



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:38 PM UTC

PDB ID : 9MWW / pdb_00009mww
Title : Structure of human endothelial nitric oxide synthase heme domain bound with N-(3-(((2-(3-(aminomethyl)-[1,1'-biphenyl]-4-yl)ethyl)amino)methyl)phenyl)thiazole-5-carboximidamide
Authors : Li, H.; Poulos, T.L.
Deposited on : 2025-01-17
Resolution : 1.80 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

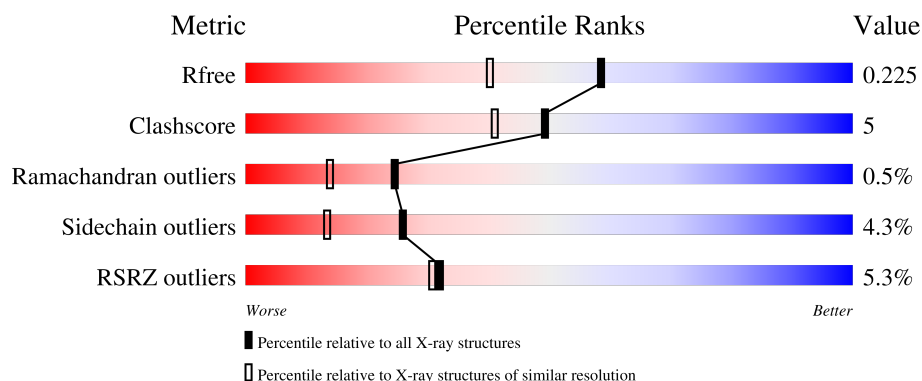
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	2% 79% 11% • 9%
1	B	440	2% 81% 9% • 9%
1	C	440	13% 74% 15% • 9%
1	D	440	2% 82% 8% • 9%

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 14209 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.

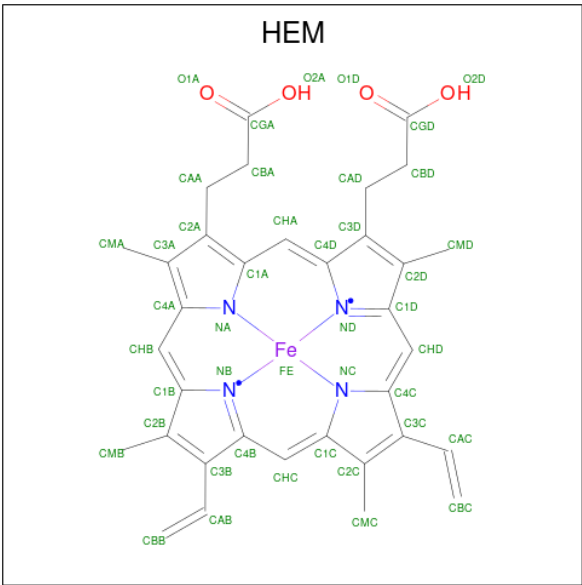
- Molecule 1 is a protein called Nitric oxide synthase, endothelial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	401	Total	C	N	O	S	0	1	0
			3207	2043	564	584	16			
1	B	401	Total	C	N	O	S	0	1	0
			3203	2040	563	584	16			
1	C	401	Total	C	N	O	S	0	1	0
			3207	2043	564	584	16			
1	D	402	Total	C	N	O	S	0	2	0
			3217	2049	566	586	16			

There are 4 discrepancies between the modelled and reference sequences:

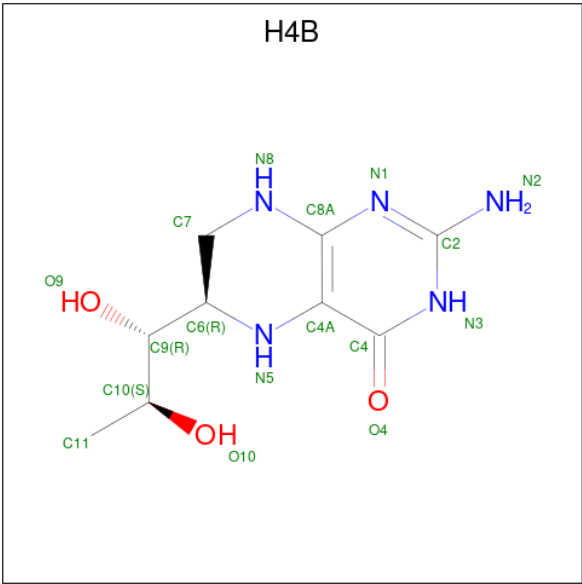
Chain	Residue	Modelled	Actual	Comment	Reference
A	298	GLU	ASP	variant	UNP P29474
B	298	GLU	ASP	variant	UNP P29474
C	298	GLU	ASP	variant	UNP P29474
D	298	GLU	ASP	variant	UNP P29474

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



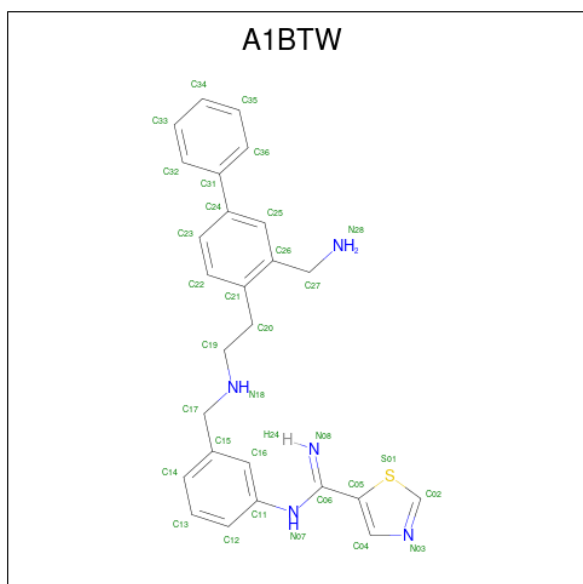
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is 5,6,7,8-TETRAHYDROBIOPTERIN (CCD ID: H4B) (formula: C₉H₁₅N₅O₃).



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 N-{3-[(2-[3-(aminomethyl)[1,1'-biphenyl]-4-yl]ethyl)amino)methyl]phenyl}-1,3-thiazole-5-carboximidamide (CCD ID: A1BTW) (formula: C₂₆H₂₇N₅S) (labeled as "Ligand of Interest" by depositor).



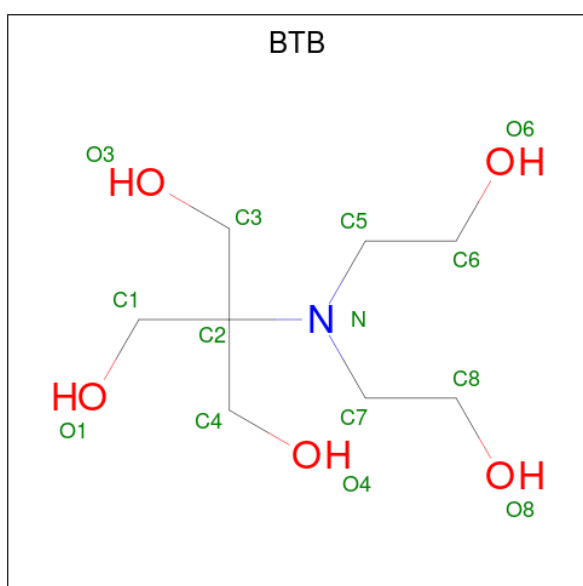
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	S	0	0
			32	26	5	1		
4	B	1	Total	C	N	S	0	0
			32	26	5	1		
4	C	1	Total	C	N	S	0	0
			32	26	5	1		
4	D	1	Total	C	N	S	0	0
			32	26	5	1		

- Molecule 5 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



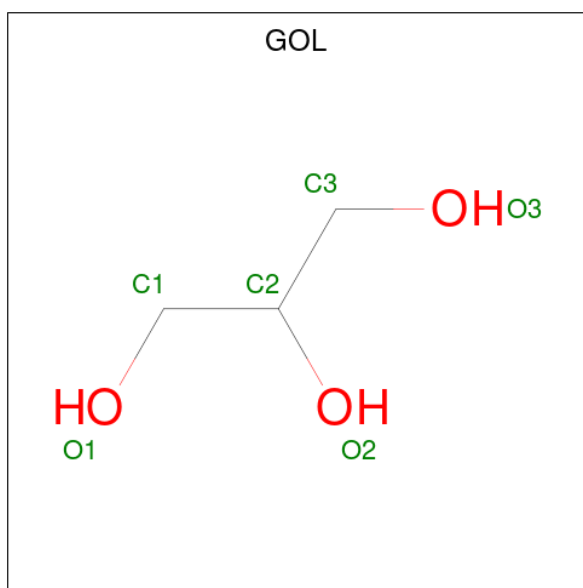
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 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
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	D	1	Total	C	N	O	0	0
			14	8	1	5		
6	D	1	Total	C	N	O	0	0
			14	8	1	5		

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



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

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

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

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

- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 10 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total Ca 1 1	0	0
10	B	1	Total Ca 1 1	0	0

- Molecule 11 is GADOLINIUM ATOM (CCD ID: GD) (formula: Gd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	B	1	Total 1	Gd 1	0	0
11	C	1	Total 1	Gd 1	0	0
11	D	2	Total 2	Gd 2	0	0

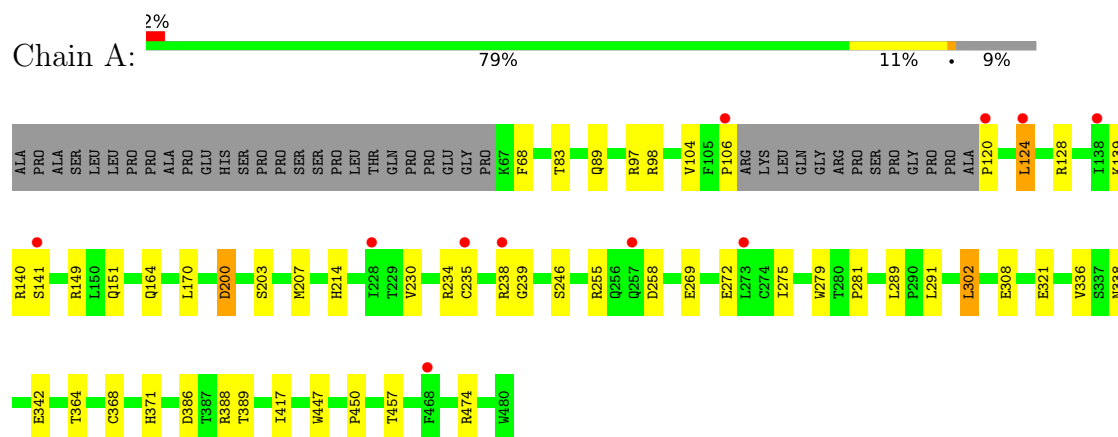
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	172	Total 172	O 172	0	0
12	B	249	Total 249	O 249	0	0
12	C	134	Total 134	O 134	0	0
12	D	246	Total 246	O 246	0	0

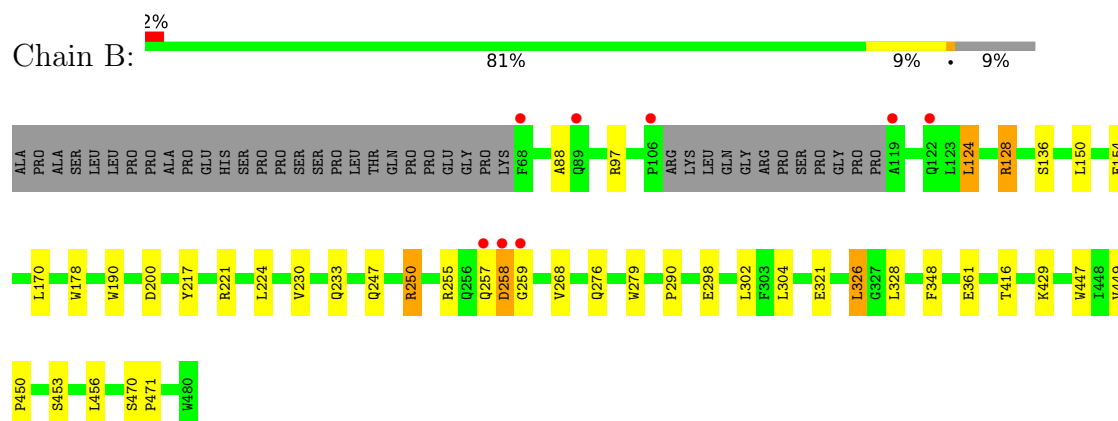
3 Residue-property plots [i](#)

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.

