



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2020 – 10:06 PM BST

PDB ID : 6NH3  
Title : Structure of human endothelial nitric oxide synthase heme domain in complex with (S)-6-(3-fluoro-5-(2-(pyrrolidin-2-yl)ethyl)phenethyl)-4-methylpyridin-2-amine  
Authors : Chreifi, G.; Li, H.; Poulos, T.L.  
Deposited on : 2018-12-21  
Resolution : 2.01 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](mailto: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.

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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	:	2.13
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)	:	2.13

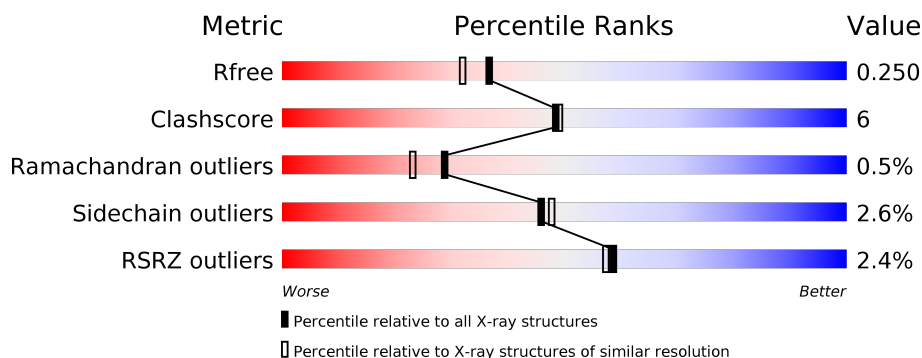
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.01 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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>5%</div> <div> <div></div> <div>75%</div> <div>15%</div> <div>• 8%</div> </div> </div>
1	B	440	<div> <div>%</div> <div> <div></div> <div>83%</div> <div>7%</div> <div>• 9%</div> </div> </div>
1	C	440	<div> <div>%</div> <div> <div></div> <div>79%</div> <div>11%</div> <div>• 9%</div> </div> </div>
1	D	440	<div> <div>%</div> <div> <div></div> <div>82%</div> <div>9%</div> <div>9%</div> </div> </div>

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 13985 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 Endothelial nitric oxide synthase splice variant eNOS13A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	404	Total	C	N	O	S	0	2	0
			3237	2062	570	589	16			
1	B	402	Total	C	N	O	S	0	3	0
			3221	2051	566	587	17			
1	C	401	Total	C	N	O	S	0	1	0
			3203	2040	563	584	16			
1	D	402	Total	C	N	O	S	0	3	0
			3221	2051	566	587	17			

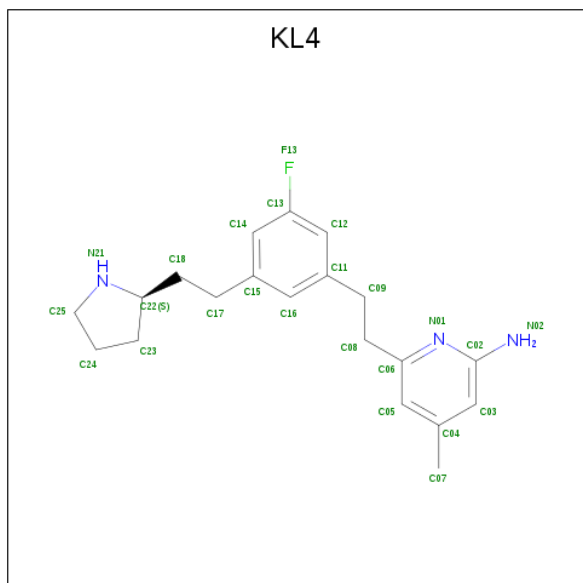
- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



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

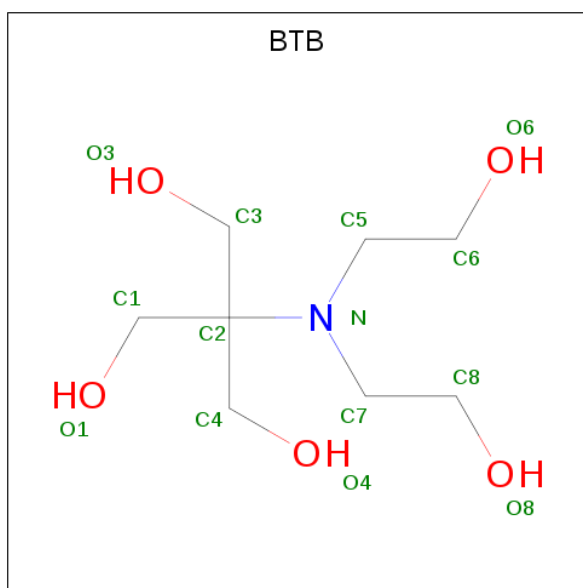
- Molecule 3 is 6-[2-(3-fluoro-5-{2-[(2S)-pyrrolidin-2-yl]ethyl}phenyl)ethyl]-4-methylpyridin-2-amine (three-letter code: KL4) (formula: C<sub>20</sub>H<sub>26</sub>FN<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	F	N	0	0
			24	20	1	3		
3	A	1	Total	C	F	N	0	0
			24	20	1	3		
3	B	1	Total	C	F	N	0	0
			24	20	1	3		
3	B	1	Total	C	F	N	0	0
			24	20	1	3		
3	C	1	Total	C	F	N	0	0
			24	20	1	3		
3	C	1	Total	C	F	N	0	0
			24	20	1	3		
3	C	1	Total	C	F	N	0	0
			24	20	1	3		
3	D	1	Total	C	F	N	0	0
			24	20	1	3		

- Molecule 4 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN

E-1,3-DIOL (three-letter code: BTB) (formula: C<sub>8</sub>H<sub>19</sub>NO<sub>5</sub>).



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

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total	Zn	0	0
			3	3		
5	C	3	Total	Zn	0	0
			3	3		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

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

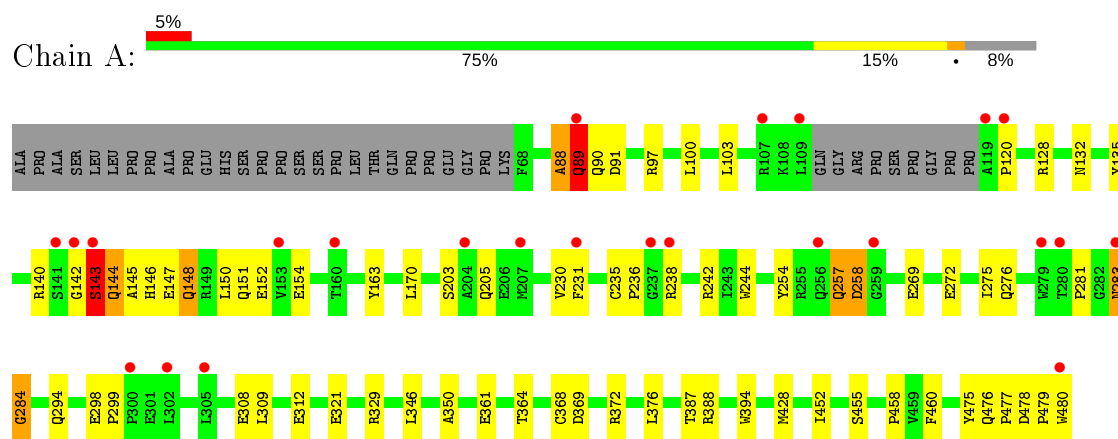
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	93	Total	O	0	0
			93	93		
9	B	164	Total	O	0	0
			164	164		
9	C	126	Total	O	0	0
			126	126		
9	D	204	Total	O	0	0
			204	204		

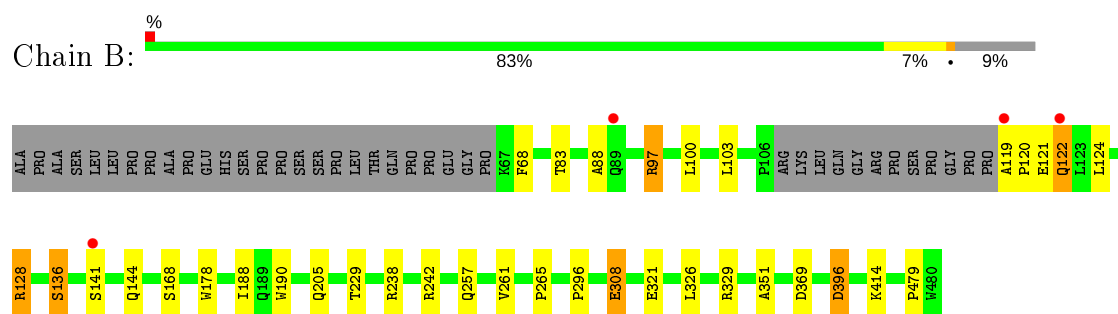
### 3 Residue-property plots [i](#)

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.

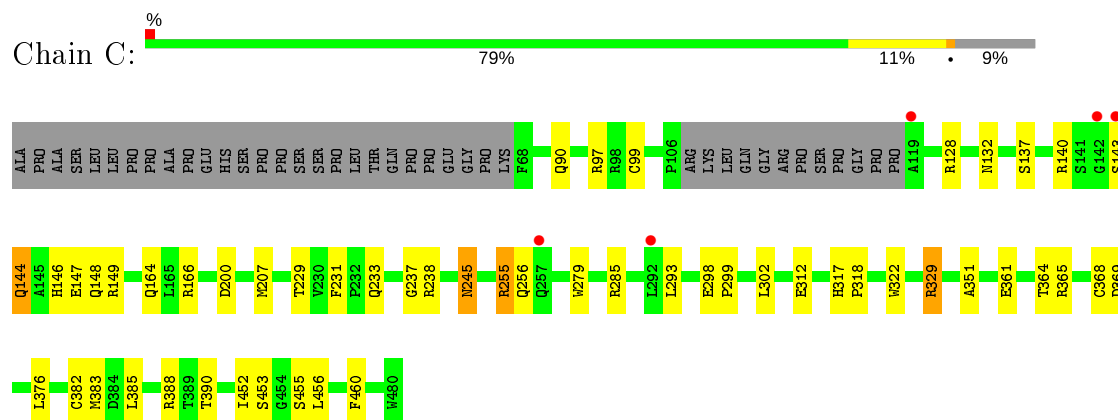
- Molecule 1: Endothelial nitric oxide synthase splice variant eNOS13A



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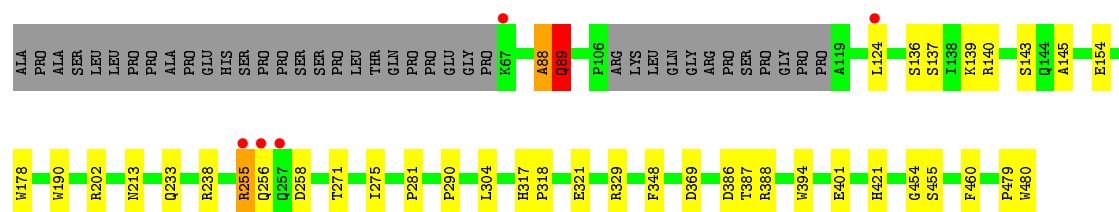
- Molecule 1: Endothelial nitric oxide synthase splice variant eNOS13A





- Molecule 1: Endothelial nitric oxide synthase splice variant eNOS13A

Chain D:  82% 9% 9%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.47Å 153.09Å 109.15Å 90.00° 90.80° 90.00°	Depositor
Resolution (Å)	88.87 – 2.01 88.87 – 2.01	Depositor EDS
% Data completeness (in resolution range)	98.4 (88.87-2.01) 99.9 (88.87-2.01)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	0.17	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.33 (at 2.02Å)	Xtriage
Refinement program	PHENIX 1.11.1-2575_1496	Depositor
R, $R_{free}$	0.206 , 0.257 0.199 , 0.250	Depositor DCC
$R_{free}$ test set	6538 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.0	Xtriage
Anisotropy	0.747	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 51.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.087 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	13985	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: GOL, ZN, CL, KL4, GD, BTB, 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	0.37	0/3335	0.55	2/4543 (0.0%)
1	B	0.41	0/3319	0.53	1/4523 (0.0%)
1	C	0.37	0/3298	0.53	1/4495 (0.0%)
1	D	0.42	0/3319	0.58	1/4523 (0.0%)
All	All	0.39	0/13271	0.55	5/18084 (0.0%)

