Full wwPDB X-ray Structure Validation Report ⓘ

Sep 25, 2023 – 01:04 PM EDT

PDB ID	:	5VVD
Title	:	Structure of human endothelial nitric oxide synthase heme domain in complex with 4-(2-(((2-Amino-4-methylquinolin-7-yl)methyl)amino)ethyl)benzonitrile
Authors	:	Li, H.; Poulos, T.L.
Deposited on	:	2017-05-19
Resolution	:	2.25 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:

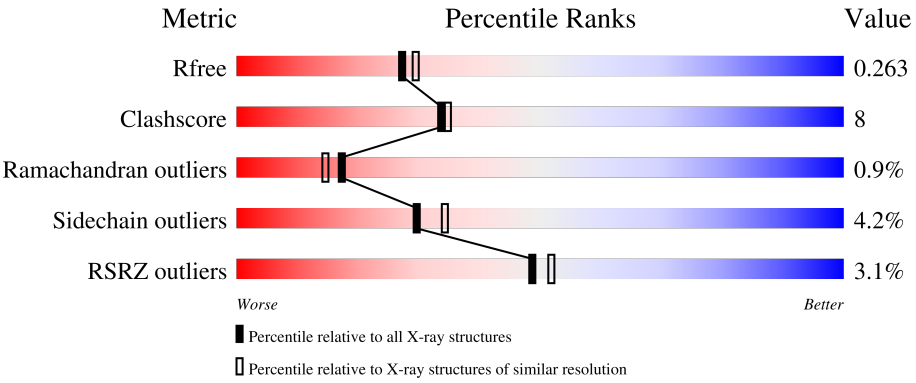
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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% 67% 21% • • 8%
1	B	440	% 75% 15% • 9%
1	C	440	3% 74% 15% • 9%
1	D	440	2% 77% 13% • 9%

2 Entry composition

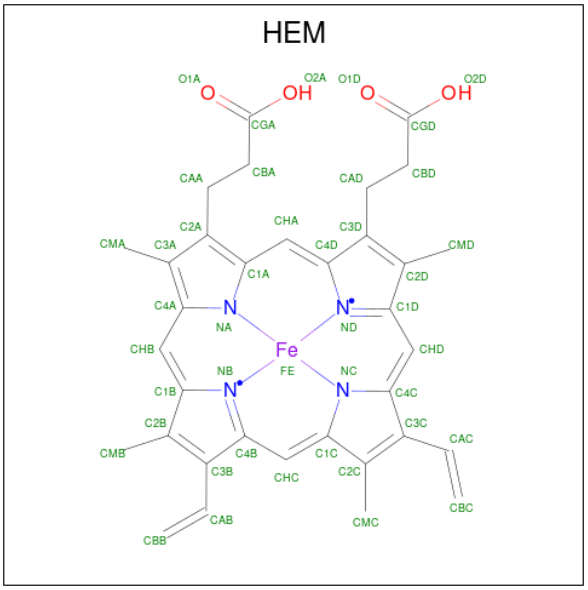
There are 10 unique types of molecules in this entry. The entry contains 13501 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	404	Total	C	N	O	S	0	3	0
			3240	2064	570	590	16			
1	B	402	Total	C	N	O	S	0	4	0
			3224	2053	566	588	17			
1	C	401	Total	C	N	O	S	0	3	0
			3212	2046	563	587	16			
1	D	402	Total	C	N	O	S	0	4	0
			3224	2053	566	588	17			

- 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		

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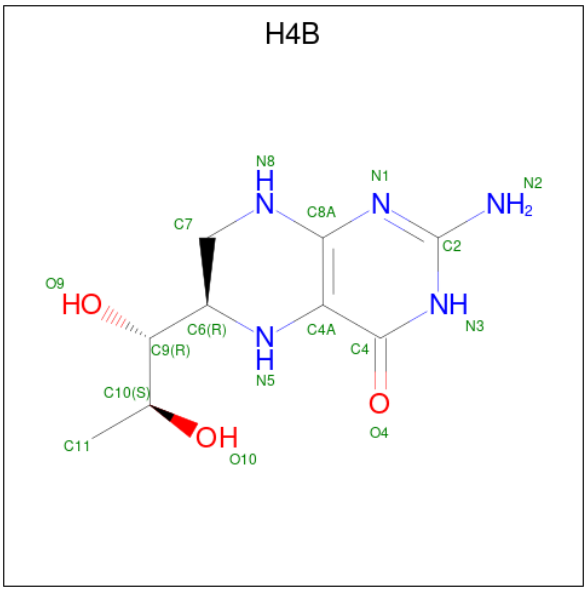
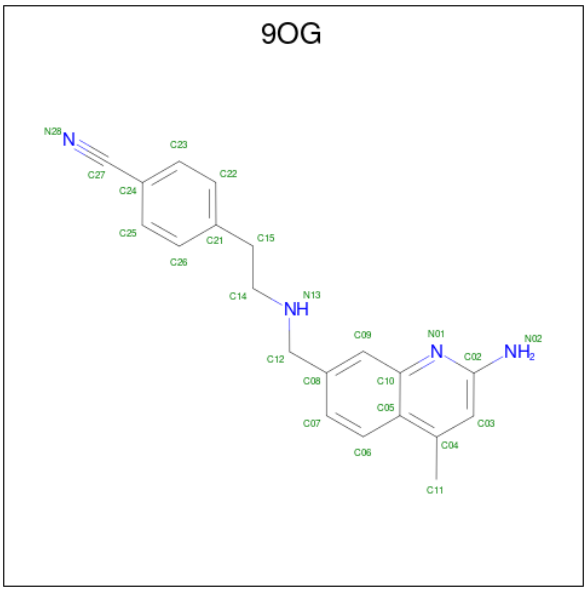
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



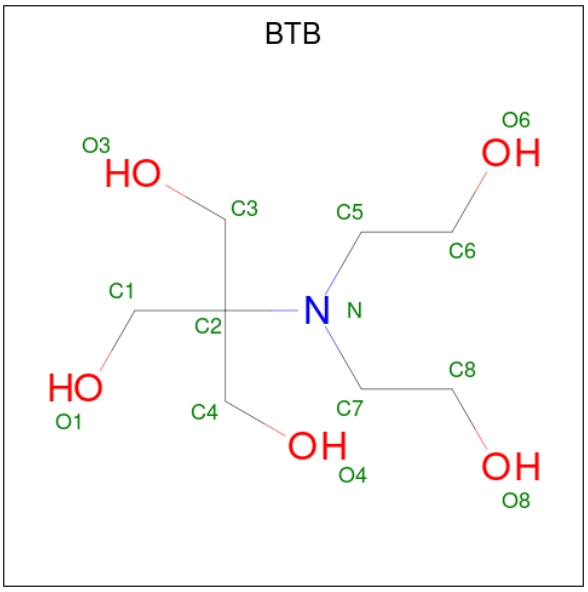
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		
3	C	1	Total	C	N	O	0	0
			17	9	5	3		
3	D	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 4 is 4-(2-{[(2-amino-4-methylquinolin-7-yl)methyl]amino}ethyl)benzonitrile (three-letter code: 9OG) (formula: $C_{20}H_{20}N_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N 24 20 4	0	0
4	B	1	Total C N 24 20 4	0	0
4	C	1	Total C N 24 20 4	0	0
4	D	1	Total C N 24 20 4	0	0

- Molecule 5 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: BTB) (formula: $C_8H_{19}NO_5$).

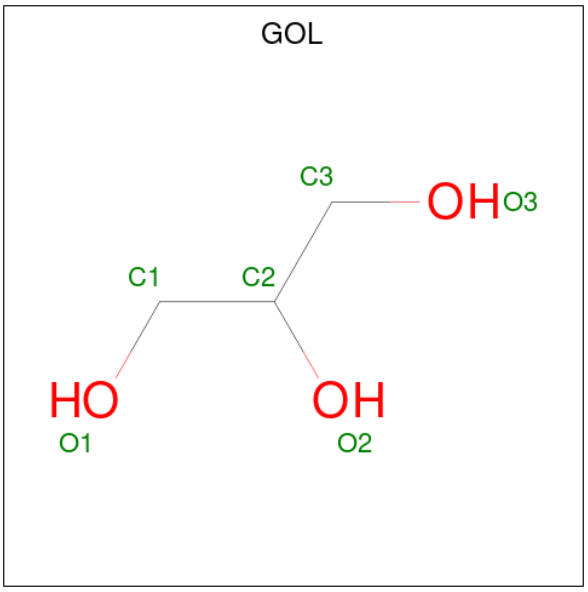


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 14 8 1 5	0	0
5	A	1	Total C N O 14 8 1 5	0	0
5	A	1	Total C N O 14 8 1 5	0	0
5	B	1	Total C N O 14 8 1 5	0	0
5	B	1	Total C N O 14 8 1 5	0	0
5	B	1	Total C N O 14 8 1 5	0	0
5	B	1	Total C N O 14 8 1 5	0	0
5	C	1	Total C N O 14 8 1 5	0	0
5	C	1	Total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

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Cl 1 1	0	0
8	B	1	Total Cl 1 1	0	0
8	C	1	Total Cl 1 1	0	0
8	D	1	Total Cl 1 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total Gd 1 1	0	0
9	B	2	Total Gd 2 2	0	0
9	D	1	Total Gd 1 1	0	0

- Molecule 10 is water.

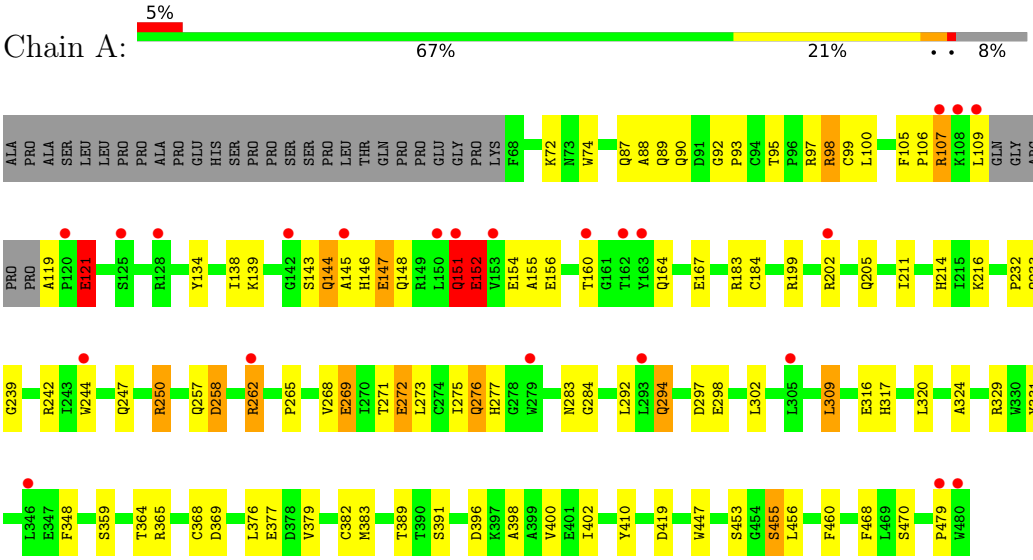
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	18	Total O 18 18	0	0
10	B	35	Total O 35 35	0	0
10	C	19	Total O 19 19	0	0
10	D	17	Total O 17 17	0	0

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.

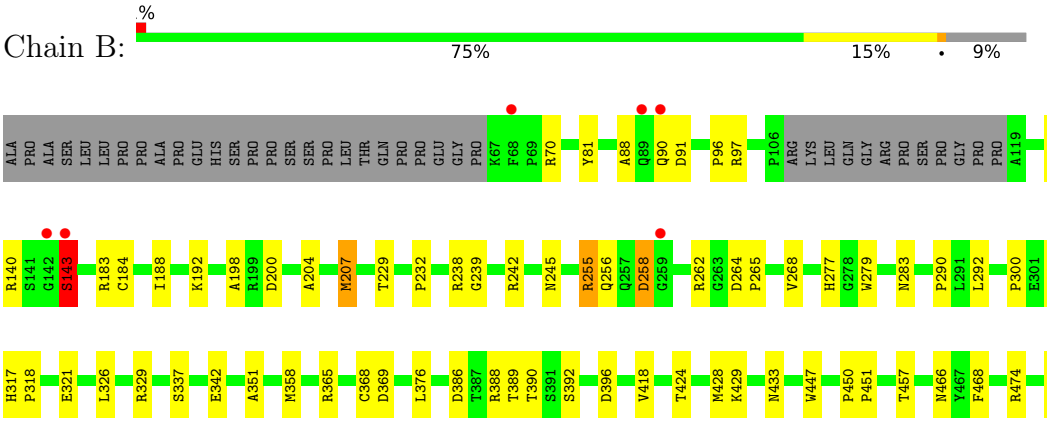
• Molecule 1: Nitric oxide synthase, endothelial

Chain A:



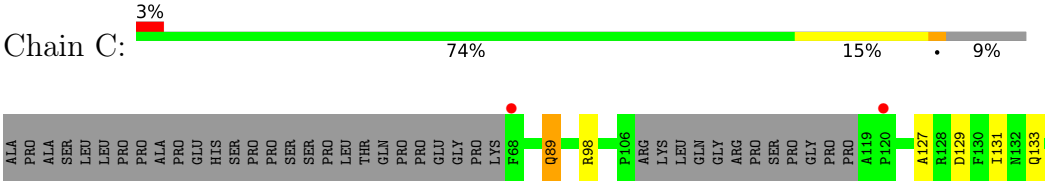
• Molecule 1: Nitric oxide synthase, endothelial

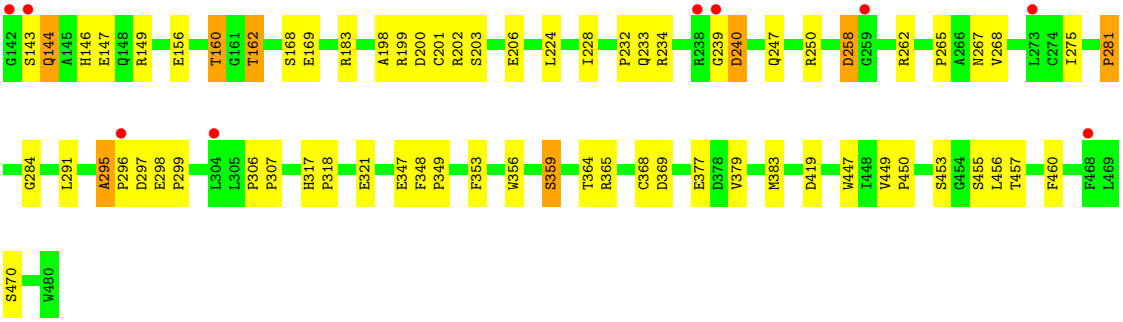
Chain B:



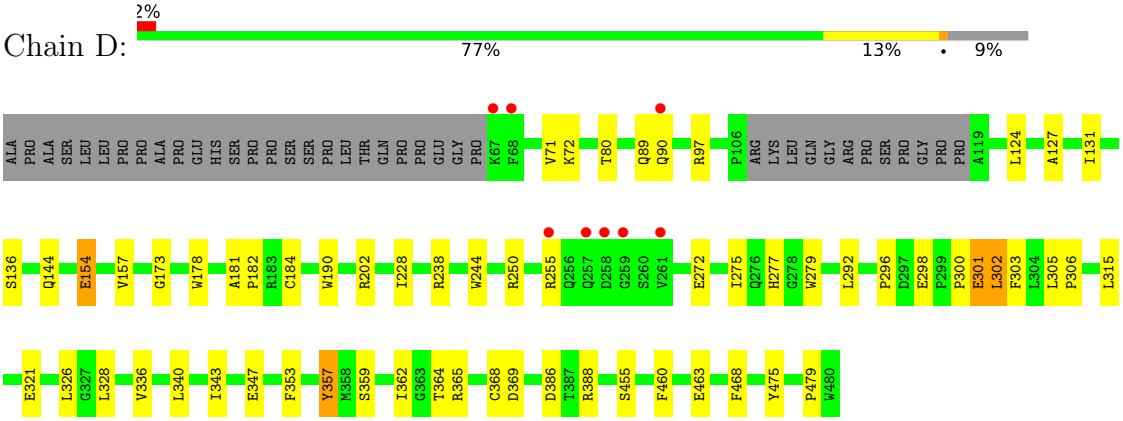
• Molecule 1: Nitric oxide synthase, endothelial

Chain C:





• Molecule 1: Nitric oxide synthase, endothelial



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	59.34Å 153.13Å 109.24Å 90.00° 90.78° 90.00°	Depositor
Resolution (Å)	39.12 – 2.25 39.12 – 2.20	Depositor EDS
% Data completeness (in resolution range)	90.8 (39.12-2.25) 90.7 (39.12-2.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	1.27 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.206 , 0.269 0.203 , 0.263	Depositor DCC
R_{free} test set	4499 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	49.9	Xtriage
Anisotropy	0.486	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 46.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.116 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	13501	wwPDB-VP
Average B, all atoms (Å^2)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% 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: BTB, GD, CL, GOL, HEM, H4B, 9OG, 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	0.38	0/3341	0.56	0/4551
1	B	0.43	0/3325	0.57	0/4531
1	C	0.42	0/3313	0.56	0/4515
1	D	0.45	0/3325	0.57	0/4531
All	All	0.42	0/13304	0.57	0/18128

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	A	0	4
1	B	0	1
1	C	0	2
1	D	0	1
All	All	0	8

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	107	ARG	Peptide
1	A	151	GLN	Peptide
1	A	152	GLU	Peptide
1	A	276	GLN	Peptide
1	B	143	SER	Peptide

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Mol	Chain	Res	Type	Group
1	C	143	SER	Peptide
1	C	144	GLN	Peptide
1	D	89	GLN	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3240	0	3151	73	0
1	B	3224	0	3131	46	0
1	C	3212	0	3114	43	0
1	D	3224	0	3131	37	0
2	A	43	0	30	5	0
2	B	43	0	30	5	0
2	C	43	0	30	1	0
2	D	43	0	30	7	0
3	A	17	0	15	1	0
3	B	17	0	15	2	0
3	C	17	0	15	1	0
3	D	17	0	15	1	0
4	A	24	0	0	1	0
4	B	24	0	0	1	0
4	C	24	0	0	0	0
4	D	24	0	0	2	0
5	A	42	0	56	12	0
5	B	56	0	72	11	0
5	C	28	0	38	5	0
5	D	28	0	36	9	0
6	A	1	0	0	0	0
6	D	1	0	0	0	0
7	A	6	0	8	1	0
7	C	6	0	8	0	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
9	A	1	0	0	0	0
9	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	D	1	0	0	0	0
10	A	18	0	0	2	0
10	B	35	0	0	1	0
10	C	19	0	0	0	0
10	D	17	0	0	1	0
All	All	13501	0	12925	223	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (223) 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:105:PHE:HB3	1:A:107:ARG:HB3	1.55	0.88
1:D:321:GLU:OE2	5:D:505:BTB:O3	1.93	0.87
1:A:152:GLU:HG2	1:A:155:ALA:HB2	1.59	0.84
1:C:89:GLN:O	1:D:97:ARG:NH1	2.12	0.82
1:B:255:ARG:HH11	1:B:268:VAL:HG11	1.45	0.81
1:C:144:GLN:HB3	1:C:147:GLU:H	1.48	0.77
1:D:365:ARG:NH2	1:D:369:ASP:OD2	2.17	0.77
1:A:97:ARG:NH1	1:B:91:ASP:OD1	2.18	0.77
5:B:504:BTB:O6	5:B:504:BTB:H82	1.86	0.75
1:A:294:GLN:NE2	1:A:298:GLU:O	2.16	0.74
1:A:453:SER:HB3	1:A:456:LEU:HD12	1.69	0.74
1:C:129:ASP:OD1	1:C:129:ASP:N	2.21	0.73
1:A:119:ALA:HB3	1:A:121:GLU:HG2	1.71	0.72
1:B:279:TRP:HB2	1:B:302:LEU:HD21	1.72	0.70
1:D:386:ASP:OD1	1:D:388:ARG:NH1	2.24	0.70
1:C:247:GLN:HB2	1:C:250:ARG:HG2	1.75	0.69
1:A:106:PRO:O	10:A:601:HOH:O	2.11	0.68
1:A:262:ARG:HH22	1:A:284:GLY:HA2	1.59	0.68
1:C:240:ASP:HB3	1:C:349:PRO:HG2	1.76	0.67
1:A:90:GLN:HB3	1:A:468:PHE:CD2	2.30	0.67
1:C:377:GLU:OE1	5:C:504:BTB:O1	2.13	0.66
1:B:292:LEU:HD22	1:B:300:PRO:HB2	1.78	0.66
1:A:144:GLN:O	1:A:147:GLU:N	2.21	0.65
1:A:382:CYS:HA	5:A:506:BTB:H12	1.79	0.64
1:D:238:ARG:HD2	1:D:296:PRO:HB3	1.79	0.64
2:A:501:HEM:HMC2	2:A:501:HEM:HBC2	1.80	0.64
1:A:377:GLU:OE2	5:A:505:BTB:O1	2.16	0.61
2:A:501:HEM:HBB2	2:A:501:HEM:HHC	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:ARG:NH1	1:A:283:ASN:O	2.33	0.61
1:A:272:GLU:OE2	1:A:272:GLU:N	2.35	0.60
1:C:250:ARG:HD2	1:C:267:ASN:HD21	1.67	0.60
1:A:242:ARG:NH2	1:A:479:PRO:HD3	2.17	0.59
1:A:239:GLY:N	1:A:297:ASP:OD2	2.34	0.59
1:D:178:TRP:CE3	1:D:190:TRP:HA	2.38	0.59
1:A:148:GLN:HA	1:A:151:GLN:HB2	1.85	0.59
1:A:97:ARG:HD2	1:B:88:ALA:HB3	1.84	0.59
1:A:244:TRP:CE2	1:A:294:GLN:HG3	2.38	0.58
1:A:144:GLN:O	1:A:146:HIS:N	2.36	0.58
5:D:505:BTB:O8	10:D:602:HOH:O	2.17	0.57
1:A:107:ARG:HB2	1:A:109:LEU:HB2	1.85	0.57
1:B:326:LEU:HD11	5:B:509:BTB:H31	1.86	0.57
1:B:258:ASP:OD1	1:B:258:ASP:N	2.36	0.57
1:D:298:GLU:OE1	5:D:506:BTB:N	2.38	0.57
1:C:450:PRO:HG2	1:C:457:THR:HG21	1.87	0.56
1:D:340:LEU:HD21	1:D:347:GLU:HG2	1.86	0.56
2:C:501:HEM:HBB2	2:C:501:HEM:HHC	1.88	0.56
1:A:244:TRP:NE1	1:A:294:GLN:HG3	2.21	0.56
1:A:258:ASP:OD1	1:A:258:ASP:N	2.37	0.56
1:C:258:ASP:N	1:C:258:ASP:OD1	2.38	0.56
1:A:183:ARG:HD3	1:A:447:TRP:CD2	2.42	0.55
1:C:265:PRO:O	1:C:268:VAL:HG23	2.07	0.55
1:D:124:LEU:HG	1:D:157:VAL:HG11	1.88	0.55
1:C:359:SER:OG	1:C:419:ASP:HA	2.06	0.55
1:A:184:CYS:HB2	2:A:501:HEM:ND	2.21	0.54
5:A:504:BTB:O6	5:A:504:BTB:H82	2.08	0.54
1:D:279:TRP:HB2	1:D:302:LEU:HD21	1.88	0.54
1:A:365:ARG:NH2	1:A:369:ASP:OD2	2.34	0.54
1:D:184:CYS:HB2	2:D:502:HEM:ND	2.23	0.54
1:A:247:GLN:HB2	1:A:250:ARG:HG2	1.91	0.53
1:B:290:PRO:HB3	1:B:304:LEU:HD23	1.90	0.53
1:B:242:ARG:NH2	1:B:479:PRO:HD3	2.23	0.53
1:A:298:GLU:OE2	5:A:504:BTB:O3	2.24	0.53
1:D:315:LEU:HD12	1:D:328:LEU:HB3	1.89	0.53
1:C:364:THR:O	1:C:368:CYS:HB2	2.09	0.52
1:A:95:THR:HG23	1:A:98:ARG:NH2	2.25	0.52
1:A:455:SER:HB3	1:B:451:PRO:HB2	1.92	0.52
1:C:133:GLN:HA	1:C:136[B]:SER:HB3	1.91	0.52
1:D:326:LEU:HB3	1:D:328:LEU:HG	1.91	0.52
1:B:450:PRO:HG2	1:B:457:THR:HG21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:364:THR:O	1:D:368:CYS:HB2	2.10	0.52
1:A:147:GLU:HB2	1:A:148:GLN:NE2	2.25	0.52
1:D:228:ILE:HG13	1:D:353:PHE:HB3	1.92	0.51
1:B:70:ARG:HG3	1:B:81:TYR:CZ	2.46	0.51
1:B:326:LEU:CD1	5:B:509:BTB:H31	2.40	0.51
1:A:152:GLU:HG3	1:A:154:GLU:HG2	1.92	0.50
1:C:275:ILE:HD11	1:C:281:PRO:HB3	1.93	0.50
1:A:265:PRO:HA	1:A:268:VAL:HG23	1.93	0.50
1:C:379:VAL:O	1:C:383:MET:HG3	2.11	0.50
3:D:503:H4B:O10	3:D:503:H4B:H71	2.10	0.50
1:B:321:GLU:OE1	5:B:504:BTB:H62	2.12	0.50
1:C:295:ALA:HB1	1:C:296:PRO:HD3	1.94	0.49
1:A:379:VAL:O	1:A:383:MET:HG3	2.12	0.49
1:A:419:ASP:OD2	1:B:390:THR:OG1	2.18	0.49
2:B:501:HEM:HBC2	2:B:501:HEM:HMC2	1.93	0.49
1:A:156:GLU:O	1:A:160:THR:HG22	2.12	0.49
1:C:365:ARG:HH12	3:C:502:H4B:C4	2.25	0.49
1:D:244:TRP:HB2	1:D:292:LEU:HB2	1.95	0.49
1:D:321:GLU:CD	5:D:505:BTB:HO6	2.16	0.49
1:D:173:GLY:HA3	1:D:343:ILE:HD13	1.94	0.48
5:D:506:BTB:H72	5:D:506:BTB:H61	1.63	0.48
1:C:453:SER:HB3	1:C:456:LEU:HD12	1.94	0.48
2:D:502:HEM:HHC	2:D:502:HEM:HBB2	1.93	0.48
1:A:273:LEU:O	1:A:277:HIS:ND1	2.45	0.48
1:D:184:CYS:HB2	2:D:502:HEM:C4D	2.47	0.48
1:B:262:ARG:NE	1:B:283:ASN:O	2.36	0.48
1:C:298:GLU:HG3	1:C:299:PRO:HD2	1.95	0.48
2:B:501:HEM:HHC	2:B:501:HEM:HBB2	1.94	0.48
1:D:475:TYR:OH	2:D:502:HEM:O2D	2.27	0.48
1:A:167:GLU:OE2	7:A:508:GOL:O1	2.17	0.48
1:A:455:SER:HA	1:A:460:PHE:CG	2.49	0.48
1:C:228:ILE:HG13	1:C:353:PHE:HB3	1.96	0.48
1:A:98:ARG:NH1	1:A:100:LEU:HG	2.28	0.47
1:A:364:THR:O	1:A:368:CYS:HB2	2.15	0.47
1:C:359:SER:HG	1:C:419:ASP:HA	1.78	0.47
1:A:93:PRO:O	1:A:98:ARG:NH2	2.38	0.47
1:A:298:GLU:OE1	5:A:504:BTB:O8	2.22	0.47
1:D:124:LEU:HD21	1:D:154:GLU:HA	1.94	0.47
1:D:475:TYR:HH	2:D:502:HEM:CGD	2.25	0.47
1:B:184:CYS:HB2	2:B:501:HEM:ND	2.30	0.47
1:A:316[B]:GLU:HG2	1:A:324:ALA:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:277:HIS:CD2	1:D:300:PRO:HG2	2.50	0.47
2:D:502:HEM:HBA1	4:D:504:9OG:C09	2.45	0.47
1:C:250:ARG:HD2	1:C:267:ASN:ND2	2.30	0.46
1:A:72:LYS:HD3	1:A:74:TRP:CZ2	2.51	0.46
1:A:87:GLN:O	1:A:87:GLN:NE2	2.47	0.46
1:C:160:THR:HG23	1:C:162:THR:H	1.80	0.46
1:A:331:TYR:O	1:A:410:TYR:OH	2.29	0.46
3:B:502:H4B:O10	3:B:502:H4B:H71	2.15	0.46
1:D:321:GLU:OE1	5:D:505:BTB:O6	2.33	0.46
1:C:233:GLN:HB3	1:C:348:PHE:CE2	2.50	0.46
1:D:455:SER:HA	1:D:460:PHE:CG	2.51	0.46
1:A:272:GLU:HA	1:A:275:ILE:HB	1.98	0.46
5:A:504:BTB:H41	5:A:504:BTB:H71	1.47	0.46
1:B:321:GLU:OE1	5:B:504:BTB:C6	2.64	0.46
1:C:262:ARG:HE	1:C:284:GLY:HA2	1.80	0.46
5:B:504:BTB:H42	5:B:504:BTB:H71	1.71	0.45
1:D:90:GLN:HB3	1:D:468:PHE:CD2	2.52	0.45
1:D:336:VAL:HG21	4:D:504:9OG:C07	2.46	0.45
5:B:504:BTB:O3	5:B:504:BTB:O4	2.32	0.45
1:B:90:GLN:HB3	1:B:468:PHE:CD2	2.52	0.45
1:B:317:HIS:CG	1:B:318:PRO:HD2	2.52	0.45
1:A:292:LEU:HA	1:A:292:LEU:HD23	1.74	0.45
5:D:506:BTB:H11	5:D:506:BTB:H51	1.71	0.45
1:A:398:ALA:O	1:A:402:ILE:HG13	2.17	0.45
5:D:505:BTB:H42	5:D:505:BTB:H71	1.77	0.45
1:A:309:LEU:HD12	1:A:309:LEU:HA	1.80	0.44
1:B:368:CYS:SG	1:B:376:LEU:HD13	2.57	0.44
1:B:342:GLU:OE1	1:B:474:ARG:NH1	2.50	0.44
1:A:269:GLU:HA	1:A:272:GLU:OE1	2.18	0.44
1:D:301:GLU:HB3	1:D:303:PHE:CE1	2.52	0.44
1:A:396:ASP:O	1:A:400:VAL:HG23	2.18	0.44
1:B:283:ASN:OD1	1:B:283:ASN:N	2.49	0.44
1:C:149:ARG:NE	1:C:169:GLU:OE2	2.42	0.44
1:C:183:ARG:HD3	1:C:447:TRP:CD2	2.53	0.44
1:D:244:TRP:CZ2	1:D:300:PRO:HG3	2.53	0.44
1:B:358:MET:HA	1:B:418:VAL:O	2.18	0.43
1:C:89:GLN:NE2	1:C:470:SER:H	2.16	0.43
1:B:124:LEU:O	1:B:128:ARG:HG3	2.18	0.43
5:B:506:BTB:H41	5:B:506:BTB:H71	1.84	0.43
1:D:181:ALA:HA	1:D:182:PRO:HD3	1.86	0.43
1:A:257:GLN:NE2	10:A:604:HOH:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:GLU:OE2	5:A:504:BTB:N	2.51	0.43
1:A:317:HIS:CD2	1:A:320:LEU:HD12	2.53	0.43
1:A:97:ARG:NE	1:B:88:ALA:O	2.52	0.43
1:B:256:GLN:HB3	10:B:611:HOH:O	2.18	0.43
1:B:429:LYS:HE2	1:B:433:ASN:HD21	1.83	0.43
2:A:501:HEM:HBC2	2:A:501:HEM:CMC	2.48	0.43
1:B:198:ALA:O	1:B:232:PRO:HD3	2.18	0.43
1:D:238:ARG:HD2	1:D:296:PRO:CB	2.49	0.43
1:A:92:GLY:N	1:B:96:PRO:O	2.50	0.43
1:B:229:THR:O	1:B:351:ALA:HA	2.19	0.43
1:B:365:ARG:HE	1:B:369:ASP:CG	2.21	0.43
1:B:264:ASP:HA	1:B:265:PRO:HD3	1.93	0.43
1:A:359:SER:OG	1:A:419:ASP:HA	2.18	0.43
1:A:382:CYS:HA	5:A:506:BTB:C1	2.49	0.43
1:C:144:GLN:HB3	1:C:146:HIS:HB3	2.00	0.43
5:C:505:BTB:H51	5:C:505:BTB:H42	1.61	0.43
1:C:224:LEU:HD12	1:C:356:TRP:HB3	2.00	0.42
1:A:341:LEU:HB3	1:A:348:PHE:HB2	2.00	0.42
1:C:306:PRO:HA	1:C:307:PRO:HD3	1.78	0.42
5:A:505:BTB:H72	5:A:505:BTB:H61	1.61	0.42
1:B:386:ASP:OD1	1:B:388:ARG:HG2	2.19	0.42
1:B:424:THR:O	1:B:428:MET:HG2	2.20	0.42
1:C:156:GLU:O	1:C:160:THR:HG22	2.19	0.42
1:C:347:GLU:O	1:C:349:PRO:HD3	2.20	0.42
5:C:505:BTB:H52	5:C:505:BTB:H11	1.75	0.42
1:A:134:TYR:O	1:A:138:ILE:HG12	2.19	0.42
5:A:506:BTB:H31	5:A:506:BTB:H52	1.75	0.42
1:C:199:ARG:O	1:C:232:PRO:HG3	2.20	0.42
5:D:506:BTB:H71	5:D:506:BTB:H32	1.74	0.42
1:B:245:ASN:O	1:B:337:SER:OG	2.35	0.42
1:C:291:LEU:HD23	1:C:291:LEU:HA	1.84	0.42
1:D:305:LEU:HA	1:D:306:PRO:HD3	1.79	0.42
1:A:152:GLU:HG2	1:A:155:ALA:CB	2.40	0.42
1:A:211:ILE:O	1:A:214:HIS:HB3	2.20	0.41
1:A:336:VAL:HG21	4:A:503:9OG:C07	2.50	0.41
1:C:298:GLU:OE2	5:C:505:BTB:H81	2.19	0.41
1:C:317:HIS:CG	1:C:318:PRO:HD2	2.54	0.41
5:C:505:BTB:H71	5:C:505:BTB:H31	1.84	0.41
1:A:199:ARG:O	1:A:232:PRO:HG3	2.21	0.41
1:B:188:ILE:HD11	1:B:429:LYS:HD3	2.01	0.41
5:B:505:BTB:H31	5:B:505:BTB:H71	1.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:ALA:HA	1:B:207:MET:HB2	2.02	0.41
2:B:501:HEM:CGA	3:B:502:H4B:HN3	2.32	0.41
1:C:449:VAL:HA	1:C:450:PRO:HD3	1.93	0.41
1:D:72:LYS:H	1:D:463:GLU:HB2	1.85	0.41
1:D:357:TYR:CD2	1:D:362:ILE:HD11	2.56	0.41
1:A:88:ALA:O	1:B:97:ARG:HG2	2.20	0.41
1:B:183:ARG:HD3	1:B:447:TRP:CD2	2.55	0.41
1:D:315:LEU:HB2	1:D:328:LEU:HB2	2.02	0.41
1:A:99:CYS:HB3	1:B:466:ASN:HB3	2.03	0.41
1:A:235:CYS:SG	1:A:238:ARG:NE	2.91	0.41
1:C:127:ALA:O	1:C:131:ILE:HG12	2.21	0.41
2:A:501:HEM:CGA	3:A:502:H4B:HN22	2.34	0.41
1:A:151:GLN:O	1:A:152:GLU:HB2	2.21	0.41
1:A:368:CYS:SG	1:A:376:LEU:HD13	2.61	0.41
5:A:505:BTB:H51	5:A:505:BTB:H32	1.83	0.41
1:B:321:GLU:CD	5:B:504:BTB:H62	2.41	0.41
1:C:365:ARG:NH2	1:C:369:ASP:OD2	2.54	0.41
1:C:455:SER:HA	1:C:460:PHE:CG	2.55	0.41
1:A:233:GLN:HB3	1:A:348:PHE:CE2	2.56	0.41
2:B:501:HEM:HBA1	4:B:503:9OG:C09	2.51	0.40
5:B:509:BTB:H52	5:B:509:BTB:H12	1.79	0.40
1:C:202:ARG:HB2	1:C:206:GLU:OE2	2.22	0.40
1:B:124:LEU:HD23	1:B:124:LEU:HA	1.94	0.40
1:B:140:ARG:HG3	1:B:143:SER:HB3	2.02	0.40
1:B:238:ARG:HG2	1:B:239:GLY:O	2.22	0.40
1:C:198:ALA:O	1:C:201:CYS:HB2	2.21	0.40
1:D:127:ALA:O	1:D:131:ILE:HG12	2.21	0.40
1:D:475:TYR:OH	2:D:502:HEM:CGD	2.70	0.40
1:A:271:THR:O	1:A:275:ILE:HG13	2.21	0.40
5:A:506:BTB:H12	5:A:506:BTB:H71	1.76	0.40
1:B:277:HIS:O	1:B:302:LEU:HD22	2.22	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	403/440 (92%)	380 (94%)	15 (4%)	8 (2%)	7 4
1	B	402/440 (91%)	388 (96%)	13 (3%)	1 (0%)	47 55
1	C	400/440 (91%)	384 (96%)	12 (3%)	4 (1%)	15 13
1	D	402/440 (91%)	384 (96%)	17 (4%)	1 (0%)	47 55
All	All	1607/1760 (91%)	1536 (96%)	57 (4%)	14 (1%)	17 14

