



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:05 AM UTC

PDB ID : 6PP3 / pdb_00006pp3
Title : Structure of human endothelial nitric oxide synthase heme domain in complex with 7-(3-(Aminomethyl)-4-(pyridin-2-ylmethoxy)phenyl)-4-methylquinolin-2-amine
Authors : Li, H.; Poulos, T.L.
Deposited on : 2019-07-05
Resolution : 1.95 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

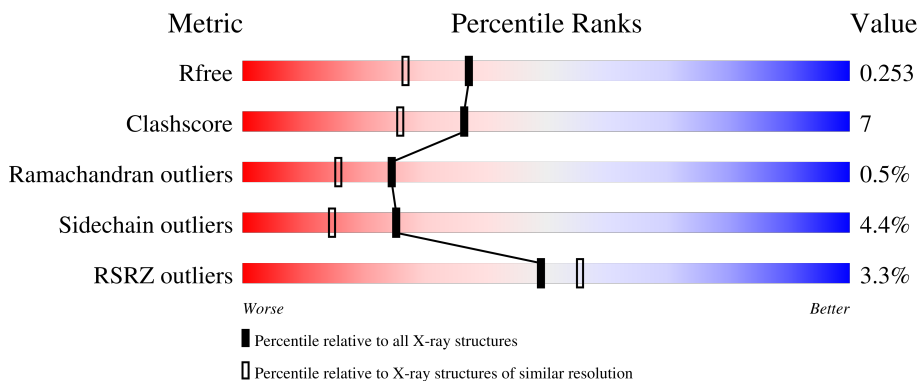
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	<div style="display: flex; align-items: center;"> <div style="width: 9%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 66%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 22%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">9% 66% 22% • 9%</p>
1	B	440	<div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 75%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 14%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">% 75% 14% • 9%</p>
1	C	440	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 79%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">2% 79% 10% • 9%</p>
1	D	440	<div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 79%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">% 79% 12% 9%</p>

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 13906 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
			Total	C	N	O	S			
1	A	401	3215	2047	566	586	16	0	2	0
1	B	402	3225	2054	566	589	16	0	4	0
1	C	401	3209	2044	563	586	16	0	2	0
1	D	401	3206	2042	563	585	16	0	2	0

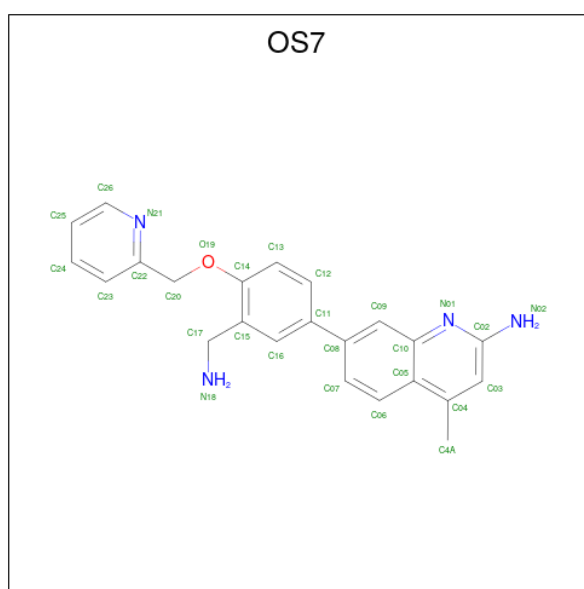
There are 4 discrepancies between the modelled and reference sequences:

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: $C_{34}H_{32}FeN_4O_4$).

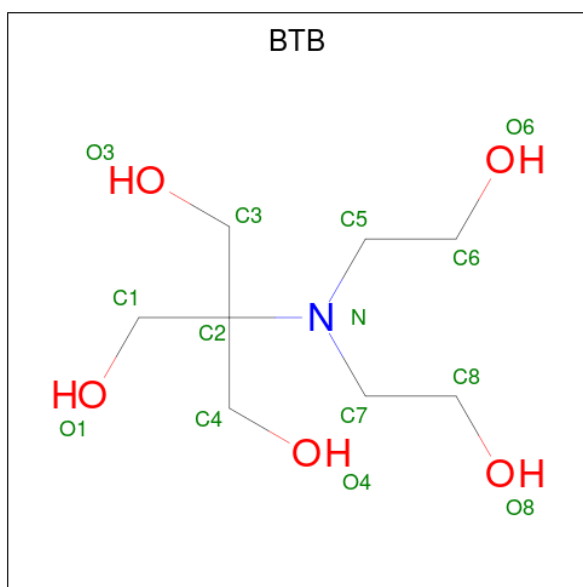
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		
3	C	1	Total	C	N	O	0	0
			17	9	5	3		
3	D	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 4 is 7-{3-(aminomethyl)-4-[(pyridin-2-yl)methoxy]phenyl}-4-methylquinolin-2-amine (CCD ID: OS7) (formula: C₂₃H₂₂N₄O) (labeled as "Ligand of Interest" by depositor).



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

- 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
			Total	C	N	O		
5	A	1	14	8	1	5	0	0
5	A	1	14	8	1	5	0	0
5	A	1	14	8	1	5	0	0
5	B	1	14	8	1	5	0	0
5	B	1	14	8	1	5	0	0
5	B	1	14	8	1	5	0	0
5	B	1	14	8	1	5	0	0
5	B	1	14	8	1	5	0	0
5	C	1	14	8	1	5	0	0
5	D	1	14	8	1	5	0	0
5	D	1	14	8	1	5	0	0

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

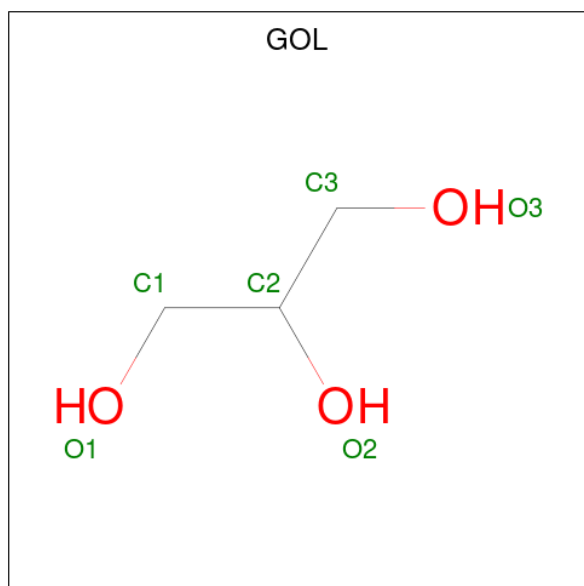
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
6	A	1	1	1	0	0

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

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 8 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

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

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

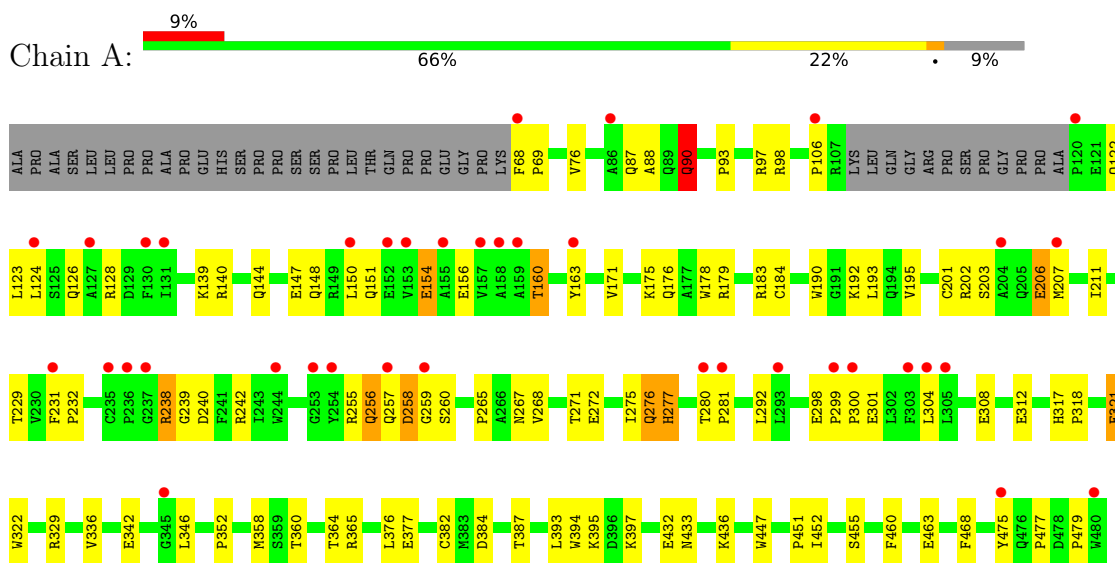
- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	66	Total O 66 66	0	0
10	B	168	Total O 168 168	0	0
10	C	121	Total O 121 121	0	0
10	D	168	Total O 168 168	0	0

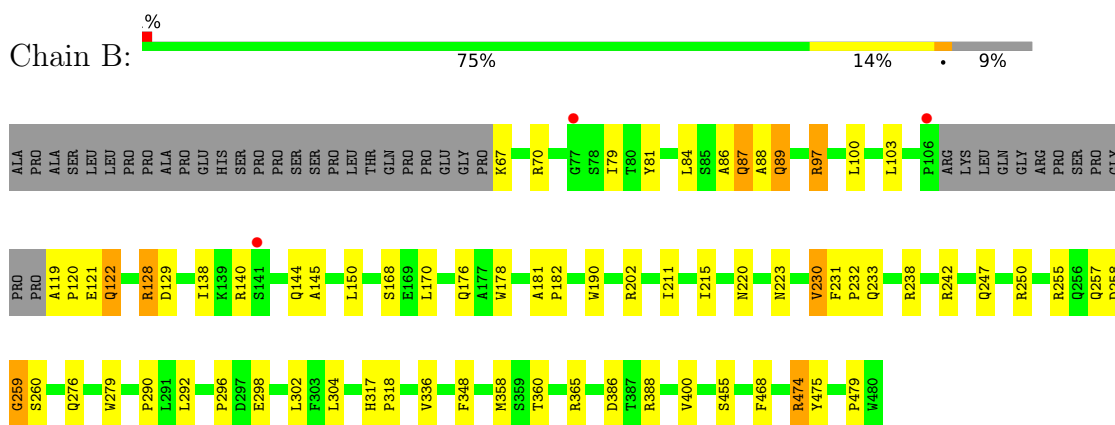
3 Residue-property plots i

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.