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	A	0	3
1	C	0	1
1	D	0	2
All	All	0	6

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	369	ASP	CB-CG-OD1	6.49	124.14	118.30
1	B	369	ASP	CB-CG-OD1	6.20	123.88	118.30
1	A	369	ASP	CB-CG-OD1	5.80	123.52	118.30
1	A	144	GLN	N-CA-C	5.41	125.62	111.00
1	C	369	ASP	CB-CG-OD1	5.27	123.04	118.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	143	SER	Peptide
1	A	88	ALA	Peptide
1	A	89	GLN	Peptide
1	C	144	GLN	Peptide
1	D	88	ALA	Peptide
1	D	89	GLN	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3237	0	3146	56	0
1	B	3221	0	3126	30	0
1	C	3203	0	3103	33	0
1	D	3221	0	3126	26	0
2	A	43	0	30	3	0
2	B	43	0	30	2	0
2	C	43	0	30	1	0
2	D	43	0	30	0	0
3	A	48	0	0	1	0
3	B	48	0	0	0	0
3	C	72	0	0	0	0
3	D	24	0	0	0	0
4	A	28	0	38	2	0
4	B	42	0	54	4	0
4	C	28	0	38	9	0
4	D	28	0	36	5	0
5	A	3	0	0	0	0
5	C	3	0	0	0	0
6	A	6	0	8	0	0
6	C	6	0	8	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	1	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	A	93	0	0	2	0
9	B	164	0	0	2	0
9	C	126	0	0	2	0
9	D	204	0	0	3	0
All	All	13985	0	12803	156	0

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

All (156) 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)
4:A:503:BTB:HO4	4:A:503:BTB:HO8	1.19	0.88
1:D:213:ASN:ND2	9:D:601:HOH:O	2.10	0.85
1:A:144:GLN:HG3	1:A:146:HIS:H	1.48	0.77
1:D:321:GLU:OE2	4:D:503:BTB:O4	2.02	0.77
1:B:124:LEU:HD22	1:B:128:ARG:HH12	1.51	0.76
2:C:501:HEM:HBB2	2:C:501:HEM:HHC	1.77	0.67
1:A:89:GLN:HE21	1:B:97:ARG:HD3	1.61	0.65
2:A:501:HEM:HBB2	2:A:501:HEM:HHC	1.77	0.65
2:A:501:HEM:HBC2	2:A:501:HEM:HMC2	1.79	0.64
1:A:298:GLU:HG3	1:A:299:PRO:HD2	1.80	0.64
1:B:188:ILE:O	9:B:901:HOH:O	2.15	0.63
1:B:238:ARG:HG2	1:B:296:PRO:HB3	1.82	0.61
1:A:89:GLN:OE1	1:A:91:ASP:HA	2.01	0.61
1:B:100:LEU:HB3	1:B:103:LEU:HD22	1.82	0.61
1:D:124:LEU:HD21	1:D:154:GLU:HG3	1.83	0.60
1:A:145:ALA:HA	1:A:148:GLN:HG2	1.83	0.60
1:A:144:GLN:HG3	1:A:146:HIS:N	2.17	0.59
1:D:290:PRO:HB3	1:D:304:LEU:HD23	1.84	0.59
1:A:128:ARG:O	1:A:132:ASN:ND2	2.35	0.59
1:B:326:LEU:HD23	4:C:504:BTB:H52	1.85	0.59
1:A:89:GLN:CD	1:B:97:ARG:HA	2.23	0.59
4:D:503:BTB:O8	4:D:503:BTB:H62	2.02	0.58
1:C:298:GLU:HG3	1:C:299:PRO:HD2	1.86	0.58
1:A:135:TYR:CG	1:A:146:HIS:HB2	2.39	0.57
1:A:242:ARG:NH2	1:A:477:PRO:O	2.38	0.57
1:B:308:GLU:CD	1:B:308:GLU:H	2.06	0.57
1:A:144:GLN:O	1:A:148:GLN:NE2	2.38	0.56
4:A:504:BTB:O3	4:A:504:BTB:O1	2.13	0.56
1:A:88:ALA:O	1:A:89:GLN:HB2	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:GLU:CD	1:A:321:GLU:H	2.08	0.56
1:C:144:GLN:HB3	1:C:147:GLU:HG2	1.86	0.56
1:D:317:HIS:NE2	1:D:401:GLU:OE1	2.36	0.56
1:D:386:ASP:OD1	1:D:388:ARG:HG2	2.06	0.55
2:B:802:HEM:HHC	2:B:802:HEM:HBB2	1.88	0.55
1:D:275:ILE:HD12	1:D:281:PRO:HG3	1.89	0.55
1:A:231:PHE:HD2	1:A:350:ALA:HB1	1.71	0.55
1:C:361:GLU:HB3	1:C:365:ARG:NH2	2.22	0.55
1:A:89:GLN:HG2	1:B:97:ARG:NE	2.22	0.54
1:A:144:GLN:HE21	1:A:147:GLU:HG3	1.73	0.54
1:D:317:HIS:CG	1:D:318:PRO:HD2	2.42	0.54
1:A:144:GLN:CD	1:A:146:HIS:HB3	2.28	0.54
1:C:245:ASN:OD1	1:C:245:ASN:N	2.39	0.54
1:D:255:ARG:HG3	1:D:255:ARG:O	2.08	0.53
1:A:361:GLU:OE2	3:A:502:KL4:N02	2.42	0.53
1:A:142:GLY:O	1:A:143:SER:OG	2.17	0.53
1:A:89:GLN:NE2	1:B:97:ARG:HA	2.24	0.52
1:B:242:ARG:NH2	1:B:479:PRO:HD3	2.25	0.52
1:D:271:THR:O	1:D:275:ILE:HG12	2.10	0.52
1:C:200:ASP:OD1	1:C:200:ASP:N	2.42	0.52
1:A:170:LEU:HD11	1:A:230:VAL:HG11	1.91	0.52
1:A:135:TYR:CD1	1:A:146:HIS:HB2	2.44	0.52
1:C:298:GLU:OE2	4:C:505:BTB:O8	2.19	0.52
1:D:256:GLN:HE22	1:D:258:ASP:CG	2.12	0.51
4:B:808:BTB:H41	4:B:808:BTB:O8	2.10	0.51
1:D:178:TRP:CE3	1:D:190:TRP:HA	2.46	0.51
1:C:149:ARG:NH2	1:C:164:GLN:O	2.39	0.51
1:A:236:PRO:O	1:A:238:ARG:HG3	2.11	0.50
1:A:242:ARG:NH1	1:A:479:PRO:HD3	2.27	0.50
1:A:89:GLN:HA	1:A:89:GLN:NE2	2.25	0.50
1:A:478:ASP:O	1:A:480:TRP:N	2.40	0.50
1:C:128:ARG:O	1:C:132:ASN:ND2	2.45	0.50
1:B:119:ALA:N	1:B:122:GLN:HE22	2.09	0.49
4:C:505:BTB:H12	4:C:505:BTB:H61	1.93	0.49
1:A:163:TYR:CE1	1:A:346:LEU:HD11	2.47	0.49
1:B:121:GLU:H	1:B:121:GLU:CD	2.15	0.49
1:A:242:ARG:HH21	1:A:476:GLN:CD	2.16	0.49
1:D:88:ALA:O	1:D:89:GLN:HB2	2.13	0.48
1:D:233:GLN:HB3	1:D:348:PHE:CE2	2.48	0.48
1:A:364:THR:HG21	1:A:452:ILE:HG23	1.95	0.48
4:B:808:BTB:H52	4:B:808:BTB:H82	1.59	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:233:GLN:NE2	9:C:602:HOH:O	2.24	0.47
1:A:100:LEU:HB3	1:A:103:LEU:HD22	1.96	0.47
1:B:321:GLU:HG2	1:C:285:ARG:NH2	2.29	0.47
1:B:261:VAL:HG11	1:B:265:PRO:HA	1.96	0.47
1:A:312:GLU:OE2	1:A:329:ARG:HD3	2.15	0.47
1:B:68:PHE:CD2	1:B:83:THR:HG22	2.50	0.47
1:C:207:MET:HG3	1:C:231:PHE:CZ	2.49	0.47
1:A:475:TYR:OH	2:A:501:HEM:O1D	2.21	0.46
1:A:147:GLU:HA	1:A:150:LEU:HD12	1.96	0.46
1:C:207:MET:HG2	1:C:293:LEU:HD13	1.98	0.46
1:C:382:CYS:HA	4:C:504:BTB:H42	1.96	0.46
1:A:455:SER:HA	1:A:460:PHE:CG	2.50	0.46
1:B:136:SER:HA	1:B:141[B]:SER:OG	2.16	0.46
1:B:257:GLN:CD	1:B:257:GLN:H	2.18	0.46
1:D:238:ARG:HD2	9:D:742:HOH:O	2.16	0.46
1:A:368:CYS:SG	1:A:376:LEU:HD13	2.56	0.46
1:C:364:THR:O	1:C:368:CYS:HB2	2.16	0.45
1:A:154:GLU:HG3	9:A:620:HOH:O	2.16	0.45
1:C:148:GLN:OE1	1:C:166:ARG:NH2	2.49	0.45
1:C:322:TRP:CH2	1:C:382:CYS:HB2	2.51	0.45
1:A:242:ARG:HE	1:A:476:GLN:NE2	2.15	0.45
4:C:505:BTB:H51	4:C:505:BTB:H42	1.49	0.45
1:D:479:PRO:HD2	1:D:480:TRP:CE3	2.52	0.45
1:A:143:SER:O	1:A:144:GLN:HG2	2.17	0.44
1:A:309:LEU:HA	1:A:309:LEU:HD12	1.80	0.44
1:D:124:LEU:HD21	1:D:154:GLU:CG	2.47	0.44
1:C:255:ARG:NH1	1:C:255:ARG:HB3	2.33	0.44
1:A:376:LEU:HB2	9:A:611:HOH:O	2.18	0.44
1:A:387:THR:HA	1:A:394:TRP:CD1	2.53	0.44
1:C:455:SER:HA	1:C:460:PHE:CG	2.53	0.44
1:A:151:GLN:HA	1:A:154:GLU:HG2	2.00	0.44
1:A:428:MET:HG3	1:A:458:PRO:HB2	2.00	0.44
1:A:97:ARG:HG2	1:B:88:ALA:HB3	2.00	0.44
1:D:455:SER:HA	1:D:460:PHE:CG	2.53	0.44
1:A:140:ARG:HD3	1:A:140:ARG:HA	1.87	0.43
1:C:298:GLU:OE2	4:C:505:BTB:O6	2.24	0.43
1:D:256:GLN:NE2	1:D:258:ASP:OD2	2.45	0.43
1:A:148:GLN:N	1:A:148:GLN:CD	2.72	0.43
1:C:279:TRP:HB2	1:C:302:LEU:HD21	2.01	0.43
4:C:504:BTB:H11	4:C:504:BTB:H71	1.70	0.43
1:A:364:THR:O	1:A:368:CYS:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:GLN:HG2	1:B:97:ARG:HE	1.83	0.43
1:A:89:GLN:NE2	1:B:97:ARG:HD3	2.32	0.43
4:D:503:BTB:H32	4:D:503:BTB:H51	1.68	0.43
4:C:504:BTB:H32	4:C:504:BTB:H51	1.74	0.43
1:C:390:THR:HB	1:D:421:HIS:HB2	2.00	0.43
1:A:244:TRP:NE1	1:A:294:GLN:OE1	2.44	0.43
1:B:178:TRP:CE3	1:B:190:TRP:HA	2.54	0.43
1:D:454:GLY:O	1:D:460:PHE:HB2	2.18	0.43
1:C:312:GLU:OE2	1:C:329:ARG:NH1	2.52	0.43
1:D:387:THR:HA	1:D:394:TRP:CD1	2.54	0.42
1:A:269:GLU:O	1:A:272:GLU:HG2	2.18	0.42
1:C:238:ARG:HA	1:C:238:ARG:HD3	1.87	0.42
1:A:231:PHE:HD2	1:A:350:ALA:CB	2.32	0.42
1:D:137:SER:O	1:D:139:LYS:HE3	2.19	0.42
1:B:120:PRO:HD2	1:B:121:GLU:OE2	2.19	0.42
1:A:258:ASP:N	1:A:258:ASP:OD1	2.53	0.42
1:B:229:THR:O	1:B:351:ALA:HA	2.20	0.42
4:B:805:BTB:H51	4:B:805:BTB:O3	2.20	0.42
1:D:143:SER:HB2	9:D:694:HOH:O	2.19	0.42
1:A:254:TYR:CE2	1:A:284:GLY:HA2	2.55	0.42
4:D:504:BTB:H32	4:D:504:BTB:H51	1.40	0.42
1:B:119:ALA:HB3	1:B:120:PRO:HD3	2.03	0.41
1:C:90:GLN:NE2	9:C:613:HOH:O	2.47	0.41
1:C:317:HIS:CG	1:C:318:PRO:HD2	2.55	0.41
1:C:368:CYS:SG	1:C:376:LEU:HD13	2.60	0.41
4:B:808:BTB:H71	4:B:808:BTB:O3	2.19	0.41
1:C:383:MET:HB2	1:C:385:LEU:HG	2.02	0.41
1:C:453:SER:HB3	1:C:456:LEU:HD12	2.03	0.41
2:B:802:HEM:CGA	2:B:802:HEM:HMA2	2.51	0.41
4:D:504:BTB:H81	4:D:504:BTB:H52	1.29	0.41
1:B:121:GLU:OE1	1:B:122:GLN:NE2	2.53	0.41
1:B:396:ASP:OD1	1:B:396:ASP:N	2.51	0.41
1:B:68:PHE:CG	1:B:83:THR:HG22	2.56	0.41
1:C:229:THR:O	1:C:351:ALA:HA	2.21	0.41
1:B:124:LEU:HD13	1:B:128:ARG:HH22	1.85	0.41
1:C:144:GLN:HA	1:C:146:HIS:H	1.86	0.41
1:C:255:ARG:HB3	1:C:255:ARG:HH11	1.85	0.41
1:C:364:THR:HG21	1:C:452:ILE:HG23	2.02	0.41
1:C:97:ARG:HB3	1:C:97:ARG:NH1	2.36	0.41
1:A:372:ARG:HD2	1:A:372:ARG:HA	1.90	0.41
1:B:205:GLN:HG3	9:B:977:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:140:ARG:HH21	1:D:145:ALA:HB3	1.86	0.40
1:D:124:LEU:HD12	1:D:124:LEU:HA	1.83	0.40
4:C:505:BTB:O1	4:C:505:BTB:O4	2.18	0.40
1:A:275:ILE:HD13	1:A:281:PRO:HG3	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	402/440 (91%)	372 (92%)	24 (6%)	6 (2%)	10	4
1	B	401/440 (91%)	390 (97%)	11 (3%)	0	100	100
1	C	398/440 (90%)	380 (96%)	17 (4%)	1 (0%)	41	37
1	D	401/440 (91%)	391 (98%)	9 (2%)	1 (0%)	47	44
All	All	1602/1760 (91%)	1533 (96%)	61 (4%)	8 (0%)	29	23