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	GLU
1	A	139	LYS
1	A	145	ALA
1	A	147	GLU
1	A	152	GLU
1	B	143	SER
1	C	295	ALA
1	A	144	GLN
1	C	89	GLN
1	C	239	GLY
1	C	281	PRO
1	A	143	SER
1	A	151	GLN
1	D	479	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	346/373 (93%)	323 (93%)	23 (7%)	16 15
1	B	345/373 (92%)	336 (97%)	9 (3%)	46 55
1	C	343/373 (92%)	331 (96%)	12 (4%)	36 43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	345/373 (92%)	330 (96%)	15 (4%)	29 33
All	All	1379/1492 (92%)	1320 (96%)	59 (4%)	30 33

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	98	ARG
1	A	121	GLU
1	A	151	GLN
1	A	152	GLU
1	A	164	GLN
1	A	202	ARG
1	A	205	GLN
1	A	216	LYS
1	A	250	ARG
1	A	258	ASP
1	A	262	ARG
1	A	269	GLU
1	A	272	GLU
1	A	276	GLN
1	A	294	GLN
1	A	302	LEU
1	A	309	LEU
1	A	329	ARG
1	A	389	THR
1	A	391	SER
1	A	455	SER
1	A	470	SER
1	B	192	LYS
1	B	200	ASP
1	B	207	MET
1	B	255	ARG
1	B	258	ASP
1	B	329	ARG
1	B	389	THR
1	B	392	SER
1	B	396	ASP
1	C	98	ARG
1	C	160	THR
1	C	162	THR
1	C	168	SER

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Mol	Chain	Res	Type
1	C	200	ASP
1	C	203	SER
1	C	234	ARG
1	C	240	ASP
1	C	258	ASP
1	C	297	ASP
1	C	321	GLU
1	C	359	SER
1	D	71	VAL
1	D	80	THR
1	D	136[A]	SER
1	D	136[B]	SER
1	D	144	GLN
1	D	154	GLU
1	D	202	ARG
1	D	250	ARG
1	D	255	ARG
1	D	272	GLU
1	D	275	ILE
1	D	301	GLU
1	D	302	LEU
1	D	357	TYR
1	D	359	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	148	GLN
1	A	430	HIS
1	B	247	GLN
1	C	122	GLN
1	C	267	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 35 ligands modelled in this entry, 10 are monoatomic - leaving 25 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	BTB	D	505	9	13,13,13	0.48	0	7,16,16	0.57	0
5	BTB	D	506	-	13,13,13	0.45	0	7,16,16	1.00	0
4	9OG	B	503	-	26,26,26	1.71	3 (11%)	33,35,35	1.03	1 (3%)
4	9OG	A	503	-	26,26,26	1.67	2 (7%)	33,35,35	1.07	1 (3%)
4	9OG	C	503	-	26,26,26	1.61	2 (7%)	33,35,35	1.12	4 (12%)
5	BTB	A	506	9	13,13,13	0.36	0	7,16,16	0.86	0
5	BTB	B	505	-	13,13,13	0.36	0	7,16,16	0.27	0
4	9OG	D	504	-	26,26,26	1.61	1 (3%)	33,35,35	1.02	2 (6%)
5	BTB	C	504	-	13,13,13	0.63	0	7,16,16	1.46	1 (14%)
5	BTB	B	506	-	13,13,13	0.42	0	7,16,16	0.75	0
2	HEM	D	502	1	41,50,50	1.89	6 (14%)	45,82,82	2.06	13 (28%)
3	H4B	D	503	-	16,18,18	0.83	0	11,26,26	2.82	7 (63%)
7	GOL	A	508	-	5,5,5	0.36	0	5,5,5	0.34	0
3	H4B	C	502	-	16,18,18	1.03	1 (6%)	11,26,26	2.70	7 (63%)
3	H4B	B	502	-	16,18,18	0.87	0	11,26,26	2.89	7 (63%)
2	HEM	C	501	1	41,50,50	2.03	6 (14%)	45,82,82	1.99	9 (20%)
7	GOL	C	506	-	5,5,5	0.45	0	5,5,5	0.58	0
5	BTB	A	505	-	13,13,13	0.49	0	7,16,16	1.15	1 (14%)
5	BTB	C	505	-	13,13,13	0.40	0	7,16,16	0.79	0
2	HEM	B	501	1	41,50,50	1.92	8 (19%)	45,82,82	2.14	14 (31%)
5	BTB	A	504	-	13,13,13	0.37	0	7,16,16	0.58	0
2	HEM	A	501	1	41,50,50	1.97	6 (14%)	45,82,82	1.71	7 (15%)
5	BTB	B	509	9	13,13,13	0.45	0	7,16,16	1.35	1 (14%)
5	BTB	B	504	9	13,13,13	0.49	0	7,16,16	0.78	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	H4B	A	502	-	16,18,18	0.92	0	11,26,26	2.95	7 (63%)

