Full wwPDB X-ray Structure Validation Report ⓘ

Oct 6, 2023 – 01:55 AM EDT

PDB ID	:	8FGL
Title	:	Structure of human neuronal nitric oxide synthase R354A/G357D mutant heme domain in complex with 6-(2,3-difluoro-5-(2-(4-methylpiperazin-1-yl)ethyl)phenethyl)-4-methylpyridin-2-amine
Authors	:	Li, H.; Poulos, T.L.
Deposited on	:	2022-12-12
Resolution	:	2.10 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:

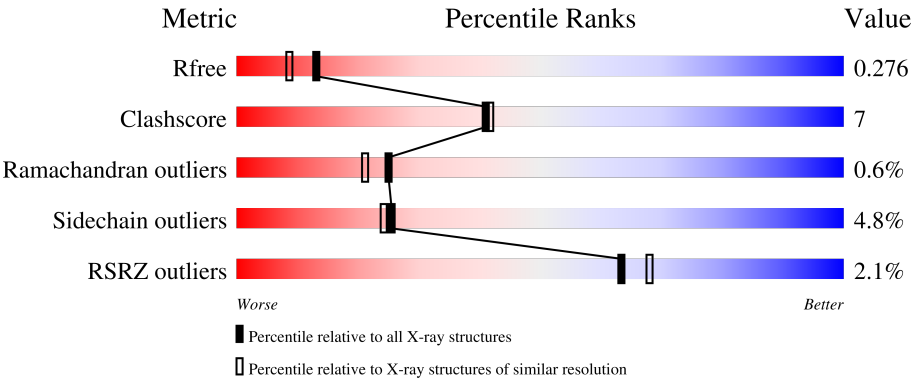
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	421	4% 77% 19%
1	B	421	% 81% 15%
1	C	421	% 79% 18%
1	D	421	2% 77% 19%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 14403 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.

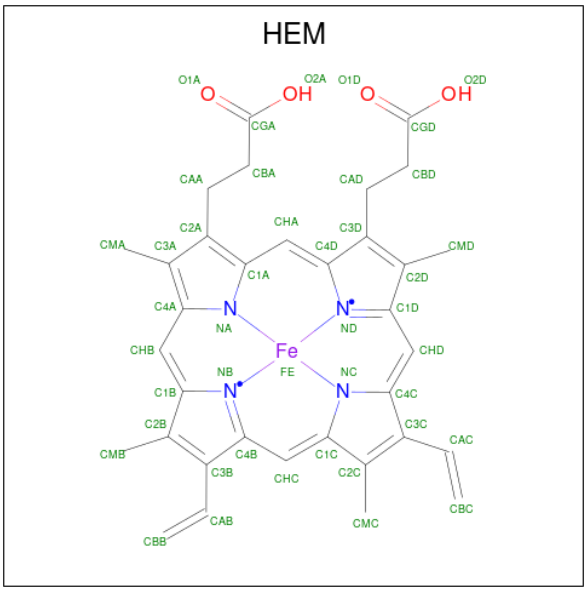
- Molecule 1 is a protein called Nitric oxide synthase, brain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	411	Total	C	N	O	S	0	4	0
			3363	2155	572	613	23			
1	B	414	Total	C	N	O	S	0	3	0
			3386	2168	575	622	21			
1	C	414	Total	C	N	O	S	0	4	0
			3388	2171	575	620	22			
1	D	411	Total	C	N	O	S	0	3	0
			3362	2154	572	615	21			

There are 8 discrepancies between the modelled and reference sequences:

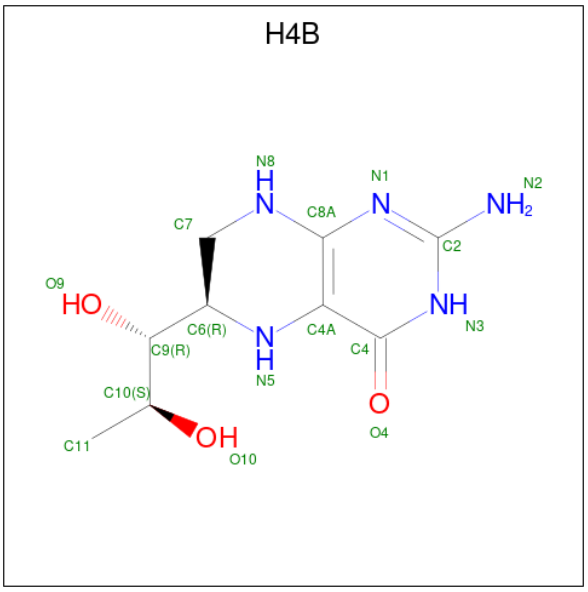
Chain	Residue	Modelled	Actual	Comment	Reference
A	354	ALA	ARG	engineered mutation	UNP P29475
A	357	ASP	GLY	engineered mutation	UNP P29475
B	354	ALA	ARG	engineered mutation	UNP P29475
B	357	ASP	GLY	engineered mutation	UNP P29475
C	354	ALA	ARG	engineered mutation	UNP P29475
C	357	ASP	GLY	engineered mutation	UNP P29475
D	354	ALA	ARG	engineered mutation	UNP P29475
D	357	ASP	GLY	engineered mutation	UNP P29475

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



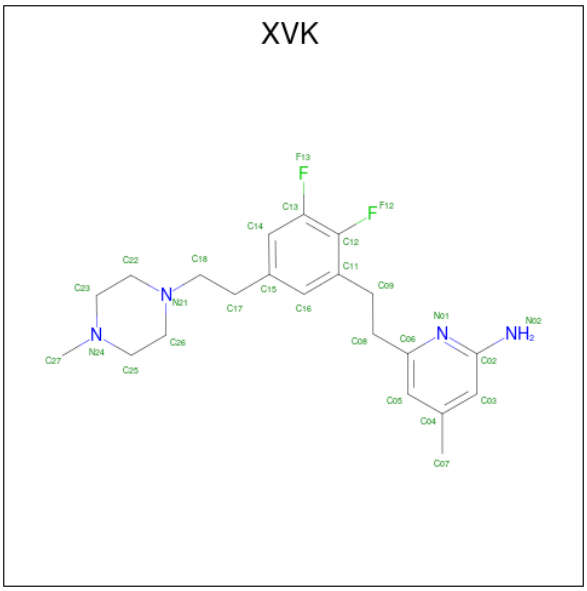
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



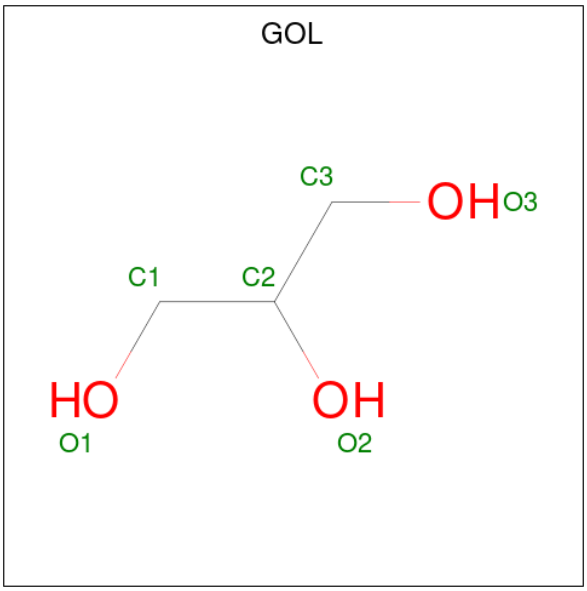
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 17 9 5 3	0	0
3	B	1	Total C N O 17 9 5 3	0	0
3	C	1	Total C N O 17 9 5 3	0	0
3	D	1	Total C N O 17 9 5 3	0	0

- Molecule 4 is 6-(2-{2,3-difluoro-5-[2-(4-methylpiperazin-1-yl)ethyl]phenyl}ethyl)-4-methylpyridin-2-amine (three-letter code: XVK) (formula: $C_{21}H_{28}F_2N_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C F N 27 21 2 4	0	0
4	B	1	Total C F N 27 21 2 4	0	0
4	C	1	Total C F N 27 21 2 4	0	0
4	D	1	Total C F N 27 21 2 4	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	91	Total O 91 91	0	0

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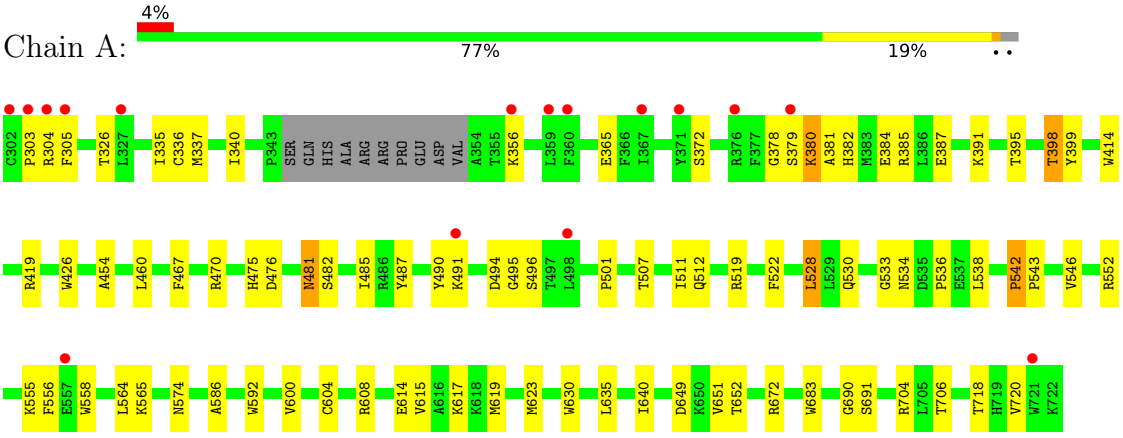
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	161	Total O 161 161	0	0
7	C	163	Total O 163 163	0	0
7	D	103	Total O 103 103	0	0

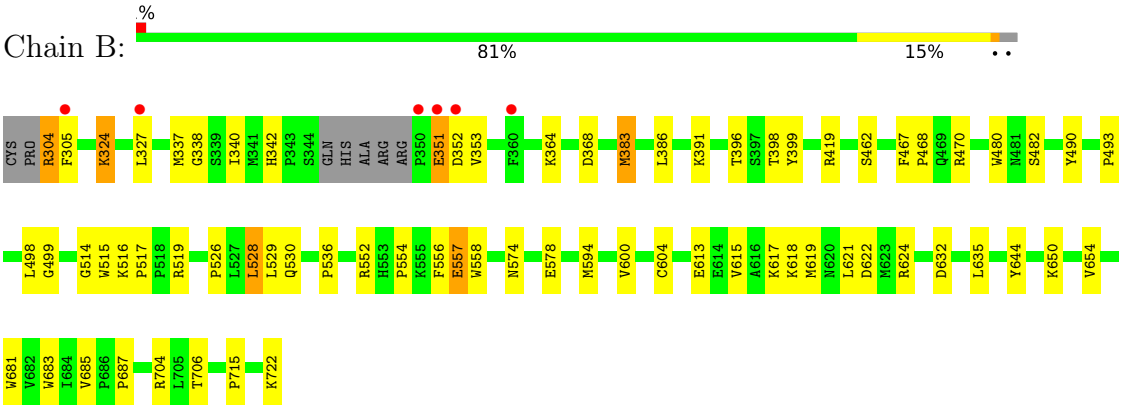
3 Residue-property plots (i)

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.

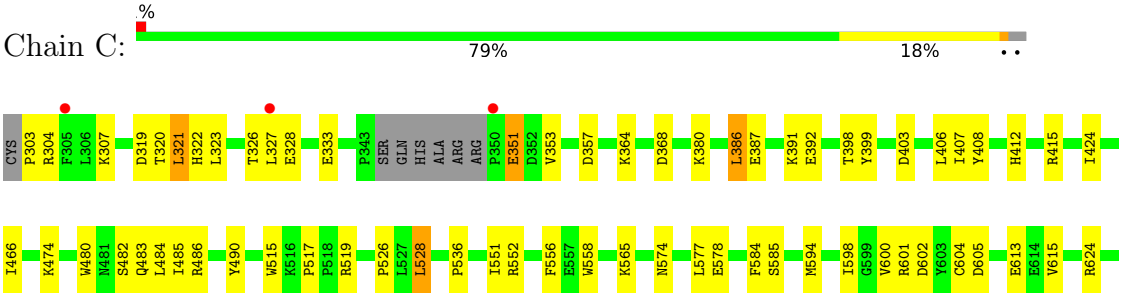
• Molecule 1: Nitric oxide synthase, brain



• Molecule 1: Nitric oxide synthase, brain

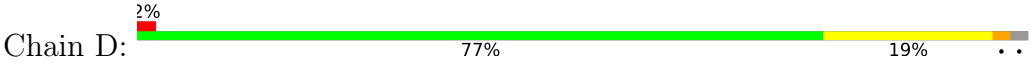


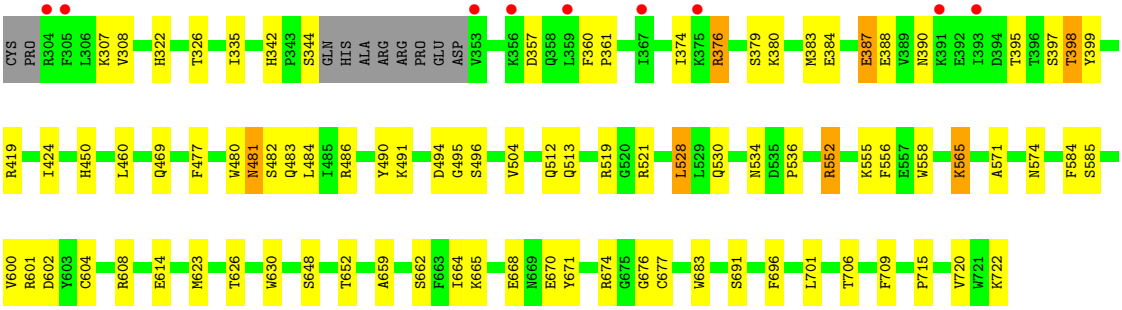
• Molecule 1: Nitric oxide synthase, brain



