Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2023 – 02:25 AM EDT

PDB ID	:	7M56
Title	:	Structure of human endothelial nitric oxide synthase heme domain in complex with 7-((3-(3-aminophenethyl)phenoxy)methyl)quinolin-2-amine
Authors	:	Li, H.; Poulos, T.L.
Deposited on	:	2021-03-22
Resolution	:	1.96 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:

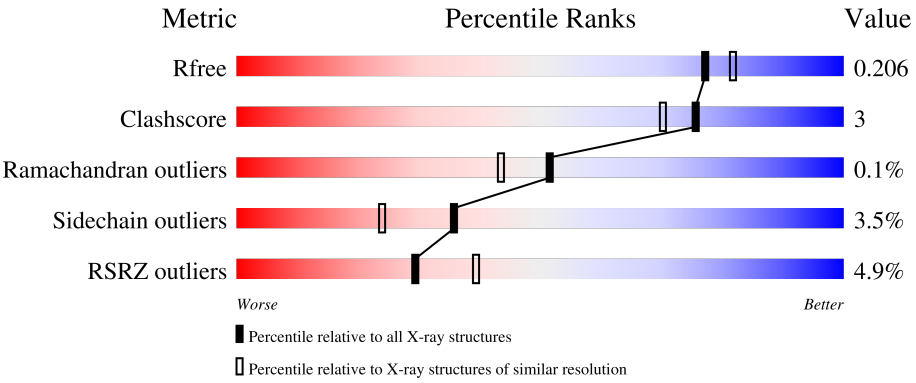
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 1.96 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	440	5% 82% 8% • 9%
1	B	440	4% 84% 7% 9%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 7263 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

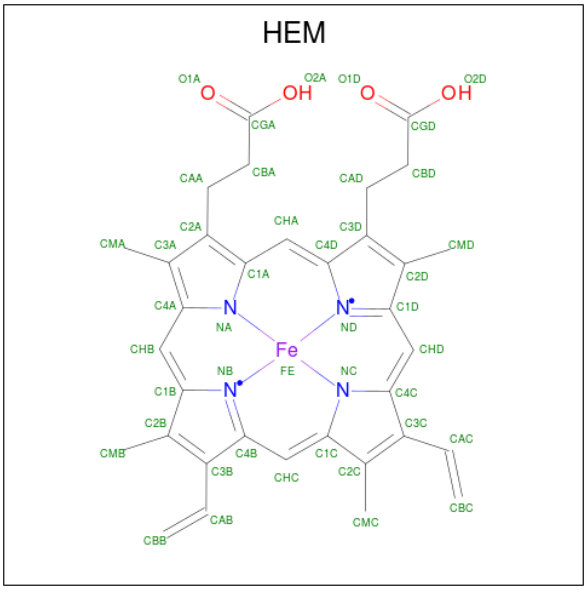
- Molecule 1 is a protein called Nitric oxide synthase, endothelial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	400	Total	C	N	O	S	0	3	0
			3206	2042	563	585	16			
1	B	402	Total	C	N	O	S	0	3	0
			3218	2050	565	587	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	298	GLU	ASP	variant	UNP P29474
B	298	GLU	ASP	variant	UNP P29474

- 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		

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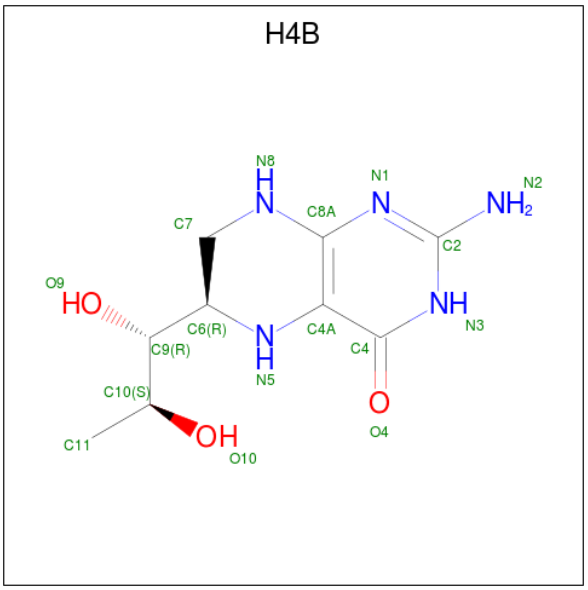
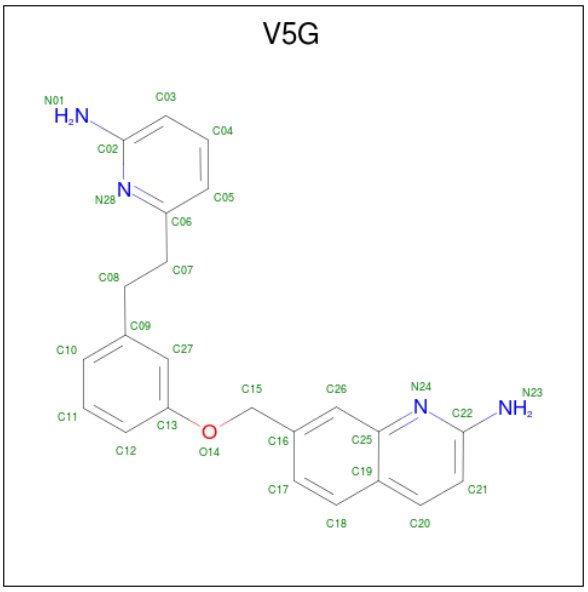
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



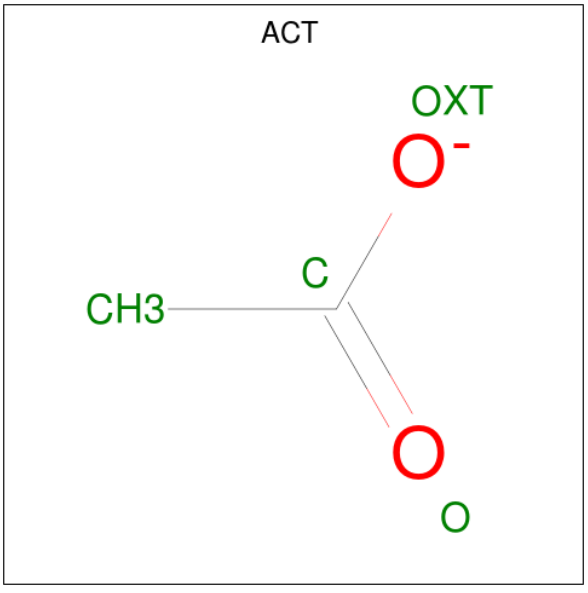
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O		0	0
			17	9	5	3			
3	B	1	Total	C	N	O		0	0
			17	9	5	3			

- Molecule 4 is 7-({3-[2-(6-aminopyridin-2-yl)ethyl]phenoxy}methyl)quinolin-2-amine (three-letter code: V5G) (formula: $C_{23}H_{22}N_4O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	28	23	4	1	0	0
			Total	C	N	O		
4	A	1	28	23	4	1	0	0
			Total	C	N	O		
4	B	1	28	23	4	1	0	0

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	4	2	2	0	0

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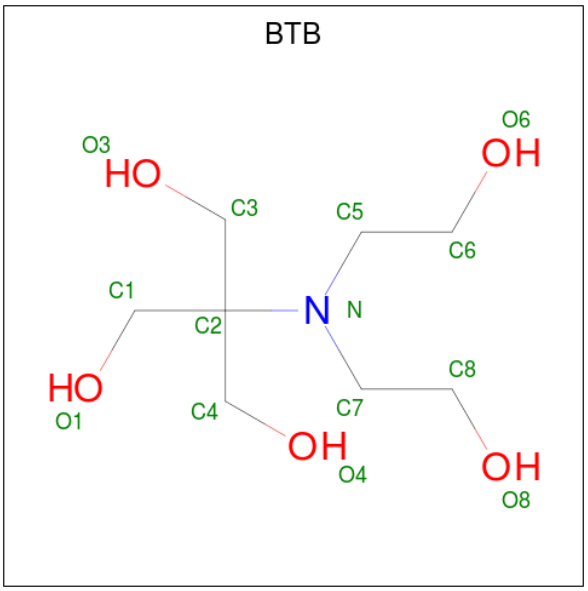
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0

- Molecule 6 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: BTB) (formula: $C_8H_{19}NO_5$).