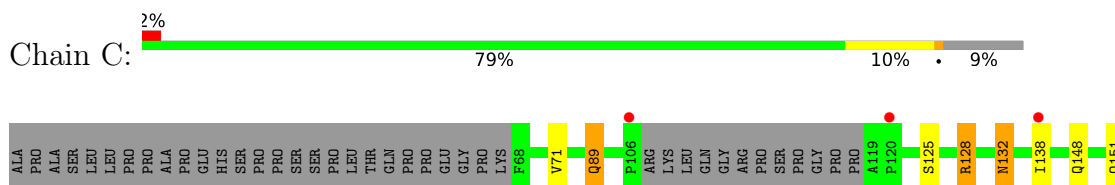
- Molecule 1: Nitric oxide synthase, endothelial

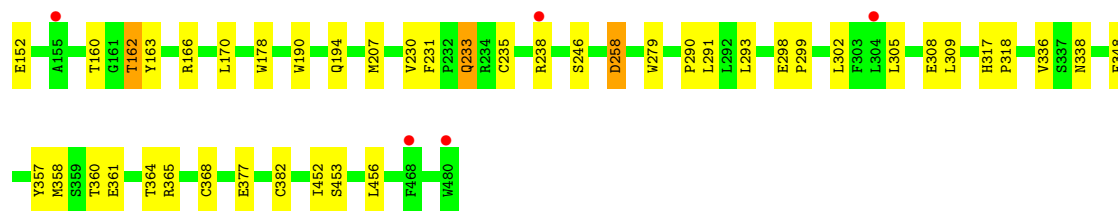


- Molecule 1: Nitric oxide synthase, endothelial

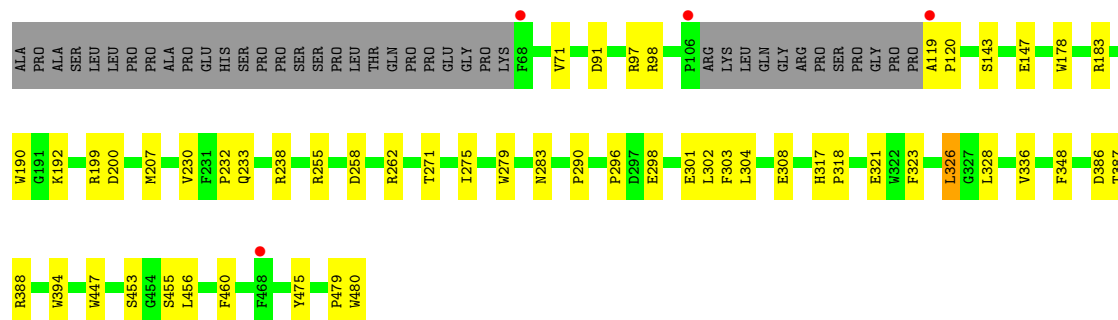
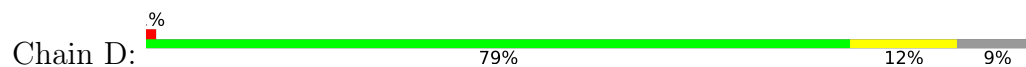


- Molecule 1: Nitric oxide synthase, endothelial





● Molecule 1: Nitric oxide synthase, endothelial



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	59.87Å 152.08Å 108.58Å 90.00° 90.91° 90.00°	Depositor
Resolution (Å)	49.86 – 1.95 49.86 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.86-1.95) 99.7 (49.86-1.95)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	0.16	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.12 (at 1.95Å)	Xtrriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.211 , 0.260 0.203 , 0.253	Depositor DCC
R_{free} test set	7064 reflections (3.81%)	wwPDB-VP
Wilson B-factor (Å ²)	36.0	Xtrriage
Anisotropy	0.552	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 50.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.107 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13906	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.05% 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: CL, HEM, ZN, H4B, GD, BTB, OS7, GOL

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	0.27	0/3313	0.49	0/4513
1	B	0.34	0/3329	0.54	0/4536
1	C	0.29	0/3307	0.48	0/4507
1	D	0.38	0/3304	0.57	0/4503
All	All	0.32	0/13253	0.52	0/18059

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	3215	0	3118	64	0
1	B	3225	0	3131	49	0
1	C	3209	0	3109	27	1
1	D	3206	0	3108	29	0
2	A	43	0	30	4	0
2	B	43	0	30	3	0
2	C	43	0	30	3	0
2	D	43	0	30	2	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	1	0
3	C	17	0	15	1	0
3	D	17	0	15	0	0
4	A	28	0	0	1	0
4	B	28	0	0	2	0
4	C	28	0	0	4	0
4	D	28	0	0	1	0
5	A	42	0	56	7	0
5	B	70	0	93	11	1
5	C	14	0	19	3	0
5	D	28	0	37	6	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
7	A	6	0	8	0	0
7	C	6	0	8	0	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
9	A	1	0	0	0	0
9	B	2	0	0	0	0
9	D	1	0	0	0	0
10	A	66	0	0	2	0
10	B	168	0	0	0	0
10	C	121	0	0	1	0
10	D	168	0	0	4	0
All	All	13906	0	12867	188	1

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

All (188) 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:257:GLN:HA	1:B:259:GLY:H	1.38	0.87
1:C:128:ARG:O	1:C:132:ASN:ND2	2.13	0.81
1:A:147:GLU:O	1:A:151:GLN:NE2	2.15	0.79
1:A:312:GLU:OE2	1:A:329:ARG:NH1	2.14	0.78
1:A:322:TRP:CD1	5:A:504:BTB:H62	2.21	0.76
1:A:433:ASN:HA	1:A:436:LYS:HE3	1.69	0.71
1:D:119:ALA:N	10:D:602:HOH:O	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:509:BTB:H12	1:C:382:CYS:HA	1.74	0.70
1:C:258:ASP:N	1:C:258:ASP:OD1	2.25	0.70
1:B:298:GLU:OE2	5:B:505:BTB:N	2.26	0.69
1:D:336:VAL:HG21	4:D:503:OS7:C07	2.22	0.68
1:B:336:VAL:HG21	4:B:503:OS7:C07	2.24	0.68
5:D:504:BTB:H61	10:D:728:HOH:O	1.92	0.67
2:A:501:HEM:HBB2	2:A:501:HEM:HHC	1.74	0.67
2:D:501:HEM:HMC2	2:D:501:HEM:HBC2	1.77	0.66
1:A:321:GLU:H	1:A:321:GLU:CD	2.03	0.66
1:C:336:VAL:HG21	4:C:503:OS7:C07	2.29	0.62
1:A:292:LEU:HD22	1:A:300:PRO:HB2	1.82	0.62
1:A:336:VAL:HG21	4:A:503:OS7:C07	2.29	0.61
1:D:91:ASP:OD1	10:D:601:HOH:O	2.16	0.61
1:B:119:ALA:HB1	1:B:122:GLN:HE21	1.65	0.61
2:B:501:HEM:HHC	2:B:501:HEM:HBB2	1.84	0.60
1:A:150:LEU:HB2	1:A:151:GLN:NE2	2.16	0.60
2:A:501:HEM:HMC2	2:A:501:HEM:HBC2	1.83	0.59
2:B:501:HEM:HBC2	2:B:501:HEM:HMC2	1.86	0.58
1:B:257:GLN:HA	1:B:259:GLY:N	2.13	0.57
1:A:377:GLU:OE1	5:A:505:BTB:H11	2.05	0.57
1:A:384:ASP:OD1	5:A:504:BTB:O3	2.21	0.57
1:B:121:GLU:OE1	1:B:122:GLN:NE2	2.38	0.56
1:C:207:MET:HE3	1:C:293:LEU:HB3	1.86	0.56
1:B:122:GLN:CD	1:B:122:GLN:H	2.13	0.56
1:C:235:CYS:SG	1:C:238:ARG:NH2	2.79	0.56
2:D:501:HEM:HBB2	2:D:501:HEM:HHC	1.87	0.56
1:C:365:ARG:HH12	3:C:502:H4B:C4	2.18	0.55
1:D:321:GLU:OE2	5:D:504:BTB:O4	2.24	0.55
1:A:258:ASP:N	1:A:258:ASP:OD1	2.40	0.54
1:C:364:THR:O	1:C:368:CYS:HB2	2.07	0.54
1:B:178:TRP:CE3	1:B:190:TRP:HA	2.43	0.54
2:C:501:HEM:HBC2	2:C:501:HEM:HMC2	1.90	0.54
1:B:138:ILE:HG13	1:B:140:ARG:HB2	1.91	0.53
1:B:386:ASP:OD1	1:B:388:ARG:HG2	2.10	0.52
1:D:326:LEU:HB3	1:D:328:LEU:HG	1.90	0.52
1:B:290:PRO:HB3	1:B:304:LEU:HD23	1.91	0.52
1:B:144:GLN:NE2	1:B:145:ALA:H	2.08	0.52
1:A:124:LEU:HD23	1:A:128:ARG:NE	2.24	0.52
1:A:148:GLN:O	1:A:151:GLN:HG2	2.10	0.51
1:C:298:GLU:HG3	1:C:299:PRO:HD2	1.91	0.51
1:A:382:CYS:HA	5:A:504:BTB:H11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:162:THR:OG1	1:C:163:TYR:N	2.43	0.51
1:B:247:GLN:HB2	1:B:250:ARG:HD3	1.93	0.51
5:B:510:BTB:H12	1:C:377:GLU:OE1	2.10	0.51
1:D:238:ARG:HG2	1:D:296:PRO:HB3	1.92	0.51
1:D:386:ASP:OD1	1:D:388:ARG:NH1	2.44	0.51
1:A:275:ILE:C	1:A:277:HIS:H	2.19	0.51
1:A:317:HIS:CG	1:A:318:PRO:HD2	2.46	0.51
1:C:233:GLN:HB3	1:C:348:PHE:CE2	2.46	0.50
5:D:505:BTB:O4	5:D:505:BTB:O1	2.13	0.50
1:A:97:ARG:NH2	1:B:86:ALA:O	2.34	0.50
1:A:124:LEU:O	1:A:128:ARG:HG3	2.11	0.50
1:A:156:GLU:O	1:A:160:THR:OG1	2.30	0.50
1:B:475:TYR:OH	2:B:501:HEM:O1D	2.24	0.49
1:D:233:GLN:HB3	1:D:348:PHE:CE2	2.47	0.49
1:B:70:ARG:HD2	1:B:79:ILE:HD13	1.93	0.49
1:B:89:GLN:NE2	1:B:129:ASP:OD2	2.46	0.49
1:B:170:LEU:HD21	1:B:230:VAL:HG11	1.93	0.49
1:D:290:PRO:HB3	1:D:304:LEU:HD23	1.94	0.49
1:C:317:HIS:CG	1:C:318:PRO:HD2	2.48	0.48
1:A:242:ARG:NH1	1:A:477:PRO:O	2.39	0.48
1:B:233:GLN:HB3	1:B:348:PHE:CE2	2.48	0.48
1:B:468:PHE:CZ	1:B:474:ARG:HD2	2.49	0.48
1:C:279:TRP:CG	1:C:290:PRO:HG3	2.49	0.48
5:B:505:BTB:O3	5:B:505:BTB:H51	2.10	0.48
1:C:361:GLU:OE2	4:C:503:OS7:N02	2.46	0.47
1:D:387:THR:HA	1:D:394:TRP:CD1	2.49	0.47
1:C:453:SER:HB3	1:C:456:LEU:HD12	1.96	0.47
1:A:124:LEU:HD23	1:A:128:ARG:HE	1.78	0.47
1:D:119:ALA:N	1:D:120:PRO:HD3	2.30	0.47
1:A:451:PRO:HB2	1:B:455:SER:OG	2.15	0.47
1:C:148:GLN:HE22	1:C:166:ARG:NH2	2.12	0.47
1:D:453:SER:HB3	1:D:456:LEU:HD12	1.96	0.47
1:B:238:ARG:HG2	1:B:296:PRO:HB3	1.97	0.47
1:A:90:GLN:HB2	1:A:468:PHE:CE2	2.50	0.46
1:A:364:THR:HG21	1:A:452:ILE:HG23	1.96	0.46
5:B:510:BTB:O3	5:B:510:BTB:O1	2.23	0.46
2:C:501:HEM:HBA2	4:C:503:OS7:C12	2.45	0.46
1:D:262:ARG:HD3	1:D:283:ASN:O	2.16	0.46
1:C:279:TRP:HB2	1:C:302:LEU:HD11	1.97	0.46
1:D:479:PRO:HD2	1:D:480:TRP:CZ3	2.51	0.46
1:A:358:MET:HE3	1:A:360:THR:OG1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:317:HIS:CG	1:D:318:PRO:HD2	2.51	0.46
1:B:242:ARG:CZ	1:B:479:PRO:HG3	2.45	0.46
1:A:183:ARG:HD3	1:A:447:TRP:CD2	2.51	0.46
1:B:358:MET:HE3	1:B:360:THR:OG1	2.16	0.46
1:C:291:LEU:HD11	1:C:305:LEU:HD21	1.97	0.46
1:A:154:GLU:H	1:A:154:GLU:HG3	1.62	0.46
1:D:178:TRP:CE3	1:D:190:TRP:HA	2.50	0.46
5:D:504:BTB:H32	5:D:504:BTB:H51	1.65	0.46
2:C:501:HEM:HBB2	2:C:501:HEM:HHC	1.98	0.45
5:D:505:BTB:H51	5:D:505:BTB:H32	1.31	0.45
1:A:256:GLN:HB3	1:A:258:ASP:H	1.80	0.45
1:B:258:ASP:O	1:B:260:SER:N	2.49	0.45
1:A:176:GLN:OE1	1:A:179:ARG:NH1	2.44	0.45
1:A:393:LEU:O	1:A:397:LYS:HG3	2.16	0.45
1:B:100:LEU:HB3	1:B:103:LEU:HD22	1.99	0.45
1:A:229:THR:O	1:A:352:PRO:HD2	2.17	0.45
1:A:455:SER:HA	1:A:460:PHE:CG	2.52	0.45
1:B:211:ILE:O	1:B:215:ILE:HG13	2.17	0.45
1:D:308:GLU:H	1:D:308:GLU:CD	2.22	0.45
1:A:267:ASN:O	1:A:271:THR:OG1	2.20	0.44
1:B:84:LEU:HD12	1:B:87:GLN:HG3	1.98	0.44
1:A:242:ARG:CZ	1:A:479:PRO:HD3	2.46	0.44
1:B:317:HIS:CG	1:B:318:PRO:HD2	2.52	0.44
1:A:201:CYS:SG	1:A:206:GLU:HB3	2.58	0.44
1:A:258:ASP:O	1:A:260:SER:N	2.51	0.44
1:A:97:ARG:HG2	1:B:88:ALA:HB3	2.00	0.44
1:B:298:GLU:OE1	5:B:505:BTB:H31	2.18	0.44
5:C:504:BTB:H41	5:C:504:BTB:H51	1.57	0.44
1:A:265:PRO:HA	1:A:268:VAL:HG23	1.99	0.44
1:B:336:VAL:HG21	4:B:503:OS7:C06	2.48	0.44
1:D:298:GLU:OE1	5:D:505:BTB:H42	2.17	0.44
1:A:88:ALA:HB3	1:B:97:ARG:HH11	1.82	0.44
1:A:275:ILE:HD11	1:A:281:PRO:HB3	2.00	0.44
5:C:504:BTB:H32	5:C:504:BTB:H71	1.54	0.44
1:D:143:SER:O	1:D:147:GLU:HG2	2.18	0.44
1:D:279:TRP:HB2	1:D:302:LEU:HD21	1.99	0.43
1:A:93:PRO:HG3	1:A:106:PRO:HB3	2.00	0.43
1:A:140:ARG:NH1	10:A:601:HOH:O	2.36	0.43
1:C:246:SER:HA	1:C:338:ASN:HB3	2.01	0.43
1:D:207:MET:HE2	1:D:207:MET:HB3	1.95	0.43
1:B:292:LEU:HD23	1:B:292:LEU:HA	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:301:GLU:HB3	1:D:303:PHE:CE1	2.54	0.43
1:D:475:TYR:HA	10:D:689:HOH:O	2.18	0.43
1:A:276:GLN:O	1:A:277:HIS:ND1	2.28	0.43
1:A:123:LEU:HD11	1:A:346:LEU:HD23	2.00	0.43
5:A:504:BTB:H52	5:A:504:BTB:H81	1.65	0.43
1:A:203:SER:H	1:A:206:GLU:HB2	1.83	0.43
1:C:357:TYR:HA	4:C:503:OS7:N02	2.34	0.43
1:A:308:GLU:H	1:A:308:GLU:CD	2.25	0.43
5:A:505:BTB:H72	5:A:505:BTB:H41	1.44	0.43
1:C:207:MET:HG3	1:C:231:PHE:CZ	2.54	0.43
1:A:68:PHE:HA	1:A:69:PRO:HD3	1.83	0.42
1:A:178:TRP:CE3	1:A:190:TRP:HA	2.54	0.42
5:B:509:BTB:H12	5:B:509:BTB:H51	1.68	0.42
1:A:163:TYR:CE1	1:A:346:LEU:HD21	2.54	0.42
1:B:250:ARG:HA	1:B:250:ARG:HD2	1.86	0.42
5:B:504:BTB:H72	5:B:504:BTB:H12	1.85	0.42
1:A:88:ALA:O	1:B:97:ARG:NH1	2.36	0.42
1:B:128:ARG:HB2	1:B:128:ARG:NH1	2.33	0.42
1:A:365:ARG:HH12	3:A:502:H4B:C4	2.32	0.42
5:B:510:BTB:H42	5:B:510:BTB:H72	1.81	0.42
1:A:238:ARG:HH21	1:A:240:ASP:HA	1.85	0.42
1:C:170:LEU:HD11	1:C:230:VAL:HG11	2.01	0.42
1:A:171:VAL:HG22	1:A:195:VAL:HB	2.02	0.42
1:A:342:GLU:HA	1:A:346:LEU:O	2.20	0.42
1:B:67:LYS:HB2	1:B:67:LYS:HE3	1.86	0.42
1:C:364:THR:HG21	1:C:452:ILE:HG23	2.01	0.42
1:C:358:MET:HE3	1:C:360:THR:OG1	2.20	0.42
5:A:506:BTB:H11	5:A:506:BTB:H72	1.60	0.41
1:D:271:THR:O	1:D:275:ILE:HG12	2.20	0.41
1:A:184:CYS:HB2	2:A:501:HEM:ND	2.35	0.41
1:A:475:TYR:OH	2:A:501:HEM:O1D	2.15	0.41
1:B:120:PRO:HD2	1:B:121:GLU:OE2	2.21	0.41
1:D:199:ARG:O	1:D:232:PRO:HG3	2.21	0.41
1:A:376:LEU:HD21	1:A:395:LYS:HB3	2.03	0.41
1:B:468:PHE:HZ	1:B:474:ARG:HH11	1.69	0.41
1:A:231:PHE:HB3	1:A:232:PRO:CD	2.51	0.41
1:A:387:THR:HA	1:A:394:TRP:CD1	2.56	0.41
1:B:181:ALA:HA	1:B:182:PRO:HD3	1.95	0.41
1:B:220:ASN:HB3	1:B:223:ASN:O	2.20	0.41
1:B:365:ARG:HH12	3:B:502:H4B:C4	2.34	0.41
1:C:194:GLN:NE2	10:C:622:HOH:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:183:ARG:HD3	1:D:447:TRP:CD2	2.55	0.41
1:D:455:SER:HA	1:D:460:PHE:CG	2.56	0.41
1:B:128:ARG:HD3	1:B:150:LEU:HD22	2.03	0.41
1:B:231:PHE:HB3	1:B:232:PRO:HD2	2.03	0.41
1:B:298:GLU:CD	5:B:505:BTB:H62	2.46	0.41
5:B:509:BTB:H41	5:B:509:BTB:H72	1.56	0.41
1:B:279:TRP:HB2	1:B:302:LEU:HD21	2.01	0.40
1:D:479:PRO:HD2	1:D:480:TRP:CE3	2.56	0.40
1:A:292:LEU:HD23	1:A:292:LEU:HA	1.93	0.40
1:A:463:GLU:HB3	1:B:103:LEU:HD12	2.04	0.40
1:B:70:ARG:HD3	1:B:81:TYR:CZ	2.56	0.40
1:D:323:PHE:O	1:D:326:LEU:HB2	2.21	0.40
1:A:298:GLU:HG2	10:A:636:HOH:O	2.22	0.40
1:A:175:LYS:HG2	1:A:193:LEU:HB3	2.03	0.40
1:A:298:GLU:HB3	1:A:299:PRO:HD2	2.04	0.40
1:C:178:TRP:CE3	1:C:190:TRP:HA	2.57	0.40
5:C:504:BTB:O6	5:C:504:BTB:H82	2.21	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:152:GLU:OE2	5:B:505:BTB:O3[2_842]	2.16	0.04