• Molecule 1: Nitric oxide synthase, brain

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	52.03Å 121.91Å 164.66Å 90.00° 90.10° 90.00°	Depositor
Resolution (Å)	39.57 – 2.10 39.57 – 2.10	Depositor EDS
% Data completeness (in resolution range)	92.8 (39.57-2.10) 93.7 (39.57-2.10)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.36 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.215 , 0.281 0.210 , 0.276	Depositor DCC
R_{free} test set	5629 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	40.6	Xtriage
Anisotropy	0.575	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 38.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.456 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	14403	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.54% 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: HEM, H4B, GOL, XVK, ZN

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	0.44	0/3471	0.58	0/4710
1	B	0.47	0/3491	0.60	0/4735
1	C	0.48	0/3497	0.59	0/4745
1	D	0.45	0/3466	0.58	0/4701
All	All	0.46	0/13925	0.59	0/18891

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	C	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	C	319	ASP	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	3363	0	3281	44	0
1	B	3386	0	3295	47	1
1	C	3388	0	3304	52	0
1	D	3362	0	3277	47	1
2	A	43	0	30	2	0
2	B	43	0	30	2	0
2	C	43	0	30	3	0
2	D	43	0	30	4	0
3	A	17	0	15	0	0
3	B	17	0	15	0	0
3	C	17	0	15	0	0
3	D	17	0	15	0	0
4	A	27	0	0	0	0
4	B	27	0	0	0	0
4	C	27	0	0	0	0
4	D	27	0	0	0	0
5	A	12	0	16	0	0
5	B	6	0	8	0	0
5	C	12	0	16	1	0
5	D	6	0	8	2	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
7	A	91	0	0	4	0
7	B	161	0	0	5	0
7	C	163	0	0	8	0
7	D	103	0	0	3	0
All	All	14403	0	13385	193	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (193) 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:528:LEU:HD22	1:A:536:PRO:HB2	1.57	0.84
1:C:387:GLU:HG3	1:C:391:LYS:HE3	1.64	0.78
1:A:305:PHE:HZ	1:D:395:THR:HA	1.48	0.78
1:D:674:ARG:HH21	5:D:804:GOL:H12	1.47	0.78
1:D:494:ASP:O	1:D:496:SER:N	2.17	0.78
1:D:528:LEU:HD22	1:D:536:PRO:HB2	1.67	0.76
1:C:392:GLU:OE2	7:C:901:HOH:O	2.05	0.74
1:C:321:LEU:N	7:C:902:HOH:O	2.09	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:494:ASP:O	1:A:496:SER:N	2.21	0.74
1:C:407:ILE:HG21	5:C:805:GOL:H31	1.71	0.73
2:D:801:HEM:HBB2	2:D:801:HEM:HHC	1.71	0.73
1:D:565:LYS:NZ	7:D:901:HOH:O	2.22	0.72
1:A:384:GLU:N	1:A:384:GLU:OE1	2.23	0.71
1:A:512:GLN:NE2	7:A:901:HOH:O	2.24	0.71
2:B:801:HEM:HMC2	2:B:801:HEM:HBC2	1.72	0.71
1:D:374:ILE:HG13	1:D:376:ARG:HG3	1.75	0.69
1:B:622:ASP:OD2	1:B:624:ARG:NH1	2.26	0.68
1:B:528:LEU:HD22	1:B:536:PRO:HB2	1.74	0.67
2:C:801:HEM:HBC2	2:C:801:HEM:HMC2	1.74	0.67
1:B:470:ARG:NH1	7:B:901:HOH:O	2.27	0.67
1:A:305:PHE:CZ	1:D:395:THR:HA	2.31	0.66
1:D:664:ILE:O	1:D:668[B]:GLU:HG2	1.96	0.66
2:A:801:HEM:HBB2	2:A:801:HEM:HHC	1.80	0.64
1:C:515:TRP:CD1	1:C:526:PRO:HG3	2.33	0.64
1:D:419:ARG:HD3	1:D:683:TRP:CD2	2.33	0.64
1:B:304:ARG:HH11	1:B:304:ARG:HB3	1.62	0.63
1:A:704:ARG:NH2	7:A:904:HOH:O	2.32	0.63
1:A:485:ILE:HD13	1:A:546:VAL:HG13	1.82	0.62
1:C:528:LEU:HD22	1:C:536:PRO:HB2	1.83	0.61
1:A:419:ARG:HD3	1:A:683:TRP:CD2	2.36	0.61
2:A:801:HEM:HMC2	2:A:801:HEM:HBC2	1.81	0.61
1:B:600:VAL:O	1:B:604:CYS:HB2	2.02	0.60
1:A:398:THR:OG1	1:A:399:TYR:N	2.32	0.59
1:D:483:GLN:OE1	1:D:486:ARG:HD2	2.03	0.58
1:B:327:LEU:HB3	1:B:704:ARG:HD2	1.85	0.58
1:B:514:GLY:O	1:B:516:LYS:NZ	2.38	0.56
1:A:600:VAL:HG22	1:A:635:LEU:HD11	1.89	0.55
1:B:364:LYS:NZ	1:B:368:ASP:OD2	2.39	0.55
1:A:522:PHE:HB2	1:A:565:LYS:HE2	1.89	0.55
1:C:364:LYS:NZ	1:C:368:ASP:OD2	2.39	0.55
2:C:801:HEM:HHC	2:C:801:HEM:HBB2	1.89	0.54
1:B:498:LEU:HD12	1:B:499:GLY:H	1.72	0.54
1:D:480:TRP:CE2	1:D:715:PRO:HB2	2.42	0.54
1:A:600:VAL:O	1:A:604:CYS:HB2	2.08	0.54
1:C:704:ARG:HG3	7:C:1040:HOH:O	2.08	0.53
1:C:519:ARG:NH2	7:C:912:HOH:O	2.43	0.52
1:D:674:ARG:NH2	5:D:804:GOL:H12	2.21	0.52
1:A:691:SER:HB3	1:B:687:PRO:HB2	1.91	0.52
1:B:554:PRO:HD3	1:B:644:TYR:CD2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:424:ILE:HB	1:C:666:HIS:HB2	1.92	0.51
1:D:600:VAL:O	1:D:604:CYS:HB2	2.11	0.51
1:B:304:ARG:HG2	1:B:305:PHE:HD1	1.74	0.51
1:D:460:LEU:HG	1:D:652:THR:HB	1.91	0.51
1:C:681:TRP:CZ2	1:C:685:VAL:HG21	2.45	0.51
1:A:460:LEU:HG	1:A:652:THR:HB	1.93	0.51
1:A:482:SER:HA	1:A:574:ASN:HB3	1.93	0.51
1:C:406:LEU:HD11	1:C:466:ILE:HG21	1.93	0.51
1:A:556:PHE:HB3	1:A:558:TRP:CE2	2.46	0.50
1:D:671:TYR:HA	1:D:676:GLY:H	1.76	0.50
1:D:322:HIS:NE2	7:D:904:HOH:O	2.35	0.50
1:D:398:THR:OG1	1:D:399:TYR:N	2.45	0.50
1:A:460:LEU:HD12	1:A:592:TRP:HB3	1.94	0.50
1:B:482:SER:HA	1:B:574:ASN:HB3	1.94	0.50
1:B:557:GLU:H	1:B:557:GLU:CD	2.14	0.50
1:A:379:SER:OG	1:A:380:LYS:N	2.45	0.49
1:C:483:GLN:HB2	1:C:486:ARG:HG2	1.94	0.49
1:D:491:LYS:HE3	1:D:504:VAL:HG11	1.93	0.49
1:A:337:MET:HB3	1:A:340:ILE:HG13	1.94	0.49
1:C:304:ARG:HA	1:C:323:LEU:HD11	1.94	0.49
1:C:327:LEU:HD23	1:C:328:GLU:O	2.13	0.49
1:B:558:TRP:HB2	1:B:618:LYS:HE2	1.96	0.48
1:B:351:GLU:O	1:B:353:VAL:N	2.47	0.48
1:B:615:VAL:O	1:B:619:MET:HG3	2.14	0.48
1:D:552:ARG:NH1	1:D:648:SER:HB2	2.28	0.48
1:C:601:ARG:HD3	7:C:965:HOH:O	2.13	0.48
1:A:304:ARG:CZ	1:A:304:ARG:HB3	2.42	0.48
1:A:501:PRO:HD2	1:A:608:ARG:HA	1.96	0.48
1:A:507:THR:O	1:A:511:ILE:HG13	2.14	0.48
1:C:303:PRO:O	1:C:322:HIS:NE2	2.47	0.48
1:D:376:ARG:O	1:D:379:SER:HB2	2.14	0.48
1:A:481:ASN:OD1	1:A:481:ASN:N	2.45	0.48
1:D:556:PHE:HB3	1:D:558:TRP:CE2	2.48	0.48
1:A:470:ARG:HG3	1:A:476:ASP:OD1	2.14	0.47
1:B:515:TRP:CD1	1:B:526:PRO:HG3	2.48	0.47
1:B:600:VAL:HG13	1:B:635:LEU:HD11	1.96	0.47
1:D:659:ALA:O	1:D:662[B]:SER:OG	2.26	0.47
1:D:709:PHE:CE1	2:D:801:HEM:CBC	2.97	0.47
1:C:598:ILE:HA	1:C:602:ASP:OD2	2.14	0.47
1:B:519:ARG:NH1	7:B:910:HOH:O	2.48	0.47
1:A:380:LYS:NZ	1:C:333:GLU:OE2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:351:GLU:C	1:C:353:VAL:H	2.18	0.47
1:D:308:VAL:HG11	1:D:701:LEU:HG	1.97	0.47
1:B:619:MET:HB2	1:B:621:LEU:HG	1.98	0.46
1:A:454:ALA:HB1	7:A:902:HOH:O	2.14	0.46
1:B:304:ARG:NH2	1:B:305:PHE:HB2	2.30	0.46
1:C:304:ARG:O	1:C:320:THR:HG22	2.16	0.46
1:C:484:LEU:O	7:C:903:HOH:O	2.20	0.46
1:C:687:PRO:HB2	1:D:691:SER:HB3	1.98	0.46
1:B:706:THR:HG23	7:B:927:HOH:O	2.15	0.46
1:C:490:TYR:HE2	1:C:517:PRO:HB2	1.80	0.46
1:C:615:VAL:HG21	1:C:638:ILE:HD11	1.97	0.46
1:A:672:ARG:NH2	7:A:912:HOH:O	2.48	0.46
1:B:498:LEU:HD12	1:B:499:GLY:N	2.31	0.46
1:C:351:GLU:OE1	1:C:474:LYS:HE3	2.15	0.46
1:C:601:ARG:NH2	1:C:605:ASP:OD2	2.39	0.46
1:D:490:TYR:CE1	1:D:519:ARG:HA	2.51	0.46
1:B:493:PRO:HG2	7:B:1005:HOH:O	2.15	0.45
1:A:487:TYR:CE2	1:A:522:PHE:HB3	2.51	0.45
1:A:460:LEU:HD12	1:A:592:TRP:CB	2.46	0.45
1:C:519:ARG:HD3	7:C:912:HOH:O	2.16	0.45
1:A:419:ARG:HD3	1:A:683:TRP:CE2	2.52	0.45
1:B:594:MET:HA	1:B:654:VAL:O	2.16	0.45
1:C:556:PHE:HB3	1:C:558:TRP:CE2	2.51	0.45
2:D:801:HEM:HBC2	2:D:801:HEM:HHD	1.99	0.45
1:C:408:TYR:CE1	1:C:412:HIS:CE1	3.05	0.45
1:D:380:LYS:O	1:D:384:GLU:HB2	2.17	0.45
1:D:387:GLU:HG3	1:D:388:GLU:N	2.29	0.45
1:B:304:ARG:HB3	1:B:304:ARG:NH1	2.28	0.44
1:A:475:HIS:HA	1:A:533:GLY:HA3	1.99	0.44
1:B:480:TRP:CE2	1:B:715:PRO:HB2	2.53	0.44
1:C:515:TRP:CG	1:C:526:PRO:HG3	2.52	0.44
1:A:615:VAL:O	1:A:619:MET:HG3	2.17	0.44
1:D:360:PHE:N	1:D:361:PRO:HD2	2.33	0.44
1:D:512:GLN:NE2	1:D:513:GLN:OE1	2.51	0.44
1:B:515:TRP:CE2	1:B:526:PRO:HD3	2.53	0.44
1:C:594:MET:HA	1:C:654:VAL:O	2.18	0.43
1:B:556:PHE:HB3	1:B:558:TRP:CE2	2.53	0.43
1:D:342:HIS:CD2	1:D:344:SER:HB3	2.54	0.43
1:D:670:GLU:CB	1:D:677:CYS:HB2	2.49	0.43
1:C:327:LEU:HB3	1:C:704:ARG:HD2	2.00	0.43
1:C:551:ILE:HG12	1:C:565:LYS:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:PRO:HA	1:A:543:PRO:HD2	1.88	0.43
1:C:689:SER:O	1:C:692:ILE:HG12	2.19	0.43
1:B:624:ARG:HB2	1:B:624:ARG:CZ	2.49	0.43
1:C:322:HIS:HB2	1:D:335:ILE:HD11	2.01	0.43
1:B:419:ARG:HD3	1:B:683:TRP:CD2	2.54	0.43
1:B:490:TYR:CE2	1:B:517:PRO:HB2	2.54	0.43
1:B:613:GLU:HB2	7:B:937:HOH:O	2.17	0.43
1:C:327:LEU:HB2	1:C:704:ARG:NH1	2.34	0.43
1:B:480:TRP:HB2	1:B:528:LEU:HB3	1.99	0.43
1:C:482:SER:HA	1:C:574:ASN:HB3	2.00	0.43
1:C:600:VAL:O	1:C:604:CYS:HB2	2.18	0.43
1:A:564:LEU:HD23	1:A:564:LEU:HA	1.84	0.43
1:D:623:MET:HA	1:D:630:TRP:CD1	2.54	0.43
1:A:414:TRP:CE3	1:A:426:TRP:HA	2.54	0.42
1:A:490:TYR:CE1	1:A:519:ARG:HA	2.55	0.42
1:A:381:ALA:O	1:A:385:ARG:N	2.39	0.42
1:B:467:PHE:HB3	1:B:468:PRO:HD2	2.01	0.42
2:B:801:HEM:HBB2	2:B:801:HEM:HHC	2.01	0.42
1:B:480:TRP:NE1	1:B:530:GLN:OE1	2.42	0.42
1:B:681:TRP:CE2	1:B:685:VAL:HG21	2.55	0.42
1:C:320:THR:O	1:C:321:LEU:HB3	2.20	0.42
1:C:327:LEU:HD11	7:C:1059:HOH:O	2.20	0.42
1:C:632:ASP:OD1	1:C:632:ASP:N	2.49	0.42
1:D:360:PHE:CE1	1:D:390:ASN:HB2	2.55	0.42
1:B:482:SER:HB2	1:B:574:ASN:ND2	2.35	0.42
1:C:515:TRP:CZ3	1:C:517:PRO:HB3	2.55	0.42
1:D:481:ASN:OD1	1:D:481:ASN:N	2.51	0.42
1:D:521:ARG:O	1:D:521:ARG:HG3	2.19	0.42
1:A:378:GLY:H	1:A:382:HIS:CE1	2.38	0.41
1:C:415:ARG:CZ	1:C:674:ARG:HD2	2.50	0.41
1:D:691:SER:HA	1:D:696:PHE:CG	2.55	0.41
1:D:709:PHE:CE1	2:D:801:HEM:HBC1	2.55	0.41
1:A:623:MET:HA	1:A:630:TRP:CD1	2.54	0.41
1:C:577:LEU:HB3	1:C:584:PHE:HB2	2.02	0.41
1:D:484:LEU:HD12	1:D:571:ALA:HB1	2.02	0.41
1:D:530:GLN:HG3	1:D:534:ASN:O	2.20	0.41
1:A:467:PHE:HB2	1:A:586:ALA:HB3	2.03	0.41
1:A:530:GLN:HG3	1:A:534:ASN:O	2.19	0.41
1:A:649:ASP:O	1:A:651:VAL:HG23	2.20	0.41
1:A:528:LEU:HG	1:A:538:LEU:HD23	2.02	0.41
1:B:529:LEU:O	1:B:536:PRO:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:383:MET:HE3	1:B:386:LEU:HD12	2.01	0.41
1:C:398:THR:OG1	1:C:399:TYR:N	2.54	0.41
1:D:450:HIS:CD2	1:D:450:HIS:C	2.93	0.41
1:D:482:SER:HA	1:D:574:ASN:HB3	2.03	0.41
1:B:398:THR:OG1	1:B:399:TYR:N	2.54	0.41
1:B:490:TYR:CZ	1:B:519:ARG:HA	2.56	0.41
1:C:480:TRP:CE2	1:C:715:PRO:HB2	2.56	0.41
2:C:801:HEM:HBB2	2:C:801:HEM:CHC	2.49	0.41
1:D:469:GLN:HB3	1:D:584:PHE:CE2	2.56	0.41
1:B:490:TYR:HE2	1:B:517:PRO:HB2	1.86	0.40
1:B:681:TRP:CZ2	1:B:685:VAL:HG21	2.56	0.40
1:D:477:PHE:O	1:D:585:SER:OG	2.25	0.40
1:C:320:THR:O	1:C:675:GLY:O	2.39	0.40
1:B:337:MET:HG2	1:B:340:ILE:HG13	2.04	0.40
1:C:320:THR:O	1:C:321:LEU:CB	2.69	0.40
1:C:386:LEU:HD12	1:C:386:LEU:HA	1.86	0.40
1:D:601:ARG:HD3	7:D:961:HOH:O	2.21	0.40
1:B:324:LYS:HE2	1:B:324:LYS:N	2.37	0.40
1:C:490:TYR:CZ	1:C:519:ARG:HA	2.57	0.40
1:C:403:ASP:O	1:C:407:ILE:HG13	2.21	0.40
1:D:602:ASP:OD1	1:D:608:ARG:NH2	2.54	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304:ARG:NH1	1:D:387:GLU:OE1[1_655]	2.15	0.05

