



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:09 PM UTC

PDB ID : 5UO8 / pdb_00005uo8
Title : Structure of human endothelial nitric oxide synthase heme domain in complex with 3-[(2-aminoquinolin-7-yl)methoxy]-5-((methylamino)methyl)benzonitrile
Authors : Chreifi, G.; Li, H.; Poulos, T.L.
Deposited on : 2017-01-31
Resolution : 2.18 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

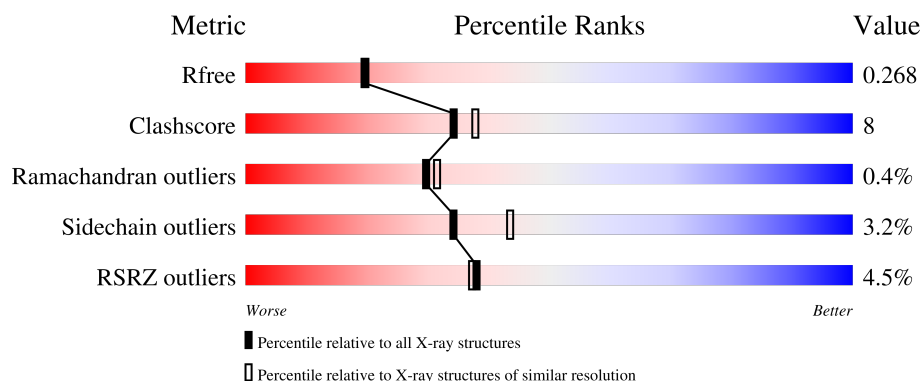
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

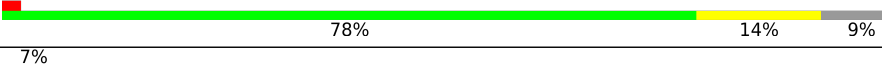
The reported resolution of this entry is 2.18 Å.

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	8975 (2.20-2.16)
Clashscore	190562	9786 (2.20-2.16)
Ramachandran outliers	187476	9664 (2.20-2.16)
Sidechain outliers	187428	9664 (2.20-2.16)
RSRZ outliers	180081	8979 (2.20-2.16)

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	
1	B	440	
1	C	440	
1	D	440	

2 Entry composition [i](#)

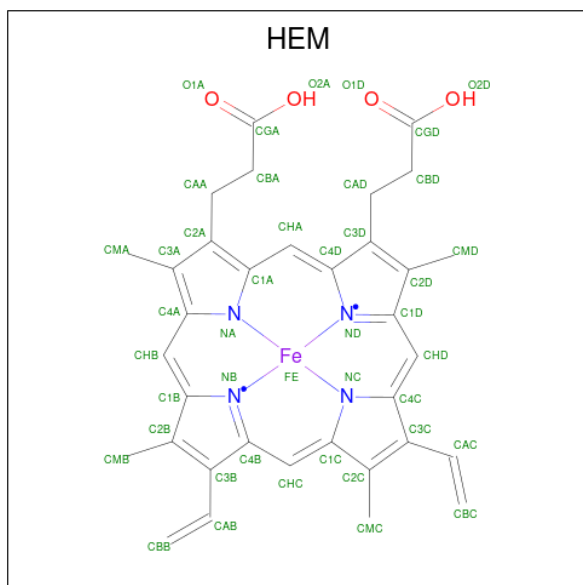
There are 9 unique types of molecules in this entry. The entry contains 13679 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	404	Total	C	N	O	S	0	2	0
			3237	2062	570	589	16			
1	B	402	Total	C	N	O	S	0	3	0
			3221	2051	566	587	17			
1	C	401	Total	C	N	O	S	0	2	0
			3209	2044	563	586	16			
1	D	402	Total	C	N	O	S	0	3	0
			3221	2051	566	587	17			

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



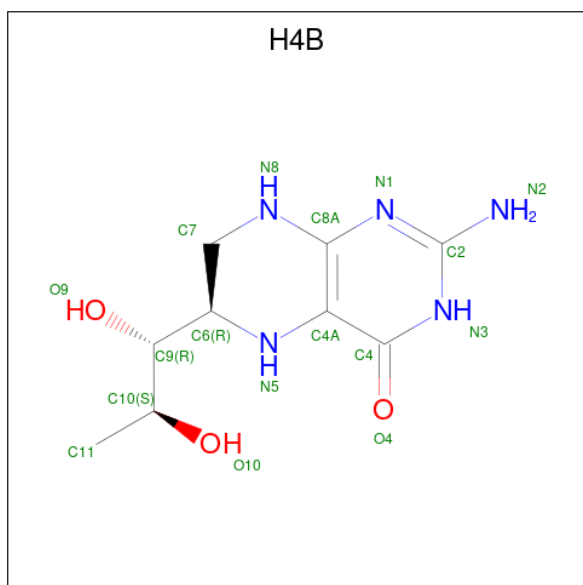
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Fe	N O	0	0
			43	34	1	4 4		
2	B	1	Total	C	Fe	N O	0	0
			43	34	1	4 4		

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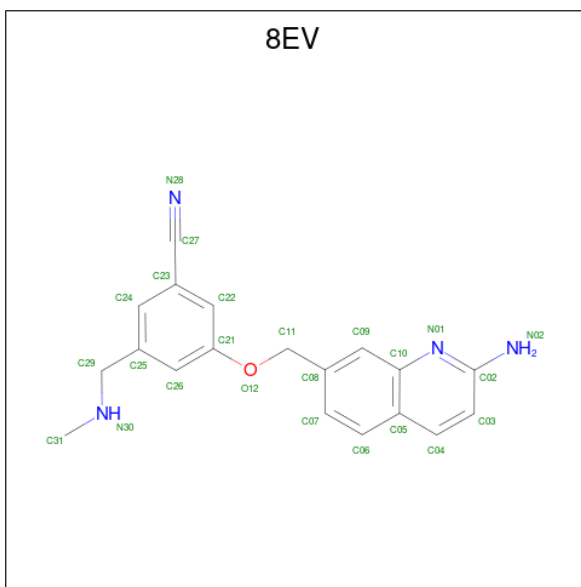
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



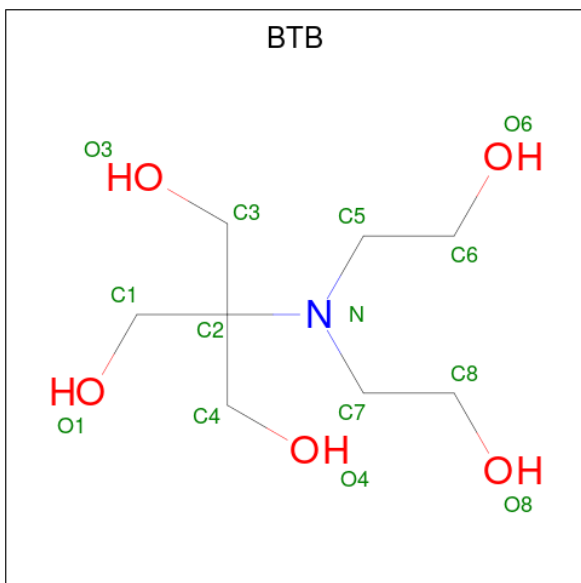
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		
3	C	1	Total	C	N	O	0	0
			17	9	5	3		
3	D	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 4 is 3-[(2-aminoquinolin-7-yl)methoxy]-5-[(methylamino)methyl]benzonitrile (CCD ID: 8EV) (formula: $C_{19}H_{18}N_4O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			24	19	4	1		
4	B	1	Total	C	N	O	0	0
			24	19	4	1		
4	C	1	Total	C	N	O	0	0
			24	19	4	1		
4	D	1	Total	C	N	O	0	0
			24	19	4	1		

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

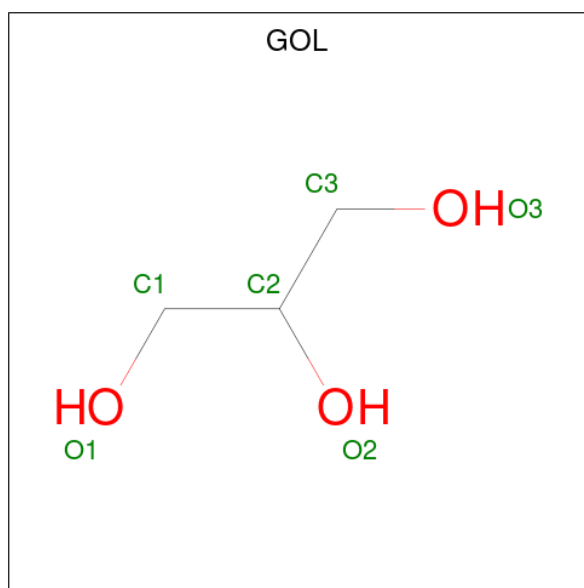


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1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

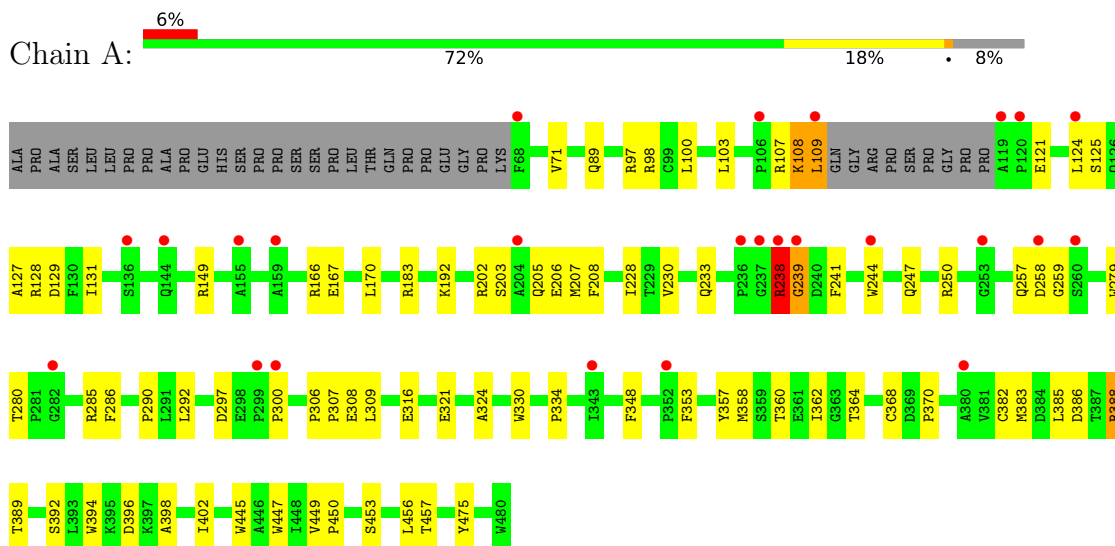
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	61	Total O 61 61	0	0
9	B	99	Total O 99 99	0	0
9	C	68	Total O 68 68	0	0
9	D	97	Total O 97 97	0	0

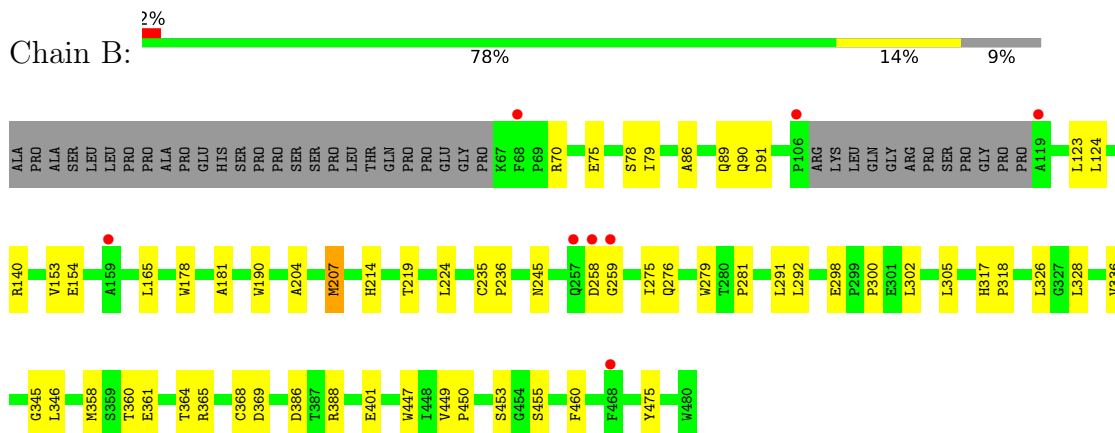
3 Residue-property plots [i](#)

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.

