



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:21 PM UTC

PDB ID : 6POV / pdb_00006pov
Title : Structure of human endothelial nitric oxide synthase heme domain in complex with 7-(3-(2-Aminoethyl)phenyl)-4-methylquinolin-2-amine
Authors : Chreifi, G.; Li, H.; Poulos, T.L.
Deposited on : 2019-07-05
Resolution : 2.05 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

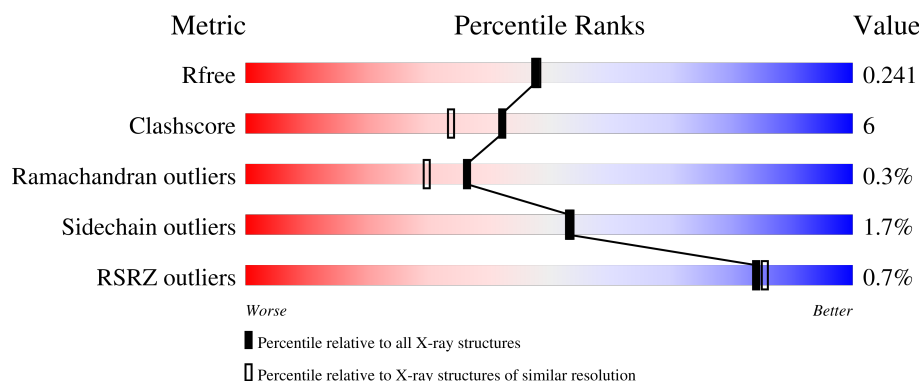
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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}	180053	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	440	% 81% 11% 8%
1	B	440	80% 11% 8%
1	C	440	% 76% 15% • 8%
1	D	440	82% 9% 8%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 13932 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.

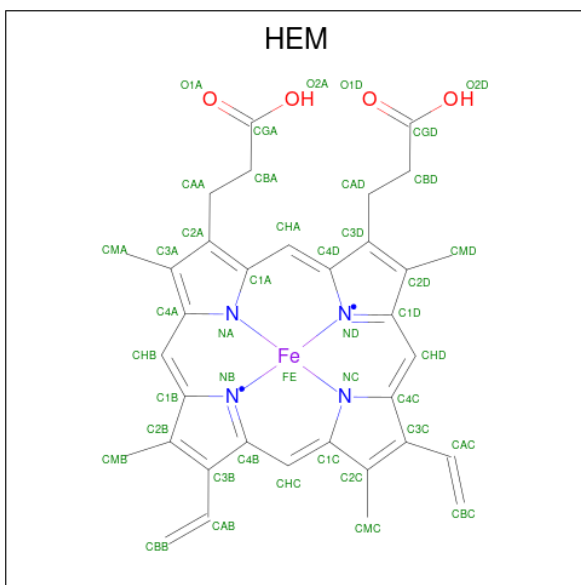
- Molecule 1 is a protein called Nitric oxide synthase, endothelial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	404	Total	C	N	O	S	0	2	0
			3234	2060	570	588	16			
1	B	403	Total	C	N	O	S	0	5	0
			3241	2063	570	591	17			
1	C	404	Total	C	N	O	S	0	3	0
			3240	2064	570	590	16			
1	D	403	Total	C	N	O	S	0	5	0
			3241	2063	570	591	17			

There are 4 discrepancies between the modelled and reference sequences:

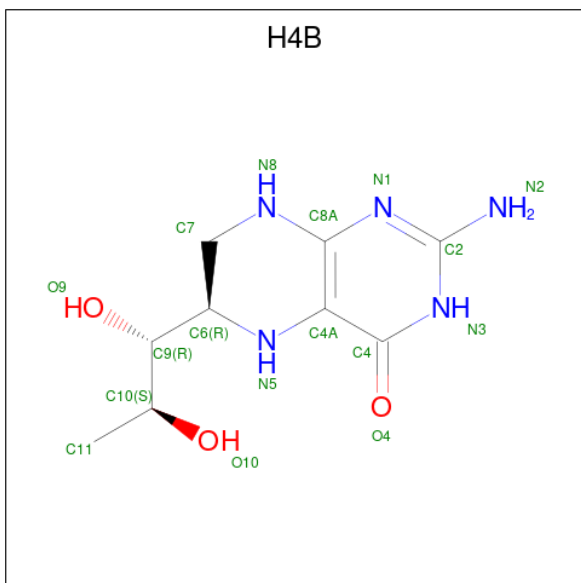
Chain	Residue	Modelled	Actual	Comment	Reference
A	298	GLU	ASP	variant	UNP P29474
B	298	GLU	ASP	variant	UNP P29474
C	298	GLU	ASP	variant	UNP P29474
D	298	GLU	ASP	variant	UNP P29474

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



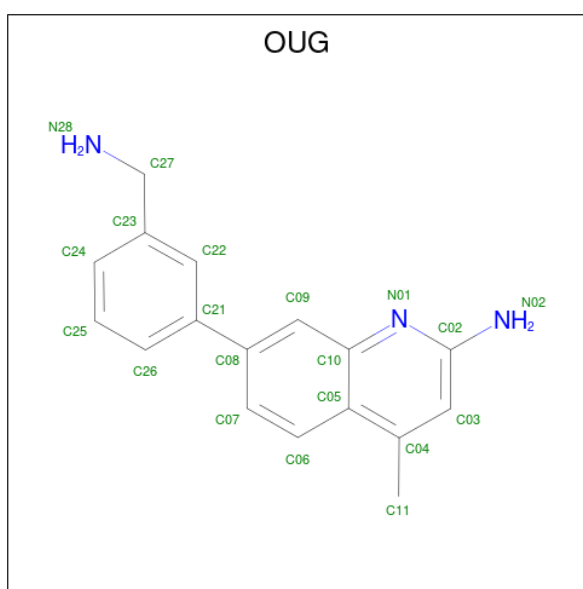
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is 5,6,7,8-TETRAHYDROBIOPTERIN (CCD ID: H4B) (formula: $\text{C}_9\text{H}_{15}\text{N}_5\text{O}_3$).



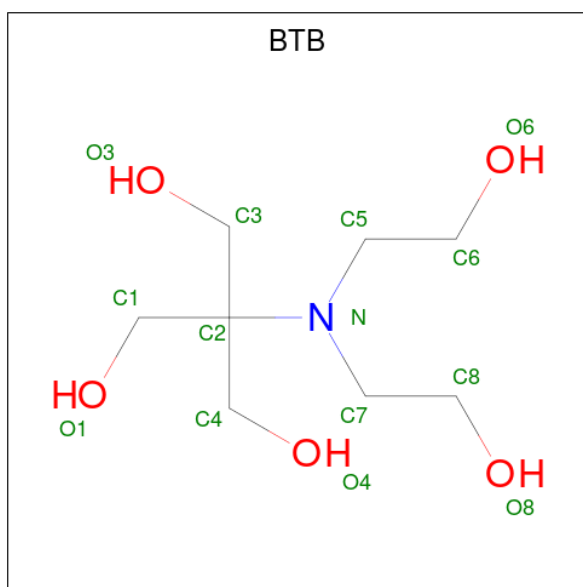
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		
3	C	1	Total	C	N	O	0	0
			17	9	5	3		
3	D	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 4 is 7-[3-(aminomethyl)phenyl]-4-methylquinolin-2-amine (CCD ID: OUG) (formula: C₁₇H₁₇N₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			20	17	3		
4	B	1	Total	C	N	0	0
			20	17	3		
4	C	1	Total	C	N	0	0
			20	17	3		
4	D	1	Total	C	N	0	0
			20	17	3		

- Molecule 5 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (CCD ID: BTB) (formula: C₈H₁₉NO₅).

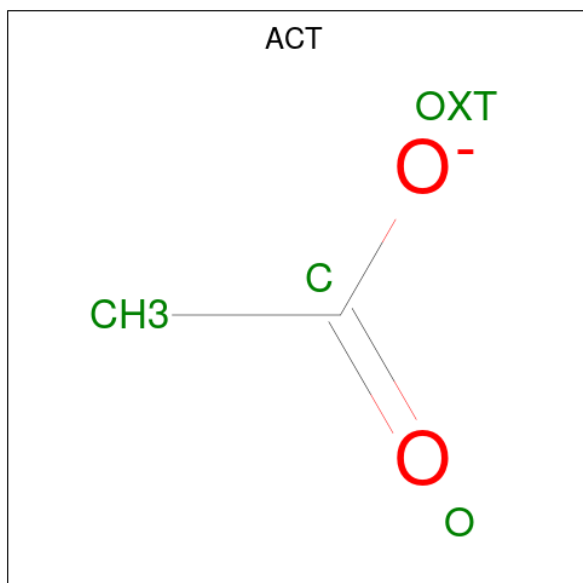


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1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

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

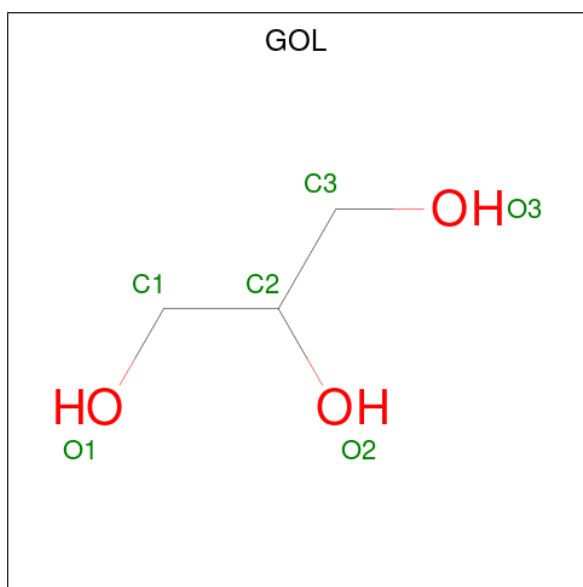
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Zn	0	0
			1	1		
6	C	1	Total	Zn	0	0
			1	1		

- Molecule 7 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 9 is GADOLINIUM ATOM (CCD ID: GD) (formula: Gd).

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

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	88	Total	O	0	0
			88	88		
10	B	137	Total	O	0	0
			137	137		
10	C	72	Total	O	0	0
			72	72		

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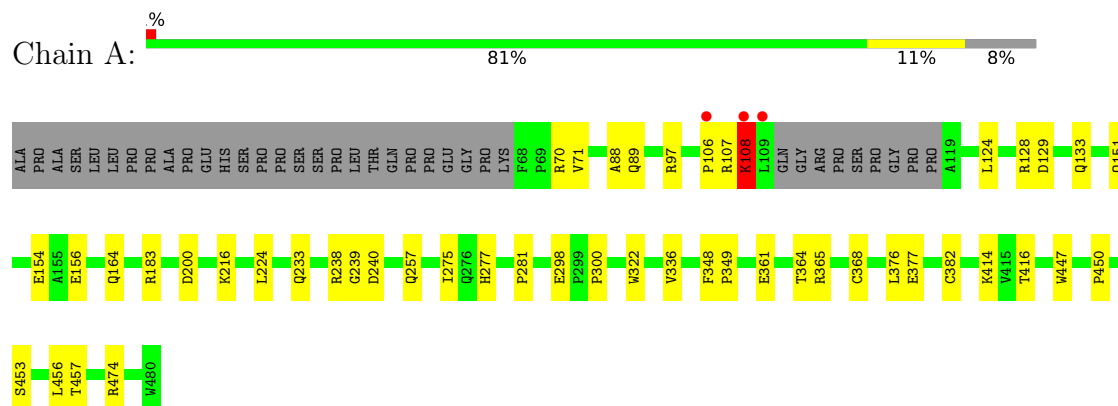
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	D	129	Total 129	O 129	0	0

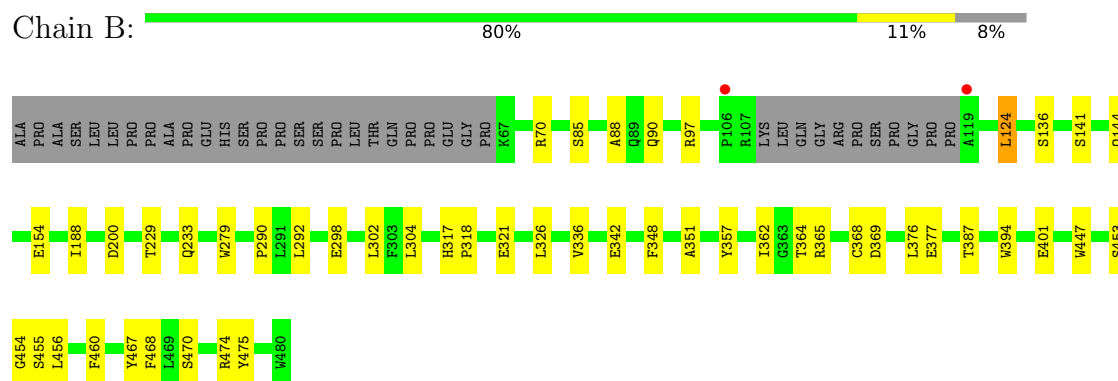
3 Residue-property plots [i](#)

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.