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	411/421 (98%)	385 (94%)	21 (5%)	5 (1%)	13 8
1	B	413/421 (98%)	395 (96%)	16 (4%)	2 (0%)	29 26
1	C	414/421 (98%)	393 (95%)	19 (5%)	2 (0%)	29 26
1	D	410/421 (97%)	393 (96%)	16 (4%)	1 (0%)	47 49
All	All	1648/1684 (98%)	1566 (95%)	72 (4%)	10 (1%)	25 21

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	495	GLY
1	D	495	GLY
1	A	380	LYS
1	B	352	ASP
1	C	321	LEU
1	C	351	GLU
1	A	356	LYS
1	A	303	PRO
1	A	690	GLY
1	B	338	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	371/376 (99%)	349 (94%)	22 (6%)	19 17
1	B	373/376 (99%)	357 (96%)	16 (4%)	29 29
1	C	374/376 (100%)	360 (96%)	14 (4%)	34 35
1	D	370/376 (98%)	350 (95%)	20 (5%)	22 20
All	All	1488/1504 (99%)	1416 (95%)	72 (5%)	25 24

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	326	THR

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Mol	Chain	Res	Type
1	A	335	ILE
1	A	336	CYS
1	A	365	GLU
1	A	372	SER
1	A	387	GLU
1	A	391	LYS
1	A	395	THR
1	A	398	THR
1	A	481	ASN
1	A	491	LYS
1	A	528	LEU
1	A	542	PRO
1	A	552	ARG
1	A	555	LYS
1	A	614	GLU
1	A	617	LYS
1	A	640	ILE
1	A	706[A]	THR
1	A	706[B]	THR
1	A	718	THR
1	A	720	VAL
1	B	304	ARG
1	B	324	LYS
1	B	342	HIS
1	B	351	GLU
1	B	383	MET
1	B	391	LYS
1	B	396	THR
1	B	462	SER
1	B	528	LEU
1	B	552	ARG
1	B	557	GLU
1	B	578	GLU
1	B	617	LYS
1	B	632	ASP
1	B	650	LYS
1	B	722	LYS
1	C	307	LYS
1	C	326	THR
1	C	357	ASP
1	C	380	LYS
1	C	386	LEU

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Mol	Chain	Res	Type
1	C	485	ILE
1	C	528	LEU
1	C	552	ARG
1	C	578	GLU
1	C	585	SER
1	C	613	GLU
1	C	624	ARG
1	C	627	SER
1	C	632	ASP
1	D	307	LYS
1	D	326	THR
1	D	357	ASP
1	D	376	ARG
1	D	383	MET
1	D	387	GLU
1	D	397	SER
1	D	398	THR
1	D	424	ILE
1	D	481	ASN
1	D	528	LEU
1	D	552	ARG
1	D	555	LYS
1	D	565	LYS
1	D	614	GLU
1	D	626	THR
1	D	665	LYS
1	D	706	THR
1	D	720	VAL
1	D	722	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	441	HIS
1	D	512	GLN
1	D	513	GLN

5.3.3 RNA

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 20 ligands modelled in this entry, 2 are monoatomic - leaving 18 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	$\#\|Z\| > 2$
5	GOL	C	804	-	5,5,5	0.45	0	5,5,5	0.49	0
4	XVK	D	803	-	29,29,29	0.54	0	39,40,40	1.96	9 (23%)
3	H4B	B	802	-	16,18,18	1.01	2 (12%)	11,26,26	2.56	6 (54%)
4	XVK	A	803	-	29,29,29	0.53	0	39,40,40	2.03	8 (20%)
3	H4B	C	802	-	16,18,18	0.92	1 (6%)	11,26,26	2.63	6 (54%)
4	XVK	C	803	-	29,29,29	0.48	0	39,40,40	2.01	9 (23%)
2	HEM	A	801	1	41,50,50	1.42	3 (7%)	45,82,82	1.63	9 (20%)
2	HEM	B	801	1	41,50,50	1.39	5 (12%)	45,82,82	1.59	8 (17%)
3	H4B	A	802	-	16,18,18	0.97	0	11,26,26	2.75	7 (63%)
5	GOL	B	804	-	5,5,5	0.41	0	5,5,5	0.38	0
5	GOL	A	804	-	5,5,5	0.39	0	5,5,5	0.54	0
4	XVK	B	803	-	29,29,29	0.46	0	39,40,40	1.95	9 (23%)
2	HEM	D	801	1	41,50,50	1.49	3 (7%)	45,82,82	1.81	9 (20%)
5	GOL	A	805	-	5,5,5	0.41	0	5,5,5	0.36	0
3	H4B	D	802	-	16,18,18	1.13	1 (6%)	11,26,26	2.72	6 (54%)
5	GOL	D	804	-	5,5,5	0.33	0	5,5,5	0.50	0
2	HEM	C	801	1	41,50,50	1.36	4 (9%)	45,82,82	1.86	9 (20%)
5	GOL	C	805	-	5,5,5	0.28	0	5,5,5	0.86	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
5	GOL	C	804	-	-	3/4/4/4	-
4	XVK	D	803	-	-	5/10/20/20	0/3/3/3
3	H4B	B	802	-	-	0/8/17/17	0/2/2/2
4	XVK	A	803	-	-	5/10/20/20	0/3/3/3
3	H4B	C	802	-	-	0/8/17/17	0/2/2/2
4	XVK	C	803	-	-	4/10/20/20	0/3/3/3
2	HEM	A	801	1	-	2/12/54/54	-
2	HEM	B	801	1	-	0/12/54/54	-
3	H4B	A	802	-	-	0/8/17/17	0/2/2/2
5	GOL	B	804	-	-	2/4/4/4	-
5	GOL	A	804	-	-	2/4/4/4	-
4	XVK	B	803	-	-	6/10/20/20	0/3/3/3
2	HEM	D	801	1	-	2/12/54/54	-
5	GOL	A	805	-	-	1/4/4/4	-
3	H4B	D	802	-	-	1/8/17/17	0/2/2/2
5	GOL	D	804	-	-	4/4/4/4	-
2	HEM	C	801	1	-	2/12/54/54	-
5	GOL	C	805	-	-	4/4/4/4	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	801	HEM	C3C-C2C	-5.30	1.33	1.40
2	C	801	HEM	C3C-C2C	-3.98	1.34	1.40
2	B	801	HEM	C3C-C2C	-3.87	1.35	1.40
2	A	801	HEM	C3C-CAC	3.76	1.55	1.47
2	A	801	HEM	C3C-C2C	-3.25	1.35	1.40
2	A	801	HEM	CAB-C3B	2.99	1.55	1.47
2	D	801	HEM	CAB-C3B	2.95	1.55	1.47
3	D	802	H4B	C4A-C4	-2.88	1.37	1.41
2	C	801	HEM	C3C-CAC	2.66	1.53	1.47
2	D	801	HEM	C3C-CAC	2.64	1.53	1.47
2	C	801	HEM	CAB-C3B	2.58	1.54	1.47
2	B	801	HEM	C3C-CAC	2.46	1.52	1.47
2	B	801	HEM	CAB-C3B	2.37	1.53	1.47
2	B	801	HEM	C3B-C2B	-2.29	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	802	H4B	C4A-C4	-2.26	1.38	1.41
3	C	802	H4B	C4A-C4	-2.06	1.38	1.41
2	C	801	HEM	C3B-C2B	-2.05	1.33	1.37
2	B	801	HEM	CMD-C2D	2.01	1.55	1.50
3	B	802	H4B	C4-N3	2.00	1.36	1.33

