



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 12:16 AM BST

PDB ID : 6POV
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 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 : 2.13.1
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) : 2.13.1

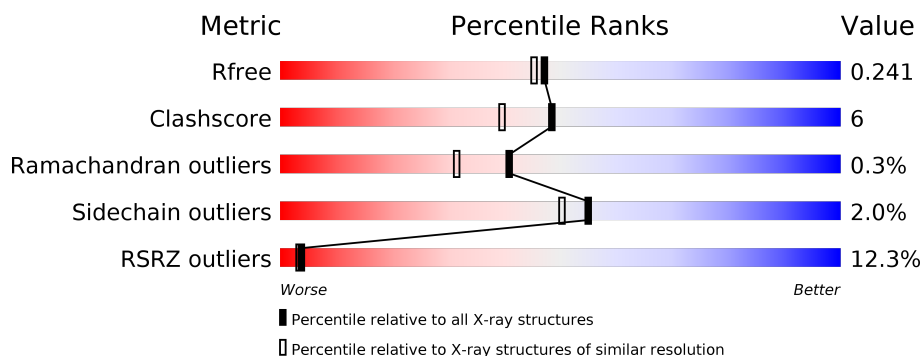
1 Overall quality at a glance

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}	130704	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (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 on 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	
1	B	440	
1	C	440	
1	D	440	

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.

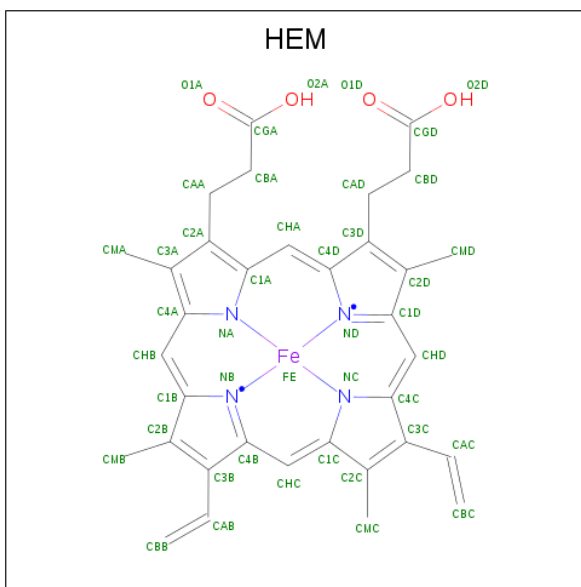
- Molecule 1 is a protein called Nitric oxide synthase, endothelial.

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:

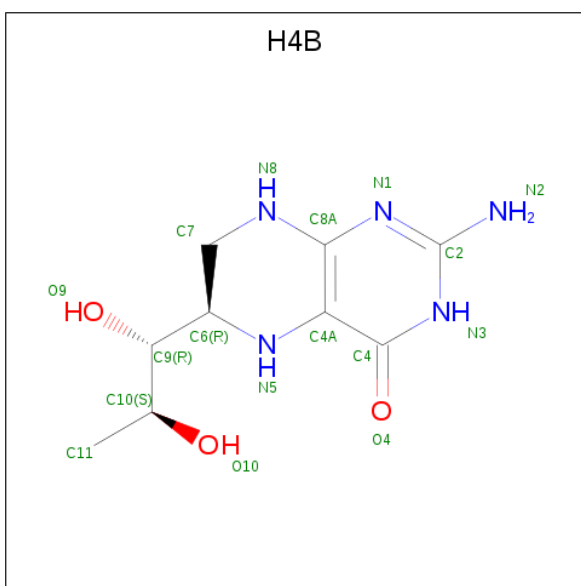
Chain	Residue	Modelled	Actual	Comment	Reference
A	298	GLU	ASP	variant	UNP P29474
B	298	GLU	ASP	variant	UNP P29474
C	298	GLU	ASP	variant	UNP P29474
D	298	GLU	ASP	variant	UNP P29474

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



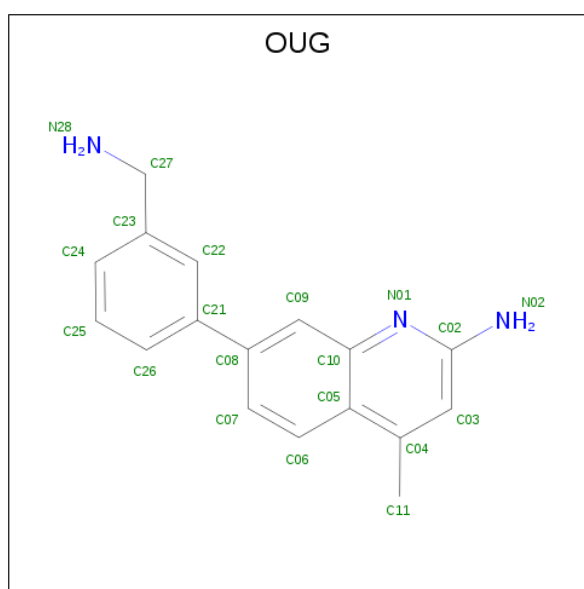
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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



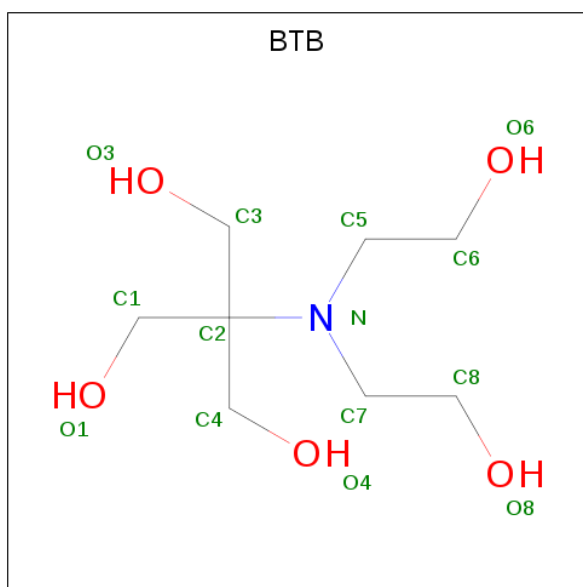
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		
3	C	1	Total	C	N	O	0	0
			17	9	5	3		
3	D	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 4 is 7-[3-(aminomethyl)phenyl]-4-methylquinolin-2-amine (three-letter code: OUG) (formula: C₁₇H₁₇N₃) (labeled as "Ligand of Interest" by author).



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 (three-letter code: BTB) (formula: C₈H₁₉NO₅).

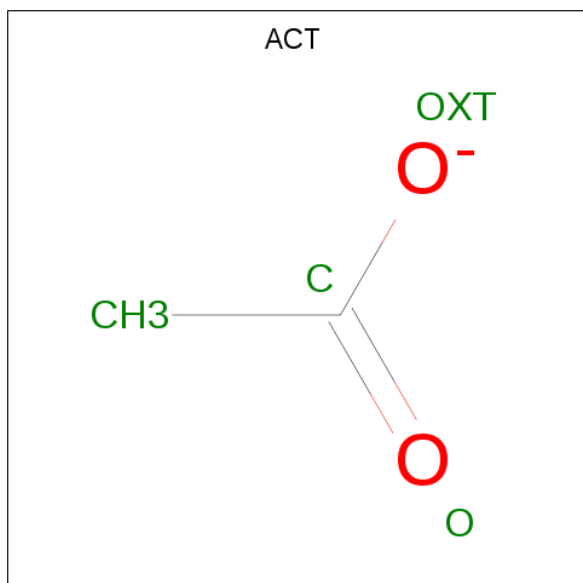


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	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 (three-letter code: ZN) (formula: Zn).

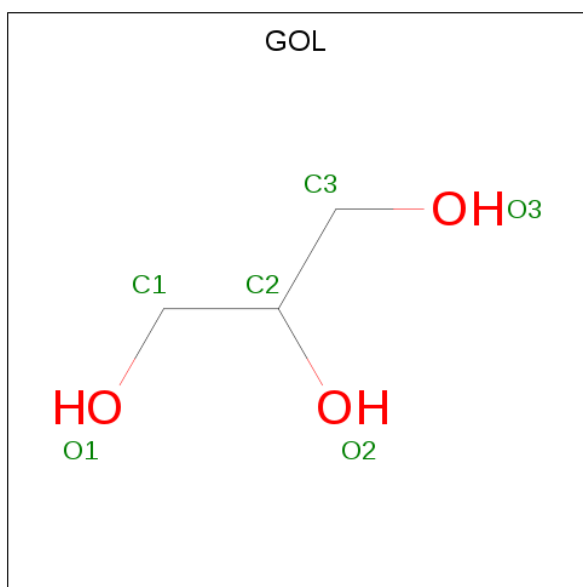
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Zn	0	0
			1	1		
6	C	1	Total	Zn	0	0
			1	1		

- Molecule 7 is ACETATE ION (three-letter code: 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 (three-letter code: 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 (three-letter code: GD) (formula: Gd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total	Gd	0	0
			1	1		
9	A	1	Total	Gd	0	0
			1	1		
9	D	1	Total	Gd	0	0
			1	1		
9	C	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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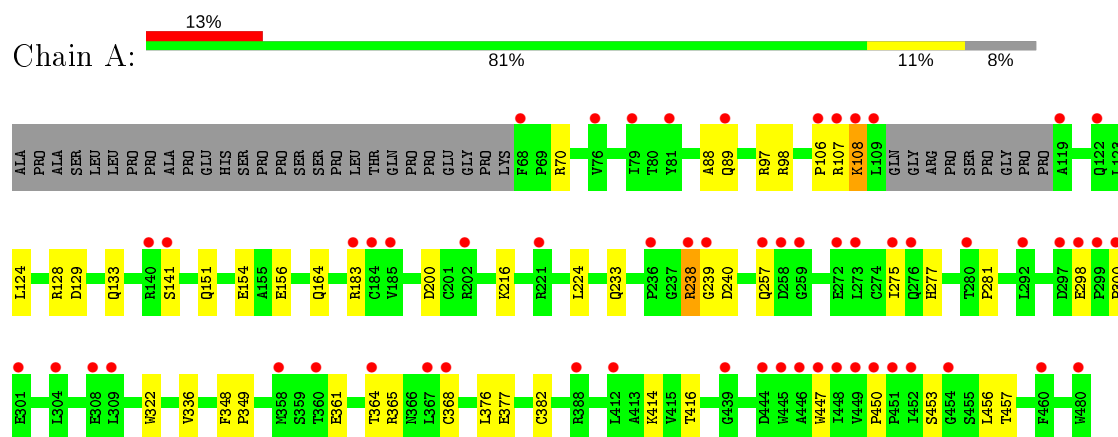
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	D	129	Total 129	O 129	0	0

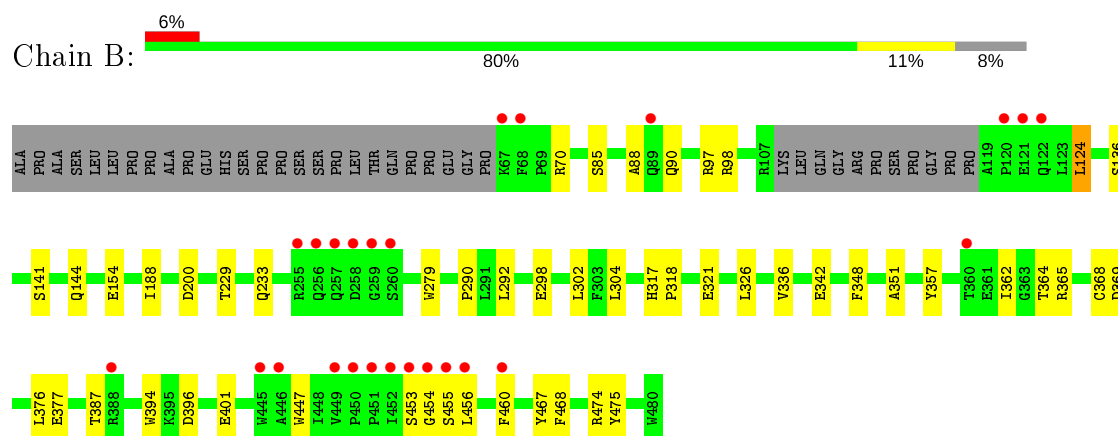
3 Residue-property plots [i](#)

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.

