



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 02:48 PM UTC

PDB ID : 5VVB / pdb_00005vvb
Title : Structure of human endothelial nitric oxide synthase heme domain in complex with 4-(2-(((2-Aminoquinolin-7-yl)methyl)amino)ethyl)-2-methylbenzonitrile
Authors : Li, H.; Poulos, T.L.
Deposited on : 2017-05-19
Resolution : 2.15 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

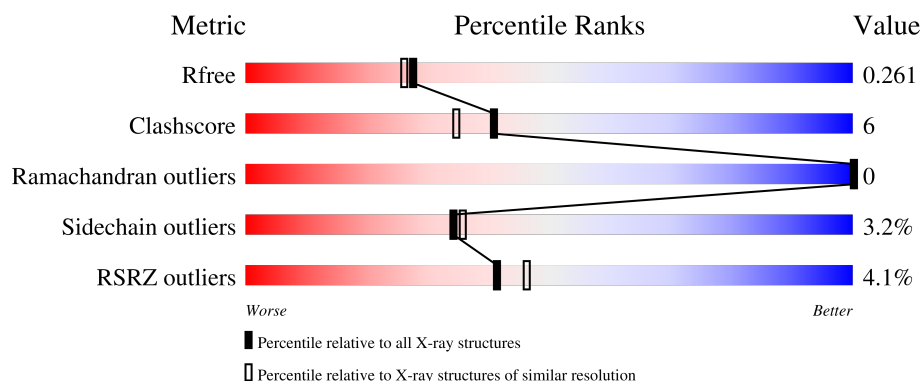
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	6% 74% 15% • 9%
1	B	440	2% 82% 9% 9%
1	C	440	5% 77% 13% • 9%
1	D	440	2% 77% 14% • 8%

2 Entry composition [i](#)

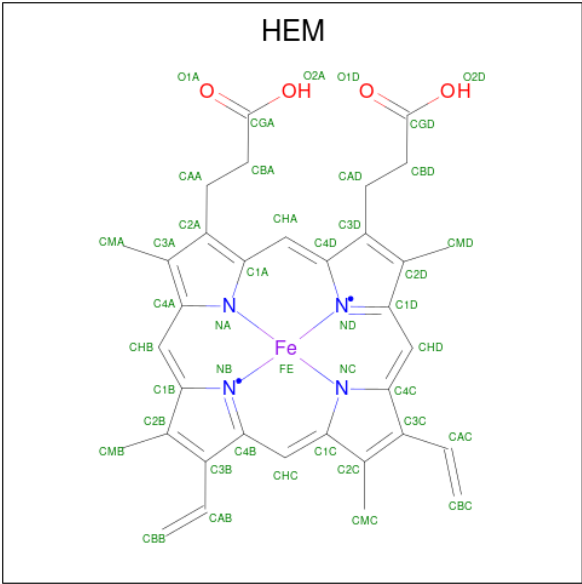
There are 10 unique types of molecules in this entry. The entry contains 13891 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	401	Total	C	N	O	S	0	3	0
			3212	2046	563	587	16			
1	B	402	Total	C	N	O	S	0	5	0
			3232	2057	568	590	17			
1	C	401	Total	C	N	O	S	0	3	0
			3212	2046	563	587	16			
1	D	403	Total	C	N	O	S	0	3	0
			3229	2056	569	588	16			

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).



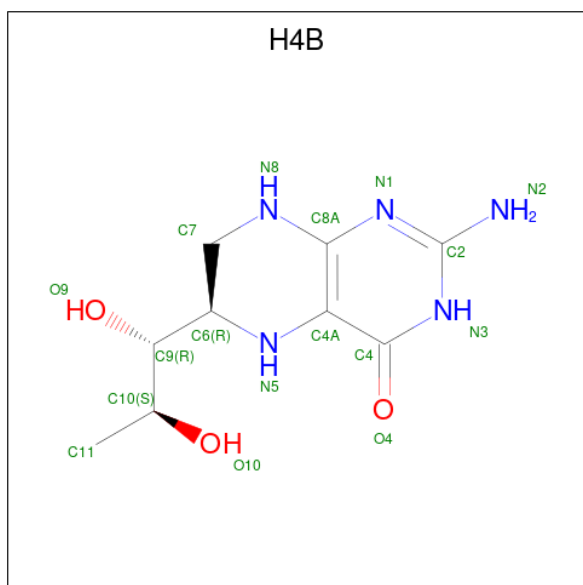
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Fe	N O	0	0
			43	34	1	4 4		
2	B	1	Total	C	Fe	N O	0	0
			43	34	1	4 4		

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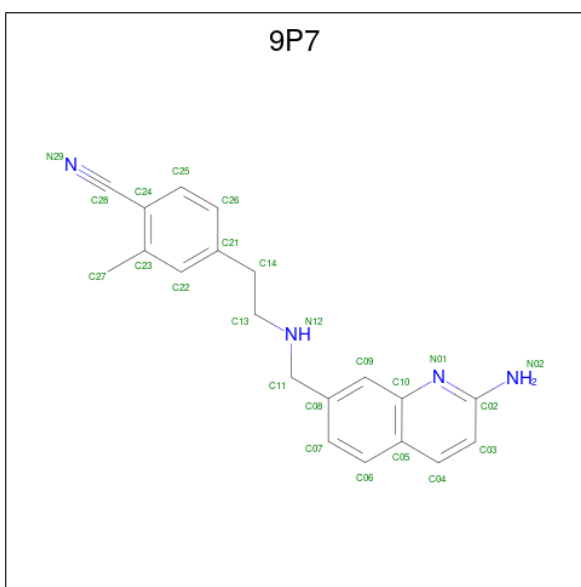
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



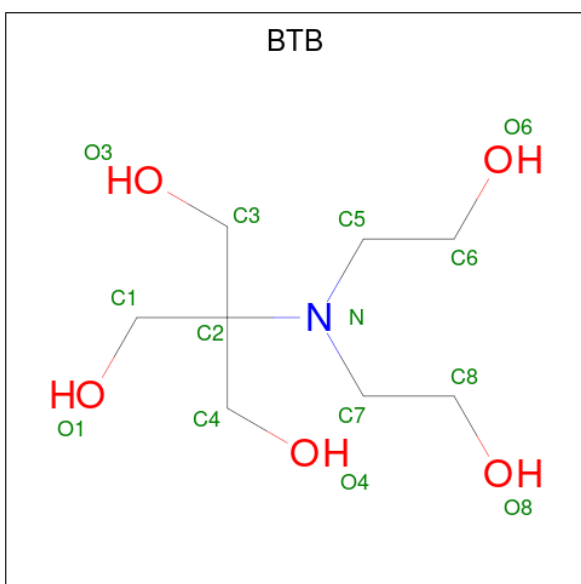
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		
3	C	1	Total	C	N	O	0	0
			17	9	5	3		
3	D	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 4 is 4-(2-[(2-aminoquinolin-7-yl)methyl]amino)ethyl)-2-methylbenzonitrile (CCD ID: 9P7) (formula: $C_{20}H_{20}N_4$).



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

- Molecule 5 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (CCD ID: BTB) (formula: $C_8H_{19}NO_5$).

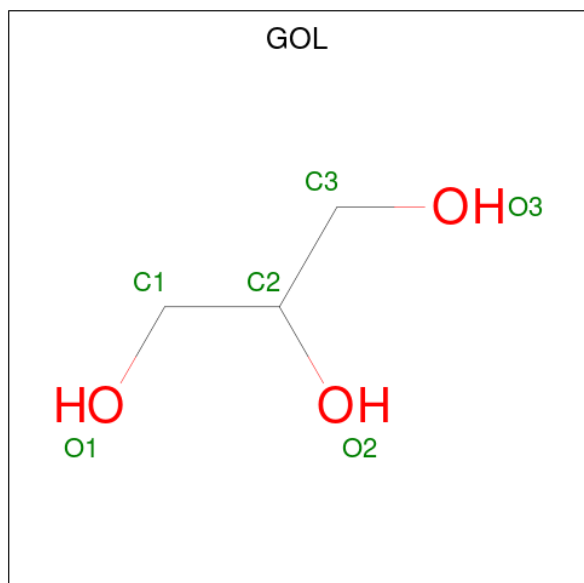


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1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

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

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

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 8 is GADOLINIUM ATOM (CCD ID: GD) (formula: Gd).

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

- Molecule 9 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

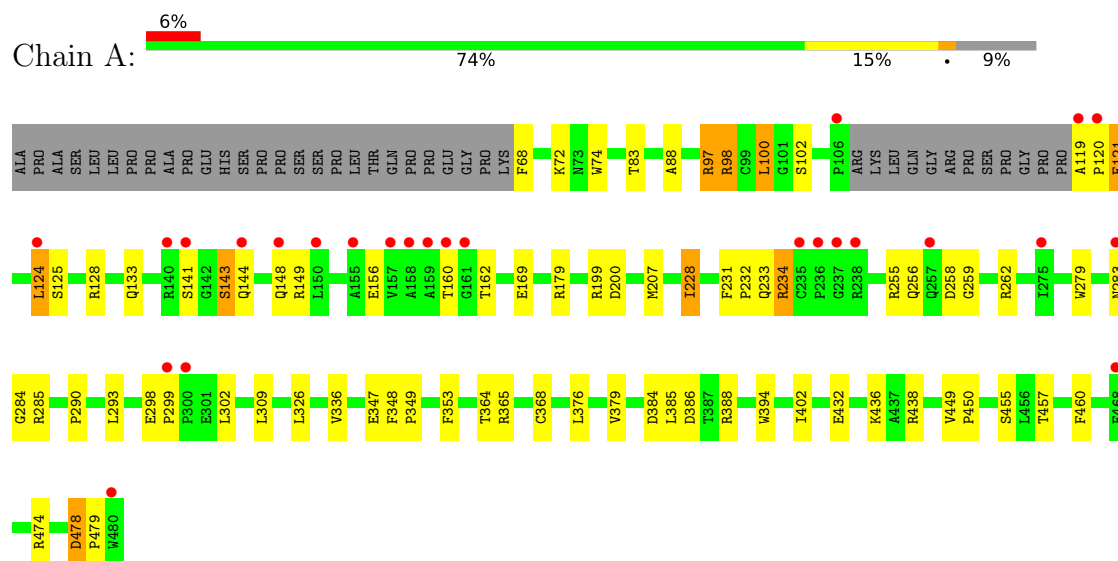
- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	123	Total O 123 123	0	0
10	B	148	Total O 148 148	0	0
10	C	99	Total O 99 99	0	0
10	D	152	Total O 152 152	0	0

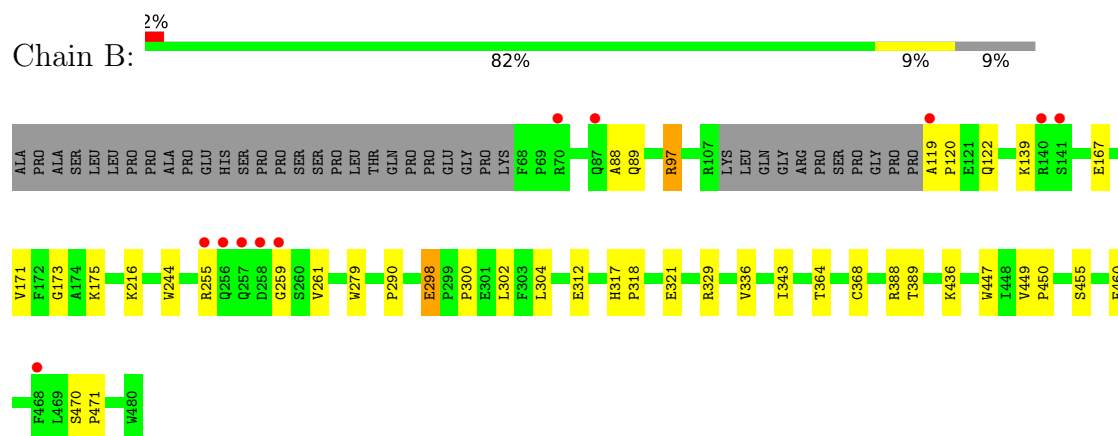
3 Residue-property plots [i](#)

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.