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	BTB	D	505	9	-	1/21/21/21	-
5	BTB	D	506	-	-	11/21/21/21	-
4	9OG	B	503	-	-	4/9/9/9	0/3/3/3
4	9OG	A	503	-	-	3/9/9/9	0/3/3/3
4	9OG	C	503	-	-	2/9/9/9	0/3/3/3
5	BTB	A	506	9	-	2/21/21/21	-
5	BTB	B	505	-	-	9/21/21/21	-
4	9OG	D	504	-	-	3/9/9/9	0/3/3/3
5	BTB	C	504	-	-	6/21/21/21	-
5	BTB	B	506	-	-	1/21/21/21	-
2	HEM	D	502	1	-	1/12/54/54	-
3	H4B	D	503	-	-	4/8/17/17	0/2/2/2
7	GOL	A	508	-	-	4/4/4/4	-
3	H4B	C	502	-	-	3/8/17/17	0/2/2/2
3	H4B	B	502	-	-	4/8/17/17	0/2/2/2
2	HEM	C	501	1	-	2/12/54/54	-
7	GOL	C	506	-	-	2/4/4/4	-
5	BTB	A	505	-	-	8/21/21/21	-
5	BTB	C	505	-	-	9/21/21/21	-
2	HEM	B	501	1	-	2/12/54/54	-
5	BTB	A	504	-	-	7/21/21/21	-
2	HEM	A	501	1	-	4/12/54/54	-
5	BTB	B	509	9	-	8/21/21/21	-
5	BTB	B	504	9	-	1/21/21/21	-
3	H4B	A	502	-	-	3/8/17/17	0/2/2/2

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	C3D-C2D	7.96	1.53	1.36
2	C	501	HEM	C3D-C2D	7.68	1.53	1.36
2	B	501	HEM	C3D-C2D	7.35	1.52	1.36
2	D	502	HEM	C3D-C2D	7.32	1.52	1.36
4	B	503	9OG	C24-C27	-7.13	1.28	1.44
4	A	503	9OG	C24-C27	-7.11	1.28	1.44
4	D	504	9OG	C24-C27	-6.79	1.29	1.44
4	C	503	9OG	C24-C27	-6.37	1.30	1.44
2	C	501	HEM	FE-NB	5.41	2.23	1.96
2	B	501	HEM	C3C-CAC	4.14	1.56	1.47
2	D	502	HEM	C3C-C2C	-4.05	1.34	1.40
2	A	501	HEM	C3C-CAC	3.88	1.55	1.47
2	D	502	HEM	C3C-CAC	3.84	1.55	1.47
2	C	501	HEM	C3C-CAC	3.80	1.55	1.47
2	A	501	HEM	C3C-C2C	-3.63	1.35	1.40
2	C	501	HEM	CAB-C3B	3.42	1.56	1.47
2	B	501	HEM	C3C-C2C	-3.36	1.35	1.40
2	C	501	HEM	C3C-C2C	-3.36	1.35	1.40
2	B	501	HEM	FE-ND	3.34	2.13	1.96
2	A	501	HEM	FE-NB	3.16	2.12	1.96
2	A	501	HEM	CAB-C3B	3.11	1.55	1.47
2	B	501	HEM	CAB-C3B	3.04	1.55	1.47
2	D	502	HEM	FE-NB	2.95	2.11	1.96
2	A	501	HEM	FE-ND	2.89	2.11	1.96
2	D	502	HEM	CAB-C3B	2.68	1.54	1.47
2	C	501	HEM	CMB-C2B	2.47	1.56	1.50
4	B	503	9OG	C09-C10	-2.33	1.38	1.41
4	B	503	9OG	C05-C10	-2.25	1.38	1.42
4	C	503	9OG	C05-C10	-2.23	1.38	1.42
2	B	501	HEM	CMB-C2B	2.22	1.55	1.50
2	B	501	HEM	FE-NB	2.13	2.07	1.96
4	A	503	9OG	C05-C10	-2.11	1.39	1.42
2	B	501	HEM	CHA-C4D	2.03	1.40	1.35
2	D	502	HEM	FE-ND	2.02	2.06	1.96
3	C	502	H4B	C4-N3	2.02	1.36	1.33

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	HEM	C4D-ND-C1D	7.40	112.72	105.07
2	C	501	HEM	C4D-ND-C1D	7.11	112.42	105.07
2	D	502	HEM	C4D-ND-C1D	6.78	112.08	105.07
2	A	501	HEM	C4D-ND-C1D	6.40	111.68	105.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	502	H4B	C8A-C4A-C4	5.68	119.62	114.57
2	C	501	HEM	CBA-CAA-C2A	-5.06	103.98	112.62
3	A	502	H4B	C8A-C4A-C4	5.06	119.06	114.57
3	A	502	H4B	C4-C4A-N5	4.66	123.03	119.12
3	B	502	H4B	C8A-C4A-C4	4.55	118.61	114.57
2	D	502	HEM	C4C-CHD-C1D	4.54	128.55	122.56
3	D	503	H4B	C4-C4A-N5	4.23	122.67	119.12
3	B	502	H4B	C4-C4A-N5	4.02	122.50	119.12
3	B	502	H4B	N1-C2-N3	-3.98	119.18	125.42
3	D	503	H4B	C8A-C4A-C4	3.88	118.02	114.57
2	B	501	HEM	C4C-CHD-C1D	3.69	127.43	122.56
3	D	503	H4B	C4A-N5-C6	-3.68	111.15	121.16
2	D	502	HEM	CMD-C2D-C1D	3.66	130.62	125.04
3	B	502	H4B	C2-N3-C4	3.58	121.62	115.93
3	A	502	H4B	N1-C2-N3	-3.55	119.85	125.42
2	C	501	HEM	CBD-CAD-C3D	-3.54	102.80	112.63
2	C	501	HEM	C4B-CHC-C1C	3.43	127.09	122.56
3	D	503	H4B	N1-C2-N3	-3.41	120.07	125.42
3	D	503	H4B	C2-N3-C4	3.37	121.28	115.93
3	C	502	H4B	N1-C2-N3	-3.27	120.28	125.42
2	B	501	HEM	CHC-C4B-C3B	3.20	129.47	124.57
2	B	501	HEM	CBA-CAA-C2A	-3.17	107.20	112.62
3	B	502	H4B	C2-N1-C8A	3.15	121.61	114.54
2	B	501	HEM	C1B-NB-C4B	3.12	108.30	105.07
2	B	501	HEM	CBD-CAD-C3D	-3.11	103.99	112.63
3	A	502	H4B	C2-N1-C8A	3.10	121.48	114.54
2	D	502	HEM	CMC-C2C-C3C	3.05	130.39	124.68
3	A	502	H4B	C2-N3-C4	3.01	120.71	115.93
3	C	502	H4B	C2-N1-C8A	2.98	121.21	114.54
2	A	501	HEM	C3B-C2B-C1B	2.97	108.69	106.49
2	D	502	HEM	CBA-CAA-C2A	-2.93	107.62	112.62
2	D	502	HEM	C3B-C2B-C1B	2.89	108.63	106.49
2	B	501	HEM	C3B-C2B-C1B	2.88	108.62	106.49
2	D	502	HEM	C4A-C3A-C2A	2.86	108.99	107.00
3	C	502	H4B	C2-N3-C4	2.85	120.46	115.93
2	B	501	HEM	C3D-C4D-ND	-2.83	107.02	110.17
2	B	501	HEM	C4B-CHC-C1C	2.79	126.24	122.56
5	C	504	BTB	O4-C4-C2	-2.78	103.84	111.44
2	B	501	HEM	CAD-CBD-CGD	-2.76	107.67	113.60
2	C	501	HEM	CMC-C2C-C3C	2.72	129.77	124.68
2	A	501	HEM	C1B-NB-C4B	2.70	107.86	105.07
3	D	503	H4B	C2-N1-C8A	2.69	120.56	114.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	503	H4B	N2-C2-N3	2.68	121.42	117.25
2	D	502	HEM	CAD-C3D-C4D	2.67	129.32	124.66
4	D	504	9OG	C12-C08-C09	-2.59	116.87	121.51
3	A	502	H4B	C4A-N5-C6	-2.55	114.23	121.16
2	D	502	HEM	CBD-CAD-C3D	-2.53	105.59	112.63
2	C	501	HEM	CMA-C3A-C4A	-2.48	124.66	128.46
2	B	501	HEM	CMD-C2D-C1D	2.46	128.79	125.04
4	C	503	9OG	C04-C05-C10	2.46	119.34	118.01
5	A	505	BTB	O4-C4-C2	-2.46	104.72	111.44
3	B	502	H4B	N2-C2-N3	2.45	121.07	117.25
2	C	501	HEM	CHC-C4B-C3B	2.45	128.32	124.57
2	C	501	HEM	C3D-C4D-ND	-2.35	107.55	110.17
4	D	504	9OG	C14-C15-C21	-2.33	107.46	112.87
2	A	501	HEM	CAD-CBD-CGD	-2.32	108.61	113.60
3	C	502	H4B	C4-C4A-N5	2.31	121.06	119.12
2	C	501	HEM	CMD-C2D-C1D	2.31	128.55	125.04
4	B	503	9OG	C12-C08-C09	-2.30	117.39	121.51
5	B	509	BTB	O4-C4-C2	2.27	117.67	111.44
4	C	503	9OG	C24-C27-N28	-2.27	171.85	177.85
2	A	501	HEM	C4C-CHD-C1D	2.25	125.53	122.56
2	D	502	HEM	CHD-C1D-ND	2.23	126.86	124.43
4	A	503	9OG	C14-C15-C21	-2.23	107.70	112.87
3	C	502	H4B	C4A-N5-C6	-2.22	115.13	121.16
4	C	503	9OG	C05-C10-N01	-2.21	120.47	122.81
2	D	502	HEM	C1B-NB-C4B	2.17	107.32	105.07
4	C	503	9OG	C25-C24-C27	-2.16	116.39	119.99
2	B	501	HEM	CMC-C2C-C3C	2.14	128.67	124.68
2	B	501	HEM	CAD-C3D-C4D	2.13	128.38	124.66
2	D	502	HEM	C3D-C4D-ND	-2.12	107.80	110.17
3	B	502	H4B	C4A-N5-C6	-2.11	115.41	121.16
2	A	501	HEM	CMC-C2C-C3C	2.10	128.62	124.68
3	C	502	H4B	N2-C2-N3	2.09	120.51	117.25
2	D	502	HEM	CHA-C4D-ND	2.09	126.97	124.38
3	A	502	H4B	N2-C2-N3	2.07	120.47	117.25
2	A	501	HEM	C4A-C3A-C2A	2.06	108.43	107.00
2	B	501	HEM	CAB-C3B-C2B	-2.01	122.00	128.60

There are no chirality outliers.

All (104) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	HEM	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
2	A	501	HEM	C3A-C2A-CAA-CBA
3	A	502	H4B	C7-C6-C9-O9
3	A	502	H4B	C7-C6-C9-C10
3	B	502	H4B	N5-C6-C9-O9
3	B	502	H4B	C7-C6-C9-O9
3	B	502	H4B	C7-C6-C9-C10
3	C	502	H4B	C7-C6-C9-O9
3	C	502	H4B	C7-C6-C9-C10
3	D	503	H4B	N5-C6-C9-O9
3	D	503	H4B	N5-C6-C9-C10
3	D	503	H4B	C7-C6-C9-O9
3	D	503	H4B	C7-C6-C9-C10
5	A	504	BTB	O1-C1-C2-N
5	A	504	BTB	C1-C2-C4-O4
5	A	504	BTB	C3-C2-C4-O4
5	A	504	BTB	N-C2-C4-O4
5	A	505	BTB	C1-C2-N-C5
5	A	505	BTB	C1-C2-N-C7
5	A	505	BTB	C3-C2-N-C5
5	A	505	BTB	C3-C2-N-C7
5	A	505	BTB	C4-C2-N-C5
5	A	505	BTB	C4-C2-N-C7
5	B	505	BTB	O1-C1-C2-C3
5	B	505	BTB	O1-C1-C2-C4
5	B	505	BTB	O1-C1-C2-N
5	B	505	BTB	C1-C2-C3-O3
5	B	505	BTB	C4-C2-C3-O3
5	B	505	BTB	N-C2-C3-O3
5	B	505	BTB	C1-C2-C4-O4
5	B	505	BTB	C3-C2-C4-O4
5	B	505	BTB	N-C2-C4-O4
5	B	509	BTB	C1-C2-C3-O3
5	B	509	BTB	C4-C2-C3-O3
5	B	509	BTB	N-C2-C3-O3
5	B	509	BTB	C1-C2-C4-O4
5	B	509	BTB	C3-C2-C4-O4
5	B	509	BTB	N-C2-C4-O4
5	C	504	BTB	C1-C2-N-C5
5	C	504	BTB	C1-C2-N-C7
5	C	504	BTB	C3-C2-N-C5
5	C	504	BTB	C3-C2-N-C7
5	C	504	BTB	C4-C2-N-C5

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Mol	Chain	Res	Type	Atoms
5	C	504	BTB	C4-C2-N-C7
5	C	505	BTB	O1-C1-C2-C3
5	C	505	BTB	O1-C1-C2-C4
5	C	505	BTB	O1-C1-C2-N
5	C	505	BTB	C1-C2-C4-O4
5	C	505	BTB	C3-C2-C4-O4
5	C	505	BTB	N-C2-C4-O4
5	C	505	BTB	C6-C5-N-C7
5	D	506	BTB	C1-C2-C3-O3
5	D	506	BTB	C4-C2-C3-O3
5	D	506	BTB	N-C2-C3-O3
5	D	506	BTB	C1-C2-C4-O4
5	D	506	BTB	C3-C2-C4-O4
5	D	506	BTB	N-C2-C4-O4
5	D	506	BTB	C6-C5-N-C7
7	A	508	GOL	O1-C1-C2-C3
7	A	508	GOL	C1-C2-C3-O3
7	C	506	GOL	O1-C1-C2-O2
7	C	506	GOL	O1-C1-C2-C3
5	A	505	BTB	N-C7-C8-O8
5	C	505	BTB	N-C7-C8-O8
4	D	504	9OG	N13-C14-C15-C21
2	A	501	HEM	C2A-CAA-CBA-CGA
4	A	503	9OG	N13-C14-C15-C21
2	D	502	HEM	C2A-CAA-CBA-CGA
7	A	508	GOL	O1-C1-C2-O2
7	A	508	GOL	O2-C2-C3-O3
5	A	505	BTB	C6-C5-N-C7
4	C	503	9OG	C15-C14-N13-C12
5	A	504	BTB	N-C5-C6-O6
5	D	506	BTB	N-C7-C8-O8
4	A	503	9OG	C14-C15-C21-C26
5	B	509	BTB	N-C5-C6-O6
4	A	503	9OG	C14-C15-C21-C22
2	B	501	HEM	C2A-CAA-CBA-CGA
5	D	505	BTB	N-C7-C8-O8
4	D	504	9OG	C14-C15-C21-C22
4	D	504	9OG	C14-C15-C21-C26
4	C	503	9OG	N13-C14-C15-C21
4	B	503	9OG	C14-C15-C21-C22
4	B	503	9OG	C14-C15-C21-C26
5	B	504	BTB	N-C7-C8-O8

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Mol	Chain	Res	Type	Atoms
2	A	501	HEM	C4B-C3B-CAB-CBB
2	B	501	HEM	C4B-C3B-CAB-CBB
2	C	501	HEM	C4B-C3B-CAB-CBB
4	B	503	9OG	N13-C14-C15-C21
5	D	506	BTB	N-C5-C6-O6
3	A	502	H4B	N5-C6-C9-O9
5	A	504	BTB	O1-C1-C2-C3
5	A	504	BTB	O1-C1-C2-C4
5	A	506	BTB	C1-C2-C4-O4
2	C	501	HEM	C2A-CAA-CBA-CGA
5	B	506	BTB	N-C2-C4-O4
5	D	506	BTB	O1-C1-C2-N
3	B	502	H4B	N5-C6-C9-C10
5	B	509	BTB	N-C7-C8-O8
5	C	505	BTB	N-C5-C6-O6
4	B	503	9OG	C15-C14-N13-C12
3	C	502	H4B	N5-C6-C9-O9
5	A	506	BTB	C3-C2-C4-O4
5	D	506	BTB	O1-C1-C2-C4

There are no ring outliers.