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	399/440 (91%)	373 (94%)	20 (5%)	6 (2%)	8 2
1	B	402/440 (91%)	393 (98%)	8 (2%)	1 (0%)	43 36
1	C	399/440 (91%)	385 (96%)	13 (3%)	1 (0%)	36 28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	399/440 (91%)	392 (98%)	7 (2%)	0	100	100
All	All	1599/1760 (91%)	1543 (96%)	48 (3%)	8 (0%)	24	16

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	144	GLN
1	A	239	GLY
1	B	259	GLY
1	A	90	GLN
1	A	276	GLN
1	A	255	ARG
1	A	259	GLY
1	C	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	343/373 (92%)	318 (93%)	25 (7%)	13	4
1	B	345/373 (92%)	331 (96%)	14 (4%)	27	17
1	C	342/373 (92%)	329 (96%)	13 (4%)	29	19
1	D	342/373 (92%)	333 (97%)	9 (3%)	40	33
All	All	1372/1492 (92%)	1311 (96%)	61 (4%)	25	15

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	VAL
1	A	87	GLN
1	A	90	GLN
1	A	98	ARG
1	A	122	GLN
1	A	126	GLN

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Mol	Chain	Res	Type
1	A	139	LYS
1	A	154	GLU
1	A	160	THR
1	A	192	LYS
1	A	202	ARG
1	A	206	GLU
1	A	207	MET
1	A	211	ILE
1	A	238	ARG
1	A	256	GLN
1	A	257	GLN
1	A	258	ASP
1	A	272	GLU
1	A	277	HIS
1	A	280	THR
1	A	301	GLU
1	A	304	LEU
1	A	321	GLU
1	A	432	GLU
1	B	87	GLN
1	B	89	GLN
1	B	97	ARG
1	B	122	GLN
1	B	128	ARG
1	B	168[A]	SER
1	B	168[B]	SER
1	B	176	GLN
1	B	202	ARG
1	B	230	VAL
1	B	255	ARG
1	B	276	GLN
1	B	400	VAL
1	B	474	ARG
1	C	71	VAL
1	C	89	GLN
1	C	125	SER
1	C	128	ARG
1	C	132	ASN
1	C	138	ILE
1	C	151	GLN
1	C	160	THR
1	C	162	THR