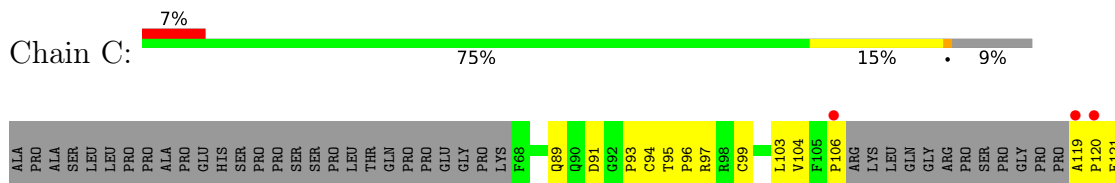
- Molecule 1: Nitric oxide synthase, endothelial



- Molecule 1: Nitric oxide synthase, endothelial

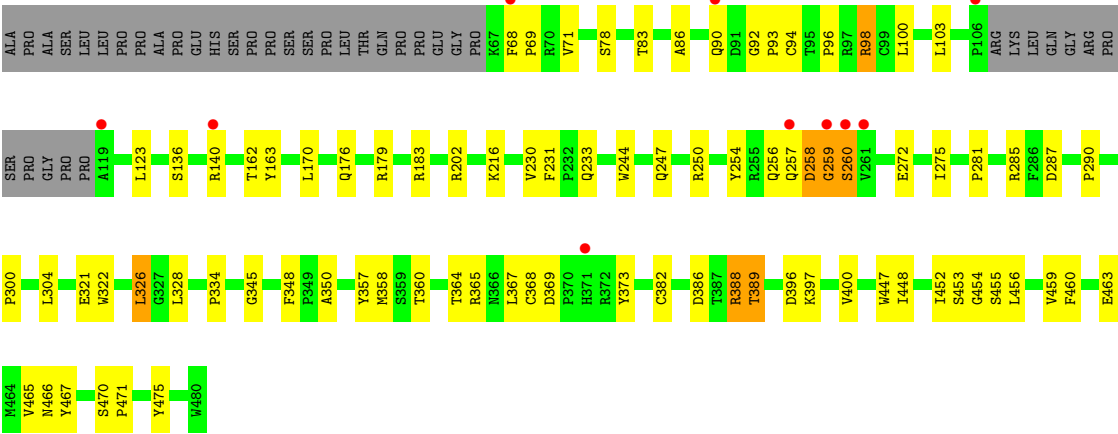


- Molecule 1: Nitric oxide synthase, endothelial





● 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	59.37Å 152.74Å 108.51Å 90.00° 90.74° 90.00°	Depositor
Resolution (Å)	49.53 – 2.18 49.53 – 2.18	Depositor EDS
% Data completeness (in resolution range)	89.4 (49.53-2.18) 89.2 (49.53-2.18)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.18Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.206 , 0.272 0.202 , 0.268	Depositor DCC
R_{free} test set	4512 reflections (2.81%)	wwPDB-VP
Wilson B-factor (Å ²)	30.0	Xtriage
Anisotropy	1.224	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 54.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.065 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13679	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% 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: 8EV, GD, BTB, ZN, GOL, H4B, HEM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.46	0/3335	0.86	4/4543 (0.1%)
1	B	0.51	0/3319	0.84	4/4523 (0.1%)
1	C	0.49	0/3307	0.82	3/4507 (0.1%)
1	D	0.54	0/3319	0.85	1/4523 (0.0%)
All	All	0.50	0/13280	0.84	12/18096 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	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	A	239	GLY	N-CA-C	8.23	123.28	112.25
1	B	259	GLY	N-CA-C	-6.92	106.22	115.21
1	A	259	GLY	N-CA-C	-6.55	106.40	114.92
1	A	207	MET	N-CA-C	-6.52	104.26	111.36
1	C	145	ALA	N-CA-C	-5.86	104.85	112.23
1	A	107	ARG	CB-CA-C	-5.82	109.32	117.23
1	C	295	ALA	CA-C-N	5.72	126.98	119.84
1	C	295	ALA	C-N-CA	5.72	126.98	119.84
1	B	181	ALA	CA-C-N	5.68	125.36	119.56
1	B	181	ALA	C-N-CA	5.68	125.36	119.56
1	B	258	ASP	N-CA-C	-5.21	106.70	113.16
1	D	259	GLY	N-CA-C	-5.14	107.17	115.08

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	138	ILE	Peptide

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	3237	0	3146	50	0
1	B	3221	0	3126	35	0
1	C	3209	0	3109	49	0
1	D	3221	0	3126	54	0
2	A	43	0	30	3	0
2	B	43	0	30	4	0
2	C	43	0	30	3	0
2	D	43	0	30	3	0
3	A	17	0	15	0	0
3	B	17	0	15	1	0
3	C	17	0	15	0	0
3	D	17	0	15	1	0
4	A	24	0	0	0	0
4	B	24	0	0	3	0
4	C	24	0	0	1	0
4	D	24	0	0	0	0
5	A	28	0	38	4	0
5	B	28	0	35	4	0
5	C	28	0	38	5	0
5	D	28	0	36	8	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	1	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	61	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	B	99	0	0	1	0
9	C	68	0	0	3	0
9	D	97	0	0	2	0
All	All	13679	0	12850	199	0