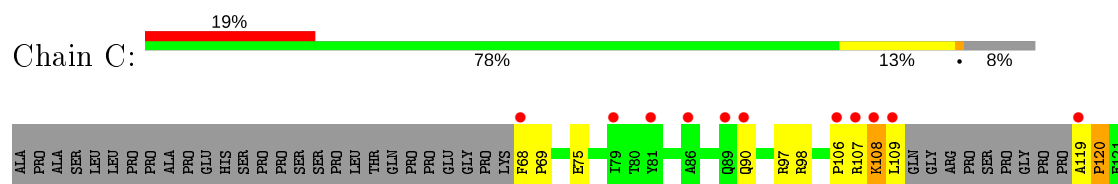
- Molecule 1: Nitric oxide synthase, endothelial

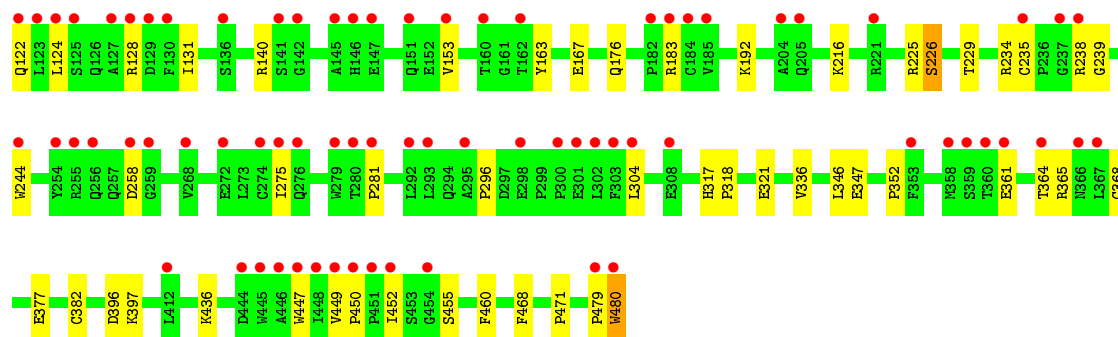


- Molecule 1: Nitric oxide synthase, endothelial

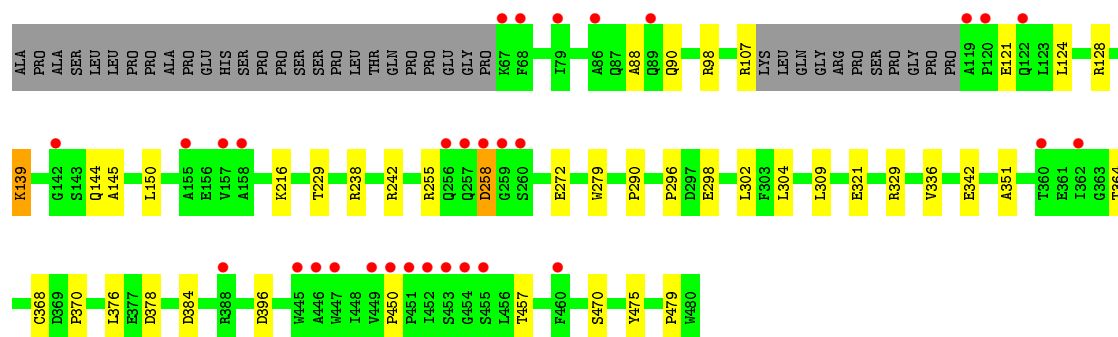
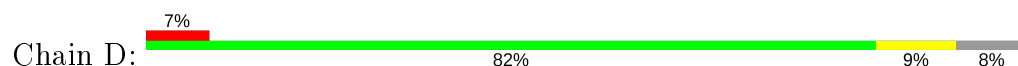


- Molecule 1: Nitric oxide synthase, endothelial





● 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) 98.6 (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 (5.02%)	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 , 67.1	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: GOL, ZN, H4B, ACT, OUG, GD, BTB, HEM

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	0.37	0/3332	0.51	0/4539
1	B	0.44	0/3345	0.56	0/4557
1	C	0.36	0/3341	0.52	0/4551
1	D	0.41	0/3345	0.54	0/4557
All	All	0.40	0/13363	0.53	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	32	0
1	C	3240	0	3151	44	0
1	D	3241	0	3150	30	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	10	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	4	0
10	D	129	0	0	2	1
All	All	13932	0	13063	159	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 (159) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B: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:H62	5:B:505:BTB:O8	1.88	0.72
1:C:480:TRP:H	1:C:480:TRP:HD1	1.36	0.72
1:C:120:PRO:HB2	1:C:122:GLN:HG2	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:322:TRP:CD1	5:A:504:BTB:H62	2.40	0.57
1:A:97:ARG:NH1	1:B:88:ALA:O	2.37	0.57
1:C:238:ARG:NH1	1:C:239:GLY:O	2.39	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
1:C:364:THR:HG21	1:C:452:ILE:HG23	1.89	0.55
2:D:501:HEM:HHC	2:D:501:HEM:HBB2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:321:GLU:H	1:C:321:GLU:CD	2.13	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:C:167:GLU:OE2	8:C:510:GOL:O3	2.22	0.51
1:D:298:GLU:CD	5:D:506:BTB:H42	2.31	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:O	1:C:108:LYS:N	2.45	0.49
5:C:506:BTB:O3	5:C:506:BTB:O4	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: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:HBC2	2:D:501:HEM:HMC2	1.94	0.47
5:A:505:BTB:H72	5:A:505:BTB:H12	1.38	0.47
1:A:128:ARG:HH22	1:A:154:GLU:CD	2.17	0.47
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:192:LYS:HZ1	1:C:225:ARG:HA	1.80	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:H51	5:D:507:BTB:H31	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:106:PRO:C	1:C:108:LYS:H	2.20	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:C:507:BTB:H72	5:C:507:BTB:H42	1.59	0.44
1:C:75:GLU:HG3	1:D:370:PRO:HG2	1.99	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:108:LYS:HB2	1:C:109:LEU:H	1.60	0.44
1:C:192:LYS:HZ1	1:C:226:SER:H	1.64	0.44
1:C:317:HIS:CG	1:C:318:PRO:HD2	2.53	0.44
5:C:507:BTB:O1	5:C:507:BTB:O4	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:N	1:C:258:ASP:OD1	2.50	0.44
1:A:238:ARG:NH1	1:A:239:GLY:O	2.51	0.43
2:B:501:HEM:HBD1	2:B:501:HEM:HMD1	2.00	0.43
1:D:258:ASP:N	1:D:258:ASP:OD1	2.51	0.43
2:B:501:HEM:HBB2	2:B:501:HEM:HHC	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:139:LYS:HB3	1:D:139:LYS:HE3	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:H52	5:A:506:BTB:H31	1.62	0.42
1:B:453:SER:HB3	1:B:456:LEU:HD12	2.01	0.42
1:C:238:ARG:HH11	1:C:296:PRO:HB3	1.84	0.42
1:C:176:GLN:HB3	1:C:471:PRO:HD2	2.01	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
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:HB3	1:D:238:ARG:HE	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:HA	1:B:292:LEU:HD23	1.88	0.41
1:D:298:GLU:OE2	5:D:506:BTB:H42	2.20	0.41
1:A:106:PRO:C	1:A:108:LYS:H	2.22	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:C:397:LYS:NZ	10:C:605:HOH:O	2.53	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: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
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

5.3.1 Protein backbone

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%)	29	18
1	B	404/440 (92%)	399 (99%)	5 (1%)	0	100	100
1	C	403/440 (92%)	385 (96%)	15 (4%)	3 (1%)	22	12
1	D	404/440 (92%)	399 (99%)	5 (1%)	0	100	100
All	All	1613/1760 (92%)	1574 (98%)	34 (2%)	5 (0%)	41	31

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

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%)	60	57
1	B	347/373 (93%)	338 (97%)	9 (3%)	46	39
1	C	346/373 (93%)	339 (98%)	7 (2%)	55	50
1	D	347/373 (93%)	340 (98%)	7 (2%)	55	50
All	All	1385/1492 (93%)	1356 (98%)	29 (2%)	55	48

