



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 5, 2022 – 04:49 PM EDT

PDB ID : 7TSH
Title : Structure of human endothelial nitric oxide synthase heme domain in complex with 4-methyl-6-(3-(methylamino)propyl)pyridin-2-amine
Authors : Li, H.; Poulos, T.L.
Deposited on : 2022-01-31
Resolution : 2.15 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at <http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.29
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.29

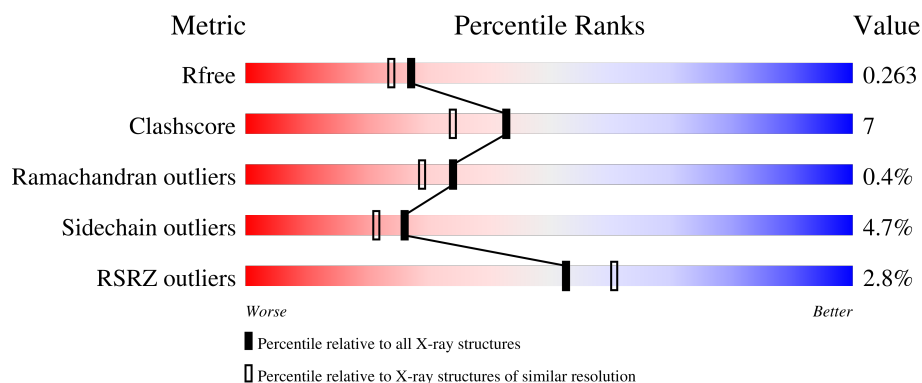
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2523 (2.16-2.12)
Clashscore	141614	2653 (2.16-2.12)
Ramachandran outliers	138981	2618 (2.16-2.12)
Sidechain outliers	138945	2617 (2.16-2.12)
RSRZ outliers	127900	2485 (2.16-2.12)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	440	<div> <div>6%</div> <div> <div></div> <div>71%</div> <div>18%</div> <div>•</div> <div>9%</div> </div> </div>
1	B	440	<div> <div>%</div> <div> <div></div> <div>77%</div> <div>13%</div> <div>•</div> <div>9%</div> </div> </div>
1	C	440	<div> <div>3%</div> <div> <div></div> <div>72%</div> <div>17%</div> <div>•</div> <div>9%</div> </div> </div>
1	D	440	<div> <div></div> <div> <div></div> <div>80%</div> <div>11%</div> <div>•</div> <div>9%</div> </div> </div>

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 13762 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.

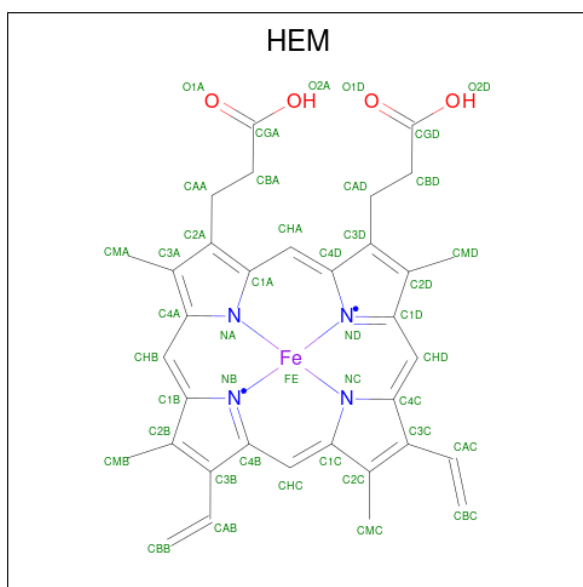
- Molecule 1 is a protein called Nitric oxide synthase, endothelial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	400	Total	C	N	O	S	0	1	0
			3198	2037	562	583	16			
1	B	402	Total	C	N	O	S	0	2	0
			3217	2048	567	586	16			
1	C	402	Total	C	N	O	S	0	1	0
			3212	2046	565	585	16			
1	D	402	Total	C	N	O	S	0	0	0
			3211	2044	567	584	16			

There are 4 discrepancies between the modelled and reference sequences:

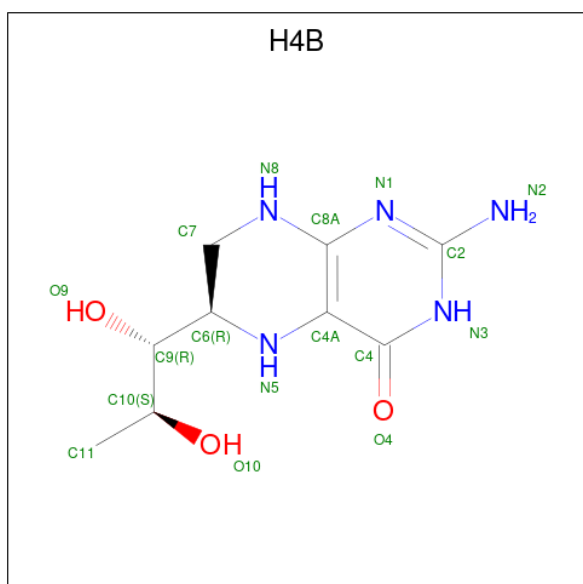
Chain	Residue	Modelled	Actual	Comment	Reference
A	298	GLU	ASP	variant	UNP P29474
B	298	GLU	ASP	variant	UNP P29474
C	298	GLU	ASP	variant	UNP P29474
D	298	GLU	ASP	variant	UNP P29474

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



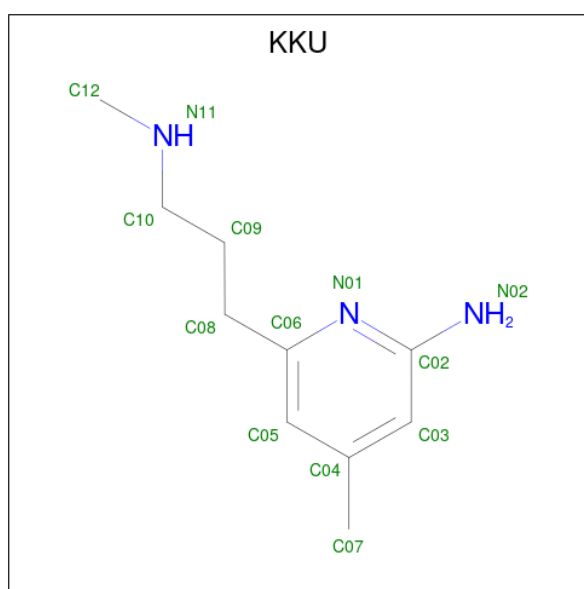
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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



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

- Molecule 4 is 4-methyl-6-[3-(methylamino)propyl]pyridin-2-amine (three-letter code: KCU) (formula: $C_{10}H_{17}N_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			13	10	3		
4	B	1	Total	C	N	0	0
			13	10	3		
4	C	1	Total	C	N	0	0
			13	10	3		
4	D	1	Total	C	N	0	0
			13	10	3		

- Molecule 5 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (three-letter code: 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	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	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 GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 8 is GADOLINIUM ATOM (three-letter code: GD) (formula: Gd).

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

- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

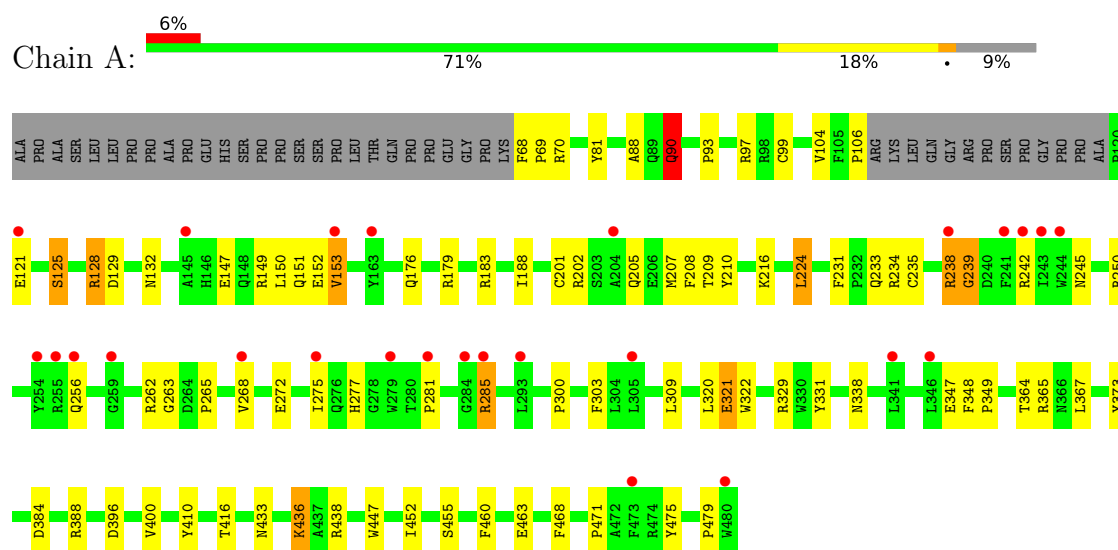
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	68	Total 68	O 68	0	0
10	B	138	Total 138	O 138	0	0
10	C	86	Total 86	O 86	0	0
10	D	142	Total 142	O 142	0	0

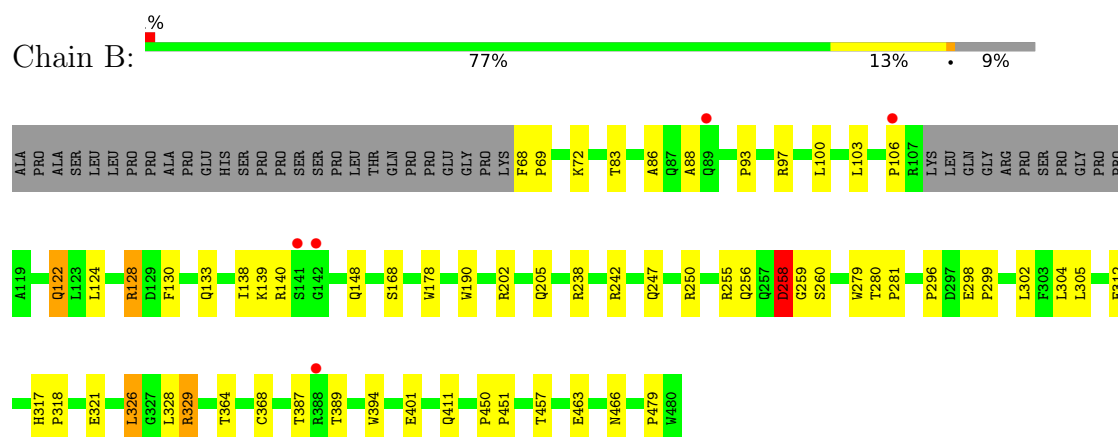
3 Residue-property plots [i](#)

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.

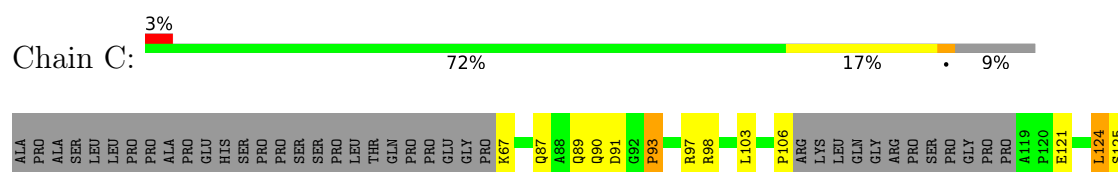
- Molecule 1: Nitric oxide synthase, endothelial

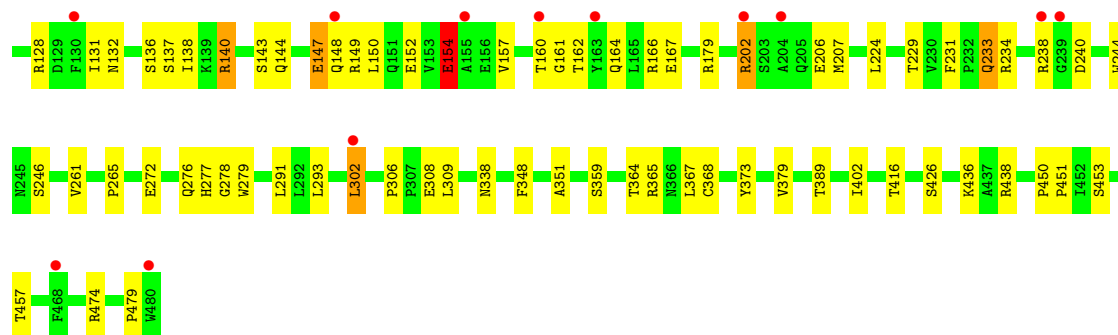


- Molecule 1: Nitric oxide synthase, endothelial



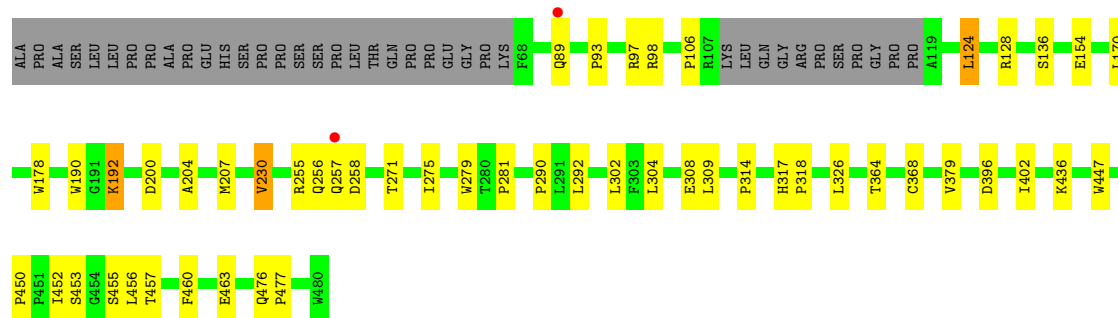
- Molecule 1: Nitric oxide synthase, endothelial