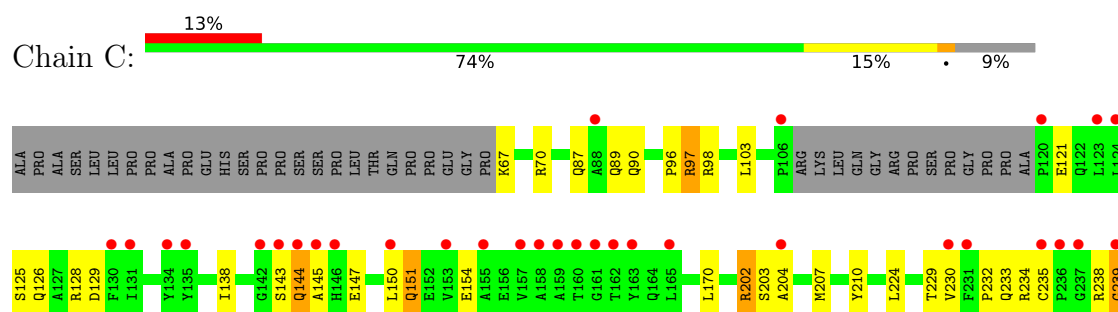
- Molecule 1: Nitric oxide synthase, endothelial

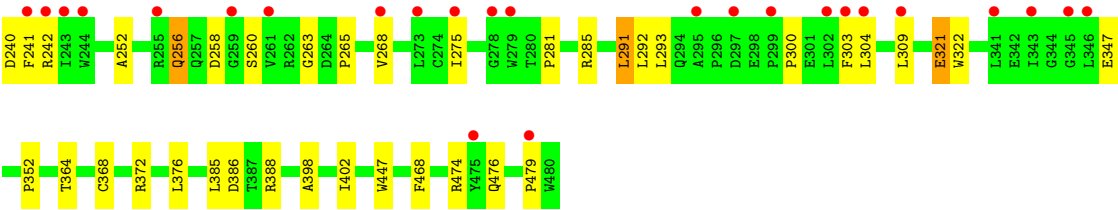


- Molecule 1: Nitric oxide synthase, endothelial

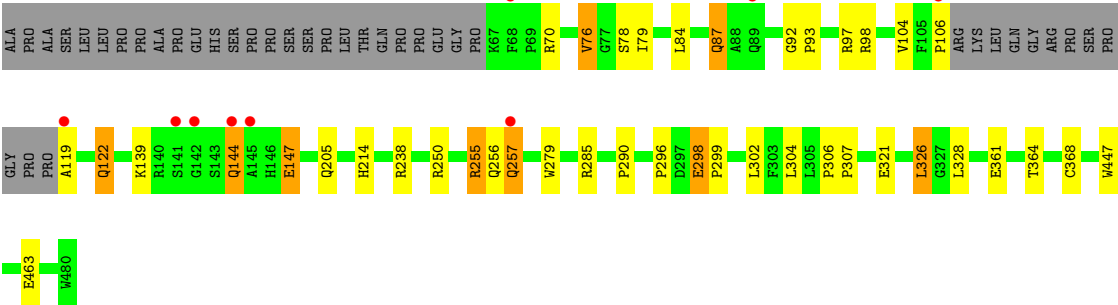
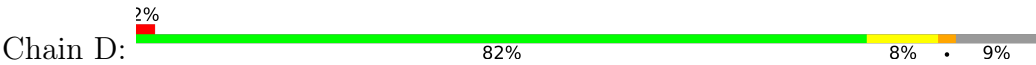


- Molecule 1: Nitric oxide synthase, endothelial





● 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	59.35Å 152.63Å 108.80Å 90.00° 90.92° 90.00°	Depositor
Resolution (Å)	49.01 – 1.80 49.01 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.9 (49.01-1.80) 99.1 (49.01-1.80)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 1.79Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.194 , 0.231 0.189 , 0.225	Depositor DCC
R_{free} test set	8892 reflections (4.21%)	wwPDB-VP
Wilson B-factor (Å ²)	29.1	Xtriage
Anisotropy	1.036	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.079 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	14209	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% 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: ACT, ZN, A1BTW, CL, H4B, HEM, CA, BTB, GOL, GD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.27	0/3302	0.46	0/4498
1	B	0.31	0/3298	0.51	0/4495
1	C	0.24	0/3302	0.47	0/4498
1	D	0.30	0/3315	0.51	0/4517
All	All	0.28	0/13217	0.48	0/18008

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
1	D	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	143	SER	Peptide
1	D	255	ARG	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	3207	0	3112	24	0
1	B	3203	0	3103	23	0
1	C	3207	0	3112	48	0
1	D	3217	0	3122	30	0
2	A	43	0	30	2	0
2	B	43	0	30	2	0
2	C	43	0	30	2	0
2	D	43	0	30	3	0
3	A	17	0	15	1	0
3	B	17	0	15	1	0
3	C	17	0	15	1	0
3	D	17	0	15	1	0
4	A	32	0	0	2	0
4	B	32	0	0	1	0
4	C	32	0	0	0	0
4	D	32	0	0	1	0
5	A	4	0	3	0	0
5	B	4	0	3	0	0
5	C	4	0	3	0	0
5	D	4	0	3	1	0
6	A	28	0	37	5	0
6	B	28	0	35	5	0
6	C	28	0	38	4	0
6	D	28	0	37	3	0
7	A	18	0	24	0	0
7	B	12	0	16	0	0
7	C	18	0	24	0	0
7	D	18	0	24	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	C	1	0	0	0	0
10	A	1	0	0	0	0
10	B	1	0	0	0	0
11	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	C	1	0	0	0	0
11	D	2	0	0	0	0
12	A	172	0	0	1	0
12	B	249	0	0	1	0
12	C	134	0	0	7	0
12	D	246	0	0	4	0
All	All	14209	0	12876	142	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 5.

All (142) 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:256:GLN:HG3	1:D:257:GLN:H	1.48	0.79
2:A:501:HEM:HBB2	2:A:501:HEM:HHC	1.63	0.78
6:B:505:BTB:O4	6:B:505:BTB:H72	1.82	0.77
1:C:233:GLN:OE1	12:C:601:HOH:O	2.04	0.73
1:A:279:TRP:HB2	1:A:302:LEU:HD11	1.70	0.73
2:C:501:HEM:HBB2	2:C:501:HEM:HHC	1.71	0.72
1:C:235:CYS:SG	12:C:604:HOH:O	2.47	0.71
1:A:200:ASP:N	1:A:200:ASP:OD1	2.22	0.71
1:C:321:GLU:H	1:C:321:GLU:CD	2.00	0.70
1:C:147:GLU:O	1:C:151:GLN:NE2	2.26	0.69
1:C:275:ILE:HD11	1:C:281:PRO:HB3	1.73	0.69
6:D:507:BTB:O1	6:D:507:BTB:O3	2.12	0.68
1:B:128:ARG:HB2	1:B:128:ARG:HH11	1.61	0.65
1:C:128:ARG:NH2	1:C:154:GLU:OE2	2.30	0.65
1:B:128:ARG:HB2	1:B:128:ARG:NH1	2.13	0.64
1:C:234:ARG:NH1	1:C:347:GLU:OE1	2.30	0.64
1:C:147:GLU:HA	1:C:150:LEU:HD12	1.79	0.64
2:C:501:HEM:HBC2	2:C:501:HEM:HMC2	1.80	0.64
1:C:70:ARG:NH2	12:C:605:HOH:O	2.31	0.63
1:C:97:ARG:HG2	1:C:98:ARG:HG2	1.80	0.62
1:B:279:TRP:HB2	1:B:302:LEU:HD21	1.81	0.62
1:D:238:ARG:NH2	12:D:603:HOH:O	2.32	0.61
1:C:210:TYR:O	12:C:602:HOH:O	2.16	0.61
2:B:501:HEM:HBC2	2:B:501:HEM:HMC2	1.83	0.61
1:C:238:ARG:NH1	1:C:239:GLY:O	2.34	0.60
1:B:128:ARG:HD3	1:B:150:LEU:HD22	1.84	0.60
1:A:342:GLU:OE1	1:A:474:ARG:NH1	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:505:BTB:H41	1:D:326:LEU:HD12	1.83	0.59
6:B:505:BTB:O4	6:B:505:BTB:C7	2.49	0.59
1:A:371:HIS:HD2	4:A:503:A1BTW:C33	2.16	0.59
1:D:298:GLU:HG3	1:D:299:PRO:HD2	1.85	0.58
1:B:217:TYR:OH	12:B:601:HOH:O	2.02	0.58
1:A:234:ARG:HA	1:A:238:ARG:HH12	1.68	0.58
2:A:501:HEM:HMC2	2:A:501:HEM:HBC2	1.86	0.58
1:B:124:LEU:HD21	1:B:154:GLU:HG2	1.88	0.56
6:C:505:BTB:O4	6:C:505:BTB:O3	2.13	0.56
1:D:279:TRP:HB2	1:D:302:LEU:HD21	1.87	0.56
1:A:149:ARG:NH2	1:A:164:GLN:O	2.36	0.55
1:C:256:GLN:HB2	1:C:260:SER:O	2.06	0.55
1:B:124:LEU:HD11	1:B:128:ARG:HH22	1.71	0.55
1:C:238:ARG:HB3	12:C:604:HOH:O	2.05	0.55
1:D:76:VAL:HG12	1:D:78:SER:H	1.73	0.54
1:D:285:ARG:NH1	12:D:601:HOH:O	2.21	0.54
1:C:97:ARG:HB2	1:C:97:ARG:HH11	1.73	0.54
1:D:144:GLN:NE2	12:D:604:HOH:O	2.33	0.54
1:D:326:LEU:HB3	1:D:328:LEU:HG	1.89	0.54
1:D:147:GLU:H	1:D:147:GLU:CD	2.16	0.54
1:B:321:GLU:OE2	6:B:505:BTB:O4	2.27	0.53
1:C:242:ARG:NH1	1:C:476:GLN:OE1	2.41	0.53
1:C:144:GLN:HG3	1:C:145:ALA:N	2.24	0.53
2:D:502:HEM:HMC2	2:D:502:HEM:HBC2	1.91	0.52
1:B:298:GLU:OE2	6:B:506:BTB:O8	2.28	0.52
1:A:447:TRP:HA	3:A:502:H4B:N1	2.25	0.51
1:C:204:ALA:HB1	1:C:303:PHE:HE1	1.75	0.51
1:A:321:GLU:H	1:A:321:GLU:CD	2.18	0.51
2:B:501:HEM:HHC	2:B:501:HEM:HBB2	1.93	0.51
1:C:265:PRO:HA	1:C:268:VAL:HG23	1.92	0.51
1:A:364:THR:O	1:A:368:CYS:HB2	2.12	0.50
6:A:506:BTB:O4	6:A:506:BTB:O3	2.17	0.50
1:C:150:LEU:HB2	1:C:151:GLN:HE21	1.77	0.50
6:B:505:BTB:H61	6:B:505:BTB:O3	2.12	0.49
1:C:292:LEU:HD22	1:C:300:PRO:HB2	1.94	0.48
1:C:252:ALA:O	1:C:263:GLY:HA3	2.12	0.48
1:C:364:THR:O	1:C:368:CYS:HB2	2.12	0.48
1:D:364:THR:O	1:D:368:CYS:HB2	2.12	0.48
1:A:386:ASP:OD2	1:A:388:ARG:HG3	2.14	0.48
1:B:326:LEU:HB3	1:B:328:LEU:HG	1.95	0.48
6:C:506:BTB:O3	6:C:506:BTB:O4	2.30	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:502:HEM:HMB3	5:D:505:ACT:H2	1.95	0.48
1:A:97:ARG:HG2	1:A:98:ARG:HG2	1.95	0.47
1:A:336:VAL:HG21	4:A:503:A1BTW:C14	2.45	0.47
6:A:505:BTB:H41	1:D:326:LEU:CD1	2.44	0.47
1:C:170:LEU:HD11	1:C:230:VAL:HG11	1.96	0.47
1:D:93:PRO:HG3	1:D:106:PRO:HB3	1.96	0.47
1:B:170:LEU:HD11	1:B:230:VAL:HG11	1.97	0.47
1:D:104:VAL:O	1:D:106:PRO:HD3	2.14	0.47
1:C:242:ARG:NE	1:C:479:PRO:HB3	2.30	0.46
6:A:506:BTB:H11	6:A:506:BTB:H51	1.67	0.46
1:B:178:TRP:CE3	1:B:190:TRP:HA	2.51	0.46
1:A:235:CYS:SG	1:A:238:ARG:HD3	2.55	0.46
1:C:322:TRP:CD1	6:C:505:BTB:H52	2.50	0.46
1:B:257:GLN:C	1:B:259:GLY:H	2.22	0.46
1:C:291:LEU:HD23	1:C:293:LEU:HD21	1.97	0.46
6:C:505:BTB:H51	6:C:505:BTB:H32	1.65	0.46
1:D:238:ARG:HG2	1:D:296:PRO:HB3	1.98	0.45
1:C:238:ARG:HD2	1:C:239:GLY:N	2.32	0.45
1:D:290:PRO:HB3	1:D:304:LEU:HD23	1.97	0.45
1:D:84:LEU:HD12	1:D:87:GLN:HG3	1.99	0.45
1:C:242:ARG:HE	1:C:479:PRO:HB3	1.81	0.45
1:D:361:GLU:OE1	4:D:504:A1BTW:N07	2.50	0.45
1:B:447:TRP:HA	3:B:502:H4B:N1	2.32	0.45
1:C:386:ASP:OD2	1:C:388:ARG:HG2	2.17	0.45
1:A:275:ILE:HD11	1:A:281:PRO:HB3	1.99	0.44
1:C:447:TRP:HA	3:C:502:H4B:N1	2.32	0.44
1:A:269:GLU:O	1:A:272:GLU:HG2	2.17	0.44
1:A:214:HIS:C	1:A:214:HIS:CD2	2.96	0.44
1:C:202:ARG:HA	1:C:241:PHE:HZ	1.81	0.44
1:A:450:PRO:HG2	1:A:457:THR:HG21	2.00	0.44
1:D:70:ARG:HD2	1:D:79:ILE:HD13	2.00	0.44
1:C:258:ASP:OD1	1:C:258:ASP:N	2.51	0.44
1:D:119:ALA:HB1	1:D:122:GLN:HG2	1.99	0.44
1:D:250:ARG:HA	1:D:250:ARG:HD2	1.74	0.43
1:D:447:TRP:HA	3:D:503:H4B:N1	2.32	0.43
1:A:104:VAL:O	1:A:106:PRO:HD3	2.18	0.43
1:C:151:GLN:HE21	1:C:151:GLN:N	2.17	0.43
1:B:470:SER:HA	1:B:471:PRO:C	2.43	0.43
1:C:234:ARG:NH2	1:C:242:ARG:HH12	2.17	0.43
1:B:290:PRO:HB3	1:B:304:LEU:HD23	2.01	0.43
1:C:372:ARG:NH2	12:C:612:HOH:O	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:255:ARG:HG2	1:D:255:ARG:HH11	1.83	0.43
1:D:321:GLU:OE2	6:D:506:BTB:O4	2.37	0.43
2:D:502:HEM:HBB2	2:D:502:HEM:HHC	2.00	0.43
1:A:120:PRO:O	1:A:124:LEU:HD12	2.19	0.43
1:D:306:PRO:HA	1:D:307:PRO:HD2	1.90	0.43
1:C:292:LEU:HD23	1:C:292:LEU:HA	1.93	0.42
1:C:202:ARG:HE	1:C:202:ARG:HB3	1.69	0.42
1:C:398:ALA:O	1:C:402:ILE:HG13	2.20	0.42
1:A:246:SER:HA	1:A:338:ASN:HB3	2.01	0.42
1:B:449:VAL:HA	1:B:450:PRO:HD3	1.91	0.42
1:D:122:GLN:CD	1:D:122:GLN:N	2.78	0.42
1:A:128:ARG:NH1	12:A:615:HOH:O	2.52	0.41
1:B:233:GLN:HB3	1:B:348:PHE:CE2	2.55	0.41
1:B:361:GLU:OE1	4:B:503:A1BTW:N07	2.54	0.41
1:C:229:THR:O	1:C:352:PRO:HD2	2.19	0.41
6:D:506:BTB:H72	6:D:506:BTB:H11	1.80	0.41
1:C:96:PRO:O	1:D:92:GLY:N	2.40	0.41
1:C:232:PRO:HA	12:C:607:HOH:O	2.20	0.41
1:B:453:SER:HB3	1:B:456:LEU:HD12	2.01	0.41
1:A:170:LEU:HD11	1:A:230:VAL:HG11	2.02	0.41
1:B:224:LEU:HB2	1:B:416:THR:HB	2.03	0.41
1:D:205:GLN:HG3	12:D:798:HOH:O	2.19	0.41
1:B:247:GLN:HB2	1:B:250:ARG:HG2	2.03	0.41
6:A:506:BTB:O4	6:A:506:BTB:H72	2.17	0.40
1:C:97:ARG:HB2	1:C:97:ARG:NH1	2.34	0.40
1:C:207:MET:HE2	1:C:207:MET:HB3	1.96	0.40
1:A:68:PHE:CD1	1:A:83:THR:HG22	2.56	0.40
1:A:97:ARG:HG3	1:B:88:ALA:HB3	2.04	0.40
1:C:90:GLN:HB3	1:C:468:PHE:CD2	2.56	0.40
1:C:368:CYS:SG	1:C:376:LEU:HD13	2.61	0.40
1:D:214:HIS:CD2	1:D:214:HIS:C	2.98	0.40
1:C:103:LEU:HD12	1:D:463:GLU:HB3	2.03	0.40
1:C:385:LEU:HD23	1:C:385:LEU:HA	1.93	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	398/440 (90%)	382 (96%)	15 (4%)	1 (0%)	36	25
1	B	398/440 (90%)	390 (98%)	6 (2%)	2 (0%)	24	14
1	C	398/440 (90%)	381 (96%)	13 (3%)	4 (1%)	12	4
1	D	400/440 (91%)	385 (96%)	14 (4%)	1 (0%)	36	25
All	All	1594/1760 (91%)	1538 (96%)	48 (3%)	8 (0%)	24	14