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

All (199) 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:D:176:GLN:HE22	1:D:179:ARG:HH11	1.19	0.89
5:C:504:BTB:O3	5:C:504:BTB:O4	1.95	0.80
1:D:365:ARG:NH2	1:D:369:ASP:OD2	2.17	0.77
1:C:256:GLN:HB3	1:C:257:GLN:HG2	1.67	0.75
2:D:501:HEM:HBB2	2:D:501:HEM:HHC	1.68	0.75
2:A:501:HEM:HBB2	2:A:501:HEM:HHC	1.71	0.71
1:A:97:ARG:HH22	1:B:86:ALA:HA	1.57	0.69
5:D:504:BTB:H82	5:D:504:BTB:O6	1.92	0.69
1:B:292:LEU:HD22	1:B:300:PRO:HB2	1.74	0.68
1:C:235:CYS:H	1:C:238:ARG:HD2	1.59	0.68
1:D:93:PRO:O	1:D:98:ARG:NH2	2.26	0.67
1:D:321:GLU:OE2	5:D:504:BTB:H62	1.94	0.67
1:A:183:ARG:HD3	1:A:447:TRP:CD2	2.30	0.66
1:C:138:ILE:O	1:C:140:ARG:N	2.28	0.66
1:D:386:ASP:OD1	1:D:388:ARG:HB2	1.96	0.66
1:C:236:PRO:HA	1:C:238:ARG:HH11	1.60	0.66
1:A:321:GLU:OE2	9:A:601:HOH:O	2.15	0.65
1:B:279:TRP:HB2	1:B:302:LEU:HD21	1.78	0.65
1:C:384:ASP:OD2	5:C:504:BTB:O3	2.15	0.65
1:A:128:ARG:NH1	1:A:129:ASP:OD1	2.30	0.64
1:C:207:MET:HE3	1:C:293:LEU:HB3	1.79	0.64
1:D:321:GLU:OE2	5:D:504:BTB:O3	2.08	0.64
1:B:365:ARG:NH2	1:B:369:ASP:OD2	2.32	0.63
1:D:397:LYS:NZ	9:D:603:HOH:O	2.31	0.63
2:B:501:HEM:HBC2	2:B:501:HEM:HMC2	1.80	0.62
2:C:501:HEM:O2A	9:C:601:HOH:O	2.16	0.61
1:A:321:GLU:H	1:A:321:GLU:CD	2.08	0.61
1:A:364:THR:O	1:A:368:CYS:HB2	2.01	0.61
5:B:504:BTB:O3	5:B:504:BTB:O4	2.18	0.61
1:B:326:LEU:HB3	1:B:328:LEU:HG	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:CYS:HA	5:A:504:BTB:H11	1.82	0.60
1:B:70:ARG:NH2	9:B:602:HOH:O	2.32	0.59
1:D:176:GLN:NE2	1:D:179:ARG:HH11	1.96	0.59
1:D:258:ASP:HB2	1:D:260:SER:HB3	1.84	0.59
1:D:475:TYR:OH	2:D:501:HEM:O1D	2.16	0.59
1:A:205:GLN:HG3	1:A:206:GLU:HG2	1.85	0.59
1:D:183:ARG:NH1	1:D:475:TYR:OH	2.36	0.59
1:C:207:MET:HG2	1:C:293:LEU:HD13	1.86	0.57
1:C:236:PRO:HA	1:C:238:ARG:NH1	2.19	0.57
1:D:364:THR:O	1:D:368:CYS:HB2	2.04	0.57
1:A:202:ARG:HA	1:A:241:PHE:HZ	1.69	0.56
2:D:501:HEM:HMC2	2:D:501:HEM:HBC2	1.87	0.56
2:B:501:HEM:HHC	2:B:501:HEM:HBB2	1.88	0.56
1:C:167:GLU:OE2	7:C:507:GOL:O2	2.23	0.56
1:A:205:GLN:O	1:A:208:PHE:HB3	2.06	0.55
1:B:70:ARG:HE	1:B:79:ILE:HG21	1.72	0.55
1:C:99:CYS:HB3	1:D:466:ASN:HB3	1.89	0.55
1:C:347:GLU:OE2	9:C:602:HOH:O	2.18	0.54
5:D:505:BTB:O8	5:D:505:BTB:O3	2.21	0.54
1:A:398:ALA:O	1:A:402:ILE:HG13	2.08	0.53
1:C:382:CYS:HA	5:C:504:BTB:H41	1.91	0.53
1:A:292:LEU:HD22	1:A:300:PRO:HB2	1.91	0.53
1:A:170:LEU:HD11	1:A:230:VAL:HG21	1.91	0.52
1:C:138:ILE:HA	1:C:139:LYS:HD2	1.90	0.52
1:A:279:TRP:CG	1:A:290:PRO:HG3	2.44	0.52
1:C:317:HIS:CG	1:C:318:PRO:HD2	2.45	0.52
1:C:463:GLU:HB3	1:D:103:LEU:HD12	1.91	0.52
1:B:178:TRP:CE3	1:B:190:TRP:HA	2.45	0.52
1:D:257:GLN:C	1:D:259:GLY:H	2.18	0.52
1:A:445:TRP:CZ2	1:A:449:VAL:HG21	2.46	0.51
1:C:104:VAL:O	1:C:106:PRO:HD3	2.11	0.51
1:D:100:LEU:HB3	1:D:103:LEU:HD22	1.91	0.51
1:D:258:ASP:OD2	1:D:258:ASP:N	2.44	0.50
1:C:94:CYS:HB3	1:D:94:CYS:HB3	1.92	0.50
1:B:358:MET:HE3	1:B:360:THR:OG1	2.12	0.50
1:D:285:ARG:HD3	9:D:601:HOH:O	2.12	0.49
1:D:275:ILE:HD11	1:D:281:PRO:HB3	1.94	0.49
2:C:501:HEM:HBB2	2:C:501:HEM:HHC	1.95	0.49
1:A:108:LYS:O	1:A:109:LEU:HB2	2.12	0.49
1:A:370:PRO:HG2	1:B:75:GLU:HG3	1.95	0.49
1:B:275:ILE:HD11	1:B:281:PRO:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:386:ASP:OD1	1:B:388:ARG:HG2	2.12	0.48
1:B:475:TYR:OH	2:B:501:HEM:O1D	2.29	0.48
1:D:455:SER:HA	1:D:460:PHE:CG	2.48	0.48
1:D:321:GLU:CD	5:D:504:BTB:H62	2.39	0.48
1:A:228:ILE:HG13	1:A:353:PHE:HB3	1.96	0.48
1:A:167:GLU:OE2	7:A:507:GOL:O1	2.21	0.47
1:A:247:GLN:HB2	1:A:250:ARG:HG2	1.96	0.47
1:A:257:GLN:NE2	1:A:258:ASP:OD1	2.48	0.47
1:A:330:TRP:CD1	1:A:362:ILE:HG12	2.50	0.47
1:B:364:THR:O	1:B:368:CYS:HB2	2.15	0.47
1:C:93:PRO:HG3	1:C:106:PRO:HB3	1.96	0.47
1:C:317:HIS:CD2	1:C:318:PRO:HD2	2.49	0.47
1:D:247:GLN:HB2	1:D:250:ARG:HG2	1.97	0.47
1:B:336:VAL:HG21	4:B:503:8EV:C07	2.44	0.47
1:A:285:ARG:HG3	1:A:286:PHE:CD2	2.50	0.47
1:B:124:LEU:HD21	1:B:154:GLU:HA	1.96	0.47
1:C:233:GLN:HB3	1:C:348:PHE:CE2	2.50	0.47
5:C:505:BTB:H11	5:C:505:BTB:H71	1.47	0.46
1:D:326:LEU:HB3	1:D:328:LEU:HG	1.97	0.46
1:A:125:SER:O	1:A:128:ARG:HG2	2.15	0.46
1:B:317:HIS:NE2	1:B:401:GLU:OE1	2.41	0.46
1:A:334:PRO:HB3	1:A:357:TYR:CZ	2.50	0.46
1:D:231:PHE:HB2	1:D:350:ALA:O	2.15	0.46
1:A:392:SER:OG	1:A:394:TRP:HD1	1.98	0.46
1:C:120:PRO:HA	1:C:123:LEU:HB3	1.97	0.46
1:B:298:GLU:CD	5:B:505:BTB:H32	2.41	0.45
1:D:244:TRP:CH2	1:D:300:PRO:HG3	2.51	0.45
1:A:308:GLU:H	1:A:308:GLU:CD	2.24	0.45
1:C:291:LEU:HB3	1:C:293:LEU:HD21	1.98	0.45
5:C:504:BTB:H62	5:C:504:BTB:H31	1.98	0.45
1:C:97:ARG:NH2	1:D:86:ALA:HA	2.32	0.45
1:D:448:ILE:HG22	1:D:459:VAL:HG21	1.98	0.45
1:B:292:LEU:HD23	1:B:292:LEU:HA	1.76	0.45
1:C:358:MET:HE1	9:C:612:HOH:O	2.17	0.45
1:C:91:ASP:HB3	1:D:96:PRO:HB3	1.98	0.45
1:D:68:PHE:CD2	1:D:83:THR:HA	2.51	0.45
1:A:233:GLN:HB3	1:A:348:PHE:CE2	2.52	0.44
1:C:247:GLN:HB2	1:C:250:ARG:HG2	1.99	0.44
1:C:364:THR:O	1:C:368:CYS:HB2	2.17	0.44
1:B:447:TRP:HA	3:B:502:H4B:N1	2.32	0.44
1:A:239:GLY:N	1:A:297:ASP:OD2	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:103:LEU:HA	1:D:463:GLU:HG2	1.99	0.44
1:A:453:SER:HB3	1:A:456:LEU:HD12	2.00	0.44
1:A:183:ARG:HB2	2:A:501:HEM:HAD2	1.99	0.44
1:A:383:MET:HB2	1:A:385:LEU:HG	1.99	0.44
1:C:359:SER:OG	1:C:419:ASP:HA	2.17	0.44
1:B:123:LEU:HD12	1:B:345:GLY:HA3	2.00	0.44
1:C:235:CYS:HB2	1:C:238:ARG:HB3	1.99	0.44
1:A:244:TRP:HB2	1:A:292:LEU:HB3	2.00	0.44
1:A:475:TYR:OH	2:A:501:HEM:O1D	2.32	0.44
1:B:214:HIS:CD2	1:B:214:HIS:C	2.96	0.44
5:B:504:BTB:H71	5:B:504:BTB:H42	1.41	0.43
1:B:298:GLU:OE2	5:B:505:BTB:N	2.51	0.43
1:D:334:PRO:HB3	1:D:357:TYR:CZ	2.54	0.43
1:A:285:ARG:H	1:A:285:ARG:HG2	1.58	0.43
1:B:219:THR:O	1:B:224:LEU:HD12	2.18	0.43
1:C:138:ILE:CA	1:C:139:LYS:HD2	2.48	0.43
1:D:290:PRO:HB3	1:D:304:LEU:HD23	2.00	0.43
1:D:388:ARG:HB3	1:D:389:THR:HG22	1.99	0.43
1:A:306:PRO:HA	1:A:307:PRO:HD3	1.91	0.43
1:D:453:SER:HB3	1:D:456:LEU:HD12	2.00	0.43
5:A:504:BTB:H42	5:A:504:BTB:H71	1.74	0.43
1:D:123:LEU:HD12	1:D:345:GLY:HA3	2.01	0.43
1:D:162:THR:OG1	1:D:163:TYR:N	2.52	0.43
1:D:170:LEU:HD11	1:D:230:VAL:HG11	2.01	0.43
1:D:233:GLN:HB3	1:D:348:PHE:CE2	2.54	0.43
5:D:505:BTB:H42	5:D:505:BTB:H71	1.46	0.43
1:A:316[B]:GLU:HG2	1:A:324:ALA:HB2	2.01	0.43
1:C:233:GLN:HG3	1:C:234:ARG:O	2.19	0.43
1:C:341:LEU:HB3	1:C:348:PHE:HB2	2.01	0.43
1:C:347:GLU:O	1:C:349:PRO:HD3	2.19	0.43
5:D:505:BTB:H11	5:D:505:BTB:H52	1.66	0.43
2:B:501:HEM:HBA2	4:B:503:8EV:C09	2.48	0.42
1:A:358:MET:HE3	1:A:360:THR:OG1	2.19	0.42
1:B:165:LEU:HG	1:B:346:LEU:HD12	2.00	0.42
1:C:387:THR:HA	1:C:394:TRP:CD1	2.55	0.42
1:C:358:MET:HE3	1:C:360:THR:OG1	2.19	0.42
1:D:322:TRP:CH2	1:D:382:CYS:HB3	2.55	0.42
1:A:247:GLN:HB2	1:A:250:ARG:CG	2.50	0.42
5:A:505:BTB:H52	5:A:505:BTB:H31	1.72	0.42
1:C:365:ARG:NH2	1:C:369:ASP:OD2	2.52	0.42
1:A:100:LEU:HB3	1:A:103:LEU:HD22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:CYS:HA	5:A:504:BTB:C1	2.50	0.42
1:D:254:TYR:OH	1:D:287:ASP:OD2	2.35	0.42
1:A:238:ARG:HD2	1:A:238:ARG:HA	1.53	0.42
1:D:68:PHE:HA	1:D:69:PRO:HD3	1.92	0.42
1:D:367:LEU:HA	1:D:373:TYR:HB2	2.01	0.42
1:A:192:LYS:HE3	1:A:192:LYS:HB2	1.85	0.42
1:A:386:ASP:OD2	1:A:388:ARG:HB2	2.19	0.42
1:B:245:ASN:OD1	1:B:291:LEU:HA	2.20	0.42
1:D:447:TRP:HA	3:D:502:H4B:N1	2.35	0.42
1:B:361:GLU:OE2	4:B:503:8EV:N02	2.53	0.41
1:C:119:ALA:HA	1:C:120:PRO:HD3	1.81	0.41
1:B:90:GLN:HG2	1:B:91:ASP:H	1.85	0.41
1:D:358:MET:HE3	1:D:360:THR:OG1	2.21	0.41
1:C:256:GLN:O	1:C:258:ASP:N	2.53	0.41
2:C:501:HEM:HBA1	4:C:503:8EV:C09	2.50	0.41
1:D:470:SER:HA	1:D:471:PRO:C	2.45	0.41
1:D:256:GLN:N	1:D:260:SER:O	2.50	0.41
1:D:465:VAL:HG12	1:D:467:TYR:HD1	1.86	0.41
1:A:127:ALA:O	1:A:131:ILE:HG12	2.21	0.41
1:B:235[B]:CYS:HA	1:B:236:PRO:HD3	1.93	0.41
1:A:149:ARG:HD3	1:A:166:ARG:CZ	2.50	0.41
1:A:445:TRP:CE2	1:A:449:VAL:HG21	2.56	0.41
1:B:317:HIS:CG	1:B:318:PRO:HD2	2.56	0.41
1:D:455:SER:HA	1:D:460:PHE:CB	2.51	0.41
1:C:194:GLN:HG2	1:C:217:TYR:CZ	2.56	0.41
1:D:396:ASP:O	1:D:400:VAL:HG23	2.21	0.41
1:B:291:LEU:HD11	1:B:305:LEU:HD21	2.03	0.41
1:B:455:SER:HA	1:B:460:PHE:CG	2.56	0.41
5:D:504:BTB:H42	5:D:504:BTB:H71	1.85	0.41
1:C:89:GLN:OE1	1:C:470:SER:HB2	2.21	0.41
1:C:183:ARG:HD3	1:C:447:TRP:CD2	2.56	0.41
1:C:235:CYS:H	1:C:238:ARG:CD	2.30	0.41
1:C:235:CYS:C	1:C:238:ARG:HD3	2.45	0.41
1:C:455:SER:HA	1:C:460:PHE:CG	2.56	0.41
1:B:204:ALA:HA	1:B:207:MET:HB2	2.02	0.41
1:C:214:HIS:CD2	1:C:214:HIS:C	2.99	0.41
1:D:364:THR:HG21	1:D:452:ILE:HG23	2.02	0.41
1:D:454:GLY:O	1:D:460:PHE:HB2	2.20	0.41
1:C:96:PRO:O	1:D:92:GLY:N	2.46	0.40
1:A:396:ASP:OD2	1:B:453:SER:OG	2.31	0.40
1:A:450:PRO:HG2	1:A:457:THR:HG21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:ARG:HG3	1:A:286:PHE:HD2	1.86	0.40
1:C:95:THR:HB	1:C:96:PRO:HD2	2.03	0.40
1:D:257:GLN:C	1:D:259:GLY:N	2.80	0.40
1:B:449:VAL:HA	1:B:450:PRO:HD3	1.95	0.40
1:C:157:VAL:HG23	1:C:163:TYR:HB3	2.04	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	402/440 (91%)	385 (96%)	14 (4%)	3 (1%)	18	17
1	B	401/440 (91%)	387 (96%)	14 (4%)	0	100	100
1	C	399/440 (91%)	375 (94%)	21 (5%)	3 (1%)	16	14
1	D	401/440 (91%)	388 (97%)	12 (3%)	1 (0%)	43	49
All	All	1603/1760 (91%)	1535 (96%)	61 (4%)	7 (0%)	30	31

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	257	GLN
1	A	89	GLN
1	A	238	ARG
1	D	388	ARG
1	A	108	LYS
1	C	235	CYS
1	C	236	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	345/373 (92%)	334 (97%)	11 (3%)	34	43
1	B	344/373 (92%)	338 (98%)	6 (2%)	53	66
1	C	342/373 (92%)	329 (96%)	13 (4%)	29	37
1	D	344/373 (92%)	331 (96%)	13 (4%)	29	37
All	All	1375/1492 (92%)	1332 (97%)	43 (3%)	34	45

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

Mol	Chain	Res	Type
1	A	71	VAL
1	A	98	ARG
1	A	109	LEU
1	A	121	GLU
1	A	124	LEU
1	A	203	SER
1	A	238	ARG
1	A	280	THR
1	A	309	LEU
1	A	388	ARG
1	A	389	THR
1	B	78	SER
1	B	89	GLN
1	B	140	ARG
1	B	153	VAL
1	B	207	MET
1	B	276	GLN
1	C	121	GLU
1	C	133	GLN
1	C	138	ILE
1	C	140	ARG
1	C	151	GLN
1	C	160	THR
1	C	192	LYS

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Mol	Chain	Res	Type
1	C	200	ASP
1	C	258	ASP
1	C	292	LEU
1	C	309	LEU
1	C	359	SER
1	C	388	ARG
1	D	71	VAL
1	D	78	SER
1	D	90	GLN
1	D	98	ARG
1	D	136	SER
1	D	140	ARG
1	D	202	ARG
1	D	216	LYS
1	D	258	ASP
1	D	260	SER
1	D	272	GLU
1	D	326	LEU
1	D	389	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	151	GLN
1	B	213	ASN
1	B	267	ASN
1	C	189	GLN
1	C	194	GLN
1	C	403	ASN
1	D	176	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 6 are monoatomic - leaving 22 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	C	505	-	13,13,13	0.62	0	7,16,16	1.47	2 (28%)
2	HEM	B	501	1	50,50,50	2.15	9 (18%)	67,82,82	1.60	11 (16%)
4	8EV	B	503	-	26,26,26	1.70	2 (7%)	33,35,35	0.80	0
5	BTB	A	504	8	13,13,13	0.47	0	7,16,16	1.07	1 (14%)
7	GOL	A	507	-	5,5,5	0.32	0	5,5,5	0.50	0
4	8EV	D	503	-	26,26,26	1.63	2 (7%)	33,35,35	0.95	3 (9%)
5	BTB	B	505	-	13,13,13	0.47	0	7,16,16	0.48	0
3	H4B	D	502	-	17,18,18	0.78	0	14,26,26	1.86	5 (35%)
5	BTB	D	504	8	13,13,13	0.53	0	7,16,16	0.28	0
3	H4B	B	502	-	17,18,18	0.90	0	14,26,26	1.86	4 (28%)
5	BTB	D	505	-	13,13,13	0.42	0	7,16,16	1.42	1 (14%)
5	BTB	A	505	-	13,13,13	0.40	0	7,16,16	0.84	0
2	HEM	C	501	1	50,50,50	2.18	9 (18%)	67,82,82	1.41	10 (14%)
5	BTB	C	504	8	13,13,13	0.58	0	7,16,16	0.60	0
3	H4B	A	502	-	17,18,18	0.78	0	14,26,26	1.89	5 (35%)
2	HEM	D	501	1	50,50,50	2.16	9 (18%)	67,82,82	1.51	10 (14%)
2	HEM	A	501	1	50,50,50	2.04	10 (20%)	67,82,82	1.47	7 (10%)
3	H4B	C	502	-	17,18,18	0.78	0	14,26,26	1.81	4 (28%)
7	GOL	C	507	-	5,5,5	0.47	0	5,5,5	0.79	0
4	8EV	A	503	-	26,26,26	1.74	1 (3%)	33,35,35	0.82	1 (3%)
4	8EV	C	503	-	26,26,26	1.74	1 (3%)	33,35,35	0.90	0
5	BTB	B	504	8	13,13,13	0.65	0	7,16,16	0.57	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BTB	C	505	-	-	14/21/21/21	-
2	HEM	B	501	1	-	2/14/54/54	-
4	8EV	B	503	-	-	2/10/19/19	0/3/3/3
5	BTB	A	504	8	-	4/21/21/21	-
7	GOL	A	507	-	-	4/4/4/4	-
4	8EV	D	503	-	-	0/10/19/19	0/3/3/3
5	BTB	B	505	-	-	10/21/21/21	-
3	H4B	D	502	-	-	3/8/17/17	0/2/2/2
5	BTB	D	504	8	-	1/21/21/21	-
3	H4B	B	502	-	-	2/8/17/17	0/2/2/2
5	BTB	D	505	-	-	11/21/21/21	-
5	BTB	A	505	-	-	8/21/21/21	-
2	HEM	C	501	1	-	3/14/54/54	-
5	BTB	C	504	8	-	4/21/21/21	-
3	H4B	A	502	-	-	1/8/17/17	0/2/2/2
2	HEM	D	501	1	-	1/14/54/54	-
2	HEM	A	501	1	-	1/14/54/54	-
3	H4B	C	502	-	-	3/8/17/17	0/2/2/2
7	GOL	C	507	-	-	2/4/4/4	-
4	8EV	A	503	-	-	0/10/19/19	0/3/3/3
4	8EV	C	503	-	-	1/10/19/19	0/3/3/3
5	BTB	B	504	8	-	10/21/21/21	-