- Molecule 1: Nitric oxide synthase, endothelial

Chain D: 80% 11% 9%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	59.80Å 152.74Å 108.59Å 90.00° 90.72° 90.00°	Depositor
Resolution (Å)	39.11 – 2.15 39.10 – 2.15	Depositor EDS
% Data completeness (in resolution range)	96.5 (39.11-2.15) 97.0 (39.10-2.15)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.01 (at 2.14Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.214 , 0.270 0.205 , 0.263	Depositor DCC
R_{free} test set	5147 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	40.6	Xtriage
Anisotropy	0.507	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.149 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13762	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, BTB, CL, H4B, KGU, GD, GOL, 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	0.38	0/3293	0.53	0/4487
1	B	0.41	0/3315	0.56	0/4517
1	C	0.38	0/3307	0.54	0/4506
1	D	0.45	0/3303	0.60	1/4501 (0.0%)
All	All	0.40	0/13218	0.56	1/18011 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	309	LEU	CA-CB-CG	5.14	127.12	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3198	0	3099	54	1
1	B	3217	0	3121	41	0
1	C	3212	0	3116	42	0
1	D	3211	0	3111	28	0
2	A	43	0	30	2	0
2	B	43	0	30	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	43	0	30	2	0
2	D	43	0	30	1	0
3	A	17	0	15	1	0
3	B	17	0	15	0	0
3	C	17	0	15	1	0
3	D	17	0	15	1	0
4	A	13	0	0	0	0
4	B	13	0	0	0	0
4	C	13	0	0	0	0
4	D	13	0	0	0	0
5	A	42	0	55	8	0
5	B	28	0	36	4	0
5	C	42	0	55	5	0
5	D	28	0	35	5	1
6	A	18	0	24	0	0
6	B	6	0	8	0	0
6	C	12	0	16	1	0
6	D	12	0	16	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
8	A	1	0	0	0	0
8	B	2	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	68	0	0	5	0
10	B	138	0	0	4	0
10	C	86	0	0	3	0
10	D	142	0	0	2	0
All	All	13762	0	12872	178	1

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

All (178) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:GLN:HB2	1:B:250:ARG:HD3	1.66	0.78
1:A:147:GLU:O	1:A:151:GLN:NE2	2.16	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:ARG:NH2	1:B:259:GLY:O	2.22	0.72
1:A:201:CYS:SG	10:A:638:HOH:O	2.48	0.71
2:C:501:HEM:HBB2	2:C:501:HEM:HHC	1.72	0.70
1:A:128:ARG:O	1:A:132:ASN:ND2	2.26	0.68
1:D:275:ILE:HD12	1:D:281:PRO:HG3	1.76	0.68
2:A:501:HEM:HBB2	2:A:501:HEM:HHC	1.76	0.66
2:D:501:HEM:HBB2	2:D:501:HEM:HHC	1.77	0.65
5:C:504:BTB:O4	5:C:504:BTB:H72	1.97	0.64
1:D:89:GLN:NE2	10:D:603:HOH:O	2.27	0.64
1:A:265:PRO:HA	1:A:268:VAL:HG23	1.81	0.63
1:A:275:ILE:HD11	1:A:281:PRO:HB3	1.81	0.63
1:A:250:ARG:HA	1:A:250:ARG:HE	1.63	0.62
1:A:93:PRO:HB3	1:A:106:PRO:HB3	1.81	0.62
1:A:263:GLY:HA2	1:A:285:ARG:HG3	1.81	0.62
1:D:290:PRO:HB3	1:D:304:LEU:HD23	1.82	0.62
1:B:298:GLU:HG3	1:B:299:PRO:HD2	1.82	0.61
1:C:91:ASP:OD1	1:D:97:ARG:NH1	2.32	0.61
1:C:202:ARG:HH11	1:C:202:ARG:HA	1.64	0.61
1:B:298:GLU:OE2	5:B:505:BTB:N	2.35	0.60
1:B:321:GLU:OE1	5:B:504:BTB:H82	2.01	0.59
1:A:321:GLU:H	1:A:321:GLU:CD	2.05	0.59
1:B:68:PHE:CE2	1:B:86:ALA:HB2	2.38	0.59
1:A:88:ALA:O	1:B:97:ARG:NH1	2.36	0.59
1:A:384:ASP:OD1	5:A:504:BTB:O3	2.21	0.59
1:C:148:GLN:OE1	1:C:166:ARG:NH2	2.36	0.58
1:A:238:ARG:NH2	1:A:239:GLY:O	2.36	0.58
1:B:68:PHE:HE2	1:B:86:ALA:HB2	1.68	0.57
1:D:453:SER:HB3	1:D:456:LEU:HD12	1.85	0.57
1:A:70:ARG:HG3	1:A:81:TYR:CE2	2.40	0.57
1:D:279:TRP:HB2	1:D:302:LEU:HD21	1.87	0.56
1:D:271:THR:O	1:D:275:ILE:HG12	2.05	0.56
1:C:261:VAL:HG11	1:C:265:PRO:HA	1.86	0.56
1:B:68:PHE:CD1	1:B:83:THR:HG22	2.41	0.56
2:C:501:HEM:HBC2	2:C:501:HEM:HMC2	1.87	0.56
1:A:125:SER:HA	1:A:128:ARG:NH1	2.22	0.55
1:C:124:LEU:O	1:C:128:ARG:HG3	2.06	0.55
1:A:262:ARG:NH2	10:A:606:HOH:O	2.41	0.54
1:A:365:ARG:HH12	3:A:502:H4B:C4	2.20	0.54
1:D:93:PRO:HB3	1:D:106:PRO:HB3	1.89	0.54
1:A:150:LEU:HB2	1:A:151:GLN:NE2	2.23	0.53
1:D:170:LEU:HD11	1:D:230:VAL:HG21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:ARG:HD3	1:A:447:TRP:CD2	2.44	0.53
1:A:320:LEU:HD13	1:A:322:TRP:CZ2	2.43	0.52
1:C:147:GLU:HA	1:C:150:LEU:HD12	1.91	0.52
1:D:192:LYS:NZ	10:D:602:HOH:O	2.24	0.52
1:D:364:THR:O	1:D:368:CYS:HB2	2.08	0.52
1:C:144:GLN:HA	1:C:147:GLU:HG2	1.91	0.52
1:C:179:ARG:NH2	1:C:438:ARG:HG3	2.24	0.51
1:D:455:SER:HA	1:D:460:PHE:CG	2.46	0.51
1:A:475:TYR:OH	2:A:501:HEM:O1D	2.22	0.51
1:D:124:LEU:HD11	1:D:154:GLU:HG3	1.93	0.51
1:C:160:THR:HG23	1:C:162:THR:H	1.75	0.51
1:A:331:TYR:O	1:A:410:TYR:OH	2.27	0.50
5:D:505:BTB:O4	5:D:505:BTB:H51	2.11	0.50
1:A:128:ARG:HH11	1:A:128:ARG:HB2	1.76	0.50
1:C:365:ARG:HH12	3:C:502:H4B:C4	2.25	0.50
1:A:210:TYR:HD2	10:A:638:HOH:O	1.96	0.49
1:A:207:MET:HG2	1:A:231:PHE:CE1	2.47	0.49
1:C:131:ILE:HD12	1:C:149:ARG:HG3	1.94	0.49
1:A:97:ARG:HG3	1:B:88:ALA:HB3	1.93	0.48
1:A:99:CYS:HB3	1:B:466:ASN:HB3	1.94	0.48
1:A:433:ASN:O	1:A:436:LYS:HE2	2.13	0.48
1:B:312:GLU:CD	1:B:329:ARG:HH21	2.16	0.48
1:A:234:ARG:NH1	1:A:347:GLU:OE1	2.46	0.48
1:C:97:ARG:NH2	10:C:602:HOH:O	2.13	0.48
1:B:72:LYS:O	1:B:463:GLU:HG3	2.13	0.48
1:D:447:TRP:HA	3:D:502:H4B:N1	2.28	0.48
1:A:433:ASN:O	1:A:436:LYS:HG3	2.13	0.48
1:D:255:ARG:O	1:D:256:GLN:NE2	2.43	0.48
1:C:279:TRP:HB2	1:C:302:LEU:HD11	1.94	0.47
1:B:279:TRP:HB2	1:B:302:LEU:HD21	1.94	0.47
1:C:234:ARG:HB3	1:C:240:ASP:OD1	2.15	0.47
1:C:246:SER:HA	1:C:338:ASN:HB3	1.96	0.47
1:A:224:LEU:HB2	1:A:416:THR:HB	1.97	0.47
1:A:104:VAL:O	1:A:106:PRO:HD3	2.14	0.47
1:B:298:GLU:OE2	5:B:505:BTB:O6	2.21	0.47
1:C:103:LEU:HA	1:D:463:GLU:HG2	1.96	0.47
5:C:506:BTB:O4	5:C:506:BTB:O1	2.30	0.47
1:B:178:TRP:CE3	1:B:190:TRP:HA	2.49	0.47
1:C:364:THR:O	1:C:368:CYS:HB2	2.13	0.46
5:C:505:BTB:O8	5:C:505:BTB:O3	2.30	0.46
2:B:501:HEM:HHC	2:B:501:HEM:HBB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:505:BTB:O4	5:B:505:BTB:H72	2.15	0.46
1:C:224:LEU:HD12	1:C:416:THR:HB	1.97	0.46
1:D:308:GLU:H	1:D:308:GLU:CD	2.18	0.46
1:B:411:GLN:NE2	10:B:610:HOH:O	2.48	0.46
1:A:90:GLN:HB2	1:A:468:PHE:CD2	2.51	0.46
1:A:201:CYS:SG	1:A:202:ARG:N	2.89	0.46
1:B:238:ARG:HG2	1:B:296:PRO:HB3	1.97	0.46
1:B:298:GLU:HG2	10:B:724:HOH:O	2.16	0.46
1:A:396:ASP:O	1:A:400:VAL:HG23	2.16	0.46
5:A:504:BTB:H32	5:A:504:BTB:H51	1.68	0.46
5:C:504:BTB:O4	5:C:504:BTB:C7	2.64	0.46
1:B:242:ARG:NH2	1:B:479:PRO:HD3	2.31	0.45
1:C:149:ARG:NH2	1:C:164:GLN:O	2.38	0.45
1:B:93:PRO:HG3	1:B:106:PRO:CB	2.47	0.45
1:C:202:ARG:HG2	1:C:206:GLU:OE1	2.16	0.45
1:C:474:ARG:NH2	10:C:603:HOH:O	2.26	0.45
1:A:338:ASN:N	10:A:607:HOH:O	2.50	0.45
1:B:450:PRO:HG2	1:B:457:THR:HG21	1.98	0.45
1:C:90:GLN:NE2	10:C:604:HOH:O	2.39	0.45
1:B:326:LEU:HB3	1:B:328:LEU:HG	1.98	0.45
1:A:388:ARG:HG2	5:A:505:BTB:H61	1.98	0.45
1:C:379:VAL:HG21	1:C:402:ILE:HD11	1.98	0.45
1:C:450:PRO:HG2	1:C:457:THR:HG21	1.99	0.45
1:A:364:THR:HG21	1:A:452:ILE:HG23	1.99	0.45
1:C:276:GLN:O	1:C:278:GLY:N	2.45	0.45
1:C:148:GLN:O	1:C:152:GLU:HB2	2.17	0.45
5:A:505:BTB:H41	5:A:505:BTB:H72	1.24	0.45
1:A:277:HIS:CD2	1:A:300:PRO:HG2	2.52	0.44
1:A:242:ARG:HD2	1:A:349:PRO:HB2	1.99	0.44
1:C:244:TRP:CD1	1:C:479:PRO:HG2	2.52	0.44
1:C:306:PRO:O	1:C:309:LEU:HB2	2.18	0.44
1:B:122:GLN:NE2	10:B:605:HOH:O	2.44	0.44
5:D:505:BTB:H11	5:D:505:BTB:H72	1.76	0.44
1:A:179:ARG:NH2	1:A:438:ARG:HG3	2.33	0.44
1:C:451:PRO:HB2	1:D:455:SER:OG	2.17	0.44
1:A:90:GLN:HB2	1:A:468:PHE:CE2	2.53	0.44
1:B:100:LEU:HB3	1:B:103:LEU:HD22	2.00	0.44
5:D:504:BTB:O3	5:D:504:BTB:O4	2.36	0.44
1:C:291:LEU:HB3	1:C:293:LEU:HD21	1.98	0.44
1:C:367:LEU:HA	1:C:373:TYR:HB2	1.99	0.44
1:B:138:ILE:HG13	1:B:140:ARG:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:LEU:HB3	1:B:128:ARG:HH12	1.82	0.43
1:B:258:ASP:HB2	1:B:259:GLY:H	1.66	0.43
1:D:275:ILE:HD13	1:D:279:TRP:HE3	1.82	0.43
1:A:463:GLU:HB3	1:B:103:LEU:HD12	2.01	0.43
1:C:124:LEU:HD11	1:C:154:GLU:OE1	2.19	0.43
1:C:157:VAL:HG13	1:C:161:GLY:C	2.38	0.43
1:A:149:ARG:O	1:A:153:VAL:HG22	2.19	0.43
1:A:455:SER:HA	1:A:460:PHE:CG	2.53	0.43
1:D:204:ALA:O	1:D:207:MET:HB2	2.18	0.43
1:A:455:SER:OG	1:B:451:PRO:HB2	2.19	0.43
1:C:132:ASN:O	1:C:136:SER:OG	2.23	0.43
1:C:167:GLU:OE2	6:C:507:GOL:O2	2.37	0.43
1:B:256:GLN:HB2	1:B:260:SER:O	2.19	0.43
1:B:317:HIS:CG	1:B:318:PRO:HD2	2.54	0.42
1:C:93:PRO:HB3	1:C:106:PRO:HB3	2.00	0.42
1:C:229:THR:O	1:C:351:ALA:HA	2.19	0.42
1:D:292:LEU:HD23	1:D:292:LEU:HA	1.88	0.42
1:B:205:GLN:HG3	10:B:677:HOH:O	2.18	0.42
5:D:505:BTB:H62	5:D:505:BTB:H82	2.00	0.42
1:B:305:LEU:HD23	1:B:305:LEU:HA	1.82	0.42
1:B:317:HIS:NE2	1:B:401:GLU:OE1	2.49	0.42
1:A:367:LEU:HA	1:A:373:TYR:HB2	2.01	0.42
5:A:504:BTB:O3	5:A:504:BTB:O4	2.36	0.42
1:B:387:THR:HA	1:B:394:TRP:CD1	2.54	0.42
1:C:276:GLN:C	1:C:278:GLY:H	2.23	0.42
1:A:242:ARG:NH2	1:A:479:PRO:HD3	2.35	0.42
1:B:364:THR:O	1:B:368:CYS:HB2	2.20	0.42
1:D:379:VAL:HG21	1:D:402:ILE:HD11	2.02	0.42
1:A:147:GLU:HA	1:A:150:LEU:HD12	2.01	0.42
1:A:208:PHE:CD1	1:A:303:PHE:HB3	2.54	0.42
1:B:280:THR:HA	1:B:281:PRO:HD3	1.92	0.42
1:A:234:ARG:HG2	1:A:235:CYS:N	2.34	0.41
5:D:504:BTB:H41	5:D:504:BTB:H72	1.79	0.41
5:A:506:BTB:H11	5:A:506:BTB:H51	1.36	0.41
1:B:130:PHE:O	1:B:133:GLN:HB2	2.19	0.41
1:C:453:SER:HA	1:D:452:ILE:HG22	2.02	0.41
1:D:317:HIS:CG	1:D:318:PRO:HD2	2.55	0.41
1:A:233:GLN:HB3	1:A:348:PHE:CE2	2.56	0.41
5:C:505:BTB:H72	5:C:505:BTB:H41	1.26	0.41
1:D:178:TRP:CE3	1:D:190:TRP:HA	2.55	0.41
1:A:70:ARG:HG3	1:A:81:TYR:CZ	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:GLN:HB2	1:A:471:PRO:HG2	2.02	0.41
5:A:504:BTB:O3	10:A:601:HOH:O	2.21	0.41
5:A:506:BTB:H41	5:A:506:BTB:H72	1.32	0.41
1:C:138:ILE:O	1:C:140:ARG:HG2	2.21	0.41
1:D:450:PRO:HG2	1:D:457:THR:HG21	2.02	0.41
1:B:68:PHE:HA	1:B:69:PRO:HD3	1.84	0.40
1:D:476:GLN:HB2	1:D:477:PRO:HD2	2.03	0.40
1:C:233:GLN:HB3	1:C:348:PHE:CE2	2.55	0.40
1:A:68:PHE:HA	1:A:69:PRO:HD3	1.96	0.40
1:C:207:MET:HG3	1:C:231:PHE:CZ	2.56	0.40
1:D:124:LEU:HD22	1:D:128:ARG:CZ	2.52	0.40
1:B:250:ARG:HA	1:B:250:ARG:HD2	1.89	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:GLU:OE2	5:D:505:BTB:O4[2_851]	2.13	0.07