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	143	SER
1	A	257	GLN
1	A	283	ASN
1	D	89	GLN
1	A	120	PRO
1	C	237	GLY
1	A	284	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	345/373 (92%)	332 (96%)	13 (4%)	33	31
1	B	344/373 (92%)	333 (97%)	11 (3%)	39	38
1	C	341/373 (91%)	332 (97%)	9 (3%)	46	48
1	D	344/373 (92%)	340 (99%)	4 (1%)	71	76
All	All	1374/1492 (92%)	1337 (97%)	37 (3%)	46	46

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	90	GLN
1	A	148	GLN
1	A	152	GLU
1	A	203	SER
1	A	205	GLN
1	A	235	CYS
1	A	257	GLN
1	A	258	ASP
1	A	276	GLN
1	A	283	ASN
1	A	308	GLU
1	A	388	ARG
1	B	97	ARG
1	B	122	GLN
1	B	128	ARG
1	B	136	SER
1	B	144	GLN
1	B	168[A]	SER
1	B	168[B]	SER
1	B	308	GLU
1	B	329	ARG
1	B	396	ASP
1	B	414	LYS

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Mol	Chain	Res	Type
1	C	99	CYS
1	C	137	SER
1	C	140	ARG
1	C	143	SER
1	C	245	ASN
1	C	255	ARG
1	C	256	GLN
1	C	329	ARG
1	C	388	ARG
1	D	136	SER
1	D	202	ARG
1	D	255	ARG
1	D	329	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	148	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 37 ligands modelled in this entry, 14 are monoatomic - leaving 23 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	KL4	C	511	-	25,26,26	1.19	3 (12%)	32,35,35	1.39	4 (12%)
3	KL4	B	803	-	25,26,26	1.23	3 (12%)	32,35,35	1.85	8 (25%)
6	GOL	C	507	-	5,5,5	0.39	0	5,5,5	0.34	0
3	KL4	B	801	-	25,26,26	1.22	3 (12%)	32,35,35	1.32	4 (12%)
3	KL4	C	502	-	25,26,26	1.19	3 (12%)	32,35,35	1.55	6 (18%)
3	KL4	A	502	-	25,26,26	1.22	3 (12%)	32,35,35	1.52	3 (9%)
3	KL4	D	502	-	25,26,26	1.29	3 (12%)	32,35,35	1.63	8 (25%)
4	BTB	D	504	-	13,13,13	0.50	0	7,16,16	0.68	0
4	BTB	C	505	-	13,13,13	0.38	0	7,16,16	0.43	0
3	KL4	A	509	-	25,26,26	1.21	3 (12%)	32,35,35	1.27	4 (12%)
4	BTB	C	504	8	13,13,13	0.41	0	7,16,16	0.51	0
4	BTB	A	504	-	13,13,13	0.40	0	7,16,16	0.61	0
2	HEM	B	802	1	27,50,50	1.82	6 (22%)	17,82,82	2.25	7 (41%)
2	HEM	C	501	1	27,50,50	1.95	5 (18%)	17,82,82	2.20	5 (29%)
4	BTB	B	805	-	13,13,13	0.42	0	7,16,16	0.65	0
2	HEM	D	501	1	27,50,50	1.96	7 (25%)	17,82,82	2.16	7 (41%)
6	GOL	A	506	-	5,5,5	0.34	0	5,5,5	0.40	0
3	KL4	C	503	-	25,26,26	1.20	3 (12%)	32,35,35	1.36	4 (12%)
2	HEM	A	501	1	27,50,50	1.97	5 (18%)	17,82,82	1.73	4 (23%)
4	BTB	B	804	8	13,13,13	0.52	0	7,16,16	0.72	0
4	BTB	D	503	8	13,13,13	0.43	0	7,16,16	0.57	0
4	BTB	A	503	-	13,13,13	0.39	0	7,16,16	0.52	0
4	BTB	B	808	-	13,13,13	0.83	1 (7%)	7,16,16	0.98	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
3	KL4	C	511	-	-	3/10/17/17	0/3/3/3
3	KL4	B	803	-	-	2/10/17/17	0/3/3/3
6	GOL	C	507	-	-	4/4/4/4	-
3	KL4	B	801	-	-	3/10/17/17	0/3/3/3
3	KL4	C	502	-	-	4/10/17/17	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	KL4	A	502	-	-	3/10/17/17	0/3/3/3
3	KL4	D	502	-	-	4/10/17/17	0/3/3/3
4	BTB	D	504	-	-	11/21/21/21	-
4	BTB	C	505	-	-	6/21/21/21	-
3	KL4	A	509	-	-	2/10/17/17	0/3/3/3
4	BTB	C	504	8	-	7/21/21/21	-
4	BTB	A	504	-	-	8/21/21/21	-
2	HEM	B	802	1	-	3/6/54/54	-
2	HEM	C	501	1	-	3/6/54/54	-
4	BTB	B	805	-	-	7/21/21/21	-
2	HEM	D	501	1	-	2/6/54/54	-
6	GOL	A	506	-	-	4/4/4/4	-
3	KL4	C	503	-	-	1/10/17/17	0/3/3/3
2	HEM	A	501	1	-	3/6/54/54	-
4	BTB	B	804	8	-	4/21/21/21	-
4	BTB	D	503	8	-	7/21/21/21	-
4	BTB	A	503	-	-	11/21/21/21	-
4	BTB	B	808	-	-	7/21/21/21	-

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	C3B-C2B	-5.17	1.33	1.40
2	B	802	HEM	C3B-C2B	-4.41	1.34	1.40
2	C	501	HEM	C3B-CAB	4.26	1.56	1.47
2	C	501	HEM	C3B-C2B	-4.23	1.34	1.40
2	D	501	HEM	C3C-C2C	-4.13	1.34	1.40
2	B	802	HEM	C3C-CAC	4.02	1.56	1.47
2	C	501	HEM	C3C-CAC	3.99	1.56	1.47
3	D	502	KL4	C25-N21	-3.80	1.35	1.49
2	D	501	HEM	C3C-CAC	3.76	1.55	1.47
3	A	502	KL4	C25-N21	-3.73	1.35	1.49
3	B	803	KL4	C25-N21	-3.72	1.35	1.49
2	A	501	HEM	C3C-C2C	-3.67	1.35	1.40
2	A	501	HEM	C3C-CAC	3.63	1.55	1.47
3	C	502	KL4	C25-N21	-3.62	1.36	1.49
2	D	501	HEM	C3B-C2B	-3.59	1.35	1.40
3	A	509	KL4	C25-N21	-3.58	1.36	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	801	KL4	C25-N21	-3.58	1.36	1.49
3	C	511	KL4	C25-N21	-3.57	1.36	1.49
3	C	503	KL4	C25-N21	-3.56	1.36	1.49
2	A	501	HEM	C3B-CAB	3.55	1.55	1.47
2	D	501	HEM	C3B-CAB	3.49	1.55	1.47
2	B	802	HEM	C3B-CAB	3.38	1.54	1.47
3	D	502	KL4	C24-C23	-3.31	1.38	1.51
2	C	501	HEM	C3C-C2C	-3.29	1.35	1.40
3	C	502	KL4	C24-C23	-3.23	1.38	1.51
2	D	501	HEM	CAA-C2A	3.23	1.56	1.52
3	B	803	KL4	C24-C23	-3.21	1.38	1.51
3	A	502	KL4	C24-C23	-3.21	1.38	1.51
3	C	511	KL4	C24-C23	-3.19	1.38	1.51
3	C	503	KL4	C24-C23	-3.14	1.38	1.51
3	A	509	KL4	C24-C23	-3.06	1.39	1.51
3	B	801	KL4	C24-C23	-3.05	1.39	1.51
2	A	501	HEM	CAA-C2A	3.04	1.56	1.52
2	B	802	HEM	C3C-C2C	-3.03	1.36	1.40
2	C	501	HEM	CAA-C2A	2.76	1.56	1.52
3	A	502	KL4	C24-C25	-2.57	1.38	1.51
3	D	502	KL4	C24-C25	-2.52	1.38	1.51
3	B	803	KL4	C24-C25	-2.50	1.38	1.51
3	C	502	KL4	C24-C25	-2.48	1.39	1.51
3	C	503	KL4	C24-C25	-2.45	1.39	1.51
3	A	509	KL4	C24-C25	-2.43	1.39	1.51
3	B	801	KL4	C24-C25	-2.43	1.39	1.51
2	B	802	HEM	CAA-C2A	2.41	1.55	1.52
3	C	511	KL4	C24-C25	-2.39	1.39	1.51
2	D	501	HEM	C1D-ND	2.37	1.41	1.36
2	D	501	HEM	CMD-C2D	2.13	1.56	1.51
2	B	802	HEM	CMB-C2B	2.12	1.56	1.51
4	B	808	BTB	C1-C2	-2.06	1.50	1.53