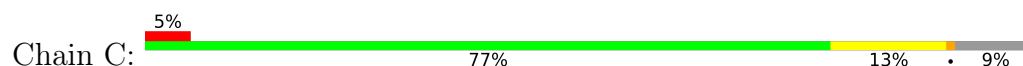
- Molecule 1: Nitric oxide synthase, endothelial

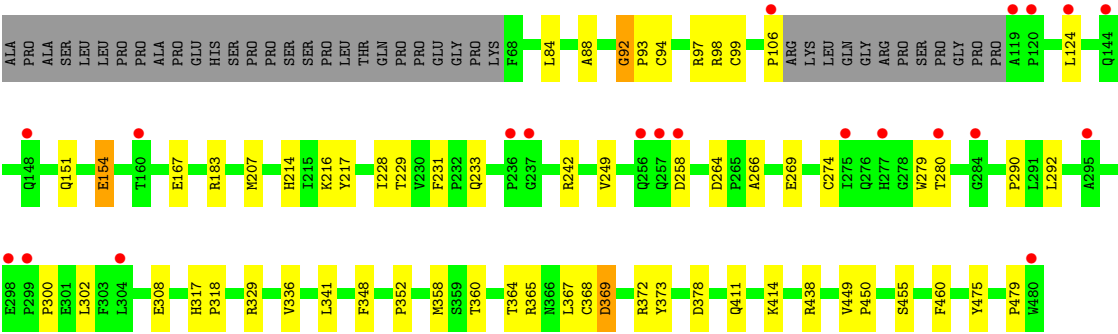


- Molecule 1: Nitric oxide synthase, endothelial

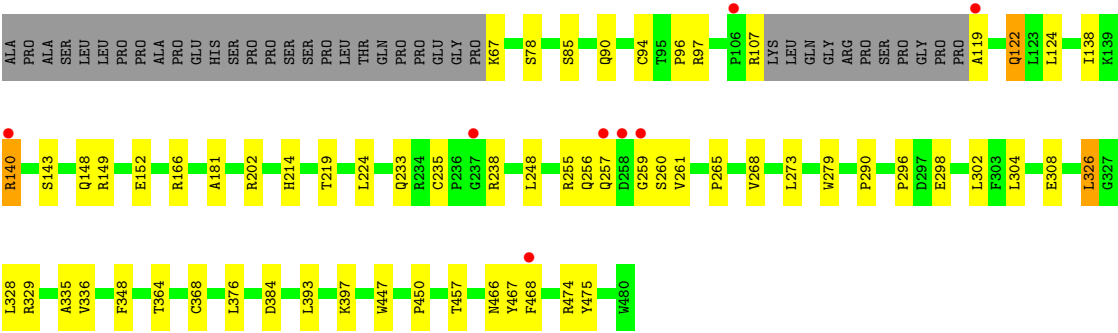
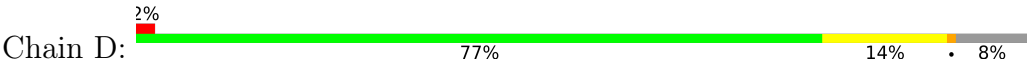


- Molecule 1: Nitric oxide synthase, endothelial





● 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	59.31Å 153.05Å 108.68Å 90.00° 90.75° 90.00°	Depositor
Resolution (Å)	55.30 – 2.15 55.30 – 2.15	Depositor EDS
% Data completeness (in resolution range)	92.5 (55.30-2.15) 91.8 (55.30-2.15)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 2.14Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.202 , 0.268 0.196 , 0.261	Depositor DCC
R_{free} test set	4831 reflections (2.96%)	wwPDB-VP
Wilson B-factor (Å ²)	30.7	Xtriage
Anisotropy	0.845	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 57.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.117 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13891	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.92% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GD, H4B, GOL, BTB, HEM, ZN, 9P7, CL

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	0.47	0/3313	0.81	0/4515
1	B	0.54	0/3336	0.82	1/4546 (0.0%)
1	C	0.45	0/3313	0.82	6/4515 (0.1%)
1	D	0.52	0/3330	0.86	5/4536 (0.1%)
All	All	0.50	0/13292	0.83	12/18112 (0.1%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	259	GLY	N-CA-C	-8.80	102.87	115.27
1	D	235	CYS	CA-C-N	7.32	127.36	119.90
1	D	235	CYS	C-N-CA	7.32	127.36	119.90
1	D	181	ALA	CA-C-N	6.46	126.38	119.28
1	D	181	ALA	C-N-CA	6.46	126.38	119.28
1	B	259	GLY	N-CA-C	-6.39	106.61	114.92
1	C	369	ASP	CA-C-N	5.42	125.25	119.28
1	C	369	ASP	C-N-CA	5.42	125.25	119.28
1	C	264	ASP	CA-C-N	5.22	124.88	119.56
1	C	264	ASP	C-N-CA	5.22	124.88	119.56
1	C	92	GLY	CA-C-N	5.16	126.18	120.45
1	C	92	GLY	C-N-CA	5.16	126.18	120.45

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3212	0	3114	50	0
1	B	3232	0	3137	21	0
1	C	3212	0	3114	35	0
1	D	3229	0	3139	45	0
2	A	43	0	30	3	0
2	B	43	0	30	1	0
2	C	43	0	30	4	0
2	D	43	0	30	2	0
3	A	17	0	15	2	0
3	B	17	0	15	1	0
3	C	17	0	15	1	0
3	D	17	0	15	1	0
4	A	24	0	0	2	0
4	B	24	0	0	1	0
4	C	24	0	0	1	0
4	D	24	0	0	1	0
5	A	28	0	37	7	0
5	B	42	0	56	12	0
5	C	28	0	38	1	0
5	D	28	0	37	7	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
7	A	6	0	8	1	0
7	C	6	0	8	0	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
9	A	1	0	0	0	0
9	B	1	0	0	0	0
9	C	1	0	0	0	0
9	D	1	0	0	0	0
10	A	123	0	0	6	0
10	B	148	0	0	1	0
10	C	99	0	0	1	0
10	D	152	0	0	2	0
All	All	13891	0	12868	170	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (170) 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)
2:A:501:HEM:HBB2	2:A:501:HEM:HHC	1.69	0.74
1:B:279:TRP:HB2	1:B:302:LEU:HD21	1.73	0.71
5:D:504:BTB:H82	5:D:504:BTB:O6	1.91	0.70
1:A:298:GLU:HG3	1:A:299:PRO:HD2	1.74	0.70
1:A:347:GLU:OE2	10:A:601:HOH:O	2.10	0.69
1:A:160:THR:HG23	1:A:162:THR:H	1.57	0.69
1:D:298:GLU:OE2	5:D:505:BTB:O8	2.09	0.68
1:B:321:GLU:OE2	5:B:504:BTB:O3	2.11	0.67
2:C:501:HEM:HBB2	2:C:501:HEM:HHC	1.76	0.67
2:C:501:HEM:HBC2	2:C:501:HEM:HMC2	1.78	0.66
1:B:298:GLU:OE2	5:B:505:BTB:N	2.28	0.66
1:D:90:GLN:OE1	1:D:474:ARG:NH2	2.29	0.65
2:B:501:HEM:HHC	2:B:501:HEM:HBB2	1.77	0.65
7:A:507:GOL:O2	10:A:602:HOH:O	2.14	0.64
2:D:501:HEM:HMC2	2:D:501:HEM:HBC2	1.79	0.63
1:A:124:LEU:O	1:A:128:ARG:HG2	1.97	0.63
1:D:90:GLN:HB2	1:D:468:PHE:CD2	2.34	0.62
1:A:97:ARG:NH1	1:B:88:ALA:O	2.32	0.62
1:A:156:GLU:O	1:A:160:THR:HG22	2.00	0.61
1:A:207:MET:HE3	1:A:293:LEU:HB3	1.83	0.61
5:B:505:BTB:O4	5:B:505:BTB:O3	2.20	0.59
1:B:447:TRP:HA	3:B:502:H4B:N1	2.18	0.59
1:D:290:PRO:HB3	1:D:304:LEU:HD23	1.83	0.59
1:C:292:LEU:HD22	1:C:300:PRO:HB2	1.84	0.58
1:C:378:ASP:OD1	10:C:601:HOH:O	2.17	0.58
2:A:501:HEM:HMC2	2:A:501:HEM:HBC2	1.86	0.57
5:A:505:BTB:H62	1:D:384:ASP:OD2	2.04	0.57
1:C:92:GLY:N	1:D:96:PRO:O	2.28	0.57
1:B:336:VAL:HG21	4:B:503:9P7:C07	2.34	0.56
1:C:97:ARG:HG2	1:C:98:ARG:HG2	1.87	0.56
1:D:279:TRP:HB2	1:D:302:LEU:HD21	1.87	0.56
1:A:258:ASP:N	10:A:603:HOH:O	2.38	0.56
1:A:124:LEU:HD13	1:A:128:ARG:HE	1.72	0.55
1:A:228:ILE:HG13	1:A:353:PHE:HB3	1.88	0.54
1:C:336:VAL:HG21	4:C:503:9P7:C07	2.37	0.54
1:D:336:VAL:HG21	4:D:503:9P7:C07	2.37	0.54
1:C:94:CYS:HB3	1:D:94:CYS:HB3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:393:LEU:O	1:D:397:LYS:HG3	2.07	0.54
1:A:200:ASP:OD1	1:A:200:ASP:N	2.37	0.54
1:B:122:GLN:HE22	5:B:506:BTB:H71	1.73	0.54
1:A:256:GLN:HB2	1:A:258:ASP:OD1	2.09	0.53
1:A:478:ASP:OD2	1:A:479:PRO:HD2	2.09	0.52
1:B:173:GLY:HA3	1:B:343:ILE:HD13	1.92	0.52
1:C:99:CYS:HB3	1:D:466:ASN:HB3	1.92	0.51
1:D:138:ILE:HG13	1:D:140:ARG:HB3	1.92	0.51
5:B:504:BTB:O6	5:B:504:BTB:H82	2.11	0.51
1:D:326:LEU:HB3	1:D:328:LEU:HG	1.93	0.51
2:A:501:HEM:O2D	4:A:503:9P7:N12	2.45	0.50
1:C:364:THR:O	1:C:368:CYS:HB2	2.10	0.50
1:D:261:VAL:HG11	1:D:265:PRO:HA	1.93	0.50
1:C:93:PRO:HB3	1:C:106:PRO:HB3	1.93	0.50
1:B:455:SER:HA	1:B:460:PHE:CG	2.47	0.50
1:A:432:GLU:O	1:A:436:LYS:HG2	2.12	0.49
1:A:364:THR:O	1:A:368:CYS:HB2	2.12	0.49
1:C:358:MET:HE3	1:C:360:THR:OG1	2.12	0.49
1:A:207:MET:HG3	1:A:231:PHE:CZ	2.48	0.49
1:A:450:PRO:HG2	1:A:457:THR:HG21	1.94	0.49
1:D:233:GLN:HB3	1:D:348:PHE:CE2	2.48	0.49
1:D:447:TRP:HA	3:D:502:H4B:N1	2.28	0.49
5:A:504:BTB:H42	5:A:504:BTB:H71	1.47	0.49
1:C:367:LEU:HA	1:C:373:TYR:HB2	1.95	0.48
1:C:229:THR:O	1:C:352:PRO:HD2	2.14	0.48
1:D:149:ARG:NH1	1:D:152:GLU:OE1	2.46	0.48
1:D:256:GLN:N	1:D:260:SER:O	2.47	0.48
1:B:167:GLU:OE1	10:B:601:HOH:O	2.20	0.47
1:C:365:ARG:HH12	3:C:502:H4B:C4	2.27	0.47
5:A:505:BTB:O8	5:A:505:BTB:H12	2.13	0.47
1:B:290:PRO:HB3	1:B:304:LEU:HD23	1.97	0.47
1:A:68:PHE:CD2	1:A:83:THR:HA	2.49	0.47
1:A:233:GLN:HB3	1:A:348:PHE:CE2	2.50	0.47
1:A:255:ARG:NH1	1:A:259:GLY:O	2.48	0.47
5:B:506:BTB:H52	5:B:506:BTB:H12	1.40	0.47
5:B:506:BTB:H82	5:B:506:BTB:H51	1.52	0.47
5:B:504:BTB:O3	5:B:504:BTB:O4	2.24	0.47
1:A:233:GLN:NE2	10:A:605:HOH:O	2.48	0.47
1:A:98:ARG:HG3	1:A:98:ARG:HH11	1.79	0.46
1:C:279:TRP:CG	1:C:290:PRO:HG3	2.50	0.46
1:A:72:LYS:HD3	1:A:74:TRP:CE2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:67:LYS:N	10:D:607:HOH:O	2.48	0.46
1:A:262:ARG:NH1	1:A:283:ASN:O	2.48	0.46
1:A:290:PRO:HB2	1:A:302:LEU:HD22	1.97	0.46
1:D:475:TYR:OH	2:D:501:HEM:O1D	2.29	0.46
1:C:207:MET:HG3	1:C:231:PHE:CZ	2.51	0.46
1:A:336:VAL:HG21	4:A:503:9P7:C07	2.45	0.46
1:C:411:GLN:O	1:C:414:LYS:HD2	2.16	0.46
1:D:140:ARG:HD2	1:D:143:SER:HB3	1.97	0.46
1:A:386:ASP:OD2	1:A:388:ARG:HG2	2.16	0.45
1:D:298:GLU:CD	5:D:505:BTB:H31	2.41	0.45
5:D:505:BTB:H42	5:D:505:BTB:H71	1.36	0.45
1:B:364:THR:O	1:B:368:CYS:HB2	2.16	0.45
5:B:505:BTB:H51	5:B:505:BTB:H81	1.61	0.45
1:C:266:ALA:HB2	1:C:372:ARG:NE	2.32	0.45
1:A:365:ARG:HH12	3:A:502:H4B:C4	2.29	0.45
5:B:505:BTB:H12	5:B:505:BTB:H52	1.68	0.45
5:C:505:BTB:H32	5:C:505:BTB:H52	1.36	0.44
1:A:149:ARG:NE	1:A:169:GLU:OE2	2.42	0.44
1:C:341:LEU:HB3	1:C:348:PHE:HB2	1.99	0.44
1:C:151:GLN:HA	1:C:154:GLU:OE2	2.17	0.44
1:D:202:ARG:CZ	1:D:202:ARG:HB2	2.46	0.44
1:D:233:GLN:O	1:D:238:ARG:NH2	2.50	0.44
1:B:122:GLN:NE2	5:B:506:BTB:H71	2.32	0.44
1:B:244:TRP:CH2	1:B:300:PRO:HG3	2.53	0.44
1:A:98:ARG:NH1	1:A:100:LEU:HD22	2.33	0.44
1:C:242:ARG:NH2	1:C:479:PRO:HD3	2.33	0.44
1:D:248:LEU:HB2	1:D:335:ALA:HB3	2.00	0.44
1:A:347:GLU:O	1:A:349:PRO:HD3	2.18	0.44
10:A:626:HOH:O	5:D:504:BTB:H12	2.17	0.43
1:A:88:ALA:HB3	1:B:97:ARG:HG2	2.00	0.43
1:A:119:ALA:HA	1:A:120:PRO:HD3	1.92	0.43
1:C:233:GLN:HB3	1:C:348:PHE:CE2	2.53	0.43
1:C:274:CYS:O	1:C:302:LEU:HD11	2.18	0.43
1:D:119:ALA:O	1:D:122:GLN:HG3	2.17	0.43
1:B:470:SER:HA	1:B:471:PRO:C	2.43	0.43
1:A:368:CYS:SG	1:A:376:LEU:HD13	2.58	0.43
1:A:449:VAL:HA	1:A:450:PRO:HD3	1.92	0.43
1:C:317:HIS:CG	1:C:318:PRO:HD2	2.54	0.43
1:C:269:GLU:N	1:C:269:GLU:OE1	2.52	0.43
1:D:219:THR:O	1:D:224:LEU:HD12	2.18	0.43
1:A:285:ARG:NH2	1:A:326:LEU:O	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:LEU:HD22	1:C:438:ARG:HB3	2.01	0.43
1:D:138:ILE:HG13	1:D:140:ARG:CB	2.48	0.43
1:B:317:HIS:CG	1:B:318:PRO:HD2	2.53	0.43
1:B:171:VAL:O	1:B:175:LYS:HG3	2.19	0.42
1:D:326:LEU:HD12	1:D:326:LEU:HA	1.83	0.42
1:B:312:GLU:CD	1:B:329:ARG:HH21	2.27	0.42
1:C:214:HIS:CD2	1:C:214:HIS:C	2.97	0.42
1:D:214:HIS:C	1:D:214:HIS:CD2	2.97	0.42
1:A:98:ARG:HG3	1:A:98:ARG:NH1	2.34	0.42
1:A:384:ASP:OD1	5:A:504:BTB:O4	2.38	0.42
1:C:475:TYR:OH	2:C:501:HEM:O1D	2.30	0.42
1:B:449:VAL:HA	1:B:450:PRO:HD3	1.91	0.42
1:C:449:VAL:HA	1:C:450:PRO:HD3	1.86	0.42
1:A:279:TRP:CG	1:A:290:PRO:HG3	2.55	0.42
1:B:119:ALA:HB3	1:B:120:PRO:HD3	2.02	0.42
1:C:365:ARG:O	1:C:369:ASP:HB2	2.20	0.42
1:A:199:ARG:O	1:A:232:PRO:HG3	2.20	0.42
1:C:183:ARG:HB2	2:C:501:HEM:HAD2	2.01	0.42
1:C:88:ALA:HB3	1:D:97:ARG:HG3	2.01	0.42
1:D:90:GLN:HB3	10:D:603:HOH:O	2.19	0.42
1:A:102:SER:O	3:A:502:H4B:O10	2.38	0.41
1:A:143:SER:OG	1:A:144:GLN:N	2.53	0.41
5:A:505:BTB:H32	5:A:505:BTB:H52	1.65	0.41
1:D:124:LEU:HD23	1:D:124:LEU:HA	1.86	0.41
1:A:284:GLY:HA3	10:A:616:HOH:O	2.20	0.41
1:D:238:ARG:HG2	1:D:296:PRO:HB3	2.02	0.41
1:D:364:THR:O	1:D:368:CYS:HB2	2.19	0.41
1:D:255:ARG:HE	1:D:268:VAL:HG11	1.86	0.41
1:C:292:LEU:HD23	1:C:292:LEU:HA	1.85	0.41
1:D:450:PRO:HG2	1:D:457:THR:HG21	2.01	0.41
5:D:504:BTB:H71	5:D:504:BTB:H42	1.57	0.41
1:A:121:GLU:O	1:A:124:LEU:HG	2.20	0.41
1:A:379:VAL:HG21	1:A:402:ILE:HD11	2.03	0.41
5:A:504:BTB:H31	1:D:326:LEU:HD11	2.03	0.41
1:C:151:GLN:O	1:C:154:GLU:HG2	2.20	0.41
1:A:234:ARG:HE	1:A:234:ARG:HB2	1.64	0.41
5:A:504:BTB:H52	5:A:504:BTB:H12	1.74	0.41
1:D:85:SER:HB3	1:D:467:TYR:CE1	2.56	0.41
1:D:140:ARG:HA	1:D:140:ARG:HD3	1.62	0.41
1:A:124:LEU:HD12	1:A:125:SER:N	2.36	0.41
1:A:179:ARG:NH2	1:A:438:ARG:HG3	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:LEU:HD13	1:A:394:TRP:HA	2.02	0.41
1:C:217:TYR:CD2	1:C:217:TYR:C	2.99	0.40
1:C:455:SER:HA	1:C:460:PHE:CG	2.56	0.40
1:D:122:GLN:HE21	1:D:122:GLN:HB2	1.68	0.40
1:D:149:ARG:HD3	1:D:166:ARG:CZ	2.52	0.40
1:A:455:SER:HA	1:A:460:PHE:CG	2.56	0.40
1:D:273:LEU:HA	1:D:273:LEU:HD23	1.91	0.40
1:D:298:GLU:OE1	5:D:505:BTB:H31	2.20	0.40
1:D:368:CYS:SG	1:D:376:LEU:HD13	2.62	0.40
5:B:506:BTB:H41	5:B:506:BTB:H72	1.58	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	400/440 (91%)	389 (97%)	11 (3%)	0	100	100
1	B	403/440 (92%)	391 (97%)	12 (3%)	0	100	100
1	C	400/440 (91%)	388 (97%)	12 (3%)	0	100	100
1	D	402/440 (91%)	386 (96%)	16 (4%)	0	100	100
All	All	1605/1760 (91%)	1554 (97%)	51 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	343/373 (92%)	329 (96%)	14 (4%)	27	26
1	B	346/373 (93%)	336 (97%)	10 (3%)	37	39
1	C	343/373 (92%)	333 (97%)	10 (3%)	37	39
1	D	345/373 (92%)	336 (97%)	9 (3%)	40	43
All	All	1377/1492 (92%)	1334 (97%)	43 (3%)	34	37