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	98	ARG
1	A	141	SER
1	A	151	GLN
1	A	216	LYS
1	A	238	ARG
1	A	414	LYS
1	B	98	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	B	396	ASP
1	C	98	ARG
1	C	216	LYS
1	C	226	SER
1	C	235	CYS
1	C	304	LEU
1	C	396	ASP
1	C	480	TRP
1	D	90	GLN
1	D	98	ARG
1	D	121	GLU
1	D	139	LYS
1	D	258	ASP
1	D	329	ARG
1	D	396	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
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 [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 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$
7	ACT	A	509	-	1,3,3	1.05	0	0,3,3	0.00	-
4	OUG	D	503	-	22,22,22	0.97	0	30,31,31	1.01	2 (6%)
8	GOL	A	510	-	5,5,5	0.30	0	5,5,5	0.47	0
5	BTB	A	504	9	13,13,13	0.52	0	7,16,16	1.00	0
2	HEM	A	501	1	27,50,50	1.90	4 (14%)	17,82,82	1.85	3 (17%)
2	HEM	C	502	1	27,50,50	1.93	5 (18%)	17,82,82	1.95	5 (29%)
8	GOL	C	510	-	5,5,5	0.36	0	5,5,5	0.40	0
5	BTB	A	506	-	13,13,13	1.06	1 (7%)	7,16,16	1.61	2 (28%)
7	ACT	D	504	-	1,3,3	1.62	0	0,3,3	0.00	-
2	HEM	D	501	1	27,50,50	1.85	4 (14%)	17,82,82	2.20	4 (23%)
5	BTB	D	508	-	13,13,13	0.36	0	7,16,16	0.37	0
5	BTB	A	507	-	13,13,13	0.49	0	7,16,16	0.61	0
4	OUG	A	503	-	22,22,22	0.92	1 (4%)	30,31,31	1.00	2 (6%)
3	H4B	D	502	-	16,18,18	0.88	0	11,26,26	2.76	6 (54%)
5	BTB	C	507	-	13,13,13	0.39	0	7,16,16	0.47	0
5	BTB	C	505	9	13,13,13	0.34	0	7,16,16	0.64	0
5	BTB	C	506	-	13,13,13	0.73	0	7,16,16	1.79	3 (42%)
7	ACT	B	504	-	1,3,3	1.34	0	0,3,3	0.00	-
3	H4B	A	502	-	16,18,18	0.99	0	11,26,26	2.74	5 (45%)
7	ACT	C	509	-	1,3,3	1.47	0	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	BTB	A	505	-	13,13,13	0.75	0	7,16,16	1.25	0
3	H4B	C	503	-	16,18,18	0.96	0	11,26,26	2.59	5 (45%)
4	OUG	B	503	-	22,22,22	0.90	1 (4%)	30,31,31	1.74	7 (23%)
5	BTB	D	505	9	13,13,13	0.46	0	7,16,16	0.45	0
5	BTB	B	506	-	13,13,13	0.58	0	7,16,16	1.45	2 (28%)
2	HEM	B	501	1	27,50,50	1.84	5 (18%)	17,82,82	2.17	5 (29%)
4	OUG	C	504	-	22,22,22	0.89	0	30,31,31	1.49	4 (13%)
5	BTB	B	507	-	13,13,13	0.39	0	7,16,16	0.54	0
5	BTB	D	507	-	13,13,13	0.52	0	7,16,16	0.62	0
3	H4B	B	502	-	16,18,18	0.77	0	11,26,26	2.70	6 (54%)
5	BTB	D	506	-	13,13,13	0.44	0	7,16,16	0.86	0
5	BTB	B	505	9	13,13,13	0.38	0	7,16,16	0.60	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	OUG	D	503	-	-	0/6/6/6	0/3/3/3
8	GOL	A	510	-	-	2/4/4/4	-
5	BTB	A	504	9	-	4/21/21/21	-
2	HEM	A	501	1	-	1/6/54/54	-
2	HEM	C	502	1	-	3/6/54/54	-
8	GOL	C	510	-	-	4/4/4/4	-
5	BTB	A	506	-	-	7/21/21/21	-
2	HEM	D	501	1	-	0/6/54/54	-
5	BTB	D	508	-	-	5/21/21/21	-
5	BTB	A	507	-	-	9/21/21/21	-
4	OUG	A	503	-	-	0/6/6/6	0/3/3/3
3	H4B	D	502	-	-	3/8/17/17	0/2/2/2
5	BTB	C	507	-	-	11/21/21/21	-
5	BTB	C	505	9	-	10/21/21/21	-
5	BTB	C	506	-	-	5/21/21/21	-
3	H4B	A	502	-	-	0/8/17/17	0/2/2/2
5	BTB	A	505	-	-	15/21/21/21	-
3	H4B	C	503	-	-	0/8/17/17	0/2/2/2
4	OUG	B	503	-	-	0/6/6/6	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BTB	D	505	9	-	4/21/21/21	-
5	BTB	B	506	-	-	12/21/21/21	-
2	HEM	B	501	1	-	2/6/54/54	-
4	OUG	C	504	-	-	0/6/6/6	0/3/3/3
5	BTB	B	507	-	-	4/21/21/21	-
5	BTB	D	507	-	-	9/21/21/21	-
3	H4B	B	502	-	-	3/8/17/17	0/2/2/2
5	BTB	D	506	-	-	10/21/21/21	-
5	BTB	B	505	9	-	7/21/21/21	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	HEM	C3B-C2B	-5.18	1.33	1.40
2	A	501	HEM	C3B-C2B	-4.61	1.34	1.40
2	C	502	HEM	C3B-C2B	-4.17	1.34	1.40
2	B	501	HEM	C3B-C2B	-4.10	1.34	1.40
2	C	502	HEM	C3B-CAB	4.09	1.56	1.47
2	A	501	HEM	C3B-CAB	4.00	1.56	1.47
2	C	502	HEM	C3C-CAC	3.89	1.55	1.47
2	A	501	HEM	C3C-C2C	-3.80	1.35	1.40
2	B	501	HEM	C3C-CAC	3.69	1.55	1.47
2	B	501	HEM	C3B-CAB	3.63	1.55	1.47
2	B	501	HEM	C3C-C2C	-3.62	1.35	1.40
2	D	501	HEM	C3B-CAB	3.56	1.55	1.47
2	D	501	HEM	C3C-CAC	3.45	1.54	1.47
2	C	502	HEM	C3C-C2C	-3.41	1.35	1.40
2	A	501	HEM	C3C-CAC	3.37	1.54	1.47
2	D	501	HEM	C3C-C2C	-3.03	1.36	1.40
2	C	502	HEM	CAD-C3D	2.78	1.57	1.52
5	A	506	BTB	C1-C2	-2.32	1.50	1.53
4	A	503	OUG	C05-C10	-2.18	1.38	1.42
2	B	501	HEM	CMD-C2D	2.07	1.55	1.51
4	B	503	OUG	C04-C05	-2.02	1.38	1.42

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	503	H4B	C4-C4A-C8A	5.77	119.70	114.57
3	A	502	H4B	C4-C4A-C8A	5.47	119.42	114.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	502	H4B	C4-C4A-C8A	5.30	119.28	114.57
2	D	501	HEM	CBA-CAA-C2A	-5.25	102.80	112.49
2	B	501	HEM	CMD-C2D-C1D	-4.53	121.51	128.46
3	B	502	H4B	C4-C4A-C8A	4.48	118.55	114.57
2	B	501	HEM	CBA-CAA-C2A	-4.43	104.31	112.49
2	A	501	HEM	CBA-CAA-C2A	-4.24	104.66	112.49
4	B	503	OUG	C04-C05-C10	4.23	120.30	118.01
2	D	501	HEM	CAD-CBD-CGD	-4.20	105.63	112.67
3	B	502	H4B	C4-C4A-N5	4.07	122.54	119.12
2	C	502	HEM	CBD-CAD-C3D	3.86	119.60	112.48
4	C	504	OUG	C04-C05-C10	3.79	120.06	118.01
2	D	501	HEM	CBD-CAD-C3D	-3.66	105.74	112.48
4	C	504	OUG	C05-C10-N01	-3.63	118.96	122.81
3	A	502	H4B	N3-C2-N1	-3.59	119.78	125.42
4	B	503	OUG	C05-C10-N01	-3.54	119.05	122.81
3	D	502	H4B	C4-C4A-N5	3.51	122.06	119.12
3	D	502	H4B	N3-C2-N1	-3.50	119.93	125.42
2	A	501	HEM	CAD-CBD-CGD	-3.43	106.92	112.67
3	A	502	H4B	C4-N3-C2	3.42	121.37	115.93
2	C	502	HEM	CMD-C2D-C1D	-3.27	123.44	128.46
3	B	502	H4B	C4-N3-C2	3.26	121.11	115.93
3	C	503	H4B	N3-C2-N1	-3.22	120.37	125.42
3	D	502	H4B	C2-N1-C8A	3.21	121.74	114.54
3	B	502	H4B	N3-C2-N1	-3.20	120.41	125.42
5	C	506	BTB	O3-C3-C2	-3.10	102.95	111.44
3	D	502	H4B	C4-N3-C2	3.02	120.73	115.93
2	B	501	HEM	CMD-C2D-C3D	3.02	130.63	124.94
5	A	506	BTB	O1-C1-C2	-3.00	103.22	111.44
3	C	503	H4B	C2-N1-C8A	2.95	121.15	114.54
4	A	503	OUG	C05-C10-N01	-2.91	119.73	122.81
4	D	503	OUG	C04-C05-C10	2.89	119.57	118.01
2	B	501	HEM	CMA-C3A-C4A	-2.88	124.04	128.46
3	C	503	H4B	C4-N3-C2	2.83	120.42	115.93
2	A	501	HEM	CBD-CAD-C3D	-2.81	107.31	112.48
4	B	503	OUG	C08-C09-C10	-2.79	119.00	121.44
3	A	502	H4B	C2-N1-C8A	2.79	120.78	114.54
3	B	502	H4B	C2-N1-C8A	2.73	120.65	114.54
4	B	503	OUG	C06-C05-C04	-2.63	118.65	123.66
4	B	503	OUG	C06-C05-C10	2.44	121.05	118.33
2	D	501	HEM	CMA-C3A-C4A	-2.42	124.75	128.46
3	B	502	H4B	C4A-N5-C6	-2.40	114.63	121.16
4	D	503	OUG	C05-C10-N01	-2.39	120.28	122.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	506	BTB	O4-C4-C2	-2.36	104.99	111.44
4	B	503	OUG	C07-C08-C21	-2.35	117.28	121.36
2	B	501	HEM	CMC-C2C-C3C	2.35	129.07	124.68
3	D	502	H4B	N2-C2-N3	2.33	120.88	117.25
2	C	502	HEM	C1D-C2D-C3D	2.31	108.60	107.00
5	A	506	BTB	C6-C5-N	2.29	120.53	111.59
2	C	502	HEM	C4A-C3A-C2A	2.26	108.57	107.00
3	A	502	H4B	C4-C4A-N5	2.18	120.95	119.12
4	C	504	OUG	N02-C02-N01	2.16	120.05	118.26
5	C	506	BTB	C8-C7-N	-2.15	103.19	111.59
4	B	503	OUG	C07-C06-C05	-2.11	118.20	121.13
4	A	503	OUG	C03-C04-C05	2.10	119.85	117.78
3	C	503	H4B	N2-C2-N3	2.10	120.52	117.25
2	C	502	HEM	CAD-CBD-CGD	2.08	116.16	112.67
5	B	506	BTB	O3-C3-C2	-2.08	105.76	111.44
5	C	506	BTB	O4-C4-C2	-2.05	105.82	111.44
4	C	504	OUG	C03-C04-C05	2.05	119.80	117.78

There are no chirality outliers.

All (130) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	504	BTB	C3-C2-C4-O4
5	A	504	BTB	N-C2-C4-O4
2	C	502	HEM	C2D-C3D-CAD-CBD
2	C	502	HEM	C4D-C3D-CAD-CBD
8	C	510	GOL	O1-C1-C2-C3
8	C	510	GOL	C1-C2-C3-O3
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	D	508	BTB	C1-C2-C4-O4
5	D	508	BTB	C3-C2-C4-O4
5	D	508	BTB	N-C2-C4-O4
5	A	507	BTB	C1-C2-C3-O3
5	A	507	BTB	C4-C2-C3-O3
5	A	507	BTB	N-C2-C3-O3
3	D	502	H4B	C7-C6-C9-O9
3	D	502	H4B	C7-C6-C9-C10
5	C	507	BTB	C3-C2-C4-O4
5	C	507	BTB	N-C2-C4-O4

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Mol	Chain	Res	Type	Atoms
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	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
5	C	505	BTB	C3-C2-C4-O4
5	A	505	BTB	C1-C2-C3-O3
5	A	505	BTB	C4-C2-C3-O3
5	A	505	BTB	N-C2-C3-O3
5	A	505	BTB	C1-C2-C4-O4
5	A	505	BTB	C3-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	D	505	BTB	C1-C2-C4-O4
5	D	505	BTB	C3-C2-C4-O4
5	D	505	BTB	N-C2-C4-O4
5	B	506	BTB	O1-C1-C2-C3
5	B	506	BTB	O1-C1-C2-C4
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
2	B	501	HEM	C2D-C3D-CAD-CBD
2	B	501	HEM	C4D-C3D-CAD-CBD
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	D	507	BTB	C4-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
5	D	507	BTB	N-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
3	B	502	H4B	C7-C6-C9-O9
3	B	502	H4B	C7-C6-C9-C10
5	D	506	BTB	C1-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	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	505	BTB	N-C5-C6-O6
5	A	507	BTB	N-C7-C8-O8
5	A	506	BTB	N-C7-C8-O8
5	A	505	BTB	N-C5-C6-O6
5	C	505	BTB	N-C5-C6-O6
5	D	505	BTB	N-C5-C6-O6
5	D	506	BTB	N-C5-C6-O6
8	C	510	GOL	O2-C2-C3-O3
5	D	508	BTB	N-C7-C8-O8
5	A	505	BTB	N-C7-C8-O8
5	B	506	BTB	N-C7-C8-O8
8	A	510	GOL	C1-C2-C3-O3
5	B	507	BTB	N-C5-C6-O6
2	A	501	HEM	C2A-CAA-CBA-CGA
5	D	508	BTB	N-C5-C6-O6
8	A	510	GOL	O2-C2-C3-O3
8	C	510	GOL	O1-C1-C2-O2
3	B	502	H4B	N5-C6-C9-O9
5	A	504	BTB	C1-C2-C3-O3
5	A	504	BTB	C1-C2-C4-O4
5	A	506	BTB	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
5	C	507	BTB	C4-C2-C3-O3
5	C	505	BTB	C1-C2-C4-O4
5	B	506	BTB	C4-C2-C3-O3
5	D	507	BTB	C1-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	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	A	505	BTB	O1-C1-C2-N
5	A	505	BTB	N-C2-C4-O4
5	B	506	BTB	O1-C1-C2-N
5	D	506	BTB	N-C2-C3-O3
5	B	505	BTB	N-C2-C4-O4
2	C	502	HEM	C2A-CAA-CBA-CGA
3	D	502	H4B	N5-C6-C9-O9
5	A	506	BTB	O1-C1-C2-C4
5	A	507	BTB	O1-C1-C2-C3
5	C	507	BTB	C1-C2-C3-O3
5	C	507	BTB	C1-C2-C4-O4
5	D	506	BTB	C4-C2-C3-O3

There are no ring outliers.