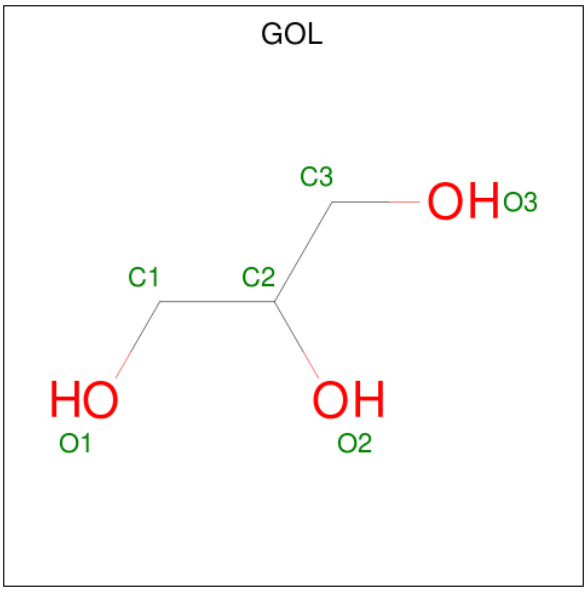


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N O 14 8 1 5	0	0
6	B	1	Total C N O 14 8 1 5	0	0

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 9 is GADOLINIUM ATOM (three-letter code: GD) (formula: Gd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total Gd 1 1	0	0

- Molecule 10 is water.

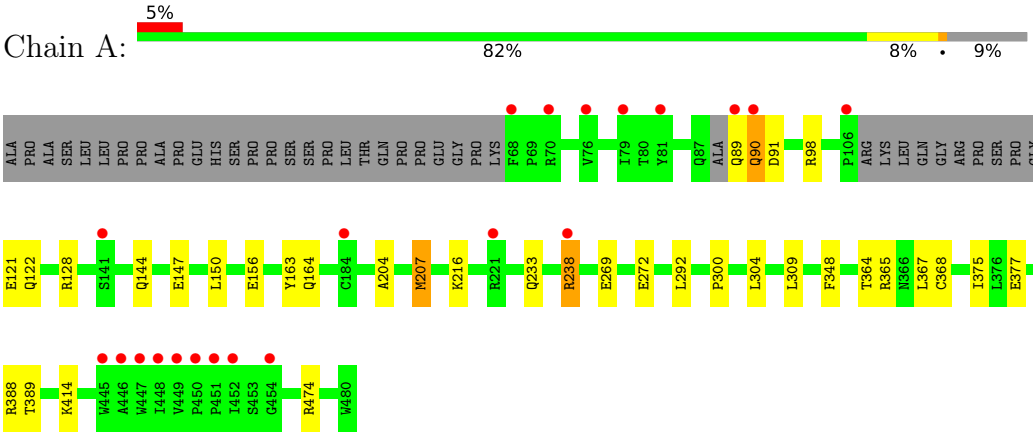
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	283	Total O 283 283	0	0
10	B	298	Total O 298 298	0	0

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.

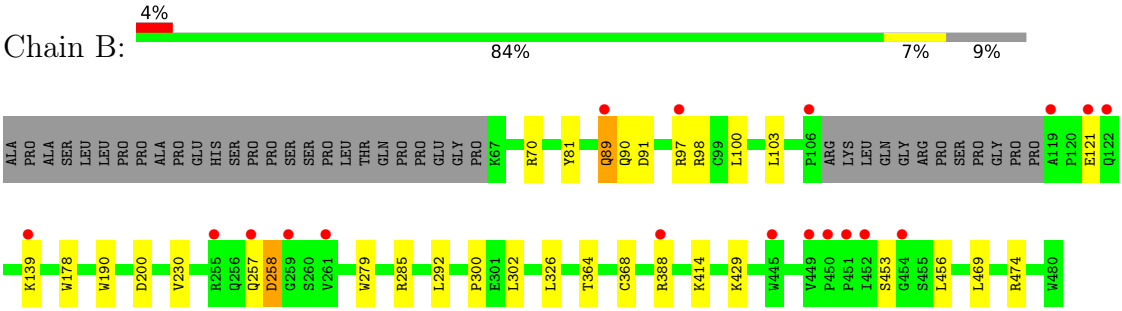
• Molecule 1: Nitric oxide synthase, endothelial

Chain A:



• Molecule 1: Nitric oxide synthase, endothelial

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	62.07Å 109.56Å 146.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.55 – 1.96 39.55 – 1.96	Depositor EDS
% Data completeness (in resolution range)	98.8 (39.55-1.96) 98.9 (39.55-1.96)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.00 (at 1.95Å)	Xtriage
Refinement program	PHENIX 1.11.1-2575_1496	Depositor
R, R_{free}	0.173 , 0.210 0.171 , 0.206	Depositor DCC
R_{free} test set	3541 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	30.4	Xtriage
Anisotropy	0.483	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 47.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	7263	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.29% 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: GOL, BTB, HEM, ACT, GD, V5G, ZN, H4B

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	0.36	0/3306	0.53	0/4504
1	B	0.38	0/3319	0.53	0/4522
All	All	0.37	0/6625	0.53	0/9026

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3206	0	3108	16	0
1	B	3218	0	3126	15	0
2	A	43	0	30	2	0
2	B	43	0	30	2	0
3	A	17	0	15	1	0
3	B	17	0	15	0	0
4	A	56	0	0	1	0
4	B	28	0	0	0	0
5	A	8	0	6	0	0
5	B	4	0	3	0	0
6	A	14	0	19	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	14	0	15	1	0
7	A	1	0	0	0	0
8	A	12	0	16	0	0
9	B	1	0	0	0	0
10	A	283	0	0	3	0
10	B	298	0	0	4	0
All	All	7263	0	6383	40	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 3.

All (40) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:GLN:HE22	1:B:469:LEU:HA	1.41	0.86
2:A:501:HEM:HBB2	2:A:501:HEM:HHC	1.79	0.65
2:B:501:HEM:HHC	2:B:501:HEM:HBB2	1.82	0.61
2:A:501:HEM:HBD2	4:A:503:V5G:C11	2.32	0.59
1:B:70:ARG:HG3	1:B:81:TYR:CE2	2.38	0.59
6:A:507:BTB:O1	6:A:507:BTB:O3	2.21	0.59
1:A:128:ARG:HG3	1:A:150:LEU:HD22	1.85	0.58
1:B:279:TRP:HB2	1:B:302:LEU:HD21	1.84	0.58
1:A:292:LEU:HD22	1:A:300:PRO:HB2	1.87	0.57
1:A:386:ASP:OD2	1:A:388:ARG:HG2	2.05	0.57
1:A:204:ALA:HA	1:A:207:MET:HE3	1.86	0.56
1:B:285:ARG:NH1	10:B:605:HOH:O	2.34	0.56
1:A:90:GLN:HG3	1:A:91:ASP:H	1.74	0.53
1:A:474:ARG:HD3	10:A:601:HOH:O	2.09	0.52
1:B:89:GLN:NE2	1:B:469:LEU:HA	2.20	0.51
2:B:501:HEM:O1A	10:B:601:HOH:O	2.19	0.51
1:A:367:LEU:O	1:A:375:ILE:HG13	2.14	0.48
1:A:364:THR:O	1:A:368:CYS:HB2	2.15	0.47
1:B:453:SER:HB3	1:B:456:LEU:HD12	1.96	0.46
1:A:269:GLU:HB2	10:A:712:HOH:O	2.15	0.46
6:A:507:BTB:H11	6:A:507:BTB:H71	1.56	0.46
6:A:507:BTB:H52	6:A:507:BTB:H82	1.57	0.46
1:B:474:ARG:HD3	10:B:606:HOH:O	2.16	0.45
1:B:257:GLN:HG2	1:B:258:ASP:N	2.32	0.45
1:B:90:GLN:HG3	1:B:91:ASP:N	2.32	0.44
1:A:233:GLN:HB3	1:A:348:PHE:CE2	2.53	0.44
1:A:156:GLU:HG2	1:A:163:TYR:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:507:BTB:H31	6:A:507:BTB:H51	1.27	0.43
1:B:200:ASP:HB2	10:B:711:HOH:O	2.17	0.43
1:B:388:ARG:HE	1:B:388:ARG:HB2	1.60	0.43
1:B:100:LEU:HB3	1:B:103:LEU:HD22	2.00	0.42
1:A:238:ARG:NH1	10:A:618:HOH:O	2.52	0.42
6:B:505:BTB:H11	6:B:505:BTB:H72	1.87	0.42
1:A:377:GLU:OE1	6:A:507:BTB:H32	2.20	0.42
1:B:178:TRP:CE3	1:B:190:TRP:HA	2.55	0.41
1:A:216:LYS:HB2	1:A:309:LEU:HD11	2.02	0.41
1:B:292:LEU:HD22	1:B:300:PRO:HB2	2.03	0.41
1:A:377:GLU:OE2	6:A:507:BTB:H41	2.21	0.41
1:A:365:ARG:HH12	3:A:502:H4B:C4	2.34	0.40
1:B:364:THR:O	1:B:368:CYS:HB2	2.20	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	397/440 (90%)	392 (99%)	4 (1%)	1 (0%)	41 30
1	B	401/440 (91%)	392 (98%)	9 (2%)	0	100 100
All	All	798/880 (91%)	784 (98%)	13 (2%)	1 (0%)	51 43