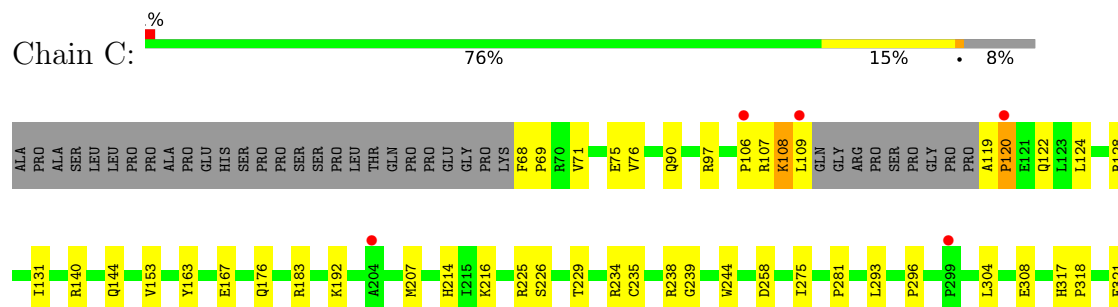
- Molecule 1: Nitric oxide synthase, endothelial



- Molecule 1: Nitric oxide synthase, endothelial

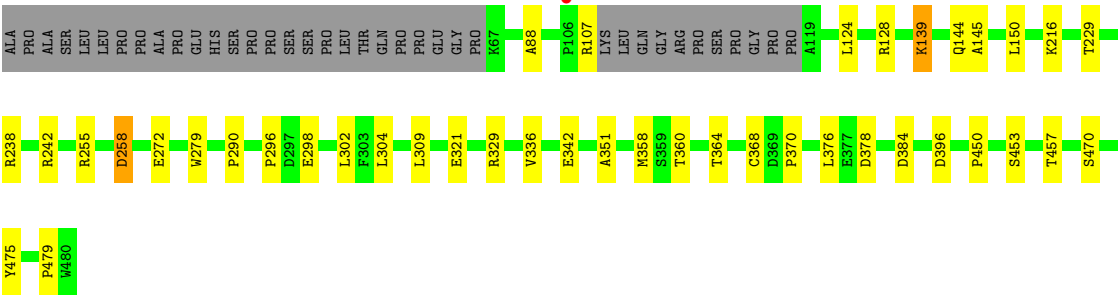
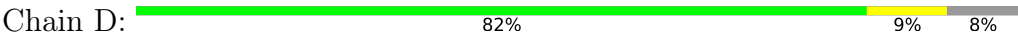


- Molecule 1: Nitric oxide synthase, endothelial





● Molecule 1: Nitric oxide synthase, endothelial



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	59.82Å 152.96Å 108.99Å 90.00° 90.80° 90.00°	Depositor
Resolution (Å)	39.21 – 2.05 39.21 – 2.05	Depositor EDS
% Data completeness (in resolution range)	98.5 (39.21-2.05) 98.5 (39.21-2.05)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 2.05Å)	Xtriage
Refinement program	PHENIX (1.11.1-2575_1496: ???)	Depositor
R, R_{free}	0.195 , 0.247 0.189 , 0.241	Depositor DCC
R_{free} test set	6084 reflections (3.50%)	wwPDB-VP
Wilson B-factor (Å ²)	40.8	Xtriage
Anisotropy	0.401	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 61.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.097 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	13932	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GD, ACT, H4B, OUG, HEM, GOL, BTB, 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	0.30	0/3332	0.48	0/4539
1	B	0.37	0/3345	0.53	0/4557
1	C	0.29	0/3341	0.47	0/4551
1	D	0.34	0/3345	0.52	0/4557
All	All	0.33	0/13363	0.50	0/18204

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 [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	3234	0	3145	32	0
1	B	3241	0	3150	33	0
1	C	3240	0	3151	48	0
1	D	3241	0	3150	32	0
2	A	43	0	30	1	0
2	B	43	0	30	6	0
2	C	43	0	30	4	0
2	D	43	0	30	4	0
3	A	17	0	15	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	17	0	15	0	0
3	C	17	0	15	1	0
3	D	17	0	15	0	0
4	A	20	0	0	2	0
4	B	20	0	0	1	0
4	C	20	0	0	3	0
4	D	20	0	0	1	0
5	A	56	0	74	11	0
5	B	42	0	55	5	0
5	C	42	0	56	6	0
5	D	56	0	74	11	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
7	A	4	0	3	0	0
7	B	4	0	3	1	0
7	C	4	0	3	0	0
7	D	4	0	3	0	0
8	A	6	0	8	0	0
8	C	6	0	8	2	0
9	A	1	0	0	0	0
9	B	1	0	0	0	0
9	C	1	0	0	0	0
9	D	1	0	0	0	0
10	A	88	0	0	2	1
10	B	137	0	0	4	0
10	C	72	0	0	3	0
10	D	129	0	0	2	1
All	All	13932	0	13063	166	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 6.

All (166) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:480:TRP:H	1:C:480:TRP:CD1	1.97	0.81
1:B:475:TYR:OH	2:B:501:HEM:O1D	2.03	0.77
1:C:382:CYS:HA	5:C:505:BTB:H11	1.68	0.74
1:B:290:PRO:HB3	1:B:304:LEU:HD23	1.69	0.74
5:B:505:BTB:O8	5:B:505:BTB:H62	1.88	0.72
1:C:480:TRP:H	1:C:480:TRP:HD1	1.36	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:PRO:HB2	1:C:122:GLN:HG2	1.72	0.71
2:B:501:HEM:HBD2	10:B:686:HOH:O	1.91	0.70
1:B:342[B]:GLU:OE1	1:B:474:ARG:NH1	2.23	0.70
1:B:365:ARG:NH2	1:B:369:ASP:OD2	2.25	0.69
2:C:502:HEM:HMC2	2:C:502:HEM:HBC2	1.76	0.68
1:D:298:GLU:OE1	5:D:506:BTB:O8	2.11	0.67
2:A:501:HEM:HBB2	2:A:501:HEM:HHC	1.76	0.67
1:C:90:GLN:HB3	1:C:468:PHE:CD1	2.30	0.66
1:B:321:GLU:OE2	5:B:505:BTB:O4	2.13	0.65
1:D:336:VAL:HG21	4:D:503:OUG:C07	2.27	0.65
2:D:501:HEM:O1A	10:D:601:HOH:O	2.14	0.65
1:B:154:GLU:OE2	10:B:601:HOH:O	2.14	0.65
1:C:183:ARG:HB2	2:C:502:HEM:CGD	2.27	0.64
1:A:365:ARG:HH12	3:A:502:H4B:C4	2.10	0.64
1:A:233:GLN:O	1:A:238:ARG:NH2	2.32	0.63
5:A:505:BTB:O6	1:D:384:ASP:OD2	2.16	0.63
2:C:502:HEM:HBB2	2:C:502:HEM:HHC	1.81	0.62
1:A:88:ALA:O	1:B:97:ARG:NH1	2.33	0.62
1:B:336:VAL:HG21	4:B:503:OUG:C07	2.29	0.62
1:C:68:PHE:N	10:C:601:HOH:O	2.33	0.61
1:D:290:PRO:HB3	1:D:304:LEU:HD23	1.81	0.61
5:A:505:BTB:O8	1:D:384:ASP:OD2	2.18	0.60
1:B:124:LEU:HD11	1:B:154:GLU:HG3	1.83	0.60
1:A:336:VAL:HG21	4:A:503:OUG:C07	2.32	0.59
1:C:163:TYR:CZ	1:C:346:LEU:HD11	2.38	0.59
1:C:192:LYS:HZ1	1:C:225:ARG:HA	1.67	0.59
1:C:97:ARG:HG2	1:D:88:ALA:HB3	1.85	0.59
2:B:501:HEM:HBC2	2:B:501:HEM:HMC2	1.84	0.58
1:C:131:ILE:HD11	1:C:153:VAL:HG21	1.85	0.58
1:B:90:GLN:HB3	1:B:468:PHE:CD1	2.38	0.58
1:C:436:LYS:NZ	10:C:602:HOH:O	2.36	0.58
1:A:97:ARG:NH1	1:B:88:ALA:O	2.37	0.57
1:A:322:TRP:CD1	5:A:504:BTB:H62	2.40	0.57
1:C:321:GLU:H	1:C:321:GLU:CD	2.13	0.57
1:C:238:ARG:NH1	1:C:239:GLY:O	2.39	0.56
1:D:298:GLU:CD	5:D:506:BTB:H42	2.31	0.56
1:D:342[A]:GLU:OE1	1:D:470:SER:OG	2.20	0.56
1:A:382:CYS:HA	5:A:504:BTB:H12	1.88	0.56
1:A:298:GLU:OE2	5:A:507:BTB:H51	2.06	0.56
1:A:70:ARG:NH1	10:A:601:HOH:O	2.37	0.55
1:D:298:GLU:OE1	5:D:506:BTB:O6	2.25	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:364:THR:HG21	1:C:452:ILE:HG23	1.89	0.55
2:D:501:HEM:HBB2	2:D:501:HEM:HHC	1.89	0.54
1:C:364:THR:O	1:C:368:CYS:HB2	2.08	0.54
1:D:107:ARG:NH2	10:D:603:HOH:O	2.28	0.53
1:A:106:PRO:HB2	1:A:108:LYS:HG2	1.90	0.53
1:A:361:GLU:OE2	4:A:503:OUG:N02	2.41	0.53
1:D:279:TRP:HB2	1:D:302:LEU:HD21	1.91	0.53
1:C:183:ARG:HD3	1:C:447:TRP:CD2	2.44	0.53
1:C:207:MET:HE3	1:C:293:LEU:HB3	1.90	0.53
1:C:361:GLU:OE2	4:C:504:OUG:N02	2.42	0.52
1:C:336:VAL:HG21	4:C:504:OUG:C07	2.39	0.52
1:C:234:ARG:NH1	1:C:347:GLU:OE2	2.43	0.52
1:D:321:GLU:OE2	5:D:505:BTB:O4	2.27	0.52
1:A:128:ARG:HH22	1:A:154:GLU:CD	2.17	0.52
1:C:167:GLU:OE2	8:C:510:GOL:O3	2.22	0.51
1:C:275:ILE:HD11	1:C:281:PRO:HB3	1.93	0.51
1:D:255:ARG:NH1	1:D:272:GLU:OE2	2.44	0.51
1:C:377:GLU:OE2	5:C:506:BTB:O1	2.21	0.50
1:D:144:GLN:NE2	1:D:145:ALA:H	2.10	0.50
1:C:106:PRO:C	1:C:108:LYS:H	2.20	0.50
1:C:106:PRO:O	1:C:108:LYS:N	2.45	0.49
5:C:506:BTB:O4	5:C:506:BTB:O3	2.24	0.49
1:A:240:ASP:HB3	1:A:349:PRO:HG2	1.93	0.49
1:A:364:THR:O	1:A:368:CYS:HB2	2.12	0.49
1:D:378:ASP:OD1	5:D:507:BTB:H41	2.12	0.49
1:A:183:ARG:HD3	1:A:447:TRP:CD2	2.48	0.49
1:B:317:HIS:NE2	1:B:401:GLU:OE1	2.41	0.49
1:C:365:ARG:HH12	3:C:503:H4B:C4	2.25	0.49
1:B:144:GLN:NE2	10:B:607:HOH:O	2.44	0.49
1:B:279:TRP:HB2	1:B:302:LEU:HD21	1.93	0.48
1:D:368:CYS:SG	1:D:376:LEU:HD13	2.53	0.48
1:B:377:GLU:OE2	5:B:507:BTB:H81	2.12	0.48
1:D:358:MET:HE3	1:D:360:THR:OG1	2.13	0.48
1:A:200:ASP:OD1	1:A:200:ASP:N	2.41	0.48
1:C:124:LEU:O	1:C:128:ARG:HG3	2.14	0.47
1:A:453:SER:HB3	1:A:456:LEU:HD12	1.95	0.47
5:A:506:BTB:H12	5:A:506:BTB:H72	1.64	0.47
1:D:450:PRO:HG2	1:D:457:THR:HG21	1.95	0.47
1:B:364:THR:O	1:B:368:CYS:HB2	2.14	0.47
2:D:501:HEM:HMC2	2:D:501:HEM:HBC2	1.94	0.47
5:A:505:BTB:H12	5:A:505:BTB:H72	1.38	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:ILE:HD11	1:A:281:PRO:HB3	1.96	0.47
1:A:450:PRO:HG2	1:A:457:THR:HG21	1.97	0.47
1:B:124:LEU:HD23	1:B:124:LEU:HA	1.75	0.47
1:C:308:GLU:H	1:C:308:GLU:CD	2.23	0.47
1:B:233:GLN:HB3	1:B:348:PHE:CE2	2.51	0.46
1:C:244:TRP:CD1	1:C:479:PRO:HG3	2.51	0.46
1:A:106:PRO:C	1:A:108:LYS:H	2.22	0.46
1:B:85:SER:HB3	1:B:467:TYR:CE1	2.49	0.46
5:C:507:BTB:O6	5:C:507:BTB:H12	2.16	0.46
1:D:216:LYS:HB2	1:D:309:LEU:HD11	1.97	0.46
1:A:224:LEU:HB2	1:A:416:THR:HB	1.97	0.46
1:A:257:GLN:HB2	5:A:506:BTB:O4	2.16	0.46
1:B:298:GLU:OE2	5:B:506:BTB:O8	2.33	0.46
5:D:507:BTB:H31	5:D:507:BTB:H51	1.47	0.46
1:D:238:ARG:HG2	1:D:296:PRO:HB3	1.97	0.45
1:B:447:TRP:NE1	10:B:604:HOH:O	2.35	0.45
1:C:455:SER:HA	1:C:460:PHE:CG	2.52	0.45
1:D:128:ARG:HG3	1:D:150:LEU:HD22	1.98	0.44
1:D:364:THR:O	1:D:368:CYS:HB2	2.16	0.44
5:A:505:BTB:O6	5:A:505:BTB:O8	2.33	0.44
1:C:75:GLU:HG3	1:D:370:PRO:HG2	1.99	0.44
5:C:507:BTB:H42	5:C:507:BTB:H72	1.59	0.44
1:B:317:HIS:CG	1:B:318:PRO:HD2	2.52	0.44
1:B:454:GLY:O	1:B:460:PHE:HB2	2.17	0.44
1:C:229:THR:O	1:C:352:PRO:HD2	2.17	0.44
1:C:238:ARG:HG2	1:C:239:GLY:N	2.33	0.44
1:C:358:MET:HE3	1:C:360:THR:OG1	2.18	0.44
1:C:108:LYS:HB2	1:C:109:LEU:H	1.60	0.44
1:C:317:HIS:CG	1:C:318:PRO:HD2	2.53	0.44
5:C:507:BTB:O4	5:C:507:BTB:O1	2.23	0.44
1:A:277:HIS:CD2	1:A:300:PRO:HG2	2.53	0.44
1:C:119:ALA:HA	1:C:120:PRO:HD3	1.86	0.44
1:D:242:ARG:NH2	1:D:479:PRO:HD3	2.33	0.44
1:B:387:THR:HA	1:B:394:TRP:CD1	2.53	0.44
1:C:258:ASP:OD1	1:C:258:ASP:N	2.50	0.44
1:A:238:ARG:NH1	1:A:239:GLY:O	2.51	0.43
2:B:501:HEM:HMD1	2:B:501:HEM:HBD1	2.00	0.43
1:D:258:ASP:OD1	1:D:258:ASP:N	2.51	0.43
2:B:501:HEM:HHC	2:B:501:HEM:HBB2	2.01	0.43
1:A:376:LEU:HB2	10:A:625:HOH:O	2.17	0.43
1:A:377:GLU:OE1	5:A:505:BTB:H72	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:PRO:O	1:A:108:LYS:N	2.52	0.43
1:B:229:THR:O	1:B:351:ALA:HA	2.18	0.43
1:B:368:CYS:SG	1:B:376:LEU:HD13	2.58	0.43
1:C:167:GLU:OE2	8:C:510:GOL:O2	2.24	0.43
5:B:506:BTB:H11	5:B:506:BTB:H72	1.29	0.43
1:A:107:ARG:HG3	1:B:70:ARG:HH22	1.84	0.43
1:D:139:LYS:HE3	1:D:139:LYS:HB3	1.40	0.43
1:A:233:GLN:HB3	1:A:348:PHE:CE2	2.54	0.42
1:C:68:PHE:HA	1:C:69:PRO:HD3	1.93	0.42
1:A:124:LEU:O	1:A:128:ARG:HG3	2.18	0.42
5:A:506:BTB:H31	5:A:506:BTB:H52	1.62	0.42
1:B:453:SER:HB3	1:B:456:LEU:HD12	2.01	0.42
1:C:176:GLN:HB3	1:C:471:PRO:HD2	2.01	0.42
1:C:238:ARG:HH11	1:C:296:PRO:HB3	1.84	0.42
1:B:357:TYR:CD2	1:B:362:ILE:HD11	2.55	0.42
1:B:455:SER:HA	1:B:460:PHE:CG	2.54	0.42
1:C:396:ASP:OD2	1:D:453:SER:OG	2.29	0.42
5:D:506:BTB:H51	5:D:506:BTB:H32	1.44	0.42
1:D:124:LEU:HD23	1:D:124:LEU:HA	1.75	0.42
1:D:238:ARG:HE	1:D:238:ARG:HB3	1.69	0.42
1:A:129:ASP:O	1:A:133:GLN:HG3	2.19	0.42
1:C:106:PRO:HB2	1:C:108:LYS:HG3	2.02	0.42
1:D:475:TYR:OH	2:D:501:HEM:O1D	2.35	0.42
1:B:292:LEU:HD23	1:B:292:LEU:HA	1.88	0.41
1:D:298:GLU:OE2	5:D:506:BTB:H42	2.20	0.41
5:D:505:BTB:H11	5:D:505:BTB:H72	1.96	0.41
1:A:156:GLU:OE2	1:A:164:GLN:HG2	2.21	0.41
1:C:140:ARG:NH1	10:C:606:HOH:O	2.53	0.41
5:D:505:BTB:H62	5:D:505:BTB:O8	2.21	0.41
1:B:188:ILE:HG22	7:B:504:ACT:H2	2.03	0.41
2:B:501:HEM:HBD1	2:B:501:HEM:CMD	2.51	0.41
1:C:214:HIS:CD2	1:C:214:HIS:C	2.97	0.41
1:D:229:THR:O	1:D:351:ALA:HA	2.20	0.41
2:C:502:HEM:HBA1	4:C:504:OUG:C09	2.51	0.40
1:C:449:VAL:HA	1:C:450:PRO:HD3	1.96	0.40
1:B:342[A]:GLU:OE1	1:B:470:SER:OG	2.29	0.40
5:D:505:BTB:H32	5:D:505:BTB:H51	1.68	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)
10:A:677:HOH:O	10:D:729:HOH:O[2_541]	2.12	0.08