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	801	HEM	CBA-CAA-C2A	-7.18	100.36	112.62
4	A	803	XVK	C02-N01-C06	6.78	123.24	118.10
4	C	803	XVK	C02-N01-C06	6.19	122.79	118.10
4	B	803	XVK	C02-N01-C06	6.10	122.72	118.10
4	A	803	XVK	C09-C11-C12	-5.93	115.97	120.73
4	D	803	XVK	C09-C08-C06	-5.67	100.28	112.99
3	D	802	H4B	C8A-C4A-C4	5.64	119.58	114.57
3	A	802	H4B	C8A-C4A-C4	5.62	119.56	114.57
4	B	803	XVK	C09-C11-C12	-5.36	116.43	120.73
3	C	802	H4B	C8A-C4A-C4	5.12	119.12	114.57
2	A	801	HEM	CBA-CAA-C2A	-4.73	104.55	112.62
4	C	803	XVK	C09-C08-C06	-4.43	103.06	112.99
2	B	801	HEM	CBA-CAA-C2A	-4.33	105.23	112.62
4	D	803	XVK	C02-N01-C06	4.24	121.31	118.10
3	B	802	H4B	C8A-C4A-C4	4.20	118.30	114.57
2	D	801	HEM	CBA-CAA-C2A	-4.15	105.55	112.62
2	D	801	HEM	C2C-C3C-C4C	4.04	109.72	106.90
2	B	801	HEM	C4B-CHC-C1C	3.88	127.67	122.56
4	C	803	XVK	C05-C06-N01	-3.83	118.84	122.90
2	A	801	HEM	C4B-CHC-C1C	3.83	127.61	122.56
4	D	803	XVK	F12-C12-C11	3.82	121.88	117.85
2	C	801	HEM	C4B-CHC-C1C	3.79	127.56	122.56
4	C	803	XVK	C09-C11-C12	-3.68	117.77	120.73
3	A	802	H4B	N1-C2-N3	-3.67	119.66	125.42
4	A	803	XVK	C05-C06-N01	-3.64	119.04	122.90
3	D	802	H4B	N1-C2-N3	-3.49	119.94	125.42
2	D	801	HEM	C4B-CHC-C1C	3.49	127.16	122.56
3	B	802	H4B	N1-C2-N3	-3.48	119.96	125.42
4	D	803	XVK	C09-C11-C12	-3.47	117.94	120.73
4	B	803	XVK	C05-C06-N01	-3.43	119.26	122.90
3	C	802	H4B	C2-N3-C4	3.43	121.37	115.93
3	C	802	H4B	N1-C2-N3	-3.33	120.20	125.42
3	D	802	H4B	C2-N3-C4	3.33	121.22	115.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	802	H4B	C2-N3-C4	3.32	121.21	115.93
4	B	803	XVK	C16-C11-C12	3.32	119.80	116.76
3	B	802	H4B	C4-C4A-N5	3.30	121.89	119.12
4	C	803	XVK	C16-C11-C12	3.27	119.76	116.76
4	A	803	XVK	C16-C11-C12	3.22	119.71	116.76
4	D	803	XVK	C16-C11-C12	3.21	119.70	116.76
2	D	801	HEM	CHA-C4D-ND	3.20	128.33	124.38
4	C	803	XVK	F12-C12-C11	3.15	121.18	117.85
3	A	802	H4B	C2-N3-C4	3.14	120.92	115.93
4	B	803	XVK	C09-C08-C06	-3.08	106.09	112.99
4	D	803	XVK	C08-C09-C11	3.07	117.78	112.81
3	A	802	H4B	C2-N1-C8A	3.07	121.41	114.54
2	D	801	HEM	C3C-C4C-NC	-2.98	105.31	110.94
3	B	802	H4B	N2-C2-N3	2.92	121.80	117.25
2	D	801	HEM	C4D-ND-C1D	2.89	108.06	105.07
2	A	801	HEM	C1B-NB-C4B	2.86	108.03	105.07
2	C	801	HEM	C3B-C2B-C1B	2.80	108.56	106.49
4	D	803	XVK	N02-C02-N01	2.71	120.78	116.49
3	C	802	H4B	N2-C2-N3	2.71	121.47	117.25
2	C	801	HEM	C2C-C3C-C4C	2.70	108.78	106.90
2	C	801	HEM	CHD-C1D-ND	2.67	127.33	124.43
2	B	801	HEM	CMC-C2C-C3C	2.64	129.61	124.68
3	C	802	H4B	C4-C4A-N5	2.62	121.32	119.12
2	D	801	HEM	C2D-C1D-ND	-2.62	106.74	109.88
3	C	802	H4B	C2-N1-C8A	2.60	120.38	114.54
3	B	802	H4B	C2-N1-C8A	2.53	120.21	114.54
2	B	801	HEM	C2C-C3C-C4C	2.53	108.66	106.90
4	C	803	XVK	C26-C25-N24	-2.50	107.98	110.80
2	A	801	HEM	C3B-C2B-C1B	2.47	108.32	106.49
4	D	803	XVK	C05-C06-N01	-2.46	120.30	122.90
4	A	803	XVK	F12-C12-C11	2.44	120.43	117.85
2	C	801	HEM	CMC-C2C-C3C	2.44	129.24	124.68
4	A	803	XVK	C09-C11-C16	2.42	124.29	119.41
3	D	802	H4B	N2-C2-N1	2.42	121.02	117.25
3	D	802	H4B	C4-C4A-N5	2.41	121.14	119.12
3	D	802	H4B	C2-N1-C8A	2.39	119.90	114.54
3	A	802	H4B	C4-C4A-N5	2.38	121.12	119.12
2	D	801	HEM	CMD-C2D-C1D	2.37	128.65	125.04
2	B	801	HEM	C3B-C2B-C1B	2.35	108.23	106.49
2	C	801	HEM	CBD-CAD-C3D	-2.32	106.19	112.63
2	A	801	HEM	C4D-ND-C1D	2.29	107.44	105.07
4	C	803	XVK	C08-C06-N01	2.28	119.34	115.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	803	XVK	C08-C06-N01	2.26	119.31	115.95
2	A	801	HEM	CHC-C4B-C3B	2.25	128.01	124.57
4	A	803	XVK	C09-C08-C06	-2.25	107.95	112.99
2	A	801	HEM	CHD-C1D-ND	2.24	126.86	124.43
2	A	801	HEM	CMC-C2C-C3C	2.22	128.83	124.68
4	C	803	XVK	C22-C23-N24	-2.19	108.33	110.80
2	C	801	HEM	C1B-NB-C4B	2.18	107.32	105.07
4	B	803	XVK	C09-C11-C16	2.16	123.77	119.41
4	B	803	XVK	C08-C09-C11	2.16	116.30	112.81
3	A	802	H4B	N2-C2-N1	2.13	120.57	117.25
4	A	803	XVK	C08-C09-C11	2.13	116.26	112.81
2	B	801	HEM	C1B-NB-C4B	2.13	107.27	105.07
4	D	803	XVK	C27-N24-C23	-2.13	107.48	110.66
2	D	801	HEM	C1B-NB-C4B	2.11	107.25	105.07
2	B	801	HEM	CBD-CAD-C3D	-2.08	106.85	112.63
4	B	803	XVK	F12-C12-C11	2.08	120.04	117.85
2	A	801	HEM	CAD-CBD-CGD	-2.03	109.23	113.60
2	C	801	HEM	CMA-C3A-C4A	-2.02	125.35	128.46
2	B	801	HEM	CAD-CBD-CGD	-2.02	109.25	113.60
3	A	802	H4B	C4A-N5-C6	-2.01	115.69	121.16

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	803	XVK	C08-C09-C11-C12
4	B	803	XVK	C08-C09-C11-C12
5	A	804	GOL	O1-C1-C2-C3
5	A	805	GOL	O1-C1-C2-C3
5	B	804	GOL	O1-C1-C2-C3
5	C	804	GOL	O1-C1-C2-C3
5	D	804	GOL	O1-C1-C2-C3
5	D	804	GOL	C1-C2-C3-O3
4	A	803	XVK	C15-C17-C18-N21
4	C	803	XVK	C17-C18-N21-C22
4	B	803	XVK	C17-C18-N21-C22
4	D	803	XVK	C17-C18-N21-C22
4	B	803	XVK	C15-C17-C18-N21
4	C	803	XVK	C17-C18-N21-C26
5	C	805	GOL	O1-C1-C2-C3
5	C	805	GOL	C1-C2-C3-O3
5	A	804	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	B	804	GOL	O1-C1-C2-O2
5	C	805	GOL	O1-C1-C2-O2
5	D	804	GOL	O1-C1-C2-O2
5	D	804	GOL	O2-C2-C3-O3
5	C	804	GOL	O1-C1-C2-O2
4	A	803	XVK	C16-C15-C17-C18
4	A	803	XVK	C14-C15-C17-C18
4	B	803	XVK	C08-C09-C11-C16
2	A	801	HEM	C4B-C3B-CAB-CBB
2	D	801	HEM	C4B-C3B-CAB-CBB
5	C	804	GOL	O2-C2-C3-O3
4	B	803	XVK	C14-C15-C17-C18
4	B	803	XVK	C16-C15-C17-C18
4	C	803	XVK	C08-C09-C11-C12
4	D	803	XVK	C08-C09-C11-C12
4	D	803	XVK	C16-C15-C17-C18
4	D	803	XVK	C14-C15-C17-C18
4	A	803	XVK	C08-C09-C11-C16
5	C	805	GOL	O2-C2-C3-O3
4	D	803	XVK	C15-C17-C18-N21
2	C	801	HEM	CAA-CBA-CGA-O2A
2	C	801	HEM	CAA-CBA-CGA-O1A
4	C	803	XVK	C08-C09-C11-C16
2	A	801	HEM	C4D-C3D-CAD-CBD
3	D	802	H4B	N5-C6-C9-O9
2	D	801	HEM	CAA-CBA-CGA-O1A

There are no ring outliers.

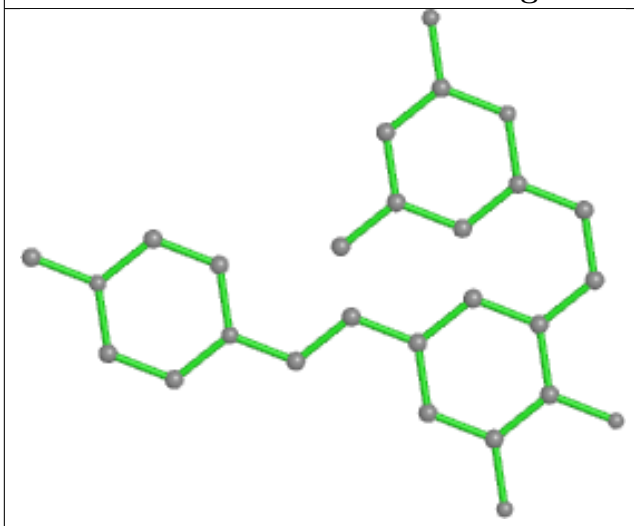
6 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	HEM	2	0
2	B	801	HEM	2	0
2	D	801	HEM	4	0
5	D	804	GOL	2	0
2	C	801	HEM	3	0
5	C	805	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 XVK D 803



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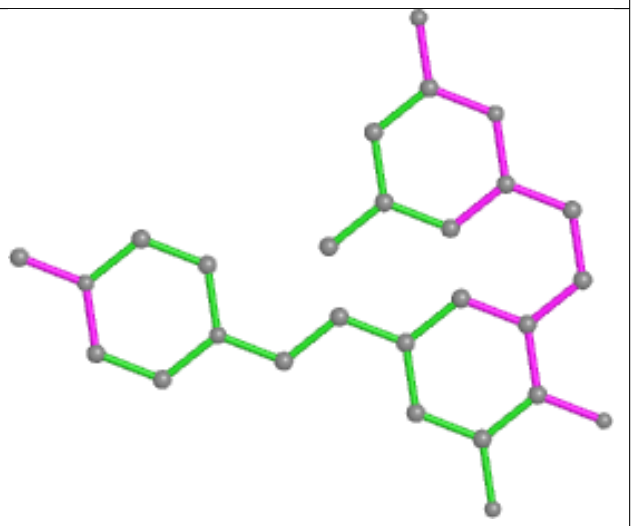
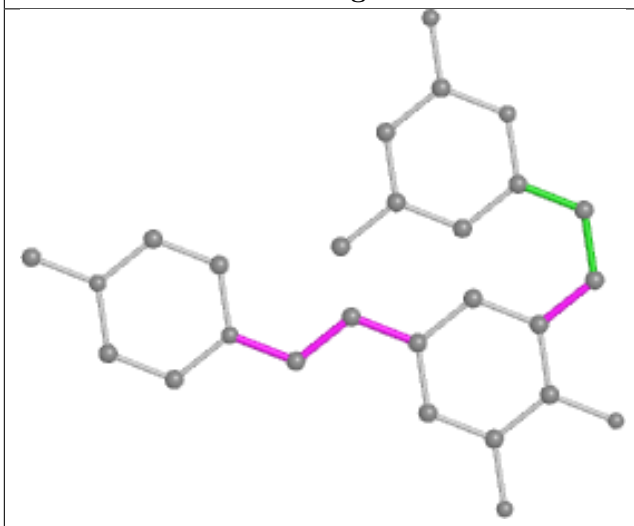
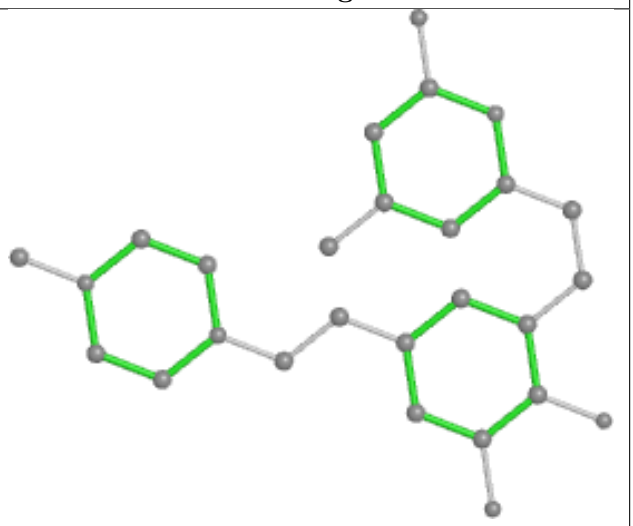


Bond angles

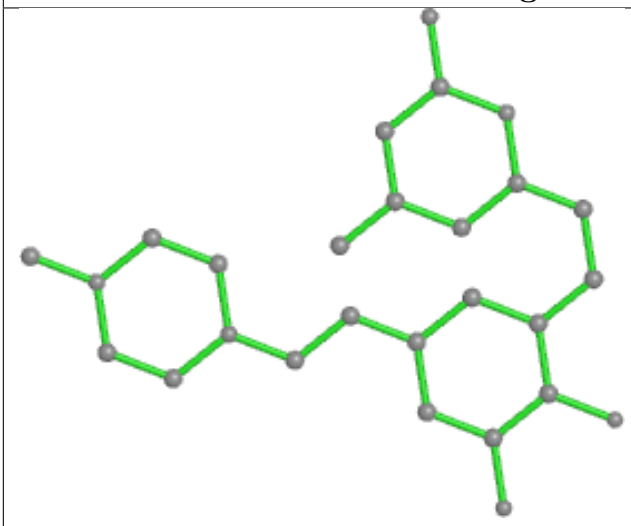


Torsions



Rings

Ligand XVK A 803



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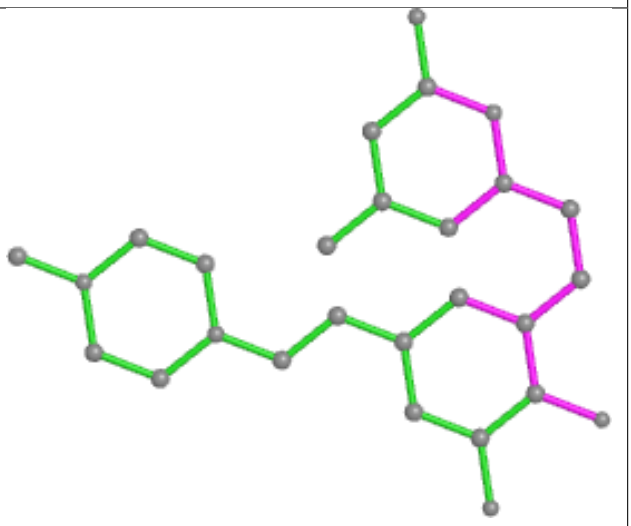