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	144	GLN
1	D	144	GLN
1	C	89	GLN
1	B	255	ARG
1	B	258	ASP
1	C	203	SER
1	A	239	GLY
1	C	239	GLY

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	342/373 (92%)	325 (95%)	17 (5%)	22	10
1	B	341/373 (91%)	329 (96%)	12 (4%)	32	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	342/373 (92%)	323 (94%)	19 (6%)	19	8
1	D	343/373 (92%)	333 (97%)	10 (3%)	37	25
All	All	1368/1492 (92%)	1310 (96%)	58 (4%)	26	14

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	124	LEU
1	A	139	LYS
1	A	140	ARG
1	A	141	SER
1	A	151	GLN
1	A	200	ASP
1	A	203	SER
1	A	207	MET
1	A	255	ARG
1	A	258	ASP
1	A	289	LEU
1	A	291	LEU
1	A	302	LEU
1	A	308	GLU
1	A	389	THR
1	A	417	ILE
1	B	97	ARG
1	B	124	LEU
1	B	128	ARG
1	B	136	SER
1	B	200	ASP
1	B	221	ARG
1	B	250	ARG
1	B	258	ASP
1	B	268	VAL
1	B	276	GLN
1	B	326	LEU
1	B	429	LYS
1	C	67	LYS
1	C	87	GLN
1	C	97	ARG
1	C	121	GLU
1	C	125	SER

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Mol	Chain	Res	Type
1	C	126	GLN
1	C	129	ASP
1	C	138	ILE
1	C	151	GLN
1	C	202	ARG
1	C	224	LEU
1	C	240	ASP
1	C	256	GLN
1	C	285	ARG
1	C	291	LEU
1	C	304	LEU
1	C	309	LEU
1	C	321	GLU
1	C	474	ARG
1	D	76	VAL
1	D	87	GLN
1	D	97	ARG
1	D	98	ARG
1	D	122	GLN
1	D	139	LYS
1	D	147	GLU
1	D	257	GLN
1	D	298	GLU
1	D	326	LEU

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	87	GLN
1	A	122	GLN
1	A	133	GLN
1	A	205	GLN
1	A	277	HIS
1	A	408	HIS
1	C	132	ASN
1	C	151	GLN
1	D	122	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 47 ligands modelled in this entry, 12 are monoatomic - leaving 35 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	A1BTW	D	504	-	35,35,35	0.99	4 (11%)	40,46,46	1.76	5 (12%)
7	GOL	B	507	-	5,5,5	0.36	0	5,5,5	0.39	0
3	H4B	C	502	-	17,18,18	0.86	1 (5%)	14,26,26	1.94	5 (35%)
7	GOL	C	507	-	5,5,5	0.40	0	5,5,5	0.28	0
2	HEM	A	501	1	50,50,50	1.76	8 (16%)	67,82,82	1.36	8 (11%)
7	GOL	C	509	-	5,5,5	0.39	0	5,5,5	0.51	0
2	HEM	B	501	1	50,50,50	1.64	10 (20%)	67,82,82	1.35	8 (11%)
6	BTB	D	507	-	13,13,13	0.61	0	7,16,16	0.88	0
7	GOL	C	508	-	5,5,5	0.35	0	5,5,5	0.48	0
7	GOL	A	508	-	5,5,5	0.37	0	5,5,5	0.34	0
7	GOL	D	508	-	5,5,5	0.38	0	5,5,5	0.21	0
4	A1BTW	C	503	-	35,35,35	0.96	3 (8%)	40,46,46	1.25	2 (5%)
6	BTB	D	506	11	13,13,13	0.40	0	7,16,16	0.69	0
7	GOL	D	509	-	5,5,5	0.33	0	5,5,5	0.87	0
2	HEM	C	501	1	50,50,50	1.65	8 (16%)	67,82,82	1.26	6 (8%)
5	ACT	A	504	-	3,3,3	0.78	0	3,3,3	0.91	0
6	BTB	B	506	-	13,13,13	0.54	0	7,16,16	1.86	2 (28%)
6	BTB	C	506	-	13,13,13	0.60	0	7,16,16	1.19	1 (14%)
6	BTB	C	505	11	13,13,13	0.44	0	7,16,16	0.60	0
4	A1BTW	B	503	-	35,35,35	1.01	4 (11%)	40,46,46	1.53	5 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	GOL	B	508	-	5,5,5	0.38	0	5,5,5	0.31	0
4	A1BTW	A	503	-	35,35,35	0.95	3 (8%)	40,46,46	1.56	7 (17%)
3	H4B	B	502	-	17,18,18	0.90	1 (5%)	14,26,26	1.88	4 (28%)
3	H4B	D	503	-	17,18,18	0.80	0	14,26,26	2.17	4 (28%)
5	ACT	D	505	-	3,3,3	0.81	0	3,3,3	0.75	0
7	GOL	A	509	-	5,5,5	0.37	0	5,5,5	0.51	0
2	HEM	D	502	1	50,50,50	1.72	8 (16%)	67,82,82	1.29	8 (11%)
6	BTB	A	506	-	13,13,13	0.80	0	7,16,16	0.96	0
6	BTB	A	505	11	13,13,13	0.40	0	7,16,16	1.48	2 (28%)
5	ACT	B	504	-	3,3,3	0.81	0	3,3,3	0.75	0
7	GOL	A	507	-	5,5,5	0.35	0	5,5,5	1.00	0
7	GOL	D	510	-	5,5,5	0.39	0	5,5,5	0.16	0
3	H4B	A	502	-	17,18,18	0.93	0	14,26,26	1.84	4 (28%)
5	ACT	C	504	-	3,3,3	0.81	0	3,3,3	0.79	0
6	BTB	B	505	11	13,13,13	0.49	0	7,16,16	0.94	1 (14%)

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	A1BTW	D	504	-	-	1/17/21/21	0/4/4/4
7	GOL	B	507	-	-	4/4/4/4	-
3	H4B	C	502	-	-	0/8/17/17	0/2/2/2
7	GOL	C	507	-	-	2/4/4/4	-
2	HEM	A	501	1	-	1/14/54/54	-
7	GOL	C	509	-	-	0/4/4/4	-
2	HEM	B	501	1	-	0/14/54/54	-
6	BTB	D	507	-	-	9/21/21/21	-
7	GOL	C	508	-	-	2/4/4/4	-
7	GOL	A	508	-	-	4/4/4/4	-
7	GOL	D	508	-	-	2/4/4/4	-
6	BTB	D	506	11	-	4/21/21/21	-
4	A1BTW	C	503	-	-	1/17/21/21	0/4/4/4
7	GOL	D	509	-	-	3/4/4/4	-
2	HEM	C	501	1	-	2/14/54/54	-
6	BTB	B	506	-	-	8/21/21/21	-
6	BTB	C	506	-	-	12/21/21/21	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BTB	C	505	11	-	5/21/21/21	-
4	A1BTW	B	503	-	-	1/17/21/21	0/4/4/4
7	GOL	B	508	-	-	1/4/4/4	-
4	A1BTW	A	503	-	-	1/17/21/21	0/4/4/4
3	H4B	B	502	-	-	0/8/17/17	0/2/2/2
3	H4B	D	503	-	-	0/8/17/17	0/2/2/2
7	GOL	A	509	-	-	3/4/4/4	-
2	HEM	D	502	1	-	0/14/54/54	-
6	BTB	A	506	-	-	12/21/21/21	-
6	BTB	A	505	11	-	1/21/21/21	-
7	GOL	A	507	-	-	4/4/4/4	-
7	GOL	D	510	-	-	3/4/4/4	-
3	H4B	A	502	-	-	0/8/17/17	0/2/2/2
6	BTB	B	505	11	-	5/21/21/21	-