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	HEM	C3D-C2D	7.81	1.53	1.36
2	C	501	HEM	FE-NB	7.79	2.18	1.94
4	C	503	8EV	C23-C27	-7.53	1.28	1.44
2	C	501	HEM	C3D-C2D	7.52	1.53	1.36
2	A	501	HEM	C3D-C2D	7.45	1.52	1.36
4	A	503	8EV	C23-C27	-7.41	1.28	1.44
4	B	503	8EV	C23-C27	-7.40	1.28	1.44
2	D	501	HEM	C3D-C2D	7.31	1.52	1.36
4	D	503	8EV	C23-C27	-7.29	1.29	1.44
2	D	501	HEM	FE-ND	6.71	2.15	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	HEM	FE-NC	6.30	2.16	1.95
2	C	501	HEM	FE-NC	6.05	2.15	1.95
2	D	501	HEM	FE-NC	5.76	2.14	1.95
2	A	501	HEM	FE-NB	5.66	2.12	1.94
2	B	501	HEM	FE-NB	5.64	2.12	1.94
2	D	501	HEM	FE-NB	5.52	2.11	1.94
2	A	501	HEM	FE-ND	5.42	2.11	1.94
2	A	501	HEM	FE-NC	5.34	2.12	1.95
2	B	501	HEM	FE-ND	5.13	2.10	1.94
2	B	501	HEM	FE-NA	3.87	2.07	1.95
2	C	501	HEM	CAB-C3B	3.35	1.56	1.47
2	B	501	HEM	CAC-C3C	3.18	1.55	1.47
2	D	501	HEM	CAC-C3C	3.16	1.55	1.47
2	C	501	HEM	FE-ND	3.15	2.04	1.94
2	B	501	HEM	CAB-C3B	3.11	1.55	1.47
2	D	501	HEM	CAB-C3B	3.07	1.55	1.47
2	C	501	HEM	CAC-C3C	3.06	1.55	1.47
2	A	501	HEM	CAC-C3C	2.93	1.55	1.47
2	A	501	HEM	CAB-C3B	2.87	1.55	1.47
2	C	501	HEM	FE-NA	2.76	2.04	1.95
2	D	501	HEM	FE-NA	2.66	2.03	1.95
2	C	501	HEM	CMB-C2B	2.51	1.55	1.50
2	A	501	HEM	FE-NA	2.40	2.03	1.95
2	A	501	HEM	CMB-C2B	2.23	1.55	1.50
2	A	501	HEM	C2A-C3A	-2.18	1.33	1.38
2	D	501	HEM	CMB-C2B	2.17	1.55	1.50
2	D	501	HEM	CMA-C3A	2.16	1.55	1.50
4	B	503	8EV	C09-C10	-2.11	1.38	1.41
2	A	501	HEM	CMC-C2C	2.10	1.55	1.50
2	C	501	HEM	CMC-C2C	2.09	1.55	1.50
4	D	503	8EV	C04-C03	2.08	1.41	1.36
2	B	501	HEM	CMB-C2B	2.01	1.54	1.50
2	B	501	HEM	CMC-C2C	2.01	1.54	1.50

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	HEM	C4D-ND-C1D	5.96	112.26	105.21
2	A	501	HEM	C4D-ND-C1D	5.80	112.08	105.21
2	C	501	HEM	C4D-ND-C1D	5.41	111.62	105.21
2	D	501	HEM	C4D-ND-C1D	5.22	111.39	105.21
3	A	502	H4B	C2-N1-C8A	4.20	120.77	113.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	502	H4B	C2-N1-C8A	4.13	120.65	113.36
3	B	502	H4B	C2-N1-C8A	4.11	120.61	113.36
3	C	502	H4B	C2-N1-C8A	4.08	120.56	113.36
2	B	501	HEM	C3B-C4B-NB	-3.47	106.98	109.47
2	D	501	HEM	C3B-C2B-C1B	3.29	108.88	106.41
2	B	501	HEM	C3B-C2B-C1B	3.23	108.84	106.41
2	A	501	HEM	CAD-C3D-C4D	3.19	130.25	124.70
2	D	501	HEM	CBA-CAA-C2A	-3.18	103.75	112.53
2	B	501	HEM	C1B-NB-C4B	3.15	108.94	105.21
2	B	501	HEM	CHA-C4D-ND	3.15	128.26	124.37
2	A	501	HEM	CBA-CAA-C2A	-3.02	104.17	112.53
2	D	501	HEM	C2A-C1A-NA	-2.95	106.88	110.15
2	A	501	HEM	C2A-C1A-NA	-2.92	106.91	110.15
5	C	505	BTB	O4-C4-C2	-2.89	104.62	111.40
5	D	505	BTB	O3-C3-C2	-2.87	104.66	111.40
2	C	501	HEM	CAD-CBD-CGD	-2.87	106.06	113.67
3	C	502	H4B	O4-C4-C4A	-2.81	120.50	127.26
3	B	502	H4B	O4-C4-C4A	-2.74	120.65	127.26
2	D	501	HEM	C1B-NB-C4B	2.72	108.42	105.21
3	B	502	H4B	C4A-C4-N3	2.67	119.47	112.13
3	D	502	H4B	C4A-C4-N3	2.66	119.42	112.13
3	A	502	H4B	C4A-C4-N3	2.63	119.36	112.13
2	D	501	HEM	CMD-C2D-C1D	2.62	129.14	125.03
2	C	501	HEM	C3B-C4B-NB	-2.52	107.66	109.47
3	C	502	H4B	C4A-C4-N3	2.50	118.99	112.13
2	A	501	HEM	C3B-C2B-C1B	2.50	108.29	106.41
2	C	501	HEM	C2A-C1A-NA	-2.42	107.47	110.15
5	A	504	BTB	O4-C4-C2	2.39	117.02	111.40
2	B	501	HEM	C2B-C1B-NB	-2.36	107.12	109.84
3	D	502	H4B	C4-C4A-N5	2.34	122.65	116.27
2	C	501	HEM	C3B-C2B-C1B	2.33	108.16	106.41
2	D	501	HEM	C2B-C1B-NB	-2.30	107.20	109.84
2	D	501	HEM	C4A-NA-C1A	2.29	109.55	105.82
3	A	502	H4B	C4-C4A-N5	2.28	122.48	116.27
3	B	502	H4B	N3-C2-N1	-2.27	119.16	123.32
3	A	502	H4B	O4-C4-C4A	-2.26	121.81	127.26
2	D	501	HEM	C3B-C4B-NB	-2.26	107.84	109.47
2	B	501	HEM	CBA-CAA-C2A	-2.25	106.32	112.53
4	D	503	8EV	C03-C02-N01	-2.23	119.42	122.09
4	D	503	8EV	C11-O12-C21	2.22	122.91	117.62
2	B	501	HEM	C4C-NC-C1C	2.21	109.43	105.82
3	D	502	H4B	O4-C4-C4A	-2.18	122.00	127.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	HEM	C3A-C4A-NA	-2.18	106.65	110.14
2	D	501	HEM	CHA-C1A-NA	2.17	127.80	123.86
3	C	502	H4B	N3-C2-N1	-2.14	119.41	123.32
2	C	501	HEM	C1B-NB-C4B	2.12	107.71	105.21
4	A	503	8EV	C03-C02-N01	-2.10	119.58	122.09
2	C	501	HEM	CMD-C2D-C1D	2.09	128.30	125.03
2	C	501	HEM	CAA-C2A-C1A	2.09	129.01	124.94
2	A	501	HEM	C1B-NB-C4B	2.07	107.66	105.21
3	D	502	H4B	C2-N3-C4	-2.07	121.36	125.11
2	A	501	HEM	CMD-C2D-C1D	2.06	128.25	125.03
3	A	502	H4B	C2-N3-C4	-2.05	121.40	125.11
2	B	501	HEM	C2A-C1A-NA	-2.05	107.88	110.15
4	D	503	8EV	C23-C27-N28	-2.04	172.84	177.87
2	C	501	HEM	CAB-C3B-C2B	-2.03	121.84	128.43
5	C	505	BTB	O1-C1-C2	-2.02	106.66	111.40
2	B	501	HEM	C2D-C1D-ND	-2.02	107.57	109.90
2	C	501	HEM	CHA-C4D-ND	2.00	126.84	124.37

There are no chirality outliers.

All (87) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	502	H4B	C7-C6-C9-O9
3	D	502	H4B	C7-C6-C9-C10
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	505	BTB	C1-C2-C4-O4
5	A	505	BTB	C3-C2-C4-O4
5	A	505	BTB	N-C2-C4-O4
5	B	504	BTB	O1-C1-C2-N
5	B	504	BTB	C1-C2-C4-O4
5	B	505	BTB	C1-C2-C4-O4
5	B	505	BTB	C3-C2-C4-O4
5	B	505	BTB	N-C2-C4-O4
5	B	505	BTB	C1-C2-N-C5
5	B	505	BTB	C1-C2-N-C7
5	B	505	BTB	C3-C2-N-C5
5	B	505	BTB	C3-C2-N-C7
5	B	505	BTB	C4-C2-N-C5
5	B	505	BTB	C4-C2-N-C7
5	C	504	BTB	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
5	C	504	BTB	C4-C2-C3-O3
5	C	504	BTB	N-C2-C3-O3
5	C	505	BTB	O1-C1-C2-C3
5	C	505	BTB	O1-C1-C2-N
5	C	505	BTB	C1-C2-C4-O4
5	C	505	BTB	C3-C2-C4-O4
5	C	505	BTB	N-C2-C4-O4
5	C	505	BTB	C1-C2-N-C5
5	C	505	BTB	C1-C2-N-C7
5	C	505	BTB	C3-C2-N-C5
5	C	505	BTB	C4-C2-N-C5
5	C	505	BTB	C4-C2-N-C7
5	D	505	BTB	C4-C2-C3-O3
5	D	505	BTB	C1-C2-N-C5
5	D	505	BTB	C1-C2-N-C7
5	D	505	BTB	C3-C2-N-C5
5	D	505	BTB	C3-C2-N-C7
5	D	505	BTB	C4-C2-N-C5
5	D	505	BTB	C4-C2-N-C7
7	A	507	GOL	O1-C1-C2-C3
7	A	507	GOL	C1-C2-C3-O3
7	C	507	GOL	C1-C2-C3-O3
2	C	501	HEM	C1A-C2A-CAA-CBA
7	A	507	GOL	O2-C2-C3-O3
7	C	507	GOL	O2-C2-C3-O3
5	D	505	BTB	N-C7-C8-O8
7	A	507	GOL	O1-C1-C2-O2
4	B	503	8EV	C22-C21-O12-C11
5	B	504	BTB	N-C7-C8-O8
4	B	503	8EV	C26-C21-O12-C11
5	B	504	BTB	N-C5-C6-O6
5	B	504	BTB	O1-C1-C2-C3
5	B	505	BTB	N-C5-C6-O6
5	C	504	BTB	N-C7-C8-O8
2	C	501	HEM	C3A-C2A-CAA-CBA
5	D	505	BTB	N-C5-C6-O6
2	A	501	HEM	C4B-C3B-CAB-CBB
2	C	501	HEM	C4B-C3B-CAB-CBB
2	D	501	HEM	C4B-C3B-CAB-CBB
5	D	504	BTB	N-C7-C8-O8
3	D	502	H4B	N5-C6-C9-O9
5	A	505	BTB	C1-C2-N-C5

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Mol	Chain	Res	Type	Atoms
5	A	505	BTB	C1-C2-N-C7
5	A	505	BTB	C3-C2-N-C5
5	A	505	BTB	C4-C2-N-C7
5	B	504	BTB	N-C2-C4-O4
5	B	504	BTB	C1-C2-N-C7
5	B	504	BTB	C4-C2-N-C7
5	C	505	BTB	C3-C2-N-C7
5	D	505	BTB	O1-C1-C2-N
3	C	502	H4B	C7-C6-C9-C10
5	B	504	BTB	C1-C2-C3-O3
3	C	502	H4B	C7-C6-C9-O9
5	C	505	BTB	N-C5-C6-O6
5	A	504	BTB	N-C5-C6-O6
5	C	505	BTB	N-C7-C8-O8
2	B	501	HEM	CAA-CBA-CGA-O2A
2	B	501	HEM	CAA-CBA-CGA-O1A
3	B	502	H4B	C7-C6-C9-O9
5	C	505	BTB	O1-C1-C2-C4
3	A	502	H4B	N5-C6-C9-O9
3	B	502	H4B	N5-C6-C9-O9
3	C	502	H4B	N5-C6-C9-O9
5	A	505	BTB	C4-C2-N-C5
5	B	504	BTB	N-C2-C3-O3
5	D	505	BTB	N-C2-C3-O3
4	C	503	8EV	C24-C23-C27-N28

There are no ring outliers.