23 monomers are involved in 61 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	505	BTB	5	0
5	D	506	BTB	4	0
4	B	503	9OG	1	0
4	A	503	9OG	1	0
5	A	506	BTB	4	0
5	B	505	BTB	1	0
4	D	504	9OG	2	0
5	C	504	BTB	1	0
5	B	506	BTB	1	0
2	D	502	HEM	7	0
3	D	503	H4B	1	0
7	A	508	GOL	1	0
3	C	502	H4B	1	0
3	B	502	H4B	2	0
2	C	501	HEM	1	0
5	A	505	BTB	3	0
5	C	505	BTB	4	0
2	B	501	HEM	5	0

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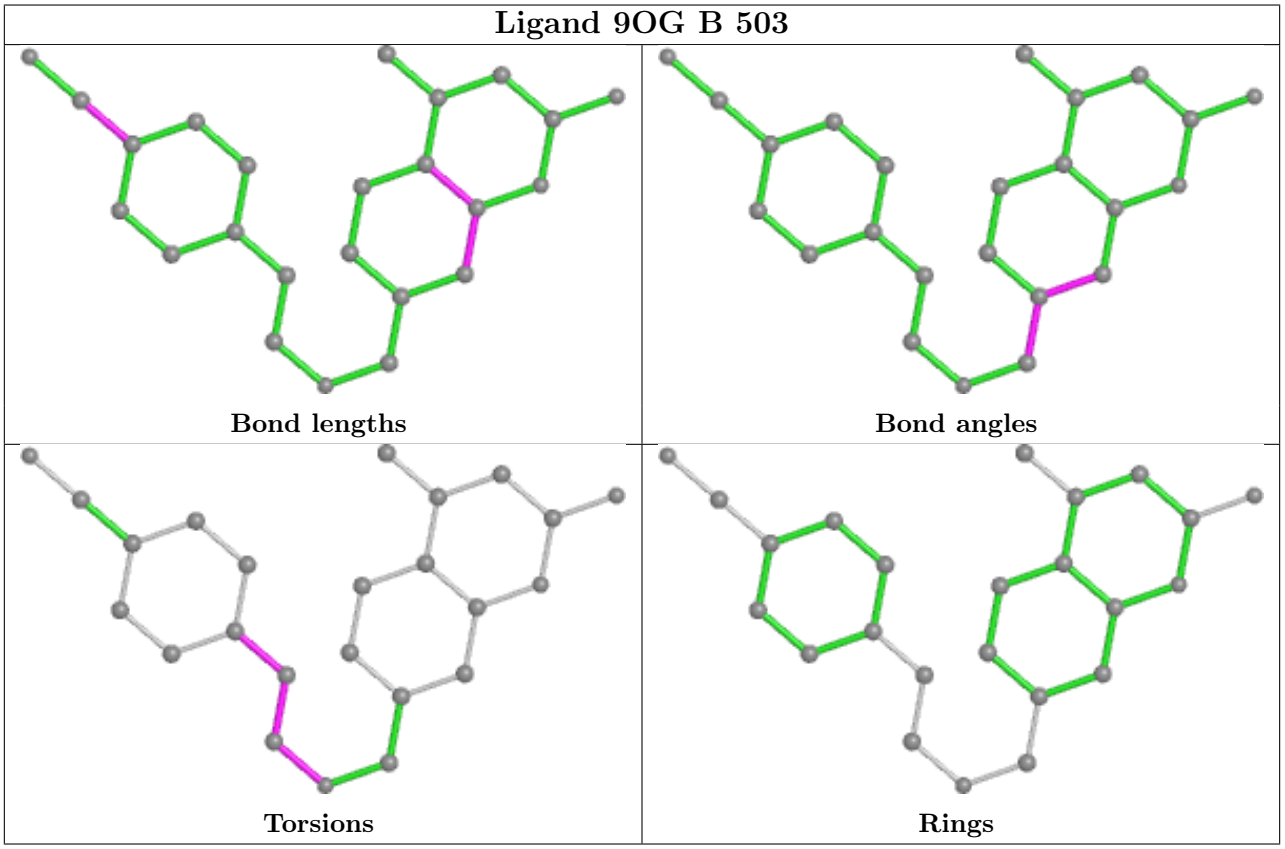
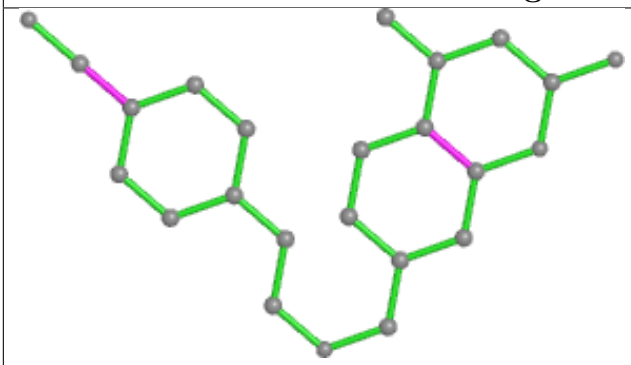
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	504	BTB	5	0
2	A	501	HEM	5	0
5	B	509	BTB	3	0
5	B	504	BTB	6	0
3	A	502	H4B	1	0

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.