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	402/440 (91%)	391 (97%)	9 (2%)	2 (0%)	24	16
1	B	404/440 (92%)	399 (99%)	5 (1%)	0	100	100
1	C	403/440 (92%)	385 (96%)	15 (4%)	3 (1%)	18	10
1	D	404/440 (92%)	399 (99%)	5 (1%)	0	100	100
All	All	1613/1760 (92%)	1574 (98%)	34 (2%)	5 (0%)	36	30

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	108	LYS
1	C	107	ARG
1	C	108	LYS
1	C	120	PRO
1	A	89	GLN

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	345/373 (92%)	339 (98%)	6 (2%)	53	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	347/373 (93%)	340 (98%)	7 (2%)	48	48
1	C	346/373 (93%)	338 (98%)	8 (2%)	44	42
1	D	347/373 (93%)	343 (99%)	4 (1%)	63	65
All	All	1385/1492 (93%)	1360 (98%)	25 (2%)	53	51

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	VAL
1	A	108	LYS
1	A	151	GLN
1	A	216	LYS
1	A	414	LYS
1	A	474	ARG
1	B	124	LEU
1	B	136[A]	SER
1	B	136[B]	SER
1	B	141[A]	SER
1	B	141[B]	SER
1	B	200	ASP
1	B	326	LEU
1	C	71	VAL
1	C	76	VAL
1	C	144	GLN
1	C	216	LYS
1	C	226	SER
1	C	235	CYS
1	C	304	LEU
1	C	480	TRP
1	D	139	LYS
1	D	258	ASP
1	D	329	ARG
1	D	396	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	133	GLN
1	A	233	GLN
1	A	257	GLN

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Mol	Chain	Res	Type
1	C	126	GLN
1	C	132	ASN
1	C	277	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 38 ligands modelled in this entry, 6 are monoatomic - leaving 32 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	$\# Z > 2$
8	GOL	C	510	-	5,5,5	0.36	0	5,5,5	0.45	0
4	OUG	C	504	-	22,22,22	0.91	0	30,31,31	1.42	3 (10%)
4	OUG	D	503	-	22,22,22	0.99	0	30,31,31	0.96	2 (6%)
2	HEM	B	501	1	50,50,50	1.79	9 (18%)	67,82,82	1.43	11 (16%)
3	H4B	B	502	-	17,18,18	0.80	0	14,26,26	1.82	5 (35%)
5	BTB	B	506	-	13,13,13	0.62	0	7,16,16	1.61	2 (28%)
5	BTB	B	505	9	13,13,13	0.43	0	7,16,16	0.65	0
2	HEM	C	502	1	50,50,50	1.76	10 (20%)	67,82,82	1.24	6 (8%)
7	ACT	D	504	-	3,3,3	0.85	0	3,3,3	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	OUG	A	503	-	22,22,22	0.94	1 (4%)	30,31,31	0.98	1 (3%)
2	HEM	D	501	1	50,50,50	1.74	9 (18%)	67,82,82	1.54	13 (19%)
3	H4B	C	503	-	17,18,18	0.86	0	14,26,26	1.94	4 (28%)
3	H4B	D	502	-	17,18,18	0.81	0	14,26,26	2.00	5 (35%)
5	BTB	D	506	-	13,13,13	0.45	0	7,16,16	0.92	0
8	GOL	A	510	-	5,5,5	0.31	0	5,5,5	0.52	0
5	BTB	A	504	9	13,13,13	0.57	0	7,16,16	1.16	0
5	BTB	C	507	-	13,13,13	0.41	0	7,16,16	0.49	0
5	BTB	A	505	-	13,13,13	0.79	1 (7%)	7,16,16	1.37	1 (14%)
7	ACT	A	509	-	3,3,3	0.74	0	3,3,3	0.95	0
5	BTB	D	507	-	13,13,13	0.53	0	7,16,16	0.71	0
5	BTB	C	506	-	13,13,13	0.77	1 (7%)	7,16,16	1.98	3 (42%)
3	H4B	A	502	-	17,18,18	0.90	0	14,26,26	1.92	4 (28%)
2	HEM	A	501	1	50,50,50	1.81	9 (18%)	67,82,82	1.55	13 (19%)
5	BTB	A	506	-	13,13,13	1.12	1 (7%)	7,16,16	1.79	2 (28%)
7	ACT	C	509	-	3,3,3	0.82	0	3,3,3	0.74	0
5	BTB	D	508	-	13,13,13	0.37	0	7,16,16	0.41	0
4	OUG	B	503	-	22,22,22	0.92	1 (4%)	30,31,31	1.62	6 (20%)
7	ACT	B	504	-	3,3,3	0.81	0	3,3,3	0.69	0
5	BTB	D	505	9	13,13,13	0.49	0	7,16,16	0.48	0
5	BTB	A	507	-	13,13,13	0.50	0	7,16,16	0.65	0
5	BTB	C	505	9	13,13,13	0.35	0	7,16,16	0.67	0
5	BTB	B	507	-	13,13,13	0.40	0	7,16,16	0.59	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
8	GOL	C	510	-	-	4/4/4/4	-
4	OUG	C	504	-	-	0/6/6/6	0/3/3/3
4	OUG	D	503	-	-	0/6/6/6	0/3/3/3
2	HEM	B	501	1	-	3/14/54/54	-
3	H4B	B	502	-	-	3/8/17/17	0/2/2/2
5	BTB	B	506	-	-	12/21/21/21	-
5	BTB	B	505	9	-	7/21/21/21	-
2	HEM	C	502	1	-	4/14/54/54	-
4	OUG	A	503	-	-	0/6/6/6	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	D	501	1	-	3/14/54/54	-
3	H4B	C	503	-	-	0/8/17/17	0/2/2/2
3	H4B	D	502	-	-	3/8/17/17	0/2/2/2
5	BTB	D	506	-	-	9/21/21/21	-
8	GOL	A	510	-	-	2/4/4/4	-
5	BTB	A	504	9	-	5/21/21/21	-
5	BTB	C	507	-	-	10/21/21/21	-
5	BTB	A	505	-	-	15/21/21/21	-
5	BTB	D	507	-	-	9/21/21/21	-
5	BTB	C	506	-	-	6/21/21/21	-
3	H4B	A	502	-	-	0/8/17/17	0/2/2/2
2	HEM	A	501	1	-	4/14/54/54	-
5	BTB	A	506	-	-	6/21/21/21	-
5	BTB	D	508	-	-	5/21/21/21	-
4	OUG	B	503	-	-	0/6/6/6	0/3/3/3
5	BTB	D	505	9	-	5/21/21/21	-
5	BTB	A	507	-	-	9/21/21/21	-
5	BTB	C	505	9	-	10/21/21/21	-
5	BTB	B	507	-	-	4/21/21/21	-