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	FE-NB	5.44	2.11	1.94
2	C	501	HEM	FE-ND	5.44	2.11	1.94
2	D	502	HEM	FE-NB	5.02	2.10	1.94
2	A	501	HEM	FE-ND	4.95	2.10	1.94
2	A	501	HEM	FE-NC	4.91	2.11	1.95
2	D	502	HEM	FE-NA	4.83	2.11	1.95
2	B	501	HEM	FE-NB	4.65	2.09	1.94
2	D	502	HEM	FE-NC	4.46	2.09	1.95
2	B	501	HEM	FE-ND	4.31	2.08	1.94
2	C	501	HEM	FE-NB	4.18	2.07	1.94
2	B	501	HEM	FE-NC	3.99	2.08	1.95
2	C	501	HEM	FE-NA	3.98	2.08	1.95
2	A	501	HEM	FE-NA	3.89	2.08	1.95
2	D	502	HEM	FE-ND	3.79	2.06	1.94
2	C	501	HEM	FE-NC	3.71	2.07	1.95
2	B	501	HEM	FE-NA	3.41	2.06	1.95
4	D	504	A1BTW	C06-N07	-3.32	1.32	1.38
4	B	503	A1BTW	C06-N07	-3.28	1.32	1.38
2	D	502	HEM	CAB-C3B	3.25	1.56	1.47
4	C	503	A1BTW	C06-N07	-3.19	1.32	1.38
2	A	501	HEM	CAB-C3B	3.10	1.55	1.47
2	C	501	HEM	CAB-C3B	3.01	1.55	1.47
2	D	502	HEM	CAC-C3C	2.90	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	503	A1BTW	C06-N07	-2.90	1.33	1.38
2	A	501	HEM	CAC-C3C	2.89	1.55	1.47
2	B	501	HEM	CAB-C3B	2.89	1.55	1.47
2	C	501	HEM	CAC-C3C	2.86	1.55	1.47
4	A	503	A1BTW	C11-N07	-2.80	1.36	1.41
4	A	503	A1BTW	C05-C06	2.78	1.50	1.45
4	C	503	A1BTW	C11-N07	-2.70	1.36	1.41
2	B	501	HEM	CAC-C3C	2.60	1.54	1.47
4	B	503	A1BTW	C11-N07	-2.53	1.36	1.41
2	A	501	HEM	CMC-C2C	2.43	1.55	1.50
2	D	502	HEM	CMD-C2D	2.43	1.55	1.50
4	D	504	A1BTW	C11-N07	-2.41	1.36	1.41
2	D	502	HEM	CMB-C2B	2.34	1.55	1.50
4	D	504	A1BTW	C05-C06	2.33	1.49	1.45
4	C	503	A1BTW	C05-C06	2.29	1.49	1.45
2	C	501	HEM	CMC-C2C	2.23	1.55	1.50
4	B	503	A1BTW	C04-C05	2.21	1.41	1.36
2	B	501	HEM	CMD-C2D	2.16	1.55	1.50
2	B	501	HEM	CMA-C3A	2.16	1.55	1.50
4	B	503	A1BTW	C05-C06	2.16	1.49	1.45
3	B	502	H4B	C4-N3	-2.13	1.34	1.38
2	B	501	HEM	CMC-C2C	2.13	1.55	1.50
4	D	504	A1BTW	C04-C05	2.12	1.40	1.36
2	A	501	HEM	CMB-C2B	2.10	1.55	1.50
2	C	501	HEM	CMB-C2B	2.07	1.55	1.50
2	B	501	HEM	CMB-C2B	2.06	1.55	1.50
3	C	502	H4B	C4-N3	-2.05	1.35	1.38

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	504	A1BTW	S01-C02-N03	-5.80	105.83	115.15
4	D	504	A1BTW	C04-N03-C02	5.22	119.46	110.24
4	C	503	A1BTW	S01-C02-N03	-5.13	106.91	115.15
4	A	503	A1BTW	S01-C02-N03	-5.11	106.95	115.15
4	B	503	A1BTW	S01-C02-N03	-4.68	107.64	115.15
4	B	503	A1BTW	C04-N03-C02	4.43	118.06	110.24
3	D	503	H4B	C2-N1-C8A	4.21	120.79	113.36
4	D	504	A1BTW	C04-C05-C06	4.16	137.12	130.64
4	D	504	A1BTW	C06-C05-S01	-4.15	113.23	120.28
3	C	502	H4B	C2-N1-C8A	4.12	120.63	113.36
3	A	502	H4B	C2-N1-C8A	4.02	120.45	113.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	503	A1BTW	C04-N03-C02	3.92	117.16	110.24
3	B	502	H4B	C2-N1-C8A	3.92	120.27	113.36
4	A	503	A1BTW	C04-N03-C02	3.84	117.02	110.24
6	B	506	BTB	O4-C4-C2	3.68	120.06	111.40
3	D	503	H4B	O4-C4-C4A	-3.62	118.52	127.26
2	D	502	HEM	C3B-C4B-NB	-3.43	107.01	109.47
2	B	501	HEM	C3B-C4B-NB	-3.39	107.03	109.47
4	B	503	A1BTW	C06-C05-S01	-3.24	114.78	120.28
6	A	505	BTB	O3-C3-C2	3.20	118.92	111.40
2	A	501	HEM	CBA-CAA-C2A	-3.16	103.80	112.53
2	B	501	HEM	C3D-C4D-ND	-3.09	106.78	110.17
2	B	501	HEM	C1B-NB-C4B	3.01	108.78	105.21
4	B	503	A1BTW	C04-C05-C06	3.00	135.31	130.64
2	A	501	HEM	C3B-C4B-NB	-2.99	107.32	109.47
3	D	503	H4B	C4A-C4-N3	2.95	120.24	112.13
2	A	501	HEM	C4D-ND-C1D	2.88	108.62	105.21
2	C	501	HEM	C3B-C2B-C1B	2.86	108.56	106.41
2	A	501	HEM	C2A-C1A-NA	-2.83	107.01	110.15
2	B	501	HEM	C4D-ND-C1D	2.79	108.52	105.21
2	D	502	HEM	C1B-NB-C4B	2.79	108.51	105.21
3	C	502	H4B	O4-C4-C4A	-2.79	120.54	127.26
3	A	502	H4B	O4-C4-C4A	-2.78	120.55	127.26
3	A	502	H4B	C2-N3-C4	-2.77	120.09	125.11
2	A	501	HEM	C3D-C4D-ND	-2.77	107.14	110.17
4	A	503	A1BTW	C04-C05-C06	2.74	134.91	130.64
3	A	502	H4B	C4A-C4-N3	2.71	119.58	112.13
2	C	501	HEM	C1B-NB-C4B	2.71	108.42	105.21
2	B	501	HEM	C3B-C2B-C1B	2.71	108.45	106.41
2	B	501	HEM	C2A-C1A-NA	-2.70	107.16	110.15
2	D	502	HEM	CHA-C4D-ND	2.70	127.70	124.37
4	A	503	A1BTW	C19-C20-C21	-2.66	107.24	112.85
4	B	503	A1BTW	C19-C20-C21	-2.65	107.26	112.85
2	C	501	HEM	C3B-C4B-NB	-2.64	107.57	109.47
3	C	502	H4B	C4A-C4-N3	2.63	119.36	112.13
2	D	502	HEM	CBA-CAA-C2A	-2.61	105.31	112.53
3	D	503	H4B	C2-N3-C4	-2.59	120.42	125.11
6	B	506	BTB	C8-C7-N	-2.57	101.54	111.59
2	D	502	HEM	CHC-C1C-NC	2.53	127.21	124.45
6	C	506	BTB	O3-C3-C2	-2.53	105.44	111.40
3	C	502	H4B	C11-C10-C9	-2.53	109.02	112.11
2	C	501	HEM	C4D-ND-C1D	2.49	108.16	105.21
3	B	502	H4B	O10-C10-C9	-2.48	105.67	109.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	503	A1BTW	C06-C05-S01	-2.46	116.09	120.28
2	B	501	HEM	CHC-C4B-NB	2.46	127.07	124.42
4	D	504	A1BTW	C19-C20-C21	-2.44	107.71	112.85
2	B	501	HEM	CBA-CAA-C2A	-2.42	105.84	112.53
2	A	501	HEM	C1B-NB-C4B	2.41	108.06	105.21
3	B	502	H4B	C4A-C4-N3	2.41	118.75	112.13
2	A	501	HEM	C3B-C2B-C1B	2.29	108.13	106.41
2	D	502	HEM	C4C-NC-C1C	2.26	109.50	105.82
4	A	503	A1BTW	C11-N07-C06	-2.24	123.25	128.41
2	D	502	HEM	C3D-C4D-ND	-2.17	107.79	110.17
4	A	503	A1BTW	C15-C17-N18	-2.14	106.05	112.79
3	B	502	H4B	O4-C4-C4A	-2.14	122.10	127.26
3	C	502	H4B	C2-N3-C4	-2.11	121.29	125.11
2	D	502	HEM	C4D-ND-C1D	2.08	107.67	105.21
2	C	501	HEM	C4C-NC-C1C	2.08	109.21	105.82
6	A	505	BTB	O4-C4-C2	2.04	116.21	111.40
2	C	501	HEM	C2A-C1A-NA	-2.04	107.89	110.15
6	B	505	BTB	O1-C1-C2	2.03	116.18	111.40
2	A	501	HEM	CAD-C3D-C2D	-2.02	124.08	127.87

There are no chirality outliers.

All (91) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	503	A1BTW	C21-C26-C27-N28
6	A	506	BTB	O1-C1-C2-C4
6	A	506	BTB	O1-C1-C2-N
6	A	506	BTB	C1-C2-C4-O4
6	A	506	BTB	C3-C2-C4-O4
6	A	506	BTB	N-C2-C4-O4
6	B	505	BTB	C1-C2-C4-O4
6	B	505	BTB	C3-C2-C4-O4
6	B	505	BTB	N-C2-C4-O4
6	B	506	BTB	C1-C2-C3-O3
6	B	506	BTB	C4-C2-C3-O3
6	B	506	BTB	N-C2-C3-O3
6	B	506	BTB	C1-C2-C4-O4
6	B	506	BTB	C3-C2-C4-O4
6	B	506	BTB	N-C2-C4-O4
6	C	505	BTB	O1-C1-C2-C3
6	C	505	BTB	O1-C1-C2-N
6	C	505	BTB	C1-C2-C4-O4

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Mol	Chain	Res	Type	Atoms
6	C	505	BTB	C3-C2-C4-O4
6	C	505	BTB	N-C2-C4-O4
6	C	506	BTB	C1-C2-C4-O4
6	C	506	BTB	C3-C2-C4-O4
6	C	506	BTB	N-C2-C4-O4
6	C	506	BTB	C1-C2-N-C5
6	C	506	BTB	C1-C2-N-C7
6	C	506	BTB	C3-C2-N-C5
6	C	506	BTB	C3-C2-N-C7
6	C	506	BTB	C4-C2-N-C5
6	C	506	BTB	C4-C2-N-C7
6	D	506	BTB	O1-C1-C2-C3
6	D	506	BTB	O1-C1-C2-C4
6	D	506	BTB	O1-C1-C2-N
6	D	507	BTB	O1-C1-C2-C3
6	D	507	BTB	O1-C1-C2-C4
6	D	507	BTB	O1-C1-C2-N
6	D	507	BTB	C1-C2-C4-O4
6	D	507	BTB	C3-C2-C4-O4
6	D	507	BTB	N-C2-C4-O4
6	D	507	BTB	C8-C7-N-C5
7	A	507	GOL	O1-C1-C2-C3
7	A	507	GOL	C1-C2-C3-O3
7	A	508	GOL	O1-C1-C2-C3
7	A	508	GOL	C1-C2-C3-O3
7	A	509	GOL	O1-C1-C2-C3
7	B	507	GOL	O1-C1-C2-C3
7	C	507	GOL	O1-C1-C2-C3
7	C	508	GOL	O1-C1-C2-C3
6	B	506	BTB	N-C7-C8-O8
6	C	506	BTB	N-C7-C8-O8
7	A	508	GOL	O2-C2-C3-O3
7	B	507	GOL	O1-C1-C2-O2
6	D	507	BTB	N-C7-C8-O8
6	A	506	BTB	N-C7-C8-O8
7	B	507	GOL	C1-C2-C3-O3
7	D	508	GOL	O1-C1-C2-C3
7	D	510	GOL	C1-C2-C3-O3
6	D	507	BTB	N-C5-C6-O6
7	B	507	GOL	O2-C2-C3-O3
7	C	507	GOL	O1-C1-C2-O2
7	A	507	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
7	A	507	GOL	O2-C2-C3-O3
7	A	509	GOL	O1-C1-C2-O2
7	C	508	GOL	O1-C1-C2-O2
7	D	508	GOL	O1-C1-C2-O2
2	C	501	HEM	C2A-CAA-CBA-CGA
6	B	505	BTB	C4-C2-C3-O3
6	C	506	BTB	O1-C1-C2-C4
7	A	508	GOL	O1-C1-C2-O2
7	D	509	GOL	O1-C1-C2-O2
7	D	509	GOL	O2-C2-C3-O3
6	B	506	BTB	N-C5-C6-O6
6	C	506	BTB	N-C5-C6-O6
7	B	508	GOL	O1-C1-C2-O2
7	D	510	GOL	O2-C2-C3-O3
4	A	503	A1BTW	C21-C26-C27-N28
4	C	503	A1BTW	C21-C26-C27-N28
4	D	504	A1BTW	C21-C26-C27-N28
2	A	501	HEM	C4B-C3B-CAB-CBB
2	C	501	HEM	C4B-C3B-CAB-CBB
6	A	505	BTB	C4-C2-C3-O3
6	A	506	BTB	C3-C2-N-C7
6	A	506	BTB	C4-C2-N-C5
6	A	506	BTB	C4-C2-N-C7
6	D	506	BTB	N-C5-C6-O6
7	D	509	GOL	C1-C2-C3-O3
7	D	510	GOL	O1-C1-C2-C3
7	A	509	GOL	O2-C2-C3-O3
6	A	506	BTB	C1-C2-N-C5
6	A	506	BTB	C1-C2-N-C7
6	A	506	BTB	C3-C2-N-C5
6	B	505	BTB	N-C2-C3-O3

There are no ring outliers.