25 monomers are involved in 58 short contacts:

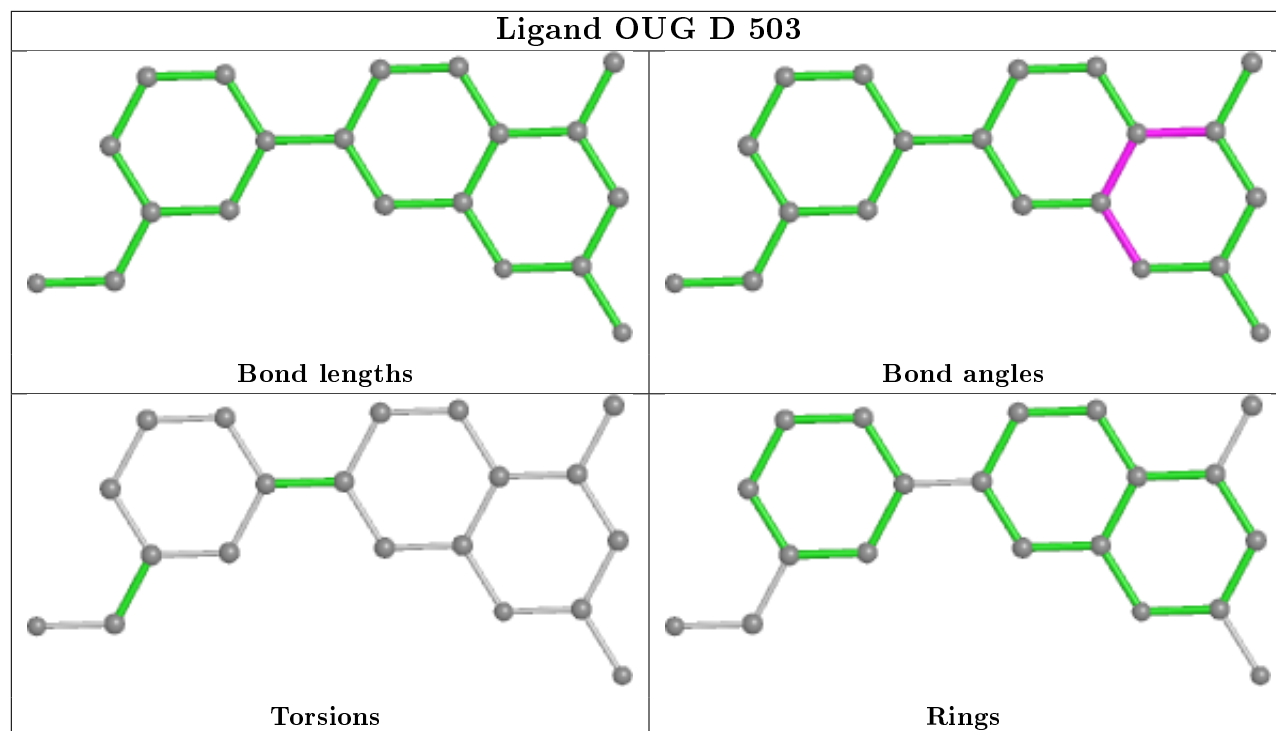
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	503	OUG	1	0
5	A	504	BTB	2	0
2	A	501	HEM	1	0
2	C	502	HEM	4	0
8	C	510	GOL	2	0
5	A	506	BTB	3	0
2	D	501	HEM	4	0
5	A	507	BTB	1	0
4	A	503	OUG	2	0
5	C	507	BTB	3	0
5	C	505	BTB	1	0

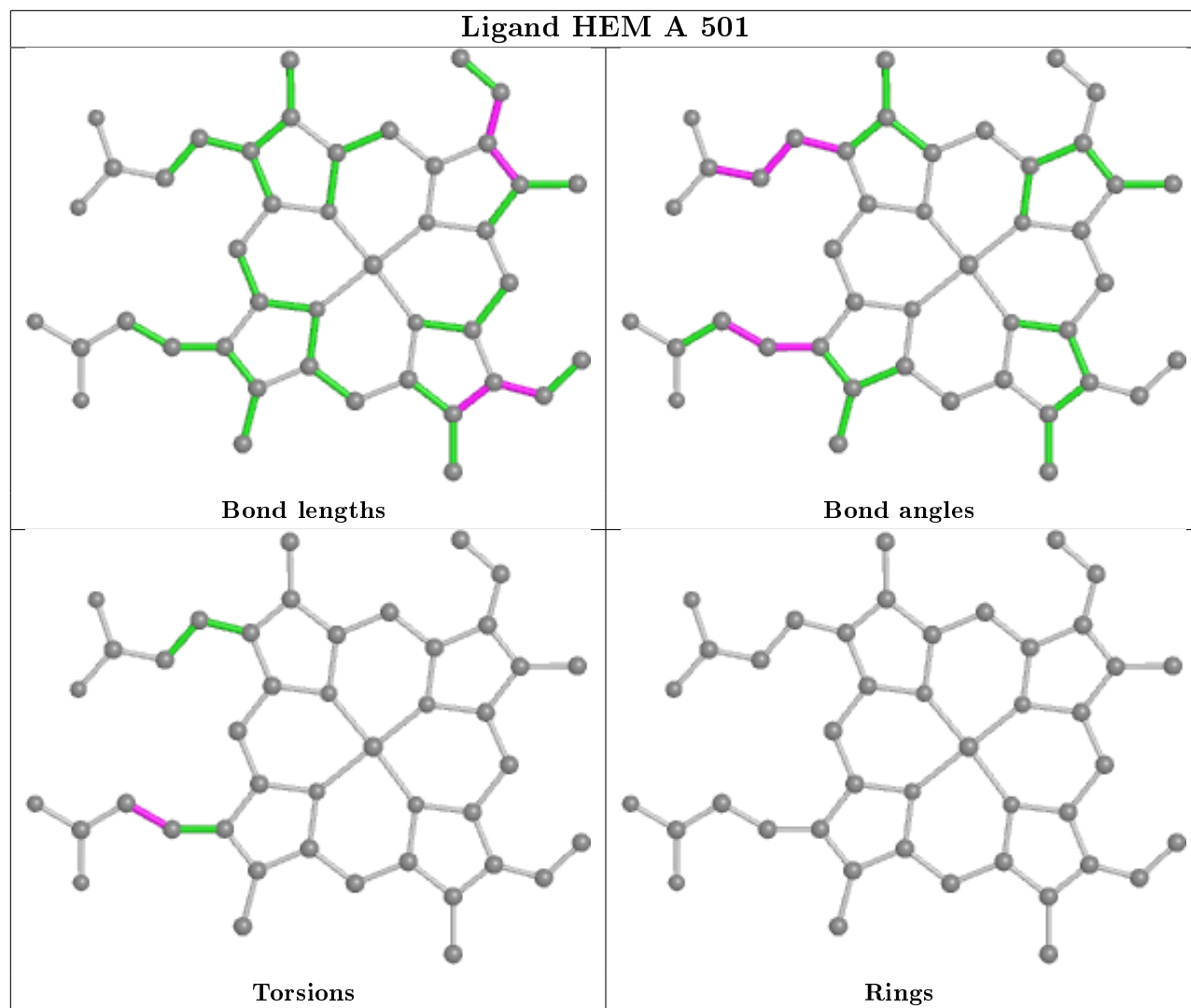
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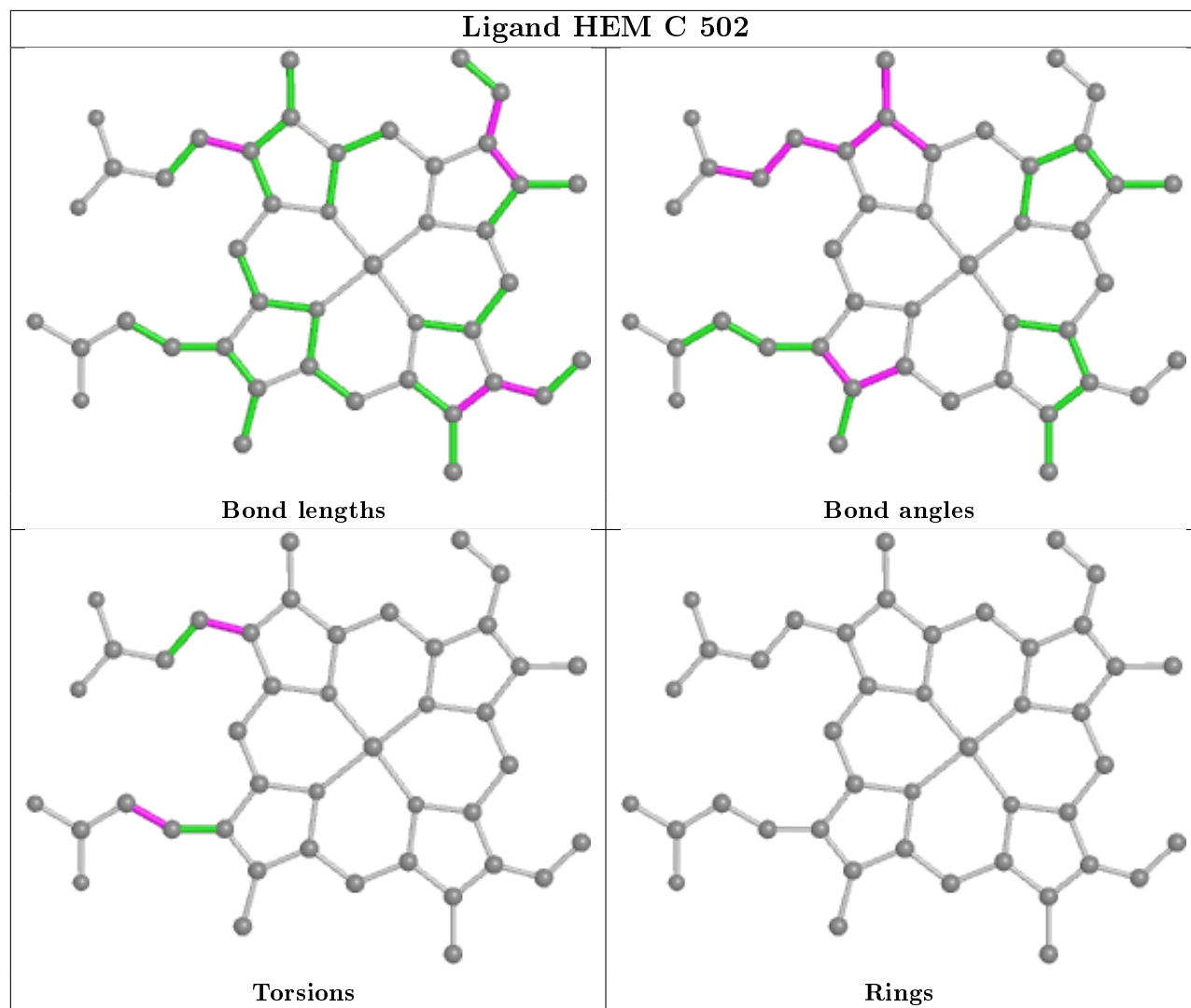
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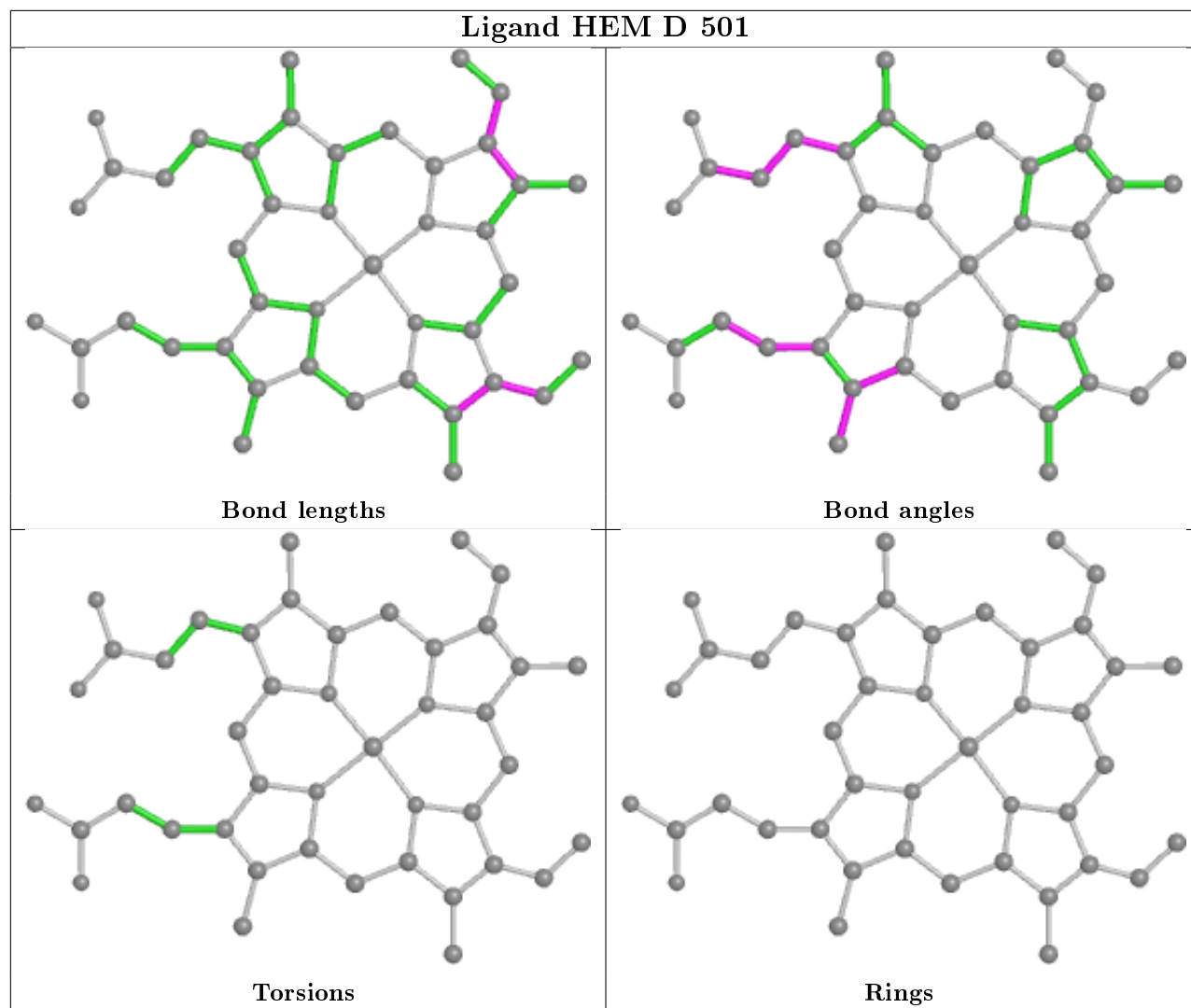
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	506	BTB	2	0
7	B	504	ACT	1	0
3	A	502	H4B	1	0
5	A	505	BTB	4	0
3	C	503	H4B	1	0
4	B	503	OUG	1	0
5	D	505	BTB	4	0
5	B	506	BTB	2	0
2	B	501	HEM	6	0
4	C	504	OUG	3	0
5	B	507	BTB	1	0
5	D	507	BTB	2	0
5	D	506	BTB	5	0
5	B	505	BTB	2	0