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	97	ARG
1	A	98	ARG
1	A	100	LEU
1	A	121	GLU
1	A	124	LEU
1	A	133	GLN
1	A	141	SER
1	A	143	SER
1	A	148	GLN
1	A	228	ILE
1	A	234	ARG
1	A	309	LEU
1	A	474	ARG
1	A	478	ASP
1	B	89	GLN
1	B	97	ARG
1	B	139	LYS
1	B	216	LYS
1	B	255	ARG
1	B	261	VAL
1	B	298	GLU
1	B	388	ARG
1	B	389	THR
1	B	436	LYS
1	C	124	LEU
1	C	154	GLU
1	C	167	GLU
1	C	216	LYS
1	C	228	ILE
1	C	249	VAL

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Mol	Chain	Res	Type
1	C	258	ASP
1	C	280	THR
1	C	308	GLU
1	C	329	ARG
1	D	78	SER
1	D	107	ARG
1	D	122	GLN
1	D	140	ARG
1	D	148	GLN
1	D	257	GLN
1	D	308	GLU
1	D	326	LEU
1	D	329	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	B	87	GLN
1	B	276	GLN
1	B	403	ASN
1	C	89	GLN
1	C	151	GLN
1	C	220	ASN
1	C	233	GLN
1	D	256	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 33 ligands modelled in this entry, 10 are monoatomic - leaving 23 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
4	9P7	C	503	-	26,26,26	2.34	1 (3%)	33,35,35	1.29	7 (21%)
2	HEM	B	501	1	50,50,50	2.20	6 (12%)	67,82,82	1.42	9 (13%)
2	HEM	D	501	1	50,50,50	2.18	7 (14%)	67,82,82	1.48	8 (11%)
2	HEM	A	501	1	50,50,50	2.23	9 (18%)	67,82,82	1.43	9 (13%)
3	H4B	D	502	-	17,18,18	0.87	0	14,26,26	2.06	5 (35%)
3	H4B	C	502	-	17,18,18	0.84	1 (5%)	14,26,26	1.78	5 (35%)
2	HEM	C	501	1	50,50,50	1.96	10 (20%)	67,82,82	1.28	6 (8%)
3	H4B	A	502	-	17,18,18	0.92	0	14,26,26	1.94	4 (28%)
4	9P7	B	503	-	26,26,26	2.35	3 (11%)	33,35,35	1.22	2 (6%)
5	BTB	B	504	8	13,13,13	0.41	0	7,16,16	1.12	1 (14%)
7	GOL	A	507	-	5,5,5	0.33	0	5,5,5	0.35	0
7	GOL	C	507	-	5,5,5	0.39	0	5,5,5	0.34	0
4	9P7	A	503	-	26,26,26	2.33	1 (3%)	33,35,35	1.32	4 (12%)
5	BTB	D	505	-	13,13,13	0.50	0	7,16,16	0.80	0
5	BTB	D	504	8	13,13,13	0.42	0	7,16,16	0.86	0
5	BTB	B	505	-	13,13,13	0.37	0	7,16,16	0.50	0
5	BTB	A	504	8	13,13,13	0.38	0	7,16,16	0.62	0
3	H4B	B	502	-	17,18,18	0.90	1 (5%)	14,26,26	1.88	5 (35%)
5	BTB	C	505	-	13,13,13	0.36	0	7,16,16	0.93	0
5	BTB	B	506	-	13,13,13	0.48	0	7,16,16	0.59	0
5	BTB	A	505	-	13,13,13	0.70	0	7,16,16	1.49	2 (28%)
5	BTB	C	504	8	13,13,13	0.41	0	7,16,16	0.63	0
4	9P7	D	503	-	26,26,26	2.35	1 (3%)	33,35,35	1.27	3 (9%)

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	9P7	C	503	-	-	2/9/18/18	0/3/3/3
2	HEM	B	501	1	-	3/14/54/54	-
2	HEM	D	501	1	-	0/14/54/54	-
2	HEM	A	501	1	-	4/14/54/54	-
3	H4B	D	502	-	-	3/8/17/17	0/2/2/2
3	H4B	C	502	-	-	3/8/17/17	0/2/2/2
2	HEM	C	501	1	-	5/14/54/54	-
3	H4B	A	502	-	-	3/8/17/17	0/2/2/2
4	9P7	B	503	-	-	0/9/18/18	0/3/3/3
5	BTB	B	504	8	-	4/21/21/21	-
7	GOL	A	507	-	-	2/4/4/4	-
7	GOL	C	507	-	-	3/4/4/4	-
4	9P7	A	503	-	-	2/9/18/18	0/3/3/3
5	BTB	D	505	-	-	12/21/21/21	-
5	BTB	D	504	8	-	4/21/21/21	-
5	BTB	B	505	-	-	9/21/21/21	-
5	BTB	A	504	8	-	7/21/21/21	-
3	H4B	B	502	-	-	3/8/17/17	0/2/2/2
5	BTB	C	505	-	-	8/21/21/21	-
5	BTB	B	506	-	-	14/21/21/21	-
5	BTB	A	505	-	-	8/21/21/21	-
5	BTB	C	504	8	-	5/21/21/21	-
4	9P7	D	503	-	-	1/9/18/18	0/3/3/3