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	HEM	CMA-C3A-C4A	-5.33	120.27	128.46
3	D	502	KL4	C02-N01-C06	4.96	121.86	118.10
2	B	802	HEM	CMA-C3A-C4A	-4.91	120.92	128.46
3	A	502	KL4	C02-N01-C06	4.77	121.72	118.10
2	D	501	HEM	CMA-C3A-C4A	-4.67	121.29	128.46
3	B	803	KL4	C02-N01-C06	4.40	121.44	118.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	HEM	CBD-CAD-C3D	-3.89	105.31	112.48
3	B	801	KL4	C02-N01-C06	3.84	121.01	118.10
3	C	502	KL4	C02-N01-C06	3.75	120.94	118.10
2	C	501	HEM	CBD-CAD-C3D	-3.73	105.61	112.48
3	B	803	KL4	C14-C13-C12	-3.70	118.85	123.52
2	A	501	HEM	CMA-C3A-C4A	-3.64	122.88	128.46
3	B	803	KL4	C04-C05-C06	-3.55	118.00	120.32
3	C	503	KL4	C02-N01-C06	3.49	120.74	118.10
2	C	501	HEM	CMA-C3A-C2A	3.48	131.51	124.94
3	C	511	KL4	C09-C08-C06	-3.39	105.40	112.99
3	B	803	KL4	C18-C17-C15	-3.34	101.56	113.18
3	A	509	KL4	C02-N01-C06	3.25	120.56	118.10
2	B	802	HEM	CMA-C3A-C2A	3.24	131.04	124.94
2	B	802	HEM	CMC-C2C-C3C	3.07	130.42	124.68
3	C	502	KL4	C08-C06-N01	3.06	120.51	115.95
2	D	501	HEM	CBA-CAA-C2A	3.05	118.11	112.49
3	C	502	KL4	C18-C17-C15	-2.99	102.78	113.18
3	C	503	KL4	C14-C13-C12	-2.97	119.76	123.52
2	A	501	HEM	CBD-CAD-C3D	-2.97	107.01	112.48
3	C	511	KL4	C02-N01-C06	2.94	120.33	118.10
3	C	511	KL4	C14-C13-C12	-2.91	119.84	123.52
2	B	802	HEM	CAA-CBA-CGA	-2.89	107.82	112.67
3	D	502	KL4	C14-C13-C12	-2.79	120.00	123.52
2	B	802	HEM	CBD-CAD-C3D	-2.78	107.35	112.48
3	A	502	KL4	C14-C13-C12	-2.78	120.00	123.52
3	A	502	KL4	C05-C06-N01	-2.77	119.97	122.90
2	D	501	HEM	CMC-C2C-C3C	2.74	129.80	124.68
2	C	501	HEM	CBA-CAA-C2A	2.68	117.42	112.49
3	A	509	KL4	C05-C06-N01	-2.64	120.10	122.90
3	A	509	KL4	C14-C13-C12	-2.63	120.19	123.52
2	D	501	HEM	CMA-C3A-C2A	2.63	129.89	124.94
2	D	501	HEM	C4A-C3A-C2A	2.62	108.82	107.00
3	B	801	KL4	C08-C06-N01	2.58	119.80	115.95
3	C	502	KL4	N02-C02-N01	2.57	120.55	116.49
3	D	502	KL4	C18-C17-C15	-2.55	104.32	113.18
3	B	801	KL4	C14-C13-C12	-2.54	120.31	123.52
3	A	509	KL4	C08-C06-N01	2.50	119.67	115.95
3	C	502	KL4	C05-C06-N01	-2.45	120.31	122.90
2	B	802	HEM	CAA-C2A-C3A	2.41	134.17	127.25
3	B	803	KL4	C15-C16-C11	-2.40	118.28	121.23
3	C	503	KL4	C08-C06-N01	2.38	119.50	115.95
3	B	801	KL4	C05-C06-N01	-2.37	120.39	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	803	KL4	C11-C12-C13	2.32	120.92	118.81
3	D	502	KL4	C05-C06-N01	-2.29	120.47	122.90
2	D	501	HEM	CAA-C2A-C3A	2.26	133.75	127.25
2	A	501	HEM	CMA-C3A-C2A	2.26	129.20	124.94
2	B	802	HEM	CMD-C2D-C1D	-2.23	125.03	128.46
3	C	503	KL4	C05-C06-N01	-2.23	120.54	122.90
3	C	511	KL4	C24-C25-N21	2.19	112.10	105.69
3	D	502	KL4	C24-C25-N21	2.18	112.05	105.69
2	A	501	HEM	CMC-C2C-C3C	2.16	128.72	124.68
3	D	502	KL4	C11-C12-C13	2.16	120.78	118.81
2	C	501	HEM	CAA-CBA-CGA	-2.10	109.16	112.67
3	C	502	KL4	C14-C13-C12	-2.09	120.88	123.52
3	D	502	KL4	C08-C06-N01	2.06	119.02	115.95
4	B	808	BTB	O1-C1-C2	-2.05	105.83	111.44
3	B	803	KL4	C16-C15-C14	2.02	121.76	118.98
3	B	803	KL4	C08-C09-C11	-2.02	106.18	113.28
3	D	502	KL4	F13-C13-C12	2.02	121.13	118.25

There are no chirality outliers.

All (109) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	511	KL4	C17-C18-C22-N21
3	B	803	KL4	C17-C18-C22-C23
3	B	803	KL4	C17-C18-C22-N21
3	B	801	KL4	C17-C18-C22-N21
3	C	502	KL4	C17-C18-C22-C23
3	C	502	KL4	C17-C18-C22-N21
3	A	502	KL4	C15-C17-C18-C22
3	D	502	KL4	C17-C18-C22-C23
3	D	502	KL4	C17-C18-C22-N21
4	D	504	BTB	O1-C1-C2-C3
4	D	504	BTB	O1-C1-C2-C4
4	D	504	BTB	O1-C1-C2-N
4	D	504	BTB	C1-C2-C3-O3
4	D	504	BTB	C4-C2-C3-O3
4	D	504	BTB	C3-C2-C4-O4
4	D	504	BTB	C8-C7-N-C5
4	C	505	BTB	C1-C2-C3-O3
4	C	505	BTB	C4-C2-C3-O3
4	C	505	BTB	N-C2-C3-O3
4	C	505	BTB	C1-C2-C4-O4

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Mol	Chain	Res	Type	Atoms
4	C	505	BTB	C3-C2-C4-O4
4	C	505	BTB	N-C2-C4-O4
3	A	509	KL4	C17-C18-C22-N21
4	C	504	BTB	O1-C1-C2-C3
4	C	504	BTB	O1-C1-C2-C4
4	C	504	BTB	O1-C1-C2-N
4	C	504	BTB	C1-C2-C4-O4
4	C	504	BTB	C3-C2-C4-O4
4	C	504	BTB	N-C2-C4-O4
4	A	504	BTB	C1-C2-C3-O3
4	A	504	BTB	C4-C2-C3-O3
4	A	504	BTB	N-C2-C3-O3
4	A	504	BTB	C1-C2-C4-O4
4	A	504	BTB	C3-C2-C4-O4
4	A	504	BTB	N-C2-C4-O4
2	B	802	HEM	C1A-C2A-CAA-CBA
2	B	802	HEM	C3A-C2A-CAA-CBA
2	C	501	HEM	C1A-C2A-CAA-CBA
2	C	501	HEM	C3A-C2A-CAA-CBA
2	C	501	HEM	C2A-CAA-CBA-CGA
4	B	805	BTB	O1-C1-C2-C4
4	B	805	BTB	C1-C2-C4-O4
4	B	805	BTB	C3-C2-C4-O4
4	B	805	BTB	N-C2-C4-O4
6	A	506	GOL	O1-C1-C2-C3
6	A	506	GOL	C1-C2-C3-O3
2	A	501	HEM	C1A-C2A-CAA-CBA
2	A	501	HEM	C3A-C2A-CAA-CBA
2	A	501	HEM	C2A-CAA-CBA-CGA
4	B	804	BTB	O1-C1-C2-C3
4	B	804	BTB	O1-C1-C2-C4
4	B	804	BTB	O1-C1-C2-N
2	D	501	HEM	C1A-C2A-CAA-CBA
2	D	501	HEM	C3A-C2A-CAA-CBA
4	D	503	BTB	O1-C1-C2-C3
4	D	503	BTB	O1-C1-C2-C4
4	D	503	BTB	O1-C1-C2-N
4	D	503	BTB	C1-C2-C4-O4
4	D	503	BTB	C3-C2-C4-O4
4	D	503	BTB	N-C2-C4-O4
4	D	503	BTB	N-C5-C6-O6
4	A	503	BTB	C1-C2-C4-O4

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Mol	Chain	Res	Type	Atoms
4	A	503	BTB	C3-C2-C4-O4
4	A	503	BTB	N-C2-C4-O4
4	A	503	BTB	C1-C2-N-C5
4	A	503	BTB	C1-C2-N-C7
4	A	503	BTB	C3-C2-N-C5
4	A	503	BTB	C3-C2-N-C7
4	A	503	BTB	C4-C2-N-C5
4	A	503	BTB	C4-C2-N-C7
4	B	808	BTB	C1-C2-C3-O3
4	B	808	BTB	C4-C2-C3-O3
4	B	808	BTB	N-C2-C3-O3
4	B	808	BTB	C1-C2-C4-O4
4	B	808	BTB	C3-C2-C4-O4
4	B	808	BTB	C8-C7-N-C5
4	A	503	BTB	N-C5-C6-O6
4	A	503	BTB	N-C7-C8-O8
6	A	506	GOL	O1-C1-C2-O2
4	C	504	BTB	N-C7-C8-O8
4	D	504	BTB	N-C7-C8-O8
4	D	504	BTB	N-C5-C6-O6
6	C	507	GOL	O1-C1-C2-C3
4	A	504	BTB	N-C5-C6-O6
6	A	506	GOL	O2-C2-C3-O3
6	C	507	GOL	O1-C1-C2-O2
6	C	507	GOL	O2-C2-C3-O3
3	C	503	KL4	C17-C18-C22-N21
4	B	805	BTB	O1-C1-C2-C3
4	D	504	BTB	N-C2-C3-O3
4	B	805	BTB	O1-C1-C2-N
4	B	808	BTB	N-C2-C4-O4
3	D	502	KL4	C14-C15-C17-C18
3	D	502	KL4	C16-C15-C17-C18
3	B	801	KL4	C14-C15-C17-C18
4	B	805	BTB	N-C5-C6-O6
3	C	511	KL4	C14-C15-C17-C18
3	B	801	KL4	C16-C15-C17-C18
3	C	511	KL4	C16-C15-C17-C18
3	A	502	KL4	C14-C15-C17-C18
4	A	504	BTB	N-C7-C8-O8
2	B	802	HEM	C2A-CAA-CBA-CGA
3	A	502	KL4	C16-C15-C17-C18
3	C	502	KL4	C14-C15-C17-C18

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Mol	Chain	Res	Type	Atoms
4	B	804	BTB	N-C7-C8-O8
6	C	507	GOL	C1-C2-C3-O3
3	C	502	KL4	C16-C15-C17-C18
4	D	504	BTB	C1-C2-C4-O4
3	A	509	KL4	C17-C18-C22-C23

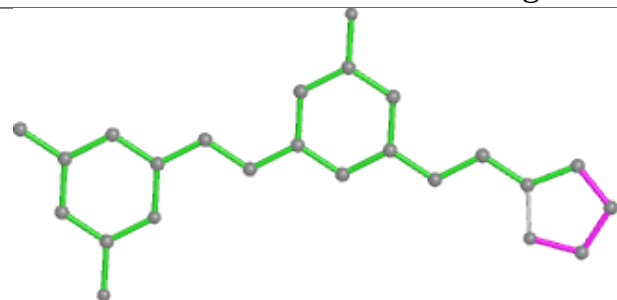
There are no ring outliers.

12 monomers are involved in 27 short contacts:

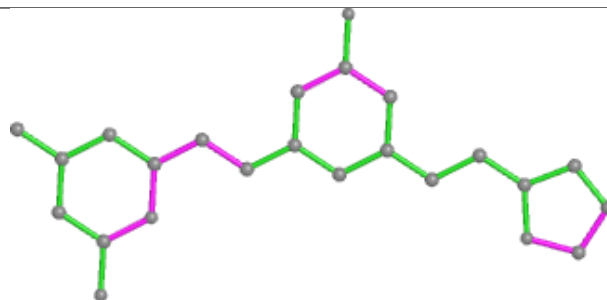
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	KL4	1	0
4	D	504	BTB	2	0
4	C	505	BTB	5	0
4	C	504	BTB	4	0
4	A	504	BTB	1	0
2	B	802	HEM	2	0
2	C	501	HEM	1	0
4	B	805	BTB	1	0
2	A	501	HEM	3	0
4	D	503	BTB	3	0
4	A	503	BTB	1	0
4	B	808	BTB	3	0

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.