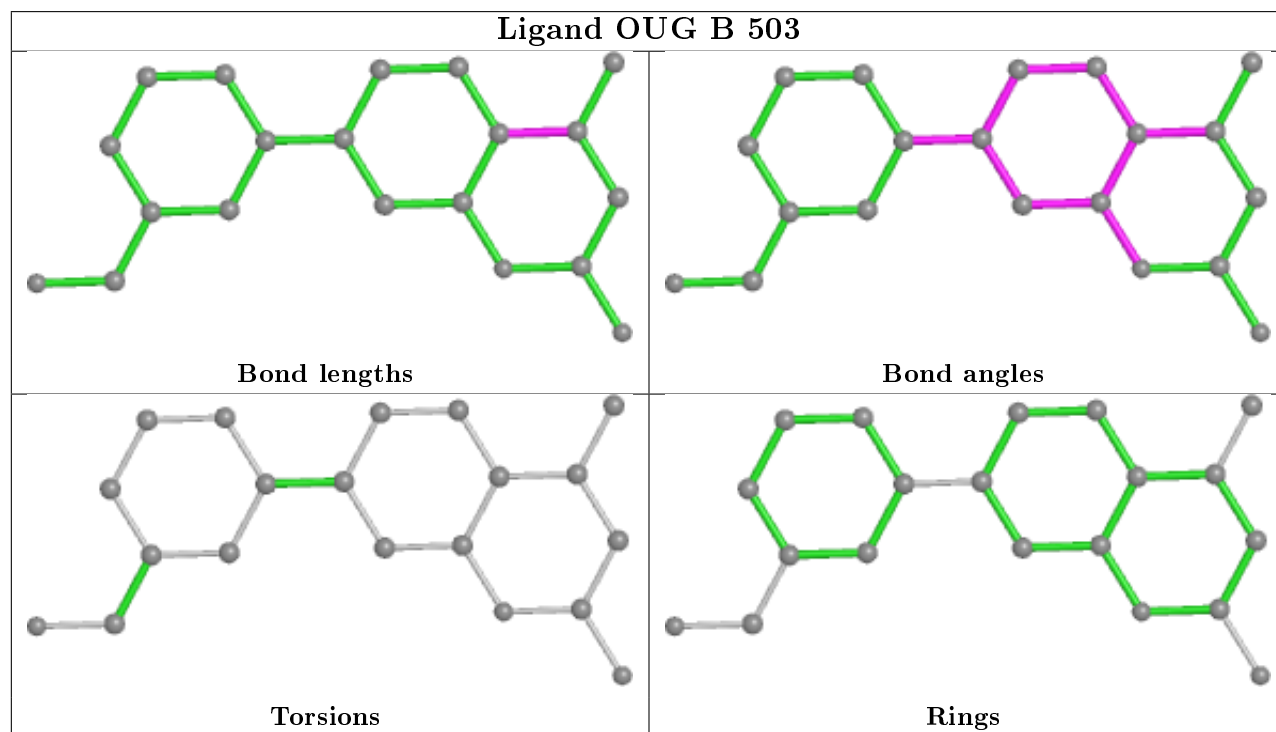
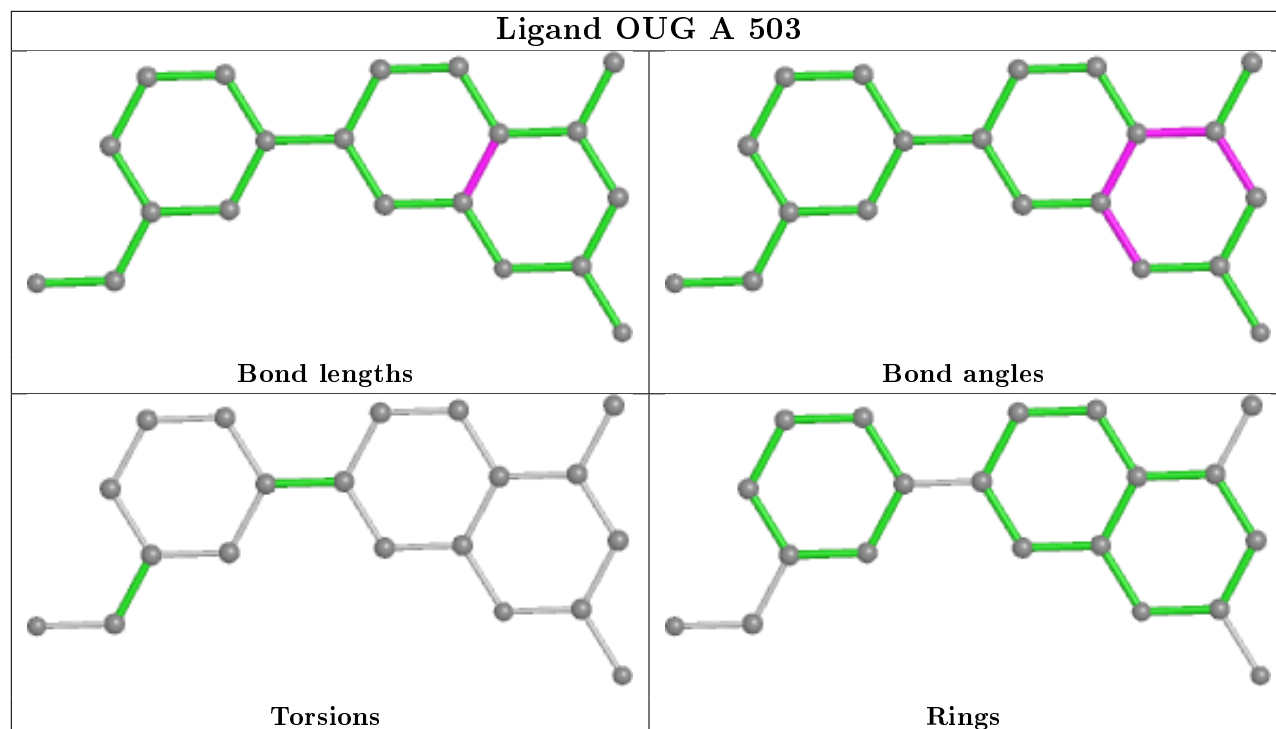
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