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	503	9P7	C24-C28	-10.90	1.28	1.44
4	A	503	9P7	C24-C28	-10.86	1.28	1.44
4	C	503	9P7	C24-C28	-10.83	1.28	1.44
4	B	503	9P7	C24-C28	-10.78	1.28	1.44
2	A	501	HEM	FE-ND	8.08	2.19	1.94
2	A	501	HEM	C3D-C2D	7.85	1.53	1.36
2	D	501	HEM	C3D-C2D	7.78	1.53	1.36
2	B	501	HEM	C3D-C2D	7.70	1.53	1.36
2	C	501	HEM	C3D-C2D	7.46	1.52	1.36
2	B	501	HEM	FE-NC	7.42	2.19	1.95
2	D	501	HEM	FE-NC	6.55	2.16	1.95
2	B	501	HEM	FE-ND	6.20	2.14	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	FE-NA	6.13	2.15	1.95
2	D	501	HEM	FE-NB	5.80	2.12	1.94
2	B	501	HEM	FE-NB	5.53	2.11	1.94
2	C	501	HEM	FE-NB	5.03	2.10	1.94
2	D	501	HEM	FE-ND	5.01	2.10	1.94
2	C	501	HEM	FE-ND	4.40	2.08	1.94
2	C	501	HEM	FE-NC	4.05	2.08	1.95
2	D	501	HEM	FE-NA	3.80	2.07	1.95
2	A	501	HEM	FE-NC	3.74	2.07	1.95
2	C	501	HEM	CAB-C3B	3.48	1.56	1.47
2	C	501	HEM	FE-NA	3.44	2.06	1.95
2	A	501	HEM	CAC-C3C	3.26	1.56	1.47
2	D	501	HEM	CAB-C3B	3.09	1.55	1.47
2	B	501	HEM	CAB-C3B	3.06	1.55	1.47
2	A	501	HEM	CAB-C3B	3.03	1.55	1.47
2	C	501	HEM	CAC-C3C	2.97	1.55	1.47
2	A	501	HEM	FE-NB	2.75	2.03	1.94
2	B	501	HEM	CAC-C3C	2.72	1.54	1.47
2	D	501	HEM	CAC-C3C	2.56	1.54	1.47
3	B	502	H4B	C4-N3	-2.45	1.34	1.38
2	C	501	HEM	CMB-C2B	2.20	1.55	1.50
2	C	501	HEM	CMC-C2C	2.17	1.55	1.50
4	B	503	9P7	C24-C23	-2.16	1.36	1.40
3	C	502	H4B	C4-N3	-2.14	1.34	1.38
4	B	503	9P7	C05-C10	-2.12	1.39	1.42
2	A	501	HEM	C2A-C3A	-2.11	1.33	1.38
2	A	501	HEM	CMC-C2C	2.11	1.55	1.50
2	C	501	HEM	CMD-C2D	2.03	1.54	1.50

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	HEM	C4D-ND-C1D	5.55	111.78	105.21
2	B	501	HEM	C4D-ND-C1D	5.30	111.49	105.21
3	D	502	H4B	C2-N1-C8A	4.91	122.03	113.36
2	C	501	HEM	C4D-ND-C1D	4.77	110.86	105.21
2	A	501	HEM	C4D-ND-C1D	4.51	110.55	105.21
3	A	502	H4B	C2-N1-C8A	4.48	121.26	113.36
3	B	502	H4B	C2-N1-C8A	4.31	120.97	113.36
3	C	502	H4B	C2-N1-C8A	4.14	120.67	113.36
2	D	501	HEM	C3B-C2B-C1B	3.65	109.15	106.41
2	B	501	HEM	C3B-C2B-C1B	3.58	109.10	106.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	HEM	C3B-C2B-C1B	3.39	108.96	106.41
2	C	501	HEM	C3B-C2B-C1B	3.34	108.92	106.41
2	B	501	HEM	C1B-NB-C4B	3.18	108.97	105.21
2	A	501	HEM	C3B-C4B-NB	-3.15	107.21	109.47
2	A	501	HEM	CBA-CAA-C2A	-3.14	103.85	112.53
2	A	501	HEM	C1B-NB-C4B	3.08	108.85	105.21
4	A	503	9P7	C23-C22-C21	-3.00	118.84	122.22
2	C	501	HEM	CBD-CAD-C3D	-2.93	104.44	112.53
3	D	502	H4B	C4A-C4-N3	2.89	120.06	112.13
3	D	502	H4B	O4-C4-C4A	-2.88	120.32	127.26
4	B	503	9P7	C22-C23-C24	2.86	121.61	117.52
3	B	502	H4B	C4A-C4-N3	2.82	119.88	112.13
4	D	503	9P7	N02-C02-N01	2.79	120.55	118.24
3	A	502	H4B	O4-C4-C4A	-2.75	120.62	127.26
4	D	503	9P7	C23-C22-C21	-2.71	119.17	122.22
2	D	501	HEM	CBD-CAD-C3D	-2.71	105.04	112.53
2	D	501	HEM	C1B-NB-C4B	2.69	108.39	105.21
4	C	503	9P7	N02-C02-N01	2.68	120.45	118.24
3	A	502	H4B	C4A-C4-N3	2.67	119.47	112.13
4	B	503	9P7	C23-C22-C21	-2.63	119.25	122.22
3	A	502	H4B	C2-N3-C4	-2.58	120.42	125.11
2	B	501	HEM	C2B-C1B-NB	-2.56	106.90	109.84
5	B	504	BTB	O3-C3-C2	-2.53	105.44	111.40
4	C	503	9P7	C23-C22-C21	-2.51	119.39	122.22
3	C	502	H4B	C4A-C4-N3	2.51	119.02	112.13
4	A	503	9P7	C03-C02-N01	-2.49	119.11	122.09
2	A	501	HEM	C2A-C1A-NA	-2.48	107.39	110.15
4	C	503	9P7	C22-C23-C24	2.47	121.06	117.52
4	A	503	9P7	C27-C23-C24	-2.41	118.35	121.44
3	C	502	H4B	C2-N3-C4	-2.39	120.77	125.11
2	A	501	HEM	C2B-C1B-NB	-2.38	107.11	109.84
4	A	503	9P7	C22-C23-C24	2.36	120.89	117.52
2	D	501	HEM	CHD-C1D-ND	2.35	126.95	124.42
3	D	502	H4B	N3-C2-N1	-2.34	119.05	123.32
2	B	501	HEM	C3B-C4B-NB	-2.30	107.82	109.47
2	C	501	HEM	CAD-C3D-C4D	2.30	128.70	124.70
2	C	501	HEM	C1B-NB-C4B	2.25	107.87	105.21
4	D	503	9P7	C11-C08-C09	-2.24	117.48	121.46
5	A	505	BTB	O3-C3-C2	-2.24	106.14	111.40
4	C	503	9P7	C11-N12-C13	-2.23	105.35	113.20
3	C	502	H4B	O4-C4-C4A	-2.23	121.89	127.26
2	D	501	HEM	C3B-C4B-NB	-2.22	107.87	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	502	H4B	C2-N3-C4	-2.22	121.09	125.11
5	A	505	BTB	O4-C4-C2	-2.20	106.24	111.40
2	C	501	HEM	CMD-C2D-C1D	2.18	128.44	125.03
4	C	503	9P7	C26-C25-C24	-2.17	117.97	120.92
2	A	501	HEM	CAD-C3D-C4D	2.15	128.45	124.70
3	B	502	H4B	C2-N3-C4	-2.14	121.23	125.11
4	C	503	9P7	C27-C23-C24	-2.13	118.72	121.44
2	D	501	HEM	C4C-NC-C1C	2.12	109.28	105.82
2	B	501	HEM	CBD-CAD-C3D	-2.11	106.69	112.53
3	B	502	H4B	O4-C4-C4A	-2.10	122.19	127.26
2	D	501	HEM	C2B-C1B-NB	-2.09	107.44	109.84
2	B	501	HEM	C4C-NC-C1C	2.08	109.20	105.82
3	C	502	H4B	C4-C4A-N5	2.06	121.89	116.27
2	B	501	HEM	CBA-CAA-C2A	-2.06	106.84	112.53
2	B	501	HEM	CMD-C2D-C1D	2.05	128.25	125.03
3	B	502	H4B	C4-C4A-N5	2.05	121.85	116.27
4	C	503	9P7	C03-C02-N01	-2.03	119.66	122.09
2	A	501	HEM	CBD-CAD-C3D	-2.03	106.92	112.53

There are no chirality outliers.

All (105) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	H4B	C7-C6-C9-O9
3	A	502	H4B	C7-C6-C9-C10
3	B	502	H4B	C7-C6-C9-O9
3	B	502	H4B	C7-C6-C9-C10
3	C	502	H4B	C7-C6-C9-O9
3	C	502	H4B	C7-C6-C9-C10
3	D	502	H4B	C7-C6-C9-O9
4	C	503	9P7	N12-C13-C14-C21
5	A	504	BTB	O1-C1-C2-C3
5	A	504	BTB	O1-C1-C2-C4
5	A	504	BTB	O1-C1-C2-N
5	A	504	BTB	C1-C2-C3-O3
5	A	504	BTB	C4-C2-C3-O3
5	A	504	BTB	N-C2-C3-O3
5	A	505	BTB	N-C2-C4-O4
5	A	505	BTB	C1-C2-N-C5
5	A	505	BTB	C1-C2-N-C7
5	A	505	BTB	C3-C2-N-C5
5	A	505	BTB	C3-C2-N-C7

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Mol	Chain	Res	Type	Atoms
5	A	505	BTB	C4-C2-N-C5
5	A	505	BTB	C4-C2-N-C7
5	B	504	BTB	O1-C1-C2-C3
5	B	504	BTB	O1-C1-C2-C4
5	B	504	BTB	O1-C1-C2-N
5	B	505	BTB	O1-C1-C2-C3
5	B	505	BTB	O1-C1-C2-C4
5	B	505	BTB	O1-C1-C2-N
5	B	505	BTB	C1-C2-C3-O3
5	B	505	BTB	C4-C2-C3-O3
5	B	505	BTB	N-C2-C3-O3
5	B	506	BTB	C1-C2-C3-O3
5	B	506	BTB	C4-C2-C3-O3
5	B	506	BTB	N-C2-C3-O3
5	B	506	BTB	C1-C2-N-C5
5	B	506	BTB	C1-C2-N-C7
5	B	506	BTB	C3-C2-N-C5
5	B	506	BTB	C3-C2-N-C7
5	B	506	BTB	C4-C2-N-C5
5	B	506	BTB	C4-C2-N-C7
5	B	506	BTB	C8-C7-N-C5
5	B	506	BTB	N-C7-C8-O8
5	C	504	BTB	O1-C1-C2-N
5	C	504	BTB	C1-C2-C4-O4
5	C	504	BTB	C3-C2-C4-O4
5	C	504	BTB	N-C2-C4-O4
5	C	505	BTB	C4-C2-C3-O3
5	C	505	BTB	N-C2-C3-O3
5	C	505	BTB	C1-C2-N-C7
5	C	505	BTB	C4-C2-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	505	BTB	O1-C1-C2-C3
5	D	505	BTB	O1-C1-C2-C4
5	D	505	BTB	O1-C1-C2-N
5	D	505	BTB	N-C2-C4-O4
5	D	505	BTB	C1-C2-N-C5
5	D	505	BTB	C4-C2-N-C7
7	A	507	GOL	O1-C1-C2-C3
7	C	507	GOL	O1-C1-C2-C3
5	B	504	BTB	N-C7-C8-O8

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Mol	Chain	Res	Type	Atoms
5	B	506	BTB	N-C5-C6-O6
5	D	504	BTB	N-C7-C8-O8
4	A	503	9P7	N12-C13-C14-C21
2	A	501	HEM	C3D-CAD-CBD-CGD
7	A	507	GOL	O1-C1-C2-O2
5	A	504	BTB	N-C5-C6-O6
7	C	507	GOL	O1-C1-C2-O2
3	D	502	H4B	C7-C6-C9-C10
2	B	501	HEM	C3D-CAD-CBD-CGD
2	C	501	HEM	C4D-C3D-CAD-CBD
2	A	501	HEM	C4B-C3B-CAB-CBB
2	B	501	HEM	C4B-C3B-CAB-CBB
2	C	501	HEM	C4B-C3B-CAB-CBB
2	A	501	HEM	C4D-C3D-CAD-CBD
5	C	504	BTB	O1-C1-C2-C3
5	D	505	BTB	C1-C2-C4-O4
3	C	502	H4B	N5-C6-C9-O9
5	B	505	BTB	N-C5-C6-O6
2	C	501	HEM	C3D-CAD-CBD-CGD
5	B	505	BTB	C1-C2-N-C5
5	C	505	BTB	C1-C2-N-C5
5	C	505	BTB	C3-C2-N-C5
5	C	505	BTB	C4-C2-N-C7
5	D	505	BTB	C1-C2-N-C7
5	D	505	BTB	C3-C2-N-C7
5	D	505	BTB	C4-C2-N-C5
2	B	501	HEM	C4D-C3D-CAD-CBD
5	A	505	BTB	C3-C2-C4-O4
4	D	503	9P7	N12-C13-C14-C21
2	A	501	HEM	C2D-C3D-CAD-CBD
5	B	506	BTB	C3-C2-C4-O4
5	D	505	BTB	N-C7-C8-O8
2	C	501	HEM	C2D-C3D-CAD-CBD
7	C	507	GOL	O2-C2-C3-O3
3	A	502	H4B	N5-C6-C9-O9
3	B	502	H4B	N5-C6-C9-O9
3	D	502	H4B	N5-C6-C9-O9
2	C	501	HEM	C1A-C2A-CAA-CBA
5	B	505	BTB	C3-C2-N-C5
5	B	506	BTB	N-C2-C4-O4
5	C	505	BTB	C3-C2-N-C7
5	D	505	BTB	C3-C2-N-C5