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Mol	Chain	Res	Type
1	C	233	GLN
1	C	258	ASP
1	C	308	GLU
1	C	309	LEU
1	D	71	VAL
1	D	97	ARG
1	D	98	ARG
1	D	192	LYS
1	D	200	ASP
1	D	230	VAL
1	D	255	ARG
1	D	258	ASP
1	D	326	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	GLN
1	A	133	GLN
1	B	90	GLN
1	B	122	GLN
1	B	256	GLN
1	C	133	GLN
1	C	247	GLN
1	C	256	GLN
1	C	267	ASN
1	D	433	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 35 ligands modelled in this entry, 10 are monoatomic - leaving 25 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	BTB	D	505	-	13,13,13	0.61	0	7,16,16	1.09	1 (14%)
2	HEM	D	501	1	50,50,50	1.73	9 (18%)	67,82,82	1.30	7 (10%)
5	BTB	B	509	9	13,13,13	0.38	0	7,16,16	1.08	1 (14%)
7	GOL	A	508	-	5,5,5	0.37	0	5,5,5	0.35	0
3	H4B	C	502	-	17,18,18	0.90	0	14,26,26	1.74	4 (28%)
7	GOL	C	506	-	5,5,5	0.40	0	5,5,5	0.29	0
4	OS7	D	503	-	31,31,31	0.90	2 (6%)	42,43,43	1.67	8 (19%)
3	H4B	B	502	-	17,18,18	0.87	0	14,26,26	1.80	3 (21%)
5	BTB	B	506	-	13,13,13	0.39	0	7,16,16	0.46	0
4	OS7	A	503	-	31,31,31	0.83	2 (6%)	42,43,43	1.54	7 (16%)
4	OS7	B	503	-	31,31,31	0.96	3 (9%)	42,43,43	1.91	10 (23%)
5	BTB	A	504	9	13,13,13	0.53	0	7,16,16	1.29	1 (14%)
5	BTB	A	506	-	13,13,13	0.35	0	7,16,16	0.49	0
2	HEM	B	501	1	50,50,50	1.69	8 (16%)	67,82,82	1.42	10 (14%)
5	BTB	A	505	-	13,13,13	0.46	0	7,16,16	0.62	0
4	OS7	C	503	-	31,31,31	0.79	0	42,43,43	1.47	5 (11%)
5	BTB	B	505	-	13,13,13	0.42	0	7,16,16	0.59	0
2	HEM	A	501	1	50,50,50	1.61	7 (14%)	67,82,82	1.36	9 (13%)
5	BTB	C	504	-	13,13,13	0.45	0	7,16,16	0.47	0
5	BTB	B	510	-	13,13,13	0.88	1 (7%)	7,16,16	1.23	1 (14%)
3	H4B	D	502	-	17,18,18	0.97	2 (11%)	14,26,26	1.74	4 (28%)
2	HEM	C	501	1	50,50,50	1.72	10 (20%)	67,82,82	1.51	10 (14%)
5	BTB	B	504	9	13,13,13	0.37	0	7,16,16	0.49	0
5	BTB	D	504	9	13,13,13	0.43	0	7,16,16	0.37	0
3	H4B	A	502	-	17,18,18	0.88	0	14,26,26	1.79	4 (28%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BTB	D	505	-	-	13/21/21/21	-
2	HEM	D	501	1	-	0/14/54/54	-
5	BTB	B	509	9	-	3/21/21/21	-
7	GOL	A	508	-	-	4/4/4/4	-
3	H4B	C	502	-	-	0/8/17/17	0/2/2/2
7	GOL	C	506	-	-	2/4/4/4	-
4	OS7	D	503	-	-	7/11/11/11	0/4/4/4
3	H4B	B	502	-	-	0/8/17/17	0/2/2/2
5	BTB	B	506	-	-	6/21/21/21	-
4	OS7	A	503	-	-	7/11/11/11	0/4/4/4
4	OS7	B	503	-	-	9/11/11/11	0/4/4/4
5	BTB	A	504	9	-	6/21/21/21	-
5	BTB	A	506	-	-	6/21/21/21	-
2	HEM	B	501	1	-	1/14/54/54	-
5	BTB	A	505	-	-	13/21/21/21	-
4	OS7	C	503	-	-	8/11/11/11	0/4/4/4
5	BTB	B	505	-	-	4/21/21/21	-
2	HEM	A	501	1	-	2/14/54/54	-
5	BTB	C	504	-	-	2/21/21/21	-
5	BTB	B	510	-	-	5/21/21/21	-
3	H4B	D	502	-	-	0/8/17/17	0/2/2/2
2	HEM	C	501	1	-	0/14/54/54	-
5	BTB	B	504	9	-	2/21/21/21	-
5	BTB	D	504	9	-	6/21/21/21	-
3	H4B	A	502	-	-	0/8/17/17	0/2/2/2

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	HEM	FE-NC	6.78	2.17	1.95
2	A	501	HEM	FE-NB	5.75	2.12	1.94
2	B	501	HEM	FE-NA	5.48	2.13	1.95
2	C	501	HEM	FE-ND	5.13	2.10	1.94
2	C	501	HEM	FE-NB	5.01	2.10	1.94
2	C	501	HEM	FE-NA	4.78	2.10	1.95
2	B	501	HEM	FE-NC	4.45	2.09	1.95
2	A	501	HEM	FE-NA	4.38	2.09	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	HEM	FE-NB	4.35	2.08	1.94
2	D	501	HEM	FE-NB	3.85	2.06	1.94
2	D	501	HEM	FE-ND	3.71	2.06	1.94
2	C	501	HEM	CAB-C3B	3.27	1.56	1.47
2	A	501	HEM	FE-NC	3.27	2.05	1.95
2	A	501	HEM	CAB-C3B	3.15	1.55	1.47
2	C	501	HEM	CAC-C3C	3.11	1.55	1.47
2	B	501	HEM	CAB-C3B	3.10	1.55	1.47
2	D	501	HEM	CAC-C3C	3.09	1.55	1.47
2	B	501	HEM	CAC-C3C	3.07	1.55	1.47
2	A	501	HEM	CAC-C3C	2.97	1.55	1.47
2	D	501	HEM	FE-NA	2.96	2.04	1.95
2	D	501	HEM	CAB-C3B	2.90	1.55	1.47
2	A	501	HEM	FE-ND	2.73	2.03	1.94
2	C	501	HEM	CMC-C2C	2.66	1.56	1.50
2	C	501	HEM	FE-NC	2.60	2.03	1.95
4	B	503	OS7	C02-N01	2.53	1.36	1.33
2	D	501	HEM	CMC-C2C	2.50	1.55	1.50
2	B	501	HEM	CMD-C2D	2.49	1.55	1.50
2	D	501	HEM	CMA-C3A	2.42	1.55	1.50
4	B	503	OS7	C05-C10	-2.39	1.38	1.42
2	B	501	HEM	CMA-C3A	2.28	1.55	1.50
2	A	501	HEM	CMC-C2C	2.27	1.55	1.50
5	B	510	BTB	C3-C2	-2.26	1.50	1.53
4	D	503	OS7	C02-N01	2.25	1.36	1.33
2	C	501	HEM	CMA-C3A	2.18	1.55	1.50
4	D	503	OS7	C05-C10	-2.17	1.39	1.42
2	C	501	HEM	CMB-C2B	2.17	1.55	1.50
3	D	502	H4B	C4-N3	-2.15	1.34	1.38
3	D	502	H4B	C7-C6	2.09	1.54	1.52
2	D	501	HEM	CMD-C2D	2.08	1.55	1.50
2	C	501	HEM	CMD-C2D	2.05	1.55	1.50
4	A	503	OS7	C05-C10	-2.04	1.39	1.42
4	B	503	OS7	C06-C05	-2.03	1.38	1.42
2	B	501	HEM	C2A-C3A	-2.02	1.33	1.38
4	A	503	OS7	C02-N01	2.02	1.36	1.33

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	503	OS7	C05-C10-N01	-5.35	117.13	122.80
4	D	503	OS7	C05-C10-N01	-4.69	117.83	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	503	OS7	C04-C05-C10	4.54	120.77	118.00
4	B	503	OS7	O19-C14-C15	4.47	121.66	115.89
2	B	501	HEM	C3B-C2B-C1B	4.35	109.68	106.41
4	A	503	OS7	O19-C14-C15	4.11	121.20	115.89
3	B	502	H4B	C2-N1-C8A	4.05	120.51	113.36
4	C	503	OS7	O19-C14-C15	4.01	121.08	115.89
4	D	503	OS7	C04-C05-C10	3.96	120.41	118.00
4	D	503	OS7	O19-C14-C15	3.94	120.98	115.89
4	A	503	OS7	C05-C10-N01	-3.91	118.66	122.80
4	C	503	OS7	C05-C10-N01	-3.87	118.70	122.80
3	D	502	H4B	C2-N1-C8A	3.85	120.15	113.36
3	A	502	H4B	C2-N1-C8A	3.77	120.02	113.36
3	C	502	H4B	C2-N1-C8A	3.75	119.97	113.36
2	B	501	HEM	CBA-CAA-C2A	-3.64	102.48	112.53
4	A	503	OS7	C04-C05-C10	3.61	120.20	118.00
4	C	503	OS7	C04-C05-C10	3.48	120.12	118.00
2	C	501	HEM	C3B-C4B-NB	-3.47	106.98	109.47
2	A	501	HEM	C3B-C2B-C1B	3.46	109.01	106.41
2	D	501	HEM	C2A-C1A-NA	-3.20	106.60	110.15
2	C	501	HEM	C3D-C4D-ND	-3.15	106.72	110.17
4	B	503	OS7	C03-C04-C05	3.15	121.02	117.84
2	A	501	HEM	C4D-ND-C1D	3.10	108.88	105.21
3	A	502	H4B	O4-C4-C4A	-3.09	119.81	127.26
2	C	501	HEM	CBA-CAA-C2A	-3.08	104.02	112.53
4	D	503	OS7	C03-C04-C05	3.04	120.91	117.84
4	B	503	OS7	C07-C08-C11	-3.00	116.07	121.25
5	A	504	BTB	O3-C3-C2	3.00	118.46	111.40
2	C	501	HEM	C4D-ND-C1D	2.90	108.65	105.21
2	D	501	HEM	CBA-CAA-C2A	-2.88	104.57	112.53
2	C	501	HEM	C1B-NB-C4B	2.88	108.61	105.21
2	A	501	HEM	C3D-C4D-ND	-2.87	107.02	110.17
2	A	501	HEM	C1B-NB-C4B	2.86	108.59	105.21
3	C	502	H4B	O4-C4-C4A	-2.77	120.58	127.26
4	D	503	OS7	C26-N21-C22	2.74	121.26	117.41
2	C	501	HEM	C3B-C2B-C1B	2.73	108.46	106.41
3	B	502	H4B	C4A-C4-N3	2.71	119.56	112.13
2	A	501	HEM	C3B-C4B-NB	-2.69	107.53	109.47
4	B	503	OS7	C26-N21-C22	2.69	121.18	117.41
5	B	509	BTB	O3-C3-C2	2.68	117.70	111.40
2	B	501	HEM	CHB-C1B-NB	2.65	127.64	124.37
2	D	501	HEM	C4A-NA-C1A	2.62	110.09	105.82
2	D	501	HEM	C3B-C2B-C1B	2.59	108.36	106.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	502	H4B	C4A-C4-N3	2.54	119.10	112.13
2	C	501	HEM	C2A-C1A-NA	-2.54	107.34	110.15
4	B	503	OS7	N02-C02-N01	2.53	120.33	118.24
4	B	503	OS7	C09-C10-N01	2.49	122.42	118.78
4	A	503	OS7	O19-C14-C13	-2.48	118.53	123.95
4	B	503	OS7	C09-C08-C11	2.48	126.62	121.05
4	C	503	OS7	C26-N21-C22	2.45	120.84	117.41
3	B	502	H4B	O4-C4-C4A	-2.43	121.40	127.26
2	A	501	HEM	C2A-C1A-NA	-2.40	107.49	110.15
2	C	501	HEM	CHA-C4D-ND	2.37	127.30	124.37
3	A	502	H4B	C4A-C4-N3	2.37	118.65	112.13
3	C	502	H4B	C4A-C4-N3	2.37	118.64	112.13
3	C	502	H4B	C2-N3-C4	-2.37	120.82	125.11
4	A	503	OS7	C07-C08-C11	-2.34	117.21	121.25
3	A	502	H4B	C2-N3-C4	-2.32	120.90	125.11
4	D	503	OS7	C09-C10-N01	2.32	122.18	118.78
2	D	501	HEM	C4D-ND-C1D	2.30	107.93	105.21
4	B	503	OS7	C04-C03-C02	-2.26	117.36	119.71
2	B	501	HEM	CAD-CBD-CGD	-2.25	107.70	113.67
4	A	503	OS7	C26-N21-C22	2.25	120.56	117.41
4	C	503	OS7	O19-C14-C13	-2.23	119.08	123.95
2	A	501	HEM	C2D-C1D-ND	-2.22	107.34	109.90
2	C	501	HEM	CHD-C1D-C2D	2.21	128.52	125.03
2	D	501	HEM	C3D-C4D-ND	-2.20	107.76	110.17
2	B	501	HEM	C3D-C4D-ND	-2.18	107.78	110.17
5	B	510	BTB	O3-C3-C2	-2.16	106.32	111.40
3	D	502	H4B	C2-N3-C4	-2.15	121.21	125.11
2	B	501	HEM	C3B-C4B-NB	-2.15	107.93	109.47
4	D	503	OS7	C04-C03-C02	-2.15	117.48	119.71
3	D	502	H4B	O4-C4-C4A	-2.14	122.11	127.26
2	A	501	HEM	CAD-CBD-CGD	-2.12	108.05	113.67
2	D	501	HEM	C1B-NB-C4B	2.11	107.71	105.21
4	A	503	OS7	C03-C04-C05	2.10	119.96	117.84
2	B	501	HEM	C3A-C4A-NA	-2.10	106.78	110.14
4	D	503	OS7	N02-C02-N01	2.10	119.97	118.24
2	B	501	HEM	C4A-NA-C1A	2.09	109.23	105.82
2	C	501	HEM	CBD-CAD-C3D	-2.07	106.80	112.53
5	D	505	BTB	O1-C1-C2	-2.07	106.54	111.40
2	B	501	HEM	C2B-C1B-NB	-2.05	107.49	109.84
2	A	501	HEM	C2B-C1B-NB	-2.05	107.49	109.84
2	B	501	HEM	C1B-NB-C4B	2.04	107.62	105.21

There are no chirality outliers.