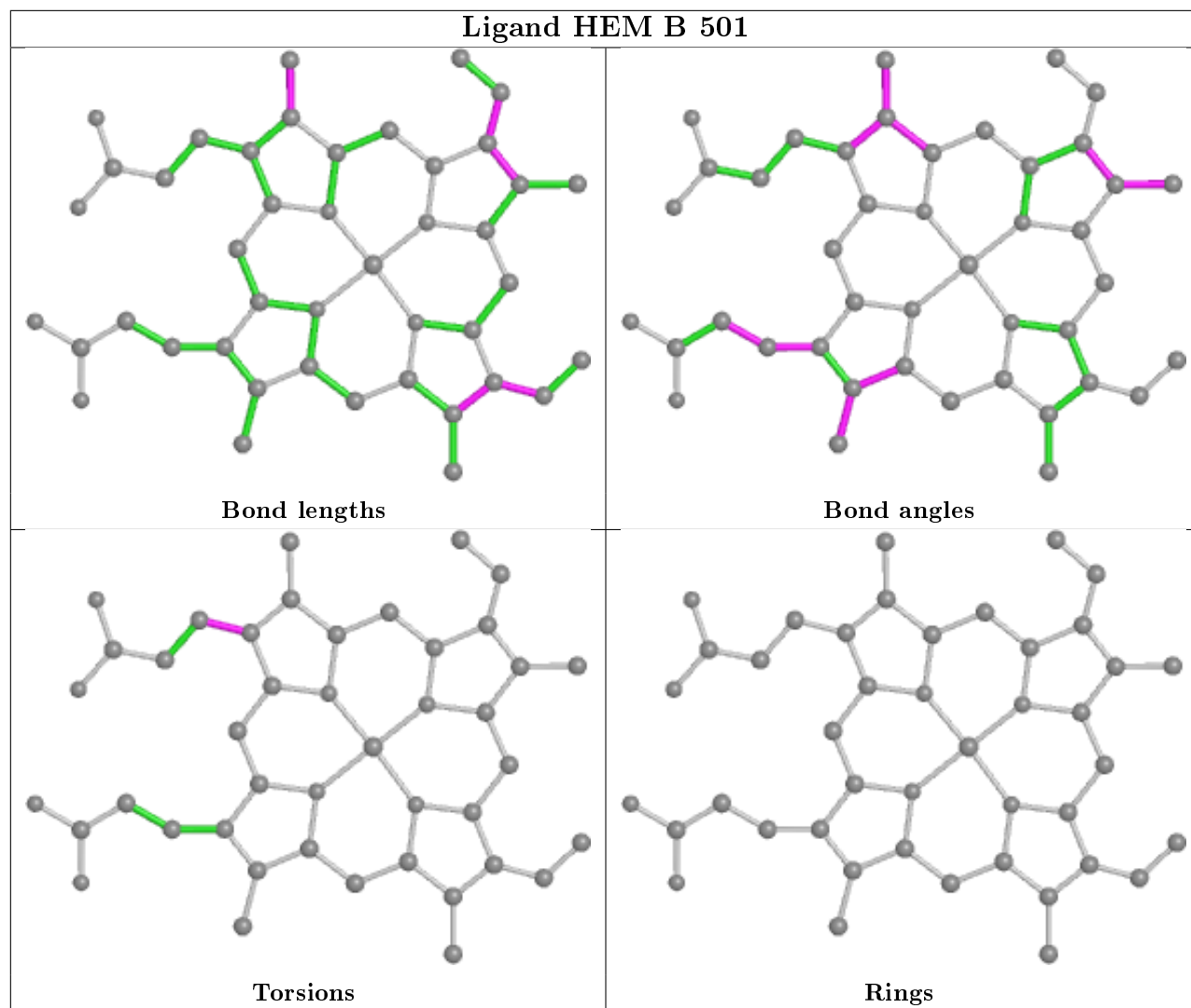


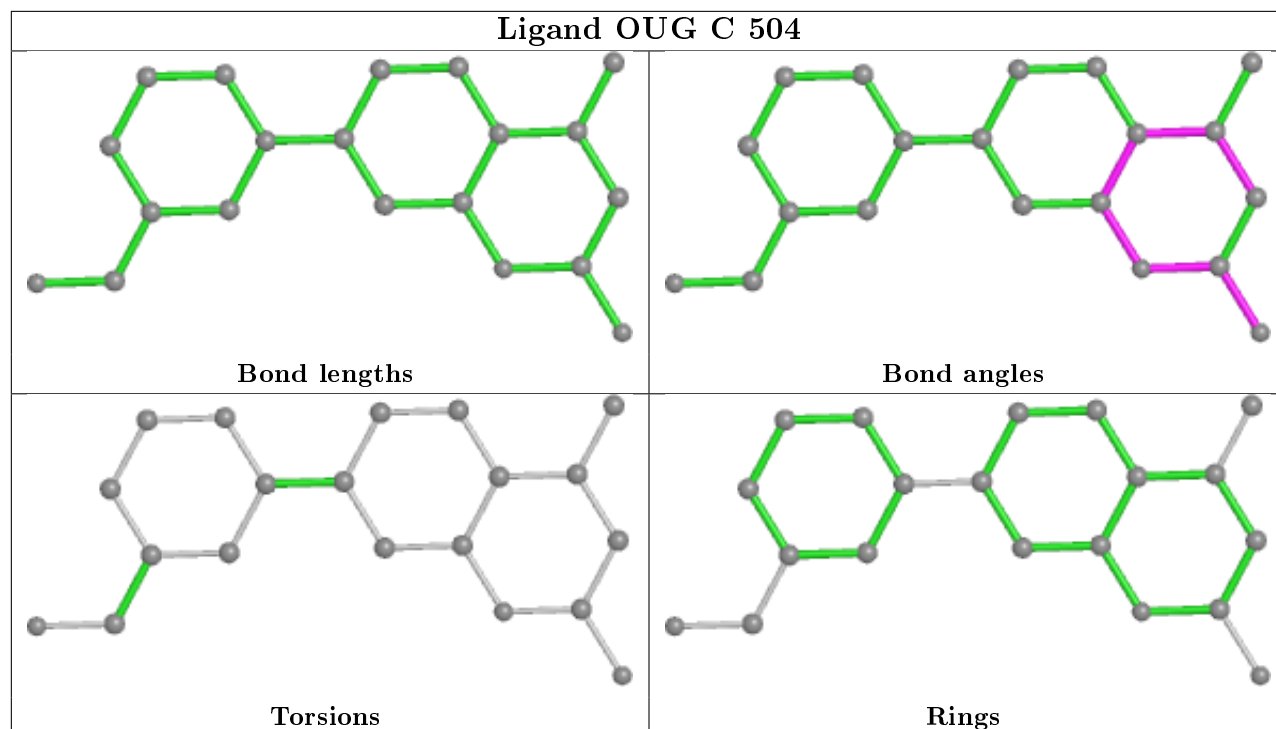












5.7 Other polymers [i](#)

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

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, 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%)	0.74	58 (14%) 2 2	35, 61, 102, 121	0
1	B	403/440 (91%)	0.22	25 (6%) 20 22	30, 47, 82, 119	0
1	C	404/440 (91%)	1.00	84 (20%) 1 0	35, 68, 116, 147	0
1	D	403/440 (91%)	0.32	31 (7%) 13 14	30, 48, 85, 129	0
All	All	1614/1760 (91%)	0.57	198 (12%) 4 3	30, 55, 103, 147	0