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	FE-NB	6.83	2.15	1.94
2	B	501	HEM	FE-NC	6.12	2.15	1.95
2	B	501	HEM	FE-NB	6.00	2.13	1.94
2	C	502	HEM	FE-NB	5.80	2.12	1.94
2	D	501	HEM	FE-NC	5.52	2.13	1.95
2	D	501	HEM	FE-NB	4.90	2.10	1.94
2	A	501	HEM	FE-NA	4.89	2.11	1.95
2	C	502	HEM	FE-ND	4.86	2.09	1.94
2	A	501	HEM	FE-NC	4.84	2.11	1.95
2	C	502	HEM	FE-NA	4.11	2.08	1.95
2	B	501	HEM	FE-NA	4.02	2.08	1.95
2	D	501	HEM	FE-ND	3.96	2.07	1.94
2	D	501	HEM	FE-NA	3.51	2.06	1.95
2	C	502	HEM	FE-NC	3.41	2.06	1.95
2	C	502	HEM	CAB-C3B	3.33	1.56	1.47
2	A	501	HEM	CAB-C3B	3.26	1.56	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	502	HEM	CAC-C3C	3.15	1.55	1.47
2	B	501	HEM	CAC-C3C	2.99	1.55	1.47
2	B	501	HEM	CAB-C3B	2.98	1.55	1.47
2	D	501	HEM	CAB-C3B	2.92	1.55	1.47
2	A	501	HEM	FE-ND	2.87	2.03	1.94
2	D	501	HEM	CAC-C3C	2.81	1.54	1.47
2	A	501	HEM	CAC-C3C	2.75	1.54	1.47
2	B	501	HEM	CMB-C2B	2.59	1.56	1.50
5	A	506	BTB	C1-C2	-2.54	1.50	1.53
2	B	501	HEM	CMC-C2C	2.54	1.56	1.50
2	B	501	HEM	CMD-C2D	2.53	1.55	1.50
2	C	502	HEM	CMC-C2C	2.45	1.55	1.50
2	D	501	HEM	CMA-C3A	2.37	1.55	1.50
4	A	503	OUG	C05-C10	-2.28	1.38	1.42
2	C	502	HEM	CMB-C2B	2.27	1.55	1.50
2	C	502	HEM	CAD-C3D	2.24	1.57	1.51
2	D	501	HEM	CMB-C2B	2.18	1.55	1.50
2	A	501	HEM	CMC-C2C	2.12	1.55	1.50
2	A	501	HEM	C3D-C2D	-2.11	1.32	1.36
4	B	503	OUG	C04-C05	-2.11	1.38	1.42
2	A	501	HEM	CMB-C2B	2.09	1.55	1.50
2	C	502	HEM	C2A-C3A	-2.07	1.33	1.38
2	B	501	HEM	FE-ND	2.03	2.01	1.94
5	A	505	BTB	C3-C2	-2.03	1.50	1.53
2	D	501	HEM	CMC-C2C	2.02	1.54	1.50
5	C	506	BTB	C3-C2	-2.01	1.50	1.53

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	502	H4B	C2-N1-C8A	4.75	121.74	113.36
3	C	503	H4B	C2-N1-C8A	4.41	121.15	113.36
3	A	502	H4B	C2-N1-C8A	4.21	120.78	113.36
3	B	502	H4B	C2-N1-C8A	4.13	120.65	113.36
4	B	503	OUG	C04-C05-C10	3.78	120.30	118.00
4	C	504	OUG	C05-C10-N01	-3.63	118.96	122.80
5	C	506	BTB	O3-C3-C2	-3.59	102.95	111.40
4	B	503	OUG	C05-C10-N01	-3.54	119.05	122.80
2	D	501	HEM	CBA-CAA-C2A	-3.52	102.80	112.53
5	A	506	BTB	O1-C1-C2	-3.48	103.22	111.40
2	D	501	HEM	C3B-C2B-C1B	3.38	108.95	106.41
4	C	504	OUG	C04-C05-C10	3.38	120.06	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	HEM	C2A-C1A-NA	-3.23	106.57	110.15
2	A	501	HEM	C3D-C4D-ND	-3.17	106.69	110.17
2	D	501	HEM	C4D-ND-C1D	3.10	108.88	105.21
2	A	501	HEM	C3B-C4B-NB	-3.05	107.28	109.47
3	C	503	H4B	O4-C4-C4A	-3.03	119.95	127.26
2	D	501	HEM	CAD-CBD-CGD	-3.03	105.63	113.67
2	C	502	HEM	C3B-C2B-C1B	3.01	108.67	106.41
2	B	501	HEM	CBA-CAA-C2A	-2.97	104.31	112.53
2	D	501	HEM	CHA-C4D-ND	2.97	128.04	124.37
4	A	503	OUG	C05-C10-N01	-2.90	119.73	122.80
2	D	501	HEM	C3D-C4D-ND	-2.85	107.05	110.17
2	A	501	HEM	CBA-CAA-C2A	-2.85	104.66	112.53
2	D	501	HEM	C3B-C4B-NB	-2.84	107.43	109.47
2	B	501	HEM	C3B-C2B-C1B	2.82	108.53	106.41
2	A	501	HEM	C3B-C2B-C1B	2.79	108.51	106.41
2	A	501	HEM	C1B-NB-C4B	2.73	108.44	105.21
5	B	506	BTB	O4-C4-C2	-2.73	104.99	111.40
3	D	502	H4B	C4A-C4-N3	2.70	119.54	112.13
3	A	502	H4B	O4-C4-C4A	-2.69	120.78	127.26
2	B	501	HEM	C3B-C4B-NB	-2.69	107.54	109.47
3	D	502	H4B	O4-C4-C4A	-2.68	120.80	127.26
2	B	501	HEM	C2A-C1A-NA	-2.67	107.19	110.15
3	C	503	H4B	C4A-C4-N3	2.65	119.40	112.13
2	C	502	HEM	C1B-NB-C4B	2.61	108.30	105.21
2	D	501	HEM	C2D-C1D-ND	-2.61	106.89	109.90
3	C	503	H4B	C2-N3-C4	-2.58	120.42	125.11
3	B	502	H4B	C4A-C4-N3	2.58	119.22	112.13
4	D	503	OUG	C04-C05-C10	2.58	119.57	118.00
2	B	501	HEM	C1B-NB-C4B	2.57	108.25	105.21
2	C	502	HEM	C3B-C4B-NB	-2.56	107.63	109.47
4	B	503	OUG	C06-C05-C04	-2.56	118.65	123.61
2	C	502	HEM	CBD-CAD-C3D	2.56	119.60	112.53
2	A	501	HEM	CAD-CBD-CGD	-2.54	106.92	113.67
2	D	501	HEM	C1B-NB-C4B	2.54	108.22	105.21
3	A	502	H4B	C4A-C4-N3	2.52	119.06	112.13
2	A	501	HEM	CHA-C4D-ND	2.46	127.41	124.37
2	D	501	HEM	CBD-CAD-C3D	-2.46	105.74	112.53
4	B	503	OUG	C06-C05-C10	2.42	121.05	118.36
3	D	502	H4B	C2-N3-C4	-2.42	120.73	125.11
5	B	506	BTB	O3-C3-C2	-2.40	105.76	111.40
2	B	501	HEM	O1D-CGD-CBD	-2.38	115.53	123.09
4	D	503	OUG	C05-C10-N01	-2.38	120.28	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	HEM	C4D-ND-C1D	2.37	108.02	105.21
5	C	506	BTB	O4-C4-C2	-2.37	105.82	111.40
2	B	501	HEM	C4A-NA-C1A	2.37	109.69	105.82
4	B	503	OUG	C07-C08-C21	-2.31	117.28	121.25
3	B	502	H4B	C4-C4A-N5	2.30	122.54	116.27
3	B	502	H4B	O4-C4-C4A	-2.29	121.73	127.26
5	A	506	BTB	C6-C5-N	2.29	120.53	111.59
2	C	502	HEM	C2A-C1A-NA	-2.28	107.62	110.15
2	A	501	HEM	CAD-C3D-C2D	-2.28	123.61	127.87
2	B	501	HEM	CMD-C2D-C1D	-2.26	121.51	125.03
2	B	501	HEM	C4D-ND-C1D	2.24	107.86	105.21
3	B	502	H4B	C2-N3-C4	-2.21	121.11	125.11
2	C	502	HEM	C4D-ND-C1D	2.19	107.80	105.21
4	C	504	OUG	N02-C02-N01	2.19	120.05	118.24
2	A	501	HEM	O1A-CGA-CBA	-2.16	116.24	123.09
5	C	506	BTB	C8-C7-N	-2.15	103.19	111.59
2	B	501	HEM	CHD-C1D-ND	2.13	126.71	124.42
3	D	502	H4B	C4-C4A-N5	2.13	122.06	116.27
2	A	501	HEM	C4A-NA-C1A	2.11	109.26	105.82
4	B	503	OUG	C07-C06-C05	-2.11	118.20	121.15
2	B	501	HEM	C4C-NC-C1C	2.11	109.25	105.82
2	D	501	HEM	C2A-C1A-NA	-2.09	107.83	110.15
2	D	501	HEM	C4C-NC-C1C	2.08	109.21	105.82
5	A	505	BTB	O3-C3-C2	-2.07	106.54	111.40
3	A	502	H4B	C2-N3-C4	-2.06	121.37	125.11
2	A	501	HEM	O2A-CGA-CBA	2.01	120.37	114.00
2	D	501	HEM	CAB-C3B-C2B	-2.01	121.89	128.43

There are no chirality outliers.

All (138) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	HEM	C2D-C3D-CAD-CBD
2	B	501	HEM	C4D-C3D-CAD-CBD
2	C	502	HEM	C2D-C3D-CAD-CBD
2	C	502	HEM	C4D-C3D-CAD-CBD
3	B	502	H4B	C7-C6-C9-O9
3	B	502	H4B	C7-C6-C9-C10
3	D	502	H4B	C7-C6-C9-O9
3	D	502	H4B	C7-C6-C9-C10
5	A	504	BTB	C3-C2-C4-O4
5	A	504	BTB	N-C2-C4-O4

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Mol	Chain	Res	Type	Atoms
5	A	505	BTB	O1-C1-C2-N
5	A	505	BTB	C4-C2-C3-O3
5	A	505	BTB	C1-C2-C4-O4
5	A	505	BTB	C3-C2-C4-O4
5	A	505	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	A	506	BTB	C1-C2-C4-O4
5	A	506	BTB	C3-C2-C4-O4
5	A	506	BTB	N-C2-C4-O4
5	A	506	BTB	C6-C5-N-C7
5	A	507	BTB	C1-C2-C3-O3
5	A	507	BTB	C4-C2-C3-O3
5	A	507	BTB	N-C2-C3-O3
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-C4-O4
5	B	505	BTB	C3-C2-C4-O4
5	B	506	BTB	O1-C1-C2-C3
5	B	506	BTB	O1-C1-C2-C4
5	B	506	BTB	O1-C1-C2-N
5	B	506	BTB	C1-C2-C3-O3
5	B	506	BTB	C1-C2-N-C5
5	B	506	BTB	C1-C2-N-C7
5	B	506	BTB	C3-C2-N-C5
5	B	506	BTB	C3-C2-N-C7
5	B	506	BTB	C4-C2-N-C5
5	B	506	BTB	C4-C2-N-C7
5	B	507	BTB	O1-C1-C2-C3
5	B	507	BTB	O1-C1-C2-C4
5	B	507	BTB	O1-C1-C2-N
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-C3-O3
5	C	505	BTB	C4-C2-C3-O3
5	C	505	BTB	N-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
5	C	505	BTB	C3-C2-C4-O4
5	C	507	BTB	C3-C2-C4-O4
5	C	507	BTB	N-C2-C4-O4
5	C	507	BTB	C1-C2-N-C5
5	C	507	BTB	C1-C2-N-C7
5	C	507	BTB	C3-C2-N-C5
5	C	507	BTB	C3-C2-N-C7
5	C	507	BTB	C4-C2-N-C5
5	C	507	BTB	C4-C2-N-C7
5	D	505	BTB	C1-C2-C4-O4
5	D	505	BTB	C3-C2-C4-O4
5	D	505	BTB	N-C2-C4-O4
5	D	506	BTB	C1-C2-C3-O3
5	D	506	BTB	N-C2-C3-O3
5	D	506	BTB	C1-C2-N-C5
5	D	506	BTB	C1-C2-N-C7
5	D	506	BTB	C3-C2-N-C5
5	D	506	BTB	C3-C2-N-C7
5	D	506	BTB	C4-C2-N-C5
5	D	506	BTB	C4-C2-N-C7
5	D	507	BTB	C4-C2-C3-O3
5	D	507	BTB	C1-C2-N-C5
5	D	507	BTB	C1-C2-N-C7
5	D	507	BTB	C3-C2-N-C5
5	D	507	BTB	C3-C2-N-C7
5	D	507	BTB	C4-C2-N-C5
5	D	507	BTB	C4-C2-N-C7
5	D	508	BTB	C3-C2-C4-O4
8	C	510	GOL	O1-C1-C2-C3
8	C	510	GOL	C1-C2-C3-O3
5	B	505	BTB	N-C5-C6-O6
5	A	507	BTB	N-C7-C8-O8
5	A	505	BTB	N-C5-C6-O6
5	A	506	BTB	N-C7-C8-O8
5	C	505	BTB	N-C5-C6-O6
8	C	510	GOL	O2-C2-C3-O3
5	D	505	BTB	N-C5-C6-O6
5	D	506	BTB	N-C5-C6-O6
2	A	501	HEM	C2A-CAA-CBA-CGA
8	A	510	GOL	C1-C2-C3-O3
5	A	505	BTB	N-C7-C8-O8
5	B	506	BTB	N-C7-C8-O8

