM	D	801	43/43	1.00	0.03	21,41,54,59	0
2	HEM	A	801	43/43	1.00	0.03	26,42,53,57	0
2	HEM	B	802	43/43	1.00	0.03	25,35,50,57	0
5	ZN	B	801	1/1	1.00	0.01	46,46,46,46	0
5	ZN	C	805	1/1	1.00	0.01	49,49,49,49	0

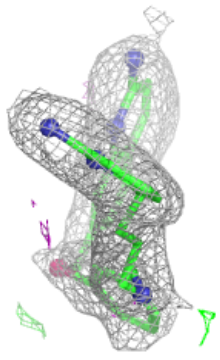
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around V5D B 803:

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

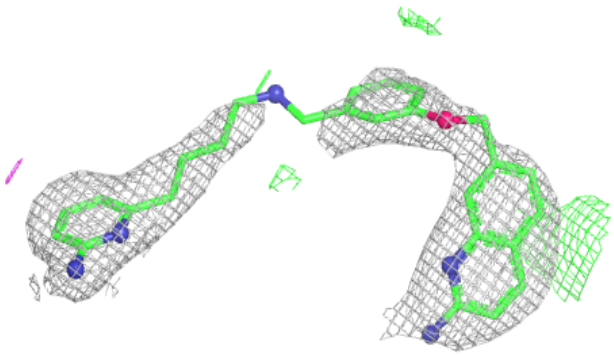


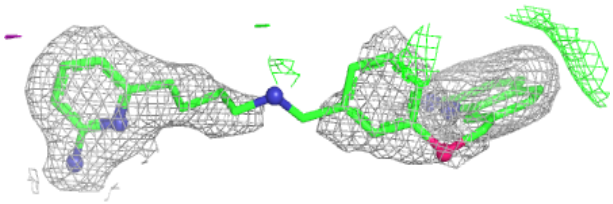


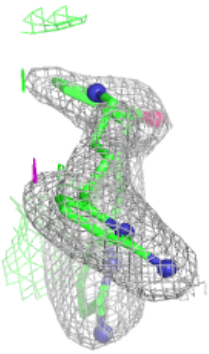


Electron density around V5D C 802:

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

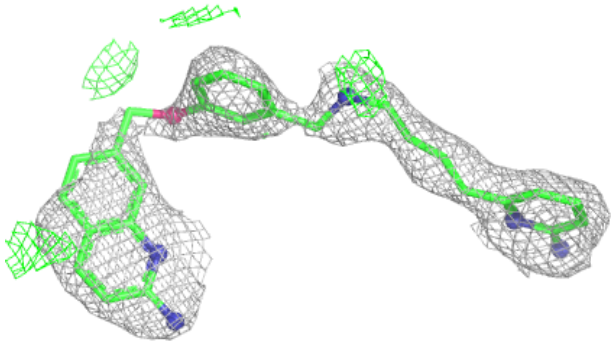


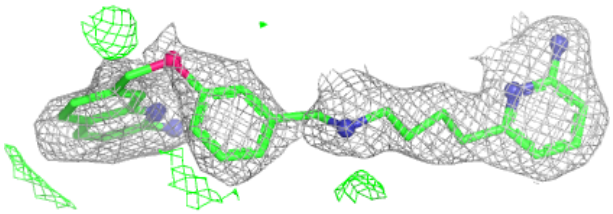


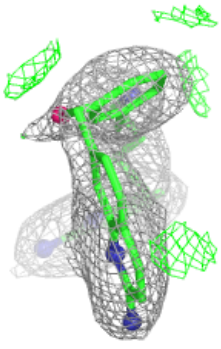


Electron density around V5D D 802:

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

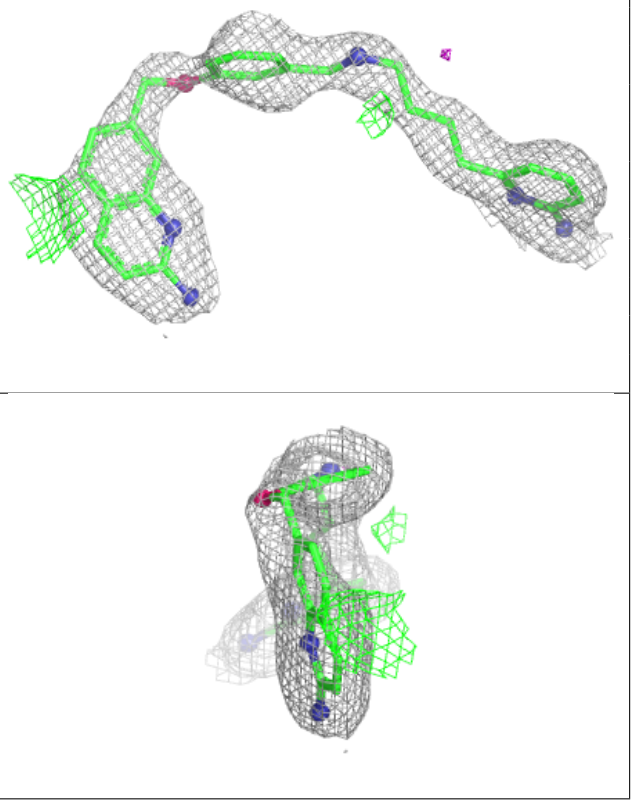






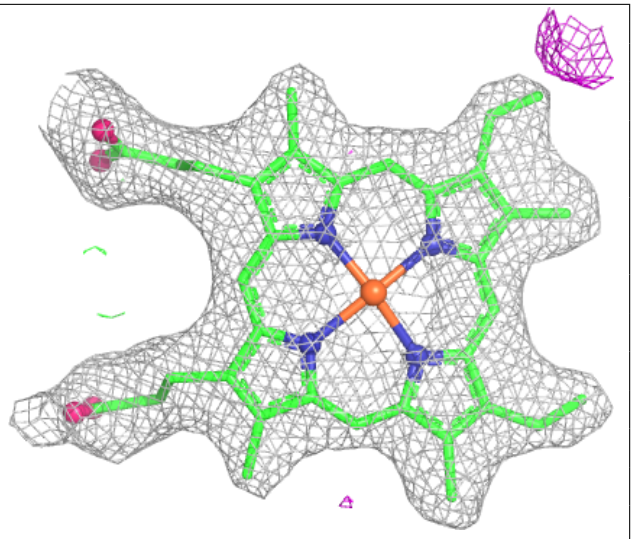
Electron density around V5D A 802:

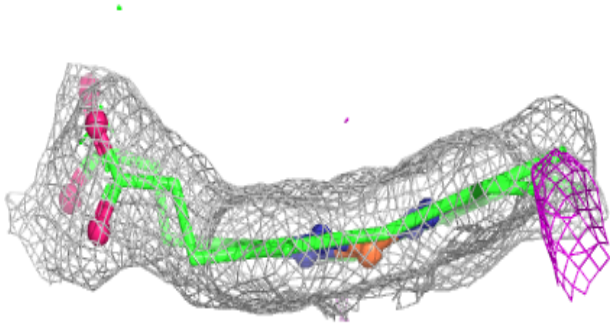
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

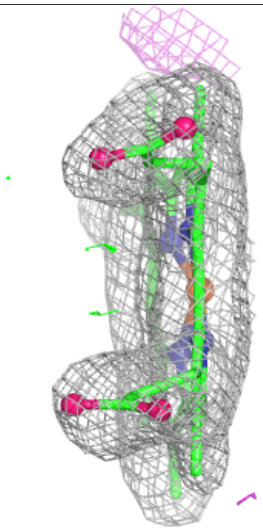


Electron density around HEM C 801:

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

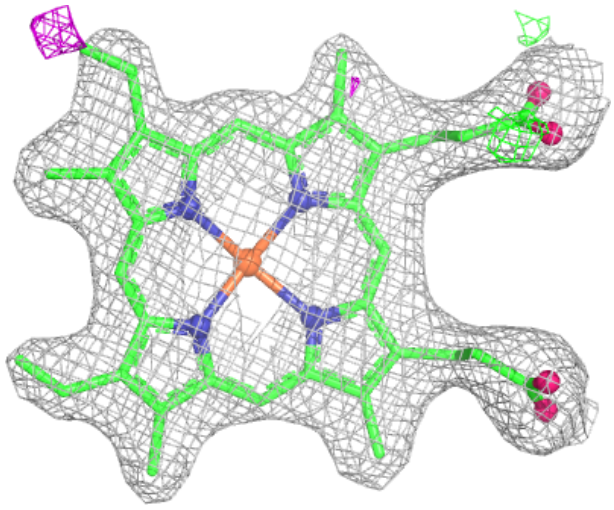


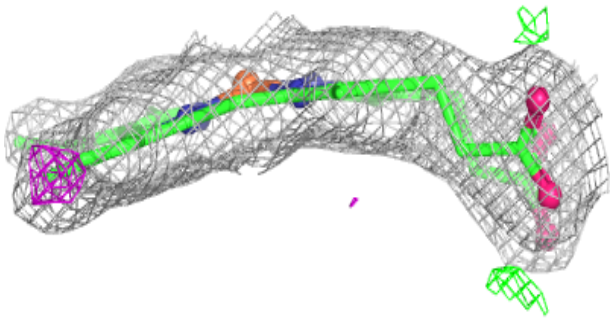


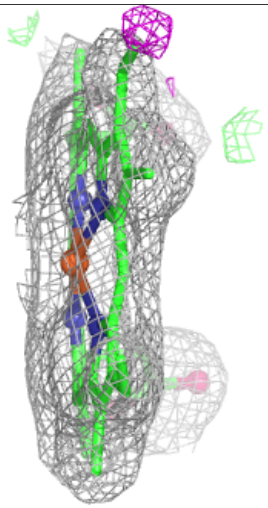


Electron density around HEM D 801:

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

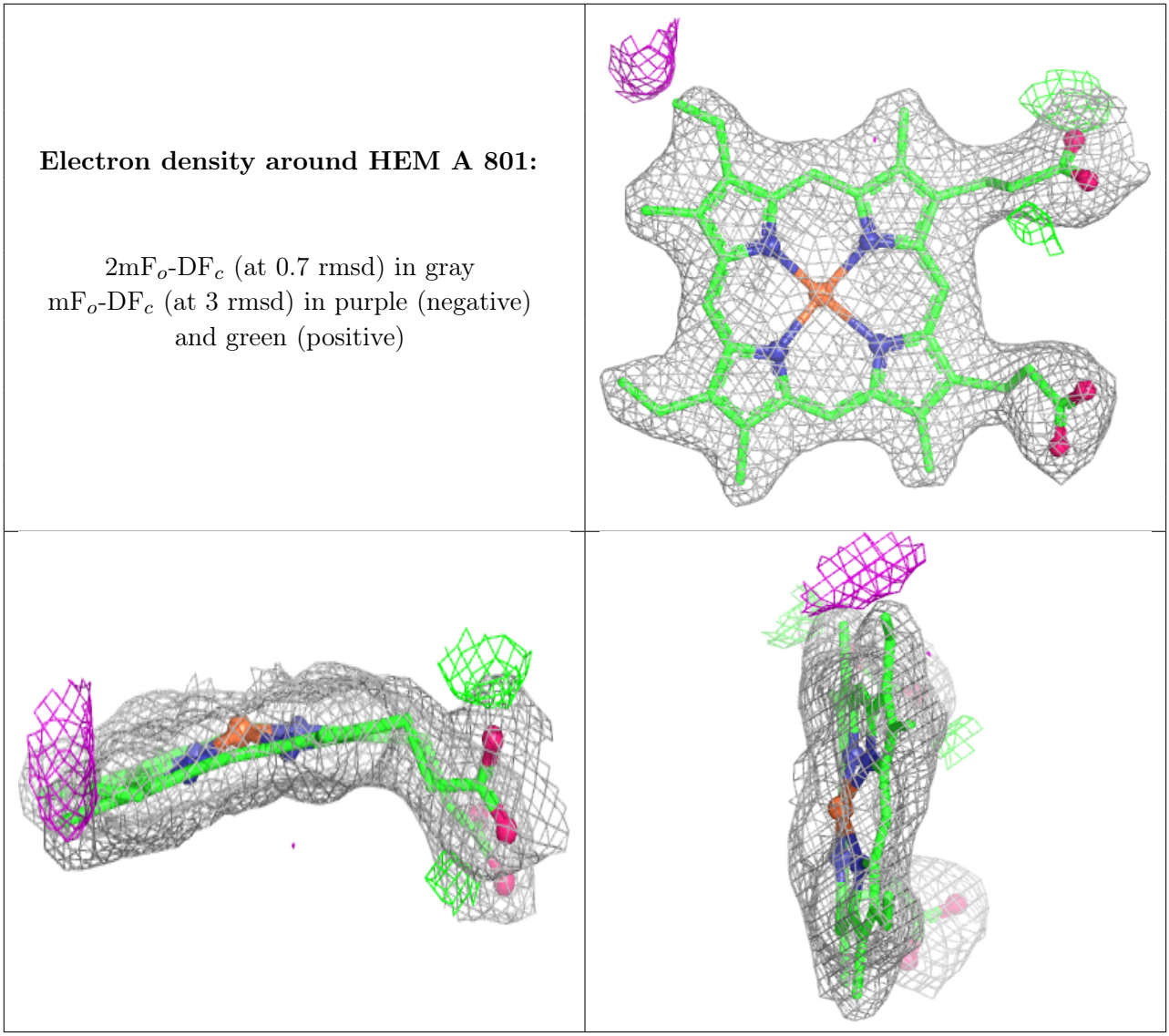






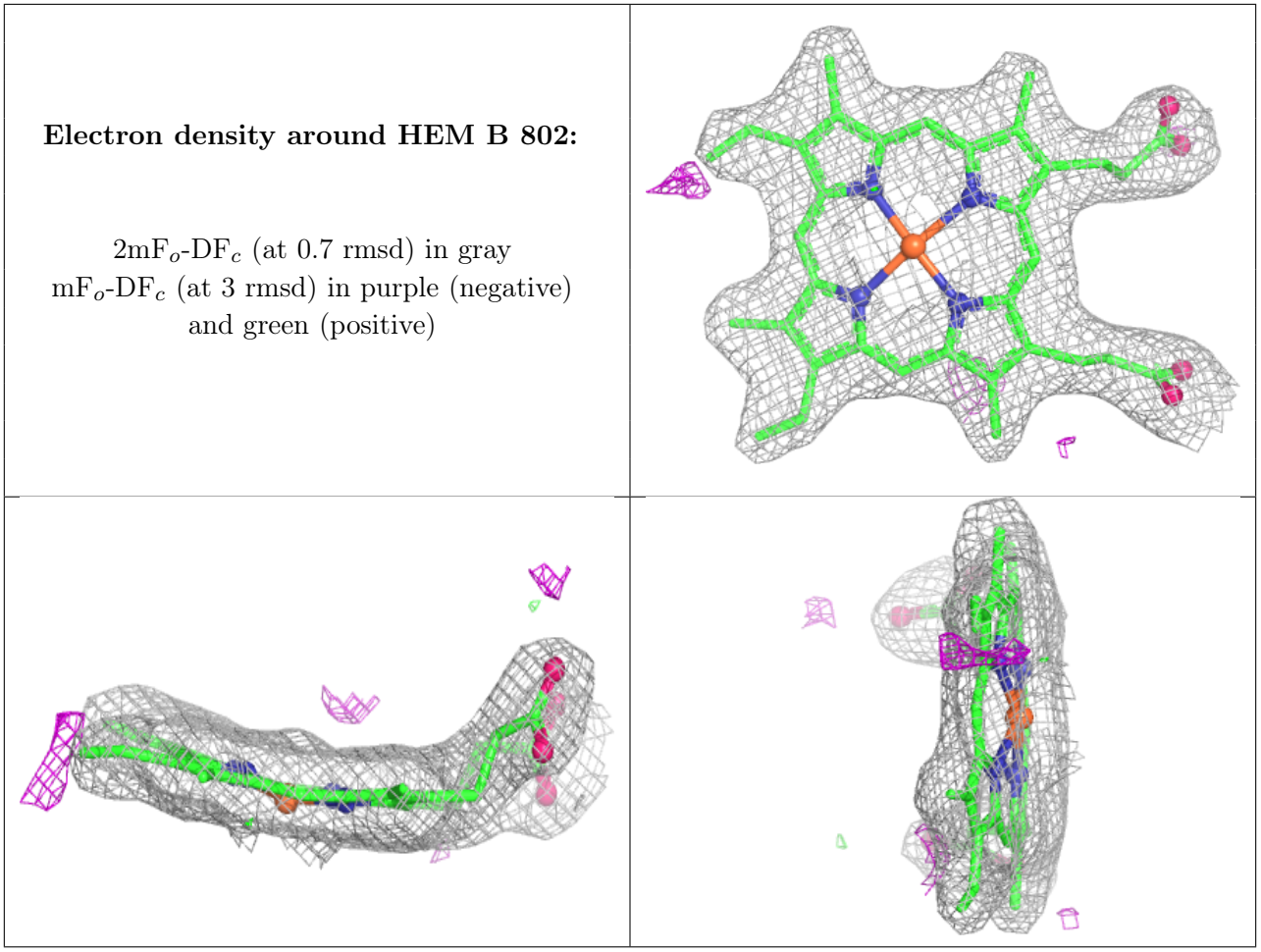
Electron density around HEM A 801:

$2mF_o$-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 802:

$2mF_o$-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.