All (106) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	504	BTB	O1-C1-C2-N
5	A	504	BTB	C1-C2-C3-O3
5	A	504	BTB	N-C2-C3-O3
5	A	505	BTB	O1-C1-C2-C4
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-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-C7
5	A	506	BTB	C1-C2-C3-O3
5	A	506	BTB	C4-C2-C3-O3
5	A	506	BTB	N-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	B	505	BTB	C1-C2-C3-O3
5	B	505	BTB	C4-C2-C3-O3
5	B	505	BTB	N-C2-C3-O3
5	B	506	BTB	O1-C1-C2-C3
5	B	506	BTB	C1-C2-C3-O3
5	B	506	BTB	C4-C2-C3-O3
5	B	506	BTB	N-C2-C3-O3
5	B	509	BTB	C1-C2-C3-O3
5	B	509	BTB	C4-C2-C3-O3
5	B	509	BTB	N-C2-C3-O3
5	B	510	BTB	O1-C1-C2-N
5	B	510	BTB	C1-C2-C3-O3
5	B	510	BTB	C4-C2-C3-O3
5	B	510	BTB	N-C2-C3-O3
5	C	504	BTB	C8-C7-N-C5
5	D	504	BTB	O1-C1-C2-C3
5	D	504	BTB	O1-C1-C2-C4
5	D	504	BTB	O1-C1-C2-N
5	D	504	BTB	C1-C2-C4-O4
5	D	504	BTB	C3-C2-C4-O4
5	D	504	BTB	N-C2-C4-O4
5	D	505	BTB	C1-C2-C3-O3
5	D	505	BTB	C4-C2-C3-O3
5	D	505	BTB	N-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
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	505	BTB	C1-C2-N-C7
5	D	505	BTB	C3-C2-N-C7
5	D	505	BTB	C4-C2-N-C7
5	D	505	BTB	C8-C7-N-C5
7	A	508	GOL	C1-C2-C3-O3
7	C	506	GOL	O1-C1-C2-C3
4	C	503	OS7	C09-C08-C11-C12
4	C	503	OS7	C09-C08-C11-C16
4	C	503	OS7	C07-C08-C11-C16
4	A	503	OS7	C09-C08-C11-C12
4	C	503	OS7	C07-C08-C11-C12
4	A	503	OS7	C07-C08-C11-C16
4	A	503	OS7	C09-C08-C11-C16
4	A	503	OS7	C07-C08-C11-C12
4	B	503	OS7	C09-C08-C11-C16
4	B	503	OS7	C07-C08-C11-C16
4	D	503	OS7	C09-C08-C11-C16
4	B	503	OS7	C07-C08-C11-C12
4	D	503	OS7	C07-C08-C11-C16
4	D	503	OS7	C07-C08-C11-C12
4	D	503	OS7	C09-C08-C11-C12
4	B	503	OS7	C09-C08-C11-C12
5	A	505	BTB	N-C5-C6-O6
2	A	501	HEM	C2A-CAA-CBA-CGA
4	A	503	OS7	C14-C15-C17-N18
4	B	503	OS7	C14-C15-C17-N18
7	A	508	GOL	O1-C1-C2-C3
7	A	508	GOL	O2-C2-C3-O3
7	C	506	GOL	O1-C1-C2-O2
4	C	503	OS7	C14-C15-C17-N18
4	B	503	OS7	C13-C14-O19-C20
4	B	503	OS7	C15-C14-O19-C20
5	B	510	BTB	O1-C1-C2-C4
7	A	508	GOL	O1-C1-C2-O2
5	B	505	BTB	N-C5-C6-O6
5	C	504	BTB	N-C7-C8-O8
4	A	503	OS7	C13-C14-O19-C20
5	A	504	BTB	N-C5-C6-O6
4	A	503	OS7	C15-C14-O19-C20

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Mol	Chain	Res	Type	Atoms
4	D	503	OS7	C14-C15-C17-N18
2	A	501	HEM	C4B-C3B-CAB-CBB
2	B	501	HEM	C4B-C3B-CAB-CBB
5	A	504	BTB	O1-C1-C2-C3
4	C	503	OS7	C13-C14-O19-C20
5	A	504	BTB	C4-C2-N-C7
5	A	505	BTB	O1-C1-C2-N
5	A	505	BTB	C4-C2-N-C5
5	B	506	BTB	O1-C1-C2-N
5	D	505	BTB	C3-C2-N-C5
5	D	505	BTB	C4-C2-N-C5
4	D	503	OS7	C13-C14-O19-C20
5	B	506	BTB	O1-C1-C2-C4
4	C	503	OS7	C15-C14-O19-C20
5	B	504	BTB	N-C5-C6-O6
4	D	503	OS7	C15-C14-O19-C20
4	C	503	OS7	C22-C20-O19-C14
5	A	505	BTB	O1-C1-C2-C3
5	B	504	BTB	C3-C2-C4-O4
4	B	503	OS7	O19-C20-C22-N21
5	D	505	BTB	C1-C2-N-C5
4	B	503	OS7	O19-C20-C22-C23

There are no ring outliers.

21 monomers are involved in 50 short contacts:

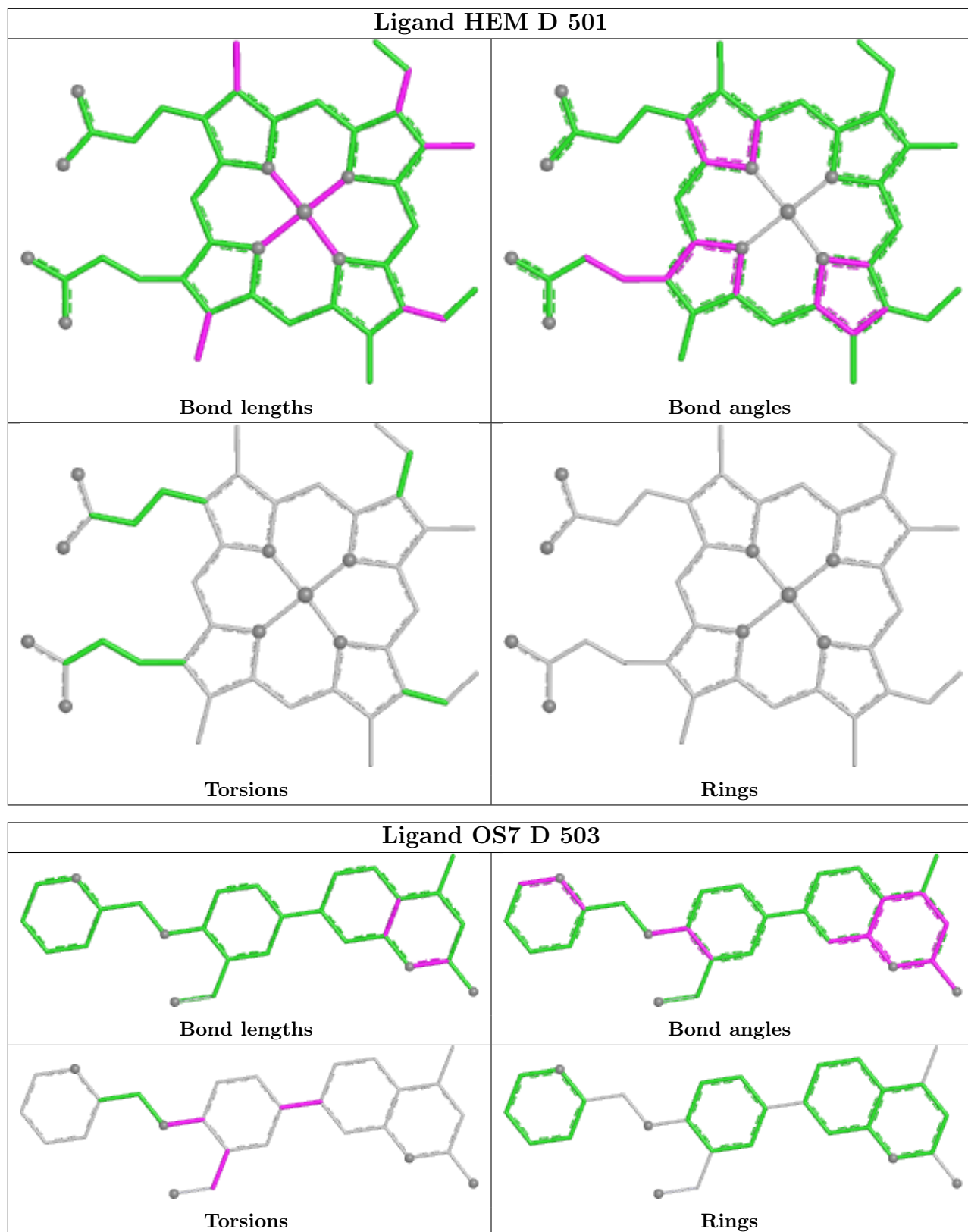
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	505	BTB	3	0
2	D	501	HEM	2	0
5	B	509	BTB	3	0
3	C	502	H4B	1	0
4	D	503	OS7	1	0
3	B	502	H4B	1	0
4	A	503	OS7	1	0
4	B	503	OS7	2	0
5	A	504	BTB	4	0
5	A	506	BTB	1	0
2	B	501	HEM	3	0
5	A	505	BTB	2	0
4	C	503	OS7	4	0
5	B	505	BTB	4	1
2	A	501	HEM	4	0