20 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	504	A1BTW	1	0
3	C	502	H4B	1	0
2	A	501	HEM	2	0
2	B	501	HEM	2	0
6	D	507	BTB	1	0
6	D	506	BTB	2	0

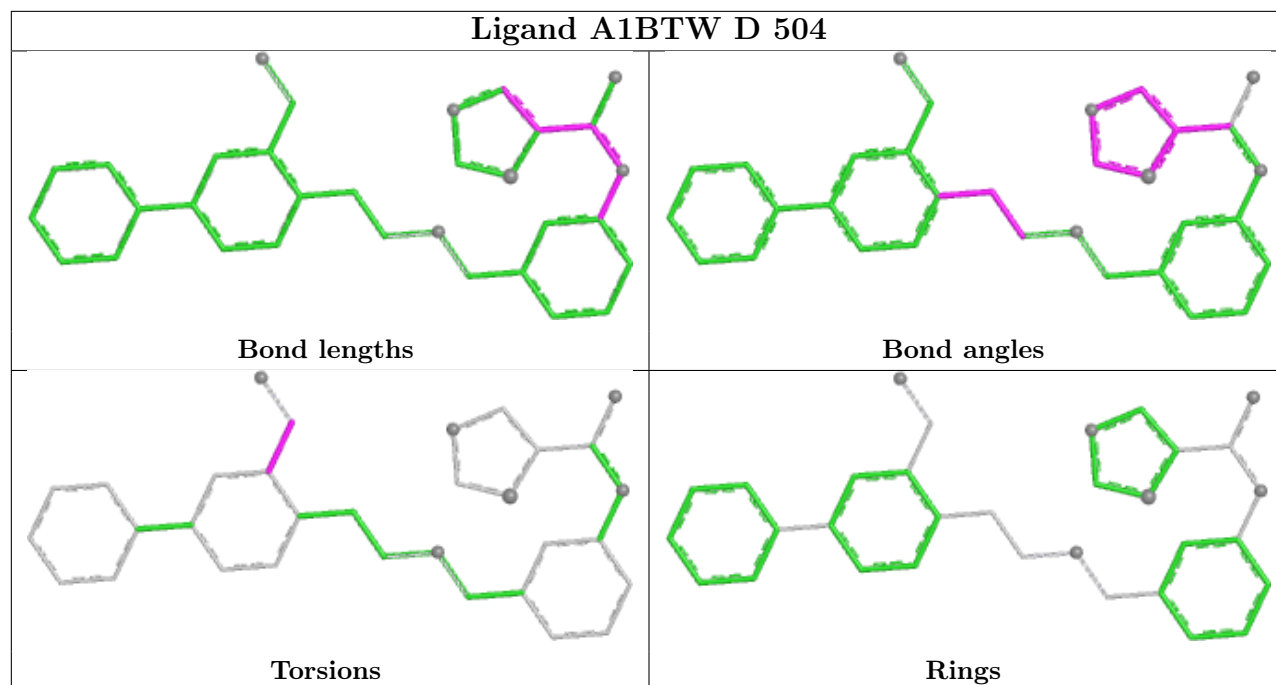
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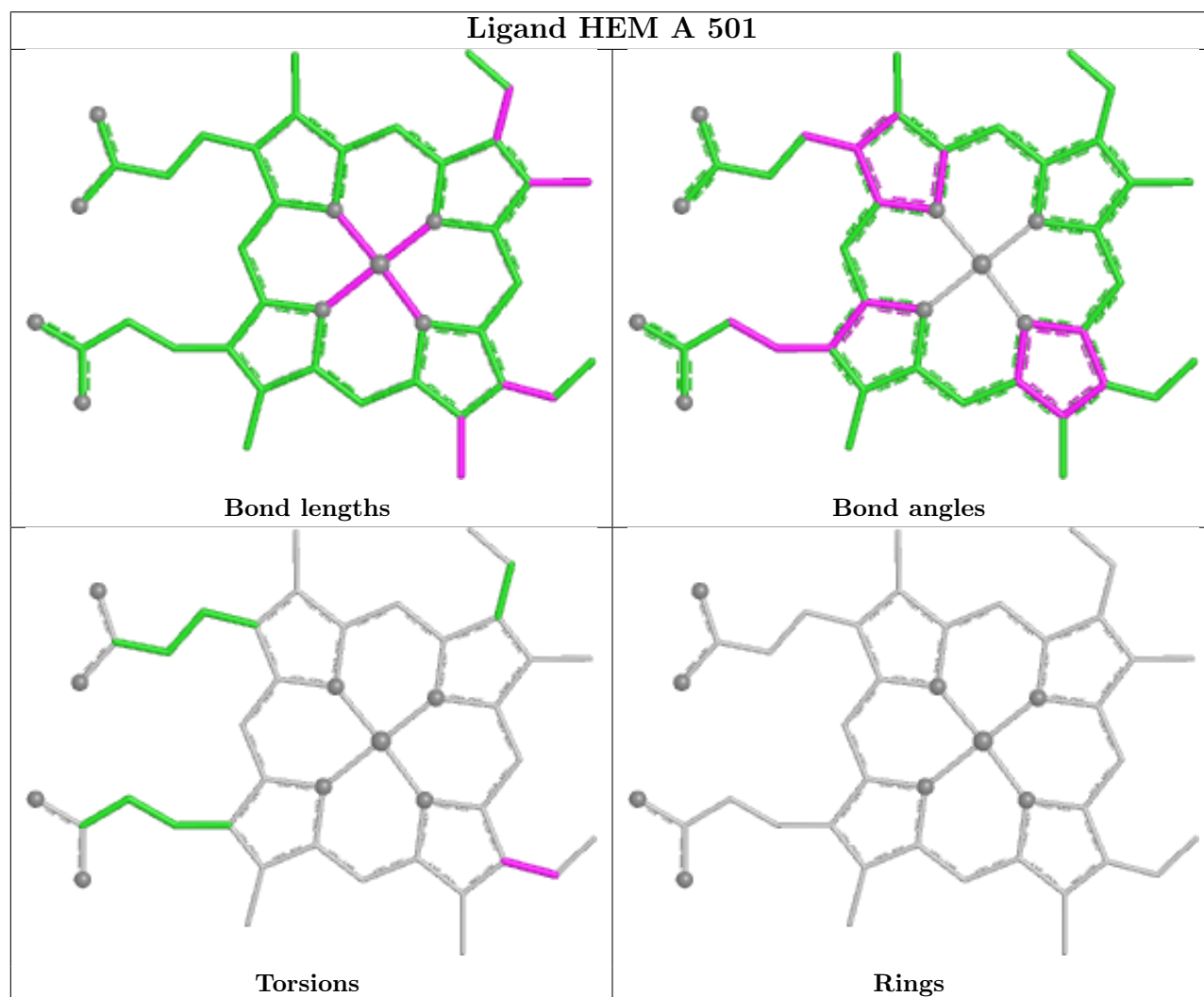
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	HEM	2	0
6	B	506	BTB	1	0
6	C	506	BTB	1	0
6	C	505	BTB	3	0
4	B	503	A1BTW	1	0
4	A	503	A1BTW	2	0
3	B	502	H4B	1	0
3	D	503	H4B	1	0
5	D	505	ACT	1	0
2	D	502	HEM	3	0
6	A	506	BTB	3	0
6	A	505	BTB	2	0
3	A	502	H4B	1	0
6	B	505	BTB	4	0

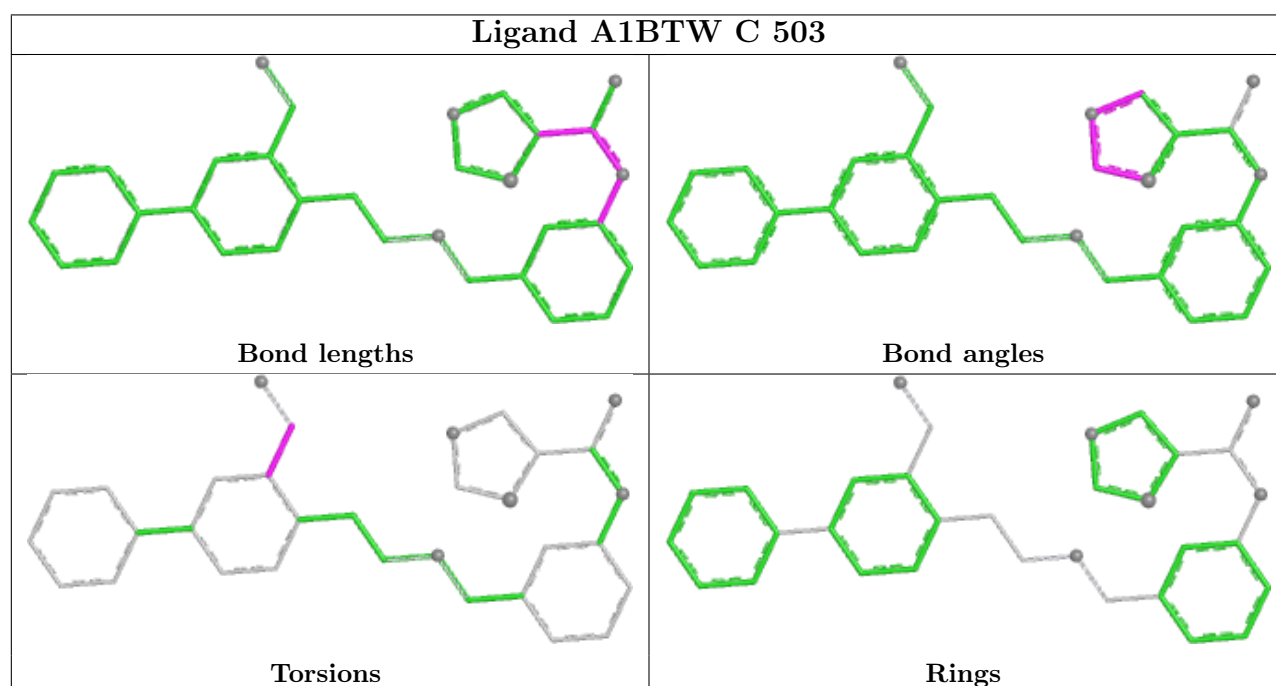
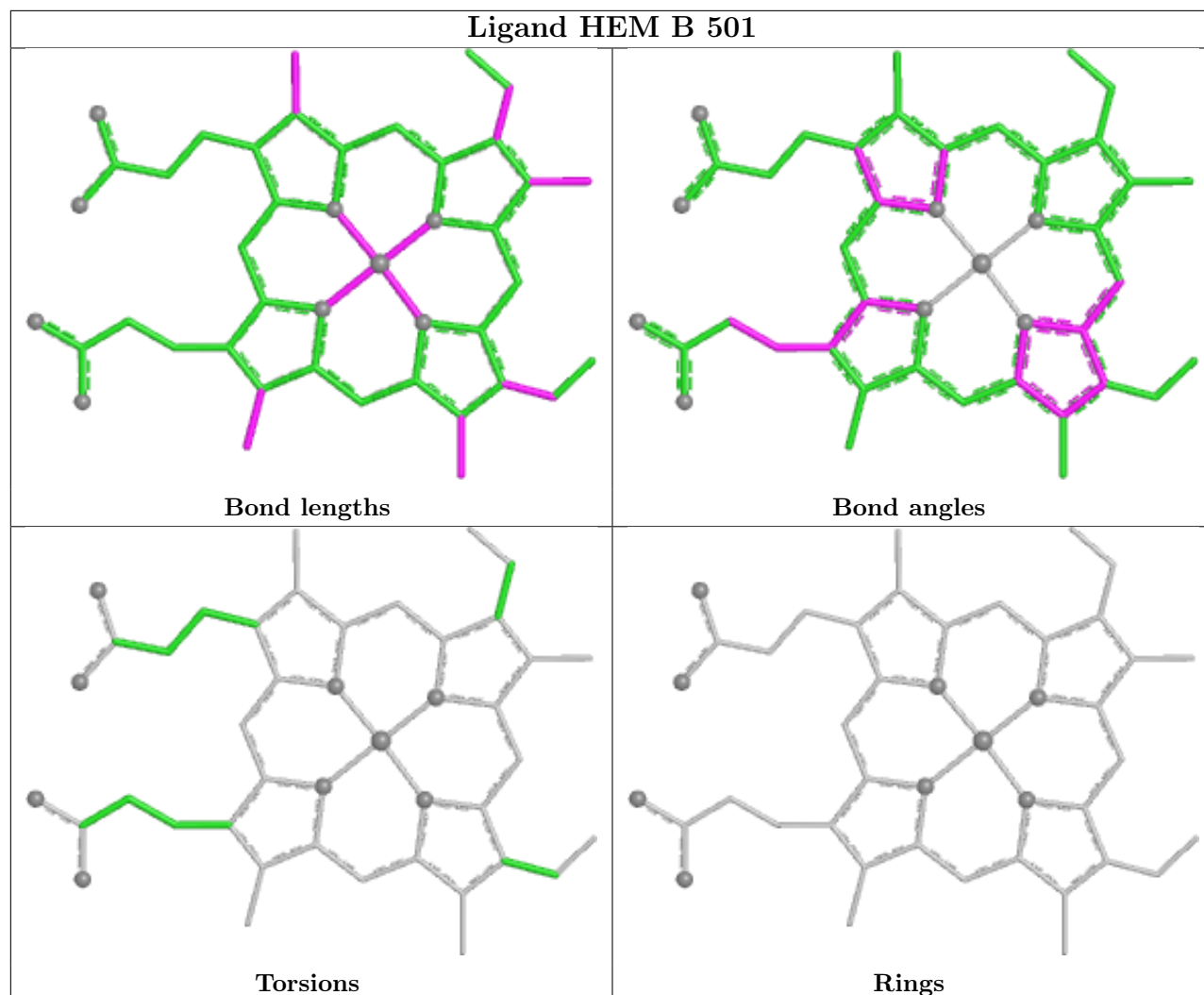
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