All (198) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	109	LEU	7.0
1	C	107	ARG	6.8
1	D	67	LYS	6.6
1	A	109	LEU	6.4
1	D	257	GLN	5.7
1	A	480	TRP	5.5
1	C	447	TRP	5.5
1	C	304	LEU	5.4
1	A	447	TRP	5.2
1	A	107	ARG	5.2
1	D	259	GLY	5.2
1	C	480	TRP	5.1
1	C	280	THR	5.0
1	C	204	ALA	4.8
1	C	108	LYS	4.7
1	C	448	ILE	4.7
1	D	452	ILE	4.5
1	A	108	LYS	4.5
1	A	451	PRO	4.4
1	A	448	ILE	4.4
1	C	119	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
1	C	451	PRO	4.3
1	A	239	GLY	4.2
1	C	153	VAL	4.2
1	C	259	GLY	4.1
1	B	452	ILE	4.1
1	B	258	ASP	4.0
1	C	452	ILE	3.9
1	D	460	PHE	3.9
1	C	302	LEU	3.8
1	A	452	ILE	3.8
1	B	255	ARG	3.8
1	C	298	GLU	3.8
1	C	141	SER	3.8
1	C	446	ALA	3.7
1	C	449	VAL	3.7
1	B	260	SER	3.7
1	A	449	VAL	3.7
1	D	449	VAL	3.7
1	A	301	GLU	3.7
1	A	68	PHE	3.7
1	C	479	PRO	3.6
1	C	142	GLY	3.6
1	C	275	ILE	3.6
1	C	293	LEU	3.6
1	C	300	PRO	3.6
1	A	280	THR	3.5
1	B	259	GLY	3.5
1	A	300	PRO	3.5
1	C	185	VAL	3.5
1	A	450	PRO	3.5
1	C	445	TRP	3.5
1	C	238	ARG	3.5
1	C	129	ASP	3.5
1	A	292	LEU	3.5
1	A	445	TRP	3.5
1	A	79	ILE	3.4
1	C	360	THR	3.4
1	D	446	ALA	3.4
1	C	450	PRO	3.4
1	C	412	LEU	3.4
1	C	122	GLN	3.3
1	D	454	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	449	VAL	3.3
1	D	258	ASP	3.2
1	C	237	GLY	3.2
1	D	260	SER	3.2
1	A	360	THR	3.2
1	A	272	GLU	3.2
1	C	254	TYR	3.2
1	B	360	THR	3.2
1	C	151	GLN	3.1
1	A	81	TYR	3.1
1	A	388	ARG	3.1
1	C	272	GLU	3.1
1	A	89	GLN	3.1
1	B	67	LYS	3.1
1	B	454	GLY	3.1
1	D	120	PRO	3.1
1	A	368	CYS	3.1
1	D	453	SER	3.0
1	D	451	PRO	3.0
1	C	276	GLN	3.0
1	D	360	THR	3.0
1	D	122	GLN	3.0
1	B	120	PRO	3.0
1	A	141	SER	3.0
1	A	185	VAL	3.0
1	B	68	PHE	3.0
1	C	184	CYS	3.0
1	A	275	ILE	2.9
1	C	279	TRP	2.9
1	A	106	PRO	2.9
1	C	268	VAL	2.9
1	D	455	SER	2.9
1	C	162	THR	2.9
1	B	446	ALA	2.9
1	C	145	ALA	2.9
1	D	89	GLN	2.9
1	A	446	ALA	2.8
1	C	89	GLN	2.8
1	D	388	ARG	2.8
1	A	304	LEU	2.8
1	D	86	ALA	2.8
1	C	444	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	257	GLN	2.8
1	A	273	LEU	2.8
1	C	244	TRP	2.8
1	B	121	GLU	2.7
1	D	450	PRO	2.7
1	A	238	ARG	2.7
1	A	439	GLY	2.7
1	C	295	ALA	2.7
1	C	292	LEU	2.7
1	D	158	ALA	2.7
1	D	447	TRP	2.6
1	C	281	PRO	2.6
1	C	125	SER	2.6
1	B	445	TRP	2.6
1	C	364	THR	2.6
1	D	79	ILE	2.6
1	C	274	CYS	2.6
1	A	364	THR	2.5
1	C	301	GLU	2.5
1	C	128	ARG	2.5
1	C	136[A]	SER	2.5
1	C	146	HIS	2.5
1	A	76	VAL	2.5
1	A	299	PRO	2.5
1	B	257	GLN	2.5
1	C	79	ILE	2.5
1	C	353	PHE	2.5
1	B	456	LEU	2.5
1	C	123	LEU	2.5
1	C	86	ALA	2.5
1	C	221	ARG	2.4
1	A	184	CYS	2.4
1	D	119	ALA	2.4
1	D	68	PHE	2.4
1	D	256	GLN	2.4
1	B	455	SER	2.4
1	A	236	PRO	2.4
1	C	359	SER	2.4
1	D	362	ILE	2.4
1	A	460	PHE	2.4
1	B	89	GLN	2.4
1	B	122	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	256	GLN	2.4
1	A	221	ARG	2.3
1	A	119	ALA	2.3
1	D	445	TRP	2.3
1	D	157	VAL	2.3
1	A	297	ASP	2.3
1	A	444	ASP	2.3
1	C	308	GLU	2.3
1	C	366	ASN	2.3
1	A	183	ARG	2.3
1	B	451	PRO	2.3
1	C	358	MET	2.3
1	A	202	ARG	2.3
1	C	256	GLN	2.3
1	C	124	LEU	2.3
1	A	276	GLN	2.3
1	C	182	PRO	2.3
1	B	453	SER	2.3
1	C	183	ARG	2.3
1	C	361	GLU	2.3
1	C	127	ALA	2.2
1	D	155	ALA	2.2
1	C	106	PRO	2.2
1	D	142	GLY	2.2
1	C	147	GLU	2.2
1	A	454	GLY	2.2
1	C	130	PHE	2.2
1	A	412	LEU	2.2
1	C	90	GLN	2.2
1	A	258	ASP	2.2
1	C	68	PHE	2.1
1	C	255	ARG	2.1
1	B	460	PHE	2.1
1	C	160	THR	2.1
1	A	122	GLN	2.1
1	A	298	GLU	2.1
1	C	81	TYR	2.1
1	C	235	CYS	2.1
1	C	367	LEU	2.1
1	B	450	PRO	2.1
1	A	140	ARG	2.1
1	A	308	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	303	PHE	2.1
1	A	259	GLY	2.1
1	A	309	LEU	2.0
1	A	367	LEU	2.0
1	C	258	ASP	2.0
1	A	358	MET	2.0
1	B	388	ARG	2.0
1	C	205	GLN	2.0
1	C	454	GLY	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, 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	A	507	14/14	0.77	0.15	86,97,105,107	0
5	BTB	B	506	14/14	0.82	0.22	78,85,97,101	0
5	BTB	B	507	14/14	0.82	0.24	79,94,103,106	0
5	BTB	D	508	14/14	0.83	0.32	92,101,105,106	0
9	GD	C	501	1/1	0.84	0.07	174,174,174,174	0
5	BTB	C	507	14/14	0.84	0.14	91,102,112,115	0
5	BTB	D	507	14/14	0.84	0.26	88,102,109,112	0
5	BTB	A	504	14/14	0.85	0.29	46,88,99,101	0
5	BTB	D	506	14/14	0.87	0.23	62,84,98,98	0
7	ACT	A	509	4/4	0.88	0.25	82,83,84,85	0
3	H4B	A	502	17/17	0.88	0.28	49,65,79,89	0
5	BTB	A	505	14/14	0.88	0.15	51,76,89,90	0
5	BTB	D	505	14/14	0.88	0.16	36,65,84,95	0
5	BTB	C	505	14/14	0.89	0.33	94,114,121,123	0

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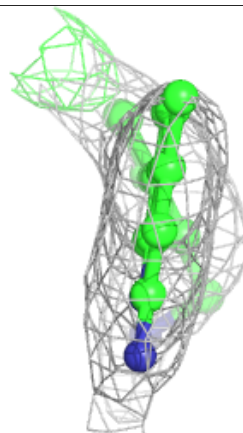
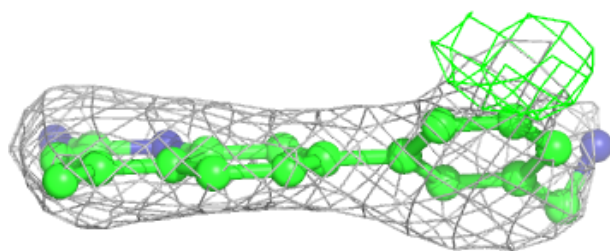
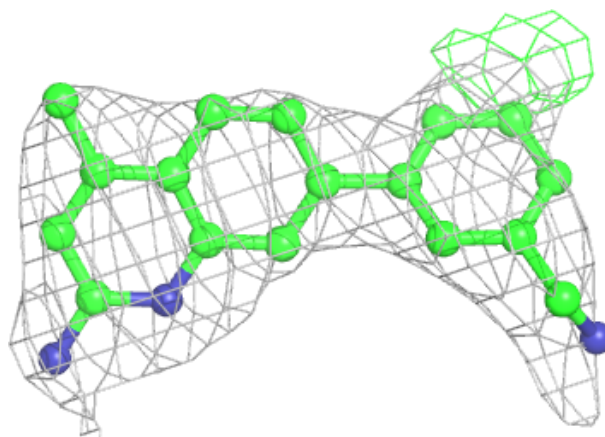
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	GOL	A	510	6/6	0.89	0.26	51,68,74,75	0
5	BTB	B	505	14/14	0.89	0.19	51,79,91,98	0
3	H4B	C	503	17/17	0.90	0.30	65,72,83,86	0
4	OUG	C	504	20/20	0.90	0.38	52,76,90,93	0
4	OUG	A	503	20/20	0.90	0.36	68,71,81,84	0
3	H4B	D	502	17/17	0.91	0.23	46,61,75,75	0
7	ACT	B	504	4/4	0.91	0.21	76,79,81,87	0
5	BTB	C	506	14/14	0.92	0.12	56,78,89,90	0
8	GOL	C	510	6/6	0.92	0.20	53,81,94,100	0
7	ACT	C	509	4/4	0.93	0.17	77,78,80,81	0
3	H4B	B	502	17/17	0.93	0.25	47,65,74,78	0
4	OUG	B	503	20/20	0.93	0.23	47,60,80,80	0
7	ACT	D	504	4/4	0.93	0.16	60,64,70,77	0
9	GD	A	511	1/1	0.94	0.06	139,139,139,139	0
4	OUG	D	503	20/20	0.94	0.22	38,62,91,94	0
2	HEM	C	502	43/43	0.96	0.25	46,64,99,104	0
2	HEM	D	501	43/43	0.97	0.14	26,39,81,87	0
2	HEM	B	501	43/43	0.97	0.14	28,39,73,83	0
5	BTB	A	506	14/14	0.97	0.19	8,69,82,86	0
2	HEM	A	501	43/43	0.97	0.24	39,53,95,102	0
6	ZN	C	508	1/1	0.99	0.12	54,54,54,54	0
9	GD	B	508	1/1	0.99	0.11	55,55,55,55	0
9	GD	D	509	1/1	0.99	0.13	54,54,54,54	0
6	ZN	A	508	1/1	1.00	0.10	47,47,47,47	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.

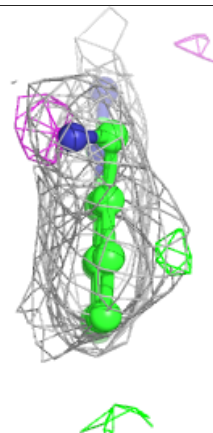
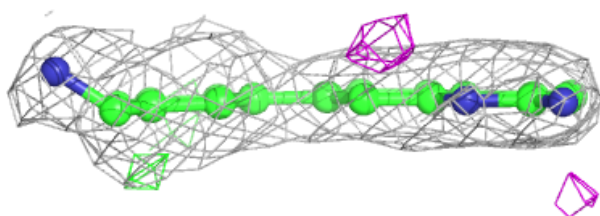
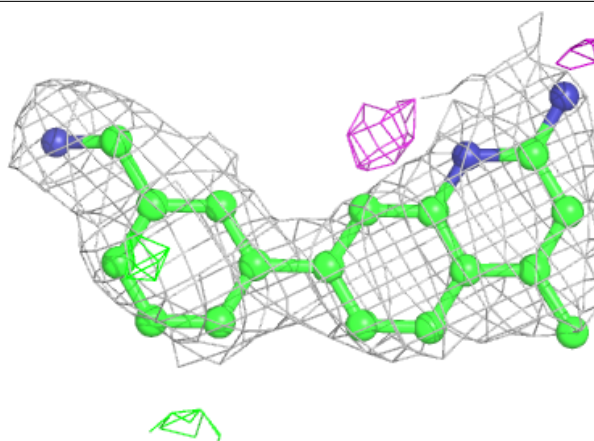
Electron density around OUG C 504:

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

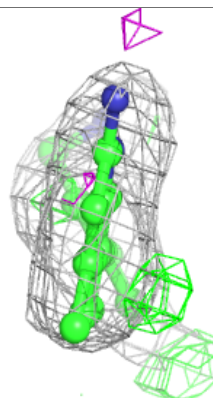
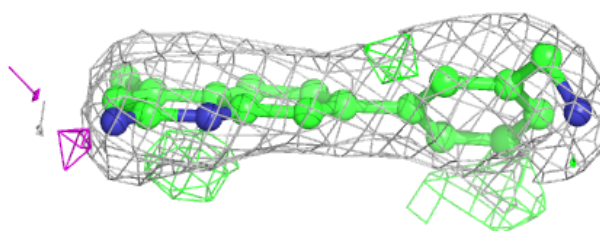
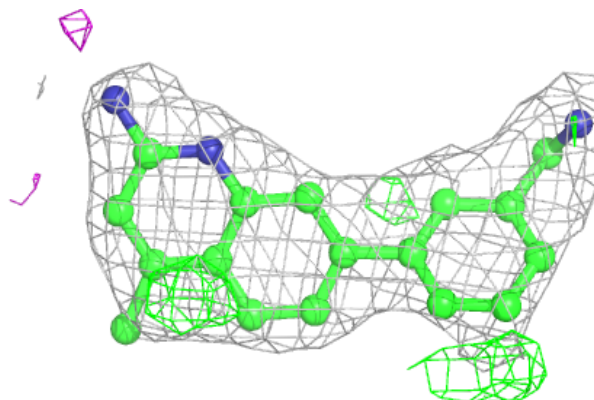


Electron density around OUG A 503:

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

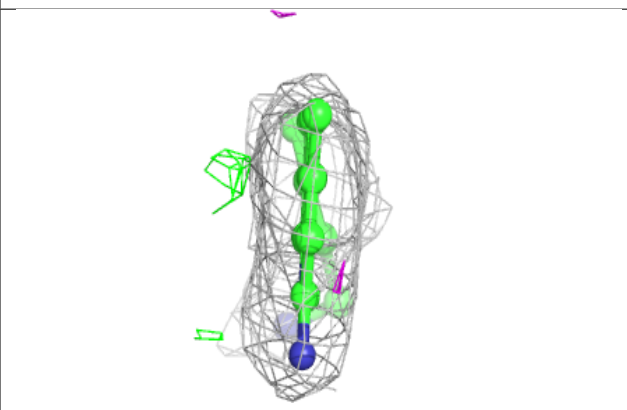
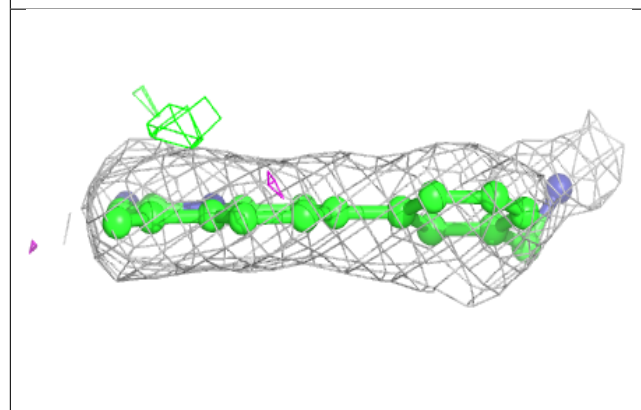
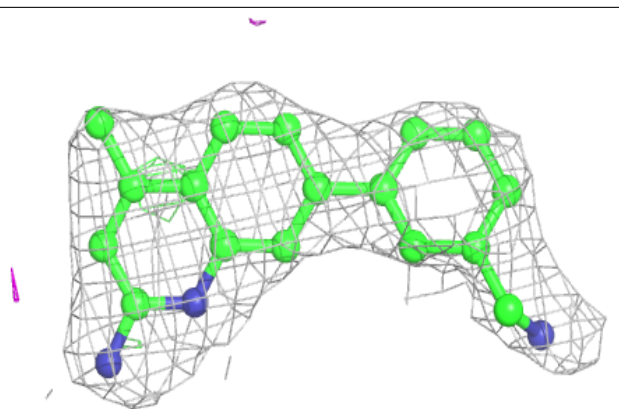
**Electron density around OUG B 503:**

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and green (positive)



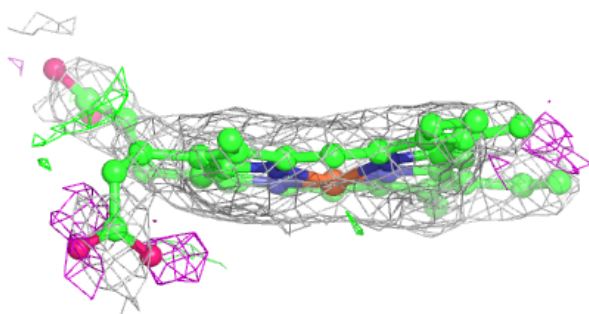
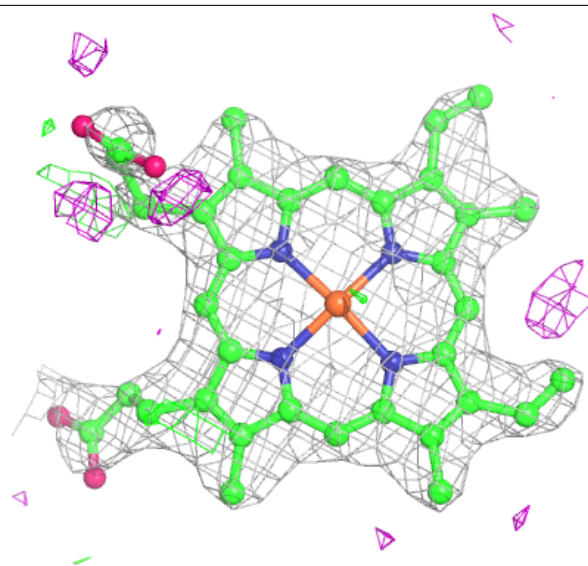
Electron density around OUG D 503:

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



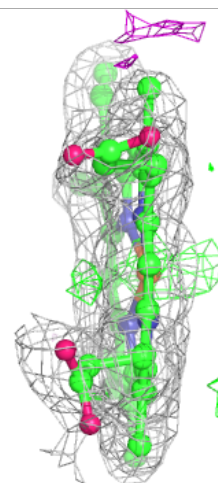
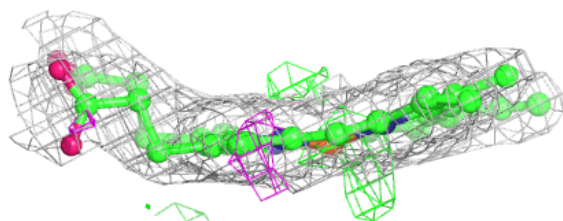
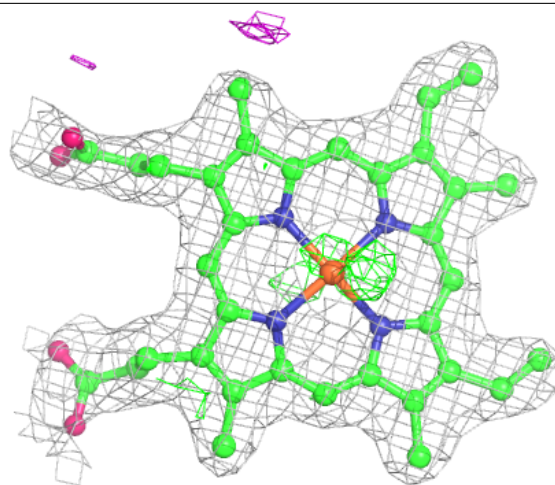
Electron density around HEM C 502:

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and green (positive)



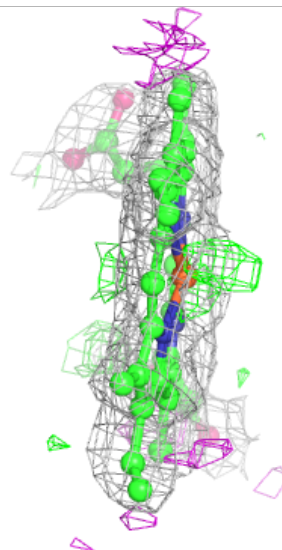
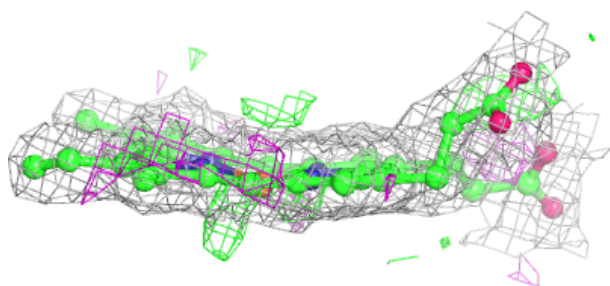
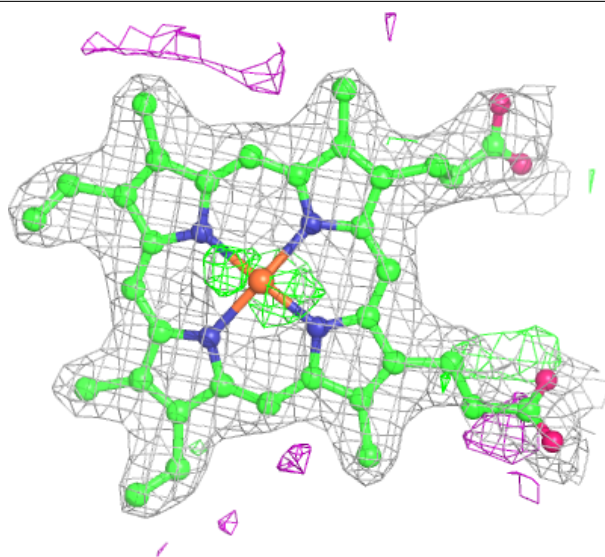
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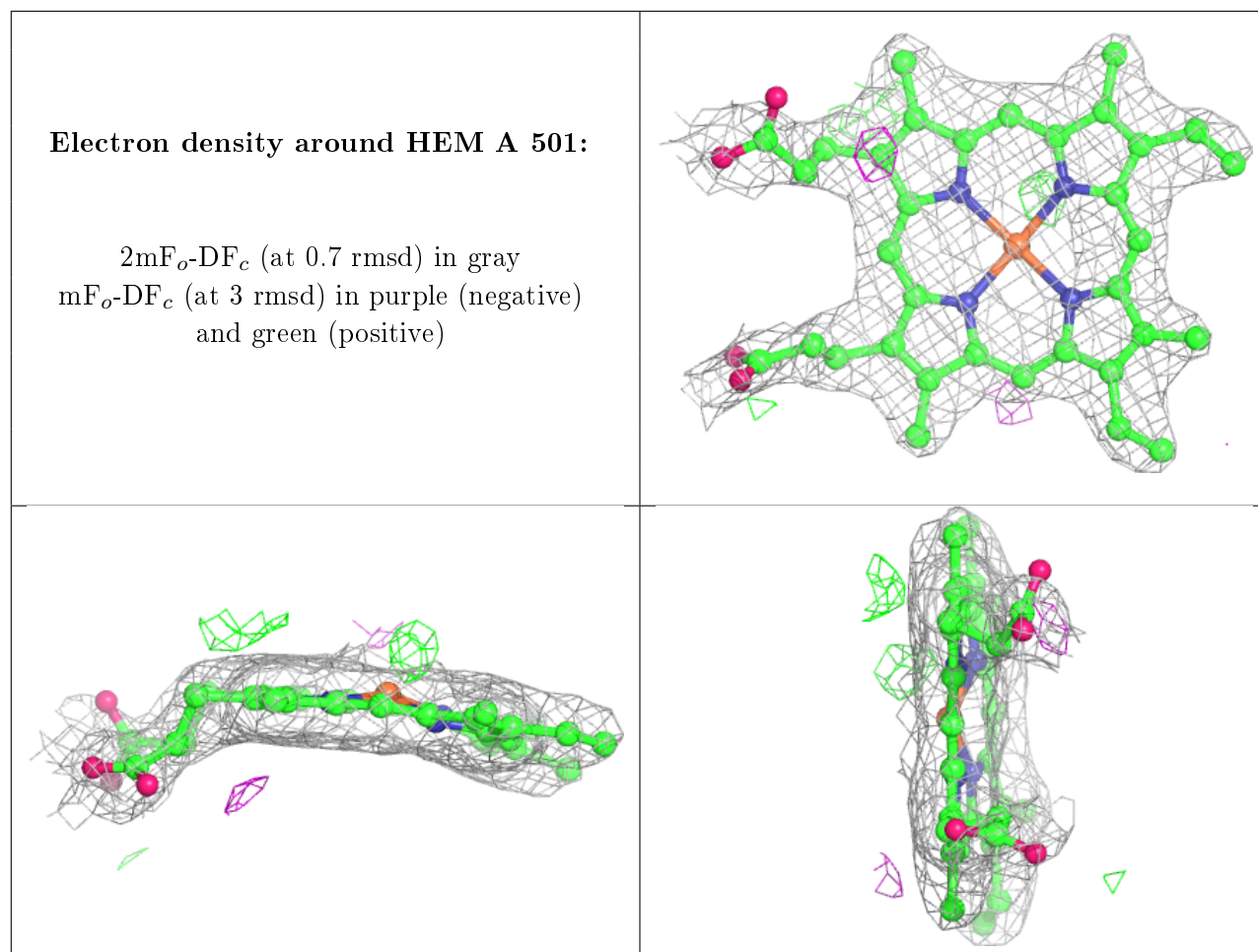
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM B 501:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.