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	238	ARG

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	343/373 (92%)	329 (96%)	14 (4%)	30	18
1	B	344/373 (92%)	334 (97%)	10 (3%)	42	31
All	All	687/746 (92%)	663 (96%)	24 (4%)	36	24

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	90	GLN
1	A	98	ARG
1	A	121	GLU
1	A	122	GLN
1	A	144	GLN
1	A	147	GLU
1	A	164	GLN
1	A	207	MET
1	A	272	GLU
1	A	304	LEU
1	A	381	VAL
1	A	389	THR
1	A	414	LYS
1	B	89	GLN
1	B	97	ARG
1	B	98	ARG
1	B	121	GLU
1	B	139	LYS
1	B	230	VAL
1	B	258	ASP
1	B	326	LEU
1	B	414	LYS
1	B	429	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	89	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides 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	$\#\|Z\| > 2$
3	H4B	B	502	-	16,18,18	0.89	0	11,26,26	2.63	6 (54%)
4	V5G	A	503	-	31,31,31	0.79	0	41,42,42	1.38	4 (9%)
6	BTB	B	505	9	13,13,13	0.60	0	7,16,16	0.83	0
8	GOL	A	509	-	5,5,5	0.42	0	5,5,5	0.60	0
5	ACT	A	505	-	3,3,3	0.75	0	3,3,3	0.79	0
8	GOL	A	510	-	5,5,5	0.35	0	5,5,5	0.55	0
2	HEM	B	501	1	41,50,50	1.72	8 (19%)	45,82,82	2.36	13 (28%)
4	V5G	A	504	-	31,31,31	0.82	1 (3%)	41,42,42	1.28	7 (17%)
3	H4B	A	502	-	16,18,18	0.91	0	11,26,26	2.76	7 (63%)
6	BTB	A	507	-	13,13,13	0.42	0	7,16,16	0.50	0
5	ACT	B	504	-	3,3,3	0.78	0	3,3,3	0.74	0
2	HEM	A	501	1	41,50,50	1.51	7 (17%)	45,82,82	1.47	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	ACT	A	506	-	3,3,3	0.78	0	3,3,3	0.65	0
4	V5G	B	503	-	31,31,31	0.77	0	41,42,42	1.24	5 (12%)

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
3	H4B	B	502	-	-	3/8/17/17	0/2/2/2
4	V5G	A	503	-	-	1/10/10/10	0/4/4/4
6	BTB	B	505	9	-	3/21/21/21	-
8	GOL	A	509	-	-	0/4/4/4	-
8	GOL	A	510	-	-	2/4/4/4	-
2	HEM	B	501	1	-	3/12/54/54	-
4	V5G	A	504	-	-	2/10/10/10	0/4/4/4
3	H4B	A	502	-	-	3/8/17/17	0/2/2/2
2	HEM	A	501	1	-	3/12/54/54	-
6	BTB	A	507	-	-	14/21/21/21	-
4	V5G	B	503	-	-	1/10/10/10	0/4/4/4

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	HEM	FE-NB	4.44	2.18	1.96
2	B	501	HEM	FE-ND	3.78	2.15	1.96
2	B	501	HEM	C3C-CAC	3.72	1.55	1.47
2	A	501	HEM	C3C-CAC	3.64	1.55	1.47
2	B	501	HEM	C3C-C2C	-3.45	1.35	1.40
2	A	501	HEM	C3C-C2C	-3.30	1.35	1.40
2	A	501	HEM	CAB-C3B	3.21	1.56	1.47
2	B	501	HEM	CAB-C3B	2.77	1.55	1.47
2	B	501	HEM	C4D-ND	-2.43	1.36	1.40
4	A	504	V5G	C26-C25	-2.39	1.38	1.41
2	B	501	HEM	C1B-NB	-2.36	1.36	1.40
2	A	501	HEM	CAA-C2A	2.18	1.55	1.52
2	B	501	HEM	CMD-C2D	2.15	1.55	1.50
2	A	501	HEM	FE-NB	2.09	2.07	1.96
2	A	501	HEM	FE-ND	2.08	2.07	1.96
2	A	501	HEM	CMA-C3A	2.05	1.55	1.51

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	HEM	C1B-NB-C4B	6.28	111.56	105.07
4	A	503	V5G	C02-N28-C06	6.22	122.81	118.10
2	B	501	HEM	C4B-CHC-C1C	5.59	129.94	122.56
2	B	501	HEM	CBA-CAA-C2A	-5.55	103.14	112.62
2	B	501	HEM	C4D-ND-C1D	5.53	110.79	105.07
3	B	502	H4B	C8A-C4A-C4	4.67	118.72	114.57
3	A	502	H4B	C8A-C4A-C4	4.62	118.68	114.57
4	B	503	V5G	C02-N28-C06	4.44	121.47	118.10
2	B	501	HEM	C4C-CHD-C1D	4.43	128.41	122.56
2	B	501	HEM	C3D-C4D-ND	-4.07	105.63	110.17
3	A	502	H4B	N1-C2-N3	-3.86	119.36	125.42
3	A	502	H4B	C2-N3-C4	3.60	121.64	115.93
3	B	502	H4B	C4-C4A-N5	3.49	122.05	119.12
3	B	502	H4B	C2-N3-C4	3.49	121.47	115.93
2	A	501	HEM	C4B-CHC-C1C	3.47	127.14	122.56
2	A	501	HEM	CBA-CAA-C2A	-3.42	106.78	112.62
3	B	502	H4B	N1-C2-N3	-3.31	120.23	125.42
2	B	501	HEM	CHC-C4B-C3B	3.30	129.62	124.57
4	A	504	V5G	C02-N28-C06	3.26	120.57	118.10
2	B	501	HEM	C2B-C1B-NB	-3.22	106.02	109.84
3	A	502	H4B	C4-C4A-N5	3.12	121.74	119.12
2	A	501	HEM	C3B-C2B-C1B	2.98	108.69	106.49
2	B	501	HEM	C3B-C2B-C1B	2.91	108.64	106.49
4	A	504	V5G	C15-C16-C26	-2.80	115.08	121.22
3	A	502	H4B	C2-N1-C8A	2.79	120.79	114.54
2	A	501	HEM	C4D-ND-C1D	2.76	107.92	105.07
4	A	503	V5G	C15-O14-C13	2.60	124.07	117.65
4	B	503	V5G	C07-C06-N28	2.55	119.75	115.95
3	B	502	H4B	N2-C2-N3	2.53	121.19	117.25
3	A	502	H4B	N2-C2-N1	2.53	121.18	117.25
3	B	502	H4B	C2-N1-C8A	2.45	120.03	114.54
4	A	503	V5G	C05-C06-N28	-2.43	119.33	122.41
4	B	503	V5G	C07-C08-C09	-2.37	104.94	113.28
4	B	503	V5G	C05-C06-N28	-2.35	119.43	122.41
4	A	504	V5G	C07-C06-N28	2.24	119.28	115.95
4	A	503	V5G	C07-C08-C09	-2.22	105.47	113.28
2	B	501	HEM	CHA-C4D-C3D	2.22	129.49	125.33
2	B	501	HEM	C2D-C1D-ND	-2.18	107.28	109.88
4	B	503	V5G	C15-O14-C13	2.13	122.91	117.65
3	A	502	H4B	C4A-N5-C6	-2.09	115.47	121.16
2	B	501	HEM	C3C-C4C-NC	-2.09	107.00	110.94
2	B	501	HEM	CMC-C2C-C3C	2.08	128.58	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	504	V5G	O14-C15-C16	2.08	115.40	109.16
4	A	504	V5G	C07-C08-C09	-2.05	106.08	113.28
4	A	504	V5G	C21-C22-N24	-2.04	119.63	122.08
4	A	504	V5G	N01-C02-N28	2.00	119.65	116.49