18 monomers are involved in 40 short contacts:

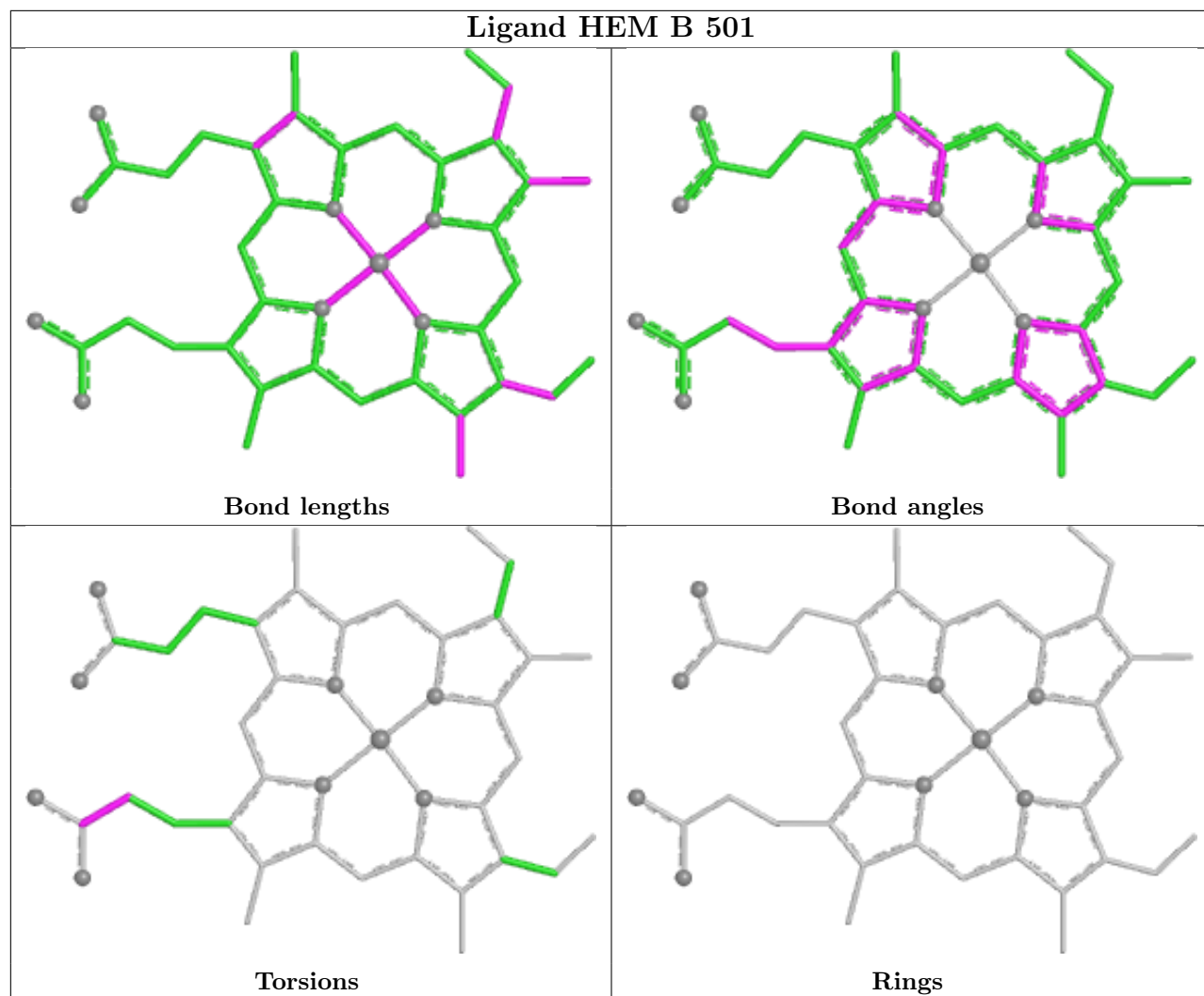
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	505	BTB	1	0
2	B	501	HEM	4	0
4	B	503	8EV	3	0
5	A	504	BTB	3	0
7	A	507	GOL	1	0
5	B	505	BTB	2	0
3	D	502	H4B	1	0
5	D	504	BTB	5	0
3	B	502	H4B	1	0
5	D	505	BTB	3	0
5	A	505	BTB	1	0
2	C	501	HEM	3	0

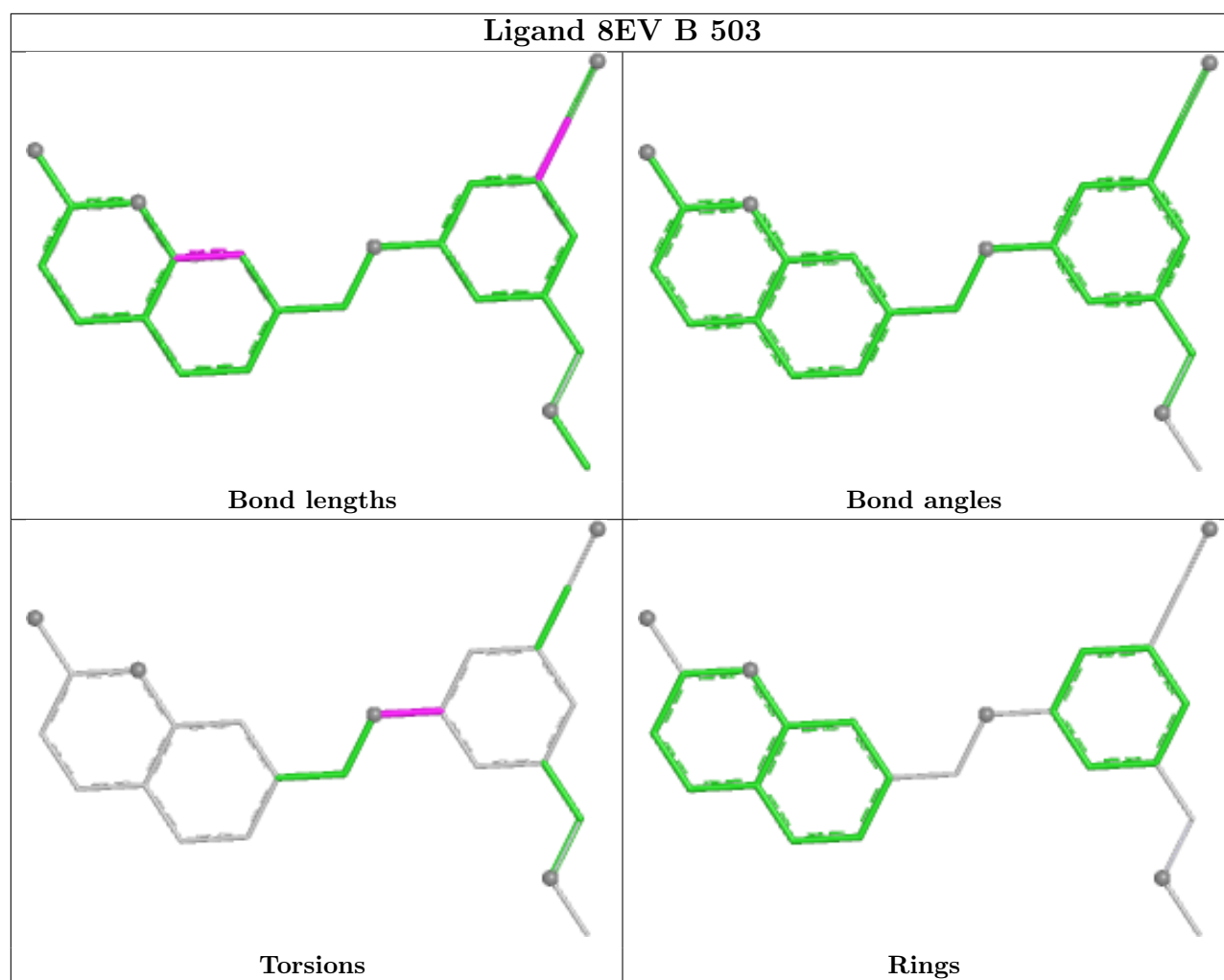
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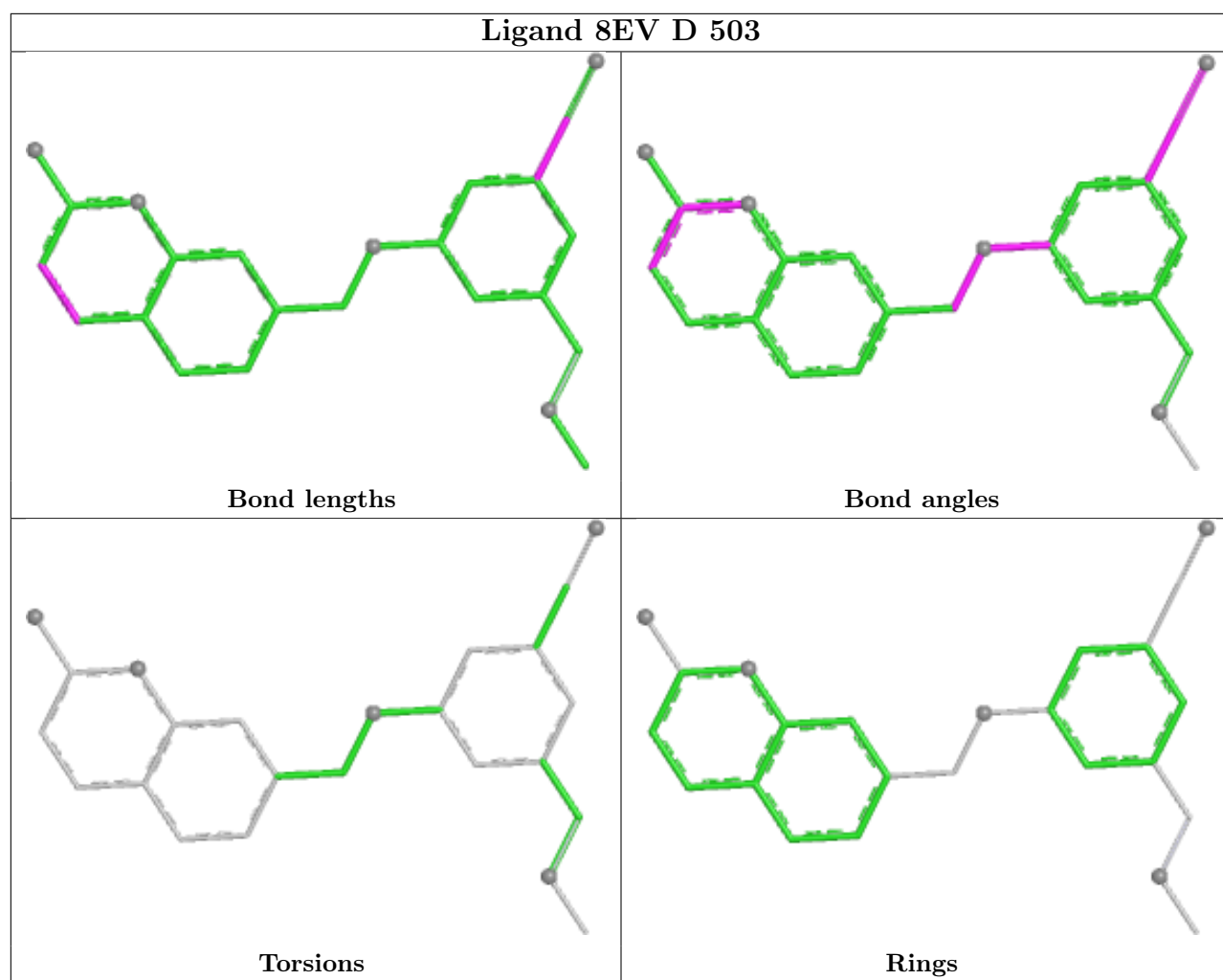
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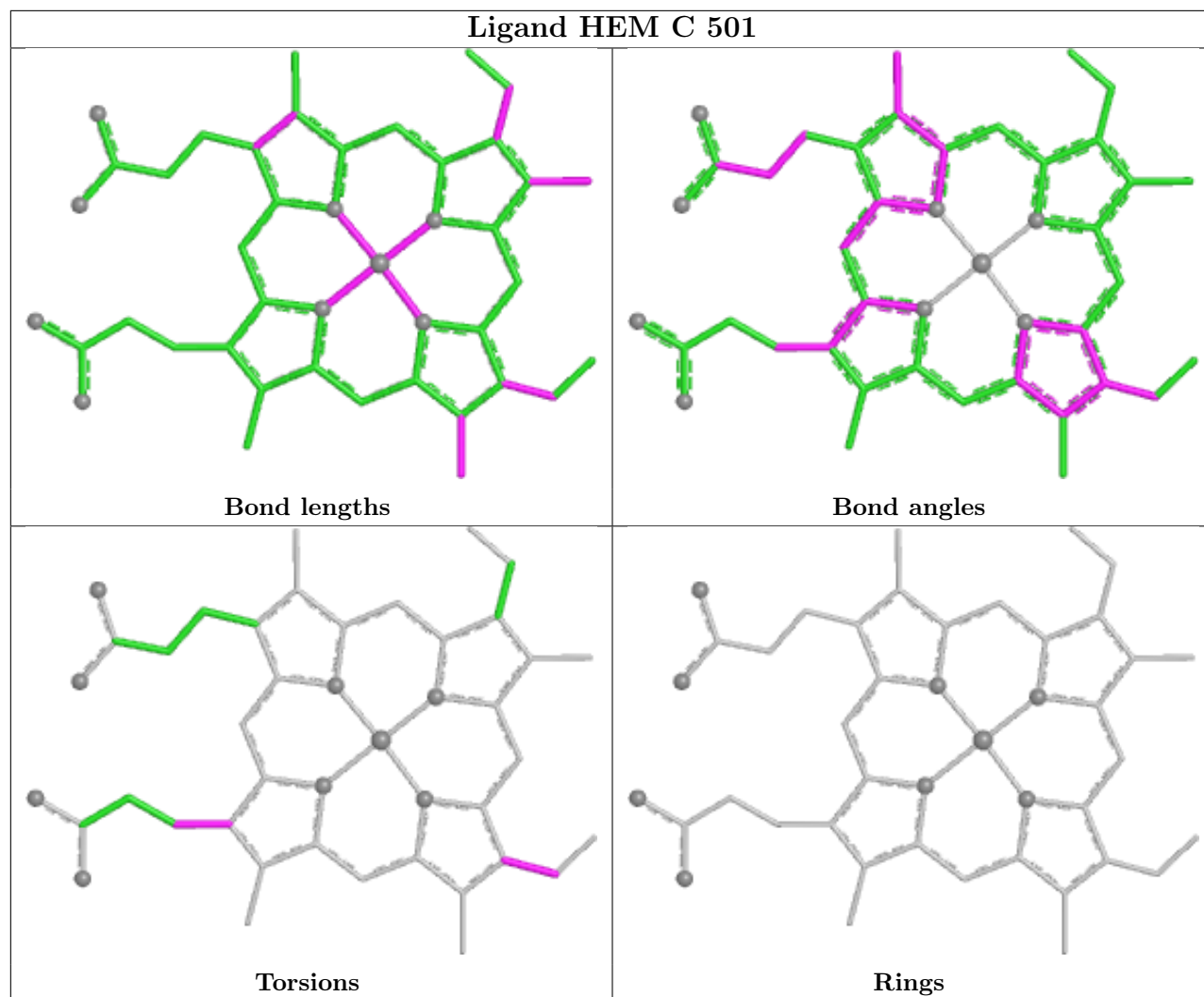
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	504	BTB	4	0
2	D	501	HEM	3	0
2	A	501	HEM	3	0
7	C	507	GOL	1	0
4	C	503	8EV	1	0
5	B	504	BTB	2	0