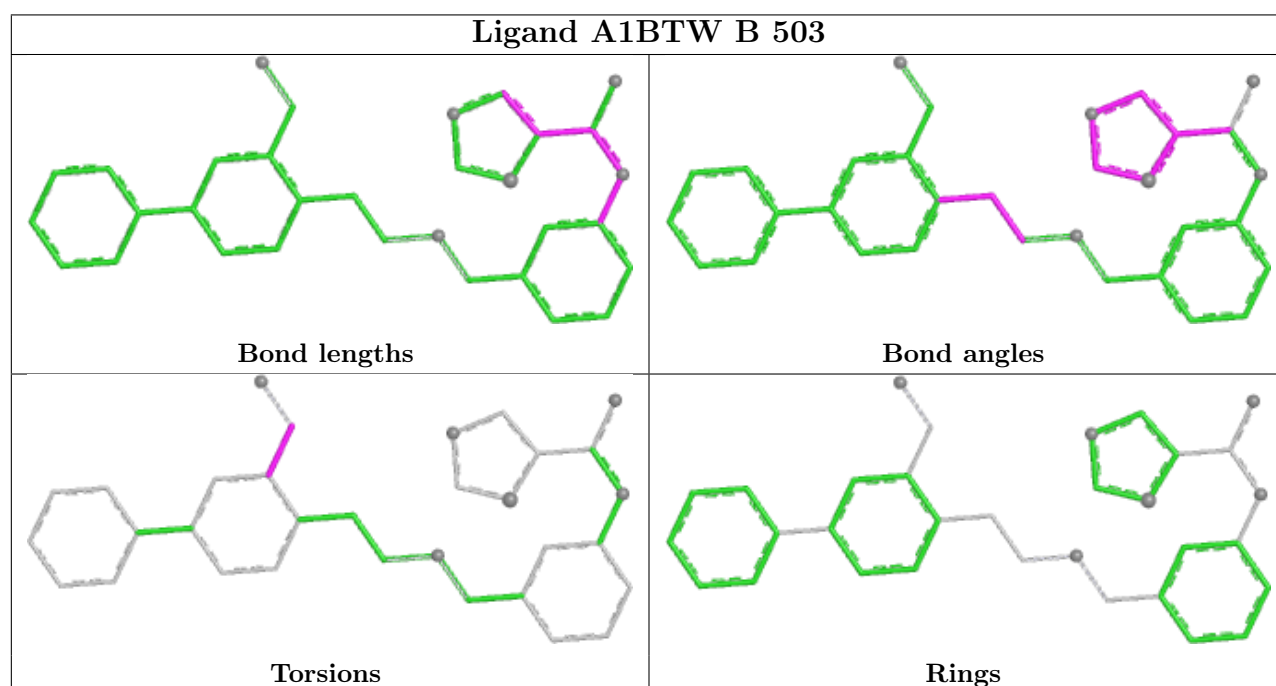
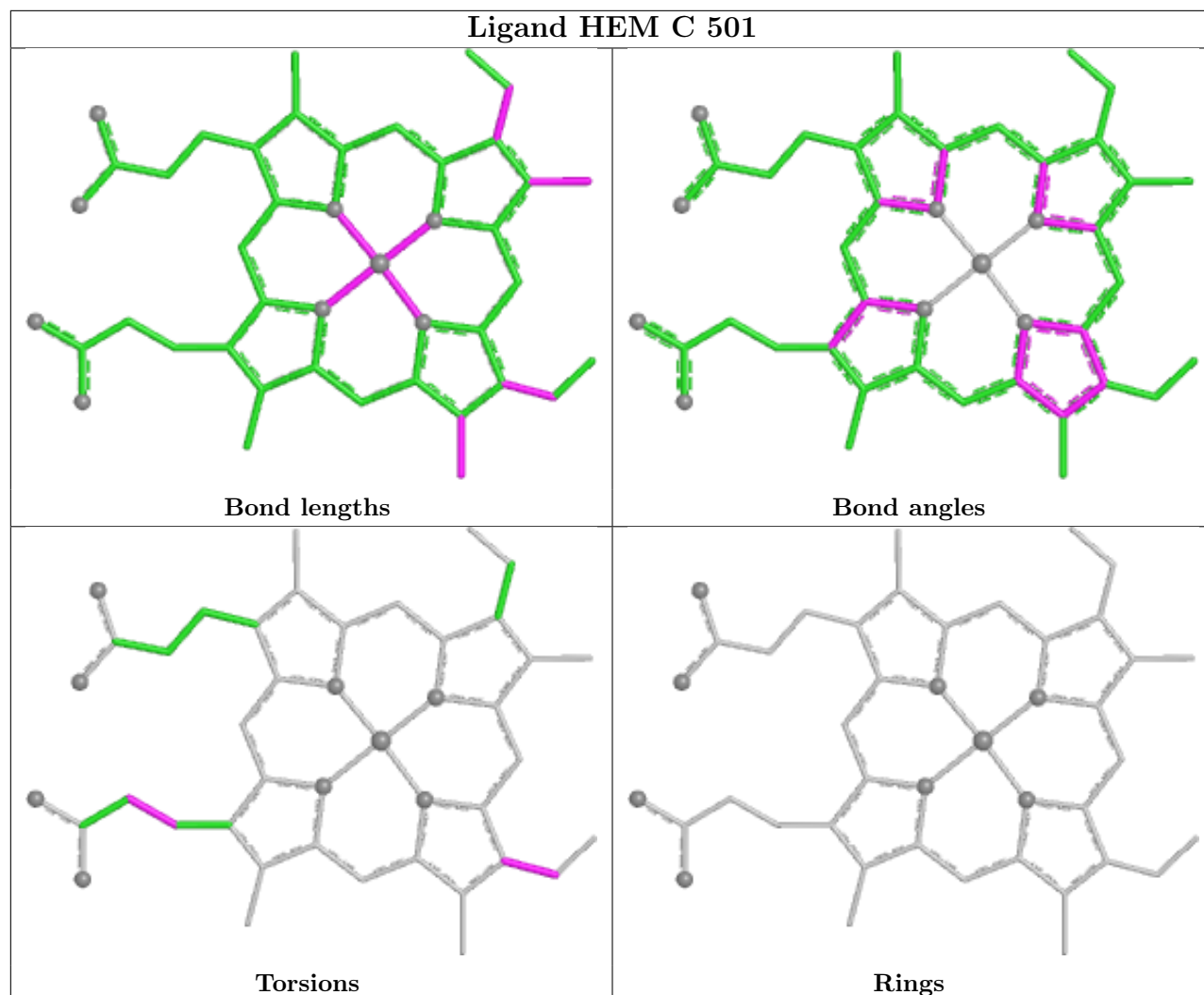
Ligand A1BTW D 504