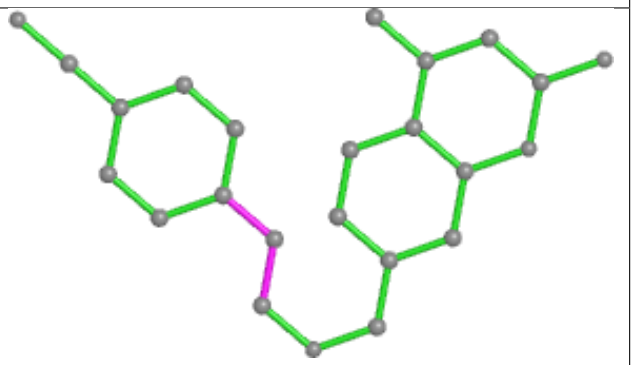
Ligand 9OG B 503



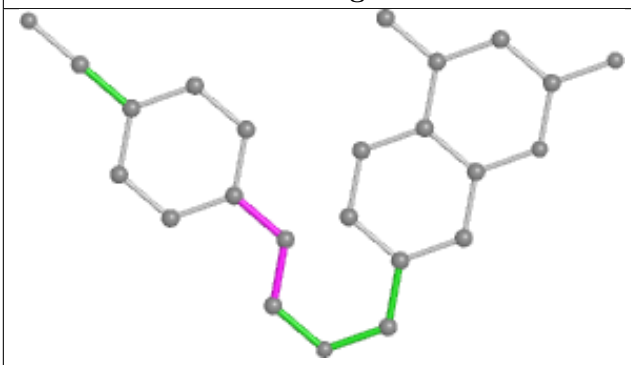
Ligand 9OG A 503



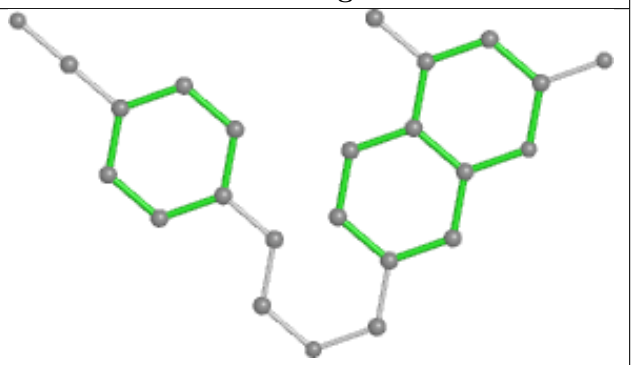
Bond lengths



Bond angles

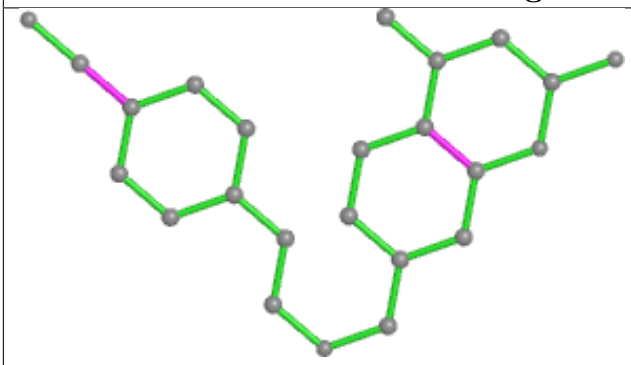


Torsions

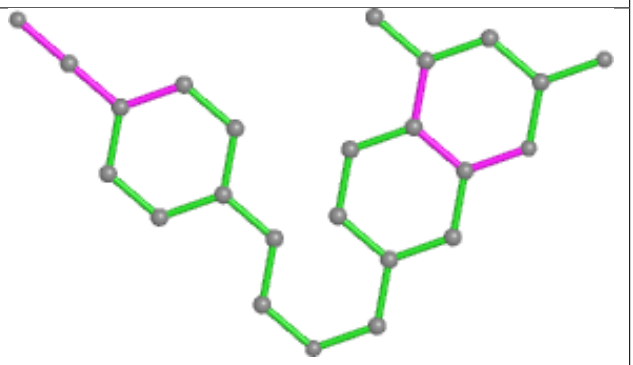


Rings

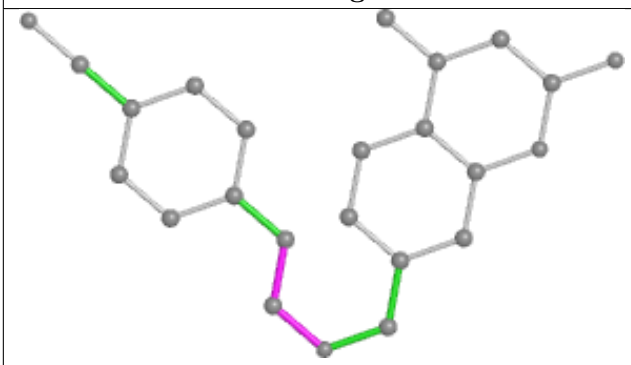
Ligand 9OG C 503



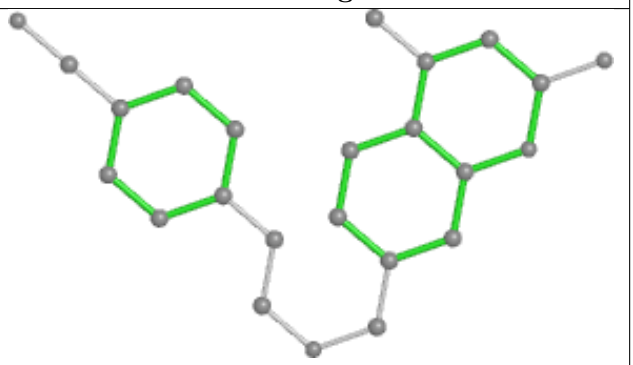
Bond lengths



Bond angles

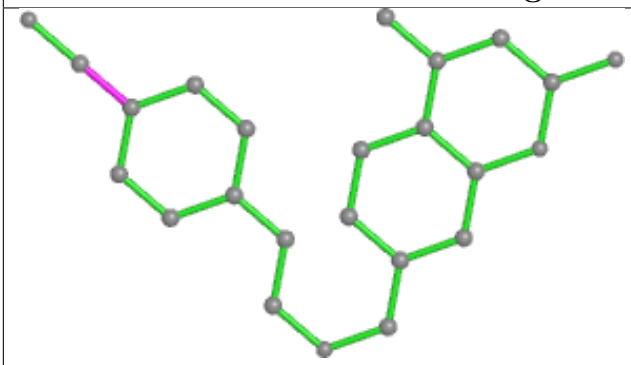


Torsions

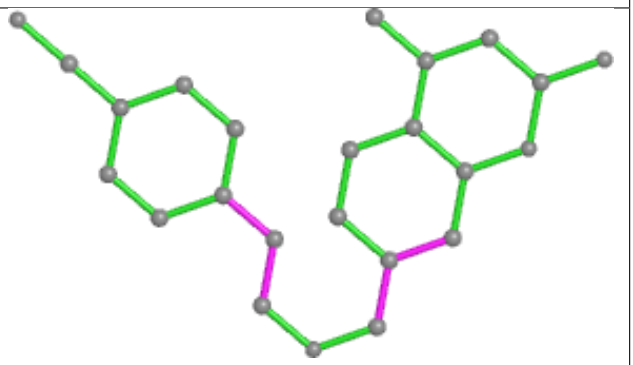


Rings

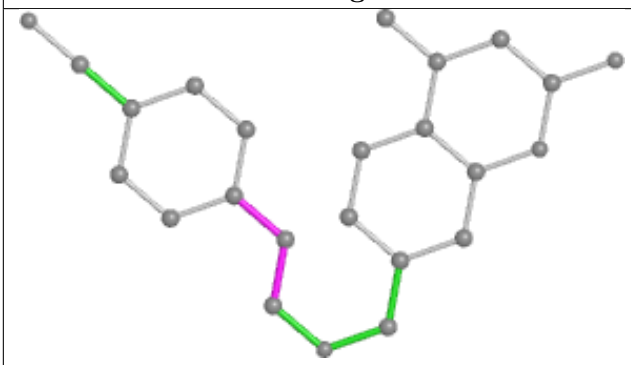
Ligand 9OG D 504



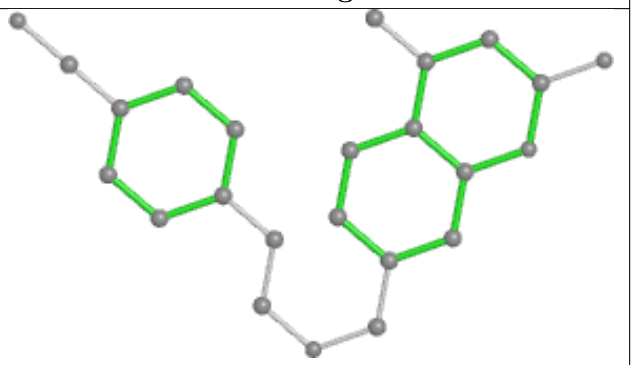
Bond lengths



Bond angles

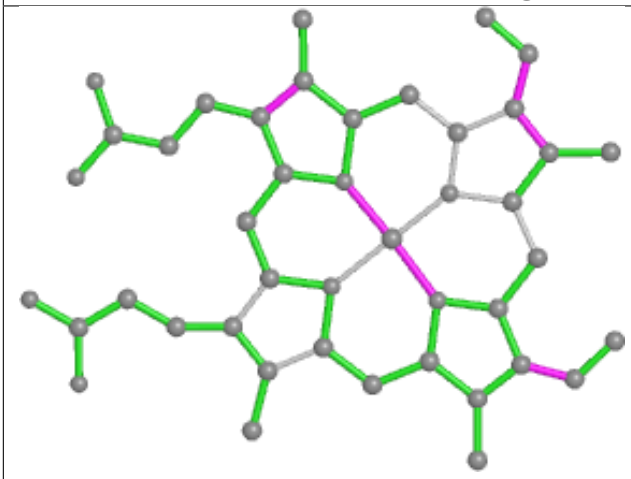


Torsions

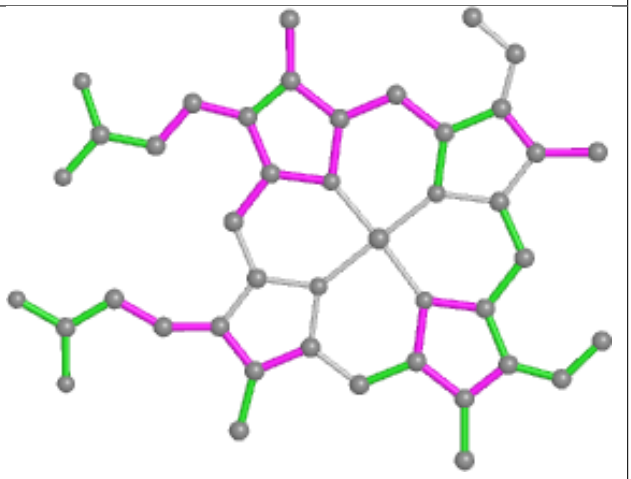


Rings

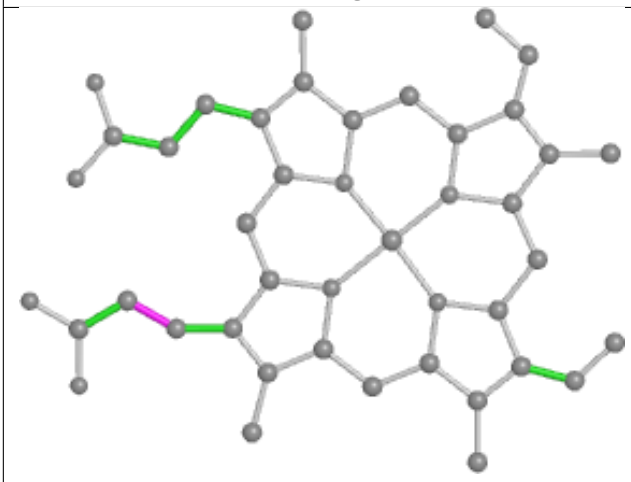
Ligand HEM D 502



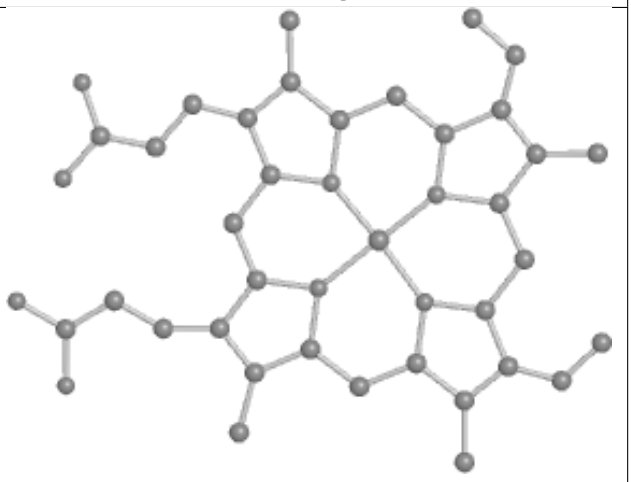
Bond lengths



Bond angles

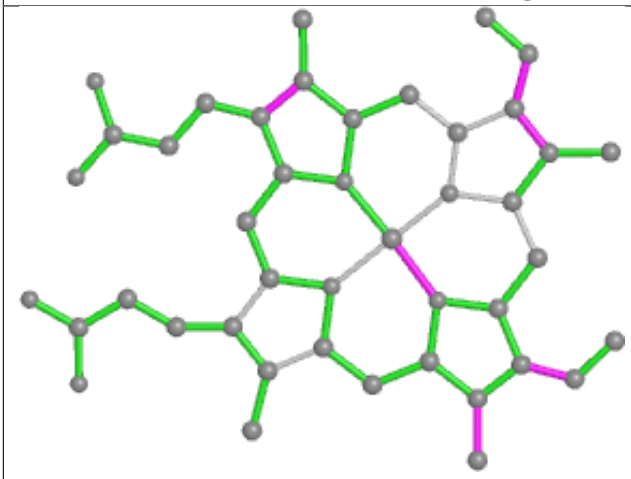


Torsions

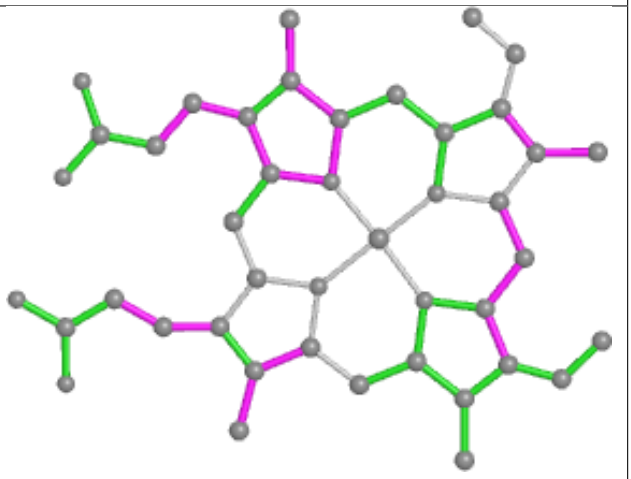


Rings

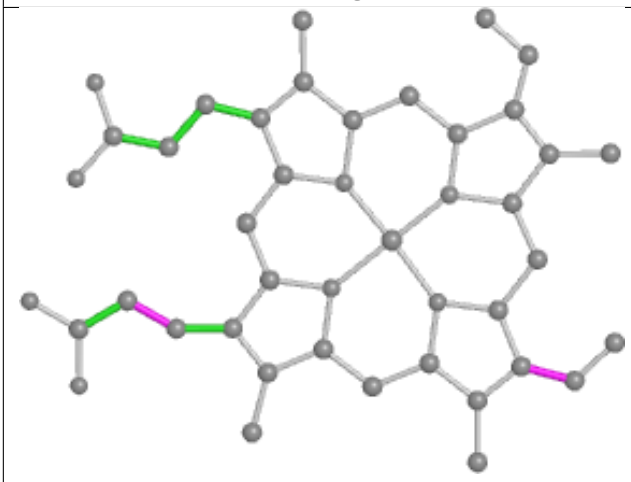
Ligand HEM C 501



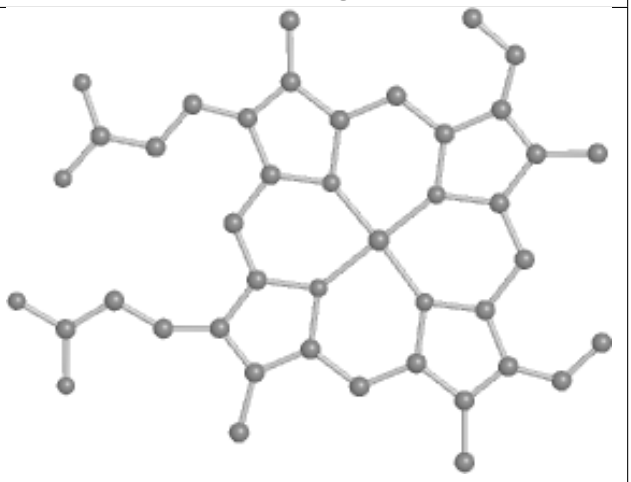
Bond lengths



Bond angles

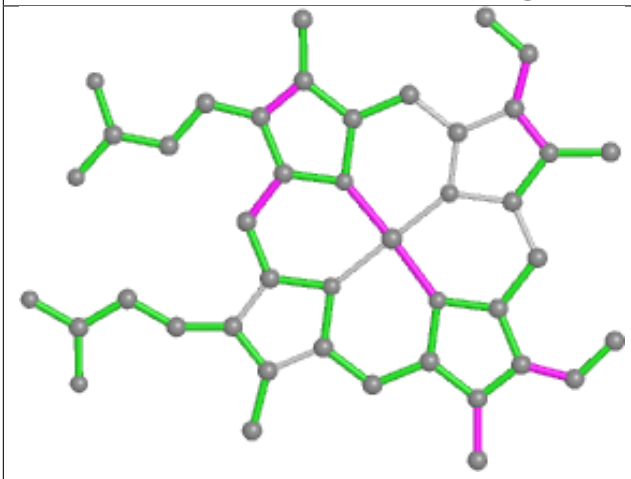


Torsions

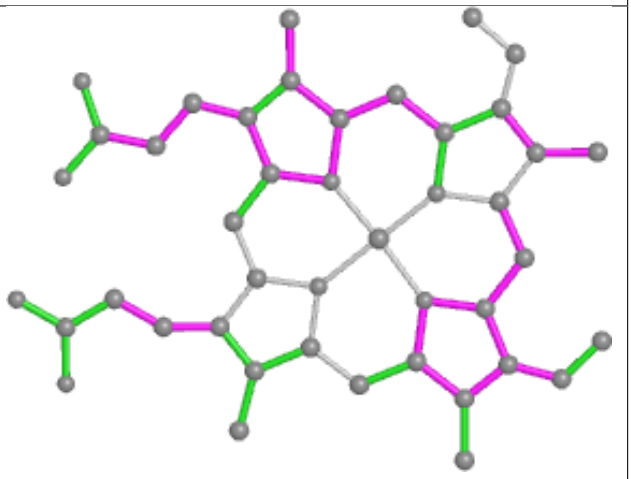


Rings

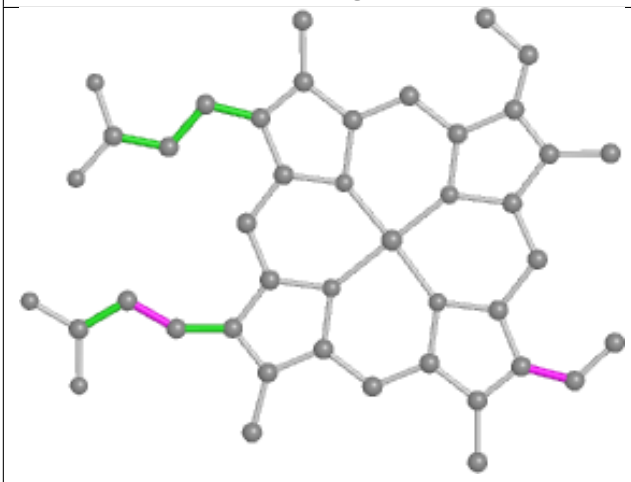
Ligand HEM B 501



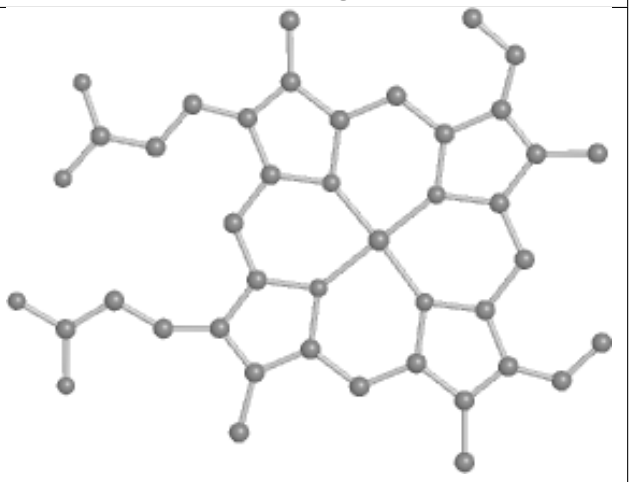
Bond lengths



Bond angles

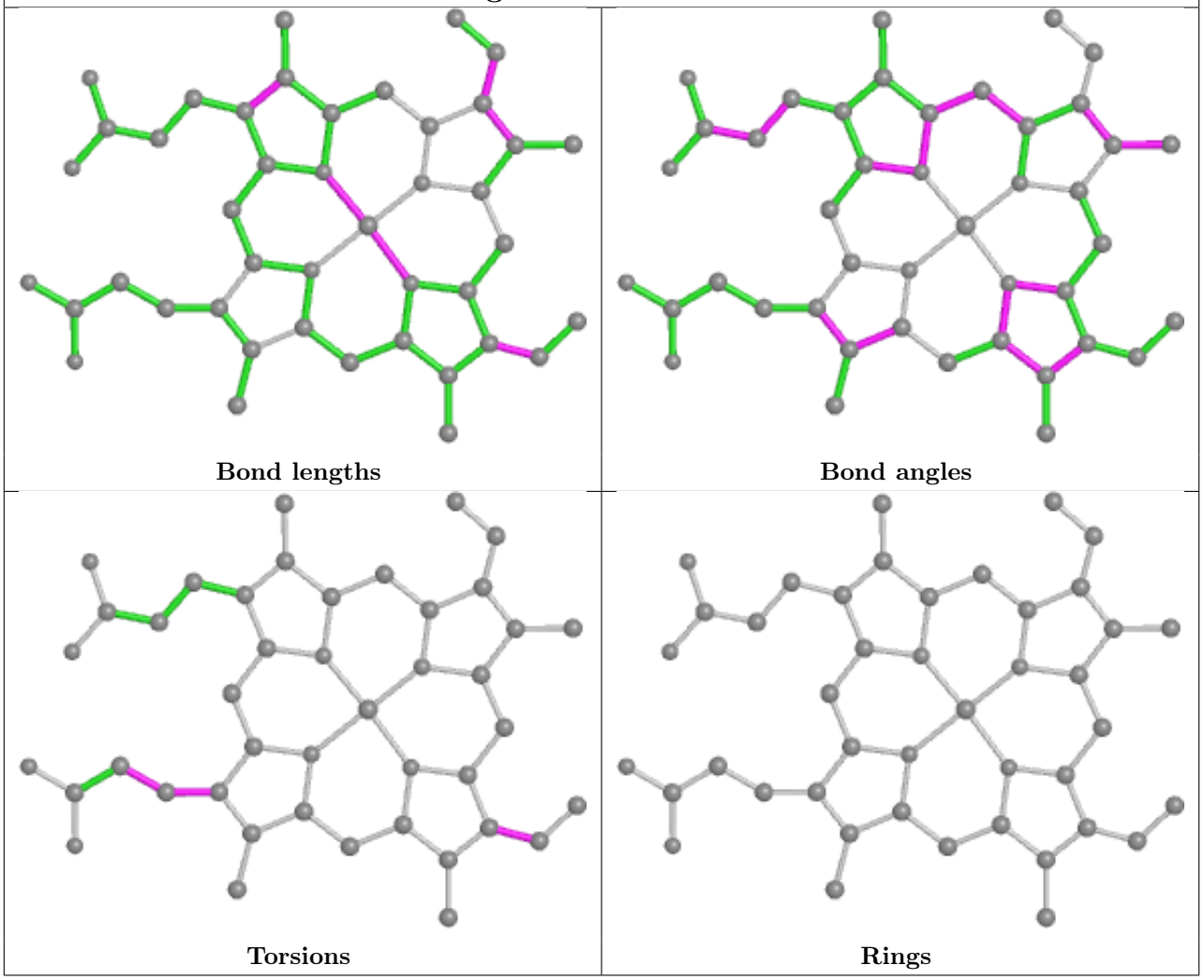


Torsions



Rings

Ligand HEM A 501



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	404/440 (91%)	0.18	24 (5%)	22	24	42, 81, 143, 185	0
1	B	402/440 (91%)	-0.20	6 (1%)	73	75	39, 60, 103, 157	0
1	C	401/440 (91%)	-0.07	12 (2%)	50	53	41, 70, 114, 160	0
1	D	402/440 (91%)	-0.20	8 (1%)	65	68	38, 63, 103, 152	0
All	All	1609/1760 (91%)	-0.07	50 (3%)	49	52	38, 68, 125, 185	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	108	LYS	7.5
1	A	109	LEU	5.7
1	B	259	GLY	5.5
1	A	153	VAL	5.1
1	A	107	ARG	5.0
1	C	142	GLY	4.6
1	A	120	PRO	4.4
1	A	163	TYR	4.1
1	C	238	ARG	4.0
1	B	68	PHE	3.8
1	B	89	GLN	3.7
1	A	293	LEU	3.6
1	D	67	LYS	3.4
1	C	259	GLY	3.4
1	A	305	LEU	3.3
1	B	142	GLY	3.3
1	A	262	ARG	3.2
1	D	255	ARG	3.2
1	A	151	GLN	3.1
1	C	239	GLY	3.1
1	C	273	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	468	PHE	3.0
1	A	162	THR	3.0
1	C	143	SER	2.9
1	A	480	TRP	2.8
1	C	296	PRO	2.7
1	D	68	PHE	2.7
1	B	90	GLN	2.7
1	A	244	TRP	2.6
1	A	238	ARG	2.6
1	A	145	ALA	2.6
1	A	150	LEU	2.6
1	D	90	GLN	2.6
1	C	120	PRO	2.5
1	A	160	THR	2.5
1	D	258	ASP	2.5
1	C	141	SER	2.5
1	A	128	ARG	2.4
1	C	304	LEU	2.3