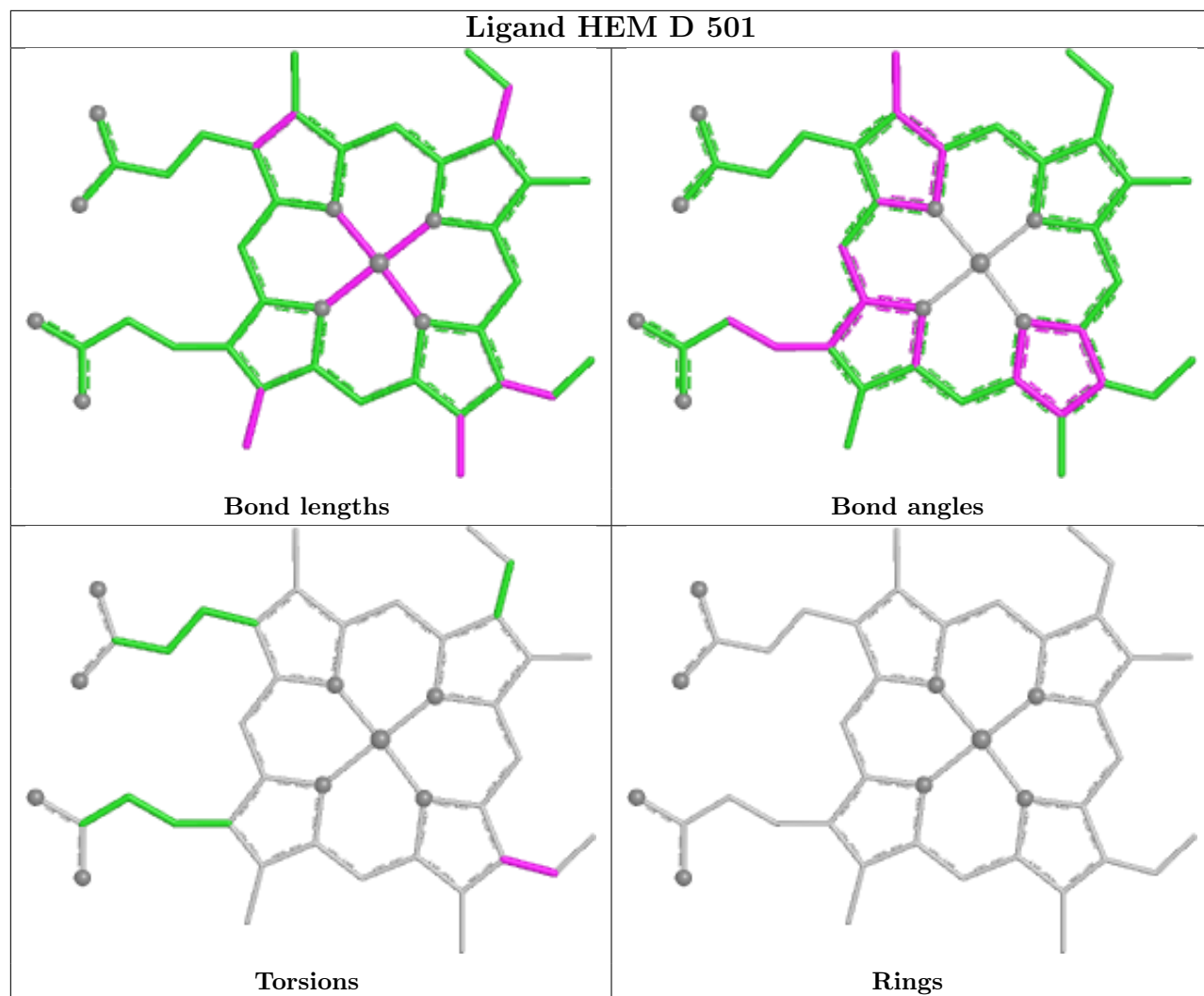
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