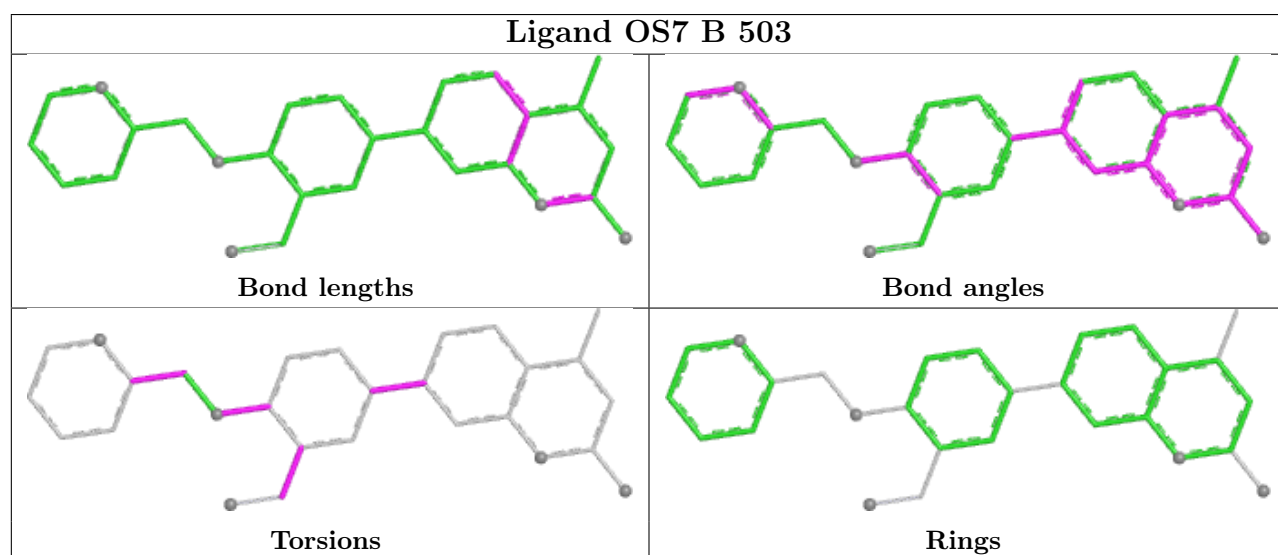
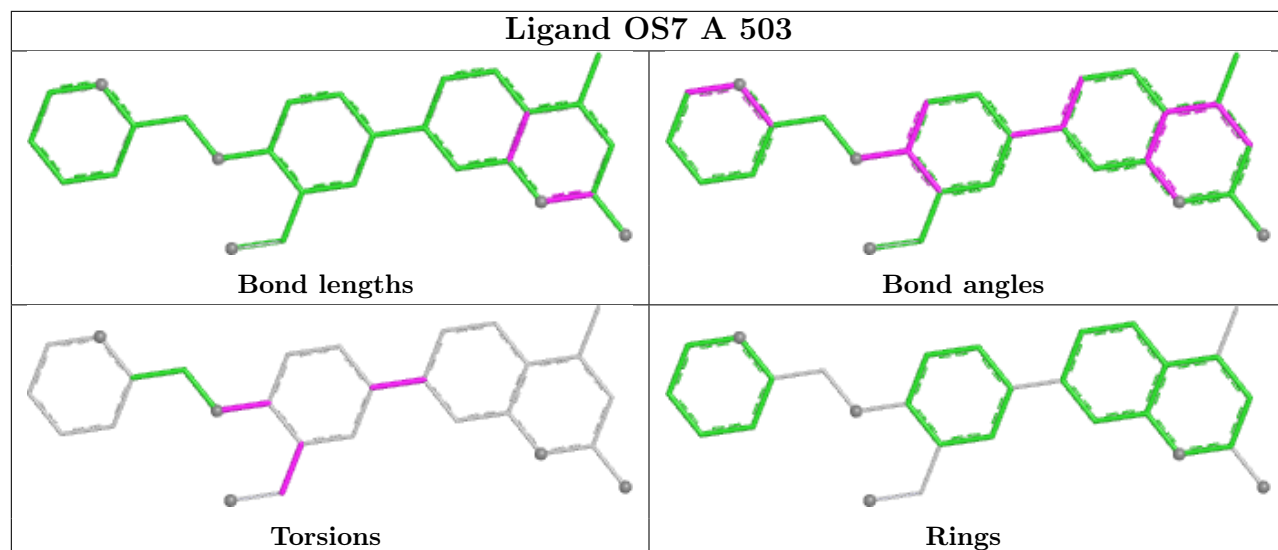
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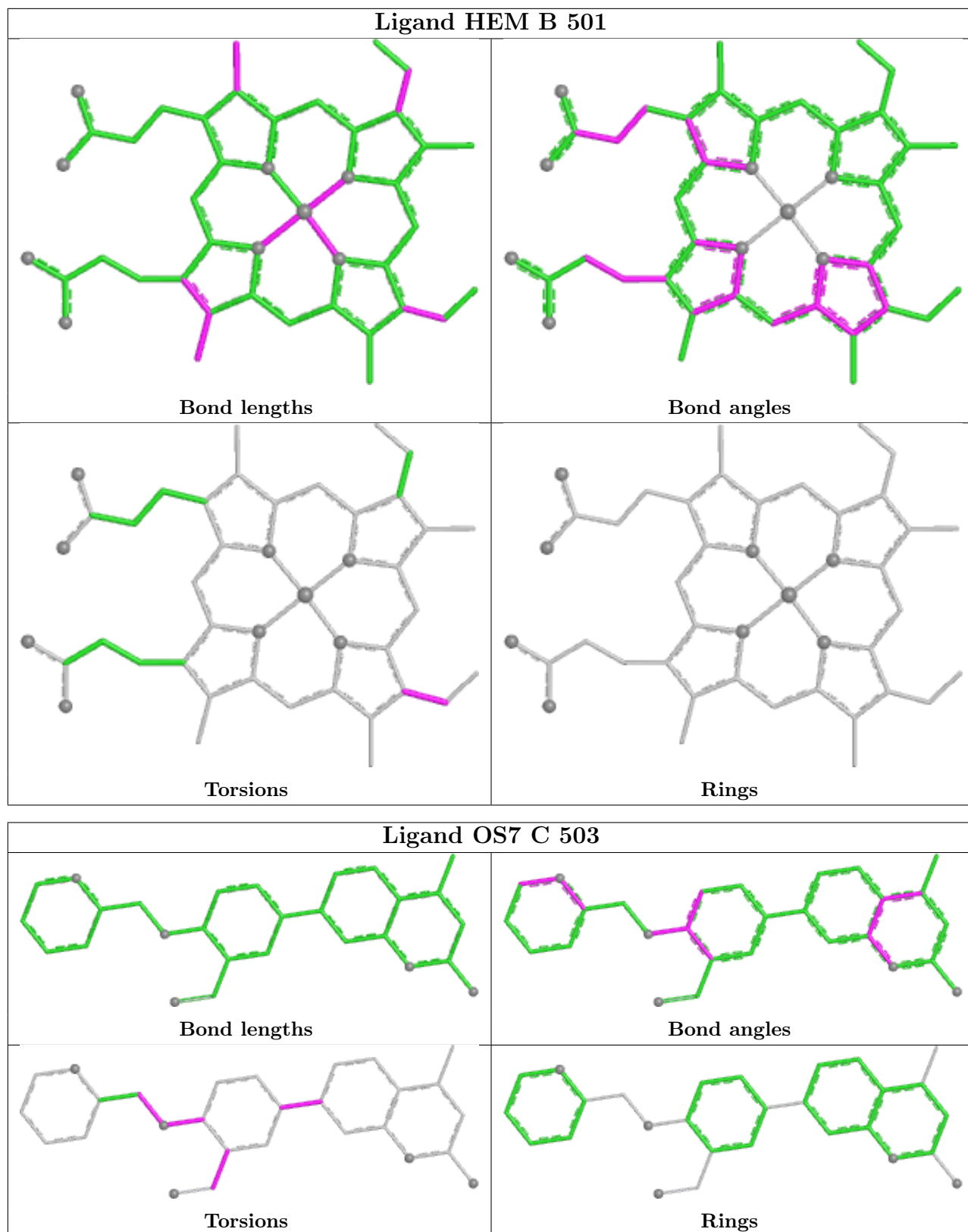
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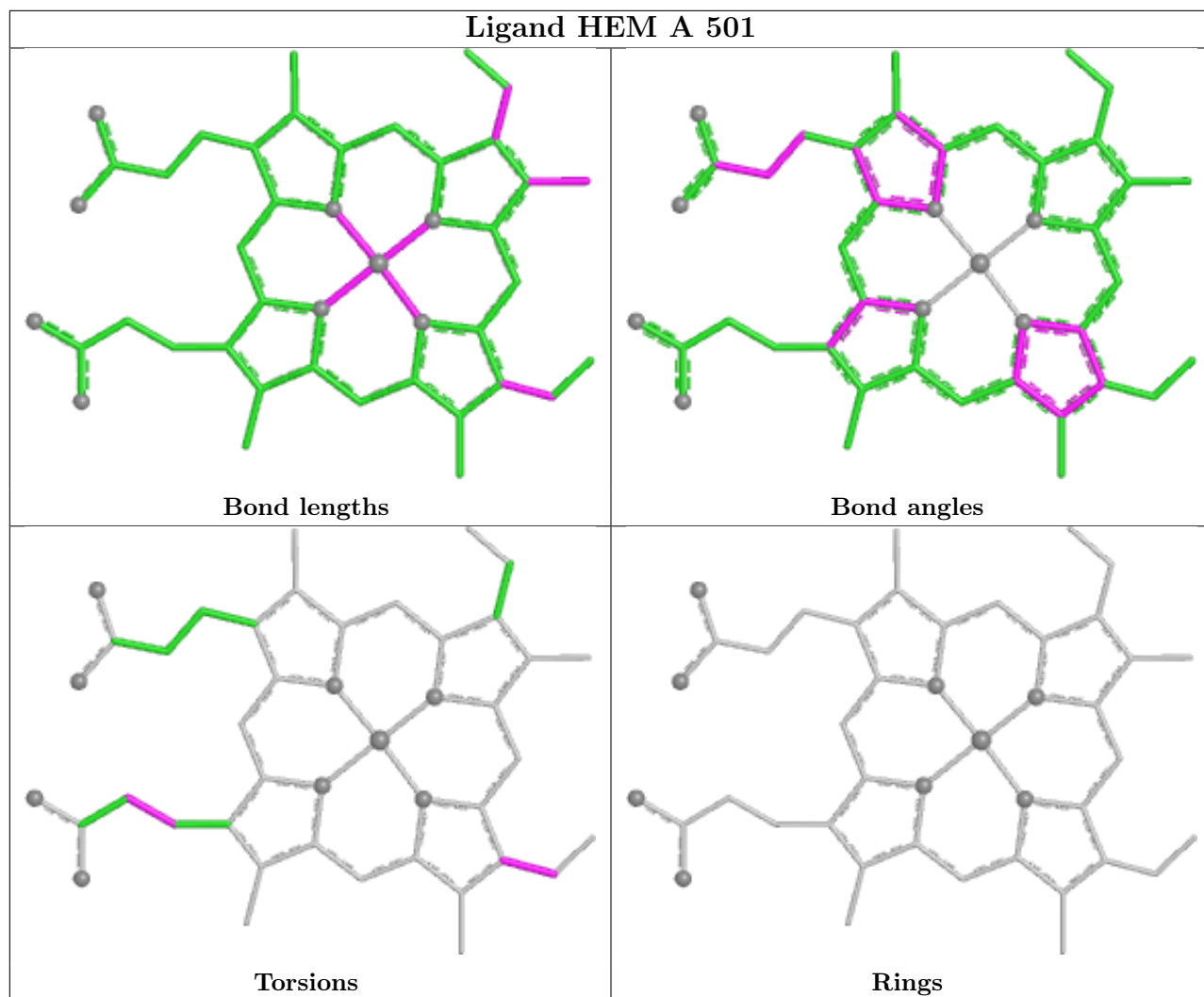
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	504	BTB	3	0
5	B	510	BTB	3	0
2	C	501	HEM	3	0
5	B	504	BTB	1	0
5	D	504	BTB	3	0
3	A	502	H4B	1	0