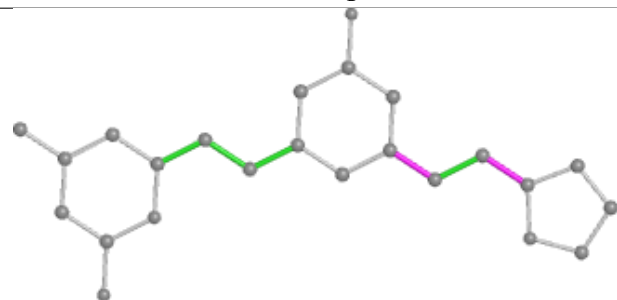
## Ligand KL4 C 511



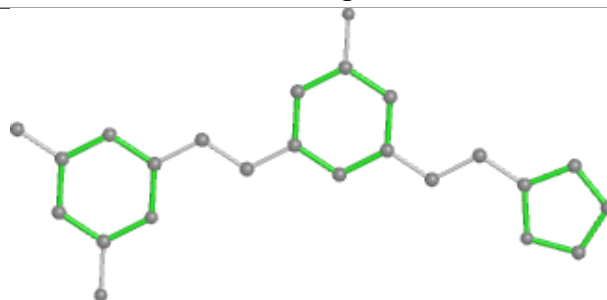
Bond lengths



Bond angles

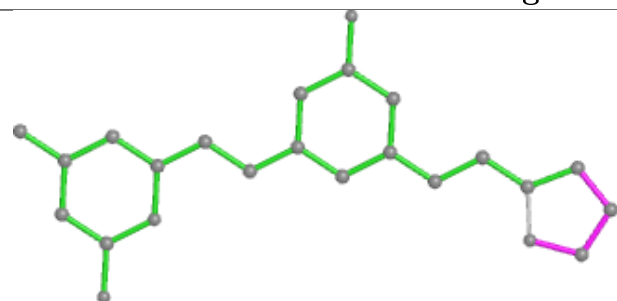


Torsions

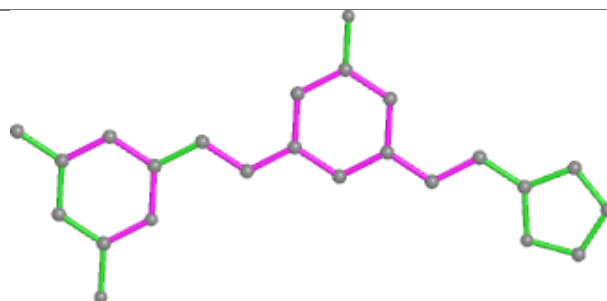


Rings

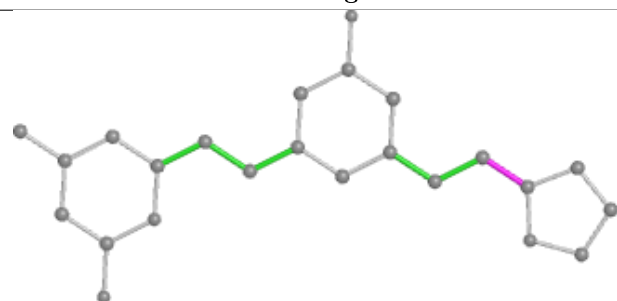
## Ligand KL4 B 803



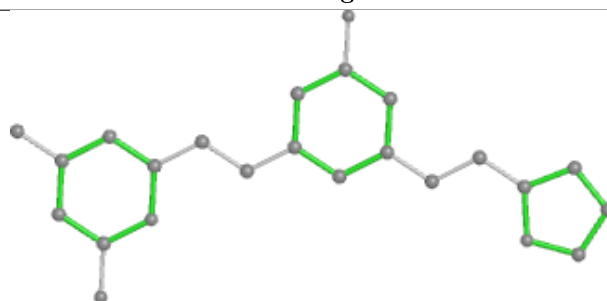
Bond lengths



Bond angles

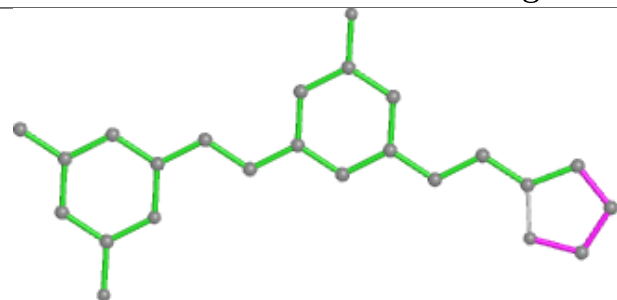


Torsions

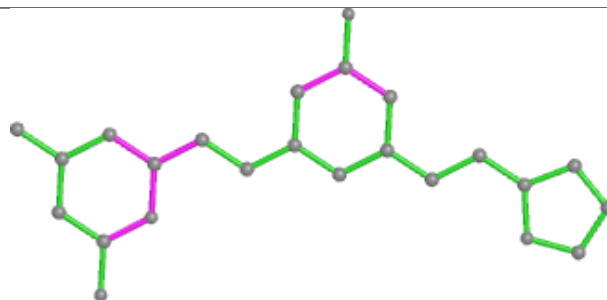


Rings

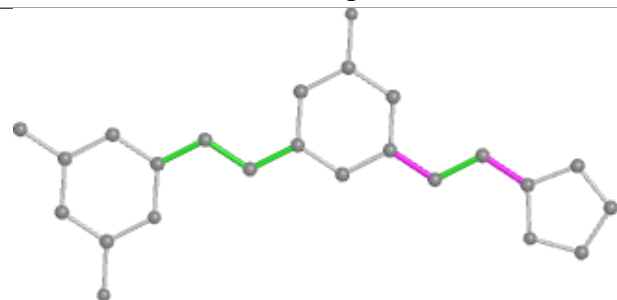
## Ligand KL4 B 801



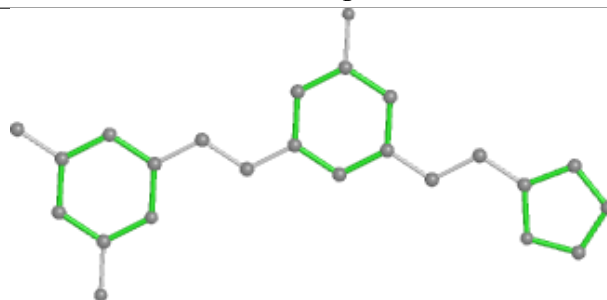
Bond lengths



Bond angles

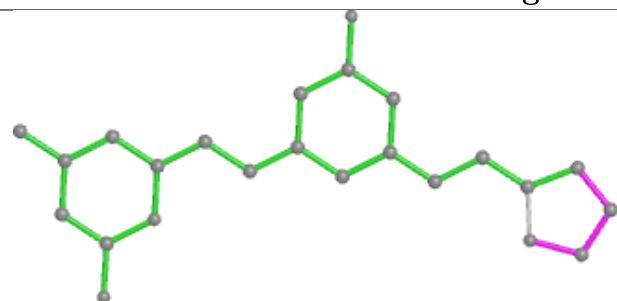


Torsions

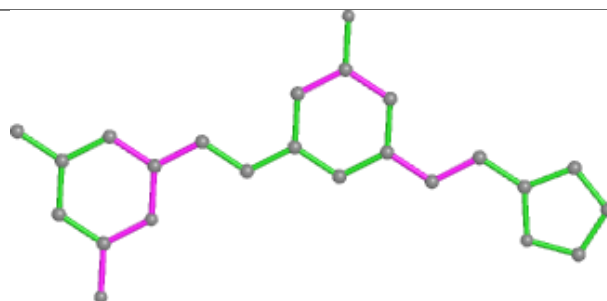


Rings

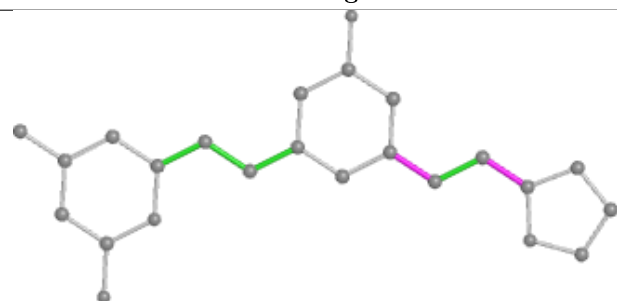
## Ligand KL4 C 502



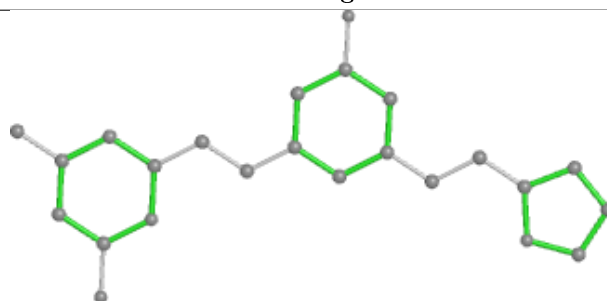
Bond lengths



Bond angles

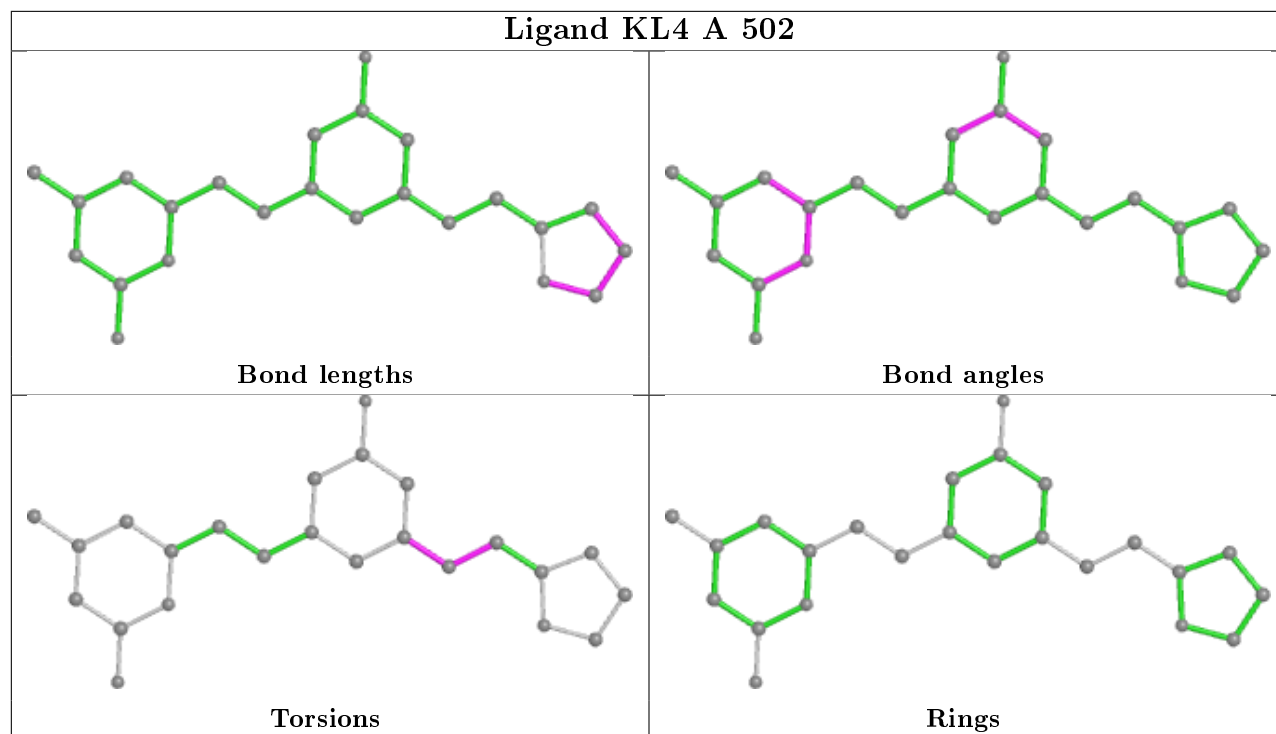


Torsions

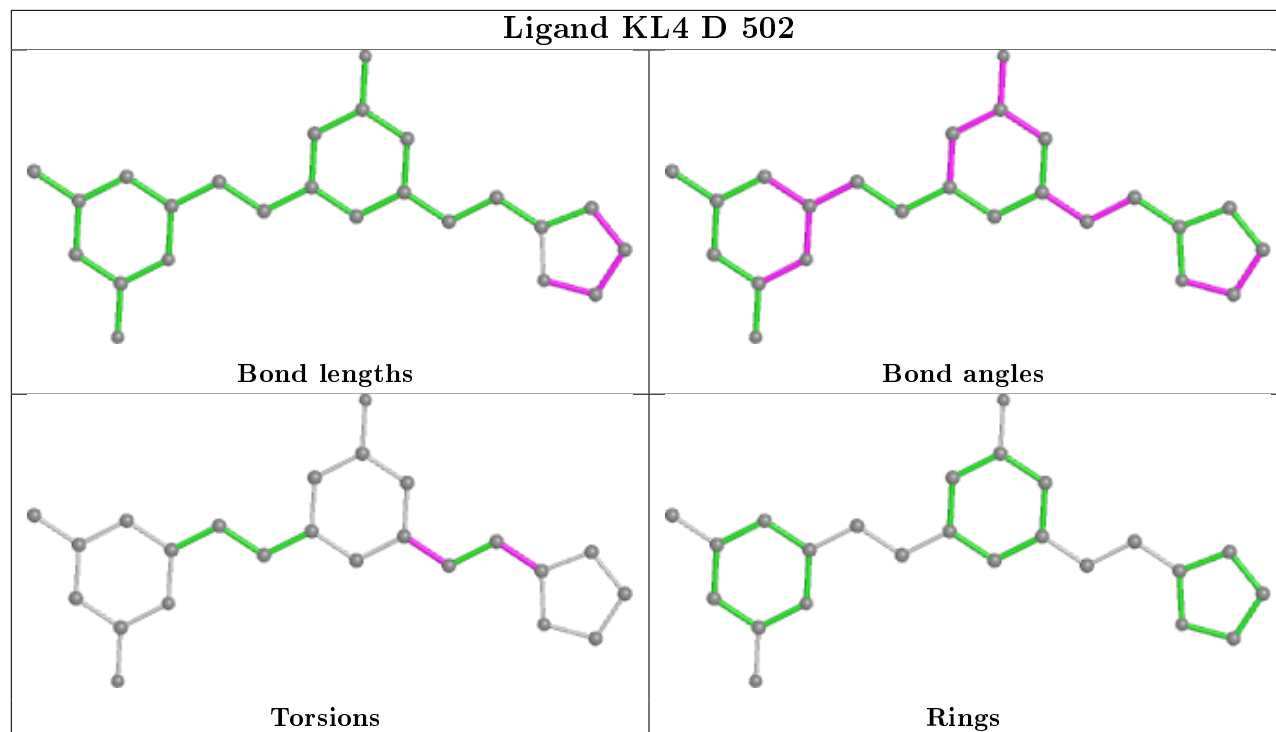


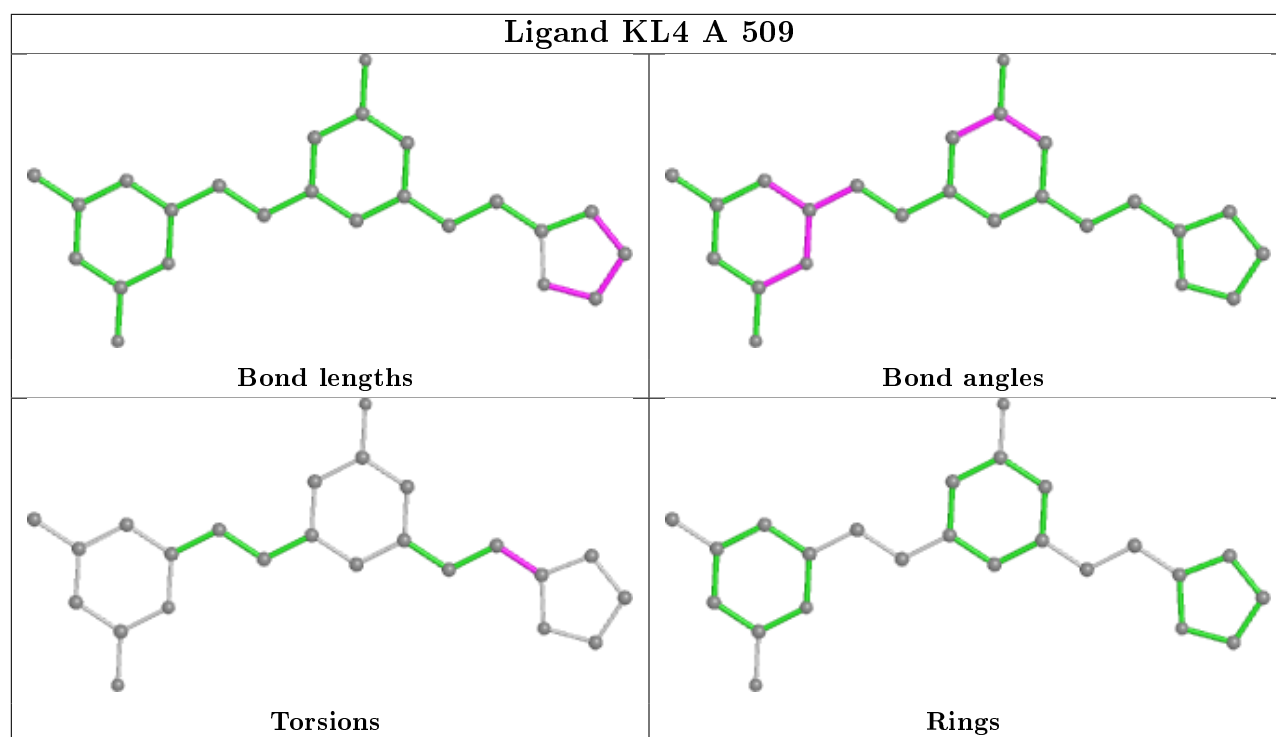
Rings

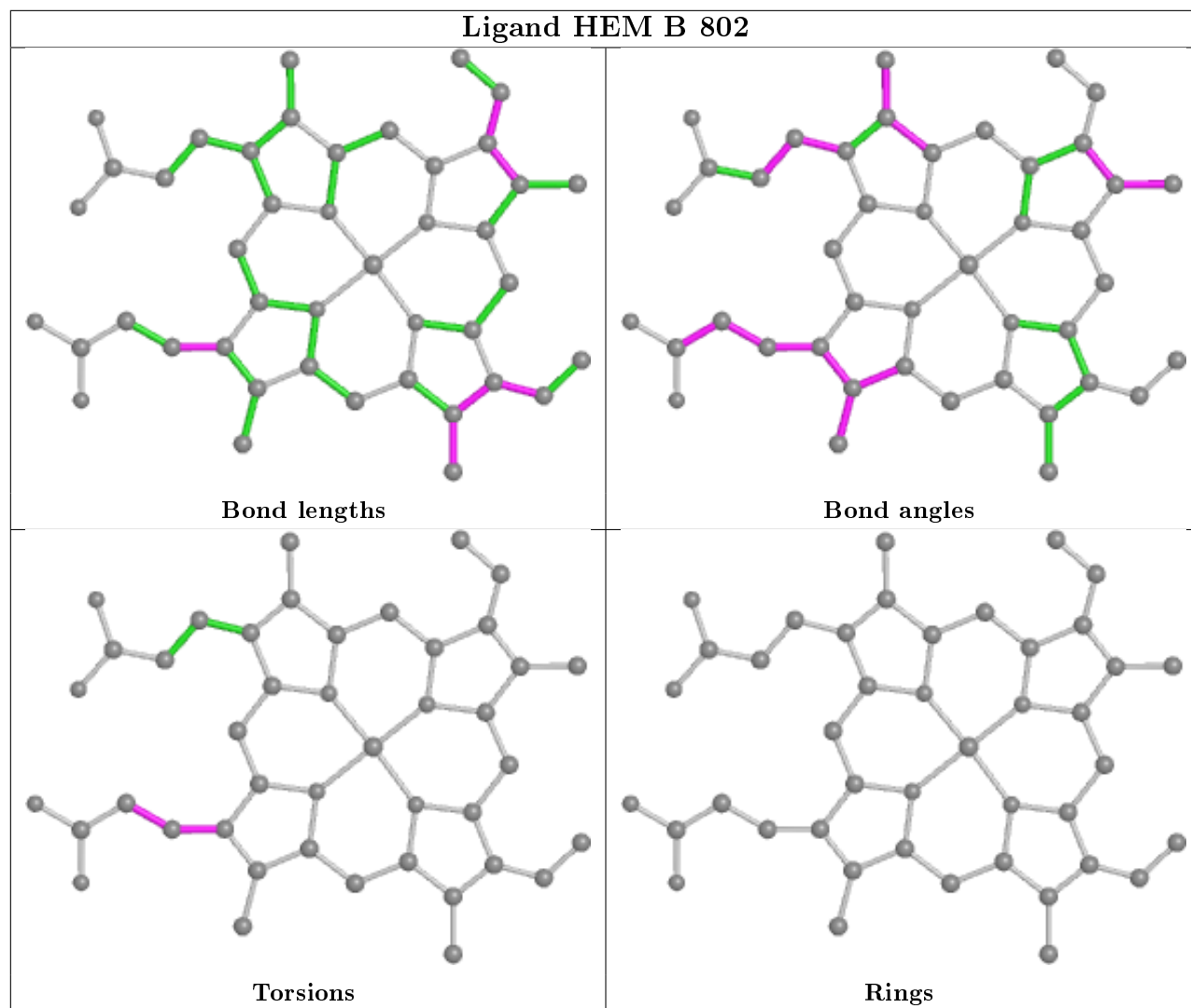
## Ligand KL4 A 502



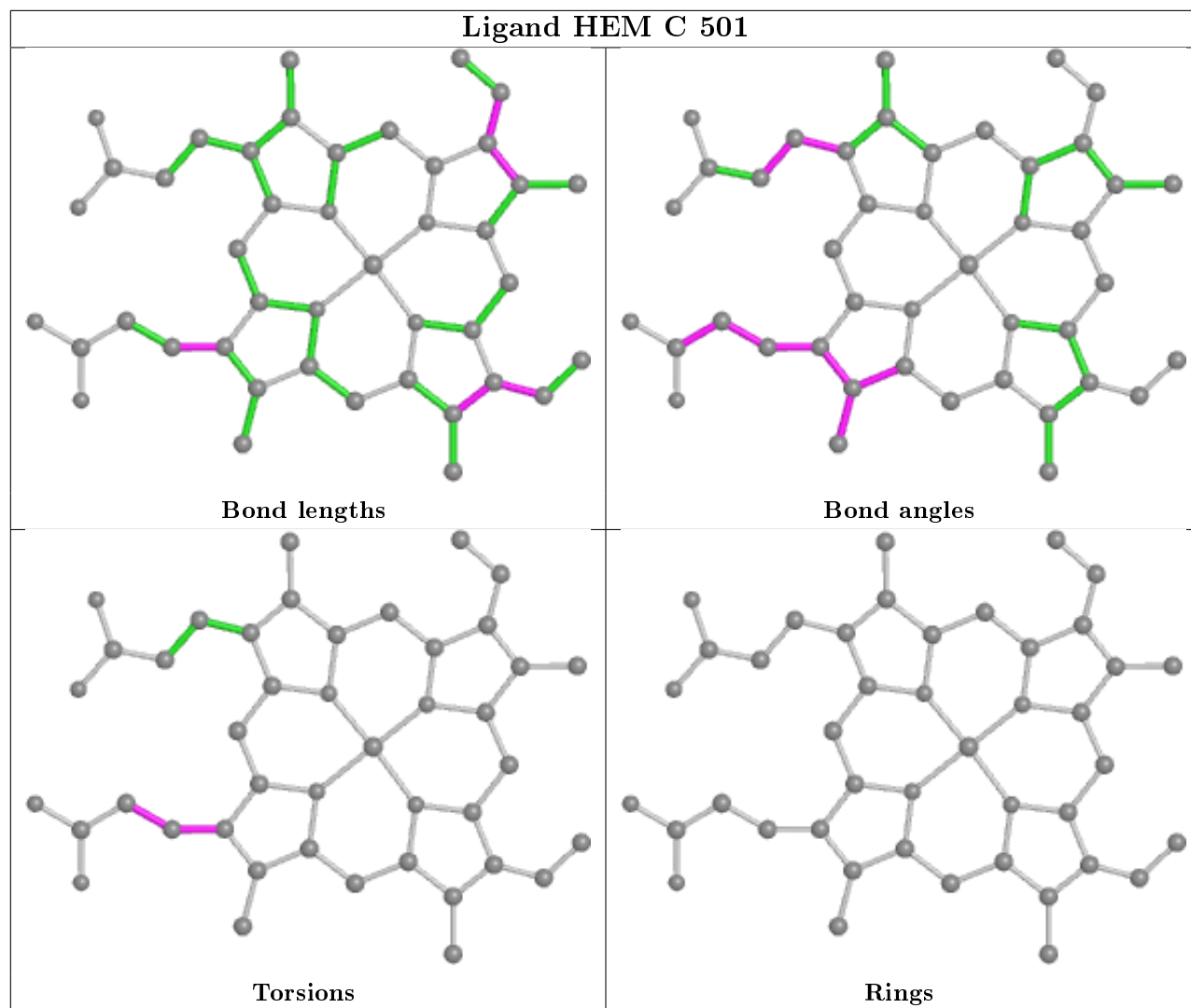
## Ligand KL4 D 502

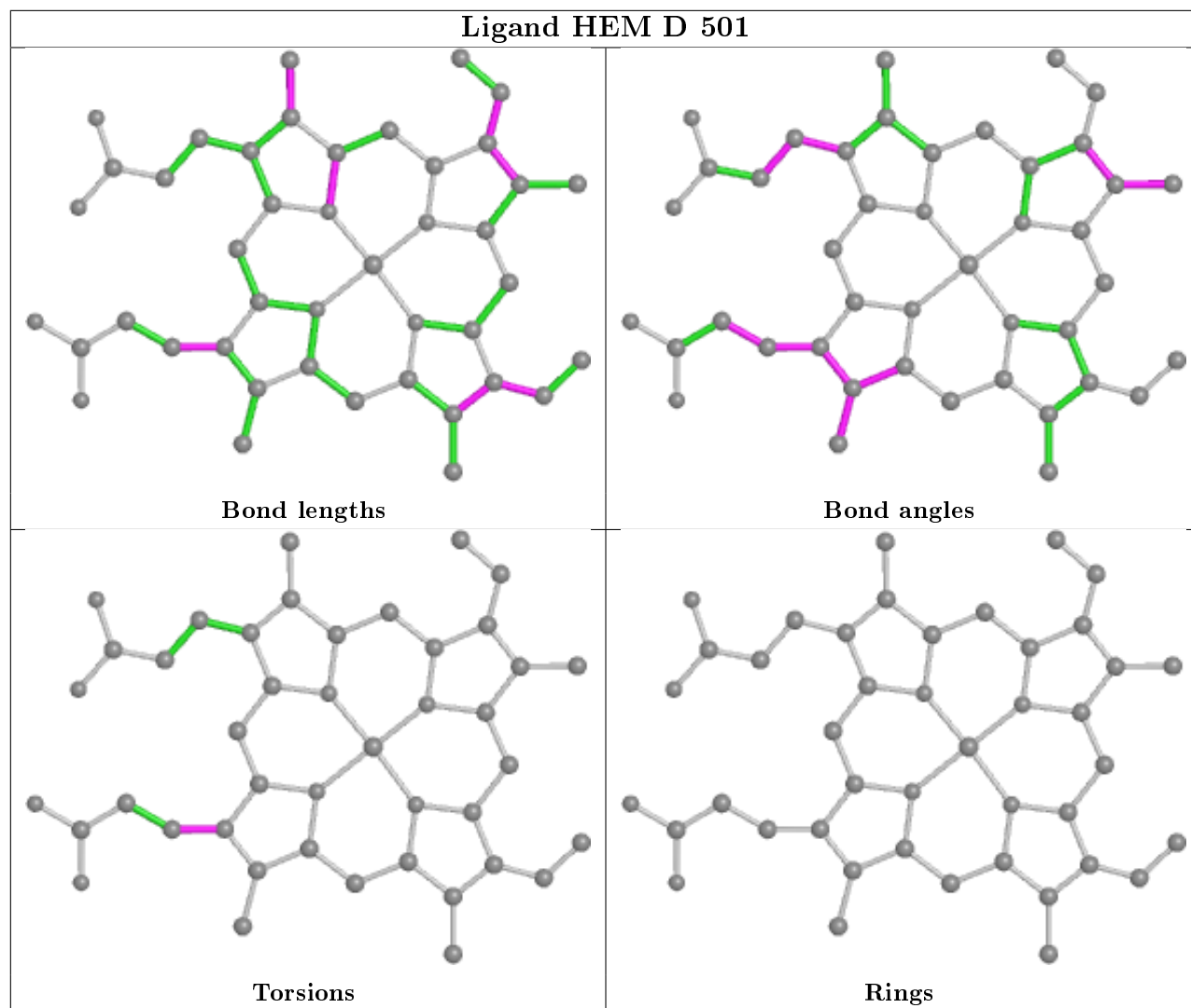


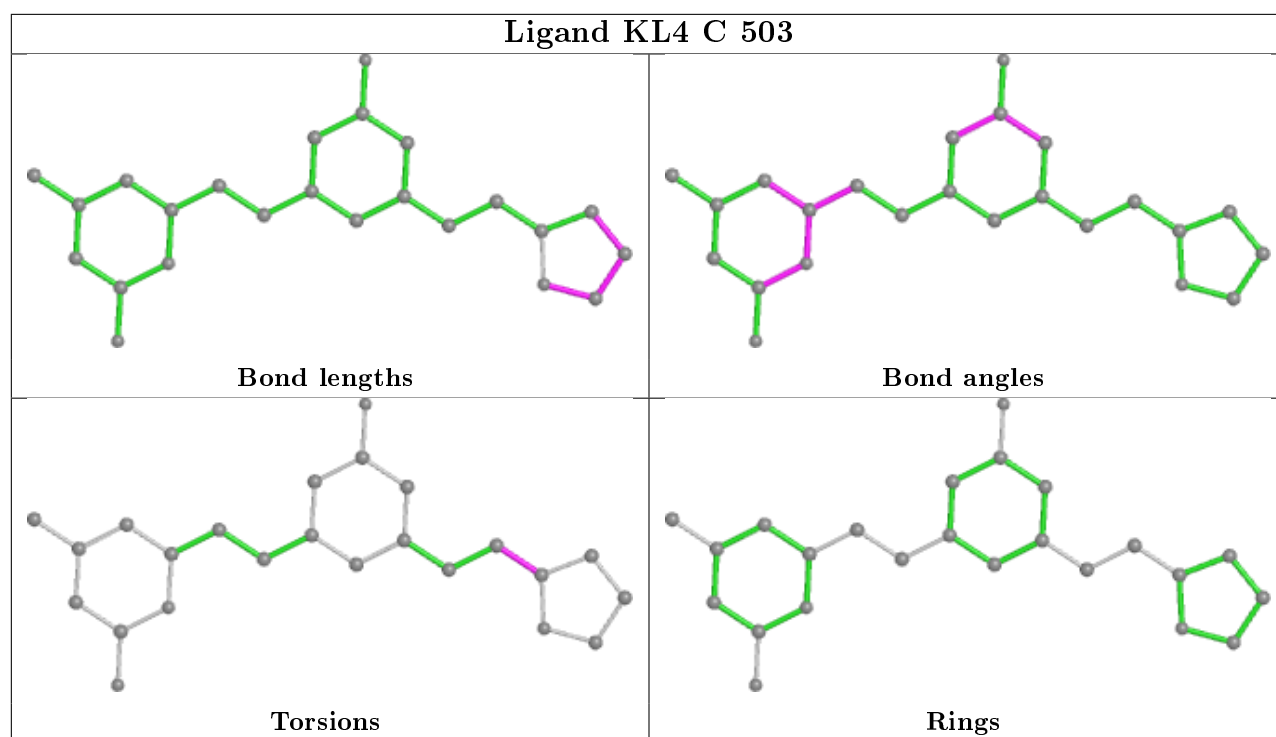


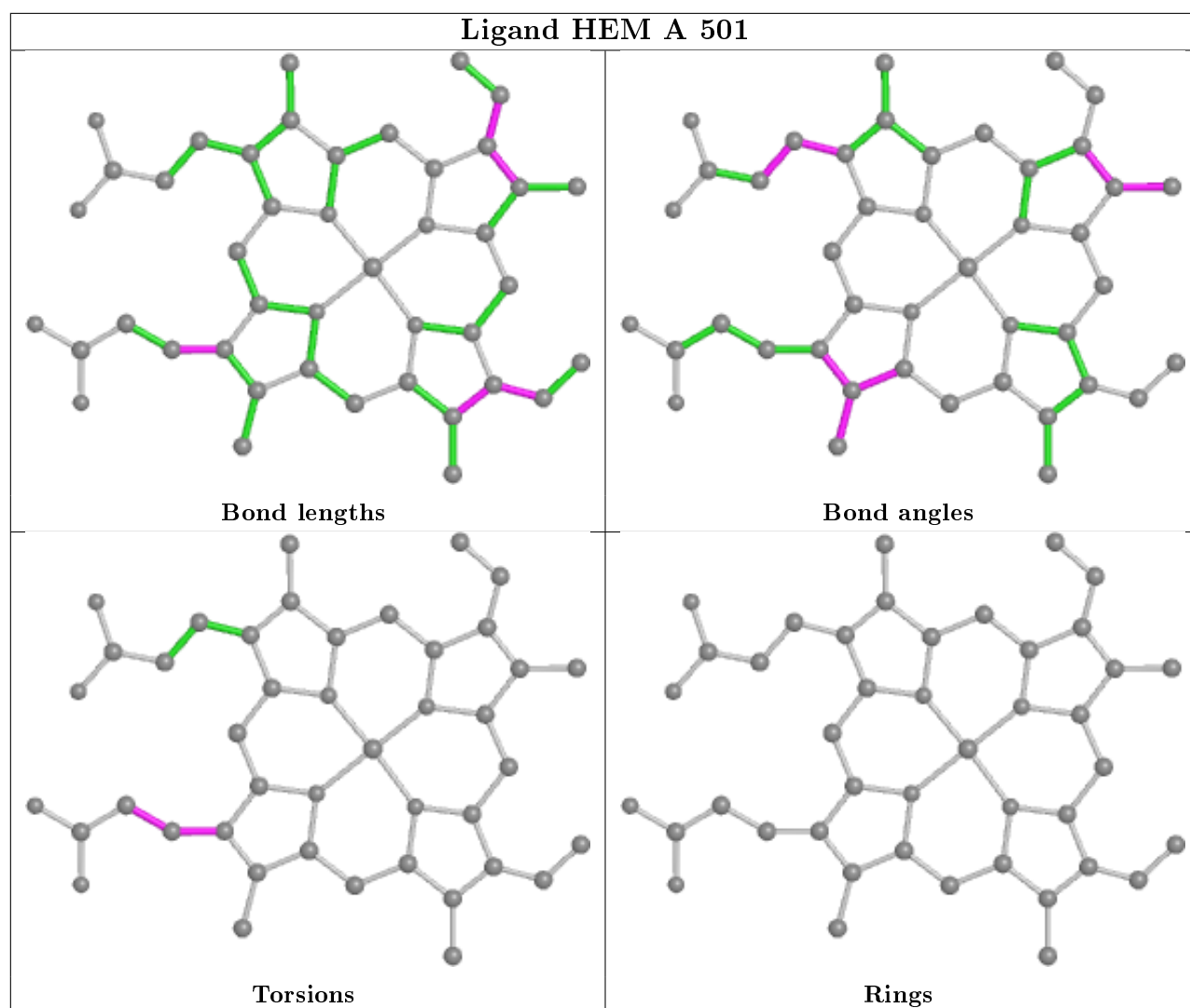