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Mol	Chain	Res	Type	Atoms
4	C	503	9P7	C23-C24-C28-N29
4	A	503	9P7	C25-C24-C28-N29

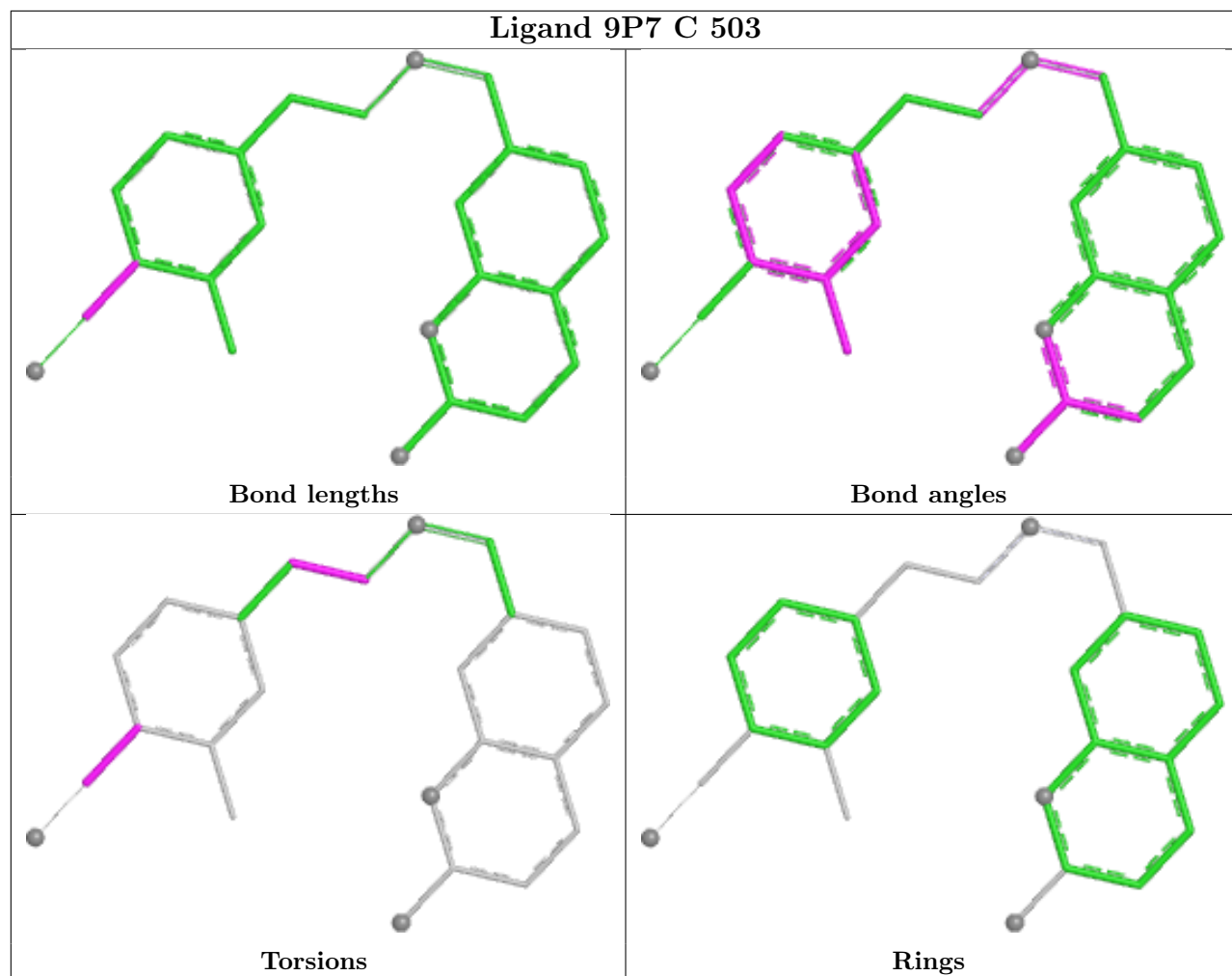
There are no ring outliers.

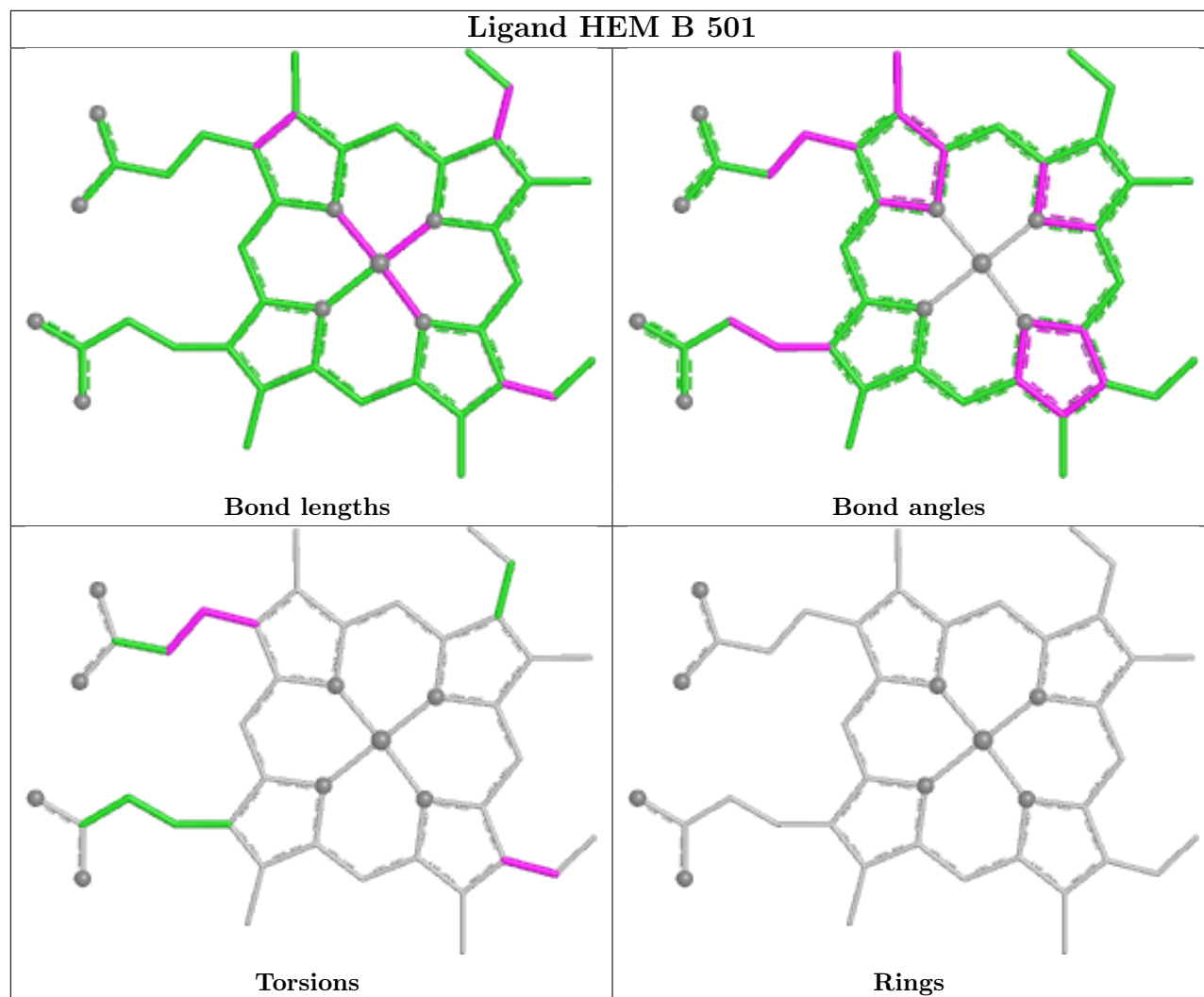
21 monomers are involved in 47 short contacts:

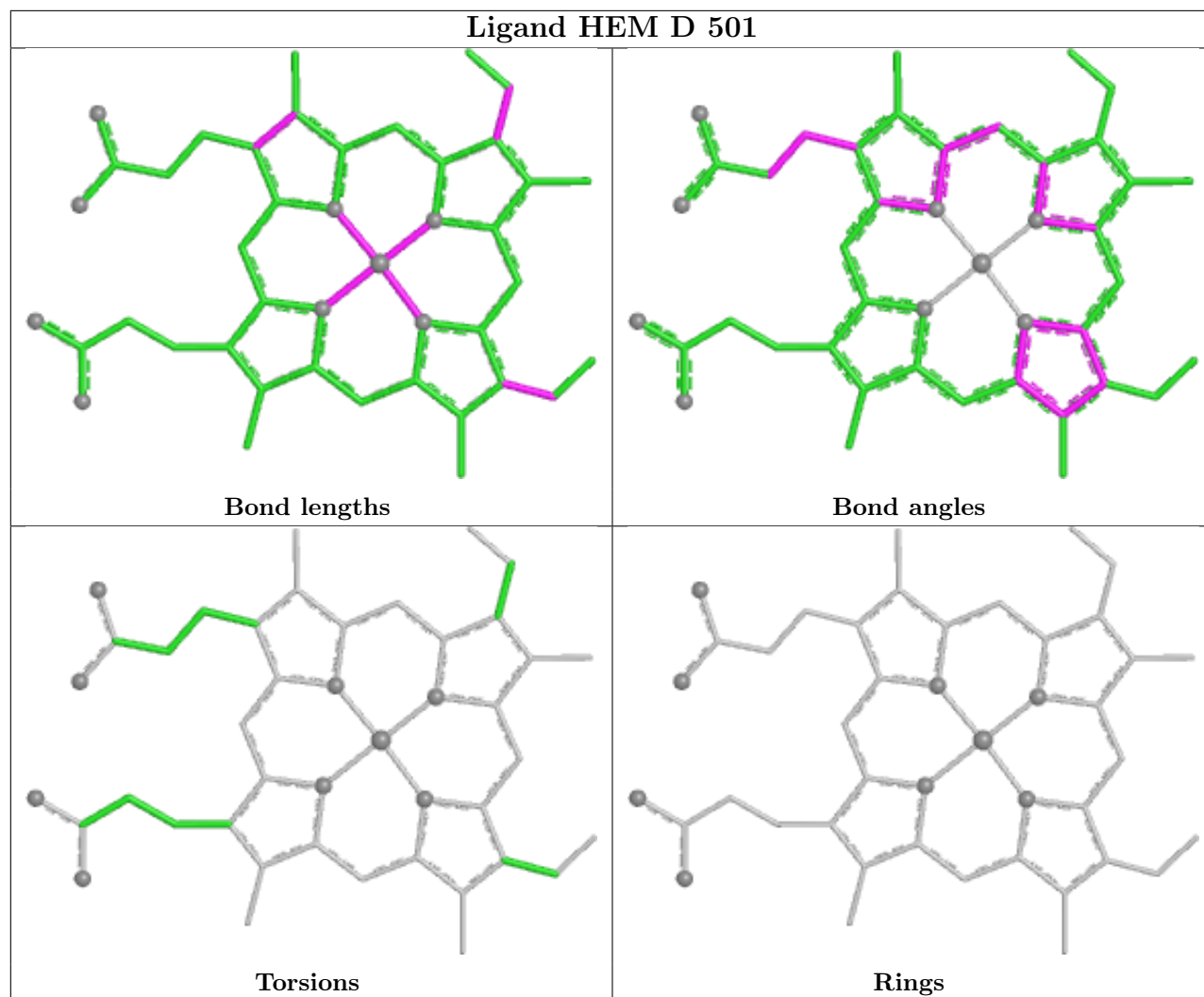
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	503	9P7	1	0
2	B	501	HEM	1	0
2	D	501	HEM	2	0
2	A	501	HEM	3	0
3	D	502	H4B	1	0
3	C	502	H4B	1	0
2	C	501	HEM	4	0
3	A	502	H4B	2	0
4	B	503	9P7	1	0
5	B	504	BTB	3	0
7	A	507	GOL	1	0
4	A	503	9P7	2	0
5	D	505	BTB	4	0
5	D	504	BTB	3	0
5	B	505	BTB	4	0
5	A	504	BTB	4	0
3	B	502	H4B	1	0
5	C	505	BTB	1	0
5	B	506	BTB	5	0
5	A	505	BTB	3	0
4	D	503	9P7	1	0