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	397/440 (90%)	373 (94%)	22 (6%)	2 (0%)	29	22
1	B	400/440 (91%)	388 (97%)	11 (3%)	1 (0%)	41	36
1	C	399/440 (91%)	376 (94%)	19 (5%)	4 (1%)	15	8
1	D	398/440 (90%)	386 (97%)	12 (3%)	0	100	100
All	All	1594/1760 (91%)	1523 (96%)	64 (4%)	7 (0%)	34	29

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	258	ASP
1	A	239	GLY
1	C	202	ARG
1	C	277	HIS
1	A	90	GLN
1	C	154	GLU
1	C	93	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	341/373 (91%)	321 (94%)	20 (6%)	19	14
1	B	343/373 (92%)	331 (96%)	12 (4%)	36	33
1	C	342/373 (92%)	320 (94%)	22 (6%)	17	12
1	D	341/373 (91%)	329 (96%)	12 (4%)	36	33
All	All	1367/1492 (92%)	1301 (95%)	66 (5%)	26	21

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	GLN
1	A	121	GLU
1	A	125	SER
1	A	128	ARG
1	A	129	ASP
1	A	153	VAL
1	A	188	ILE
1	A	205	GLN
1	A	209	THR
1	A	216	LYS
1	A	224	LEU
1	A	238	ARG
1	A	245	ASN
1	A	256	GLN
1	A	272	GLU

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Mol	Chain	Res	Type
1	A	285	ARG
1	A	309	LEU
1	A	321	GLU
1	A	329	ARG
1	A	436	LYS
1	B	122	GLN
1	B	128	ARG
1	B	139	LYS
1	B	148	GLN
1	B	168[A]	SER
1	B	168[B]	SER
1	B	202	ARG
1	B	258	ASP
1	B	304	LEU
1	B	326	LEU
1	B	329	ARG
1	B	389	THR
1	C	67	LYS
1	C	87	GLN
1	C	89	GLN
1	C	98	ARG
1	C	121	GLU
1	C	124	LEU
1	C	125	SER
1	C	137	SER
1	C	140	ARG
1	C	143	SER
1	C	147	GLU
1	C	154	GLU
1	C	233	GLN
1	C	238	ARG
1	C	272	GLU
1	C	302	LEU
1	C	308	GLU
1	C	359	SER
1	C	389	THR
1	C	426[A]	SER
1	C	426[B]	SER
1	C	436	LYS
1	D	98	ARG
1	D	124	LEU
1	D	136	SER

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Mol	Chain	Res	Type
1	D	192	LYS
1	D	200	ASP
1	D	230	VAL
1	D	257	GLN
1	D	258	ASP
1	D	314	PRO
1	D	326	LEU
1	D	396	ASP
1	D	436	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	132	ASN
1	D	122	GLN
1	D	126	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 40 ligands modelled in this entry, 10 are monoatomic - leaving 30 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	B	505	-	13,13,13	0.40	0	7,16,16	1.04	1 (14%)
5	BTB	C	506	-	13,13,13	0.40	0	7,16,16	0.36	0
6	GOL	B	506	-	5,5,5	0.38	0	5,5,5	0.41	0
3	H4B	C	502	-	16,18,18	0.83	0	11,26,26	2.98	6 (54%)
2	HEM	A	501	1	41,50,50	1.50	4 (9%)	45,82,82	1.80	12 (26%)
5	BTB	C	504	8	13,13,13	0.50	0	7,16,16	0.75	0
6	GOL	A	512	-	5,5,5	0.52	0	5,5,5	0.45	0
3	H4B	B	502	-	16,18,18	0.90	0	11,26,26	2.86	6 (54%)
6	GOL	A	508	-	5,5,5	0.46	0	5,5,5	0.50	0
4	KKU	B	503	-	13,13,13	0.44	0	16,16,16	1.76	4 (25%)
5	BTB	C	505	-	13,13,13	1.04	1 (7%)	7,16,16	1.75	3 (42%)
6	GOL	D	507	-	5,5,5	0.34	0	5,5,5	0.36	0
5	BTB	D	504	8	13,13,13	0.42	0	7,16,16	0.42	0
4	KKU	D	503	-	13,13,13	0.47	0	16,16,16	1.79	4 (25%)
6	GOL	A	507	-	5,5,5	0.36	0	5,5,5	0.38	0
6	GOL	D	506	-	5,5,5	0.70	0	5,5,5	1.27	0
5	BTB	A	504	8	13,13,13	0.36	0	7,16,16	0.89	1 (14%)
3	H4B	D	502	-	16,18,18	0.96	1 (6%)	11,26,26	2.65	6 (54%)
2	HEM	D	501	1	41,50,50	1.51	6 (14%)	45,82,82	1.92	12 (26%)
4	KKU	A	503	-	13,13,13	0.23	0	16,16,16	1.73	3 (18%)
5	BTB	D	505	-	13,13,13	0.50	0	7,16,16	0.48	0
6	GOL	C	507	-	5,5,5	0.41	0	5,5,5	0.63	0
2	HEM	C	501	1	41,50,50	1.48	5 (12%)	45,82,82	1.87	11 (24%)
2	HEM	B	501	1	41,50,50	1.58	7 (17%)	45,82,82	2.01	17 (37%)
5	BTB	A	505	-	13,13,13	0.63	0	7,16,16	1.27	0
5	BTB	B	504	8	13,13,13	0.38	0	7,16,16	0.46	0
3	H4B	A	502	-	16,18,18	0.95	1 (6%)	11,26,26	2.68	5 (45%)
5	BTB	A	506	-	13,13,13	0.45	0	7,16,16	0.57	0
6	GOL	C	508	-	5,5,5	0.48	0	5,5,5	0.40	0
4	KKU	C	503	-	13,13,13	0.30	0	16,16,16	2.12	3 (18%)

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	B	505	-	-	7/21/21/21	-
5	BTB	C	506	-	-	3/21/21/21	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	B	506	-	-	4/4/4/4	-
3	H4B	C	502	-	-	0/8/17/17	0/2/2/2
2	HEM	A	501	1	-	1/12/54/54	-
5	BTB	C	504	8	-	6/21/21/21	-
6	GOL	A	512	-	-	4/4/4/4	-
3	H4B	B	502	-	-	0/8/17/17	0/2/2/2
6	GOL	A	508	-	-	4/4/4/4	-
4	KKU	B	503	-	-	1/5/5/5	0/1/1/1
5	BTB	C	505	-	-	11/21/21/21	-
6	GOL	D	507	-	-	3/4/4/4	-
5	BTB	D	504	8	-	3/21/21/21	-
4	KKU	D	503	-	-	1/5/5/5	0/1/1/1
6	GOL	A	507	-	-	2/4/4/4	-
6	GOL	D	506	-	-	3/4/4/4	-
5	BTB	A	504	8	-	6/21/21/21	-
3	H4B	D	502	-	-	0/8/17/17	0/2/2/2
2	HEM	D	501	1	-	0/12/54/54	-
4	KKU	A	503	-	-	1/5/5/5	0/1/1/1
5	BTB	D	505	-	-	6/21/21/21	-
6	GOL	C	507	-	-	2/4/4/4	-
2	HEM	C	501	1	-	3/12/54/54	-
2	HEM	B	501	1	-	1/12/54/54	-
5	BTB	A	505	-	-	13/21/21/21	-
5	BTB	B	504	8	-	0/21/21/21	-
3	H4B	A	502	-	-	2/8/17/17	0/2/2/2
5	BTB	A	506	-	-	12/21/21/21	-
6	GOL	C	508	-	-	1/4/4/4	-
4	KKU	C	503	-	-	2/5/5/5	0/1/1/1