## 5.7 Other polymers [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	404/440 (91%)	0.36	24 (5%)	22 21	29, 56, 108, 145	0
1	B	402/440 (91%)	0.01	4 (0%)	82 81	24, 40, 75, 130	0
1	C	401/440 (91%)	0.13	5 (1%)	79 78	28, 52, 97, 127	0
1	D	402/440 (91%)	-0.04	5 (1%)	79 78	24, 39, 68, 120	0
All	All	1609/1760 (91%)	0.12	38 (2%)	59 57	24, 46, 95, 145	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	142	GLY	7.1
1	A	143	SER	6.8
1	A	480	TRP	5.8
1	A	119	ALA	5.1
1	A	109	LEU	4.9
1	A	89	GLN	4.5
1	C	142	GLY	4.4
1	C	143	SER	4.0
1	A	256	GLN	3.6
1	A	207	MET	3.5
1	A	153	VAL	3.5
1	C	257	GLN	3.4
1	A	259	GLY	3.1
1	A	231	PHE	3.0
1	B	89	GLN	3.0
1	B	122	GLN	2.9
1	B	141[A]	SER	2.8
1	C	119	ALA	2.7
1	D	257	GLN	2.7
1	A	107	ARG	2.7
1	A	237	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	283	ASN	2.6
1	A	141	SER	2.6
1	A	160	THR	2.6
1	A	280	THR	2.5
1	D	255	ARG	2.4
1	B	119	ALA	2.3
1	A	204	ALA	2.3
1	A	120	PRO	2.3
1	A	238	ARG	2.2
1	A	279	TRP	2.2
1	D	124	LEU	2.2
1	A	305	LEU	2.2
1	D	67	LYS	2.2
1	A	300	PRO	2.2
1	A	302	LEU	2.1
1	C	292	LEU	2.1
1	D	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, 95<sup>th</sup> 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
4	BTB	C	505	14/14	0.62	0.19	94,113,117,118	0
4	BTB	A	503	14/14	0.76	0.19	86,92,103,104	0