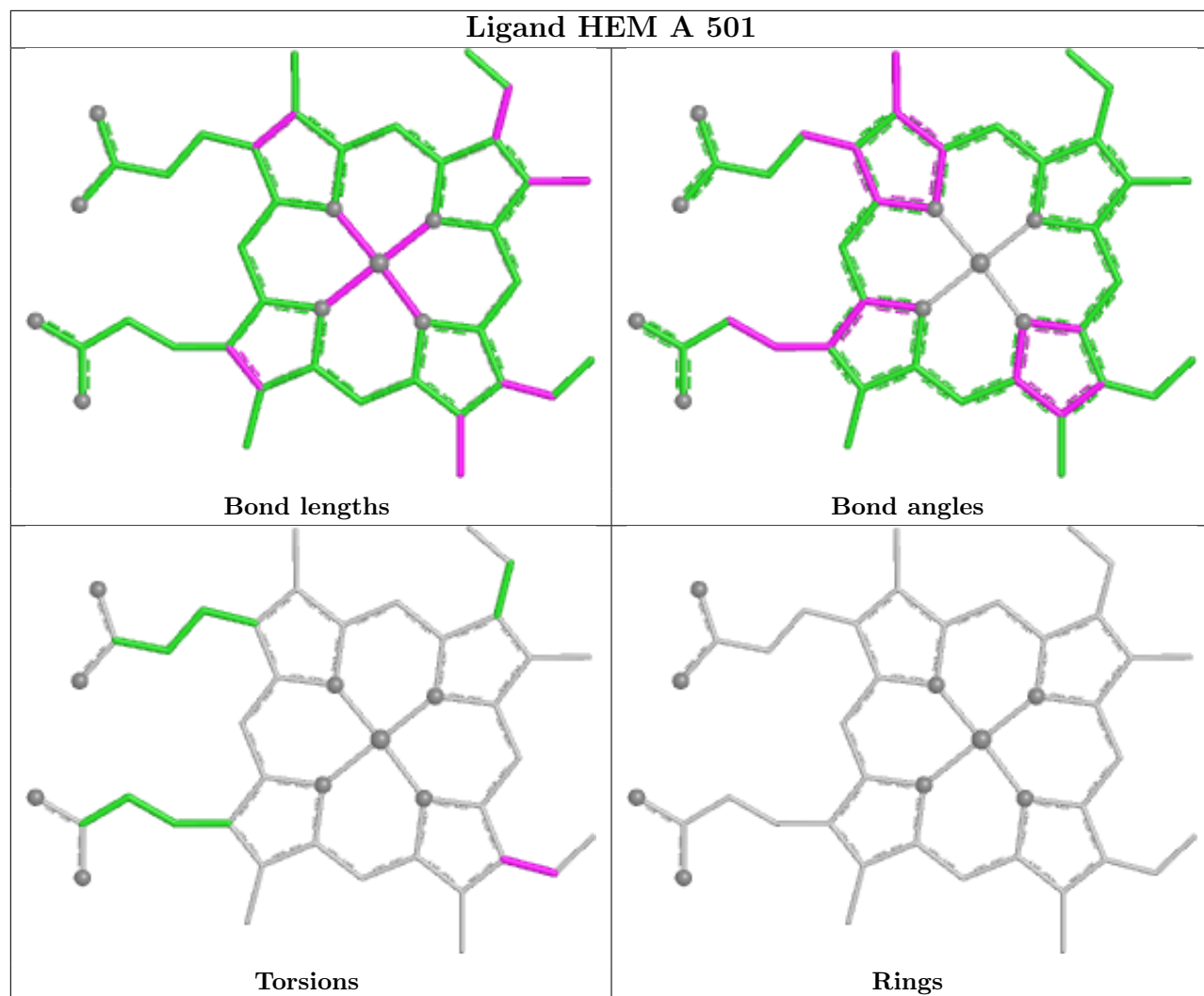


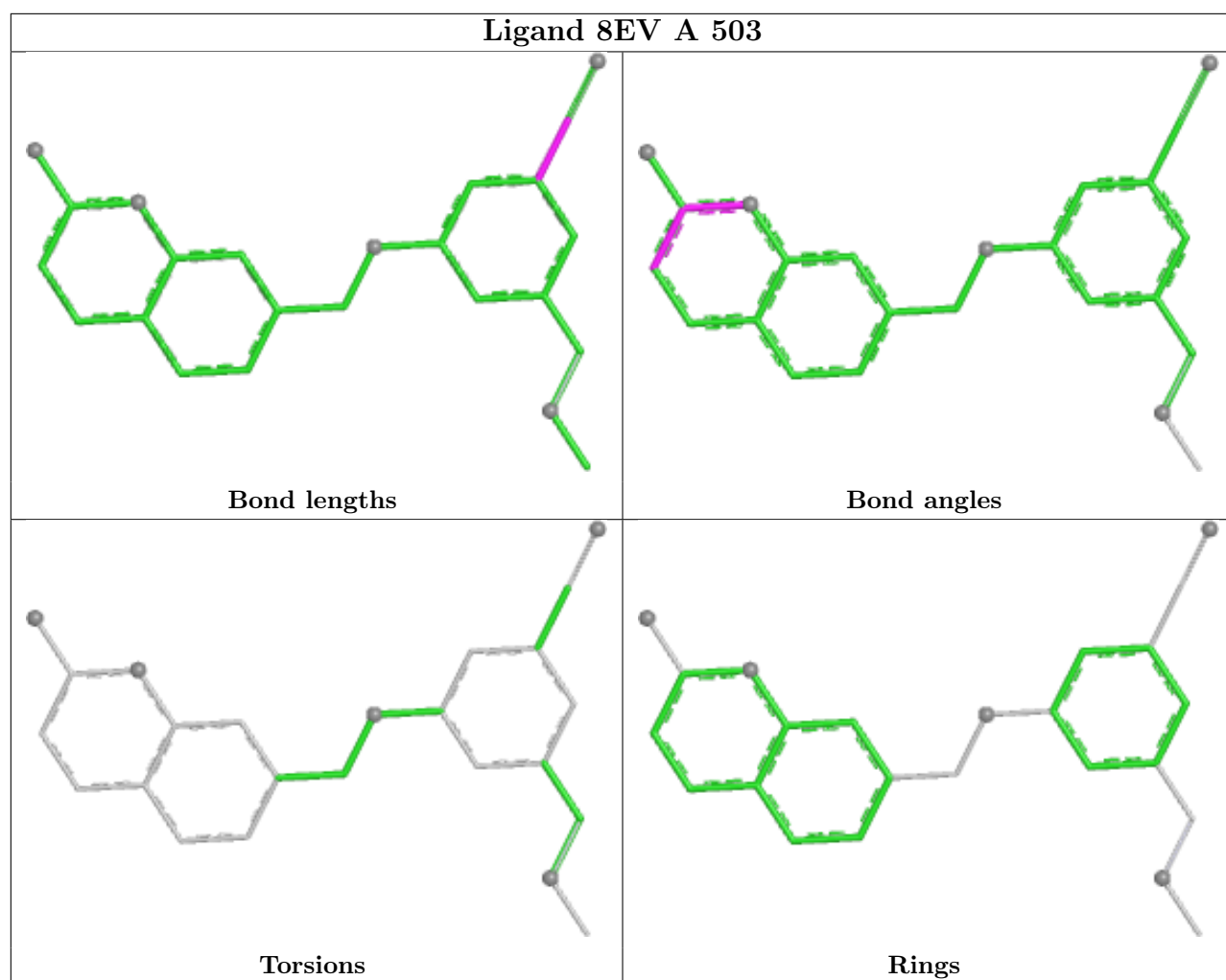


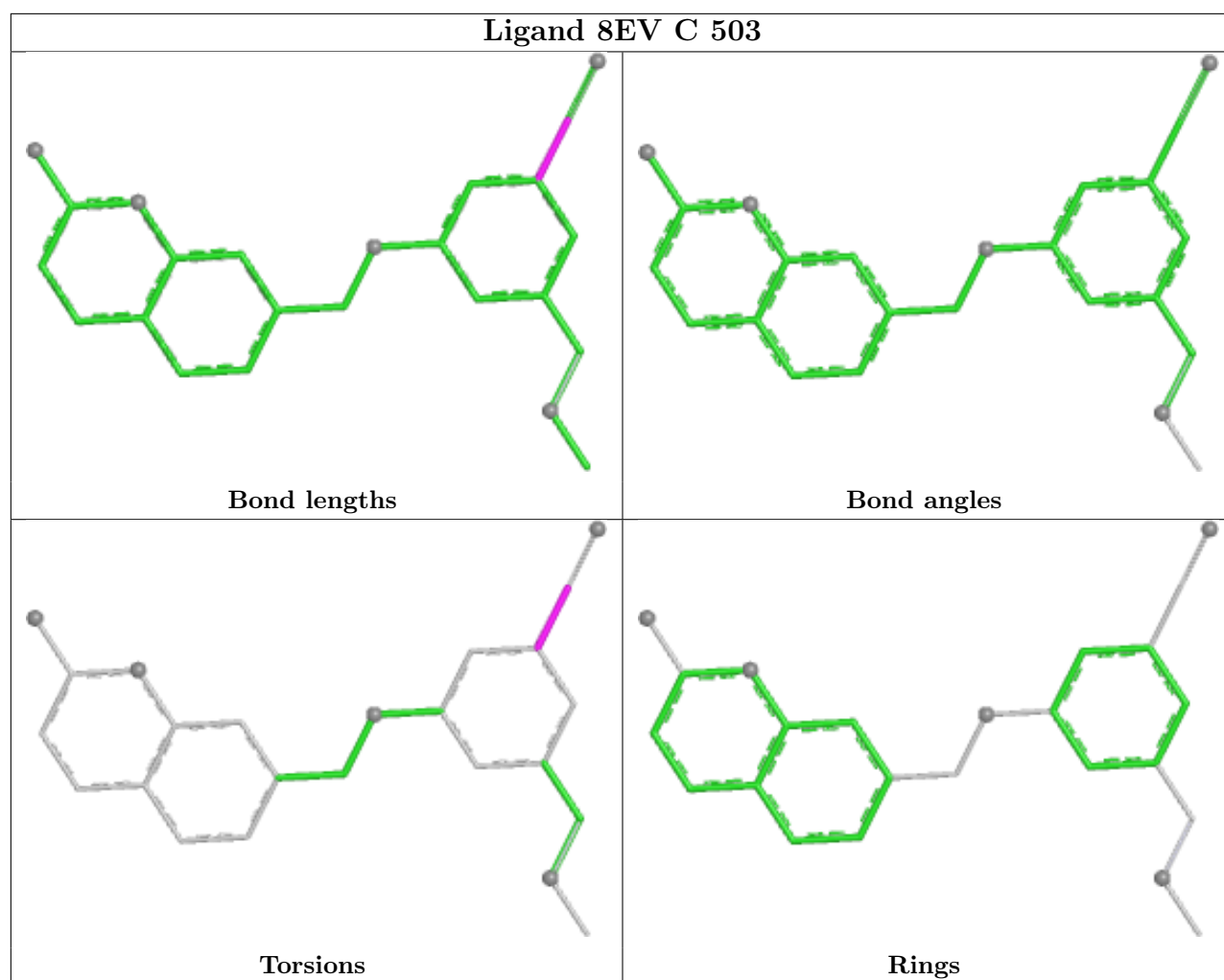












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	404/440 (91%)	0.65	25 (6%) 26 25	23, 53, 99, 142	2 (0%)
1	B	402/440 (91%)	0.26	8 (1%) 65 64	25, 40, 77, 128	3 (0%)
1	C	401/440 (91%)	0.58	29 (7%) 21 21	23, 49, 93, 140	2 (0%)
1	D	402/440 (91%)	0.23	10 (2%) 58 57	22, 40, 69, 117	3 (0%)
All	All	1609/1760 (91%)	0.43	72 (4%) 38 37	22, 45, 91, 142	10 (0%)

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	120	PRO	5.5
1	A	106	PRO	4.9
1	A	237	GLY	4.9
1	C	106	PRO	4.2
1	B	119	ALA	4.0
1	A	159	ALA	3.7
1	A	109	LEU	3.7
1	C	236	PRO	3.6
1	B	259	GLY	3.6
1	D	119	ALA	3.6
1	A	119	ALA	3.4
1	B	258	ASP	3.3
1	C	144	GLN	3.3
1	C	141	SER	3.2
1	D	259	GLY	3.2
1	C	174	ALA	3.1
1	C	139	LYS	3.0
1	A	124	LEU	2.9
1	A	204	ALA	2.9
1	B	106	PRO	2.8
1	C	140	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	239	GLY	2.8
1	A	244	TRP	2.8
1	A	258	ASP	2.8
1	C	253	GLY	2.8
1	D	260	SER	2.7
1	C	161	GLY	2.7
1	A	120	PRO	2.7
1	A	136	SER	2.7
1	C	259	GLY	2.7
1	A	144	GLN	2.6
1	A	260	SER	2.6
1	A	238	ARG	2.6
1	C	258	ASP	2.5
1	C	299	PRO	2.5
1	C	238	ARG	2.5
1	C	142	GLY	2.5
1	C	468	PHE	2.4
1	C	235	CYS	2.4
1	C	143	SER	2.4
1	D	371	HIS	2.4
1	D	261	VAL	2.4
1	A	299	PRO	2.4
1	A	300	PRO	2.4
1	C	304	LEU	2.4
1	C	157	VAL	2.3
1	A	253	GLY	2.3
1	C	309	LEU	2.3
1	D	106	PRO	2.3
1	C	282	GLY	2.3
1	C	480	TRP	2.3
1	B	257	GLN	2.2
1	A	68	PHE	2.2
1	D	68	PHE	2.2
1	C	300	PRO	2.2
1	A	352	PRO	2.2
1	A	282	GLY	2.2
1	A	380	ALA	2.2
1	B	159	ALA	2.2
1	B	68	PHE	2.2
1	A	236	PRO	2.1
1	B	468	PHE	2.1
1	D	140	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	244	TRP	2.1
1	A	155	ALA	2.1
1	C	119	ALA	2.1
1	D	257	GLN	2.1
1	A	343	ILE	2.1
1	C	303	PHE	2.1
1	C	158	ALA	2.1
1	D	90	GLN	2.0
1	A	239	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($\text{\AA}^2$)	Q<0.9
5	BTB	B	505	14/14	0.63	0.21	75,89,97,101	0
5	BTB	A	505	14/14	0.64	0.20	81,86,91,92	0
5	BTB	C	505	14/14	0.69	0.19	55,71,81,86	0
4	8EV	C	503	24/24	0.76	0.18	39,61,77,80	0
5	BTB	D	505	14/14	0.80	0.17	69,77,83,89	0
5	BTB	B	504	14/14	0.85	0.18	22,62,79,85	0
5	BTB	D	504	14/14	0.85	0.16	37,56,63,64	0
3	H4B	B	502	17/17	0.85	0.15	32,47,55,65	0
7	GOL	C	507	6/6	0.85	0.13	44,57,64,67	0
7	GOL	A	507	6/6	0.86	0.13	46,58,74,77	0
4	8EV	A	503	24/24	0.88	0.14	43,61,81,93	0
4	8EV	D	503	24/24	0.88	0.14	18,45,74,75	0
5	BTB	C	504	14/14	0.90	0.15	70,82,93,97	0
4	8EV	B	503	24/24	0.91	0.13	31,61,79,83	0

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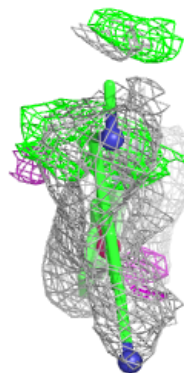
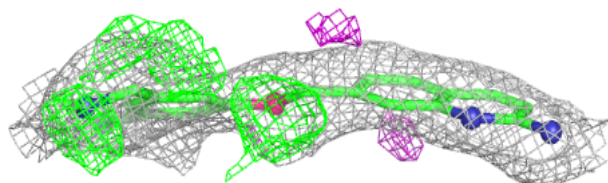
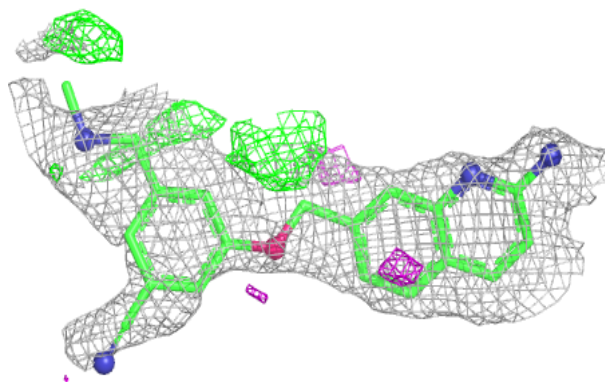
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	H4B	D	502	17/17	0.91	0.12	30,43,68,70	0
3	H4B	A	502	17/17	0.92	0.11	42,51,64,64	0
3	H4B	C	502	17/17	0.93	0.10	34,50,74,76	0
5	BTB	A	504	14/14	0.94	0.10	41,74,80,82	0
2	HEM	C	501	43/43	0.96	0.09	22,41,62,72	0
2	HEM	D	501	43/43	0.96	0.10	15,35,51,73	0
2	HEM	A	501	43/43	0.97	0.08	27,43,60,69	0
2	HEM	B	501	43/43	0.97	0.08	18,32,45,70	0
8	GD	A	508	1/1	0.98	0.05	89,89,89,89	0
8	GD	B	506	1/1	0.98	0.04	47,47,47,47	0
8	GD	D	506	1/1	0.98	0.04	47,47,47,47	0
8	GD	C	508	1/1	0.99	0.04	89,89,89,89	0
6	ZN	A	506	1/1	0.99	0.02	40,40,40,40	0
6	ZN	C	506	1/1	1.00	0.02	38,38,38,38	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.