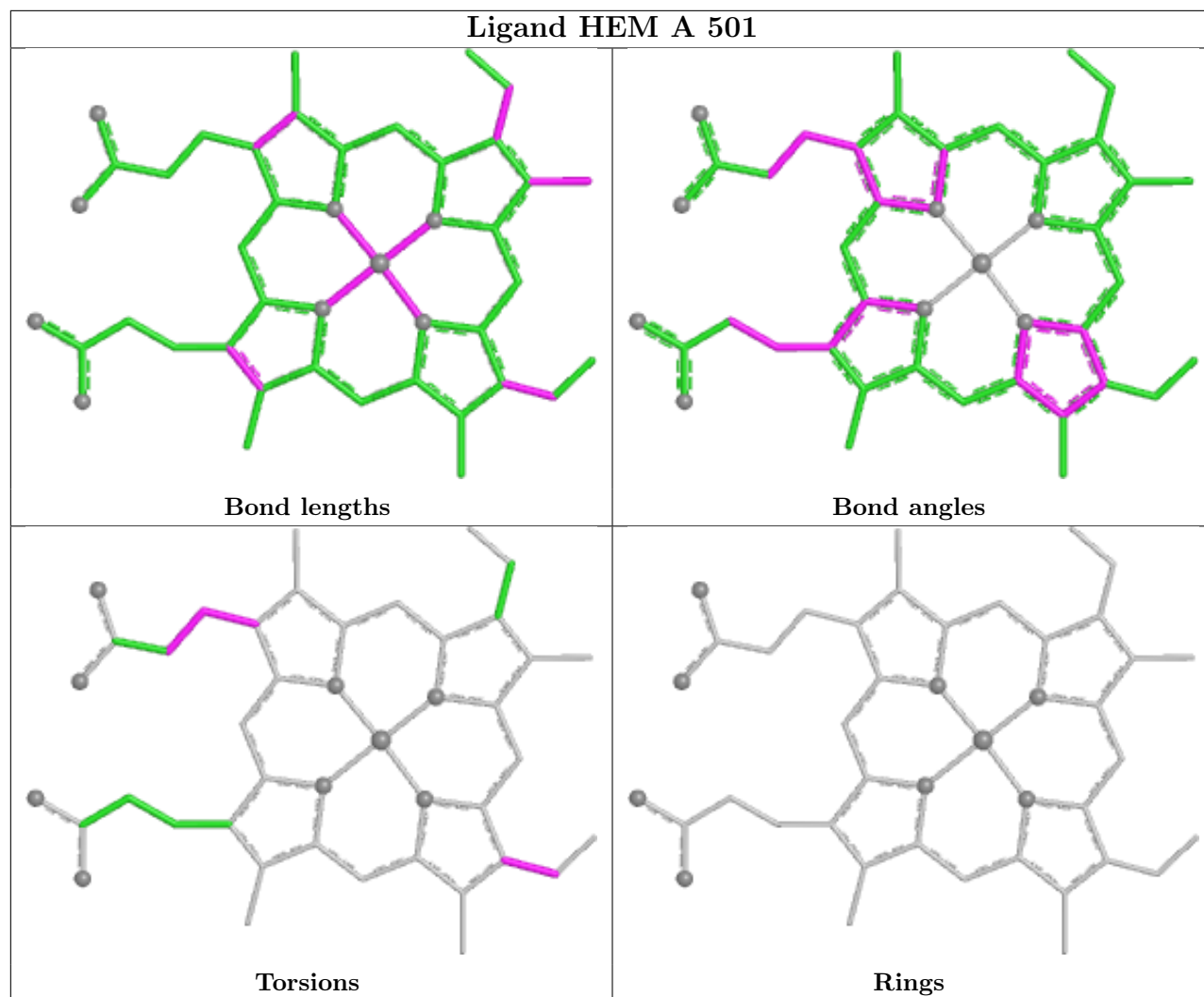
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