8	GD	C	509	1/1	0.76	0.17	237,237,237,237	0
4	BTB	C	504	14/14	0.77	0.29	85,103,122,124	0
4	BTB	B	804	14/14	0.81	0.15	27,46,74,79	0
4	BTB	D	503	14/14	0.81	0.17	45,68,78,79	0

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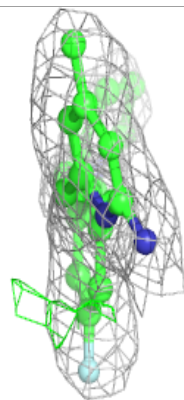
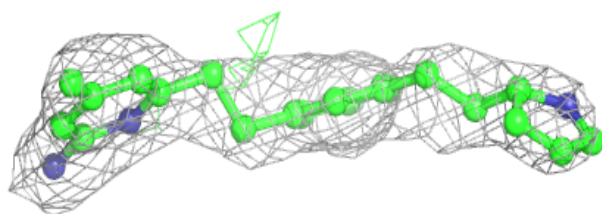
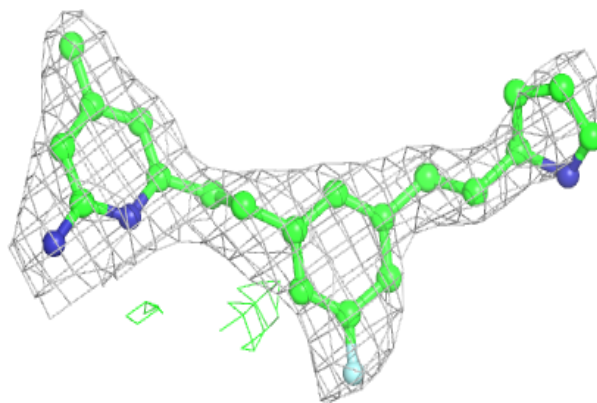
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	KL4	C	503	24/24	0.88	0.17	40,73,84,86	0
4	BTB	B	805	14/14	0.89	0.18	48,68,77,82	0
4	BTB	D	504	14/14	0.89	0.21	63,75,101,104	0
4	BTB	B	808	14/14	0.90	0.20	48,68,87,88	0
4	BTB	A	504	14/14	0.91	0.18	84,89,96,100	0
3	KL4	B	801	24/24	0.91	0.17	40,61,76,81	0
6	GOL	A	506	6/6	0.91	0.15	71,84,96,98	0
6	GOL	C	507	6/6	0.92	0.15	61,74,91,94	0
3	KL4	A	509	24/24	0.92	0.14	36,51,81,83	0
3	KL4	A	502	24/24	0.93	0.18	34,76,94,97	0
3	KL4	C	502	24/24	0.93	0.13	40,56,77,79	0
3	KL4	B	803	24/24	0.94	0.15	27,55,82,86	0
3	KL4	D	502	24/24	0.94	0.15	25,51,82,84	0
3	KL4	C	511	24/24	0.94	0.14	32,49,62,67	0
8	GD	A	511	1/1	0.95	0.07	87,87,87,87	0
8	GD	B	807	1/1	0.95	0.16	48,48,48,48	0
5	ZN	C	510	1/1	0.95	0.11	35,35,35,35	1
5	ZN	A	508	1/1	0.95	0.12	42,42,42,42	1
7	CL	B	806	1/1	0.97	0.12	37,37,37,37	0
2	HEM	C	501	43/43	0.97	0.13	27,44,83,111	0
2	HEM	A	501	43/43	0.98	0.12	33,44,69,87	0