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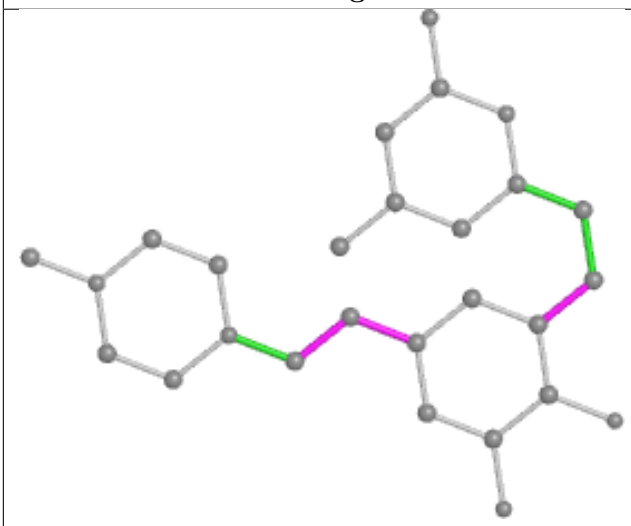

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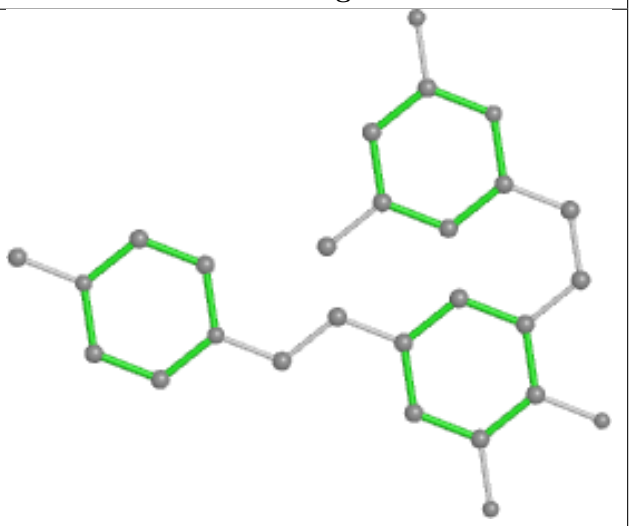

Rings

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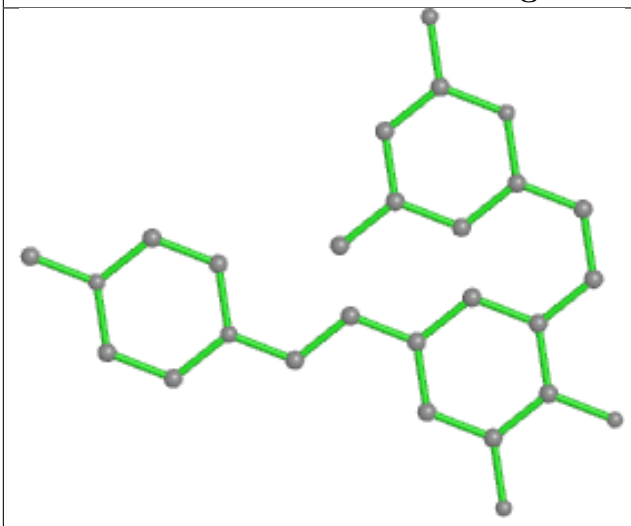

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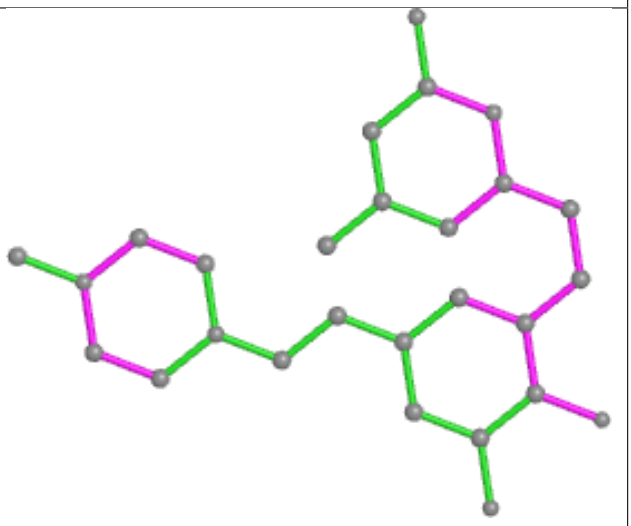

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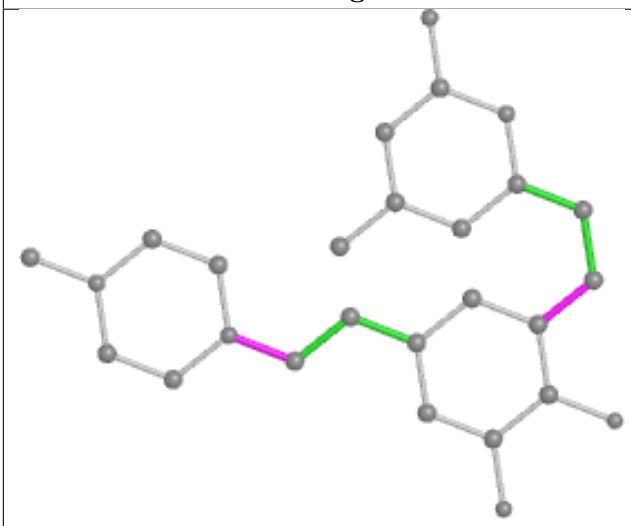

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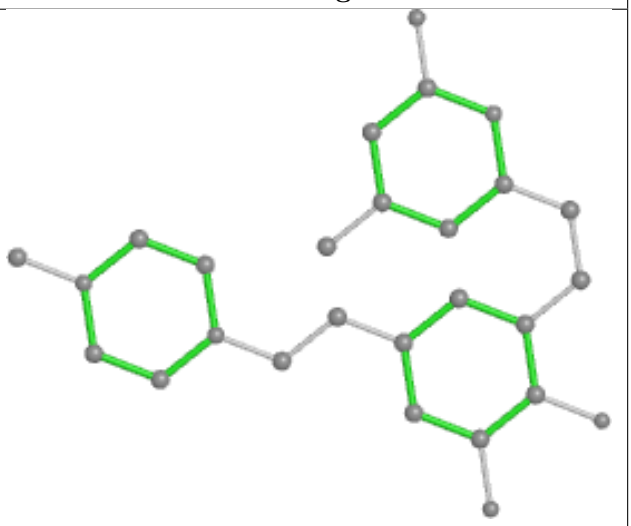
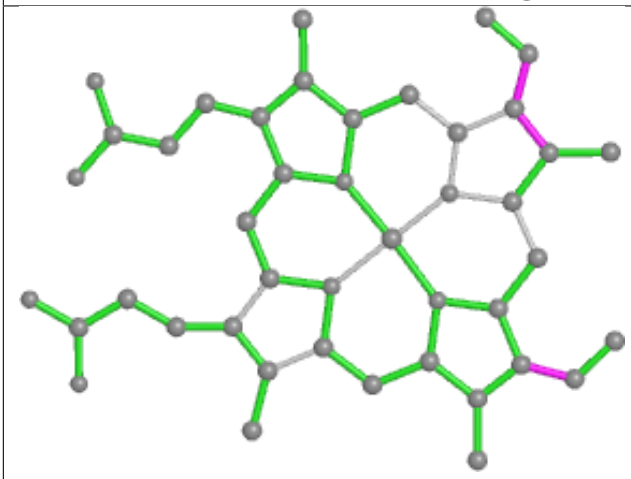


Rings

Ligand HEM A 801



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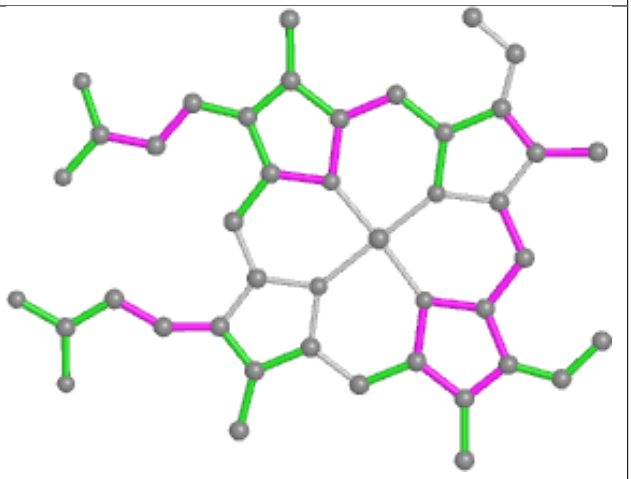

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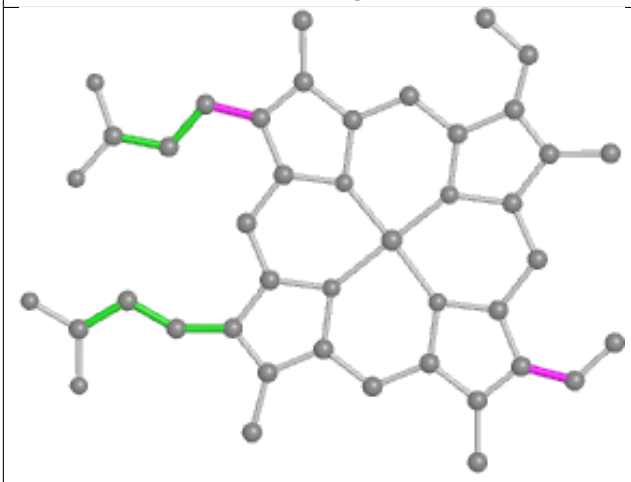

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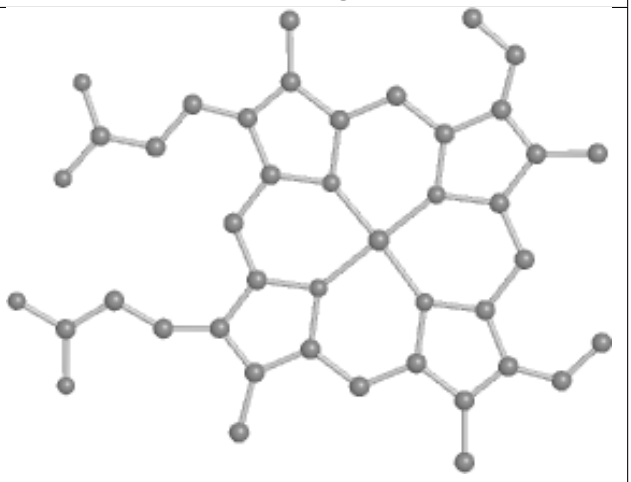

Rings

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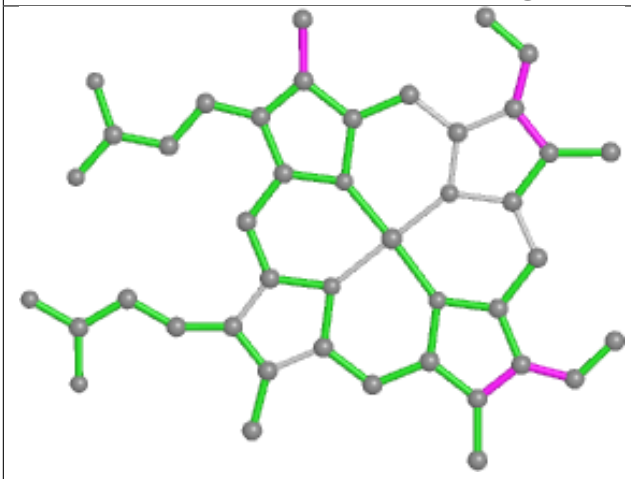

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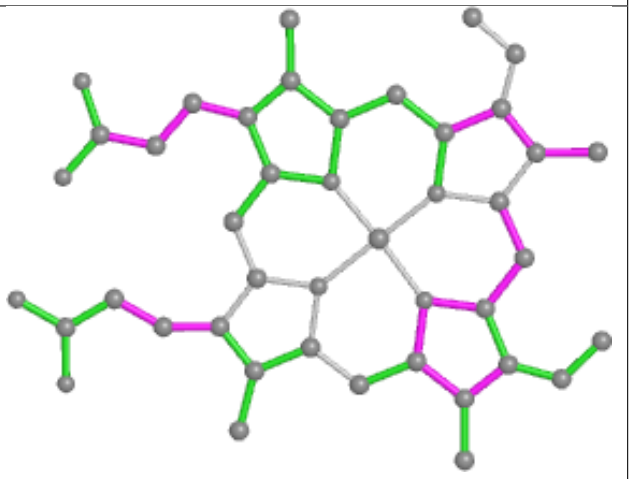

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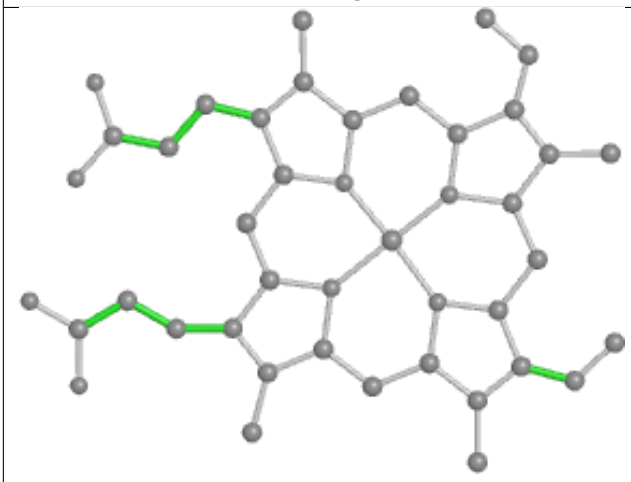