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Mol	Chain	Res	Type	Atoms
5	D	508	BTB	N-C7-C8-O8
5	B	507	BTB	N-C5-C6-O6
5	A	504	BTB	C1-C2-C4-O4
5	C	505	BTB	C1-C2-C4-O4
2	C	502	HEM	C2A-CAA-CBA-CGA
8	A	510	GOL	O2-C2-C3-O3
8	C	510	GOL	O1-C1-C2-O2
5	D	508	BTB	N-C5-C6-O6
5	C	507	BTB	C4-C2-C3-O3
2	A	501	HEM	C4B-C3B-CAB-CBB
2	C	502	HEM	C4B-C3B-CAB-CBB
2	D	501	HEM	C4B-C3B-CAB-CBB
3	B	502	H4B	N5-C6-C9-O9
5	A	505	BTB	N-C2-C3-O3
5	A	507	BTB	C1-C2-N-C5
5	A	507	BTB	C1-C2-N-C7
5	A	507	BTB	C3-C2-N-C5
5	A	507	BTB	C4-C2-N-C7
5	B	505	BTB	N-C2-C4-O4
5	C	505	BTB	N-C2-C4-O4
5	C	506	BTB	C1-C2-N-C5
5	C	506	BTB	C1-C2-N-C7
5	C	506	BTB	C3-C2-N-C5
5	C	506	BTB	C3-C2-N-C7
5	C	506	BTB	C4-C2-N-C7
5	D	507	BTB	N-C2-C3-O3
5	D	507	BTB	N-C2-C4-O4
5	D	508	BTB	N-C2-C4-O4
5	A	505	BTB	C1-C2-C3-O3
5	D	508	BTB	C1-C2-C4-O4
2	A	501	HEM	CAA-CBA-CGA-O1A
2	A	501	HEM	CAA-CBA-CGA-O2A
2	D	501	HEM	CAA-CBA-CGA-O1A
2	D	501	HEM	CAA-CBA-CGA-O2A
5	A	504	BTB	C1-C2-C3-O3
5	A	506	BTB	O1-C1-C2-C3
2	B	501	HEM	C2A-CAA-CBA-CGA
3	D	502	H4B	N5-C6-C9-O9
5	A	504	BTB	N-C2-C3-O3
5	A	507	BTB	C3-C2-N-C7
5	B	506	BTB	N-C2-C3-O3
5	C	506	BTB	C4-C2-N-C5

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Mol	Chain	Res	Type	Atoms
5	C	507	BTB	N-C2-C3-O3
5	D	505	BTB	C1-C2-N-C5

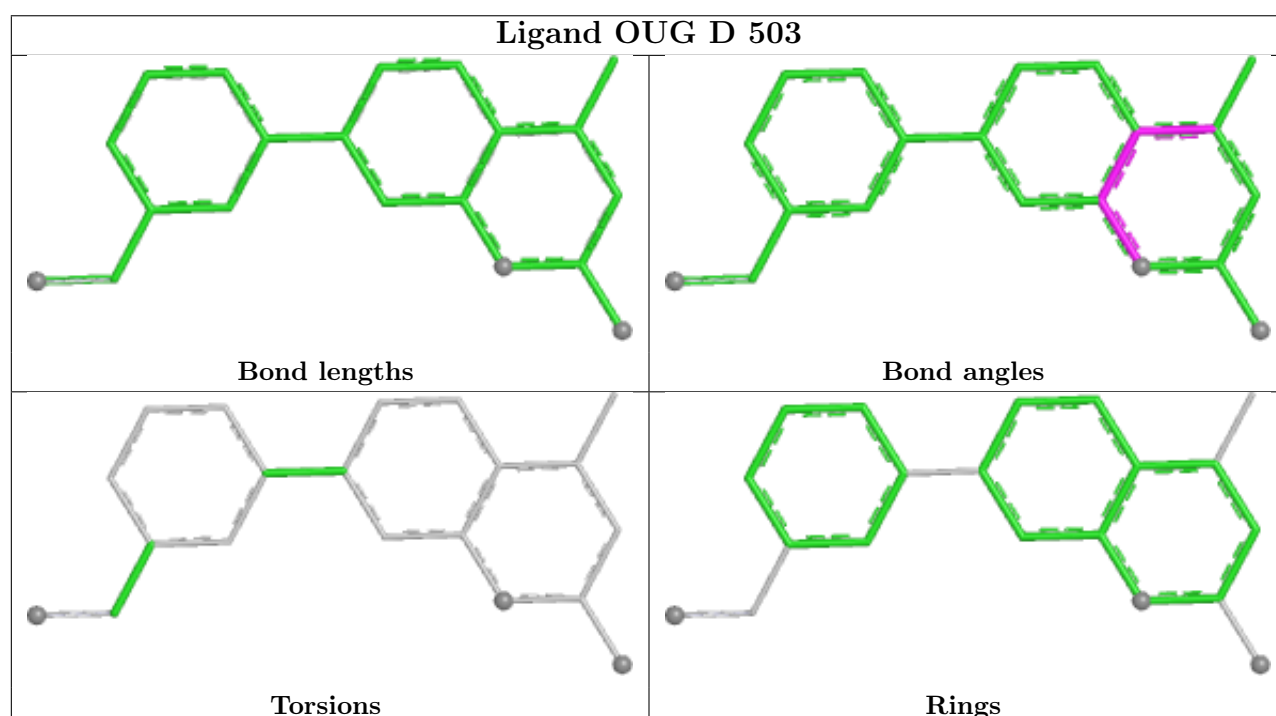
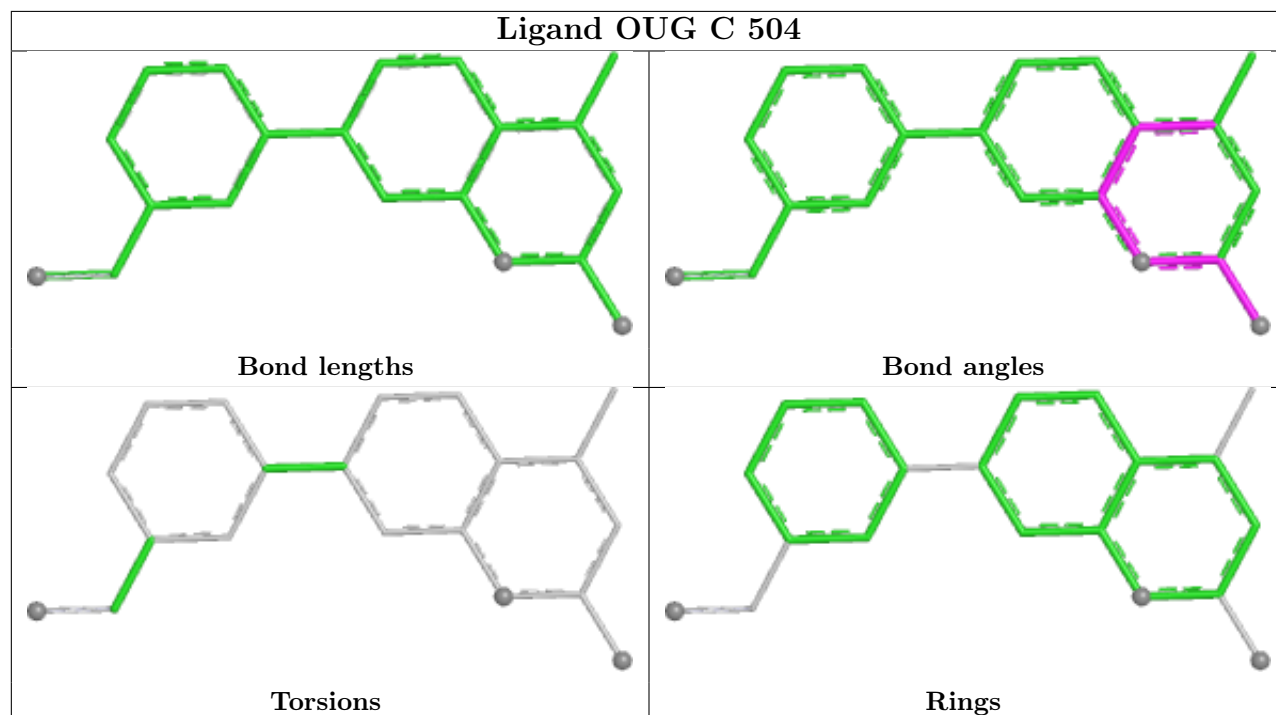
There are no ring outliers.

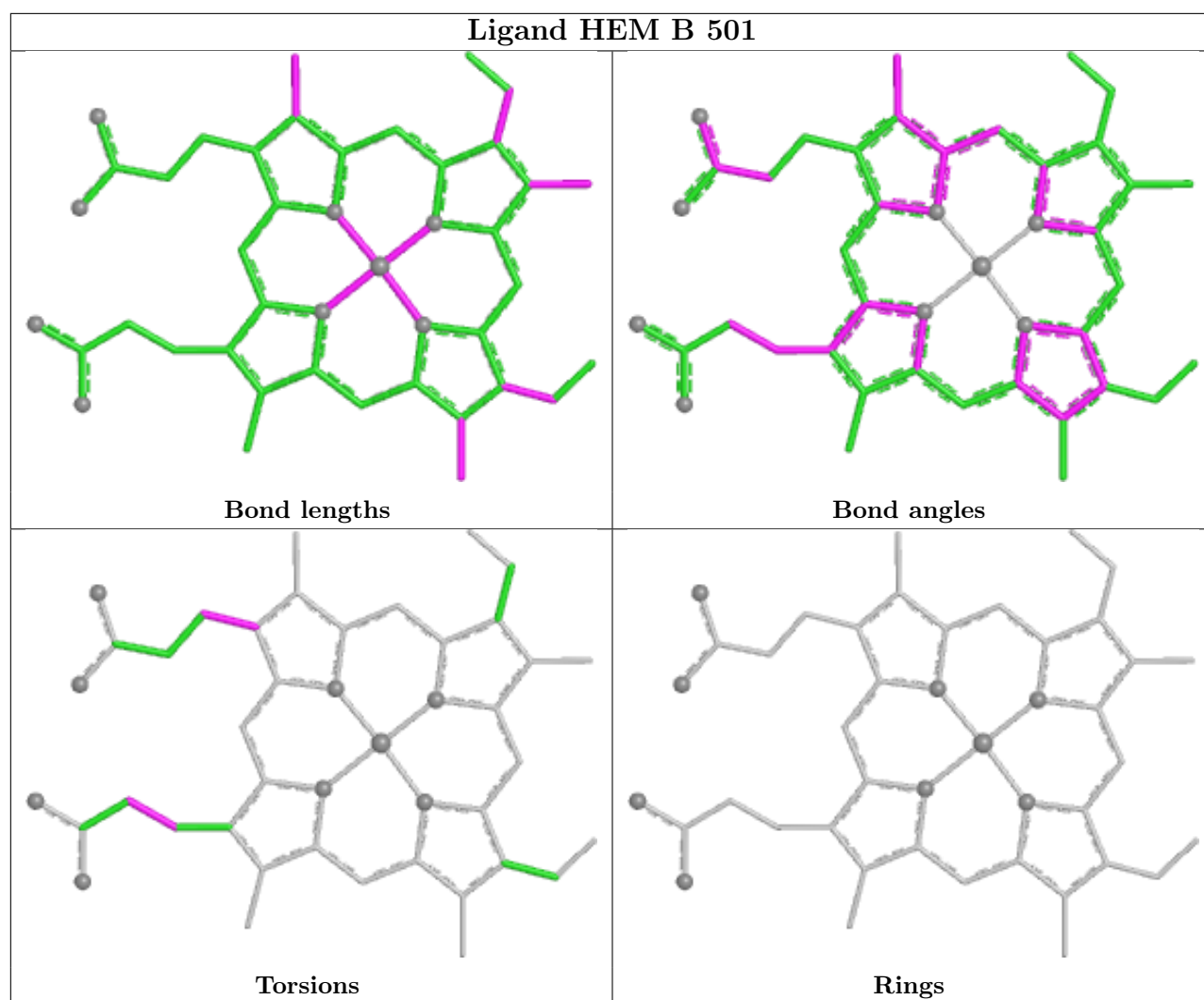
25 monomers are involved in 59 short contacts:

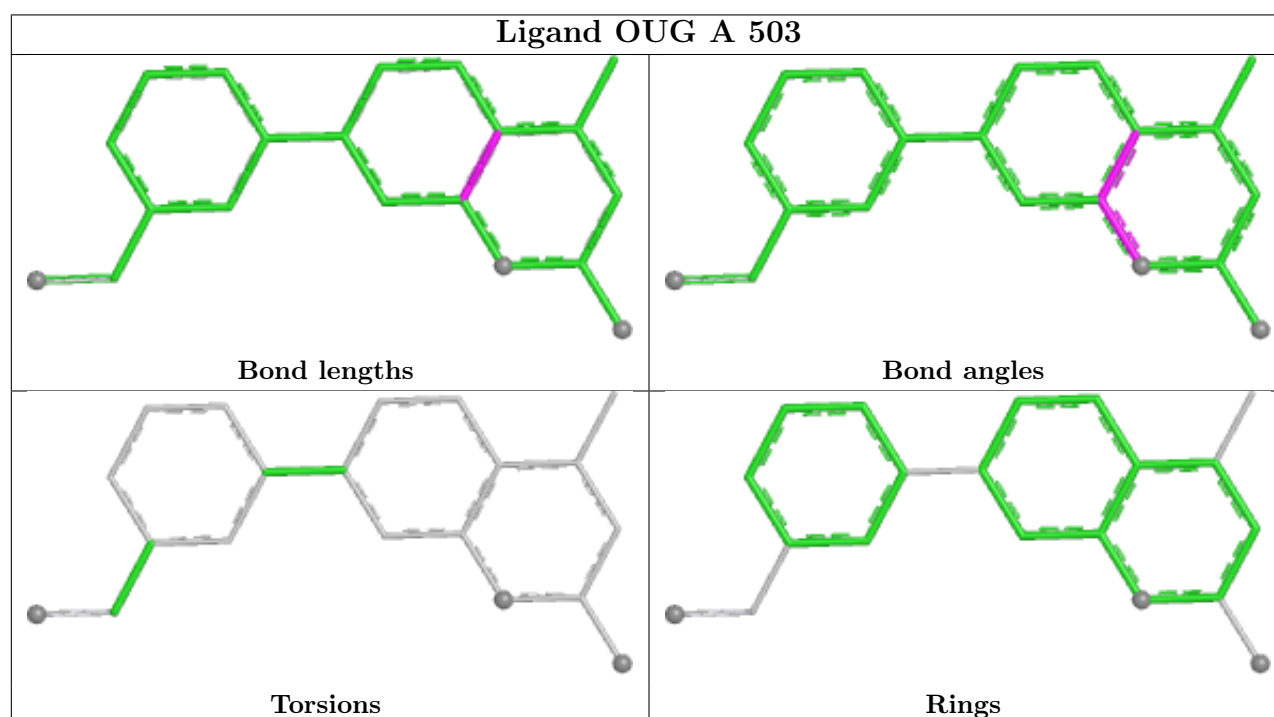
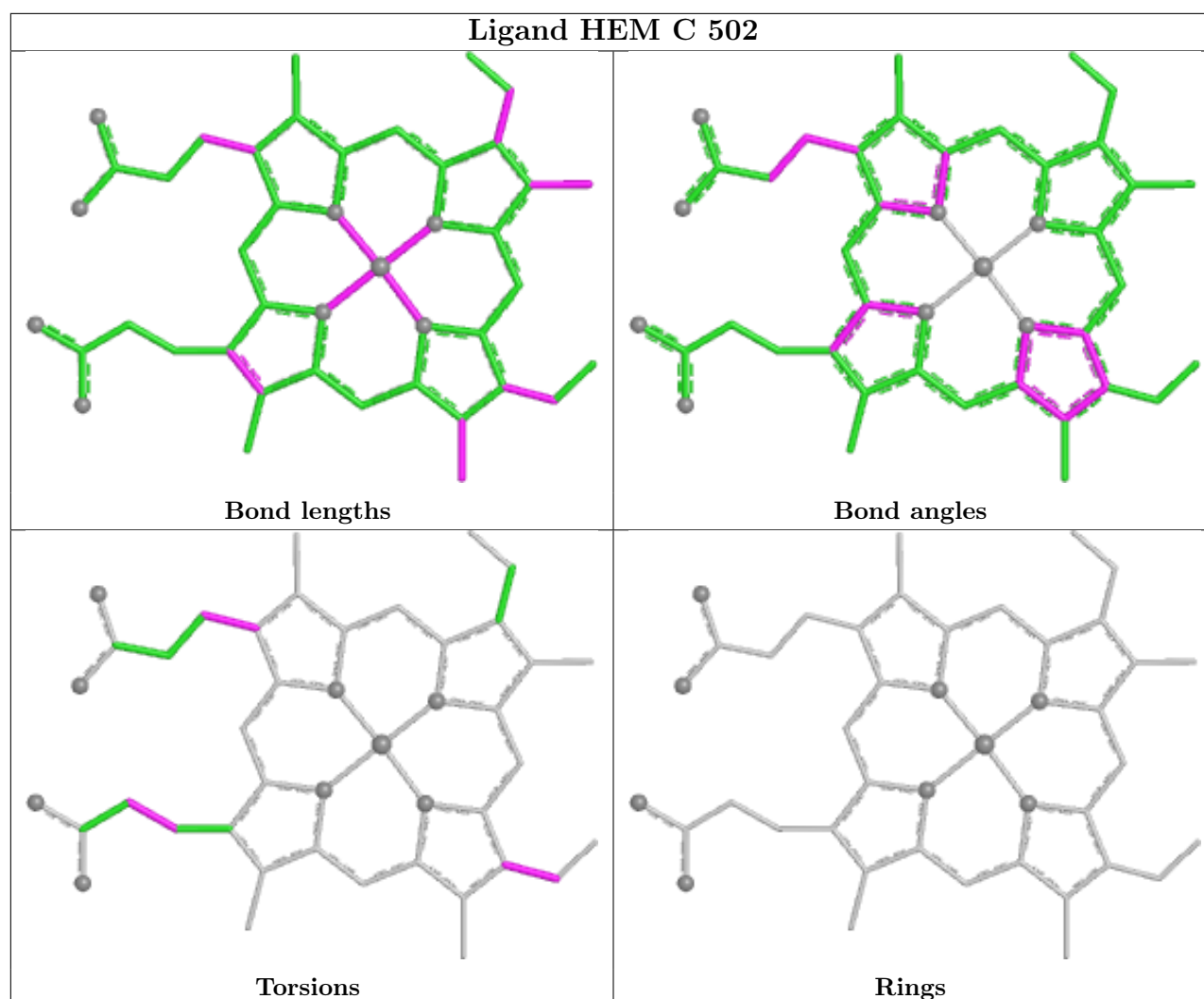
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	510	GOL	2	0
4	C	504	OUG	3	0
4	D	503	OUG	1	0
2	B	501	HEM	6	0
5	B	506	BTB	2	0
5	B	505	BTB	2	0
2	C	502	HEM	4	0
4	A	503	OUG	2	0
2	D	501	HEM	4	0
3	C	503	H4B	1	0
5	D	506	BTB	5	0
5	A	504	BTB	2	0
5	C	507	BTB	3	0
5	A	505	BTB	5	0
5	D	507	BTB	2	0
5	C	506	BTB	2	0
3	A	502	H4B	1	0
2	A	501	HEM	1	0
5	A	506	BTB	3	0
4	B	503	OUG	1	0
7	B	504	ACT	1	0
5	D	505	BTB	4	0
5	A	507	BTB	1	0
5	C	505	BTB	1	0
5	B	507	BTB	1	0

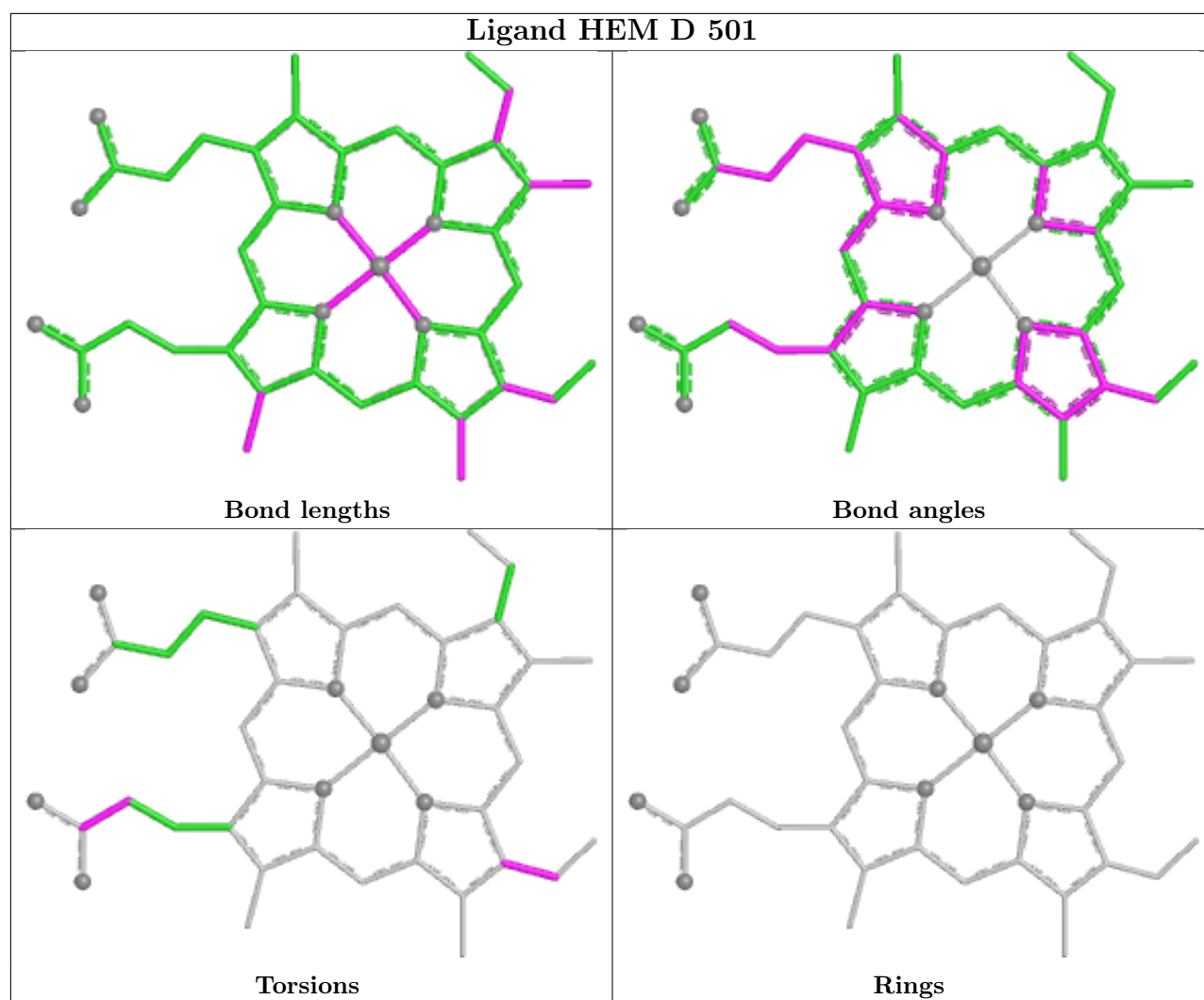
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