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	HEM	C3C-CAC	4.05	1.56	1.47
2	B	501	HEM	C3C-CAC	4.05	1.56	1.47
2	A	501	HEM	C3C-CAC	3.77	1.55	1.47
2	C	501	HEM	C3C-CAC	3.67	1.55	1.47
2	A	501	HEM	C3C-C2C	-3.46	1.35	1.40
2	B	501	HEM	FE-NB	3.45	2.13	1.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	HEM	C3C-C2C	-3.28	1.35	1.40
2	B	501	HEM	CAB-C3B	3.25	1.56	1.47
2	A	501	HEM	FE-NB	3.15	2.12	1.96
2	C	501	HEM	C3C-C2C	-3.12	1.36	1.40
2	A	501	HEM	CAB-C3B	3.07	1.55	1.47
2	C	501	HEM	CAB-C3B	3.06	1.55	1.47
2	C	501	HEM	FE-NB	2.98	2.11	1.96
2	D	501	HEM	CAB-C3B	2.96	1.55	1.47
5	C	505	BTB	C1-C2	-2.70	1.49	1.53
2	D	501	HEM	FE-NB	2.68	2.10	1.96
2	B	501	HEM	C3C-C2C	-2.66	1.36	1.40
2	B	501	HEM	FE-ND	2.30	2.08	1.96
3	D	502	H4B	C4A-C4	-2.25	1.38	1.41
2	D	501	HEM	CMC-C2C	2.23	1.56	1.51
2	B	501	HEM	CMB-C2B	2.14	1.55	1.50
2	D	501	HEM	CMD-C2D	2.13	1.55	1.50
2	B	501	HEM	CMD-C2D	2.11	1.55	1.50
2	C	501	HEM	CAA-C2A	2.03	1.55	1.52
3	A	502	H4B	C4-N3	2.01	1.36	1.33

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	503	KKU	C02-N01-C06	6.51	123.03	118.10
3	A	502	H4B	C8A-C4A-C4	6.11	120.00	114.57
3	C	502	H4B	C8A-C4A-C4	5.75	119.67	114.57
3	B	502	H4B	C8A-C4A-C4	5.66	119.59	114.57
3	D	502	H4B	C8A-C4A-C4	5.40	119.36	114.57
2	D	501	HEM	CBA-CAA-C2A	-5.08	103.95	112.62
4	A	503	KKU	C02-N01-C06	4.53	121.54	118.10
2	C	501	HEM	CBA-CAA-C2A	-4.53	104.88	112.62
2	B	501	HEM	C1B-NB-C4B	4.44	109.66	105.07
2	B	501	HEM	C4B-CHC-C1C	4.19	128.09	122.56
2	C	501	HEM	C1B-NB-C4B	4.17	109.38	105.07
2	D	501	HEM	C4C-CHD-C1D	4.06	127.91	122.56
2	B	501	HEM	C3B-C2B-C1B	3.99	109.44	106.49
4	D	503	KKU	C10-C09-C08	-3.92	105.97	112.95
2	B	501	HEM	C4D-ND-C1D	3.89	109.09	105.07
2	C	501	HEM	C4B-CHC-C1C	3.86	127.65	122.56
2	C	501	HEM	C4D-ND-C1D	3.82	109.02	105.07
3	C	502	H4B	C4-C4A-N5	3.79	122.30	119.12
4	B	503	KKU	C10-C09-C08	-3.79	106.19	112.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	HEM	CBA-CAA-C2A	-3.78	106.17	112.62
2	D	501	HEM	C4D-ND-C1D	3.76	108.95	105.07
3	C	502	H4B	N2-C2-N3	3.65	122.93	117.25
3	B	502	H4B	C4-C4A-N5	3.55	122.10	119.12
2	A	501	HEM	C3B-C2B-C1B	3.54	109.11	106.49
4	C	503	KKU	C05-C06-N01	-3.48	119.21	122.90
2	A	501	HEM	C1B-NB-C4B	3.46	108.65	105.07
4	D	503	KKU	C02-N01-C06	3.44	120.70	118.10
3	B	502	H4B	N1-C2-N3	-3.43	120.04	125.42
3	B	502	H4B	C2-N3-C4	3.41	121.35	115.93
3	D	502	H4B	C2-N3-C4	3.40	121.34	115.93
3	D	502	H4B	N1-C2-N3	-3.39	120.10	125.42
2	D	501	HEM	C1B-NB-C4B	3.38	108.57	105.07
3	C	502	H4B	N1-C2-N3	-3.30	120.24	125.42
3	C	502	H4B	C2-N3-C4	3.28	121.13	115.93
2	A	501	HEM	C4B-CHC-C1C	3.23	126.82	122.56
2	A	501	HEM	C4D-ND-C1D	3.22	108.40	105.07
2	D	501	HEM	C3D-C4D-ND	-3.21	106.59	110.17
5	C	505	BTB	O1-C1-C2	-3.19	102.72	111.44
2	B	501	HEM	C4C-CHD-C1D	3.14	126.71	122.56
2	D	501	HEM	C3B-C2B-C1B	3.13	108.81	106.49
3	B	502	H4B	C2-N1-C8A	3.02	121.30	114.54
2	B	501	HEM	CHC-C4B-C3B	3.00	129.17	124.57
3	A	502	H4B	N1-C2-N3	-2.99	120.73	125.42
2	C	501	HEM	C3D-C4D-ND	-2.96	106.87	110.17
4	A	503	KKU	C05-C06-N01	-2.94	119.78	122.90
2	D	501	HEM	C4B-CHC-C1C	2.94	126.43	122.56
4	B	503	KKU	C02-N01-C06	2.93	120.32	118.10
3	C	502	H4B	C2-N1-C8A	2.91	121.06	114.54
2	B	501	HEM	CAD-CBD-CGD	-2.87	107.43	113.60
2	B	501	HEM	C2B-C1B-NB	-2.85	106.46	109.84
3	A	502	H4B	C2-N3-C4	2.85	120.45	115.93
2	A	501	HEM	CMA-C3A-C4A	-2.82	124.13	128.46
3	D	502	H4B	C2-N1-C8A	2.78	120.77	114.54
4	A	503	KKU	C08-C06-N01	2.78	120.08	115.95
3	A	502	H4B	C2-N1-C8A	2.77	120.74	114.54
2	A	501	HEM	C4C-CHD-C1D	2.77	126.21	122.56
2	B	501	HEM	C3D-C4D-ND	-2.73	107.13	110.17
3	A	502	H4B	C4-C4A-N5	2.73	121.41	119.12
2	D	501	HEM	CBD-CAD-C3D	-2.68	105.19	112.63
2	D	501	HEM	CMC-C2C-C3C	2.63	129.59	124.68
2	B	501	HEM	CHD-C1D-C2D	2.61	129.06	124.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	HEM	CBD-CAD-C3D	-2.54	105.56	112.63
2	A	501	HEM	C4A-C3A-C2A	2.53	108.76	107.00
2	C	501	HEM	C3B-C2B-C1B	2.50	108.34	106.49
4	D	503	KKU	C04-C05-C06	-2.48	118.69	120.32
2	B	501	HEM	CBD-CAD-C3D	-2.46	105.80	112.63
2	D	501	HEM	CMA-C3A-C4A	-2.46	124.69	128.46
4	B	503	KKU	C08-C06-N01	2.45	119.59	115.95
2	C	501	HEM	CHC-C4B-C3B	2.45	128.31	124.57
2	B	501	HEM	C2D-C1D-ND	-2.43	106.97	109.88
2	C	501	HEM	CMA-C3A-C4A	-2.41	124.75	128.46
3	D	502	H4B	C4-C4A-N5	2.40	121.14	119.12
3	B	502	H4B	N2-C2-N3	2.35	120.91	117.25
2	D	501	HEM	C2B-C1B-NB	-2.32	107.09	109.84
4	B	503	KKU	C04-C05-C06	-2.29	118.82	120.32
2	A	501	HEM	C2B-C1B-NB	-2.27	107.15	109.84
2	A	501	HEM	C3D-C4D-ND	-2.24	107.67	110.17
2	C	501	HEM	CAD-CBD-CGD	-2.24	108.79	113.60
5	C	505	BTB	O3-C3-C2	-2.23	105.32	111.44
2	B	501	HEM	CHA-C4D-ND	2.22	127.13	124.38
4	C	503	KKU	C08-C06-N01	2.21	119.25	115.95
5	C	505	BTB	O4-C4-C2	-2.18	105.48	111.44
2	C	501	HEM	C2B-C1B-NB	-2.16	107.28	109.84
4	D	503	KKU	C08-C06-N01	2.15	119.15	115.95
5	B	505	BTB	O4-C4-C2	2.12	117.25	111.44
2	A	501	HEM	CMC-C2C-C3C	2.12	128.64	124.68
2	C	501	HEM	CMC-C2C-C3C	2.11	128.63	124.68
3	D	502	H4B	N2-C2-N1	2.11	120.53	117.25
2	D	501	HEM	C2D-C1D-ND	-2.08	107.39	109.88
2	B	501	HEM	C3C-C4C-NC	-2.03	107.11	110.94
5	A	504	BTB	O3-C3-C2	2.02	116.97	111.44
2	B	501	HEM	CMD-C2D-C1D	2.02	128.11	125.04
2	B	501	HEM	CMA-C3A-C4A	-2.01	125.37	128.46
2	B	501	HEM	CBA-CAA-C2A	-2.01	109.20	112.62

There are no chirality outliers.

All (102) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	504	BTB	C4-C2-C3-O3
5	A	504	BTB	N-C2-C3-O3
5	A	504	BTB	C1-C2-C4-O4
5	A	504	BTB	C3-C2-C4-O4

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

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Mol	Chain	Res	Type	Atoms
5	D	505	BTB	C4-C2-C3-O3
5	D	505	BTB	N-C2-C3-O3
6	A	507	GOL	C1-C2-C3-O3
6	A	508	GOL	O1-C1-C2-C3
6	A	512	GOL	C1-C2-C3-O3
6	A	512	GOL	O2-C2-C3-O3
6	B	506	GOL	O1-C1-C2-C3
6	B	506	GOL	C1-C2-C3-O3
6	B	506	GOL	O1-C1-C2-O2
5	A	505	BTB	N-C7-C8-O8
5	A	506	BTB	N-C5-C6-O6
5	B	505	BTB	N-C5-C6-O6
5	A	506	BTB	N-C7-C8-O8
4	D	503	KKU	C08-C09-C10-N11
6	A	508	GOL	C1-C2-C3-O3
6	A	512	GOL	O1-C1-C2-C3
6	C	507	GOL	O1-C1-C2-C3
6	D	506	GOL	O1-C1-C2-C3
6	D	507	GOL	O1-C1-C2-C3
5	C	505	BTB	N-C7-C8-O8
4	C	503	KKU	C08-C09-C10-N11
6	A	507	GOL	O2-C2-C3-O3
6	A	508	GOL	O1-C1-C2-O2
6	B	506	GOL	O2-C2-C3-O3
6	D	507	GOL	O1-C1-C2-O2
4	B	503	KKU	C08-C09-C10-N11
5	C	504	BTB	N-C7-C8-O8
6	A	508	GOL	O2-C2-C3-O3
6	A	512	GOL	O1-C1-C2-O2
6	C	507	GOL	O1-C1-C2-O2
6	D	506	GOL	O1-C1-C2-O2
6	C	508	GOL	O1-C1-C2-O2
2	A	501	HEM	C4B-C3B-CAB-CBB
2	B	501	HEM	C4B-C3B-CAB-CBB
2	C	501	HEM	C4B-C3B-CAB-CBB
4	A	503	KKU	C08-C09-C10-N11
5	A	504	BTB	C1-C2-C3-O3
5	A	505	BTB	O1-C1-C2-C4
5	C	504	BTB	C1-C2-C3-O3
2	C	501	HEM	C1A-C2A-CAA-CBA
5	A	506	BTB	O1-C1-C2-N
5	A	506	BTB	C1-C2-N-C5

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Mol	Chain	Res	Type	Atoms
5	A	506	BTB	C3-C2-N-C5
5	A	506	BTB	C4-C2-N-C7
5	C	505	BTB	N-C2-C4-O4
5	D	505	BTB	O1-C1-C2-N
6	D	506	GOL	O2-C2-C3-O3
6	D	507	GOL	C1-C2-C3-O3
3	A	502	H4B	C7-C6-C9-C10
4	C	503	KKU	C06-C08-C09-C10
2	C	501	HEM	C4D-C3D-CAD-CBD
5	C	505	BTB	C8-C7-N-C5
3	A	502	H4B	N5-C6-C9-O9
5	A	506	BTB	C3-C2-C4-O4
5	C	505	BTB	C1-C2-C4-O4
5	C	505	BTB	C3-C2-C4-O4