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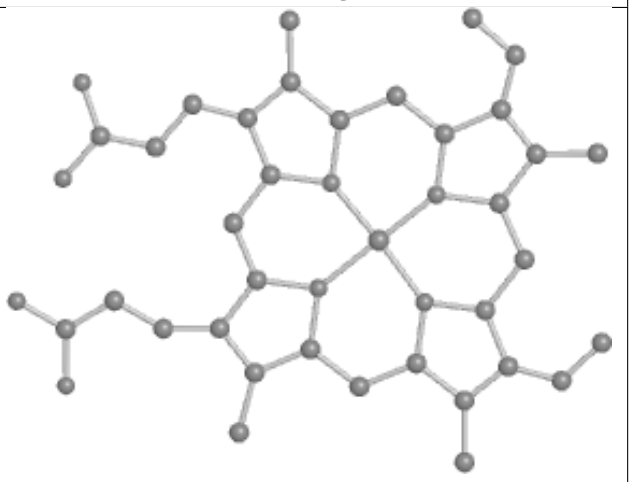

Rings

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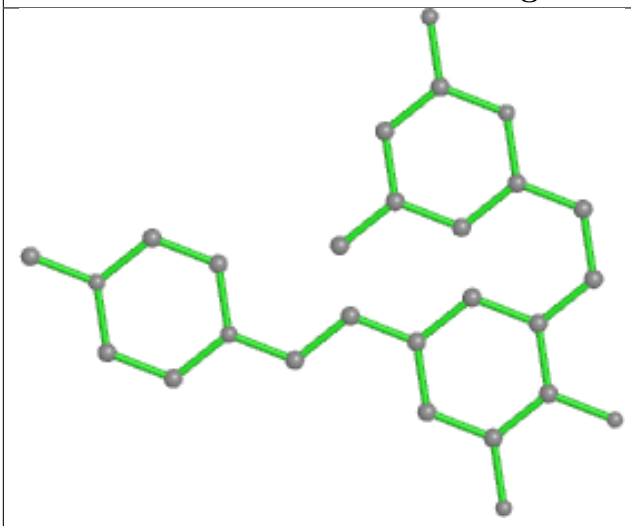

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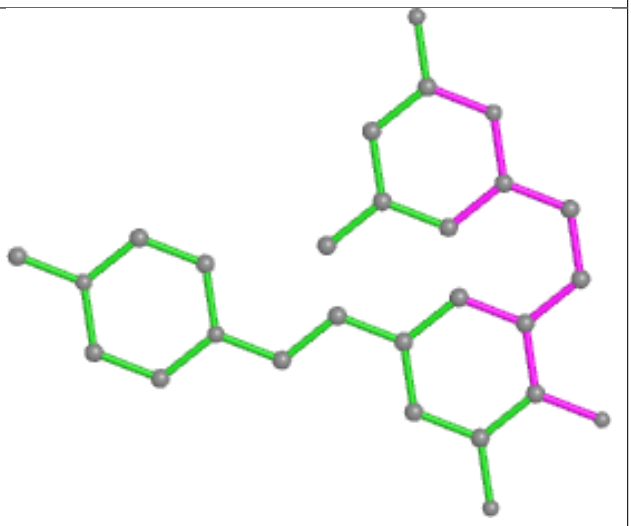

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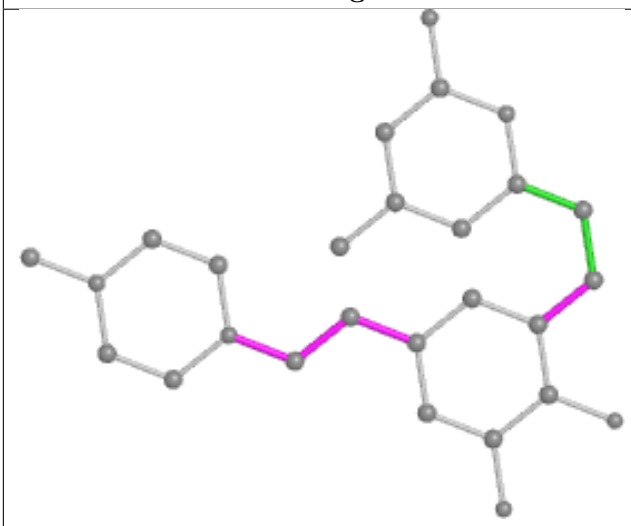

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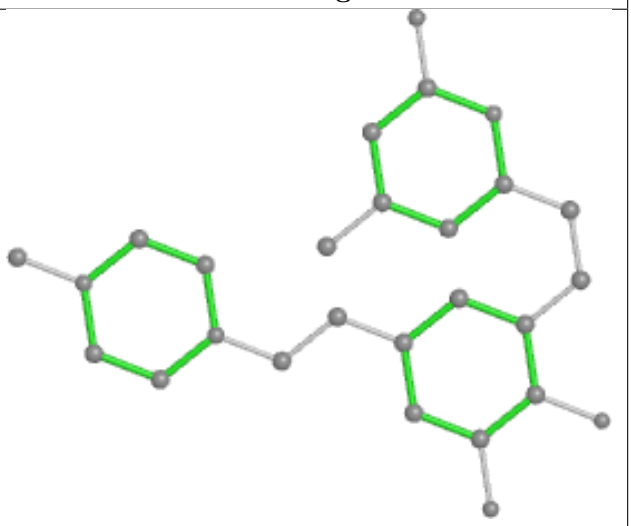

Rings

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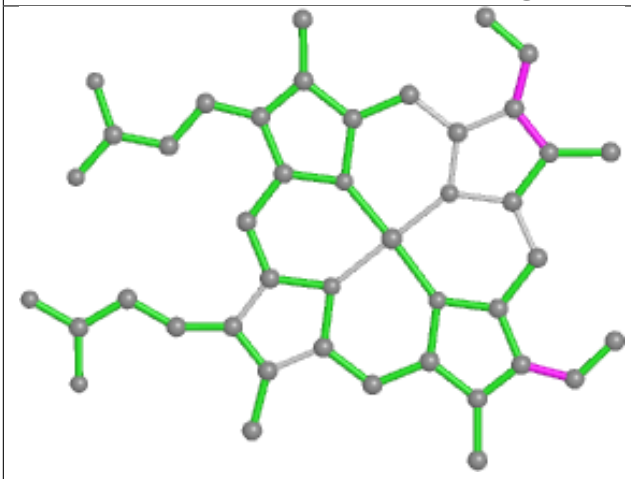

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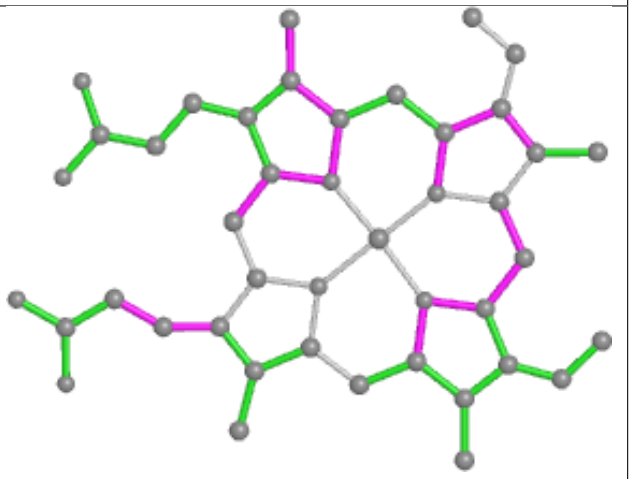

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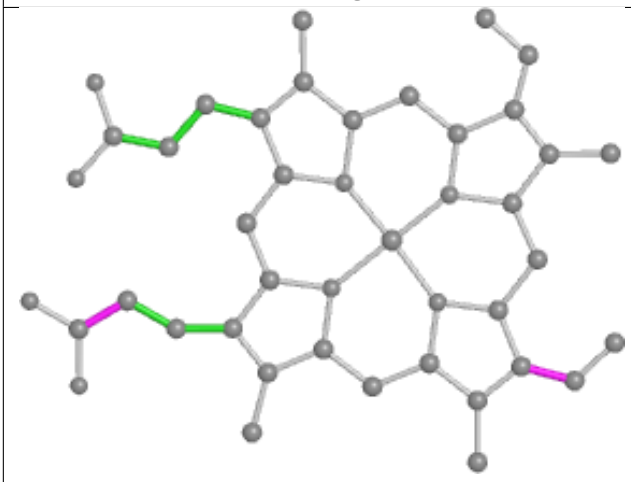
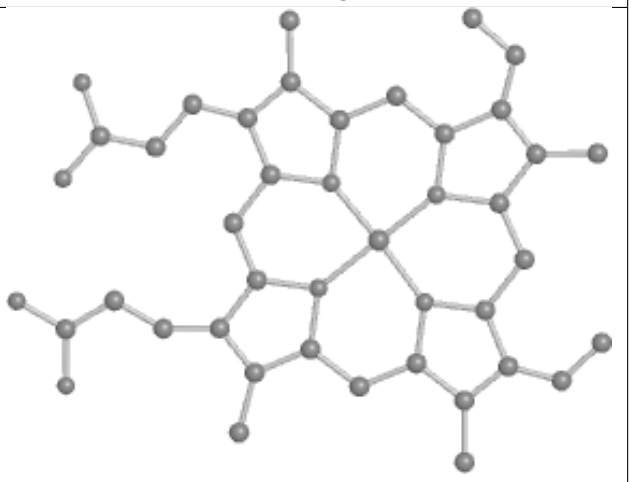
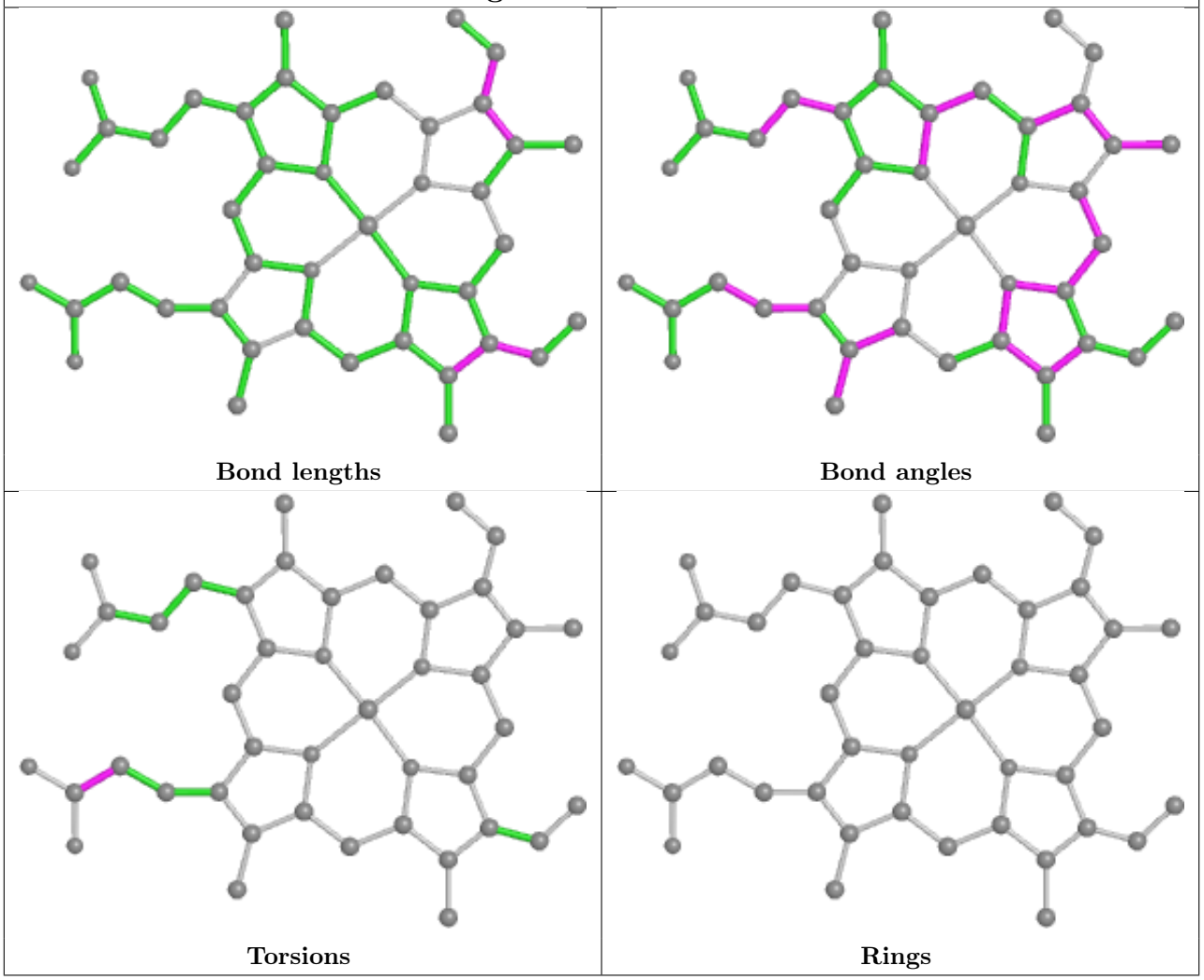