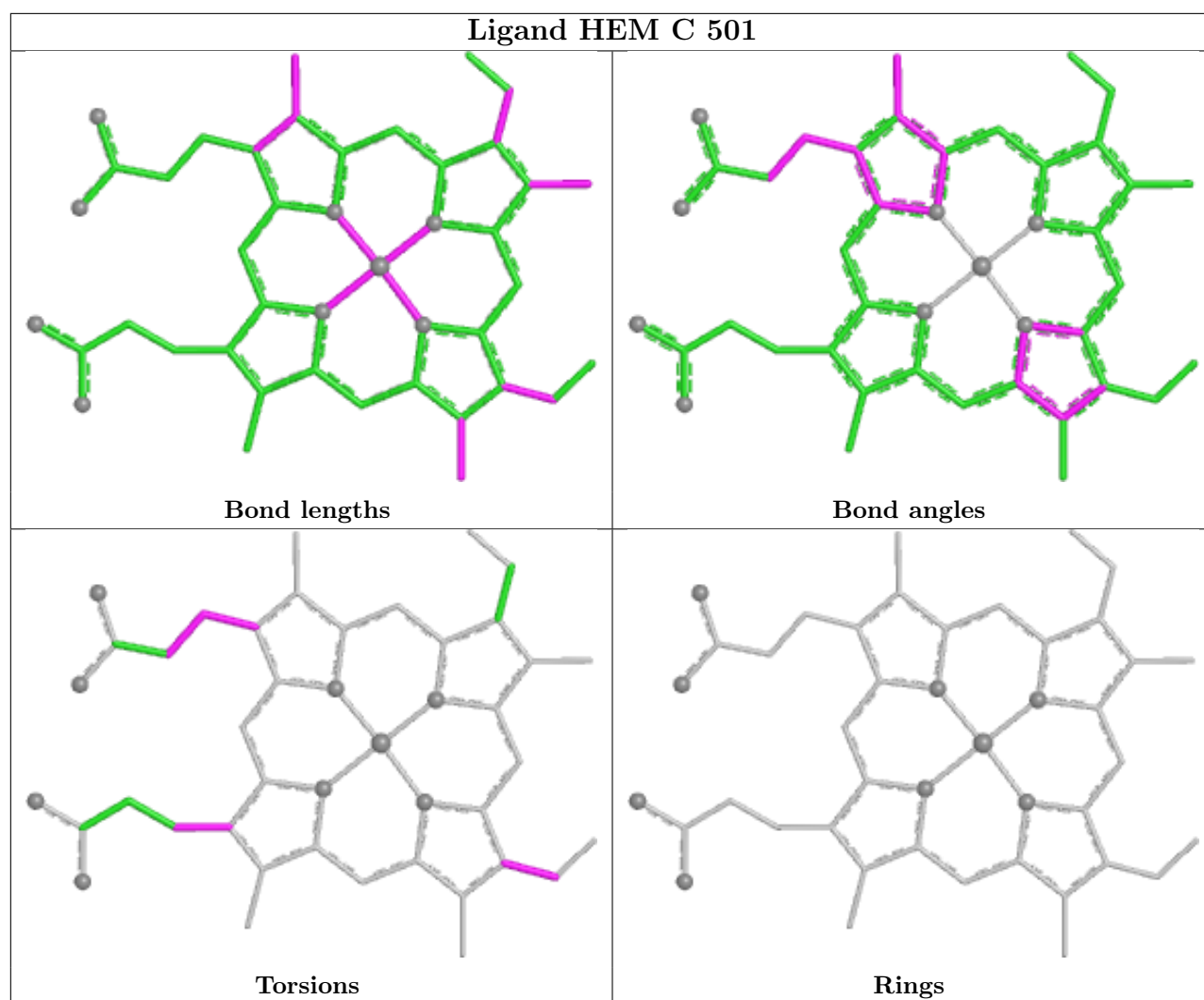
Ligand 9P7 C 503



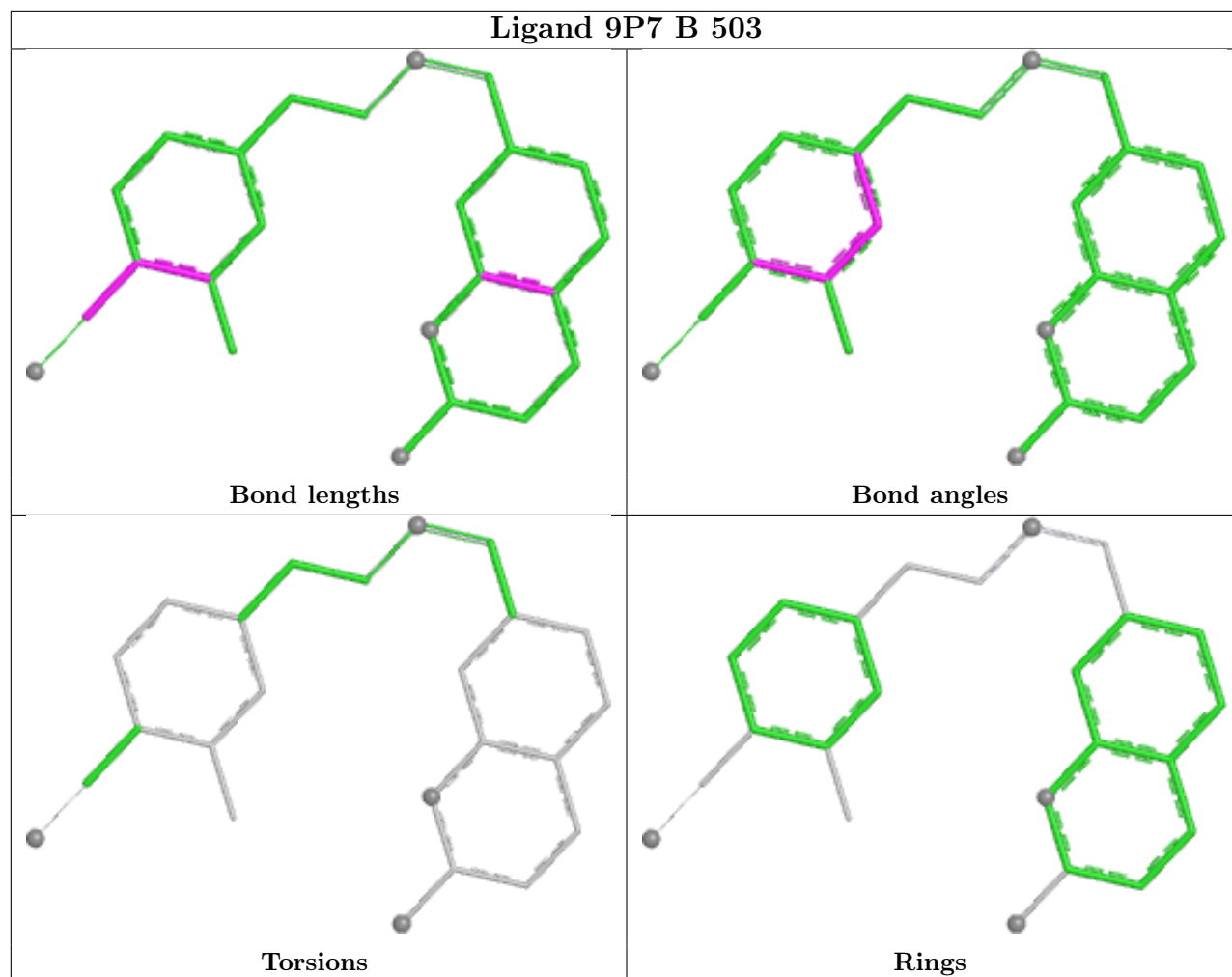




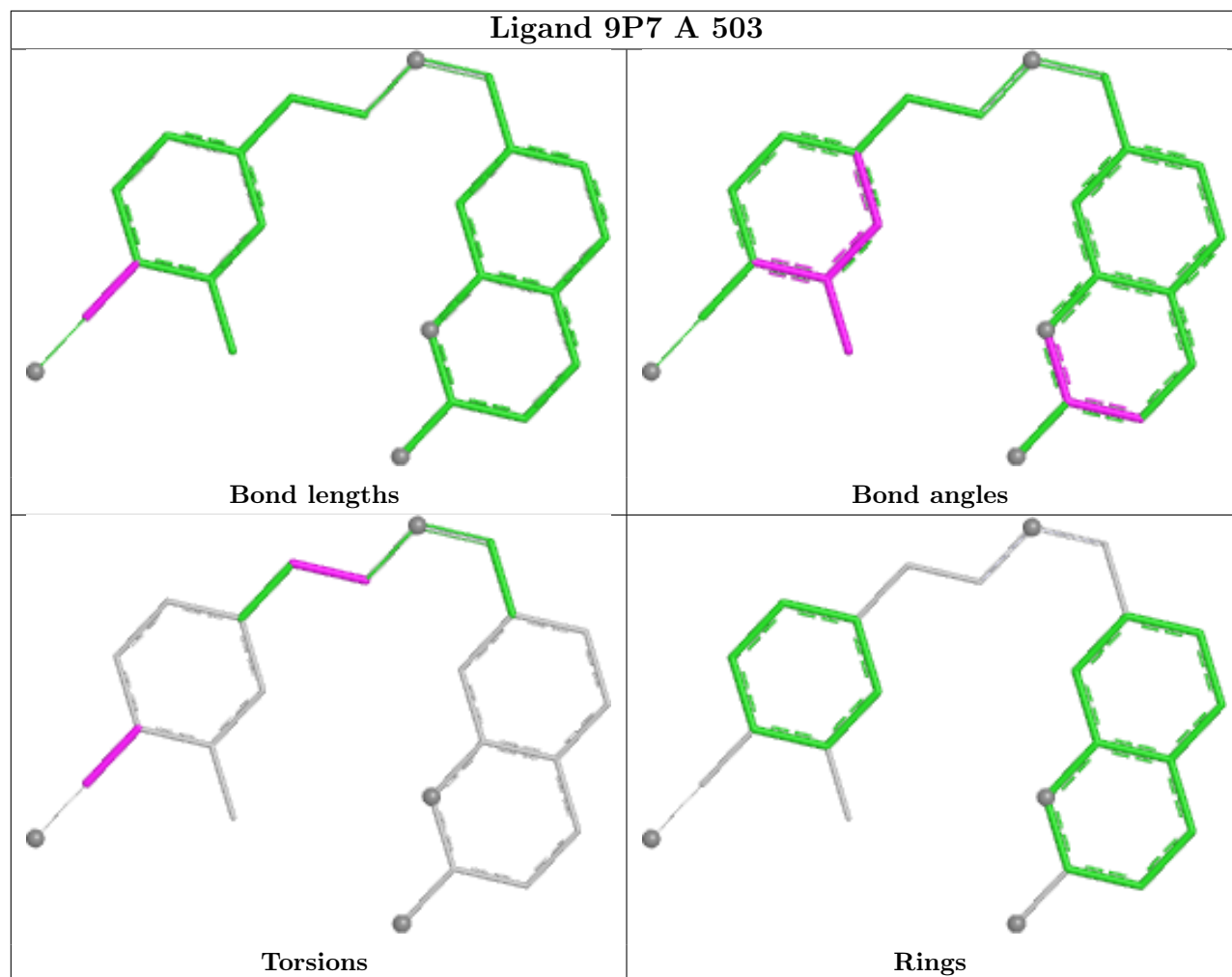


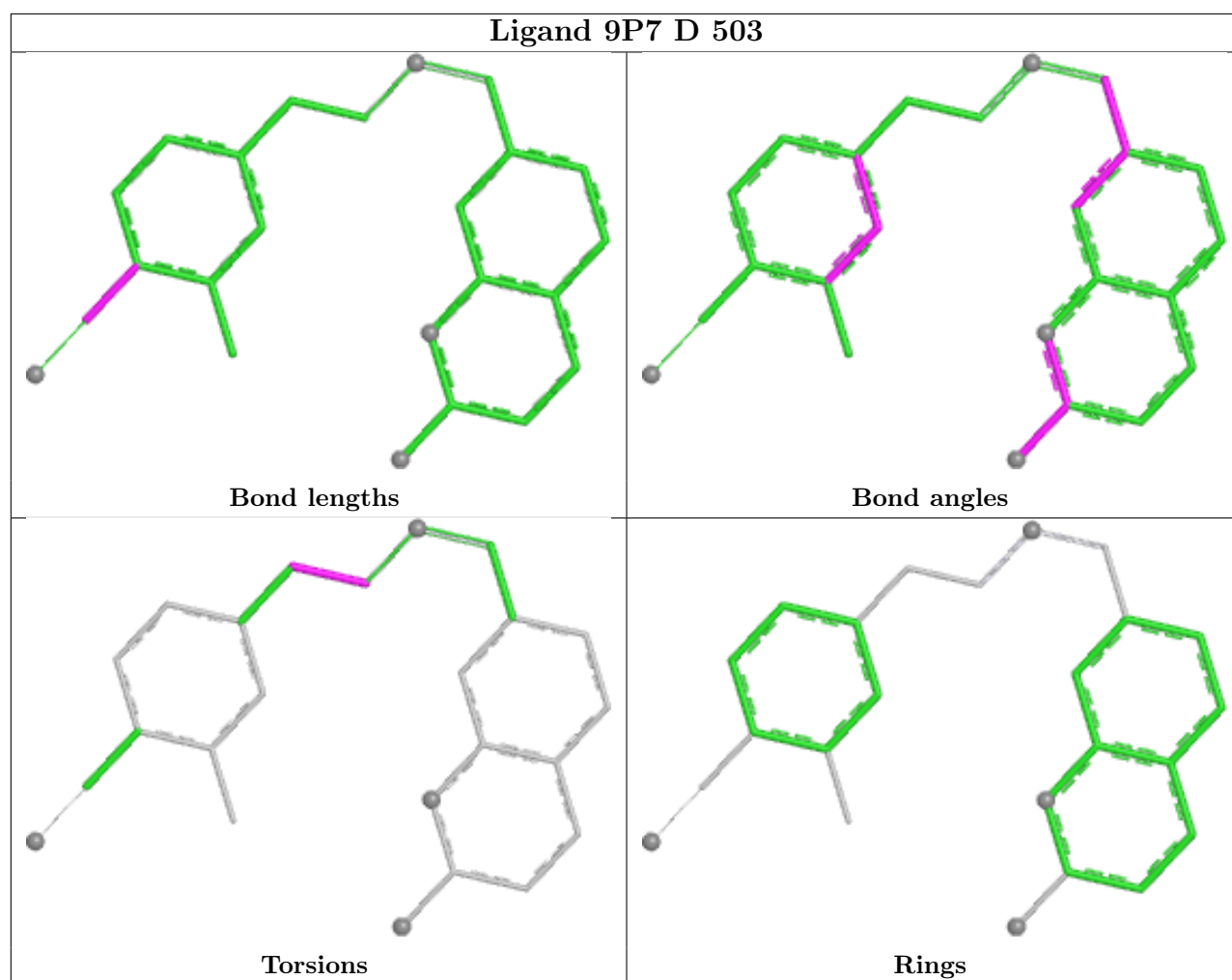


Ligand 9P7 B 503



Ligand 9P7 A 503





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.38	26 (6%) 25 28	21, 46, 93, 120	3 (0%)
1	B	402/440 (91%)	0.01	11 (2%) 56 60	19, 35, 65, 114	5 (1%)
1	C	401/440 (91%)	0.48	21 (5%) 33 36	23, 49, 93, 129	3 (0%)
1	D	403/440 (91%)	0.07	8 (1%) 65 69	20, 36, 75, 132	3 (0%)
All	All	1607/1760 (91%)	0.23	66 (4%) 41 46	19, 41, 88, 132	14 (0%)

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	106	PRO	5.0
1	B	119	ALA	4.2
1	A	119	ALA	3.7
1	C	119	ALA	3.6
1	D	140	ARG	3.5
1	C	237	GLY	3.4
1	A	124	LEU	3.3
1	A	300	PRO	3.1
1	A	106	PRO	3.1
1	A	468	PHE	3.0
1	A	158	ALA	3.0
1	C	295	ALA	3.0
1	A	283	ASN	2.9
1	C	277	HIS	2.9
1	A	120	PRO	2.8
1	C	299	PRO	2.8
1	B	257	GLN	2.8
1	C	120	PRO	2.7
1	A	237	GLY	2.7
1	C	124	LEU	2.7
1	A	155	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	259	GLY	2.6
1	B	468	PHE	2.6
1	A	275	ILE	2.6
1	A	150	LEU	2.6
1	A	299	PRO	2.6
1	D	106	PRO	2.6
1	C	148	GLN	2.5
1	B	141[A]	SER	2.5
1	A	141	SER	2.5
1	C	257	GLN	2.5
1	A	238	ARG	2.5
1	B	255	ARG	2.5
1	C	144	GLN	2.4
1	D	257	GLN	2.4
1	A	140	ARG	2.4
1	B	259	GLY	2.4
1	B	70	ARG	2.4
1	A	144	GLN	2.4
1	D	119	ALA	2.3
1	C	256	GLN	2.3
1	C	275	ILE	2.3
1	A	148	GLN	2.3
1	B	256	GLN	2.3
1	D	237	GLY	2.3
1	C	236	PRO	2.3
1	B	140	ARG	2.3
1	A	160	THR	2.3
1	A	236	PRO	2.2
1	B	258	ASP	2.2
1	A	161	GLY	2.2
1	A	235	CYS	2.2
1	A	480	TRP	2.2
1	B	87	GLN	2.2
1	C	280	THR	2.2
1	A	159	ALA	2.2
1	A	257	GLN	2.2
1	C	258	ASP	2.1
1	D	468	PHE	2.1
1	C	298	GLU	2.1
1	C	160	THR	2.1
1	C	480	TRP	2.1
1	A	157	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	304	LEU	2.0
1	D	258	ASP	2.0
1	C	284	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 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	C	505	14/14	0.60	0.23	69,76,84,88	0
5	BTB	A	505	14/14	0.63	0.25	58,71,76,84	0
5	BTB	B	506	14/14	0.64	0.17	60,67,76,78	0
5	BTB	C	504	14/14	0.71	0.15	70,84,95,100	0
5	BTB	D	505	14/14	0.75	0.19	70,78,92,99	0
5	BTB	B	505	14/14	0.83	0.18	66,76,92,95	0
5	BTB	B	504	14/14	0.89	0.13	30,60,66,70	0
4	9P7	C	503	24/24	0.90	0.11	30,44,54,76	0
7	GOL	C	507	6/6	0.90	0.11	38,51,77,82	0
3	H4B	D	502	17/17	0.91	0.10	29,34,44,45	0
8	GD	C	508	1/1	0.91	0.09	131,131,131,131	0
5	BTB	D	504	14/14	0.92	0.12	15,44,59,66	0
2	HEM	C	501	43/43	0.92	0.10	29,44,58,87	0
4	9P7	A	503	24/24	0.93	0.09	26,38,47,61	0
7	GOL	A	507	6/6	0.93	0.09	42,51,66,66	0
3	H4B	C	502	17/17	0.93	0.10	28,43,59,67	0
3	H4B	A	502	17/17	0.93	0.11	24,45,67,68	0
5	BTB	A	504	14/14	0.94	0.12	15,75,84,96	0
3	H4B	B	502	17/17	0.94	0.10	24,34,43,52	0
4	9P7	D	503	24/24	0.94	0.08	17,30,40,42	0

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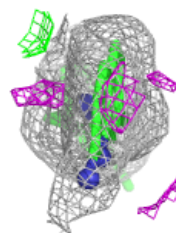
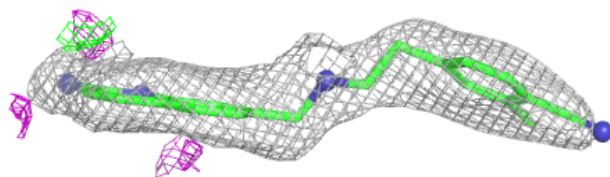
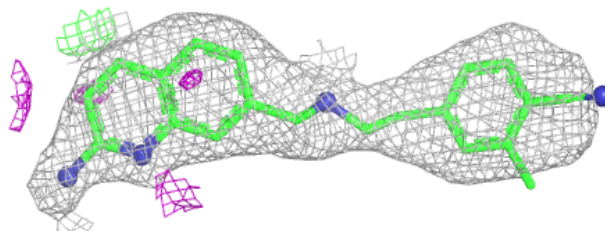
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	GD	A	508	1/1	0.95	0.07	92,92,92,92	0
4	9P7	B	503	24/24	0.95	0.08	22,31,47,56	0
9	CL	A	509	1/1	0.95	0.15	65,65,65,65	0
2	HEM	B	501	43/43	0.96	0.08	12,25,39,65	0
2	HEM	A	501	43/43	0.98	0.07	24,38,47,59	0
2	HEM	D	501	43/43	0.98	0.07	13,23,38,55	0
9	CL	C	509	1/1	0.98	0.15	66,66,66,66	0
9	CL	D	507	1/1	0.98	0.05	37,37,37,37	0
8	GD	B	507	1/1	0.99	0.04	45,45,45,45	0
9	CL	B	508	1/1	0.99	0.04	34,34,34,34	0
6	ZN	C	506	1/1	0.99	0.03	36,36,36,36	0
8	GD	D	506	1/1	0.99	0.04	43,43,43,43	0
6	ZN	A	506	1/1	1.00	0.04	26,26,26,26	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.