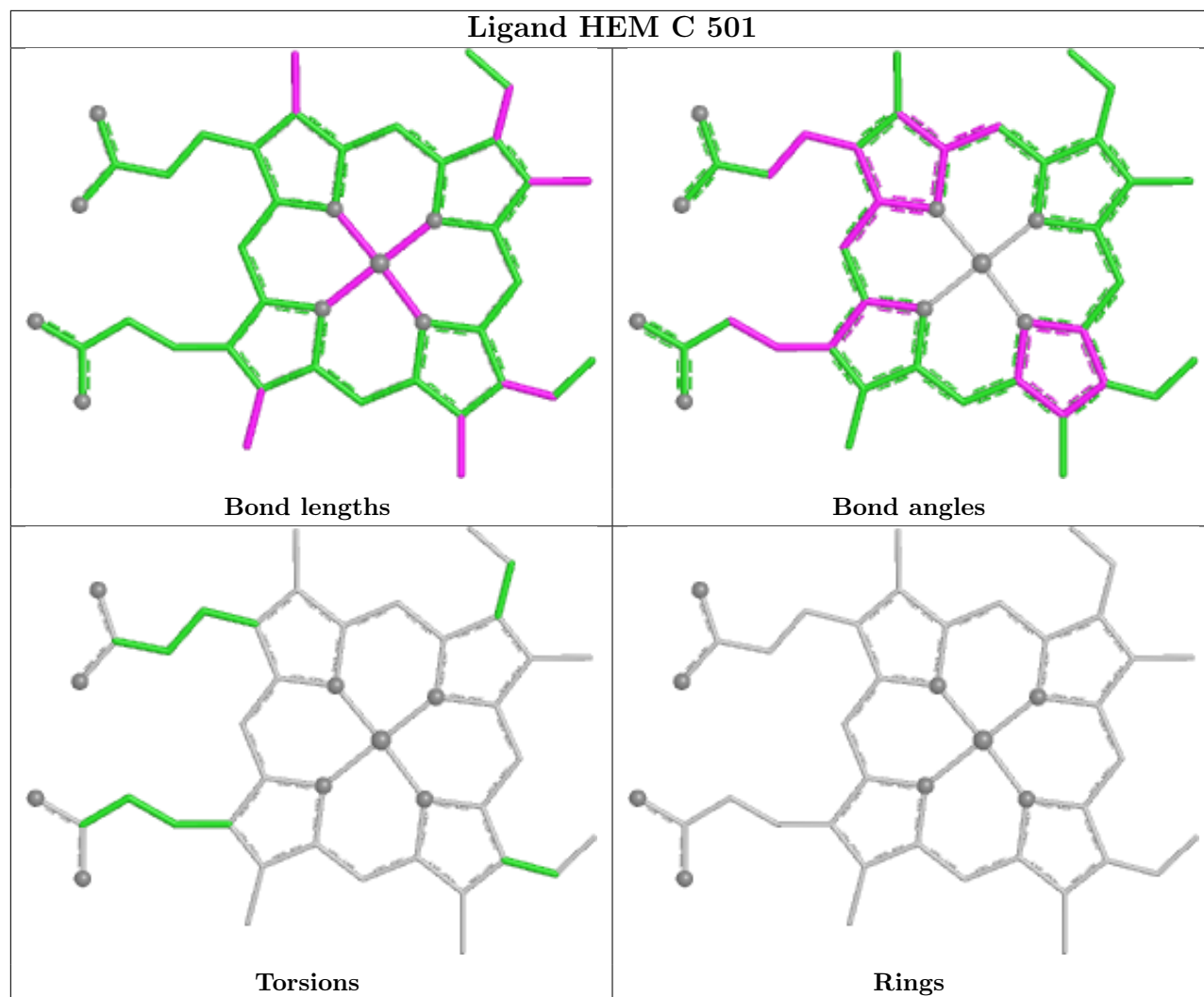
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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	401/440 (91%)	0.74	38 (9%) 14 15	27, 66, 122, 156	2 (0%)
1	B	402/440 (91%)	0.14	3 (0%) 84 88	22, 42, 78, 111	4 (0%)
1	C	401/440 (91%)	0.37	8 (1%) 65 72	26, 54, 98, 137	2 (0%)
1	D	401/440 (91%)	0.04	4 (0%) 79 84	27, 40, 65, 126	2 (0%)
All	All	1605/1760 (91%)	0.32	53 (3%) 49 55	22, 49, 102, 156	10 (0%)

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	204	ALA	4.3
1	D	119	ALA	4.3
1	D	106	PRO	4.0
1	A	120	PRO	3.8
1	A	244	TRP	3.6
1	A	480	TRP	3.5
1	A	106	PRO	3.4
1	C	106	PRO	3.4
1	A	300	PRO	3.3
1	A	153	VAL	3.1
1	A	130	PHE	3.1
1	A	293	LEU	2.9
1	A	237	GLY	2.9
1	B	106	PRO	2.8
1	A	158	ALA	2.8
1	A	345	GLY	2.8
1	B	141[A]	SER	2.8
1	A	131	ILE	2.7
1	A	254	TYR	2.7
1	A	304	LEU	2.6
1	A	235	CYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	68	PHE	2.6
1	A	257	GLN	2.6
1	A	155	ALA	2.6
1	A	159	ALA	2.6
1	C	238	ARG	2.5
1	A	207	MET	2.5
1	A	157	VAL	2.5
1	C	120	PRO	2.5
1	A	163	TYR	2.4
1	C	304	LEU	2.4
1	C	138	ILE	2.4
1	A	124	LEU	2.3
1	A	150	LEU	2.3
1	A	303	PHE	2.3
1	A	299	PRO	2.3
1	C	155	ALA	2.3
1	A	152	GLU	2.3
1	A	253	GLY	2.2
1	D	68	PHE	2.2
1	A	236	PRO	2.2
1	A	281	PRO	2.2
1	D	468	PHE	2.2
1	C	480	TRP	2.2
1	A	259	GLY	2.1
1	A	305	LEU	2.1
1	A	86	ALA	2.1
1	A	127	ALA	2.1
1	A	475	TYR	2.0
1	B	77	GLY	2.0
1	A	231	PHE	2.0
1	C	468	PHE	2.0
1	A	280	THR	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 oligosaccharides in this entry.

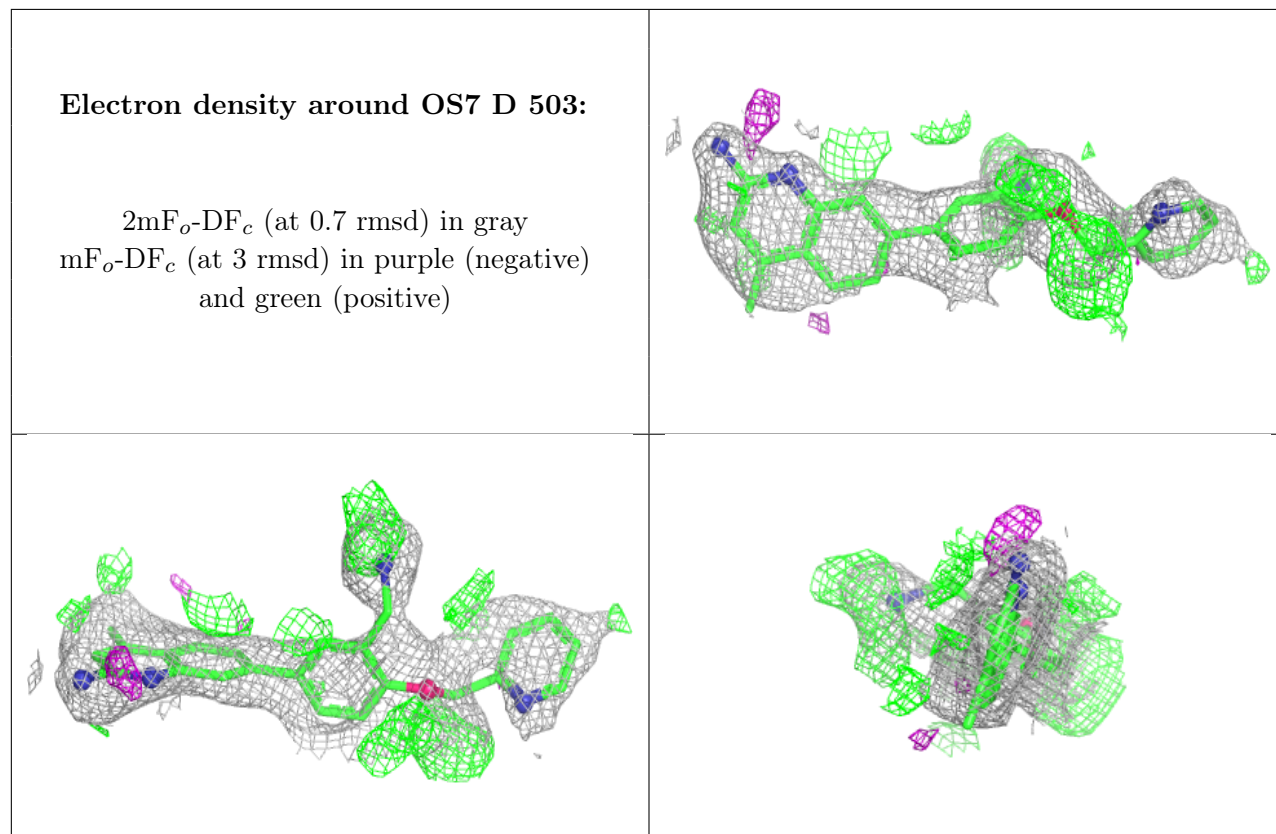
6.4 Ligands [i](#)

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	B	506	14/14	0.65	0.13	82,98,104,106	0
5	BTB	B	505	14/14	0.69	0.17	44,69,80,83	0
5	BTB	A	506	14/14	0.71	0.13	98,107,113,114	0
4	OS7	D	503	28/28	0.76	0.21	44,79,101,104	0
5	BTB	C	504	14/14	0.76	0.12	70,97,104,106	0
4	OS7	B	503	28/28	0.78	0.22	49,87,108,110	0
4	OS7	C	503	28/28	0.79	0.22	69,87,97,102	0
4	OS7	A	503	28/28	0.81	0.19	59,104,108,111	0
5	BTB	B	510	14/14	0.83	0.16	32,63,73,76	0
5	BTB	A	505	14/14	0.83	0.13	63,71,80,83	0
7	GOL	A	508	6/6	0.84	0.10	58,79,84,88	0
5	BTB	D	505	14/14	0.85	0.12	48,68,96,99	0
5	BTB	D	504	14/14	0.87	0.15	39,67,89,90	0
7	GOL	C	506	6/6	0.91	0.08	57,68,75,81	0
5	BTB	B	504	14/14	0.93	0.10	31,58,76,77	0
3	H4B	A	502	17/17	0.93	0.09	43,50,65,75	0
3	H4B	C	502	17/17	0.93	0.08	35,47,56,60	0
8	CL	A	509	1/1	0.93	0.10	58,58,58,58	0
8	CL	C	507	1/1	0.93	0.09	65,65,65,65	0
3	H4B	D	502	17/17	0.94	0.07	31,39,45,48	0
5	BTB	A	504	14/14	0.94	0.10	38,73,82,83	0
3	H4B	B	502	17/17	0.94	0.07	35,41,48,49	0
8	CL	B	507	1/1	0.95	0.09	54,54,54,54	0
5	BTB	B	509	14/14	0.95	0.10	25,66,74,76	0
8	CL	D	506	1/1	0.96	0.08	55,55,55,55	0
2	HEM	A	501	43/43	0.97	0.09	42,58,75,78	0
9	GD	A	510	1/1	0.97	0.06	94,94,94,94	0
2	HEM	D	501	43/43	0.98	0.07	24,34,45,51	0
2	HEM	B	501	43/43	0.98	0.07	21,33,47,67	0
2	HEM	C	501	43/43	0.98	0.07	31,43,67,79	0
9	GD	B	511	1/1	0.98	0.05	84,84,84,84	0
9	GD	D	507	1/1	0.98	0.04	48,48,48,48	0
6	ZN	A	507	1/1	0.99	0.03	46,46,46,46	0
9	GD	B	508	1/1	0.99	0.04	47,47,47,47	0
6	ZN	C	505	1/1	1.00	0.01	36,36,36,36	0

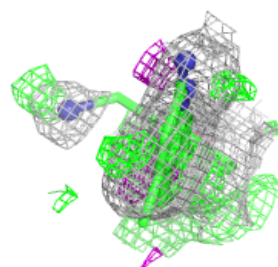
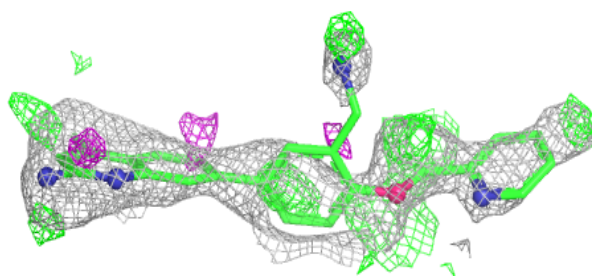
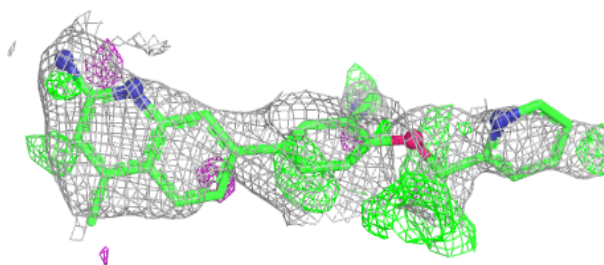
The following is a graphical depiction of the model fit to experimental electron density of all

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.