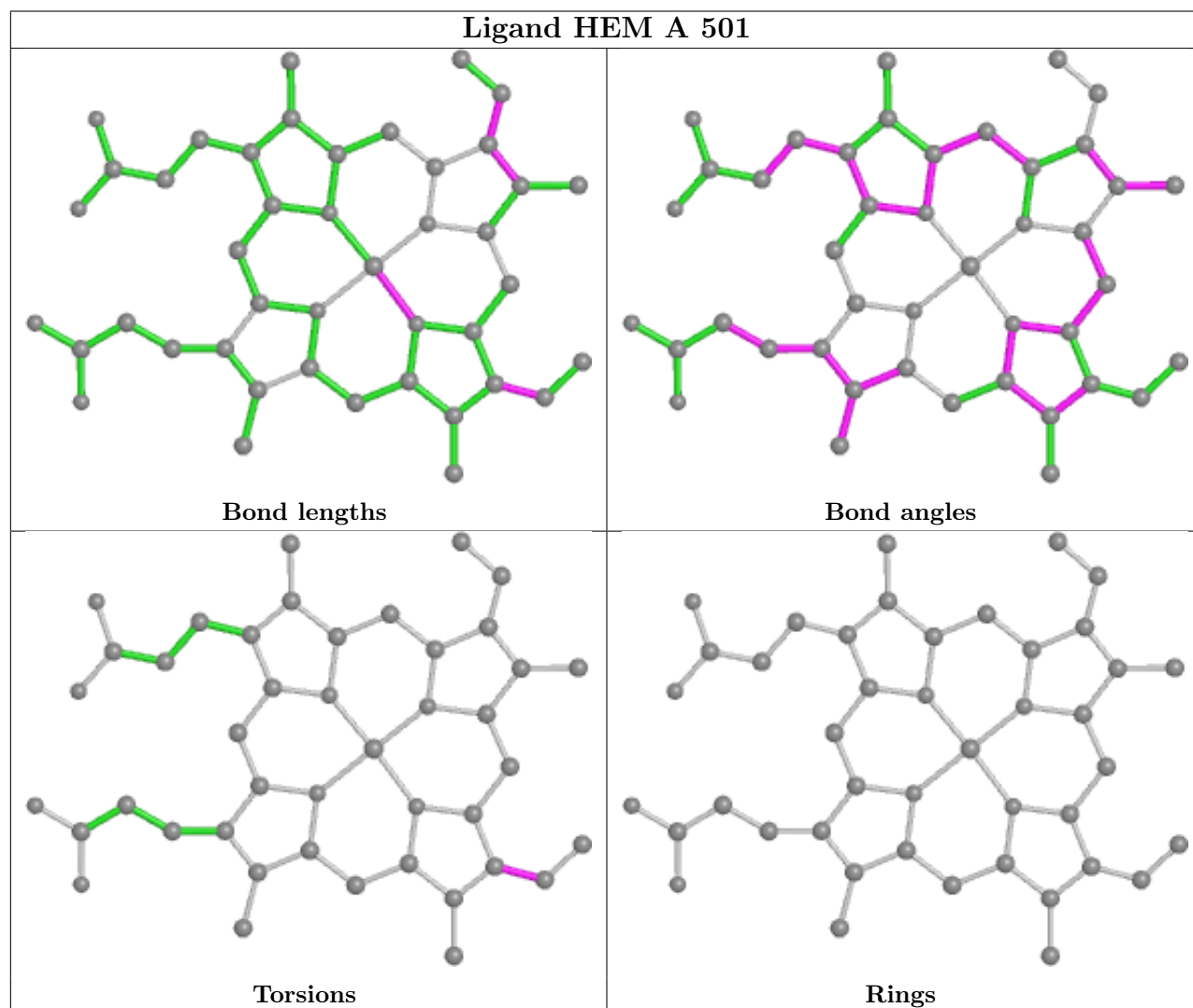
There are no ring outliers.

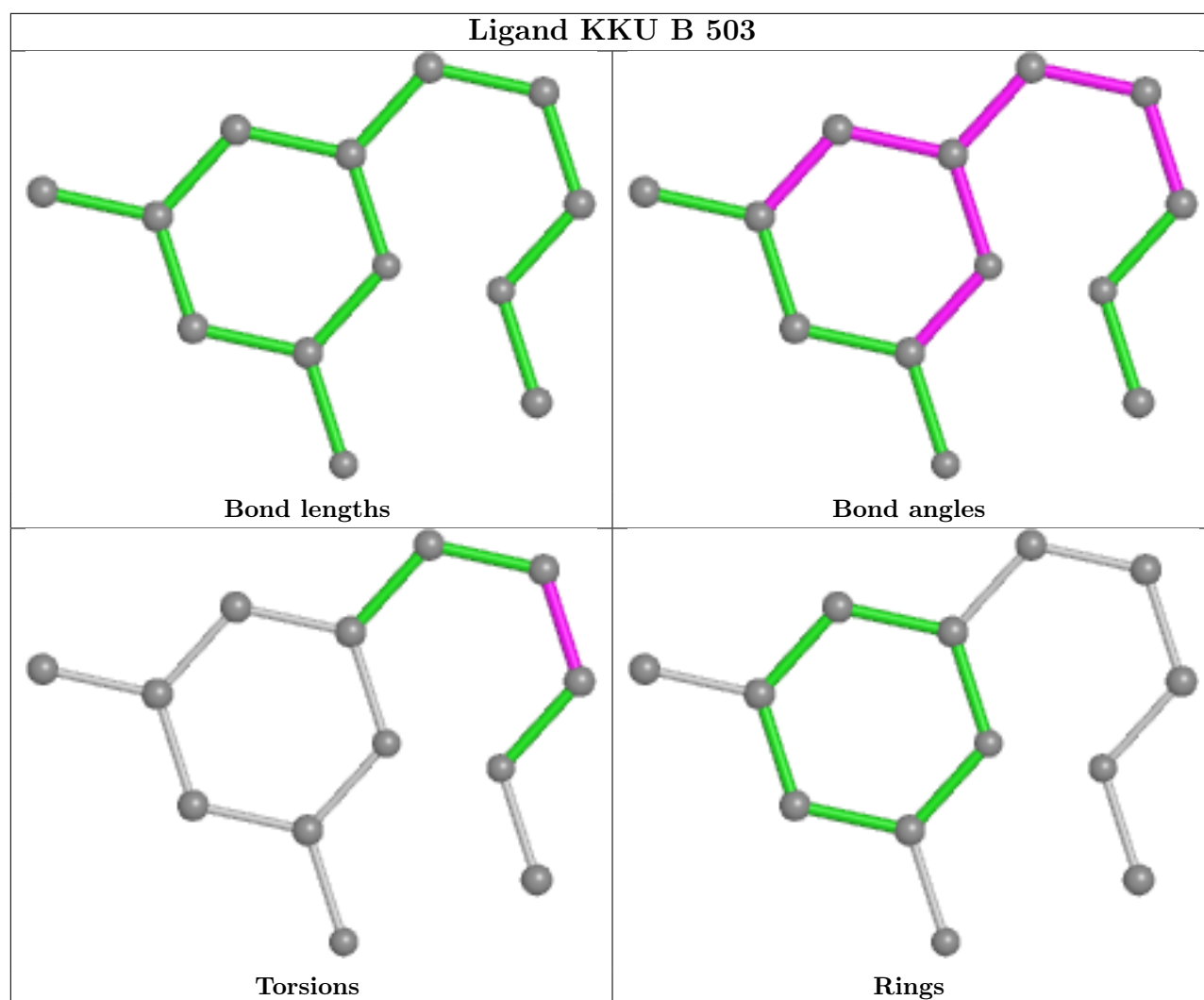
18 monomers are involved in 33 short contacts:

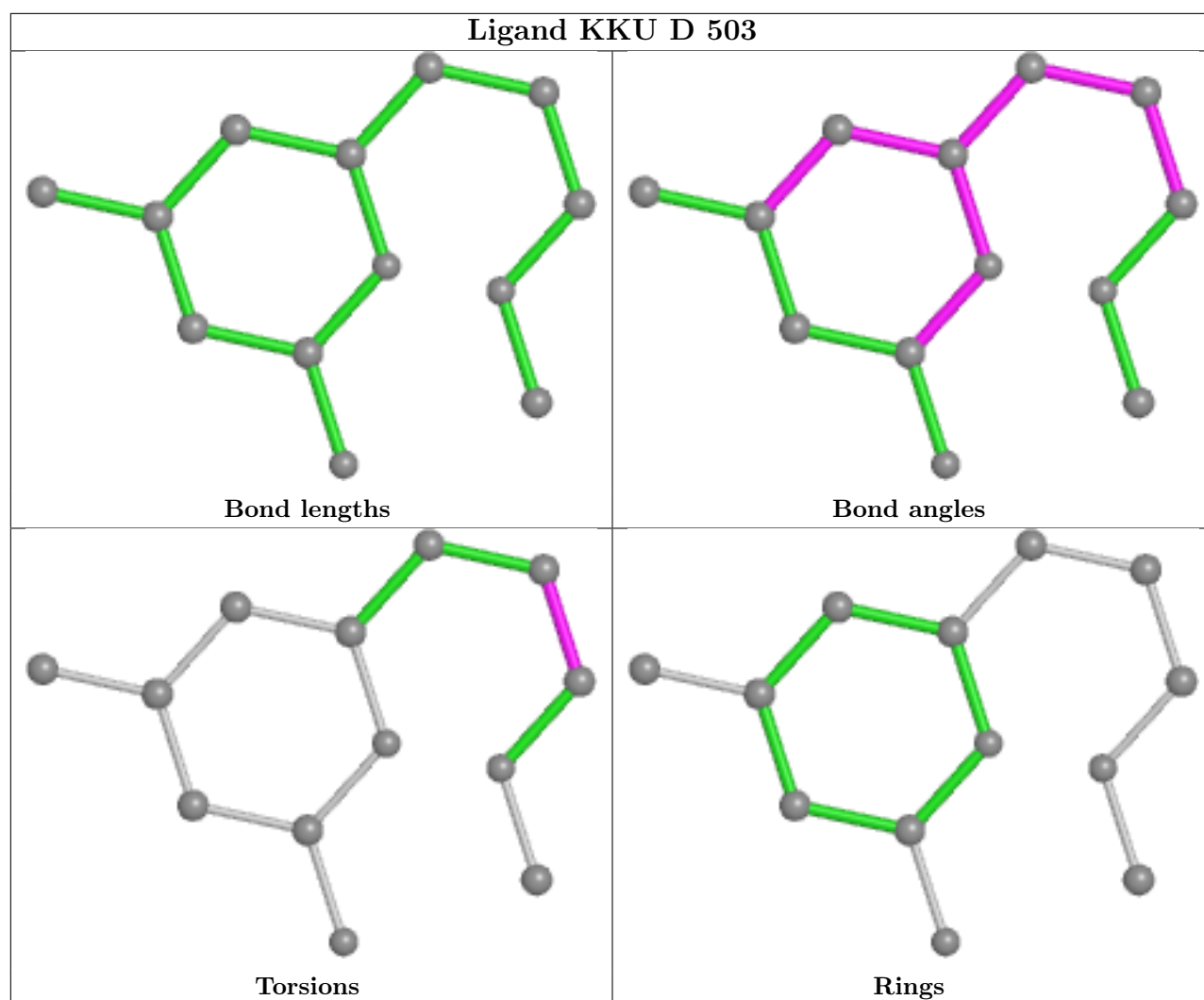
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	505	BTB	3	0
5	C	506	BTB	1	0
3	C	502	H4B	1	0
2	A	501	HEM	2	0
5	C	504	BTB	2	0
5	C	505	BTB	2	0
5	D	504	BTB	2	0
5	A	504	BTB	4	0
3	D	502	H4B	1	0
2	D	501	HEM	1	0
5	D	505	BTB	3	1
6	C	507	GOL	1	0
2	C	501	HEM	2	0
2	B	501	HEM	1	0
5	A	505	BTB	2	0
5	B	504	BTB	1	0
3	A	502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