Torsions



Rings

Ligand HEM C 801



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	411/421 (97%)	0.15	16 (3%)	39	45	36, 58, 107, 156	0
1	B	414/421 (98%)	-0.06	6 (1%)	75	78	31, 50, 83, 138	0
1	C	414/421 (98%)	-0.06	3 (0%)	87	89	31, 50, 82, 142	0
1	D	411/421 (97%)	0.09	9 (2%)	62	66	35, 59, 106, 143	0
All	All	1650/1684 (97%)	0.03	34 (2%)	63	68	31, 54, 100, 156	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	353	VAL	7.0
1	D	304	ARG	3.9
1	A	302	CYS	3.7
1	D	393	ILE	3.7
1	A	360	PHE	3.4
1	B	305	PHE	3.3
1	A	327	LEU	3.3
1	B	351	GLU	3.1
1	A	304	ARG	3.1
1	B	360	PHE	3.1
1	C	350	PRO	3.0
1	A	359	LEU	2.9
1	B	350	PRO	2.8
1	A	367	ILE	2.6
1	A	371	TYR	2.6
1	A	376	ARG	2.5
1	A	303	PRO	2.5
1	A	498	LEU	2.5
1	D	356	LYS	2.5
1	C	327	LEU	2.4
1	A	379	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	356	LYS	2.3
1	D	367	ILE	2.3
1	A	305	PHE	2.2
1	D	375	LYS	2.2
1	B	352	ASP	2.2
1	C	305	PHE	2.2
1	D	359	LEU	2.2
1	D	305	PHE	2.1
1	D	391	LYS	2.1
1	B	327	LEU	2.1
1	A	557	GLU	2.1
1	A	491	LYS	2.1
1	A	721	TRP	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, 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
5	GOL	A	805	6/6	0.77	0.24	69,76,84,93	0
5	GOL	A	804	6/6	0.81	0.18	62,69,72,73	0
5	GOL	D	804	6/6	0.82	0.20	70,75,82,82	0
5	GOL	C	804	6/6	0.86	0.21	66,72,73,74	0
5	GOL	B	804	6/6	0.89	0.14	59,66,74,74	0
5	GOL	C	805	6/6	0.92	0.10	52,57,62,64	0
4	XVK	A	803	27/27	0.93	0.17	41,74,95,100	0
4	XVK	B	803	27/27	0.94	0.15	45,66,89,95	0
4	XVK	D	803	27/27	0.94	0.15	32,75,90,95	0
4	XVK	C	803	27/27	0.95	0.18	33,65,88,90	0

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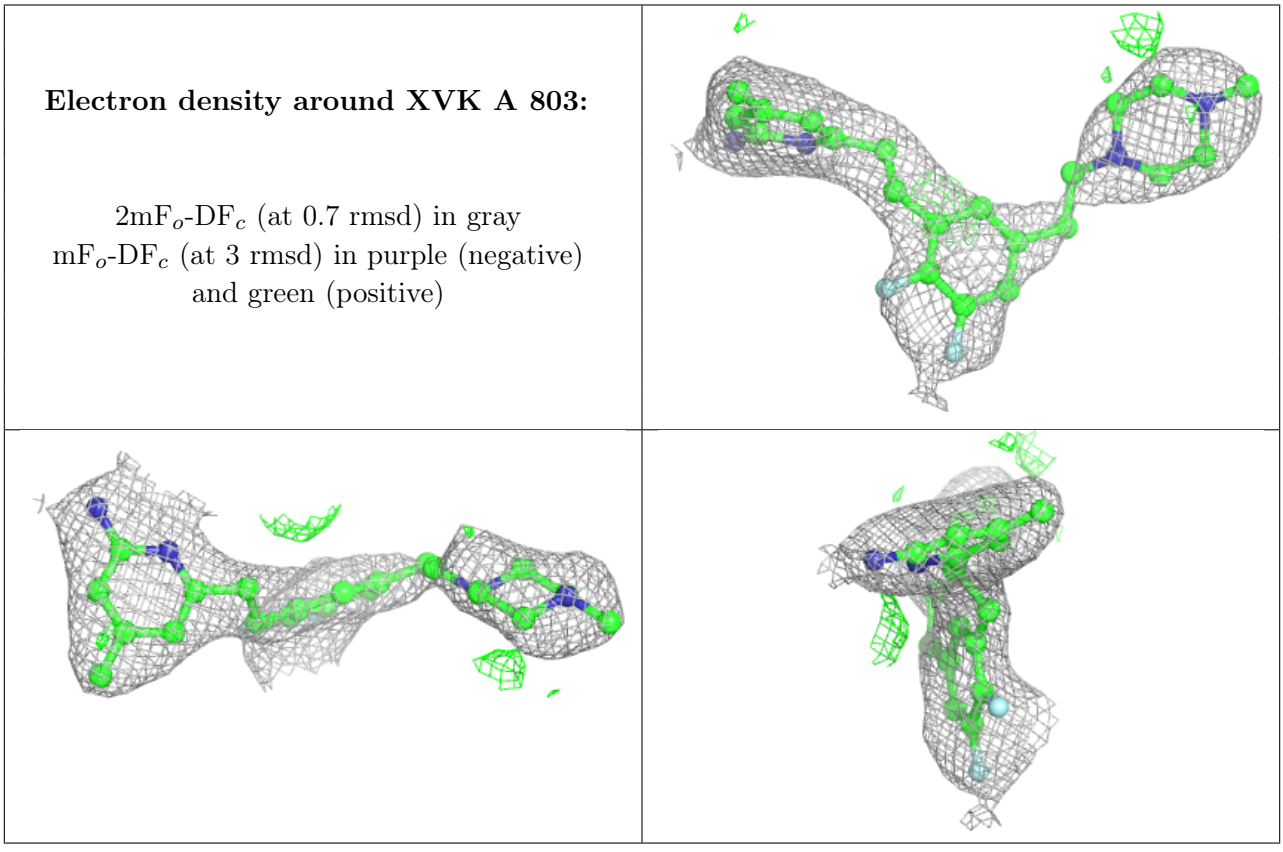
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	H4B	A	802	17/17	0.96	0.14	43,54,70,70	0
3	H4B	C	802	17/17	0.97	0.12	36,47,60,66	0
3	H4B	D	802	17/17	0.97	0.10	41,51,63,69	0
3	H4B	B	802	17/17	0.97	0.12	34,45,61,65	0
2	HEM	C	801	43/43	0.98	0.14	32,42,54,68	0
2	HEM	D	801	43/43	0.98	0.13	26,44,50,61	0
2	HEM	A	801	43/43	0.98	0.12	31,47,55,60	0
2	HEM	B	801	43/43	0.98	0.12	27,43,54,63	0
6	ZN	A	806	1/1	0.99	0.13	52,52,52,52	0
6	ZN	C	806	1/1	0.99	0.16	50,50,50,50	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.

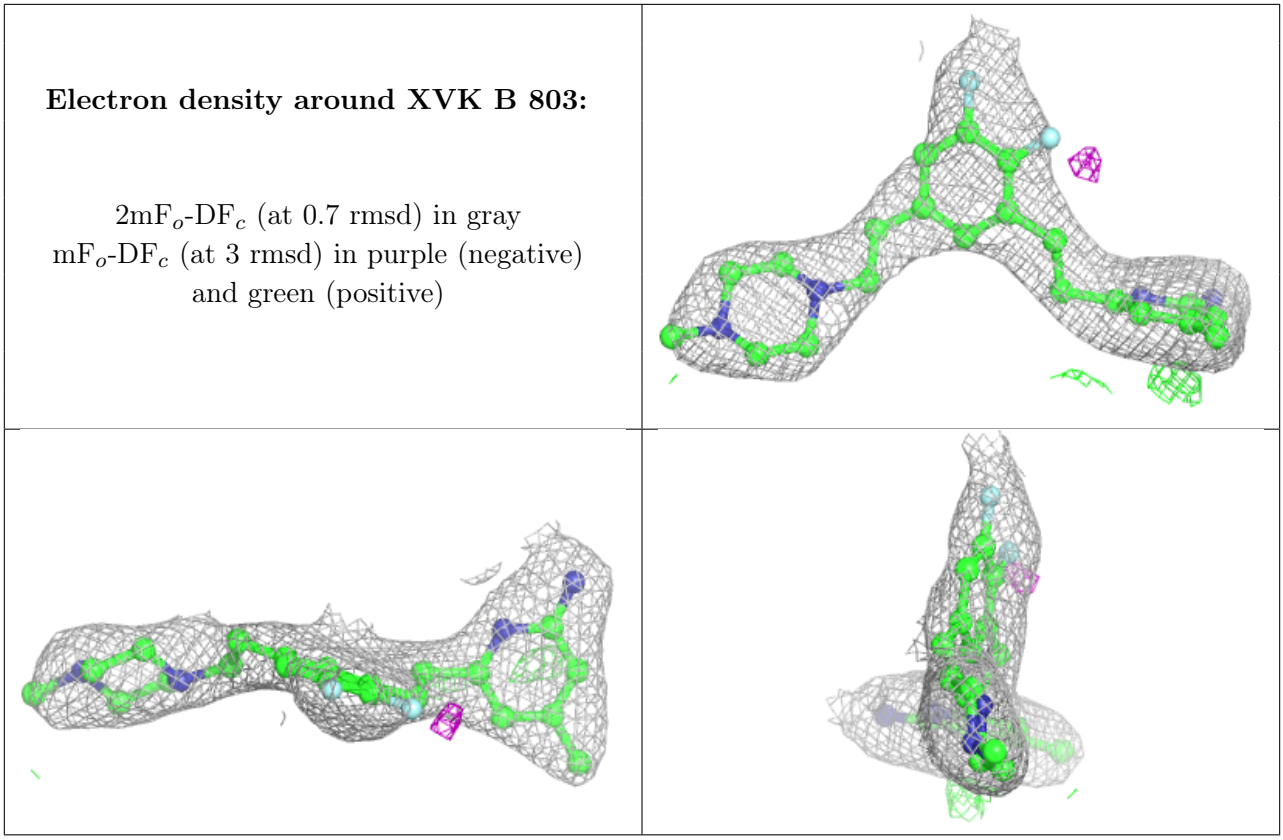
Electron density around XVK A 803:

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



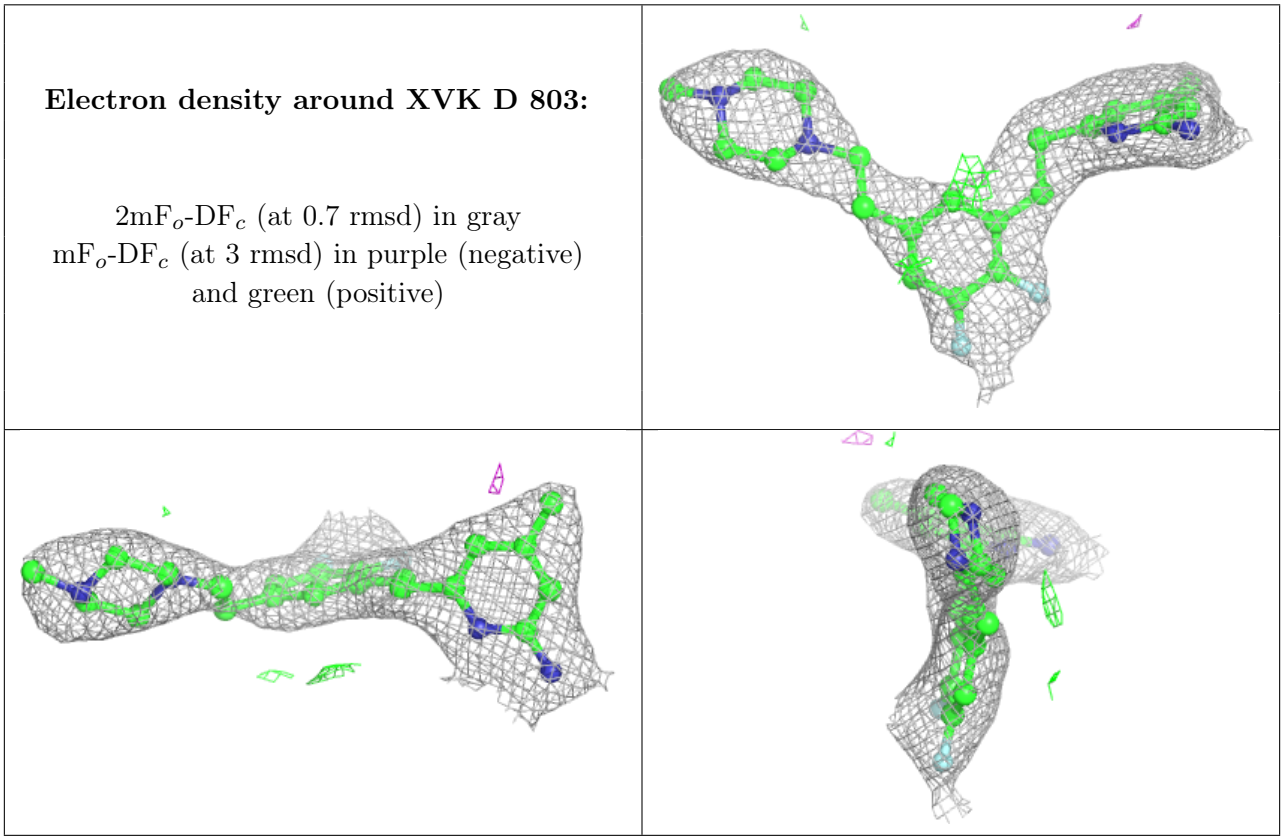
Electron density around XVK B 803:

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



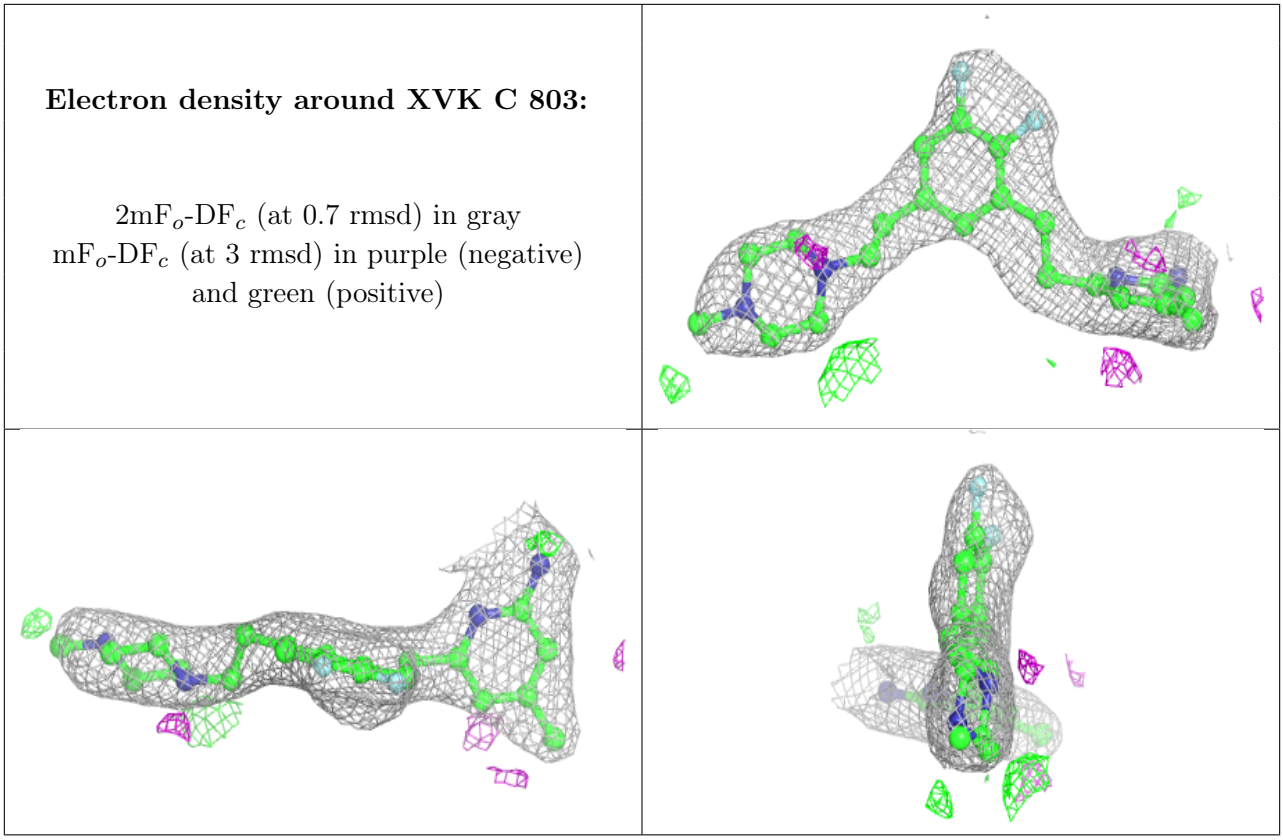
Electron density around XVK D 803:

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



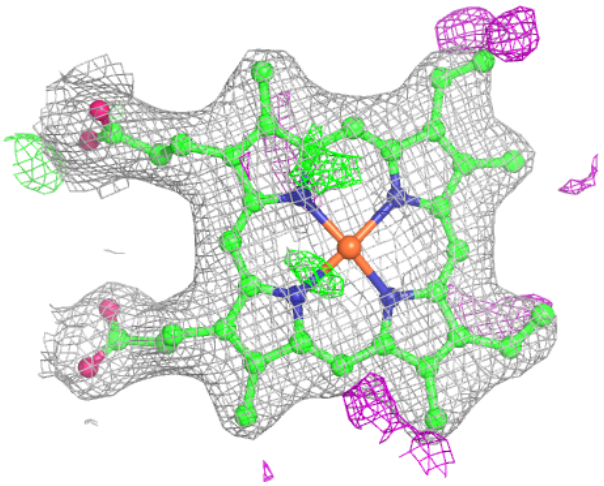
Electron density around XVK C 803:

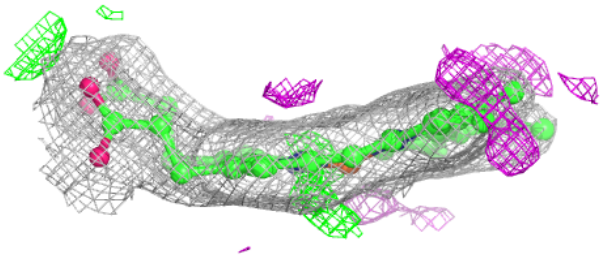
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

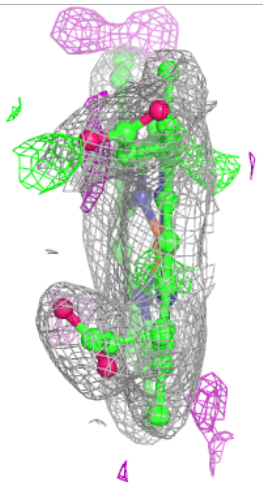


Electron density around HEM C 801:

$2mF_o$-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:

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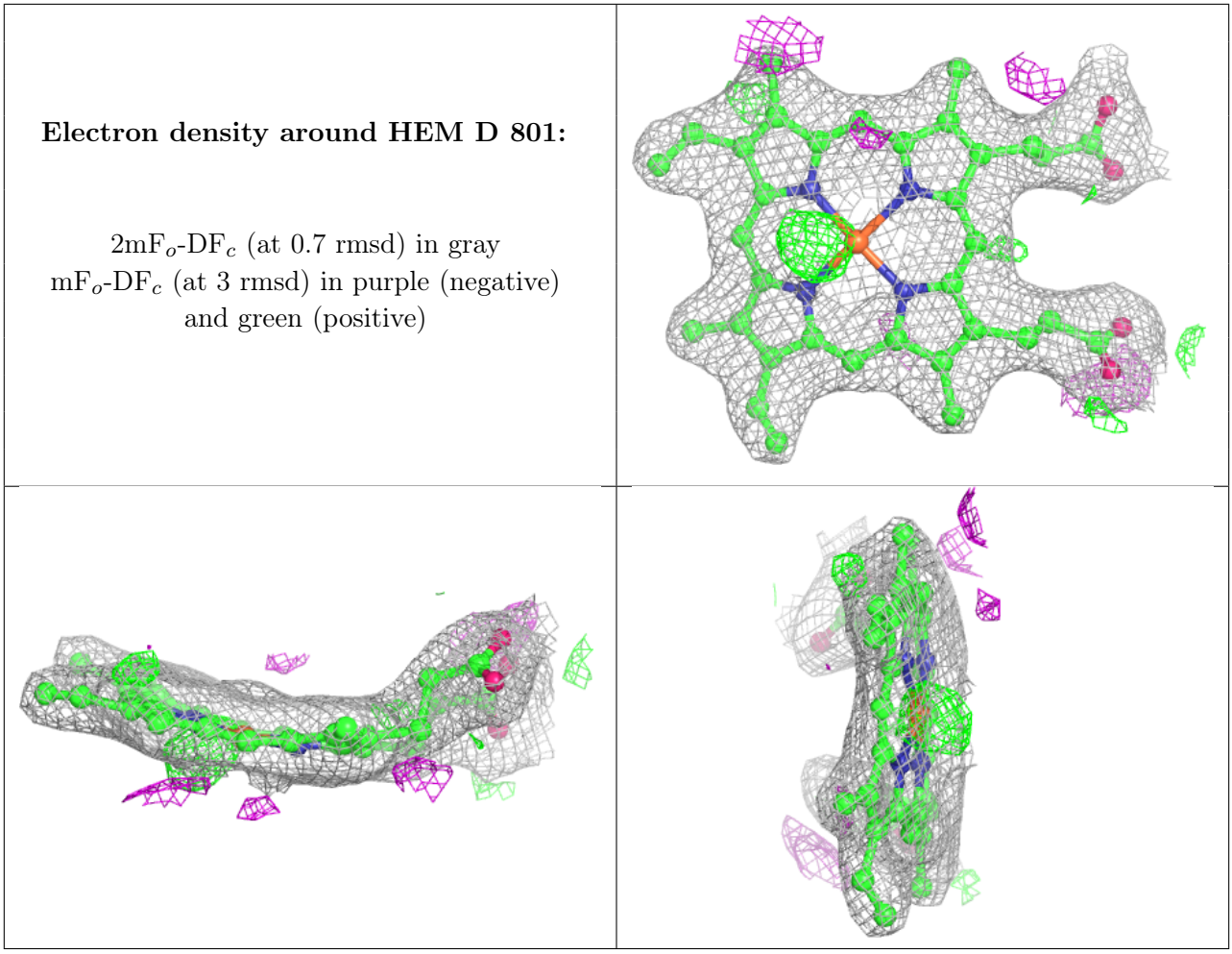
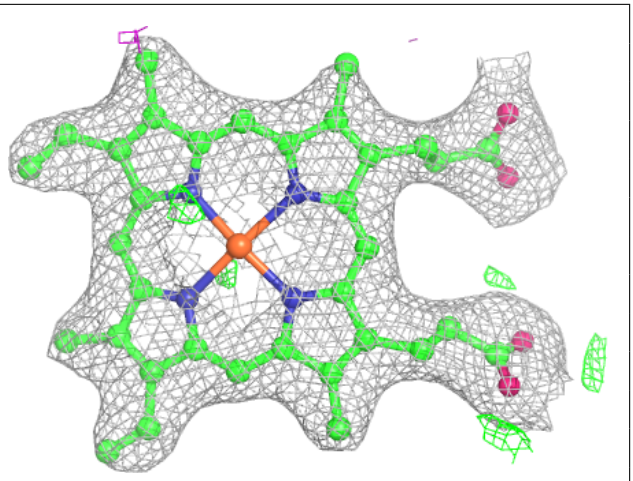
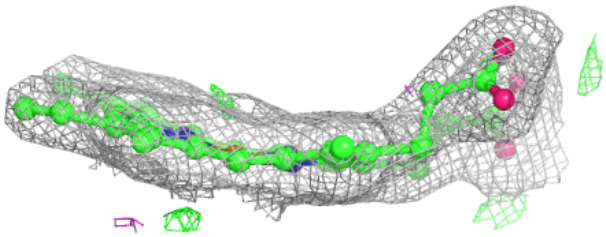
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

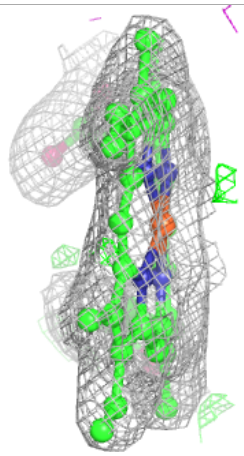


Electron density around HEM A 801:

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

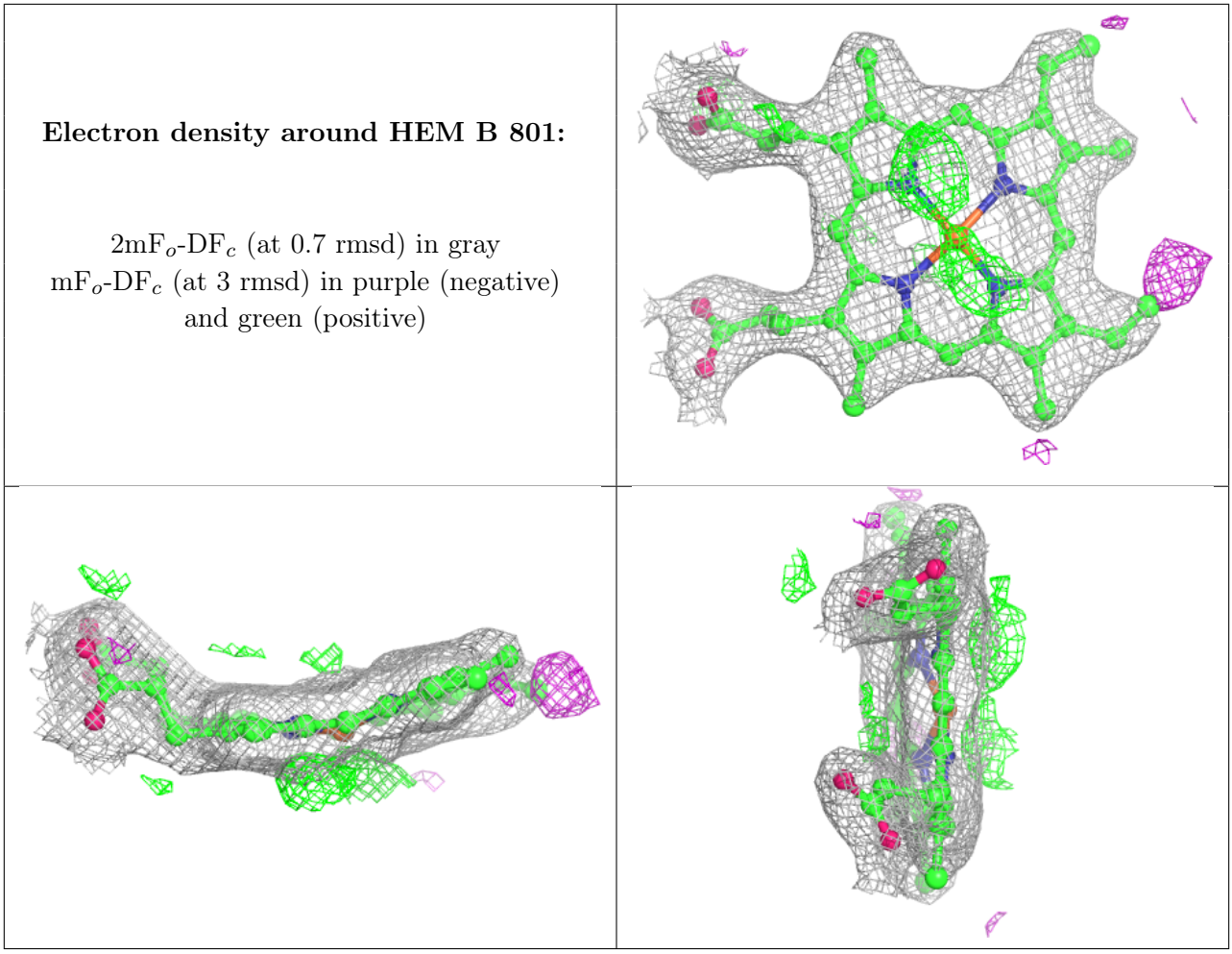






Electron density around HEM B 801:

$2mF_o$-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.