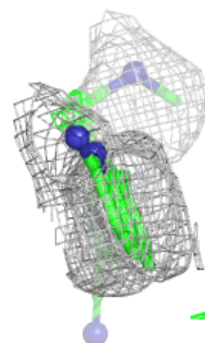
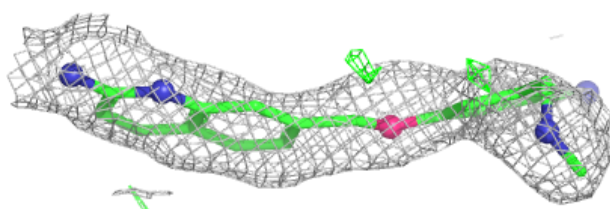
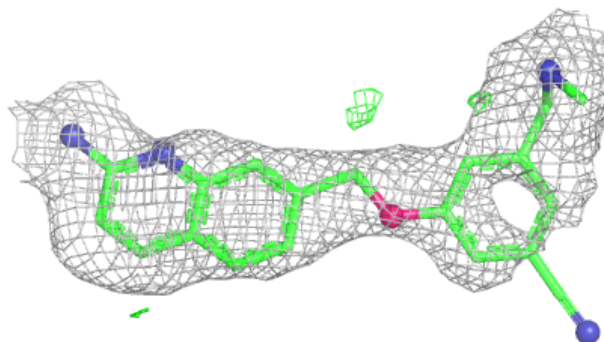
Electron density around 8EV C 503:

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

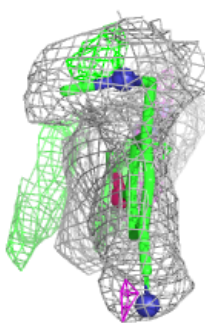
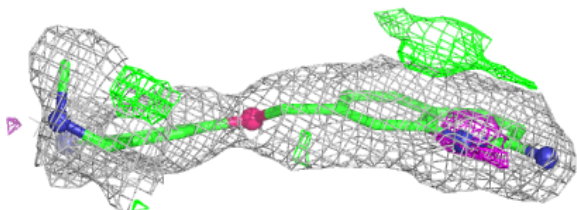
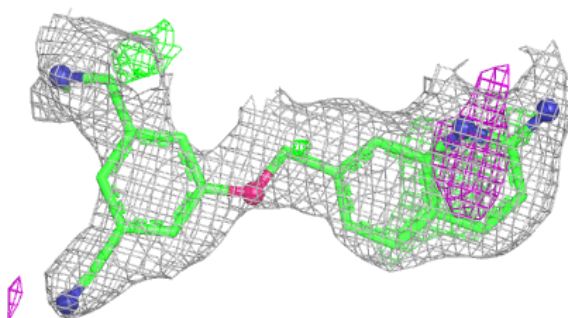


Electron density around 8EV A 503:

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

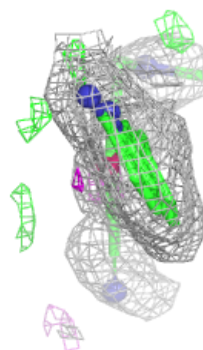
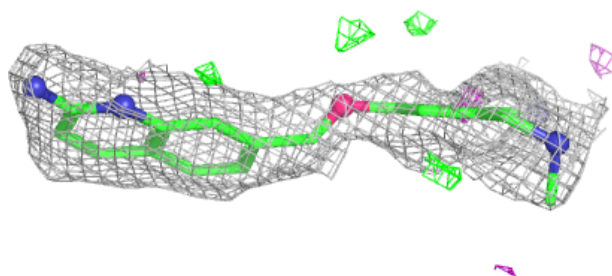
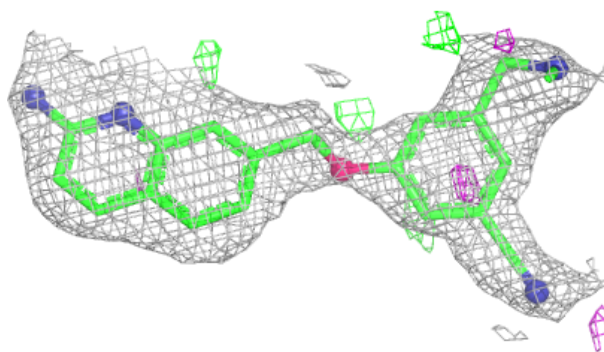
**Electron density around 8EV D 503:**

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



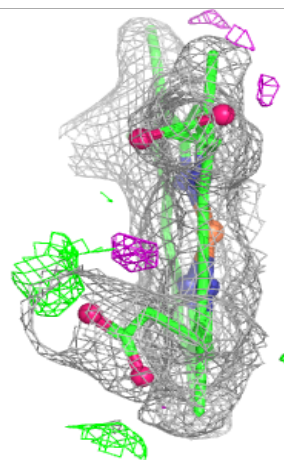
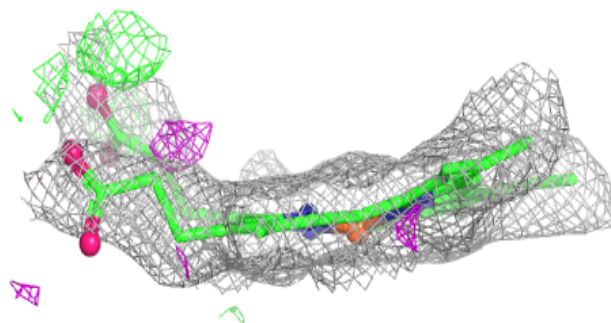
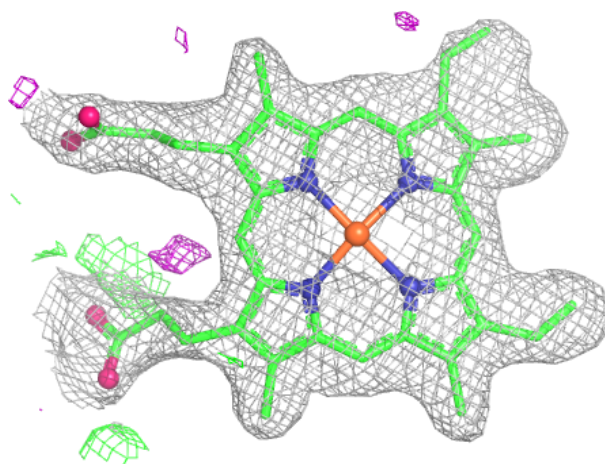
Electron density around 8EV B 503:

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



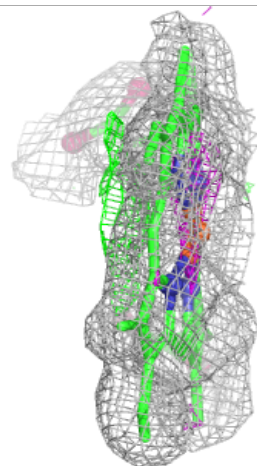
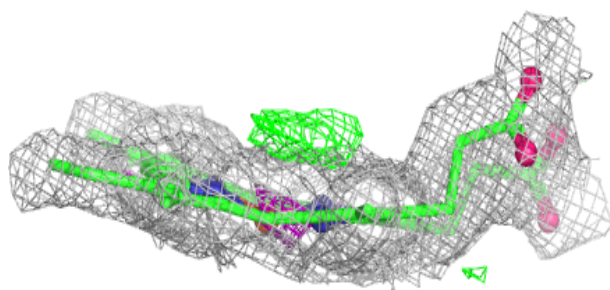
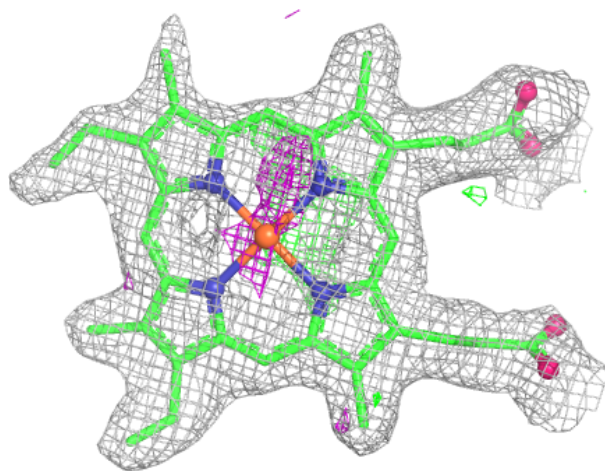
Electron density around HEM C 501:

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



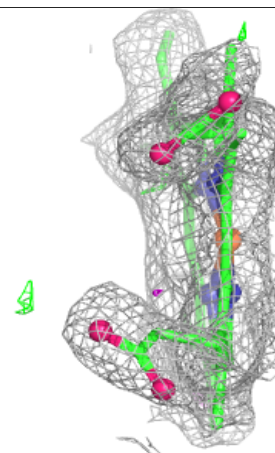
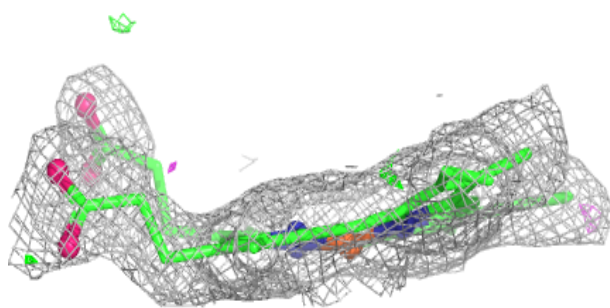
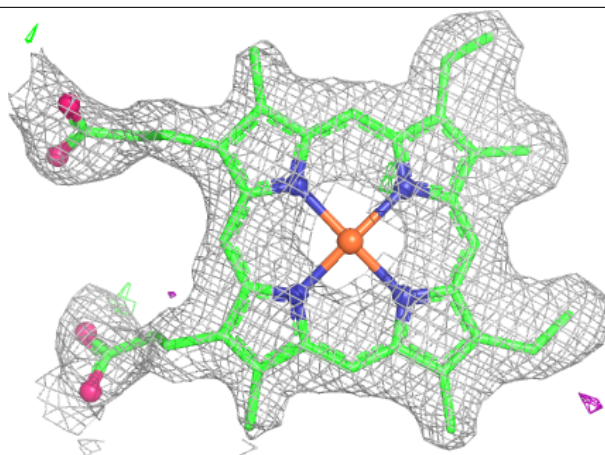
Electron density around HEM D 501:

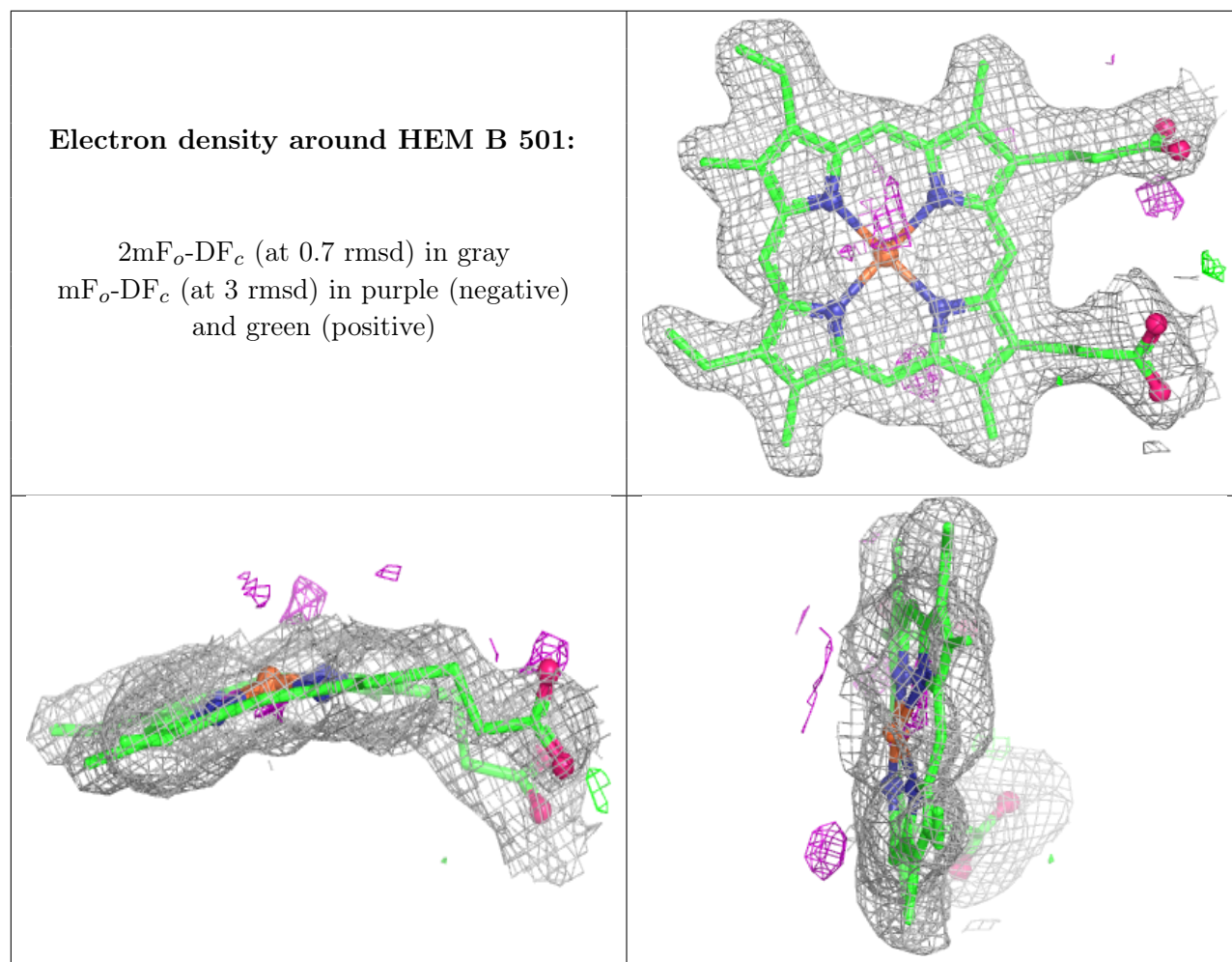
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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.