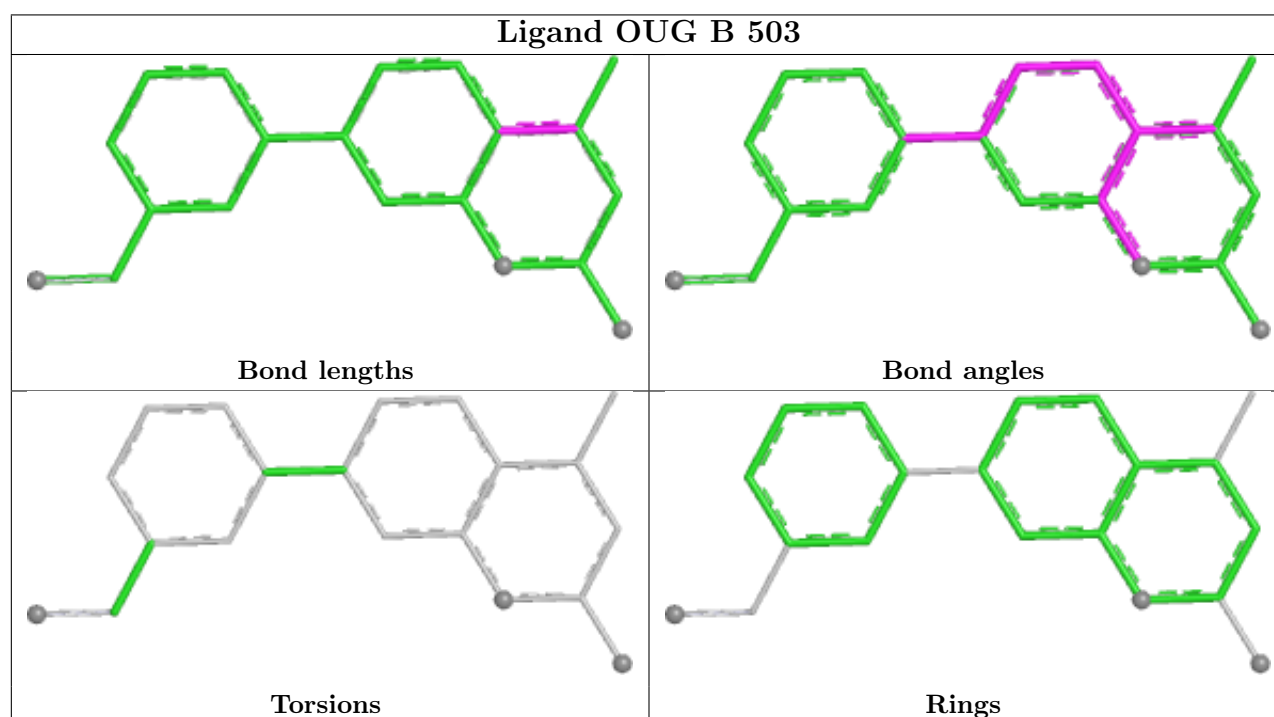
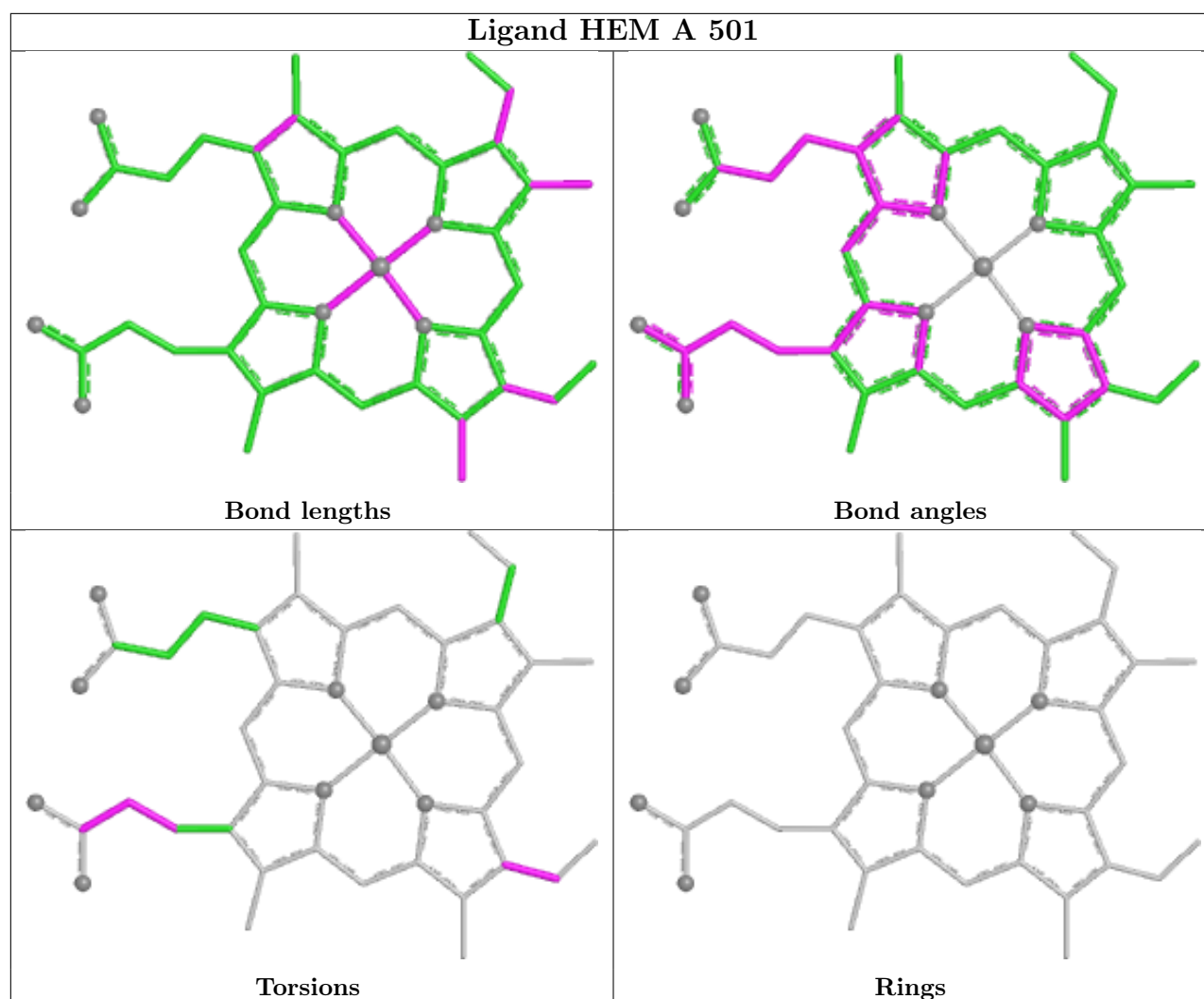
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	404/440 (91%)	-0.02	3 (0%) 84 85	30, 61, 102, 121	2 (0%)
1	B	403/440 (91%)	-0.26	2 (0%) 87 89	27, 47, 82, 119	5 (1%)
1	C	404/440 (91%)	0.20	5 (1%) 76 78	31, 68, 116, 147	3 (0%)
1	D	403/440 (91%)	-0.20	1 (0%) 91 93	30, 48, 85, 129	5 (1%)
All	All	1614/1760 (91%)	-0.07	11 (0%) 84 85	27, 55, 103, 147	15 (0%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	106	PRO	3.4
1	C	106	PRO	3.3
1	B	119	ALA	2.9
1	A	109	LEU	2.8
1	C	299	PRO	2.6
1	C	109	LEU	2.4
1	C	204	ALA	2.4
1	C	120	PRO	2.3
1	D	106	PRO	2.1
1	B	106	PRO	2.1
1	A	108	LYS	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

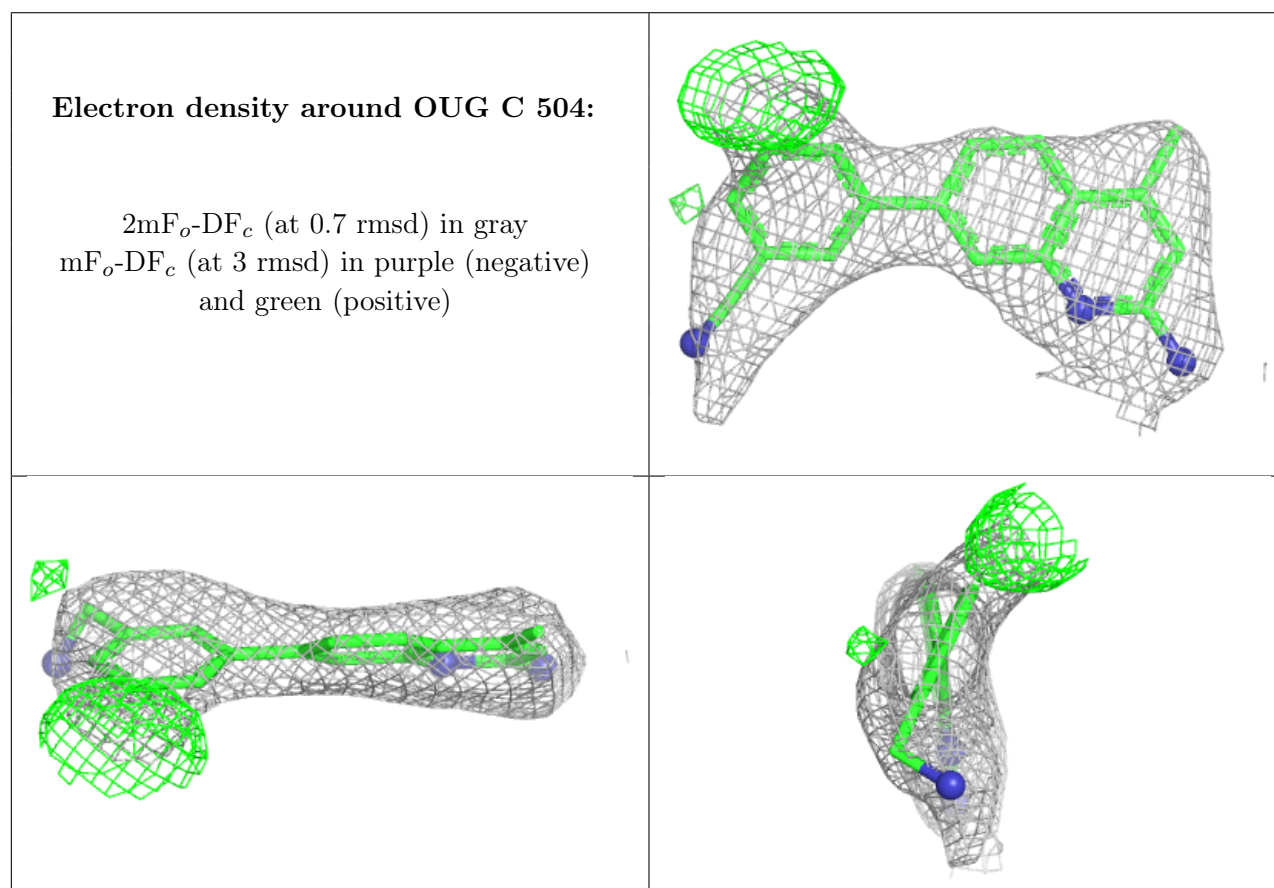
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	BTB	D	508	14/14	0.66	0.12	92,101,105,106	0
5	BTB	C	507	14/14	0.70	0.14	91,102,112,115	0
5	BTB	B	506	14/14	0.70	0.21	78,85,97,101	0
5	BTB	D	507	14/14	0.71	0.14	88,102,109,112	0
5	BTB	A	507	14/14	0.71	0.12	86,97,105,107	0
5	BTB	B	507	14/14	0.74	0.11	79,94,103,106	0
5	BTB	D	506	14/14	0.74	0.16	62,84,98,98	0
5	BTB	A	505	14/14	0.79	0.16	51,76,89,90	0
5	BTB	C	506	14/14	0.79	0.14	56,78,89,90	0
4	OUG	C	504	20/20	0.85	0.14	52,76,90,93	0
5	BTB	B	505	14/14	0.87	0.15	51,79,91,98	0
4	OUG	B	503	20/20	0.88	0.14	47,60,80,80	0
5	BTB	C	505	14/14	0.88	0.13	94,114,121,123	0
5	BTB	D	505	14/14	0.88	0.12	36,65,84,95	0
4	OUG	A	503	20/20	0.89	0.13	68,71,81,84	0
8	GOL	C	510	6/6	0.89	0.10	53,81,94,100	0
7	ACT	A	509	4/4	0.90	0.18	82,83,84,85	0
7	ACT	B	504	4/4	0.90	0.18	76,79,81,87	0
3	H4B	C	503	17/17	0.90	0.10	65,72,83,86	0
5	BTB	A	504	14/14	0.91	0.12	46,88,99,101	0
7	ACT	D	504	4/4	0.91	0.13	60,64,70,77	0
3	H4B	A	502	17/17	0.91	0.11	49,65,79,89	0
9	GD	C	501	1/1	0.91	0.07	174,174,174,174	0
8	GOL	A	510	6/6	0.92	0.08	51,68,74,75	0
3	H4B	D	502	17/17	0.92	0.10	46,61,75,75	0
4	OUG	D	503	20/20	0.92	0.11	38,62,91,94	0
9	GD	A	511	1/1	0.93	0.07	139,139,139,139	0
7	ACT	C	509	4/4	0.93	0.14	77,78,80,81	0
5	BTB	A	506	14/14	0.94	0.13	8,69,82,86	0
3	H4B	B	502	17/17	0.94	0.10	47,65,74,78	0
2	HEM	C	502	43/43	0.97	0.10	46,64,99,104	0
2	HEM	B	501	43/43	0.98	0.07	28,39,73,83	0
2	HEM	A	501	43/43	0.98	0.08	39,53,95,102	0
2	HEM	D	501	43/43	0.98	0.06	26,39,81,87	0
9	GD	B	508	1/1	0.99	0.03	55,55,55,55	0
9	GD	D	509	1/1	0.99	0.04	54,54,54,54	0
6	ZN	A	508	1/1	1.00	0.01	47,47,47,47	0

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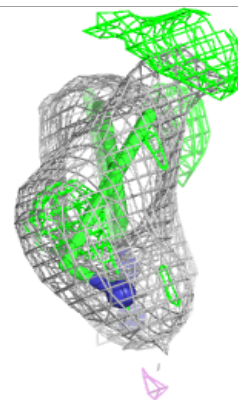
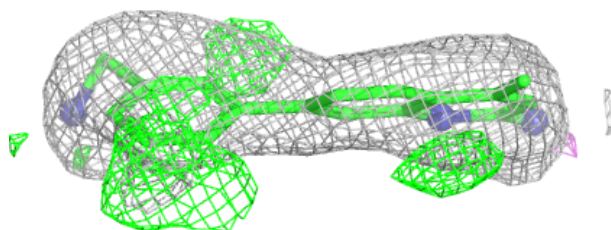
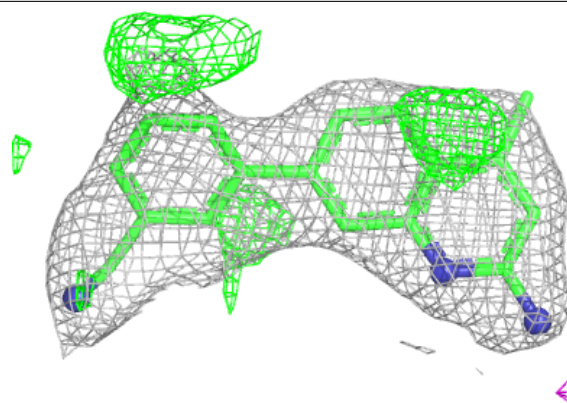
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	ZN	C	508	1/1	1.00	0.03	54,54,54,54	0

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.