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	H4B	C7-C6-C9-O9
3	A	502	H4B	C7-C6-C9-C10
3	B	502	H4B	C7-C6-C9-O9
3	B	502	H4B	C7-C6-C9-C10
6	A	507	BTB	O1-C1-C2-C3
6	A	507	BTB	O1-C1-C2-N
6	A	507	BTB	C1-C2-C3-O3
6	A	507	BTB	C4-C2-C3-O3
6	A	507	BTB	N-C2-C3-O3
6	A	507	BTB	C1-C2-N-C7
6	A	507	BTB	C3-C2-N-C5
6	A	507	BTB	C3-C2-N-C7
6	A	507	BTB	C4-C2-N-C5
6	A	507	BTB	C4-C2-N-C7
6	A	507	BTB	C8-C7-N-C5
6	B	505	BTB	O1-C1-C2-C4
6	B	505	BTB	O1-C1-C2-N
8	A	510	GOL	O1-C1-C2-C3
2	A	501	HEM	C4D-C3D-CAD-CBD
2	A	501	HEM	C4B-C3B-CAB-CBB
2	B	501	HEM	C4B-C3B-CAB-CBB
2	A	501	HEM	C2D-C3D-CAD-CBD
8	A	510	GOL	O1-C1-C2-O2
3	A	502	H4B	N5-C6-C9-O9
3	B	502	H4B	N5-C6-C9-O9
6	A	507	BTB	O1-C1-C2-C4
6	A	507	BTB	N-C5-C6-O6
6	A	507	BTB	C1-C2-N-C5
4	A	504	V5G	C07-C08-C09-C10
2	B	501	HEM	CAA-CBA-CGA-O2A
4	A	503	V5G	C06-C07-C08-C09
4	B	503	V5G	C06-C07-C08-C09
4	A	504	V5G	C07-C08-C09-C27

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Mol	Chain	Res	Type	Atoms
2	B	501	HEM	CAA-CBA-CGA-O1A
6	B	505	BTB	O1-C1-C2-C3

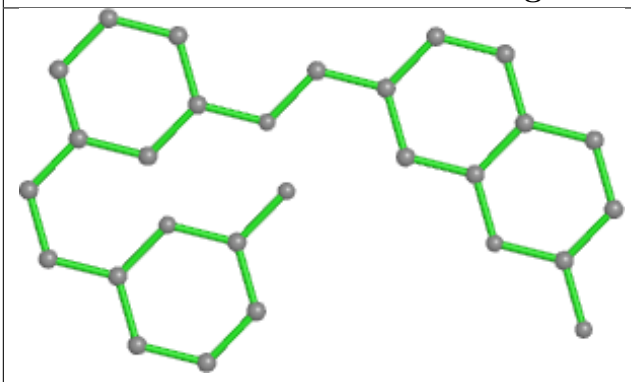
There are no ring outliers.

6 monomers are involved in 12 short contacts:

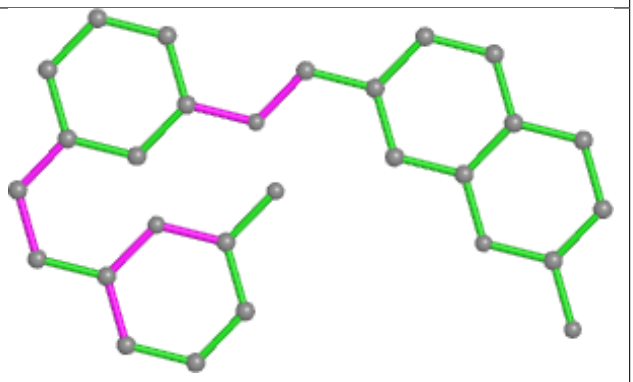
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	503	V5G	1	0
6	B	505	BTB	1	0
2	B	501	HEM	2	0
3	A	502	H4B	1	0
6	A	507	BTB	6	0
2	A	501	HEM	2	0

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.