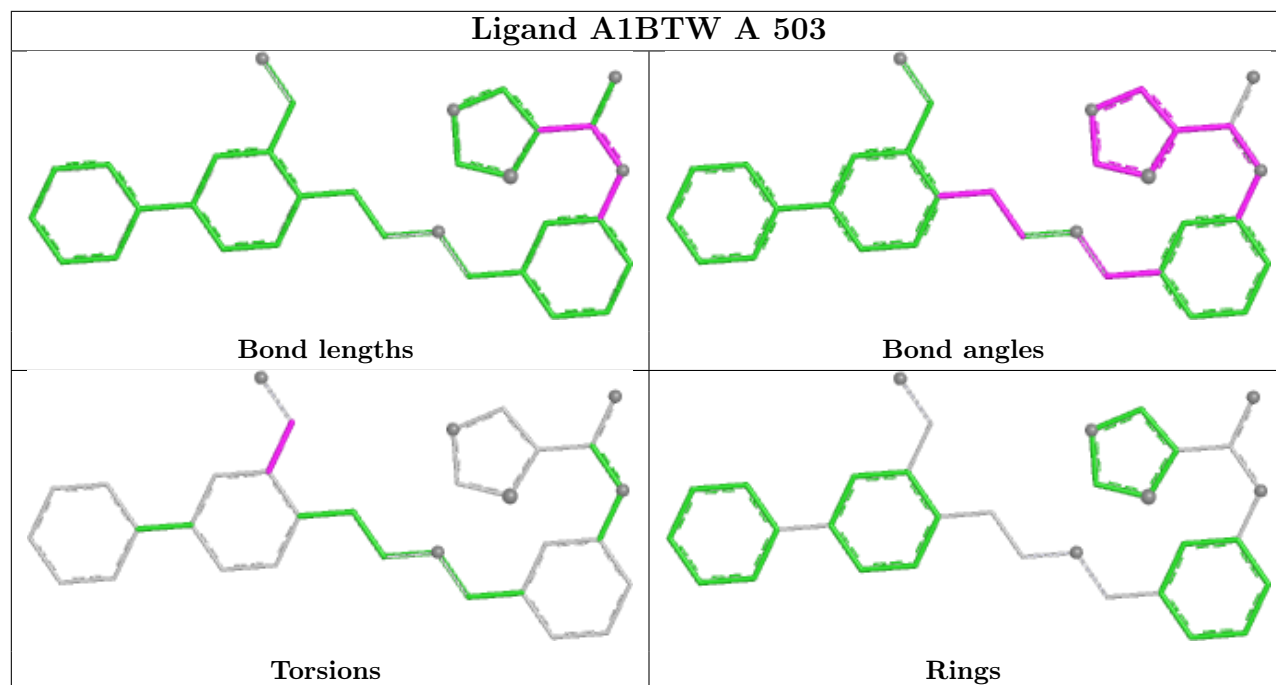
Ligand HEM A 501



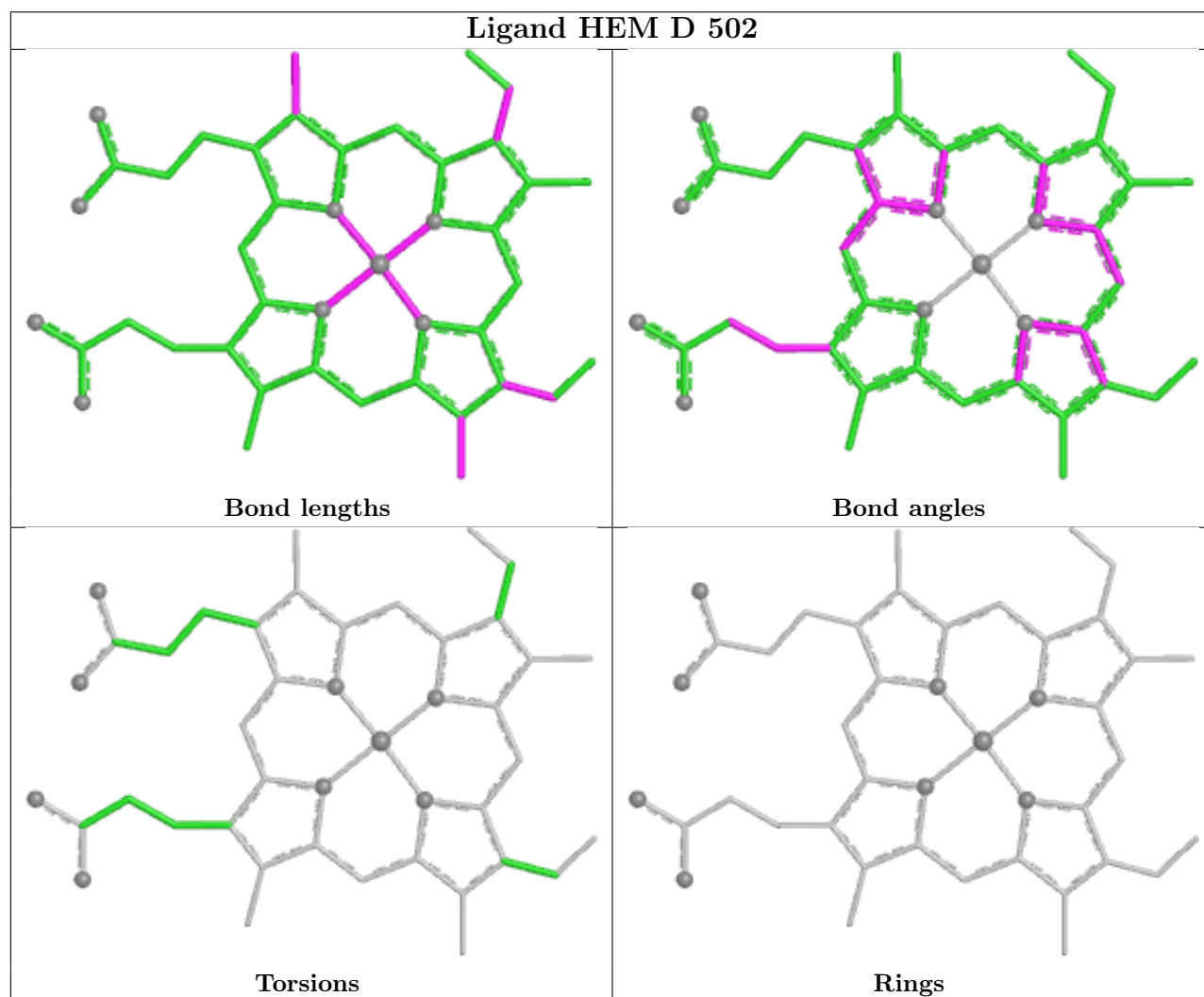




Ligand A1BTW A 503



Ligand HEM D 502



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%)	0.37	11 (2%) 56 56	28, 54, 96, 139	1 (0%)
1	B	401/440 (91%)	-0.04	8 (1%) 65 65	25, 40, 72, 118	1 (0%)
1	C	401/440 (91%)	0.79	57 (14%) 6 5	25, 63, 121, 152	1 (0%)
1	D	402/440 (91%)	0.03	9 (2%) 62 62	22, 40, 81, 117	2 (0%)
All	All	1605/1760 (91%)	0.29	85 (5%) 32 31	22, 48, 103, 152	5 (0%)

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	106	PRO	6.0
1	B	106	PRO	5.3
1	C	204	ALA	5.3
1	D	141	SER	4.8
1	A	120	PRO	4.5
1	C	106	PRO	4.4
1	C	88	ALA	4.1
1	D	106	PRO	4.0
1	C	120	PRO	4.0
1	C	124	LEU	3.3
1	C	158	ALA	3.2
1	C	159	ALA	3.2
1	C	275	ILE	3.2
1	C	279	TRP	3.1
1	C	145	ALA	3.1
1	C	242	ARG	3.1
1	B	119	ALA	3.1
1	C	346	LEU	3.1
1	C	163	TYR	3.0
1	C	244	TRP	3.0
1	C	345	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	268	VAL	3.0
1	B	68	PHE	2.9
1	C	295	ALA	2.9
1	C	302	LEU	2.9
1	C	299	PRO	2.9
1	D	145	ALA	2.9
1	C	303	PHE	2.8
1	C	131	ILE	2.8
1	C	155	ALA	2.8
1	C	161	GLY	2.8
1	C	304	LEU	2.8
1	B	122	GLN	2.7
1	C	165	LEU	2.7
1	C	241	PHE	2.6
1	C	157	VAL	2.6
1	D	142	GLY	2.6
1	C	261	VAL	2.6
1	C	150	LEU	2.6
1	C	153	VAL	2.6
1	C	143	SER	2.5
1	C	144	GLN	2.5
1	D	144	GLN	2.5
1	C	343	ILE	2.5
1	C	259	GLY	2.5
1	B	89	GLN	2.5
1	A	124	LEU	2.4
1	A	138	ILE	2.4
1	C	160	THR	2.4
1	B	257	GLN	2.4
1	C	341	LEU	2.4
1	C	123	LEU	2.3
1	C	273	LEU	2.3
1	C	236	PRO	2.3
1	C	130	PHE	2.3
1	D	68	PHE	2.3
1	C	243	ILE	2.3
1	A	141	SER	2.3
1	B	258	ASP	2.3
1	A	235	CYS	2.3
1	A	238	ARG	2.2
1	B	259	GLY	2.2
1	A	273	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	134	TYR	2.2
1	C	230	VAL	2.2
1	C	162	THR	2.2
1	C	231	PHE	2.2
1	C	255	ARG	2.2
1	C	297	ASP	2.2
1	C	235	CYS	2.2
1	C	237	GLY	2.2
1	C	278	GLY	2.1
1	C	146	HIS	2.1
1	D	119	ALA	2.1
1	D	89	GLN	2.1
1	C	475	TYR	2.1
1	C	239	GLY	2.1
1	C	309	LEU	2.1
1	C	135	TYR	2.0
1	A	257	GLN	2.0
1	A	228	ILE	2.0
1	A	468	PHE	2.0
1	C	142	GLY	2.0
1	D	257	GLN	2.0
1	C	479	PRO	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
7	GOL	C	508	6/6	0.42	0.16	88,93,94,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	GOL	A	508	6/6	0.46	0.15	94,95,95,96	0
7	GOL	C	507	6/6	0.54	0.19	87,94,94,95	0
7	GOL	B	507	6/6	0.66	0.17	86,94,98,99	0
7	GOL	D	510	6/6	0.68	0.14	83,84,87,89	0
7	GOL	D	508	6/6	0.79	0.15	62,77,83,89	0
6	BTB	B	506	14/14	0.84	0.14	50,84,90,92	0
6	BTB	C	506	14/14	0.85	0.15	48,70,76,78	0
6	BTB	D	506	14/14	0.87	0.14	53,57,77,86	0
6	BTB	D	507	14/14	0.87	0.14	29,68,79,80	0
5	ACT	A	504	4/4	0.87	0.13	55,58,60,65	0
6	BTB	A	506	14/14	0.87	0.17	16,62,69,73	0
4	A1BTW	C	503	32/32	0.88	0.16	37,63,96,98	0
5	ACT	C	504	4/4	0.88	0.16	68,70,72,74	0
6	BTB	C	505	14/14	0.88	0.15	36,87,99,104	0
6	BTB	B	505	14/14	0.90	0.11	41,57,67,67	0
7	GOL	A	507	6/6	0.90	0.11	40,49,61,64	0
4	A1BTW	A	503	32/32	0.91	0.15	24,48,109,111	0
7	GOL	C	509	6/6	0.91	0.14	58,62,67,71	0
5	ACT	D	505	4/4	0.92	0.10	47,51,53,55	0
7	GOL	A	509	6/6	0.92	0.14	56,64,66,72	0
7	GOL	B	508	6/6	0.93	0.12	40,58,66,72	0
5	ACT	B	504	4/4	0.93	0.11	46,53,54,59	0
7	GOL	D	509	6/6	0.94	0.10	41,46,47,47	0
6	BTB	A	505	14/14	0.94	0.10	27,60,67,69	0
4	A1BTW	D	504	32/32	0.95	0.10	11,41,61,66	0
4	A1BTW	B	503	32/32	0.95	0.10	9,40,73,76	0
11	GD	C	511	1/1	0.95	0.09	107,107,107,107	0
2	HEM	C	501	43/43	0.96	0.09	35,47,58,61	0
8	CL	C	510	1/1	0.96	0.08	55,55,55,55	0
11	GD	B	510	1/1	0.96	0.06	48,48,48,48	0
3	H4B	C	502	17/17	0.96	0.07	39,45,50,50	0
3	H4B	A	502	17/17	0.97	0.06	31,35,40,47	0
3	H4B	B	502	17/17	0.97	0.05	28,32,38,42	0
2	HEM	A	501	43/43	0.97	0.08	31,38,47,55	0
8	CL	A	510	1/1	0.98	0.06	45,45,45,45	0
2	HEM	D	502	43/43	0.98	0.06	23,30,37,39	0
9	ZN	C	512	1/1	0.98	0.04	39,39,39,39	0
10	CA	A	512	1/1	0.98	0.05	55,55,55,55	0
2	HEM	B	501	43/43	0.98	0.06	23,28,35,38	0
3	H4B	D	503	17/17	0.98	0.05	28,30,37,38	0
11	GD	D	501	1/1	0.98	0.09	68,68,68,68	0
11	GD	D	512	1/1	0.98	0.04	44,44,44,44	0

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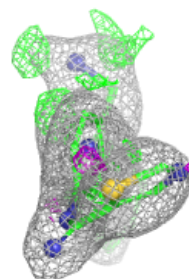
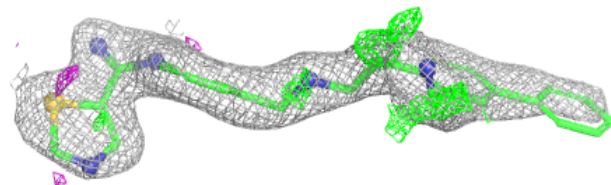
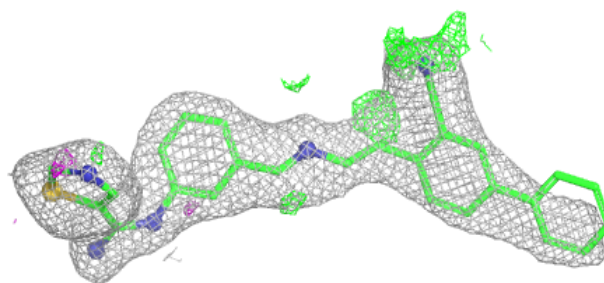
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	CL	D	511	1/1	0.99	0.04	34,34,34,34	0
10	CA	B	511	1/1	0.99	0.04	38,38,38,38	0
8	CL	B	509	1/1	0.99	0.05	37,37,37,37	0
9	ZN	A	511	1/1	1.00	0.03	34,34,34,34	0

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.