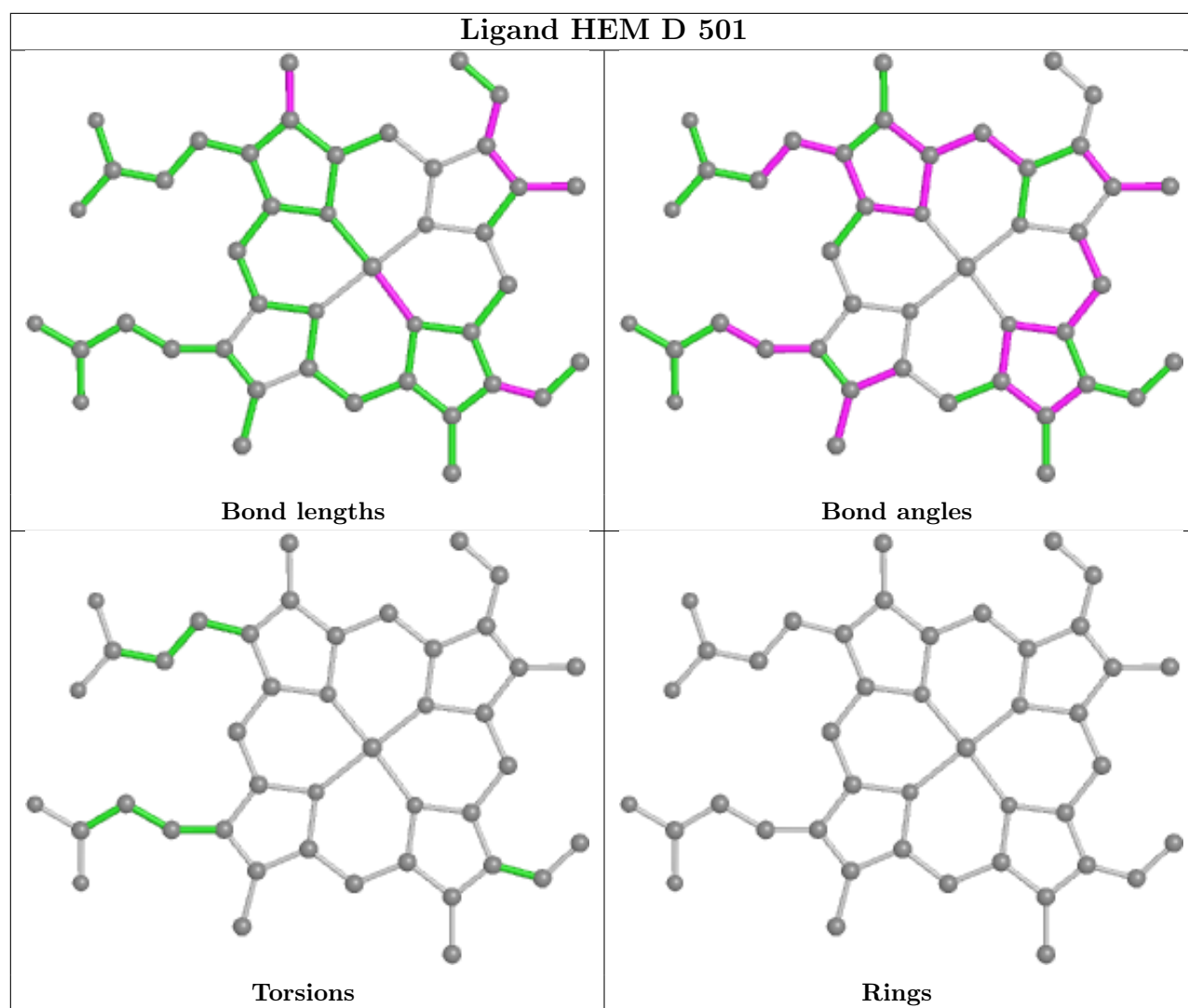
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

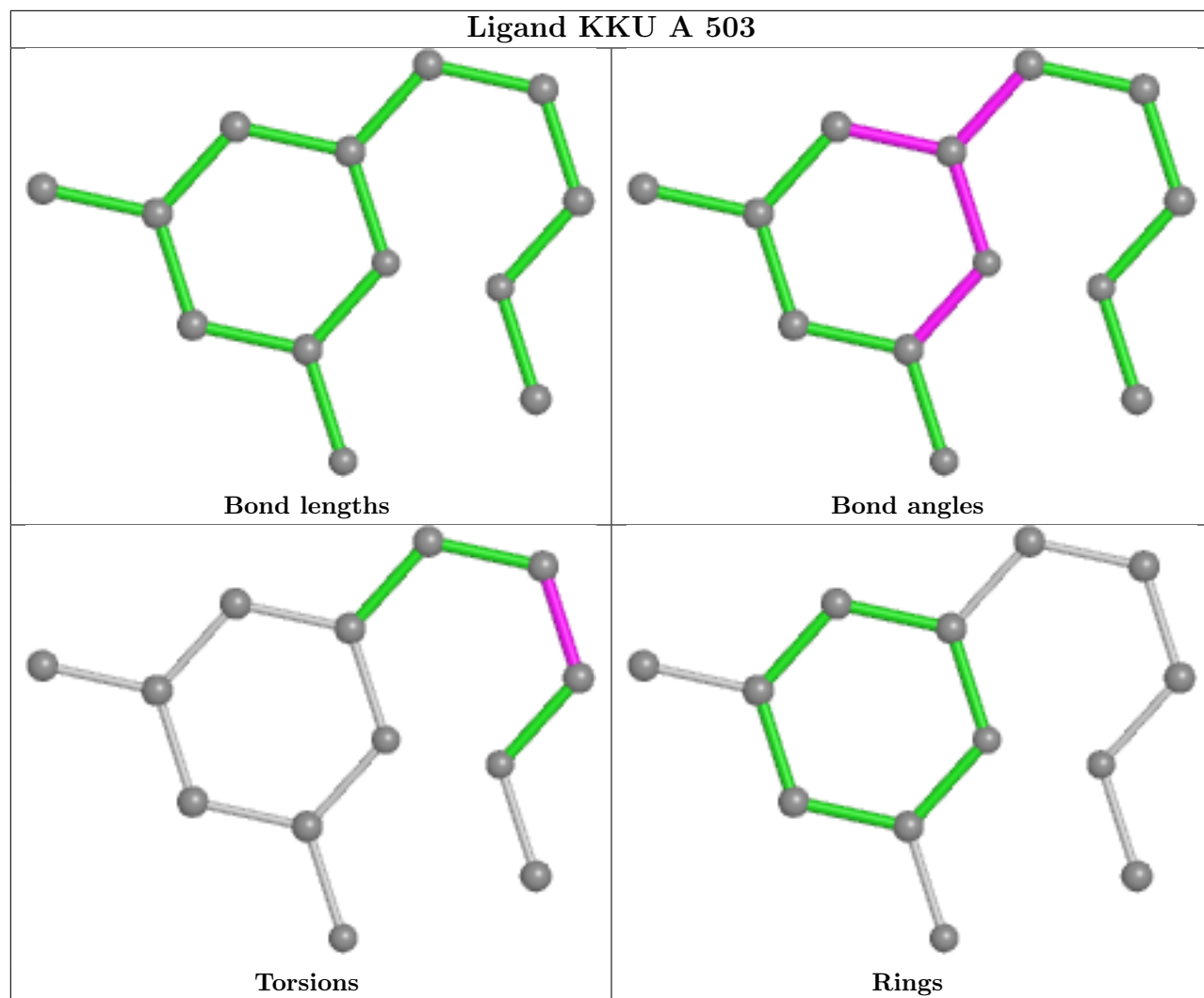
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.