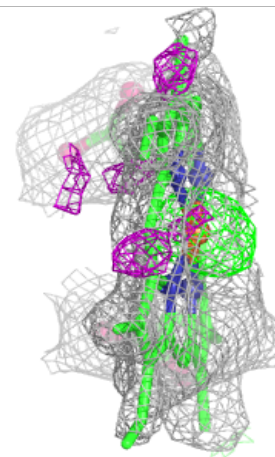
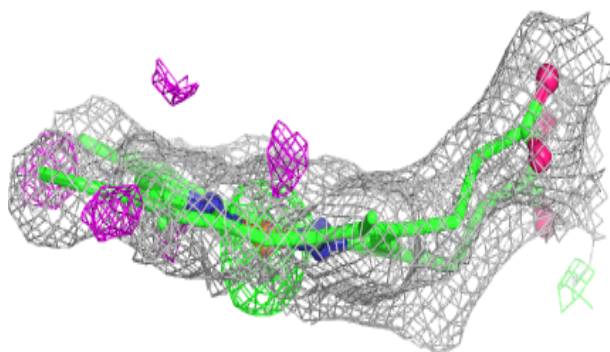
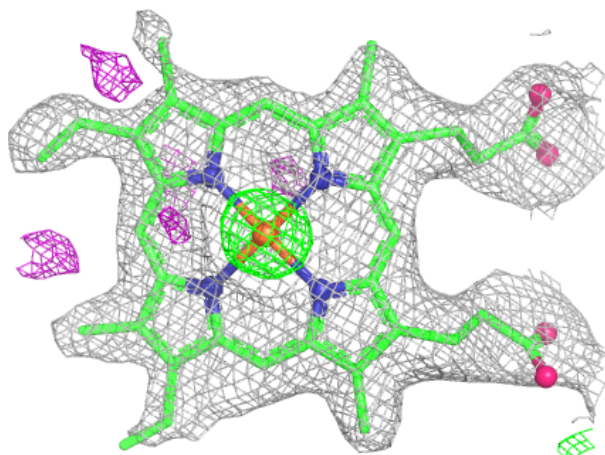
Electron density around 9P7 C 503:

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



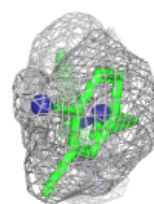
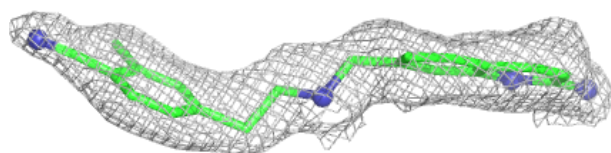
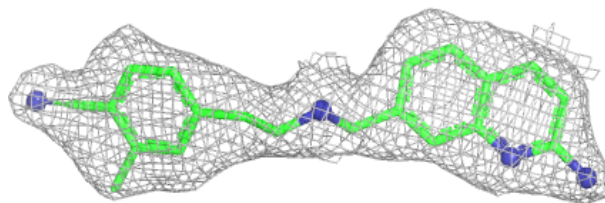
Electron density around HEM C 501:

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

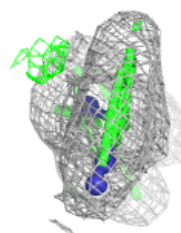
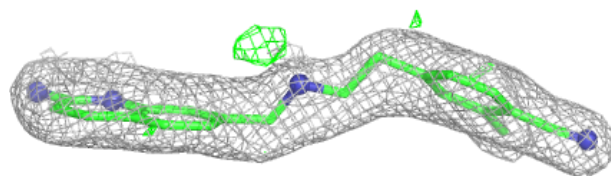
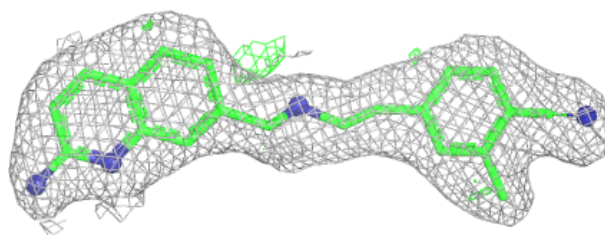


Electron density around 9P7 A 503:

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

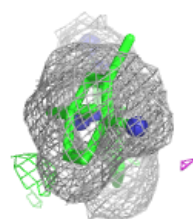
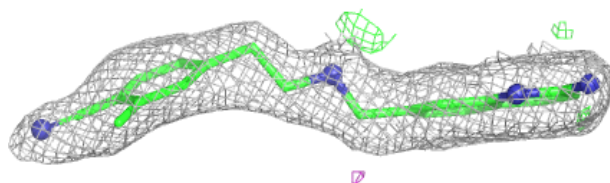
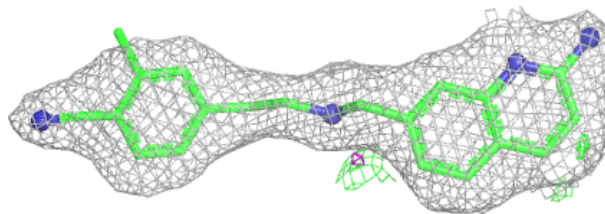
**Electron density around 9P7 D 503:**

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



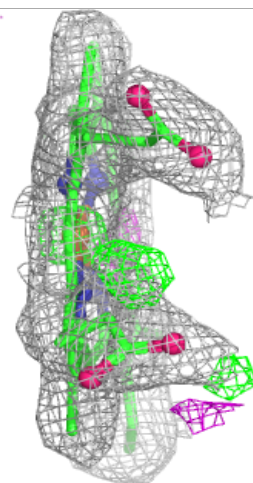
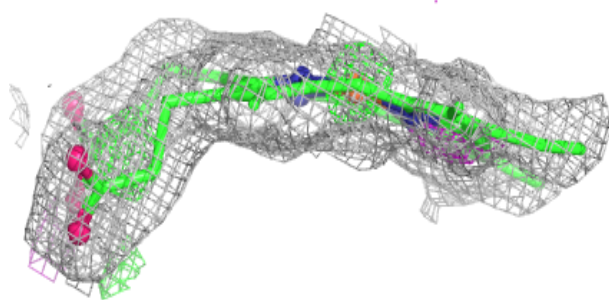
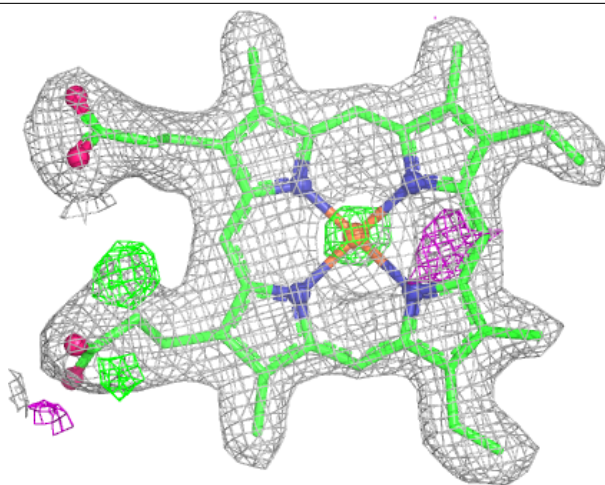
Electron density around 9P7 B 503:

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



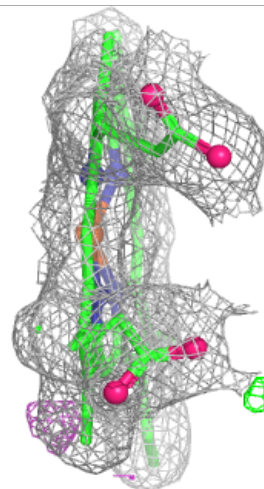
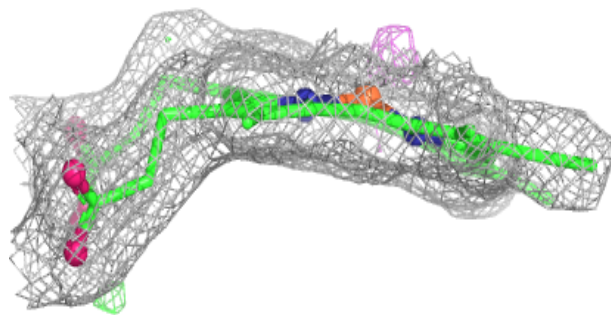
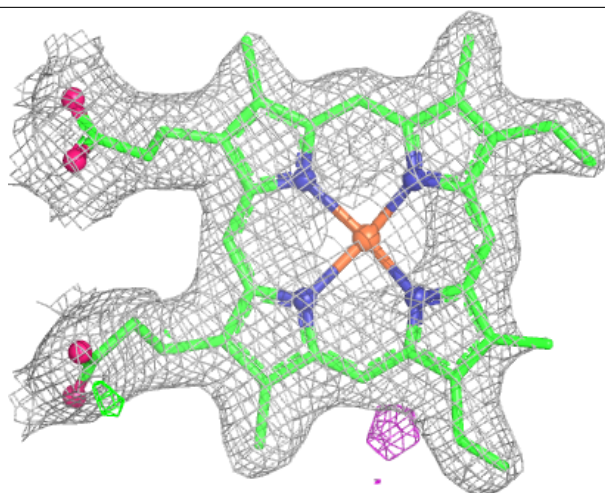
Electron density around HEM B 501:

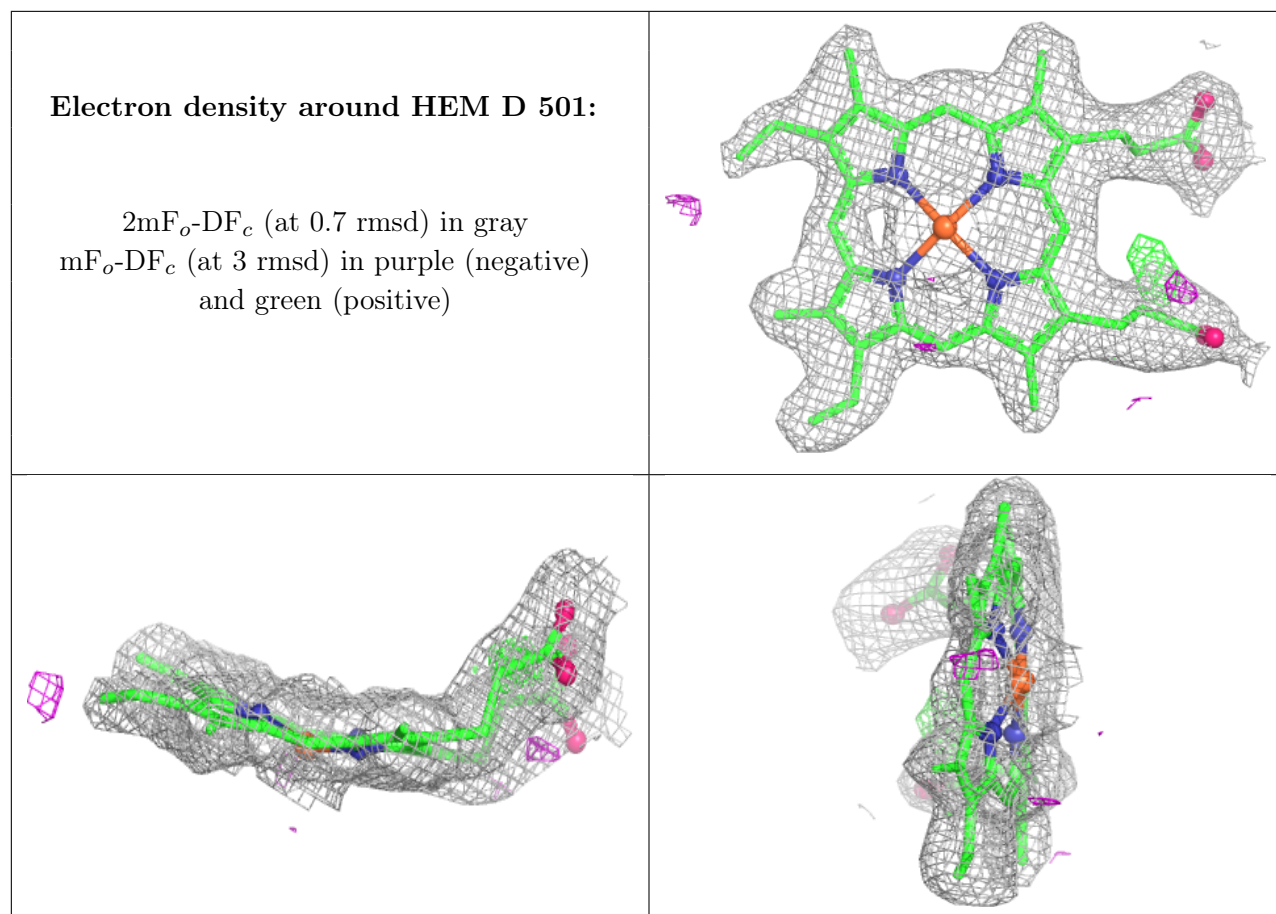
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM A 501:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.