1	A	142	GLY	2.3
1	D	257	GLN	2.3
1	A	202	ARG	2.3
1	A	479	PRO	2.3
1	C	68	PHE	2.2
1	D	261	VAL	2.1
1	A	346	LEU	2.1
1	A	279	TRP	2.1
1	D	259	GLY	2.1
1	B	143	SER	2.1
1	A	125	SER	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.

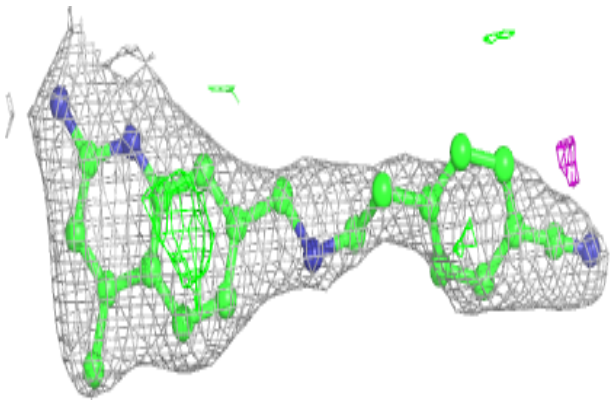
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	CL	A	509	1/1	0.61	0.12	91,91,91,91	0
5	BTB	C	505	14/14	0.79	0.13	74,96,107,109	0
8	CL	C	507	1/1	0.80	0.15	103,103,103,103	0
3	H4B	B	502	17/17	0.82	0.21	52,77,122,127	0
5	BTB	A	504	14/14	0.86	0.12	88,108,112,113	0
5	BTB	D	506	14/14	0.87	0.28	86,96,99,103	0
5	BTB	A	505	14/14	0.89	0.14	77,88,105,111	0
5	BTB	B	506	14/14	0.89	0.10	74,101,109,109	0
3	H4B	D	503	17/17	0.90	0.18	41,69,121,121	0
3	H4B	C	502	17/17	0.91	0.20	51,79,92,93	0
3	H4B	A	502	17/17	0.92	0.16	55,78,98,100	0
5	BTB	D	505	14/14	0.92	0.13	39,82,100,107	0
4	9OG	B	503	24/24	0.92	0.16	54,71,96,102	0
7	GOL	A	508	6/6	0.92	0.24	62,73,96,98	0
7	GOL	C	506	6/6	0.92	0.25	54,66,84,85	0
5	BTB	B	505	14/14	0.92	0.25	71,96,106,108	0
4	9OG	D	504	24/24	0.92	0.13	51,70,93,94	0
5	BTB	C	504	14/14	0.93	0.20	71,87,96,97	0
4	9OG	A	503	24/24	0.94	0.15	65,89,103,109	0
5	BTB	B	504	14/14	0.94	0.12	55,78,100,104	0
4	9OG	C	503	24/24	0.94	0.14	60,74,85,92	0
5	BTB	A	506	14/14	0.95	0.13	73,93,98,98	0
5	BTB	B	509	14/14	0.95	0.14	59,101,121,122	0
8	CL	D	507	1/1	0.95	0.10	69,69,69,69	0
8	CL	B	507	1/1	0.96	0.14	79,79,79,79	0
2	HEM	B	501	43/43	0.98	0.13	35,57,85,96	0
2	HEM	C	501	43/43	0.98	0.14	48,63,89,98	0
2	HEM	D	502	43/43	0.98	0.14	34,54,82,92	0
2	HEM	A	501	43/43	0.98	0.16	62,78,91,105	0
9	GD	A	510	1/1	0.99	0.18	105,105,105,105	0
9	GD	B	508	1/1	0.99	0.21	61,61,61,61	0
9	GD	B	510	1/1	0.99	0.14	102,102,102,102	0
6	ZN	D	501	1/1	1.00	0.14	60,60,60,60	0
6	ZN	A	507	1/1	1.00	0.15	73,73,73,73	0
9	GD	D	508	1/1	1.00	0.20	58,58,58,58	0

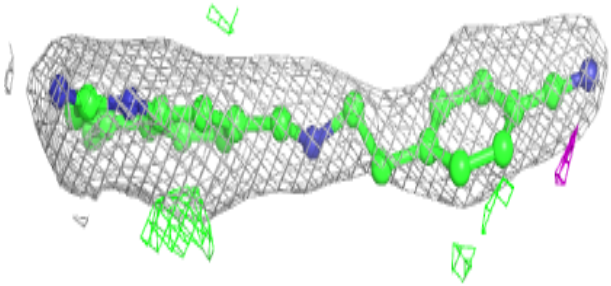
The following is a graphical depiction of the model fit to experimental electron density of all

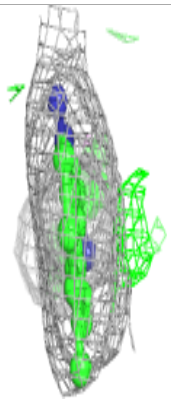
instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 9OG 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)

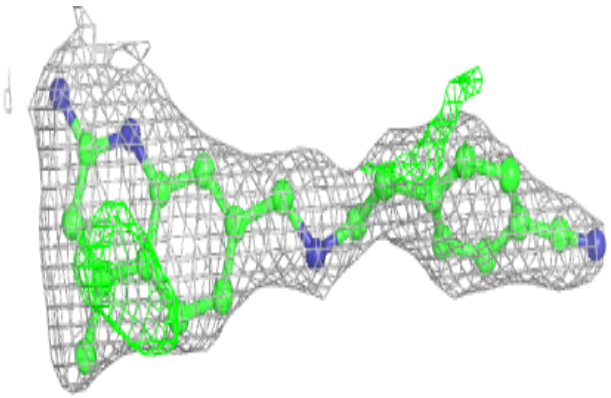


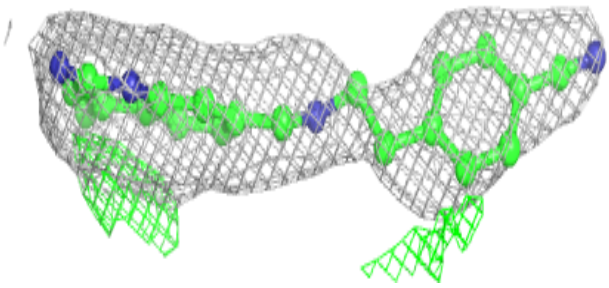


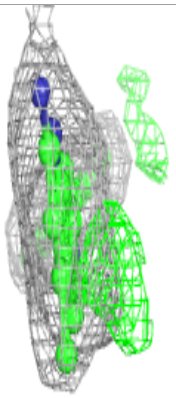


Electron density around 9OG D 504:

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

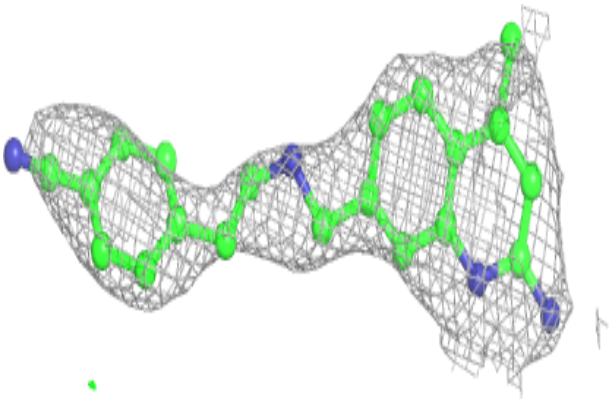


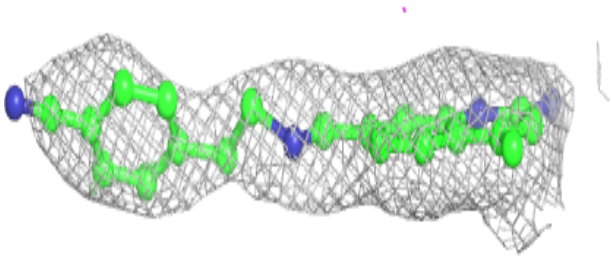


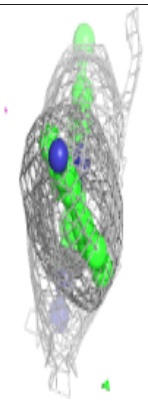


Electron density around 9OG A 503:

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

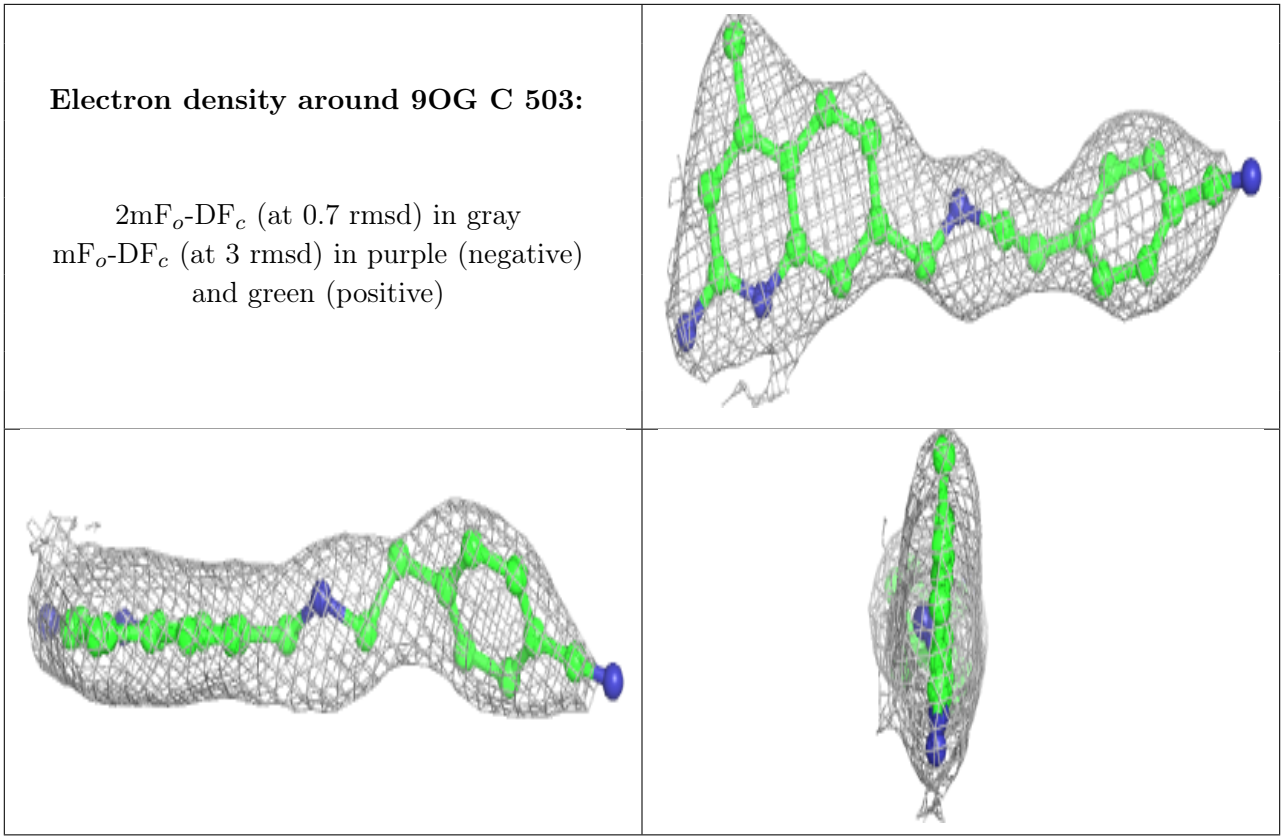






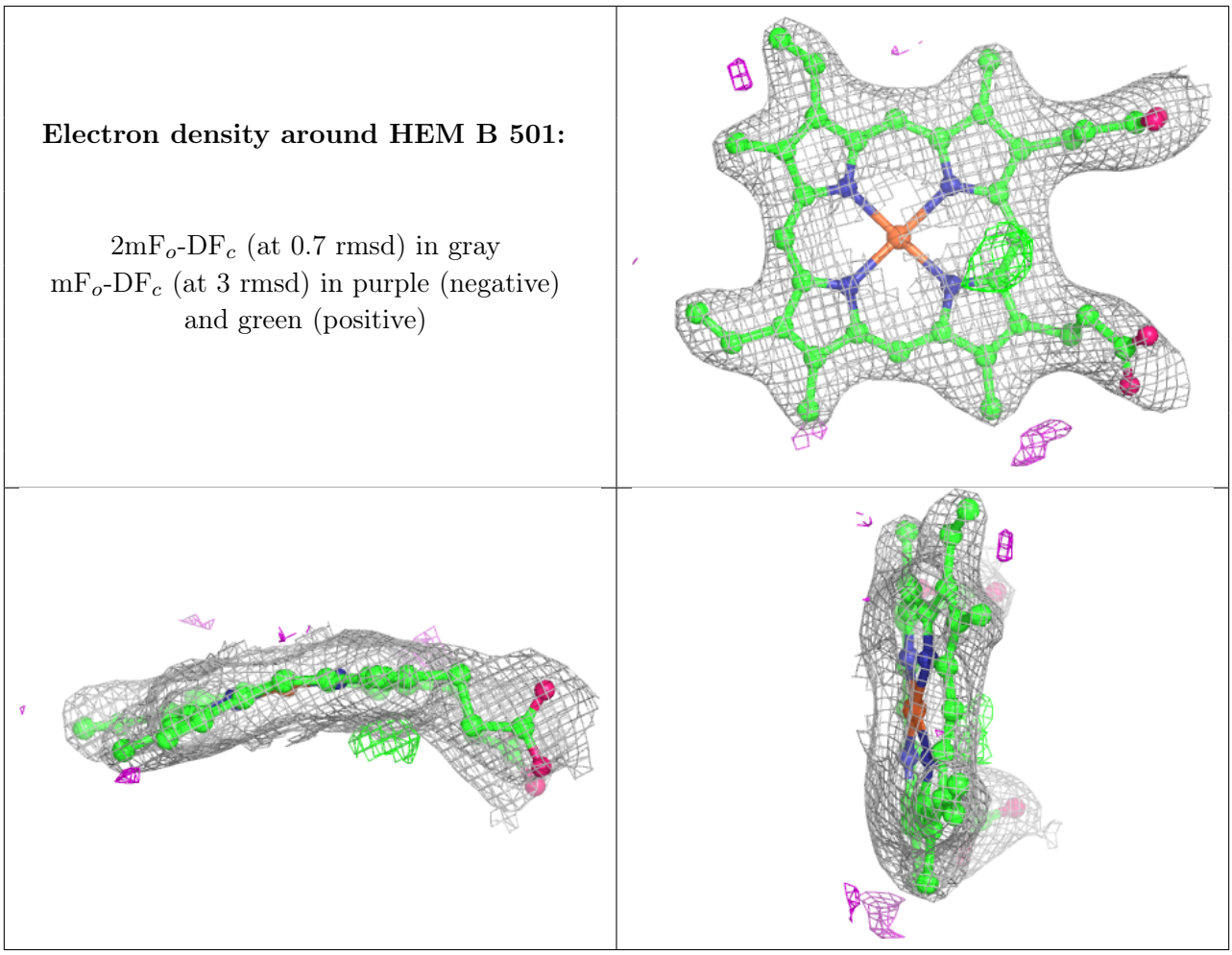
Electron density around 9OG C 503:

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



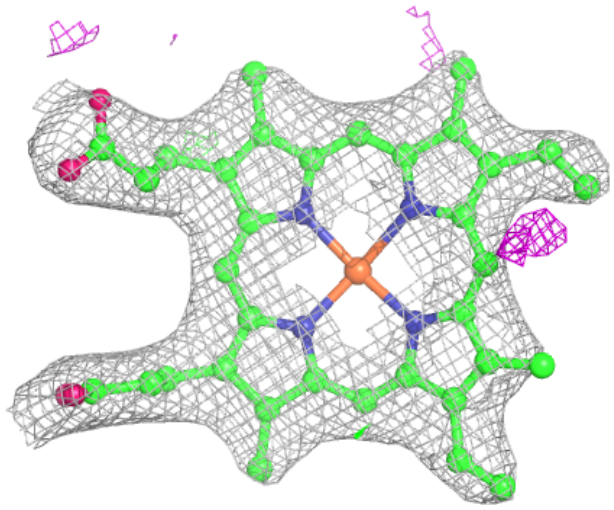
Electron density around HEM B 501:

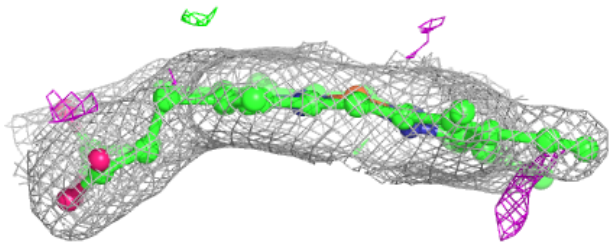
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

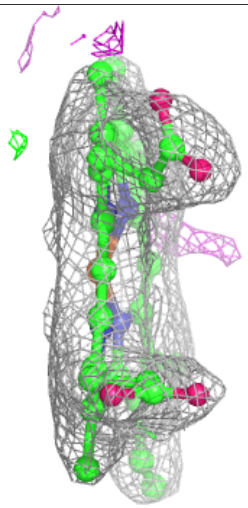


Electron density around HEM C 501:

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

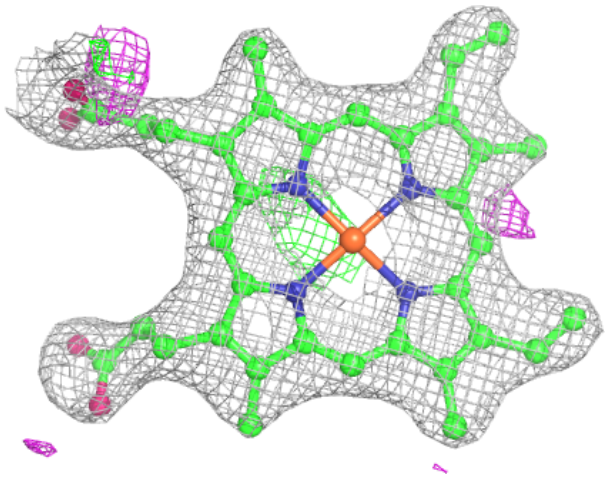


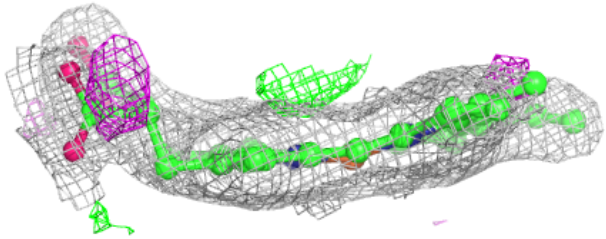


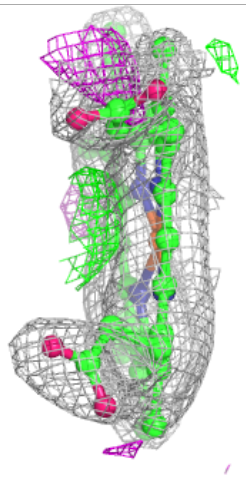


Electron density around HEM D 502:

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

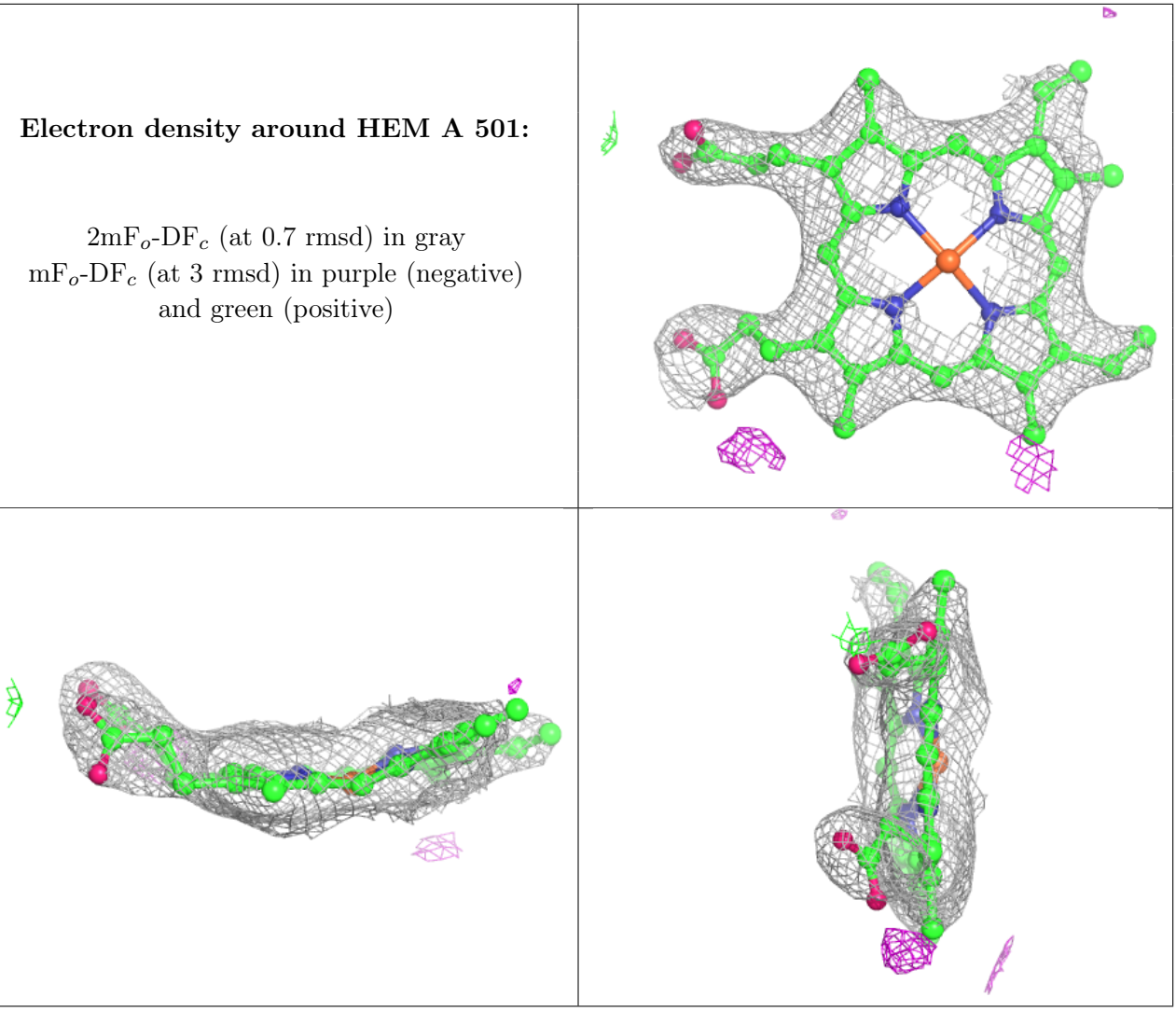






Electron density around HEM A 501:

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



6.5 Other polymers (i)

There are no such residues in this entry.