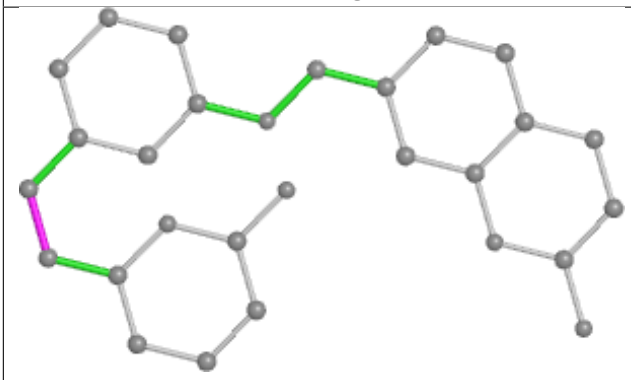
Ligand V5G A 503



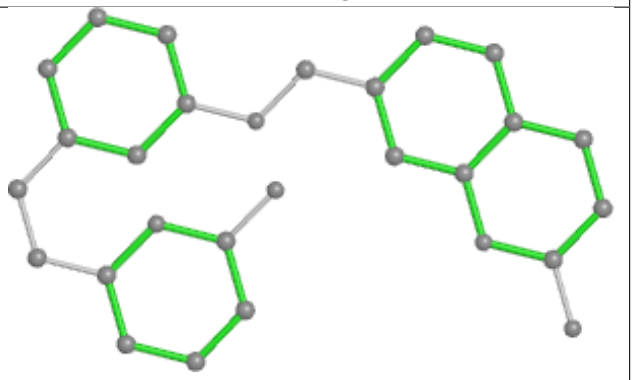
Bond lengths



Bond angles

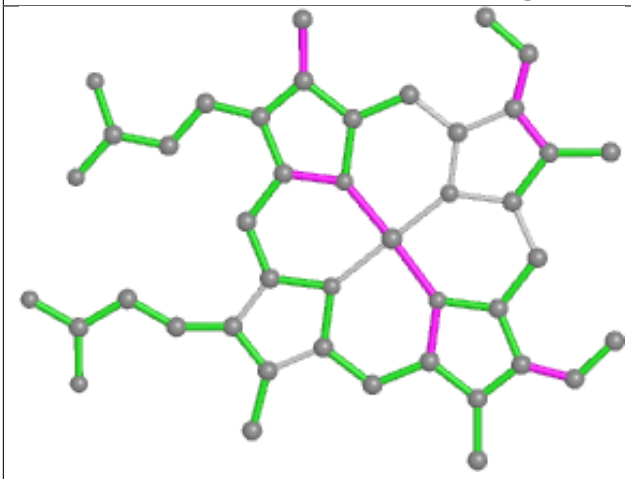


Torsions

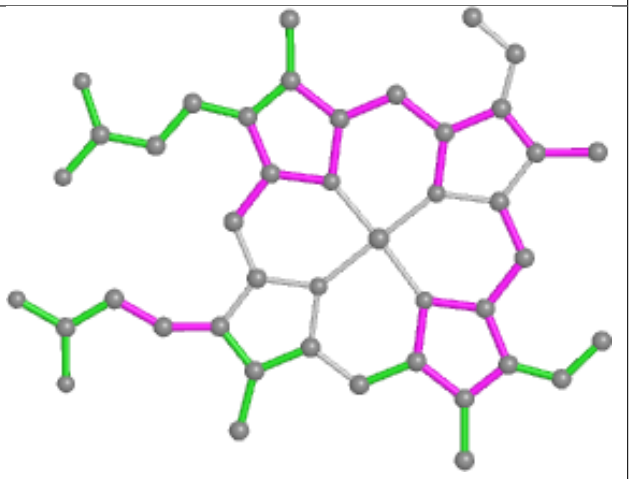


Rings

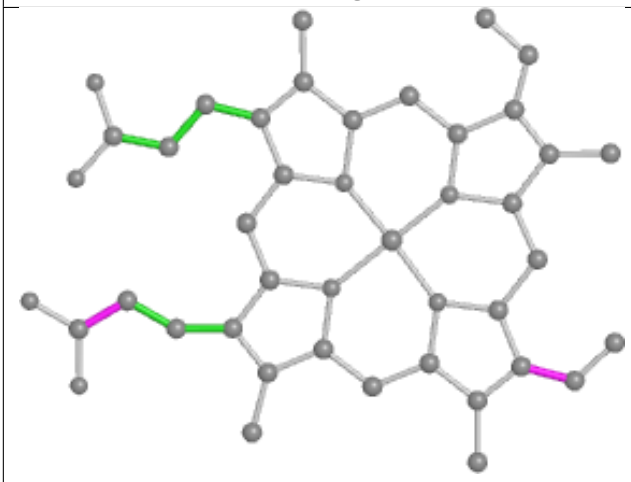
Ligand HEM B 501



Bond lengths



Bond angles



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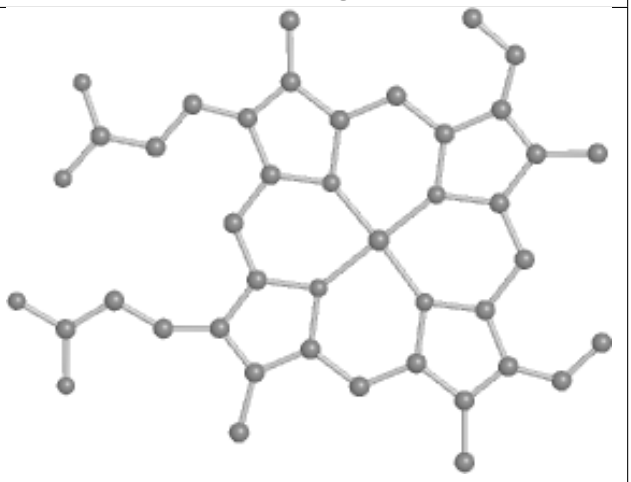
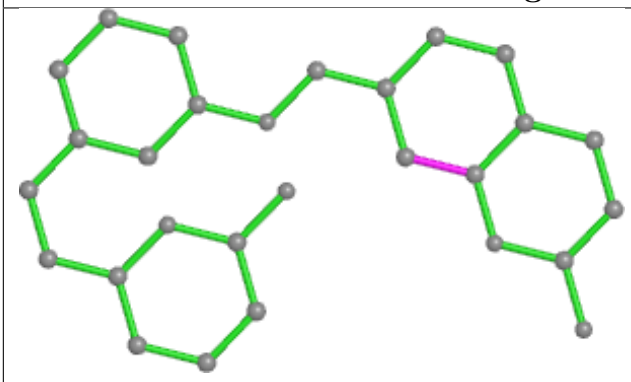
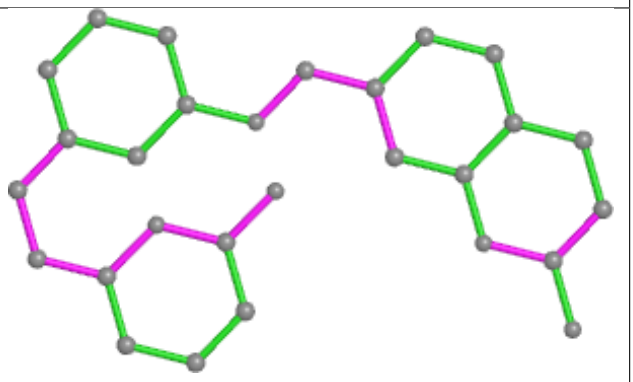