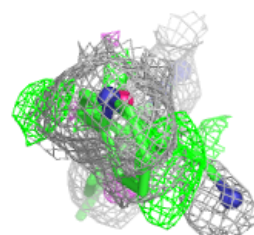
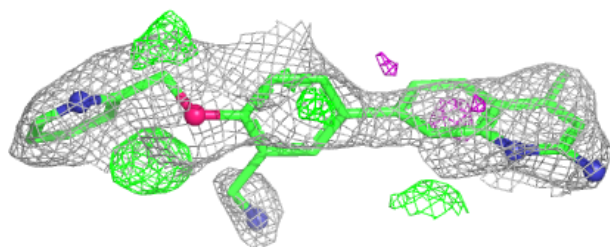
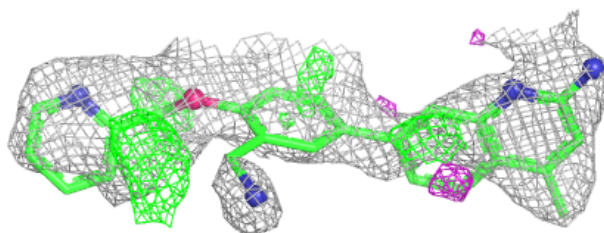


Electron density around OS7 B 503:

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

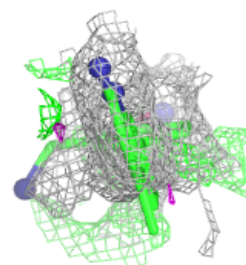
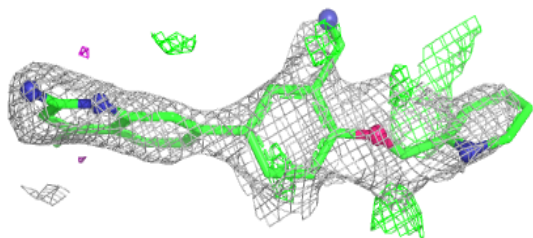
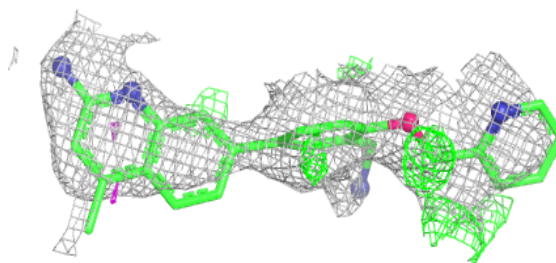
**Electron density around OS7 C 503:**

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

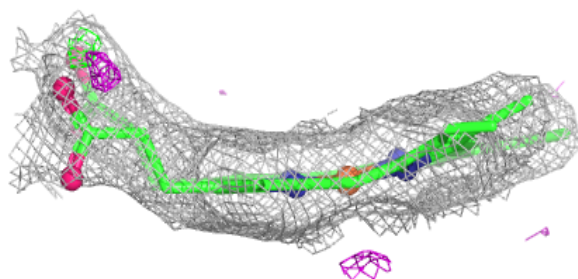
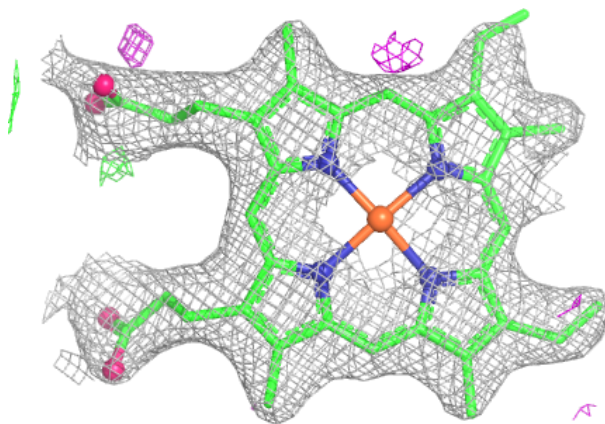


Electron density around OS7 A 503:

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

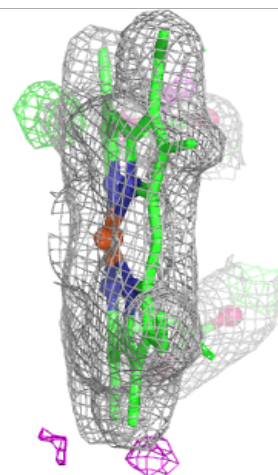
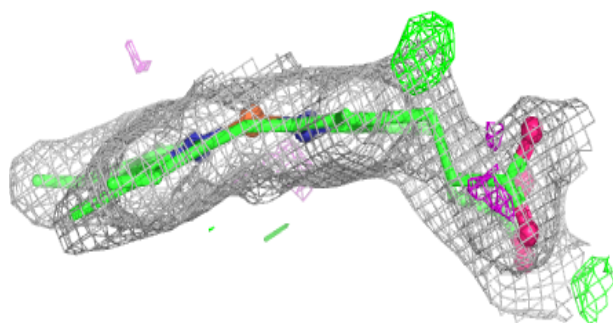
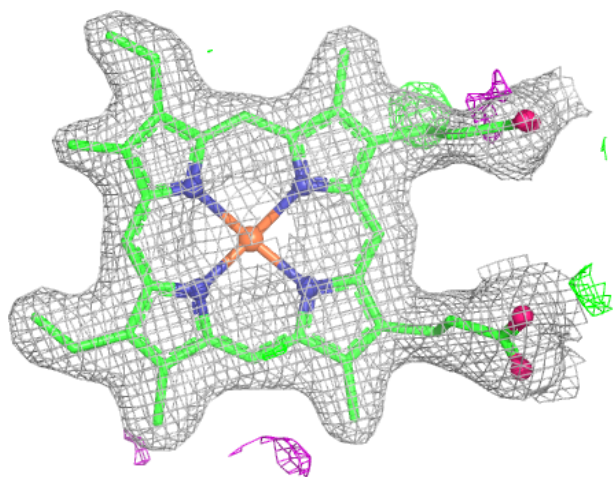
**Electron density around HEM A 501:**

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



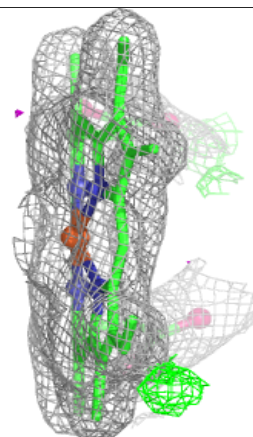
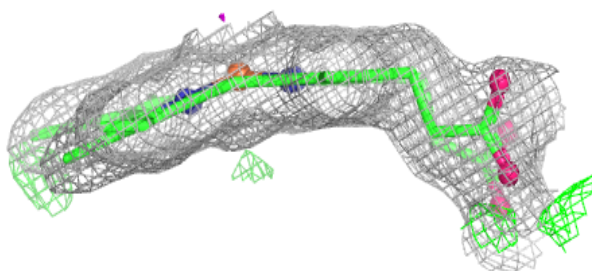
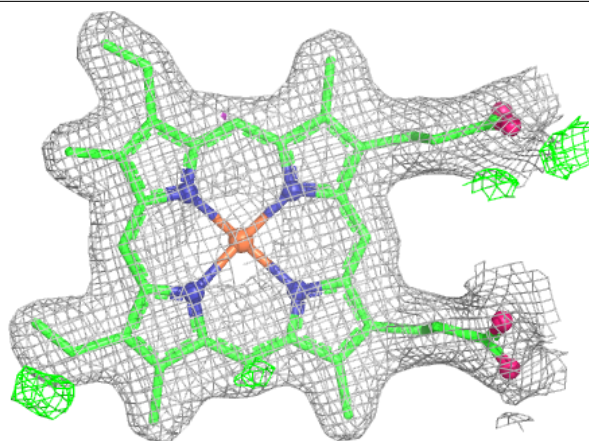
Electron density around HEM D 501:

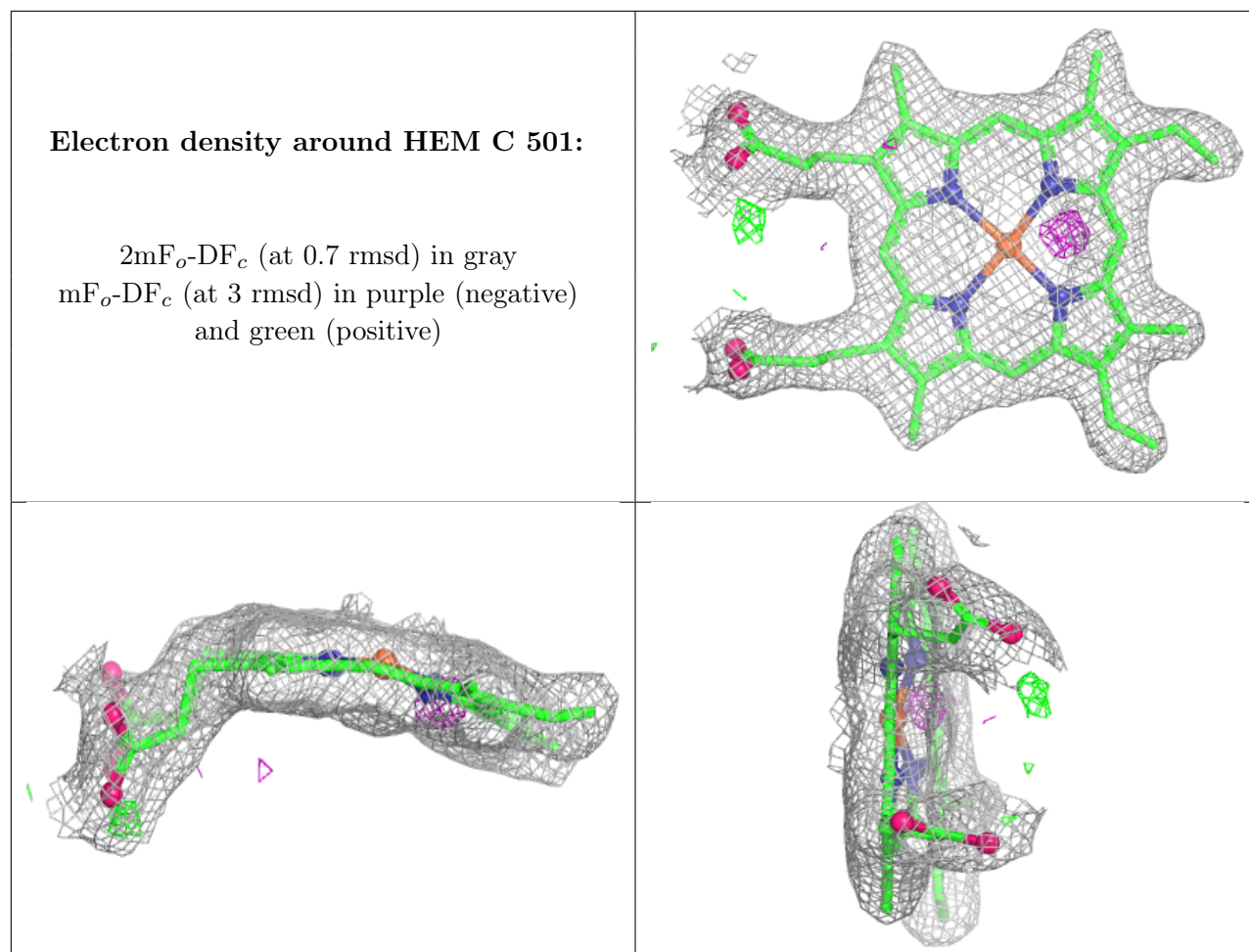
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM B 501:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.