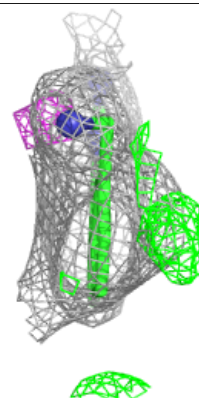
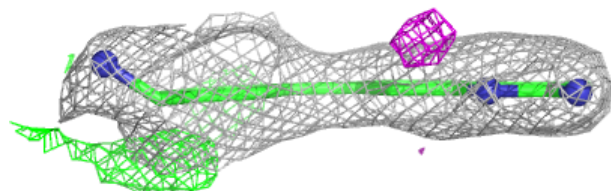
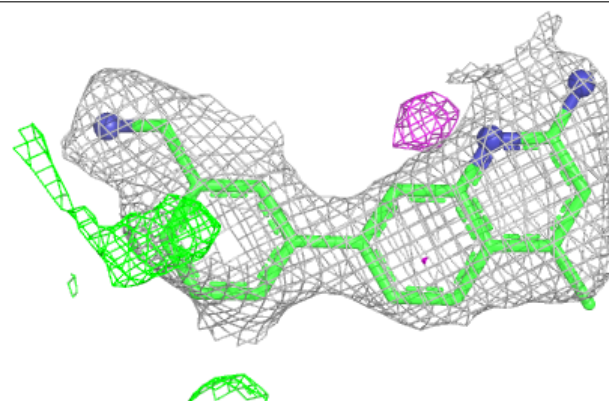


Electron density around OUG B 503:

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

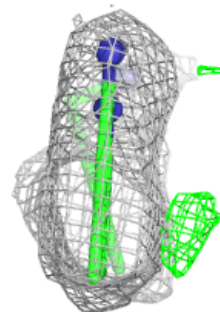
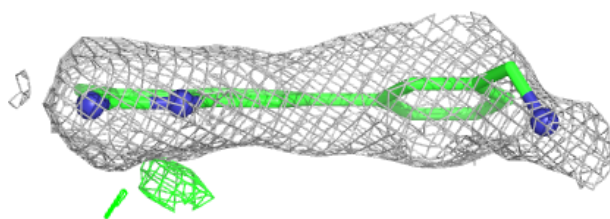
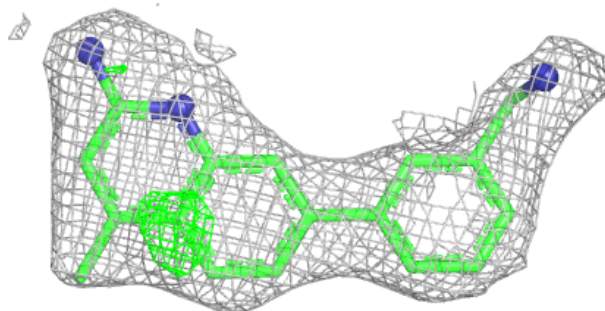
**Electron density around OUG A 503:**

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



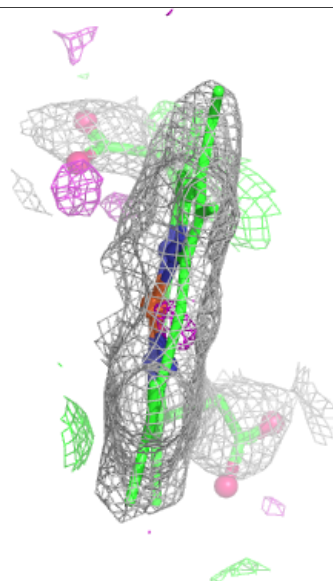
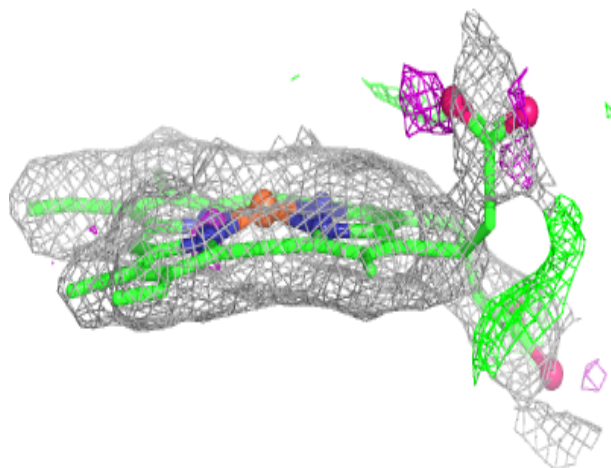
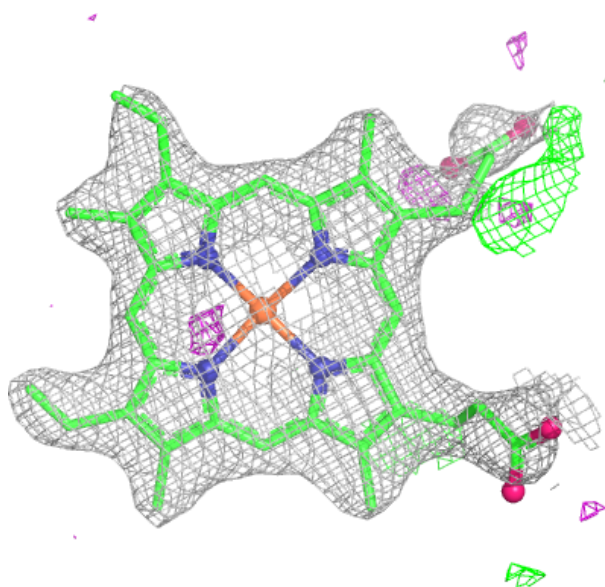
Electron density around OUG D 503:

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



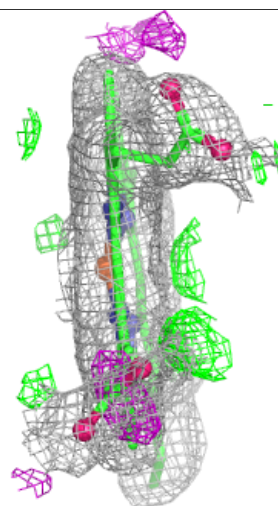
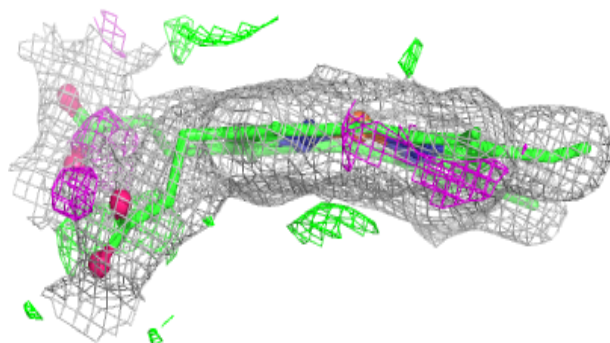
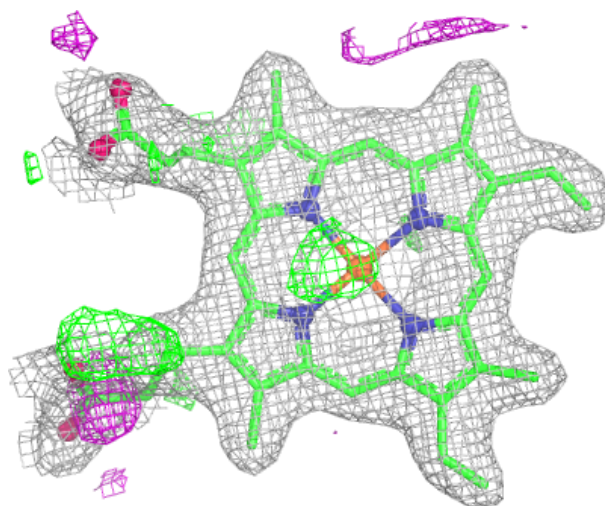
Electron density around HEM C 502:

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



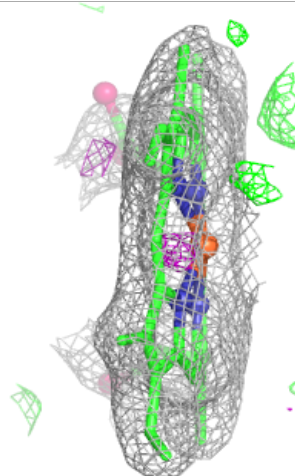
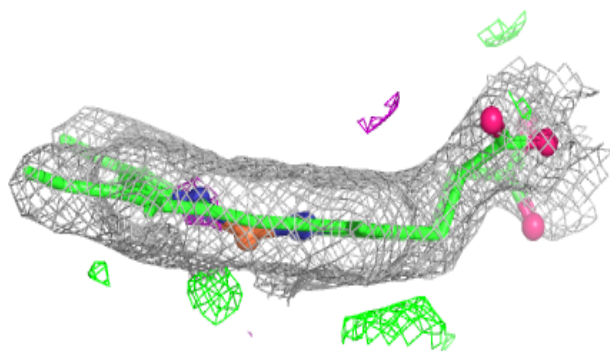
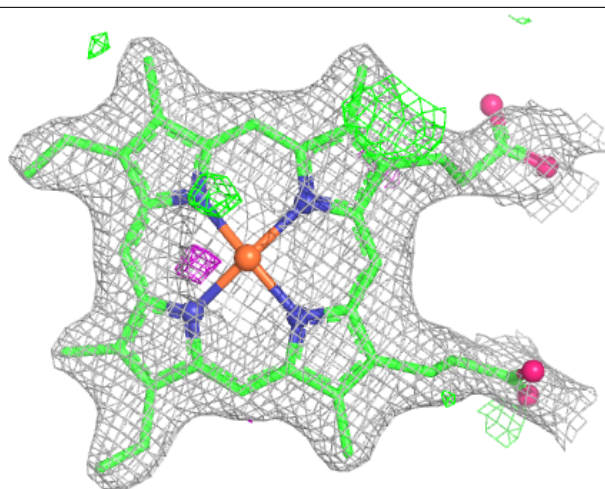
Electron density around HEM B 501:

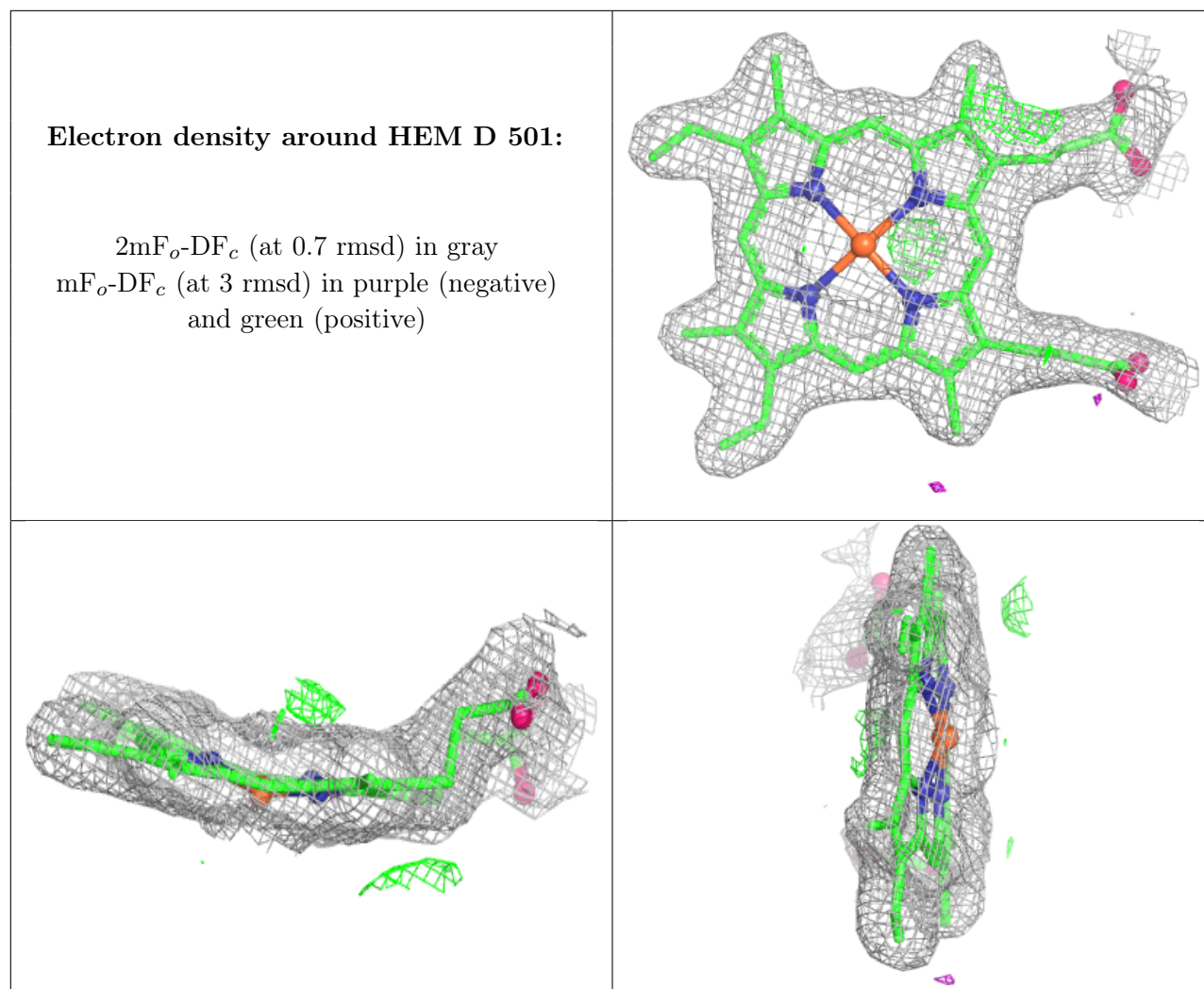
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM 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 ⓘ

There are no such residues in this entry.