Rings

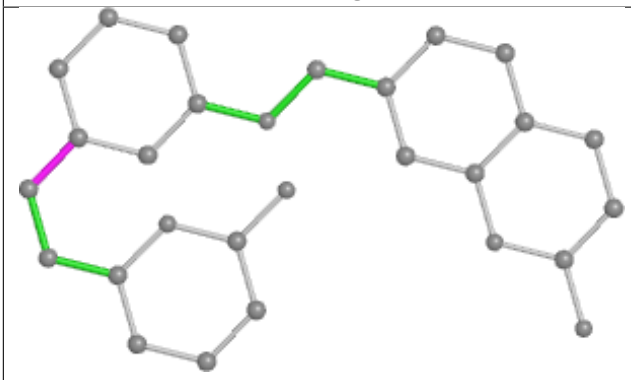
Ligand V5G A 504



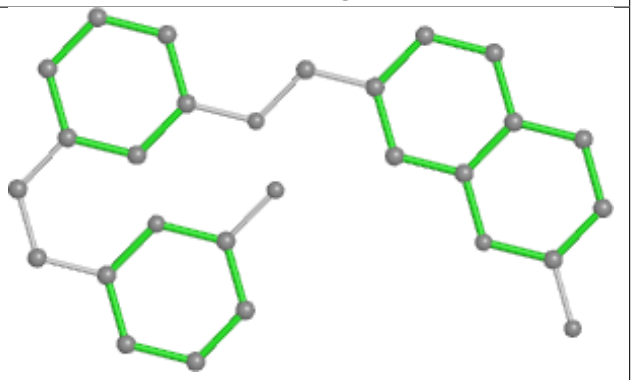
Bond lengths



Bond angles

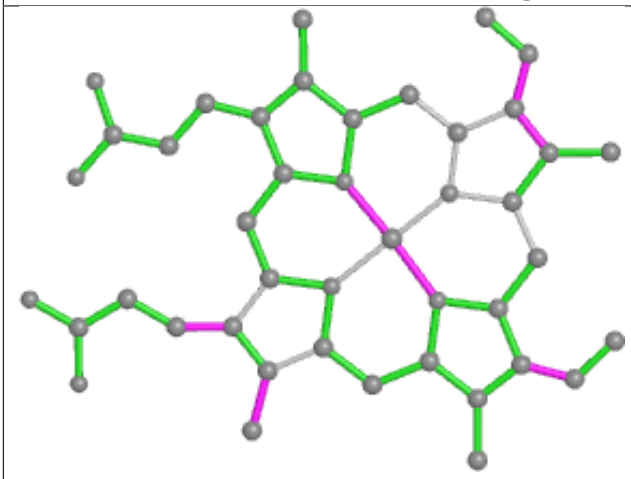


Torsions

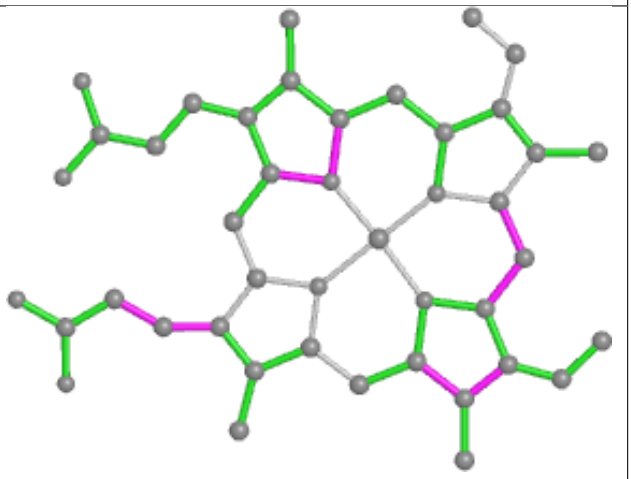


Rings

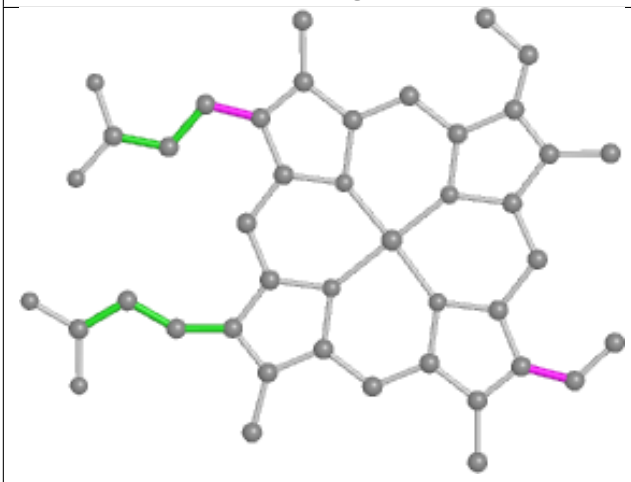
Ligand HEM A 501



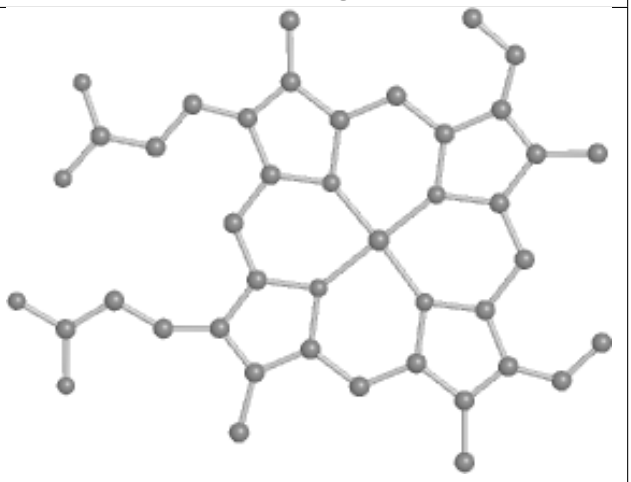
Bond lengths



Bond angles

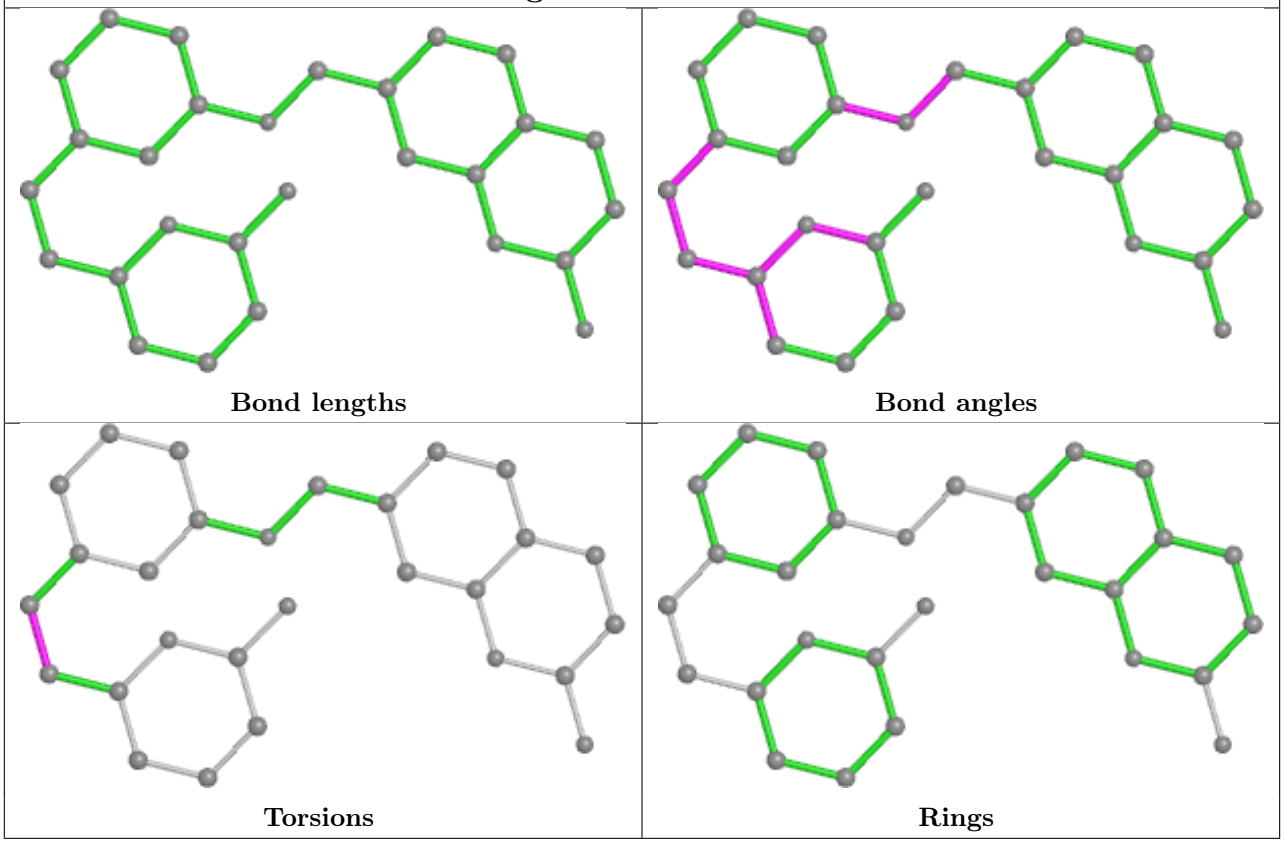


Torsions



Rings

Ligand V5G B 503



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	400/440 (90%)	0.10	21 (5%)	26	35	24, 34, 64, 96	0
1	B	402/440 (91%)	-0.02	18 (4%)	33	43	22, 33, 64, 98	0
All	All	802/880 (91%)	0.04	39 (4%)	29	39	22, 34, 64, 98	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	89	GLN	5.6
1	A	447	TRP	3.7
1	B	257	GLN	3.4
1	A	141	SER	3.3
1	A	449	VAL	3.3
1	A	448	ILE	3.3
1	A	68	PHE	3.2
1	B	122	GLN	3.2
1	B	255	ARG	2.8
1	B	452	ILE	2.7
1	A	451	PRO	2.7
1	A	106	PRO	2.7
1	A	90	GLN	2.7
1	B	89	GLN	2.6
1	B	449	VAL	2.6
1	B	388	ARG	2.6
1	A	452	ILE	2.6
1	A	446	ALA	2.5
1	B	445	TRP	2.5
1	B	106	PRO	2.5
1	A	184	CYS	2.5
1	A	238	ARG	2.5
1	B	119	ALA	2.5
1	B	450	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	79	ILE	2.4
1	A	76	VAL	2.4
1	B	451	PRO	2.4
1	A	450	PRO	2.3
1	A	445	TRP	2.3
1	A	454	GLY	2.2
1	B	121	GLU	2.2
1	B	261	VAL	2.2
1	B	454	GLY	2.2
1	A	81	TYR	2.1
1	A	70	ARG	2.1
1	A	221	ARG	2.1
1	B	139	LYS	2.1
1	B	259	GLY	2.0
1	B	97	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no 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	ACT	A	505	4/4	0.76	0.15	61,61,63,64	0
8	GOL	A	510	6/6	0.79	0.14	74,80,84,89	0
8	GOL	A	509	6/6	0.85	0.14	74,84,85,86	0
6	BTB	A	507	14/14	0.85	0.16	60,70,75,82	0
5	ACT	B	504	4/4	0.87	0.20	58,62,67,68	0
4	V5G	B	503	28/28	0.87	0.18	27,51,74,75	0
3	H4B	B	502	17/17	0.90	0.19	44,54,67,74	0
5	ACT	A	506	4/4	0.90	0.26	61,62,63,64	0