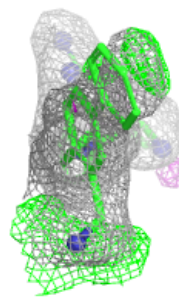
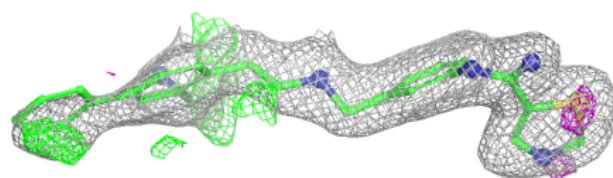
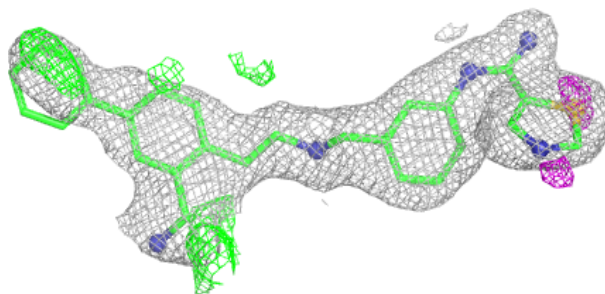
Electron density around A1BTW C 503:

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

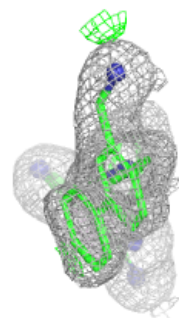
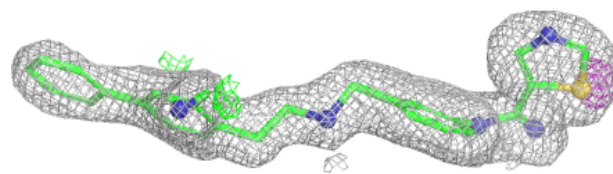
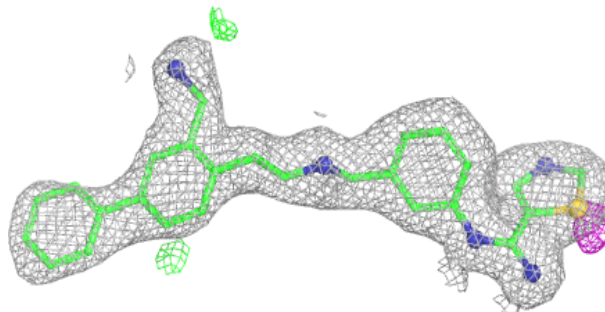


Electron density around A1BTW A 503:

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

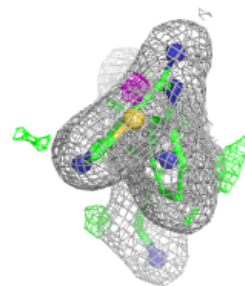
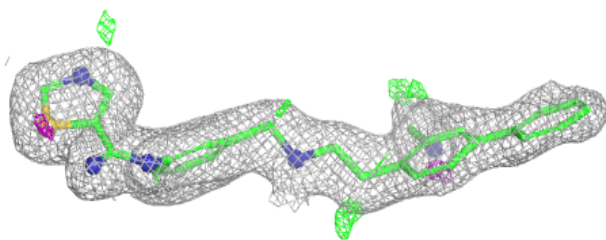
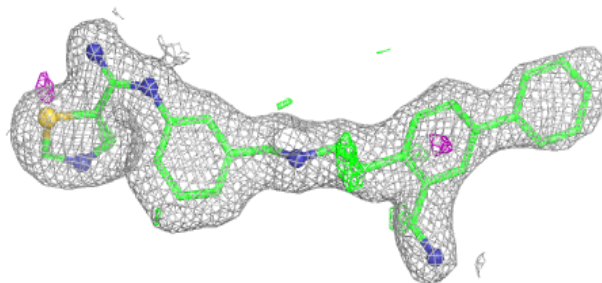
**Electron density around A1BTW D 504:**

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



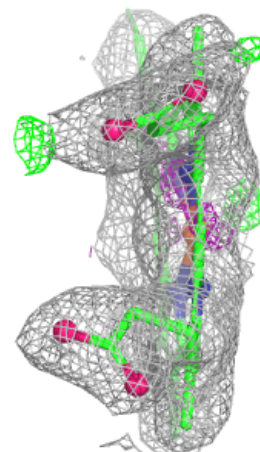
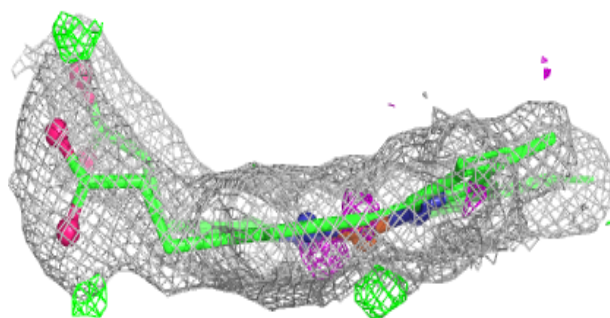
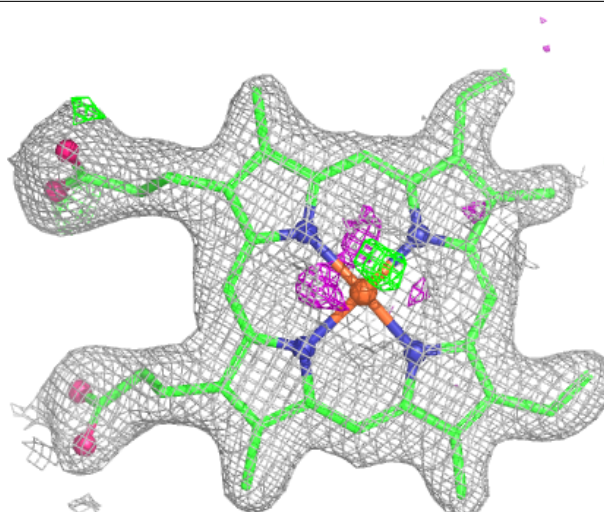
Electron density around A1BTW B 503:

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



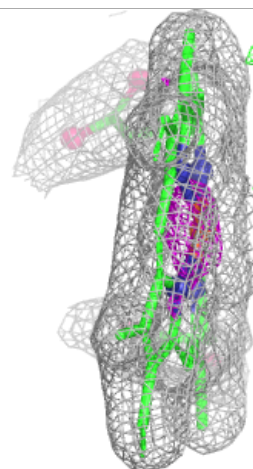
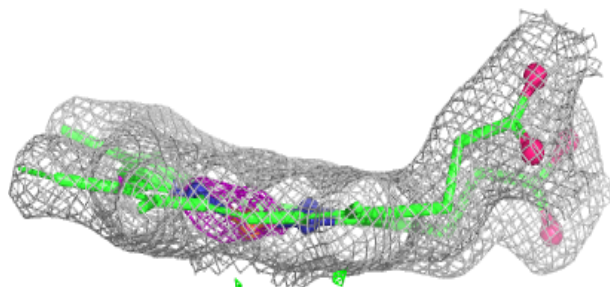
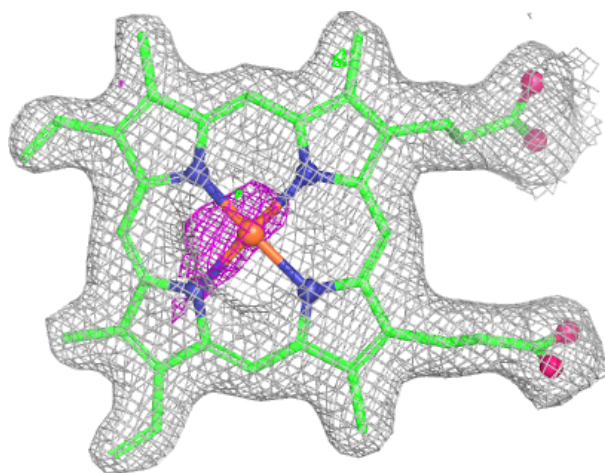
Electron density around HEM C 501:

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



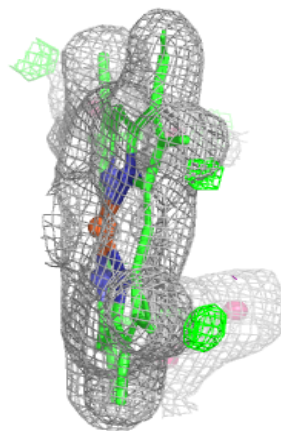
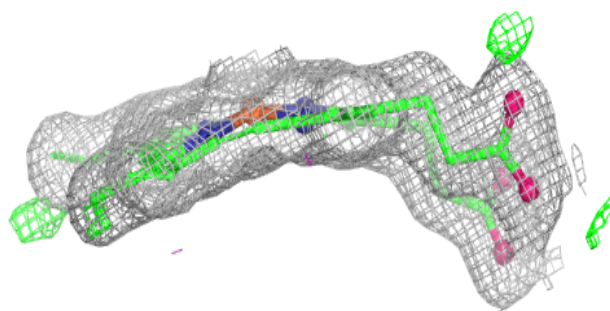
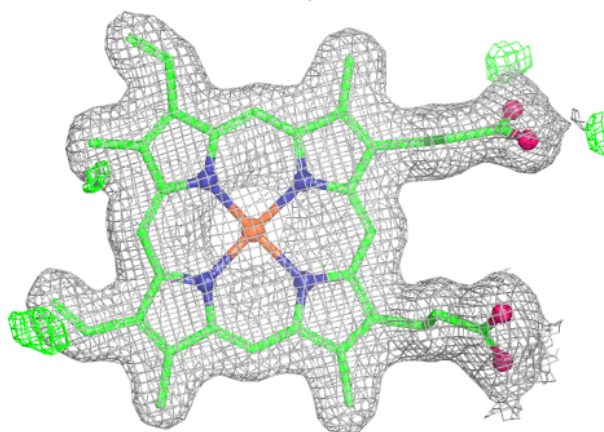
Electron density around HEM A 501:

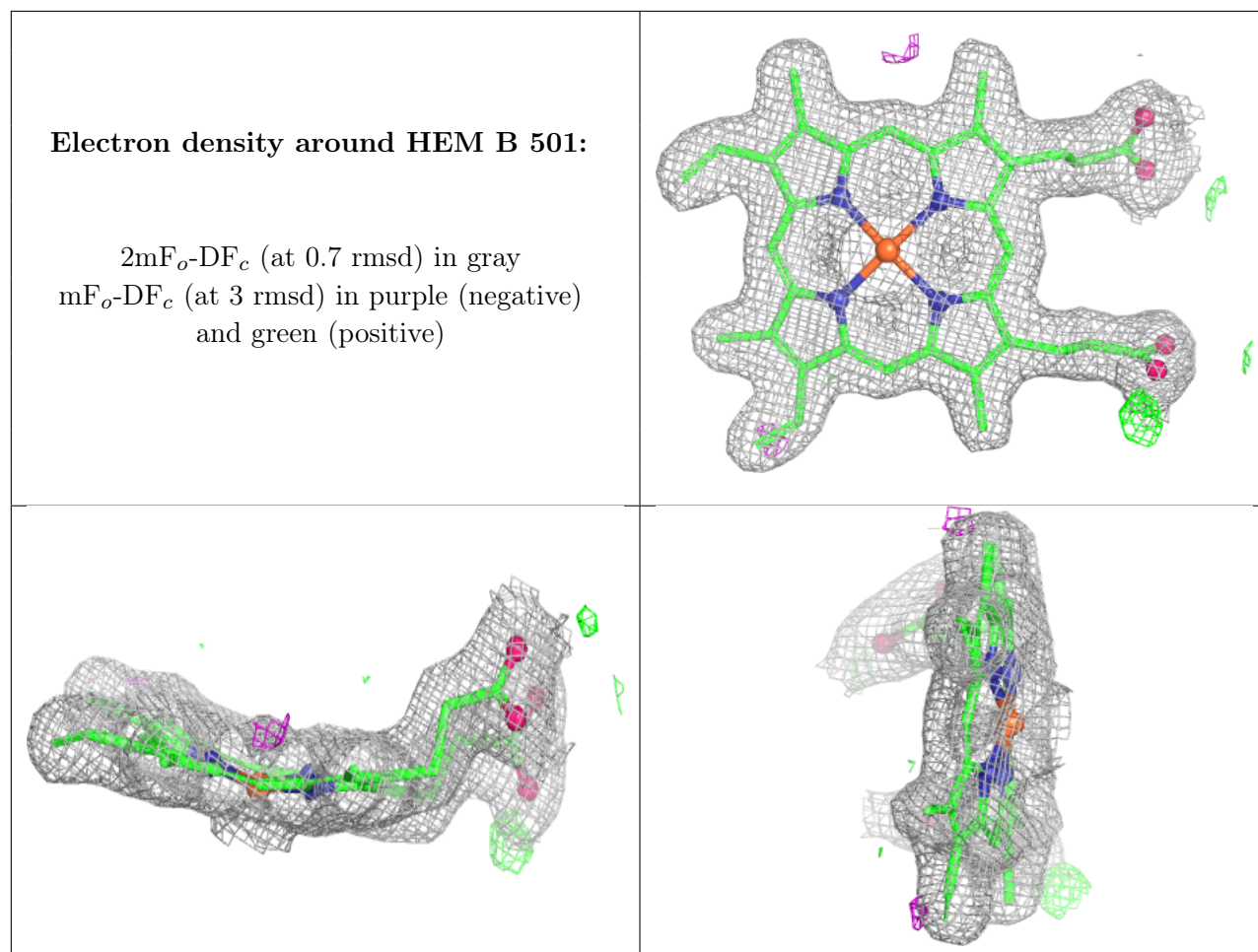
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM D 502:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.