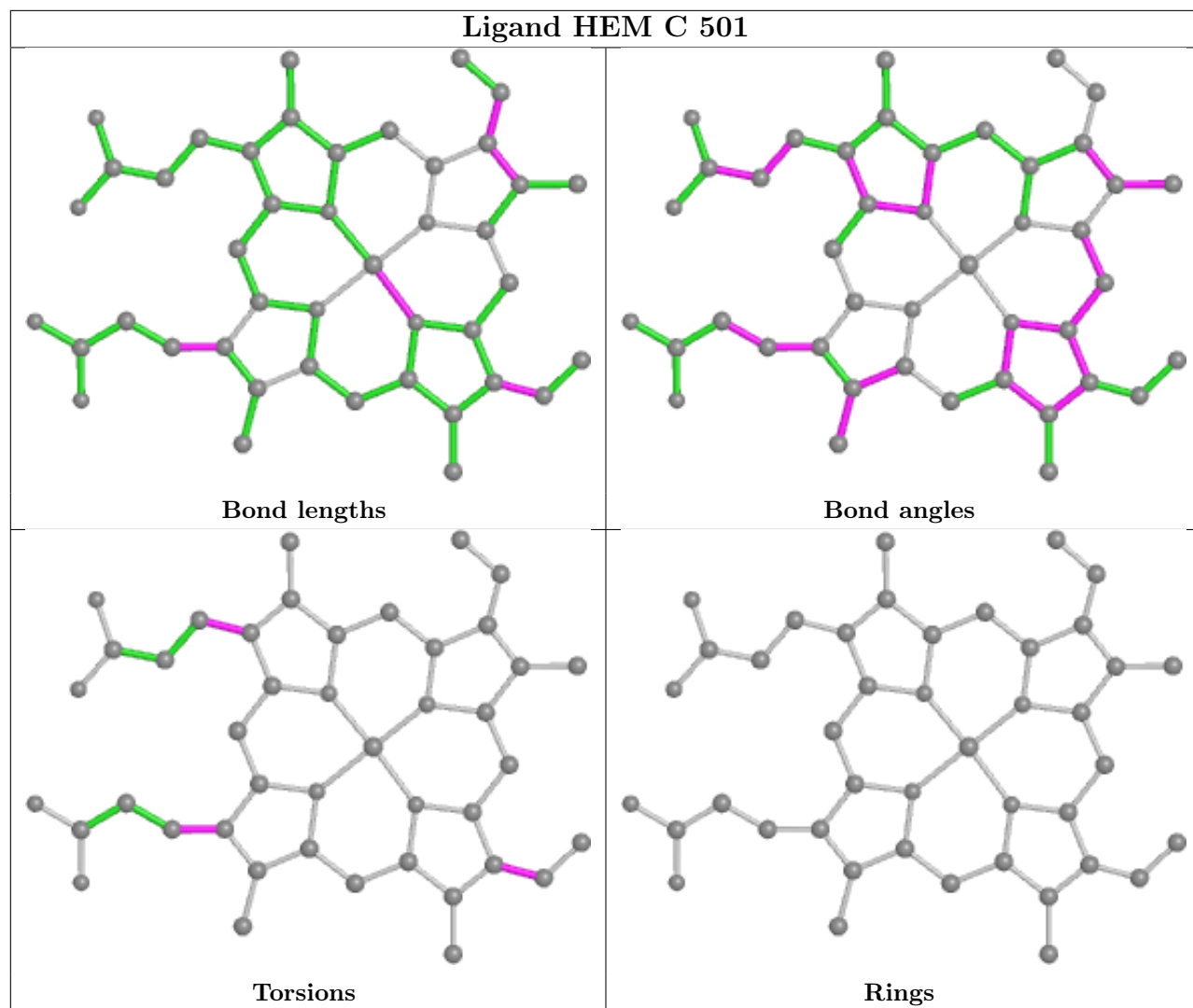


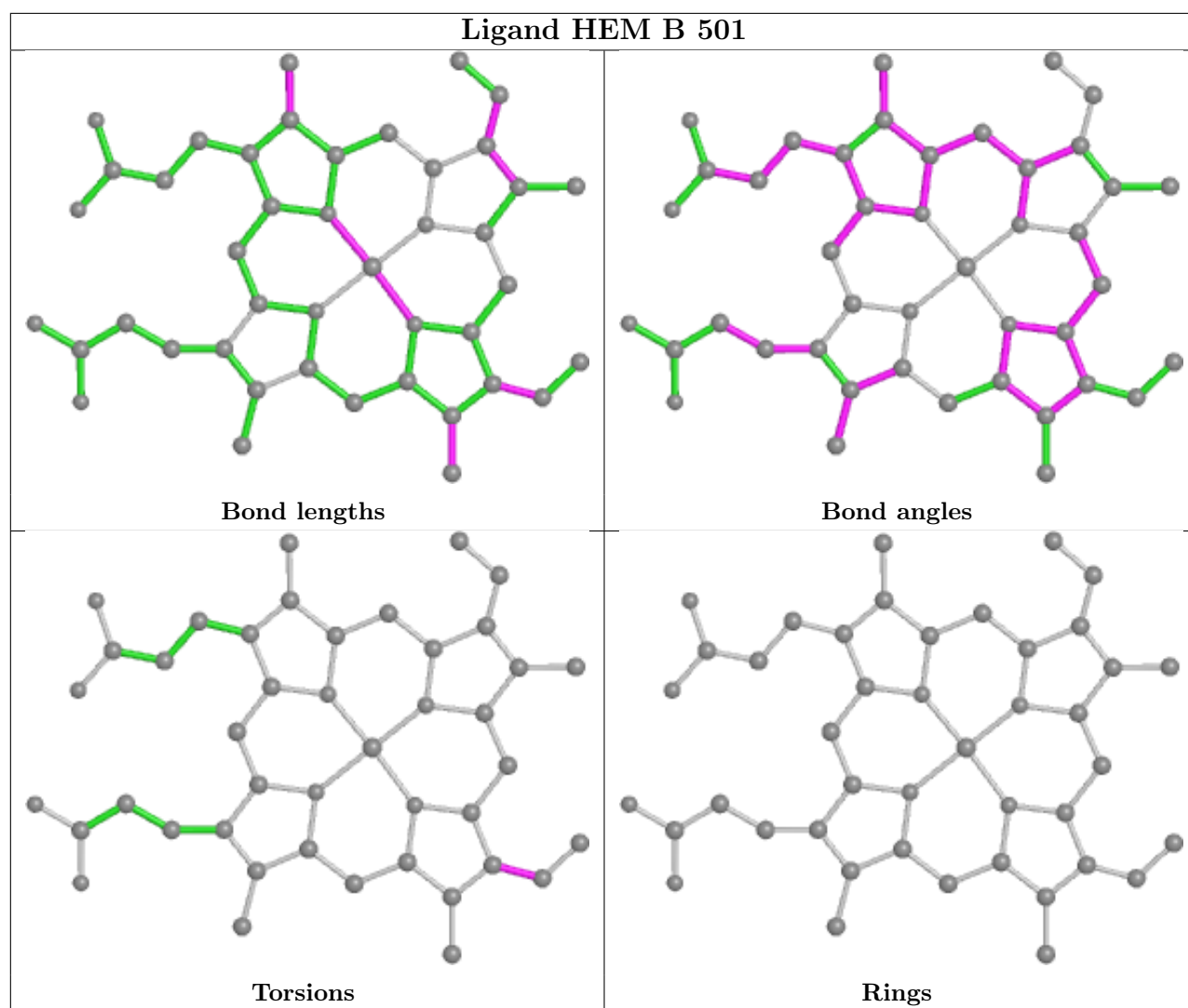


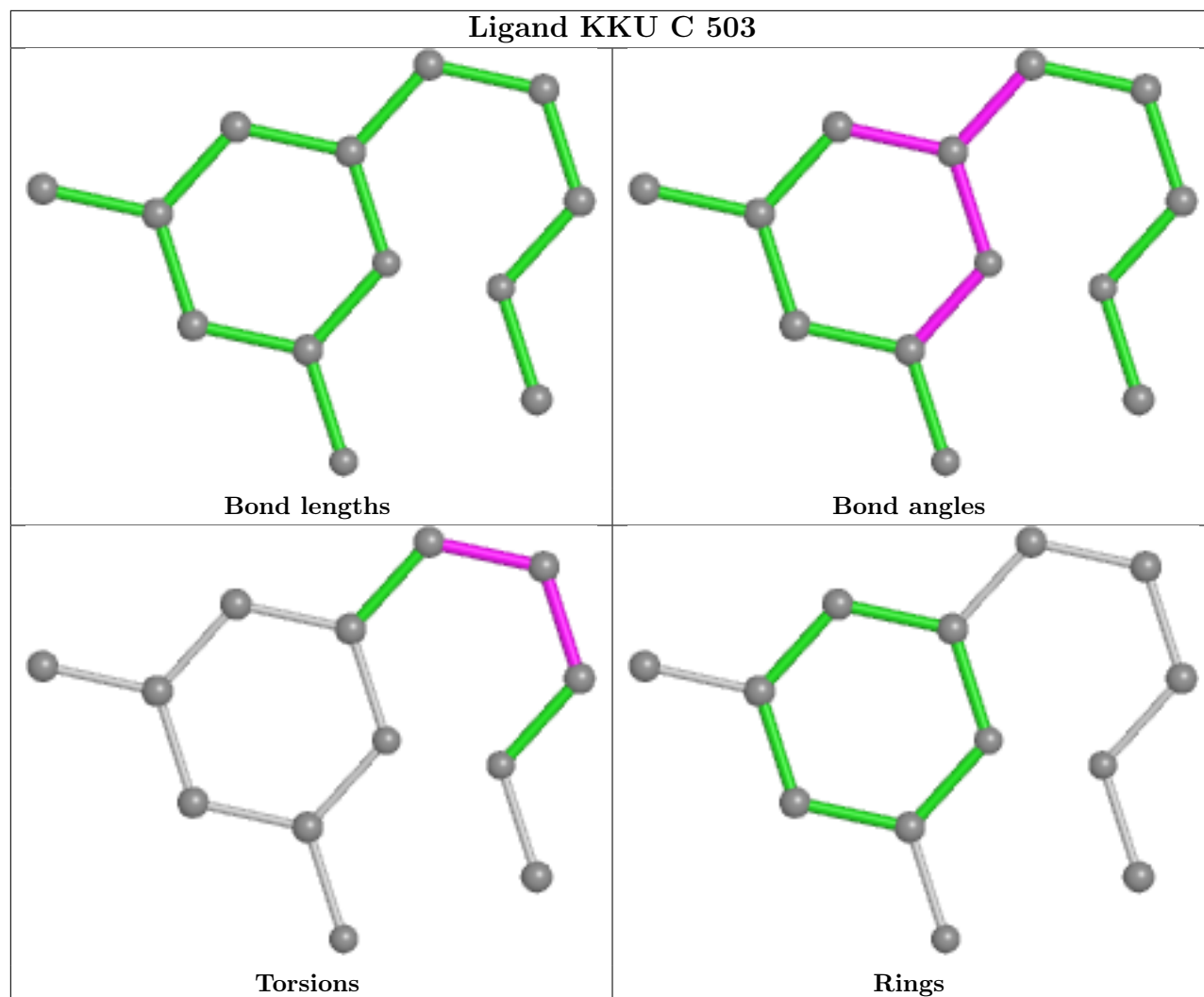












5.7 Other polymers [i](#)

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	400/440 (90%)	0.19	26 (6%) 18 23	34, 70, 122, 161	0
1	B	402/440 (91%)	-0.24	5 (1%) 79 83	30, 47, 87, 121	0
1	C	402/440 (91%)	-0.02	12 (2%) 50 58	32, 63, 107, 161	0
1	D	402/440 (91%)	-0.35	2 (0%) 91 93	30, 46, 73, 143	0
All	All	1606/1760 (91%)	-0.10	45 (2%) 53 61	30, 54, 107, 161	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	153	VAL	6.5
1	A	284	GLY	4.8
1	C	204	ALA	4.2
1	A	346	LEU	4.2
1	B	89	GLN	4.1
1	A	163	TYR	4.1
1	D	89	GLN	4.1
1	C	480	TRP	4.0
1	C	130	PHE	3.7
1	A	480	TRP	3.6
1	A	238	ARG	3.6
1	A	254	TYR	3.6
1	C	202	ARG	3.4
1	A	279	TRP	3.3
1	C	238	ARG	3.2
1	A	275	ILE	3.2
1	A	242	ARG	3.1
1	C	163	TYR	3.1
1	B	106	PRO	3.0
1	A	268	VAL	2.8
1	C	155	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	468	PHE	2.7
1	A	285	ARG	2.7
1	A	341	LEU	2.7
1	B	142	GLY	2.6
1	D	257	GLN	2.6
1	C	160	THR	2.6
1	A	259	GLY	2.6
1	A	293	LEU	2.6
1	A	473	PHE	2.5
1	A	281	PRO	2.4
1	B	141[A]	SER	2.3
1	A	243	ILE	2.3
1	C	148	GLN	2.2
1	A	241	PHE	2.2
1	A	204	ALA	2.2
1	A	305	LEU	2.2
1	A	145	ALA	2.1
1	A	255	ARG	2.1
1	A	121	GLU	2.1
1	C	239	GLY	2.1
1	B	388	ARG	2.1
1	A	244	TRP	2.1
1	C	302	LEU	2.0
1	A	256	GLN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

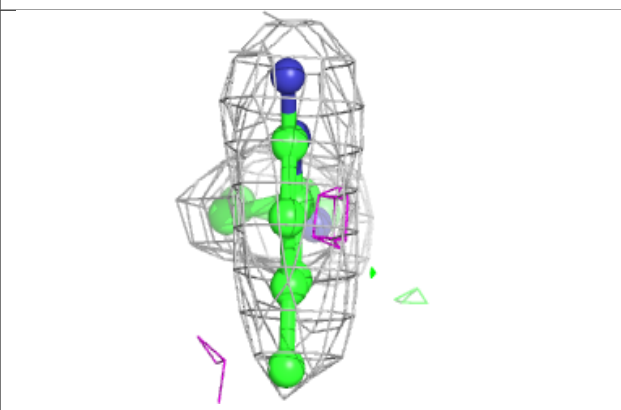
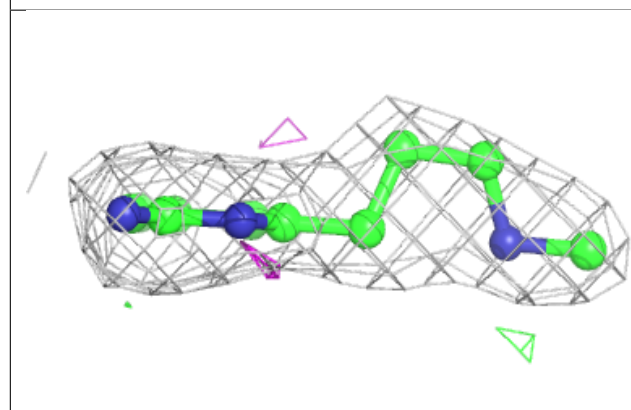
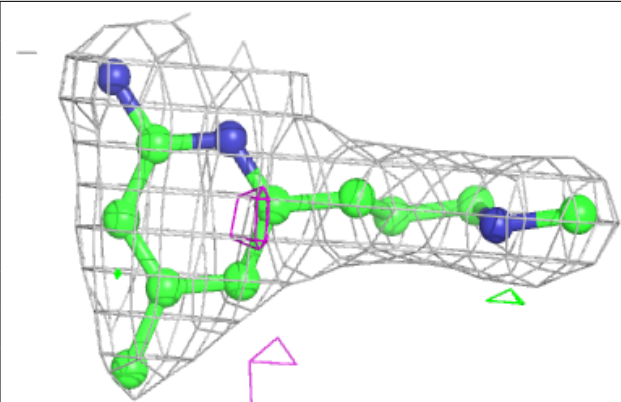
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	GOL	C	508	6/6	0.73	0.14	73,79,80,81	0
5	BTB	A	506	14/14	0.78	0.12	94,102,107,107	0
6	GOL	B	506	6/6	0.83	0.12	77,80,86,88	0
5	BTB	B	505	14/14	0.84	0.18	51,70,77,78	0
5	BTB	C	506	14/14	0.84	0.11	83,96,103,103	0
6	GOL	A	508	6/6	0.88	0.16	59,73,83,86	0
6	GOL	D	507	6/6	0.89	0.07	75,80,84,86	0
5	BTB	D	504	14/14	0.92	0.13	53,68,78,80	0
5	BTB	B	504	14/14	0.93	0.11	31,50,79,84	0
6	GOL	D	506	6/6	0.93	0.20	44,56,67,70	0
6	GOL	A	507	6/6	0.93	0.20	59,63,76,87	0
5	BTB	D	505	14/14	0.94	0.15	49,75,80,84	0
5	BTB	A	505	14/14	0.94	0.17	60,73,83,84	0
6	GOL	C	507	6/6	0.94	0.21	57,60,64,66	0
4	KKU	B	503	13/13	0.95	0.13	32,44,50,54	0
3	H4B	B	502	17/17	0.95	0.08	27,42,51,55	0
3	H4B	C	502	17/17	0.95	0.11	35,55,63,64	0
3	H4B	A	502	17/17	0.96	0.10	52,60,69,71	0
4	KKU	C	503	13/13	0.96	0.14	42,52,85,87	0
4	KKU	D	503	13/13	0.97	0.12	31,49,57,66	0
6	GOL	A	512	6/6	0.97	0.10	35,45,55,64	0
5	BTB	C	505	14/14	0.97	0.22	24,57,75,81	0
5	BTB	A	504	14/14	0.97	0.14	52,80,91,92	0
4	KKU	A	503	13/13	0.97	0.11	48,52,59,64	0
2	HEM	A	501	43/43	0.97	0.15	49,68,85,88	0
3	H4B	D	502	17/17	0.97	0.10	35,44,48,49	0
2	HEM	C	501	43/43	0.98	0.11	41,53,61,67	0
2	HEM	D	501	43/43	0.98	0.10	30,41,50,57	0
2	HEM	B	501	43/43	0.98	0.10	26,44,53,58	0
5	BTB	C	504	14/14	0.98	0.12	28,69,76,81	0
7	CL	A	509	1/1	0.98	0.06	62,62,62,62	0
7	CL	B	507	1/1	0.99	0.10	42,42,42,42	0
7	CL	C	509	1/1	0.99	0.07	49,49,49,49	0
7	CL	D	508	1/1	0.99	0.10	42,42,42,42	0
8	GD	A	510	1/1	0.99	0.15	81,81,81,81	1
8	GD	B	509	1/1	0.99	0.14	78,78,78,78	1
9	ZN	A	511	1/1	0.99	0.13	50,50,50,50	0
8	GD	D	509	1/1	1.00	0.19	56,56,56,56	0
8	GD	B	508	1/1	1.00	0.18	52,52,52,52	0
9	ZN	C	510	1/1	1.00	0.14	41,41,41,41	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.