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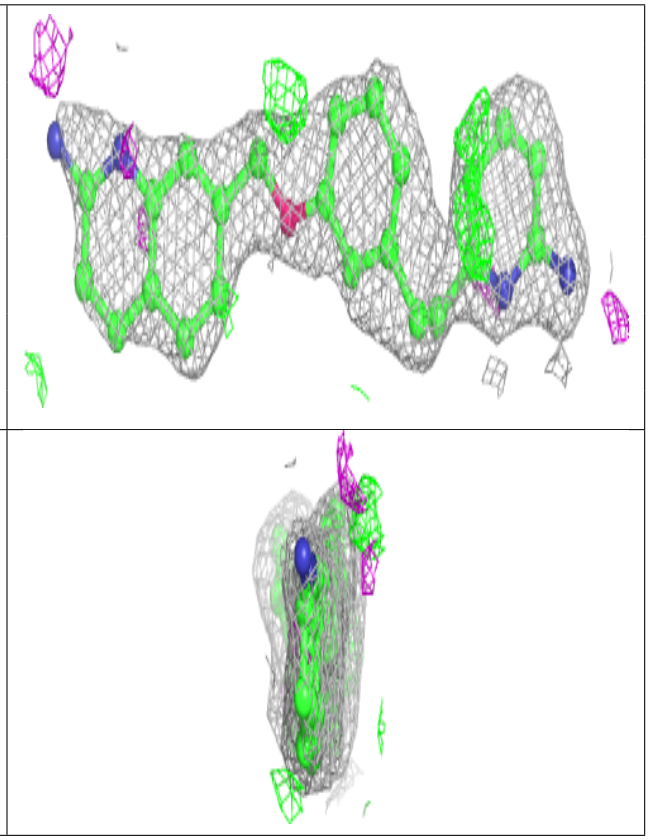
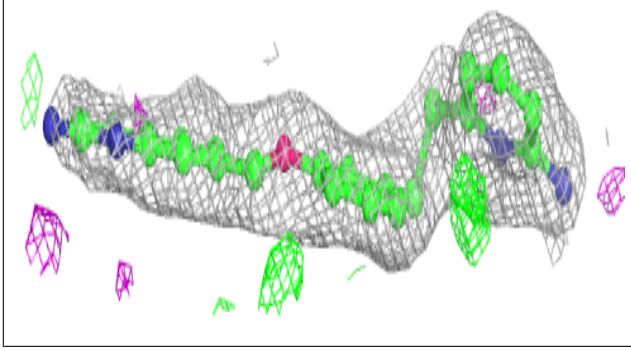
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	H4B	A	502	17/17	0.90	0.21	34,47,66,73	0
4	V5G	A	504	28/28	0.91	0.24	33,64,127,133	0
4	V5G	A	503	28/28	0.92	0.15	32,47,71,74	0
6	BTB	B	505	14/14	0.95	0.12	24,32,41,57	0
2	HEM	A	501	43/43	0.97	0.18	23,30,67,70	0
2	HEM	B	501	43/43	0.98	0.13	18,26,55,72	0
7	ZN	A	508	1/1	1.00	0.04	28,28,28,28	0
9	GD	B	506	1/1	1.00	0.09	29,29,29,29	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 V5G B 503:

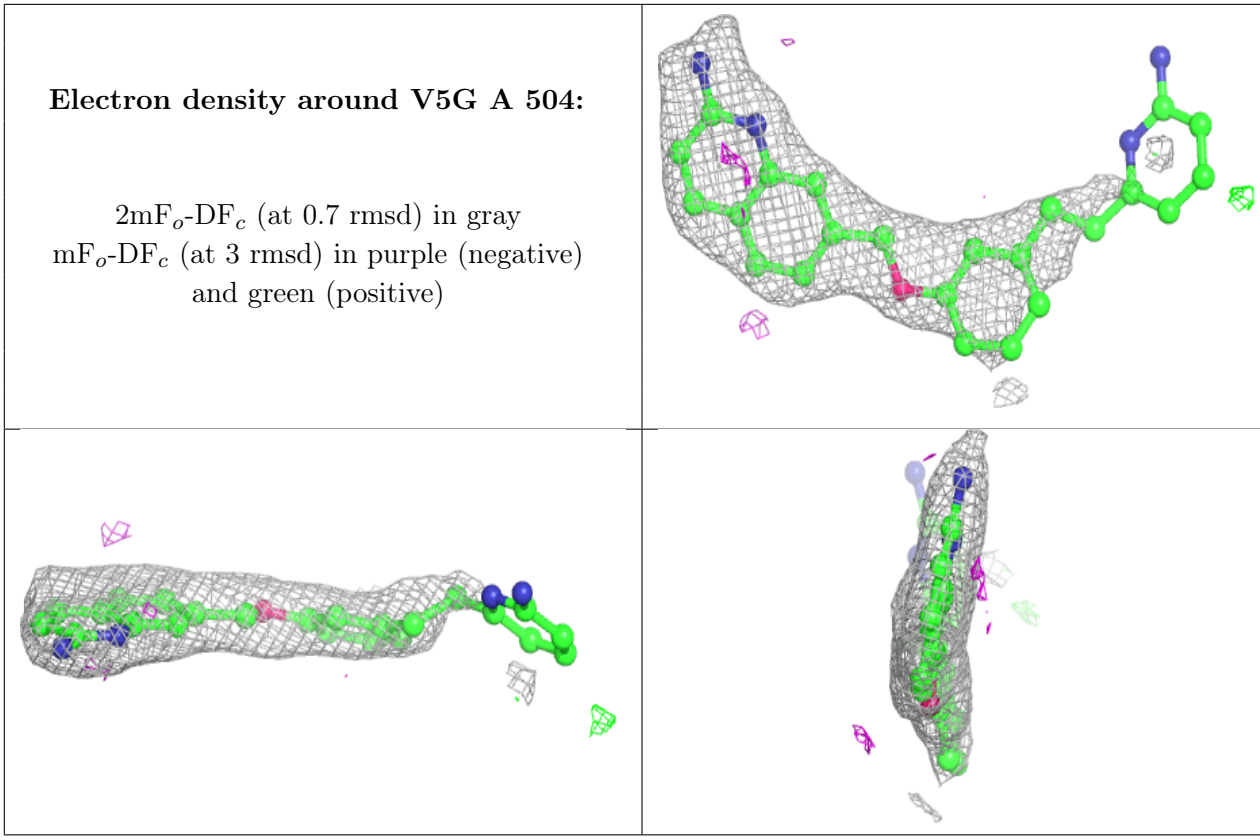
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





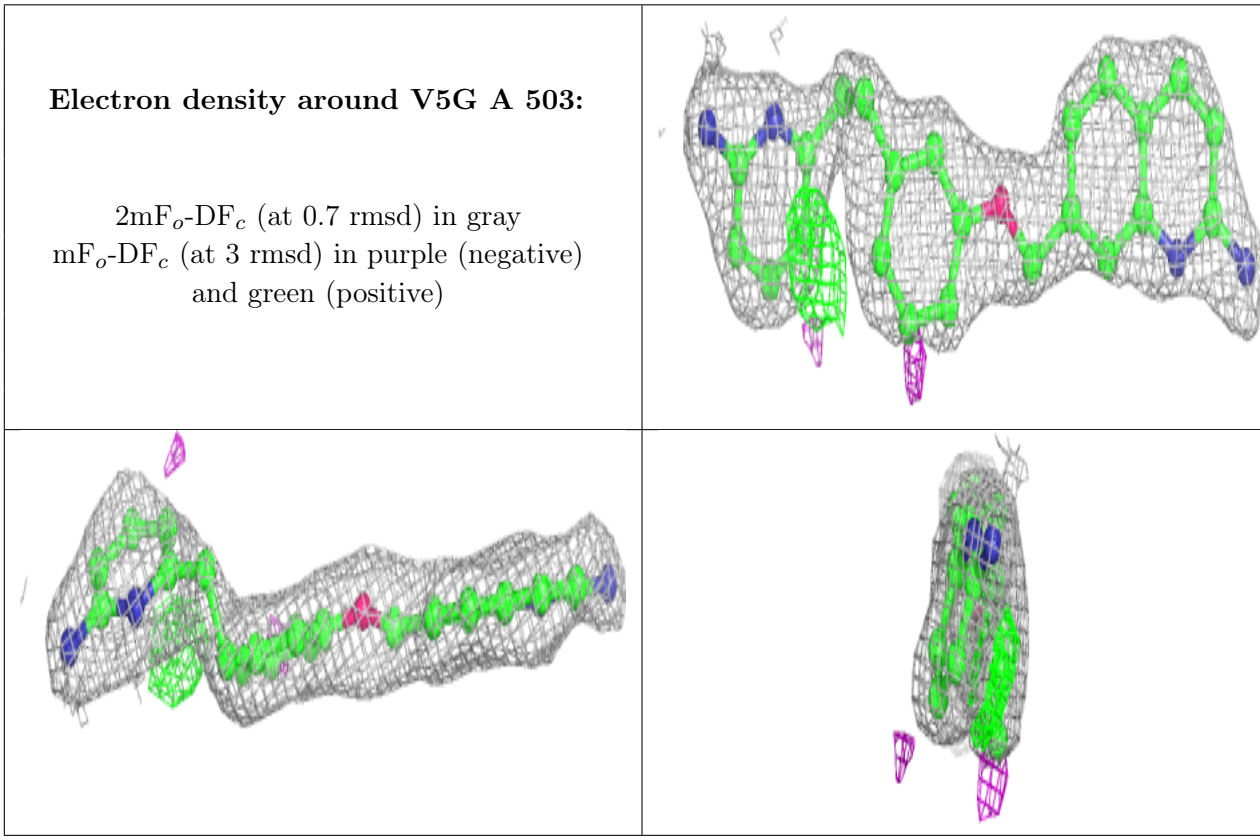
Electron density around V5G A 504:

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



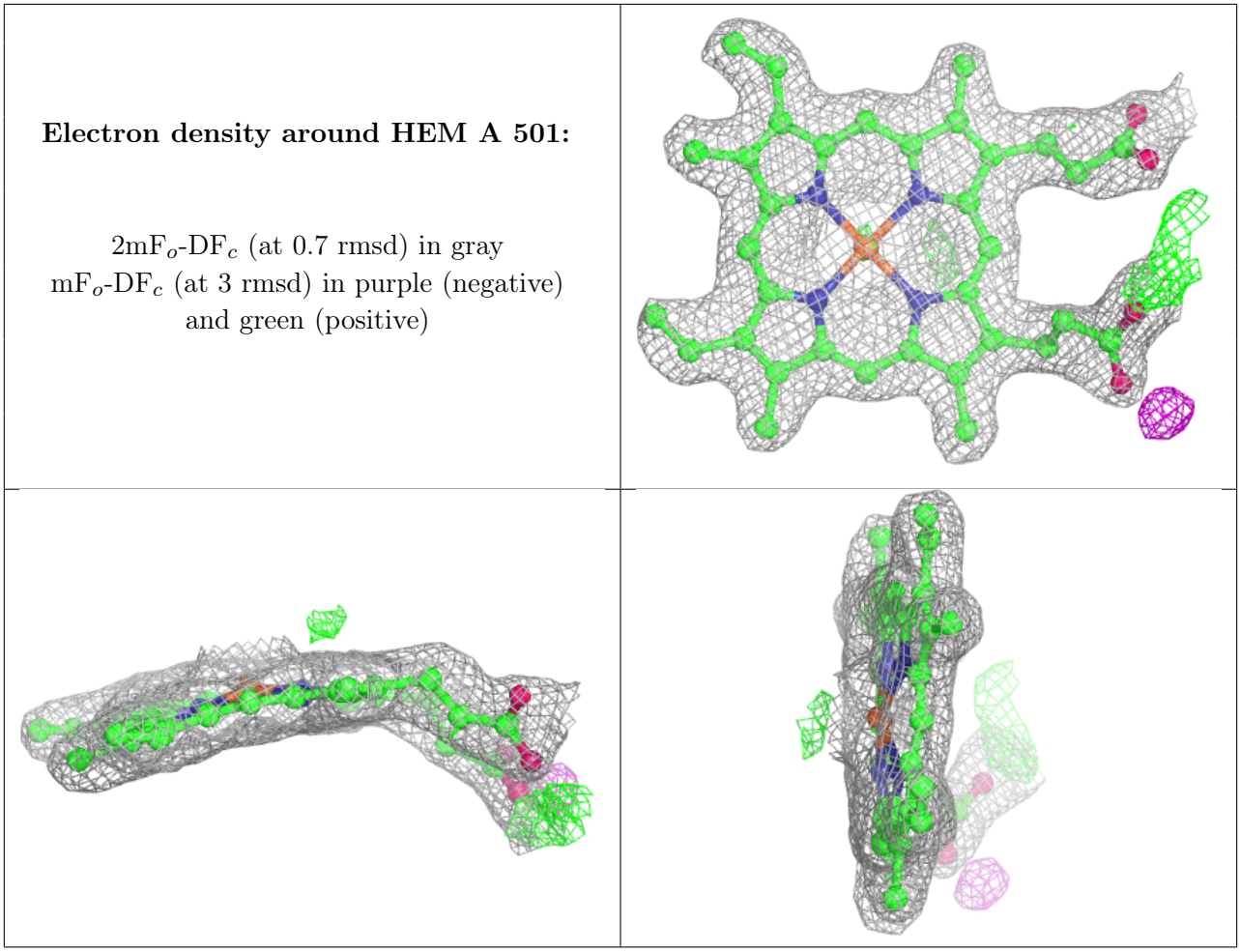
Electron density around V5G A 503:

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



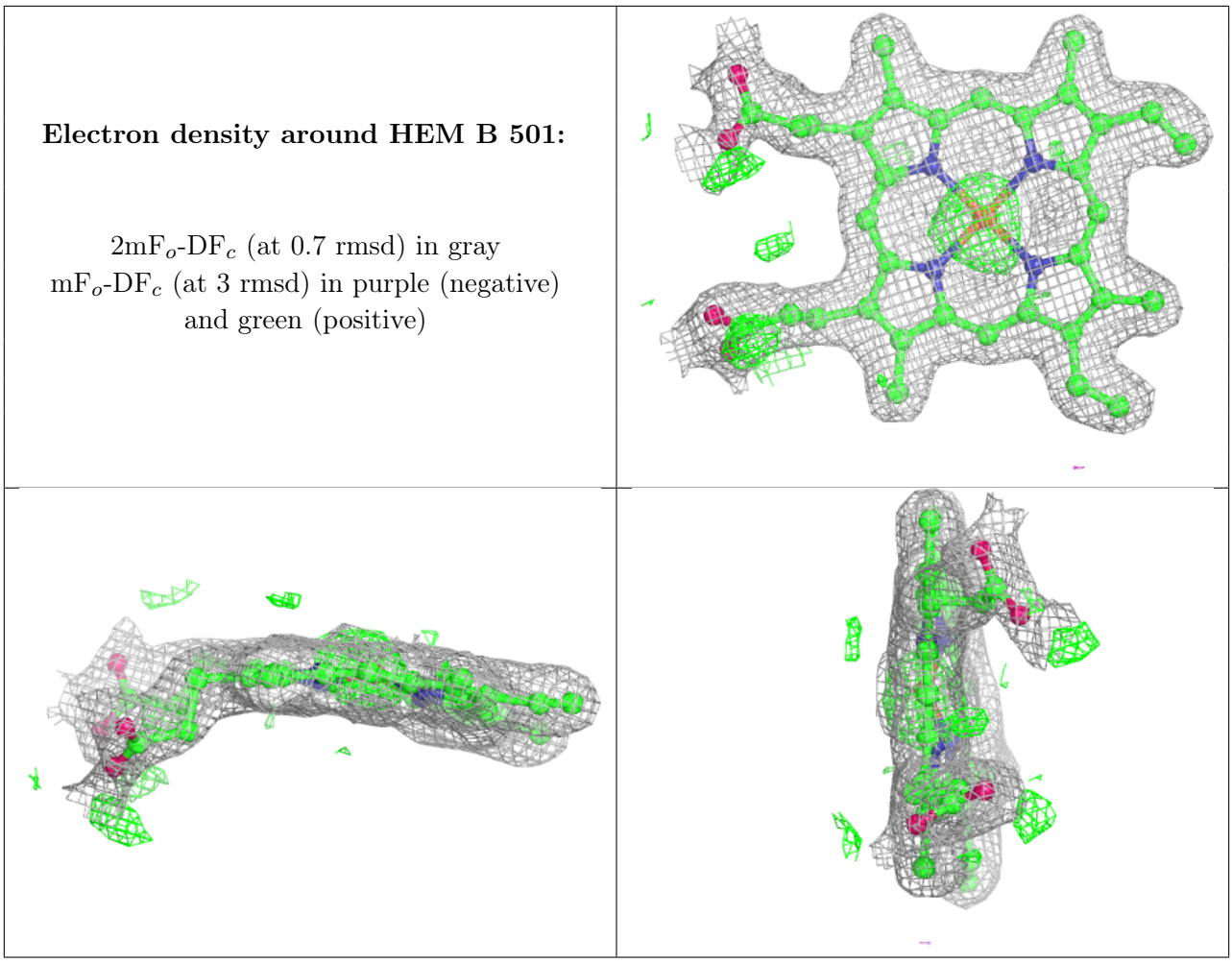
Electron density around HEM A 501:

$2mF_o$-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 501:

$2mF_o$-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.