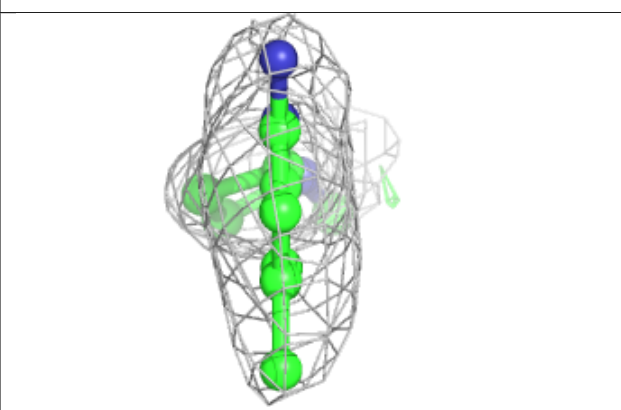
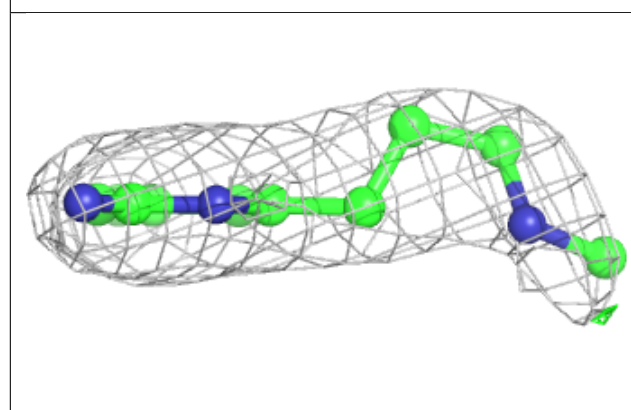
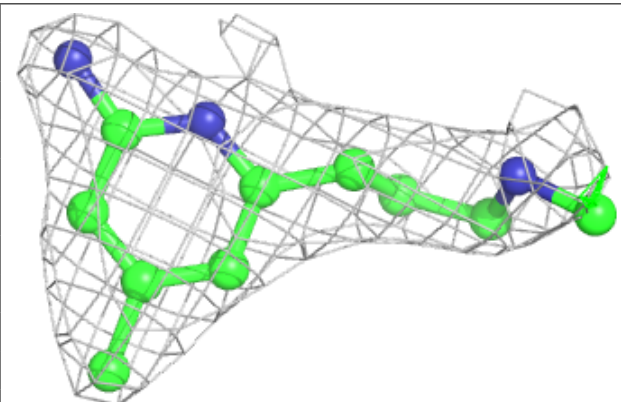
Electron density around KCU B 503:

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



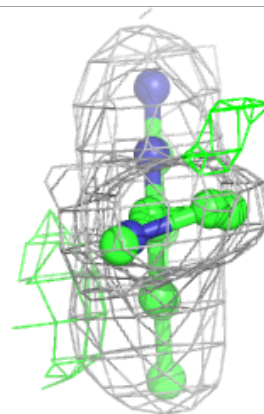
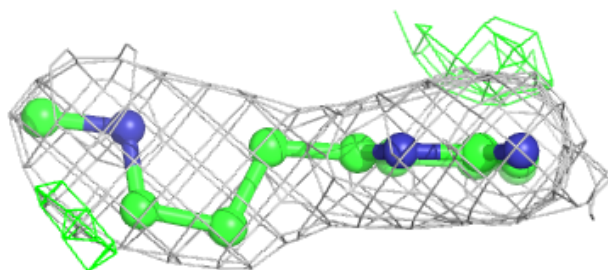
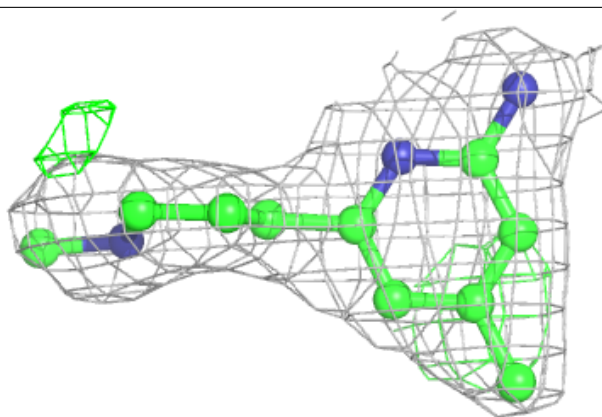
Electron density around KCU C 503:

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

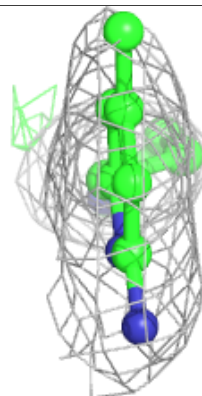
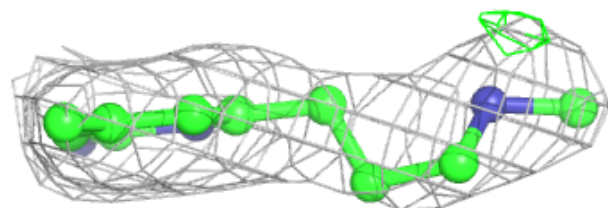
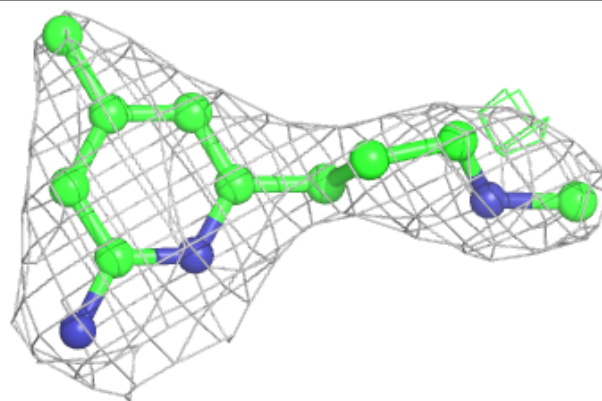


Electron density around KCU D 503:

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

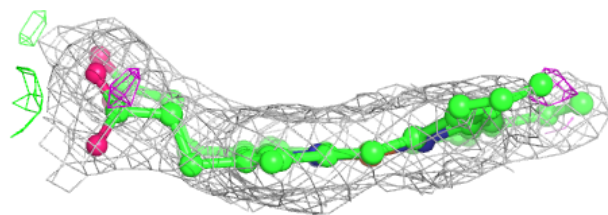
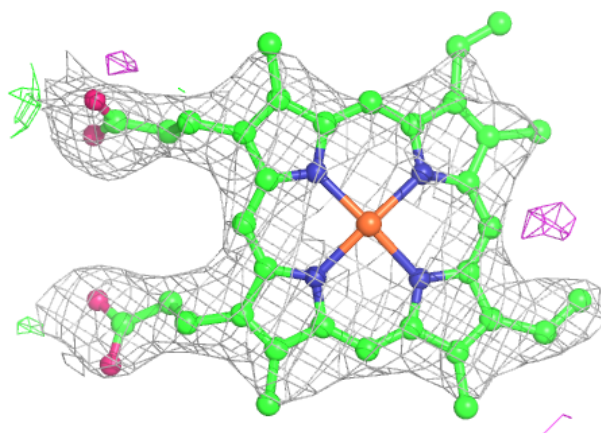
**Electron density around KCU A 503:**

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



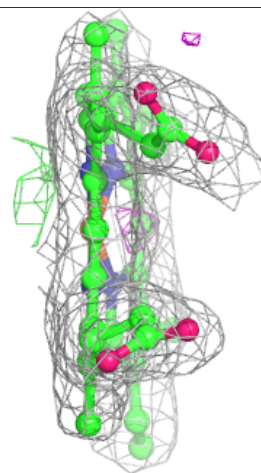
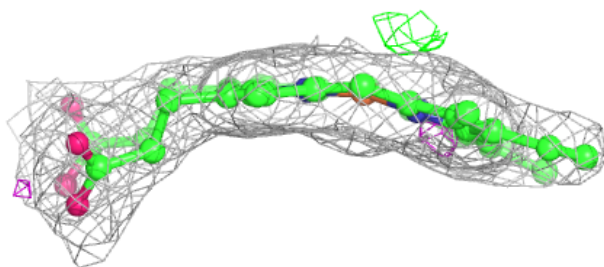
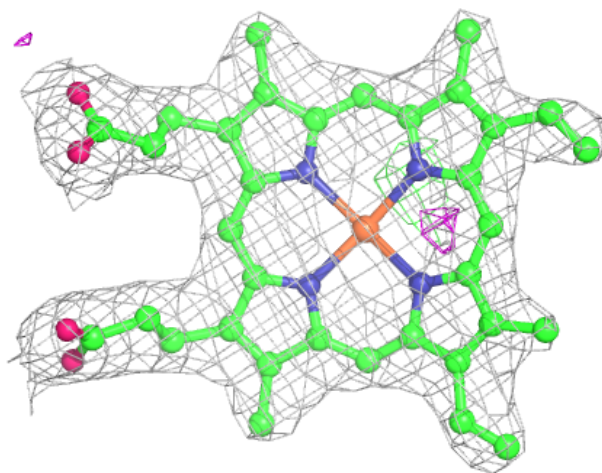
Electron density around HEM A 501:

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



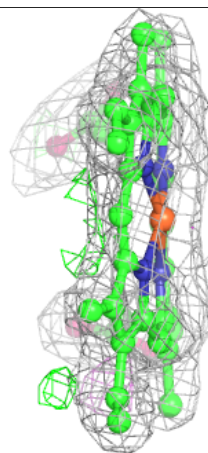
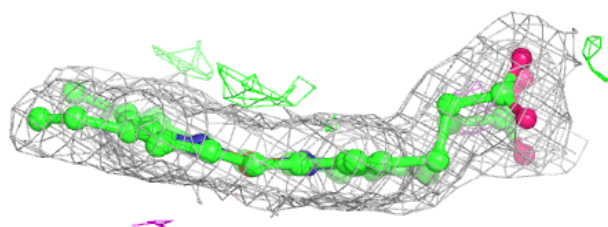
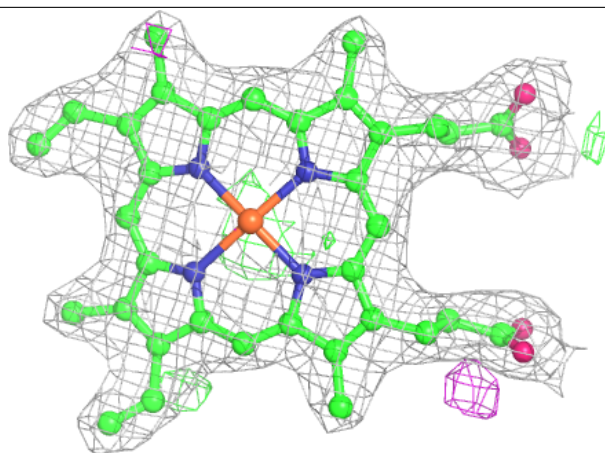
Electron density around HEM C 501:

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



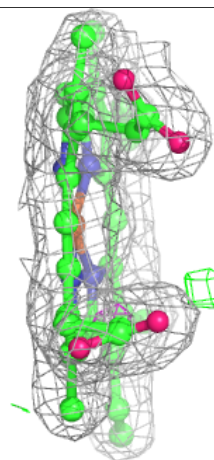
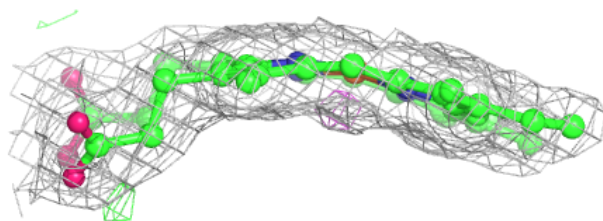
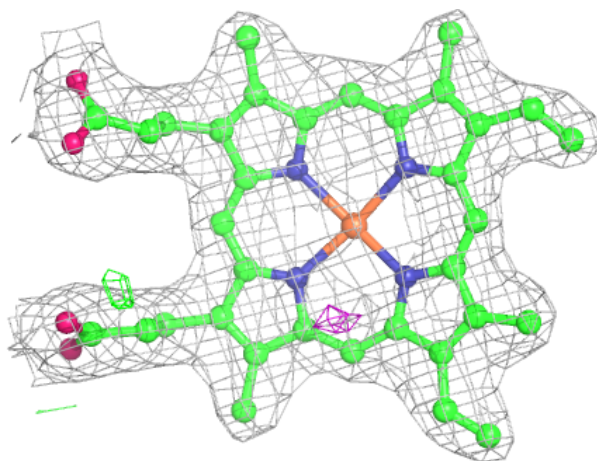
Electron density around HEM D 501:

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



Electron density around HEM B 501:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.