7	CL	C	508	1/1	0.98	0.12	54,54,54,54	0
2	HEM	D	501	43/43	0.98	0.11	21,26,48,64	0
8	GD	D	505	1/1	0.98	0.15	48,48,48,48	0
7	CL	A	507	1/1	0.99	0.07	55,55,55,55	0
2	HEM	B	802	43/43	0.99	0.10	23,29,55,77	0
5	ZN	A	510	1/1	0.99	0.11	37,37,37,37	1
5	ZN	C	512	1/1	0.99	0.10	41,41,41,41	1
7	CL	D	506	1/1	0.99	0.08	36,36,36,36	0
5	ZN	A	505	1/1	1.00	0.14	42,42,42,42	0
5	ZN	C	506	1/1	1.00	0.11	36,36,36,36	0

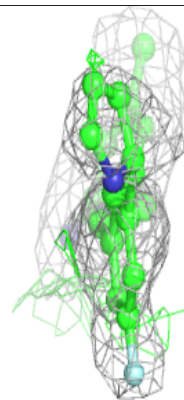
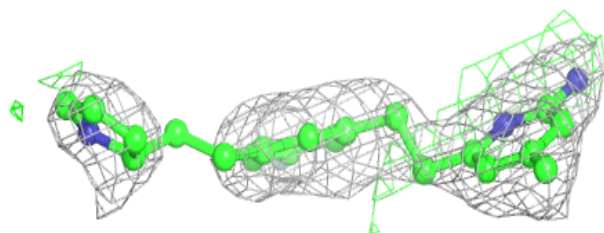
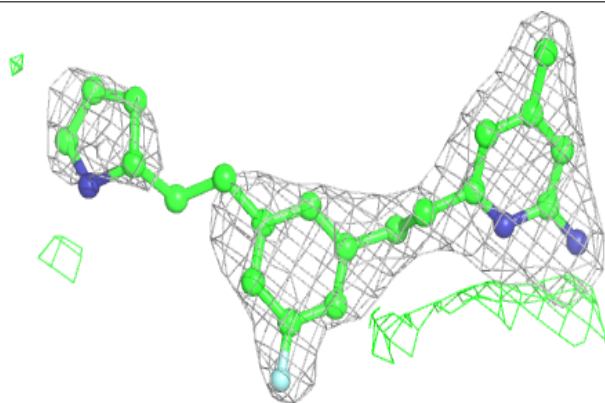
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around KL4 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 KL4 B 801:**

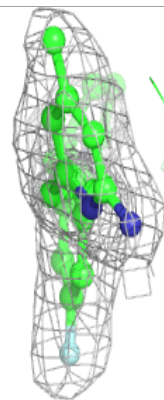
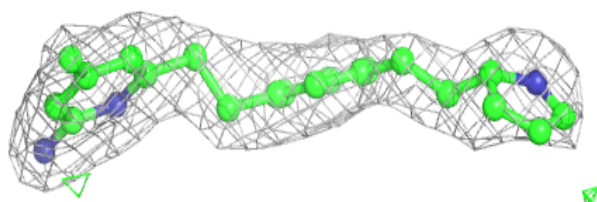
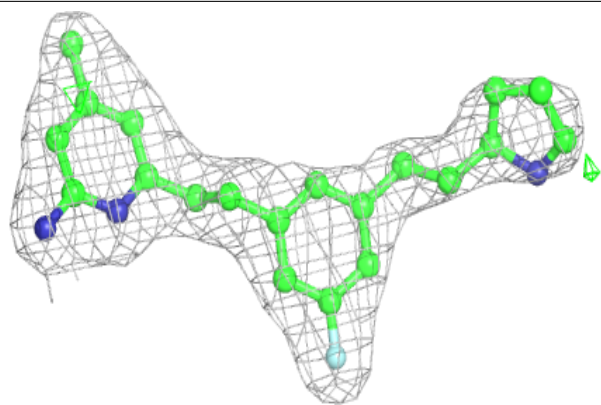
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



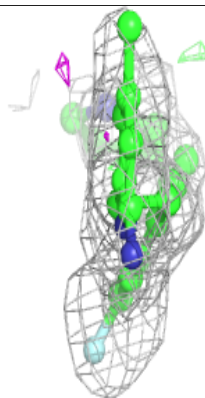
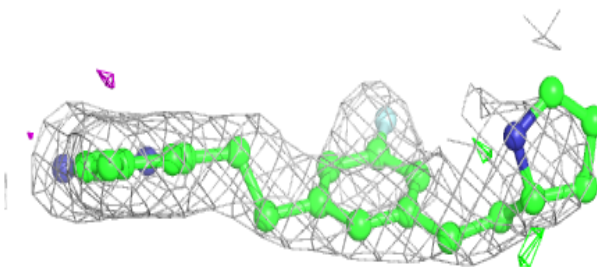
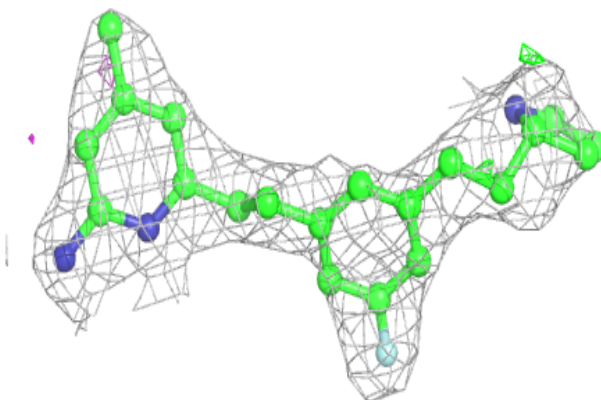


**Electron density around KL4 A 509:**

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

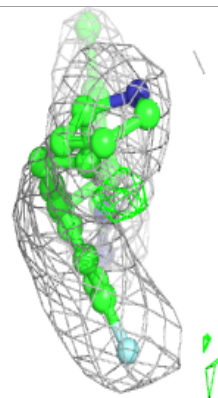
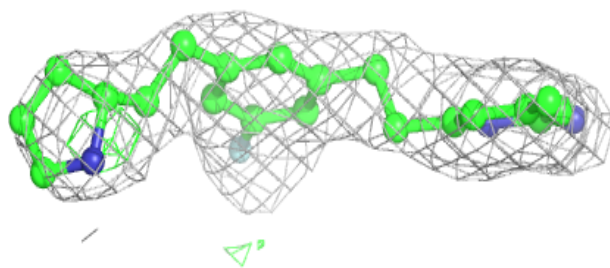
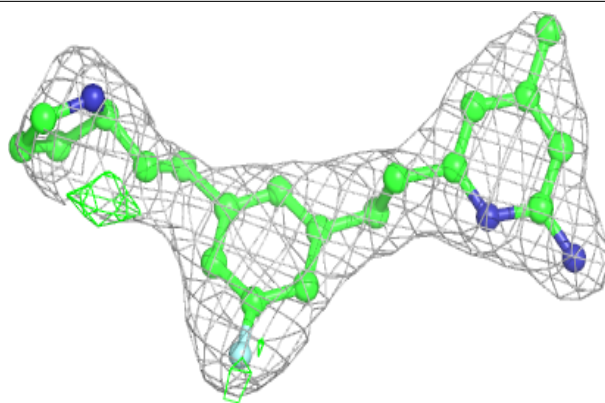
**Electron density around KL4 A 502:**

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

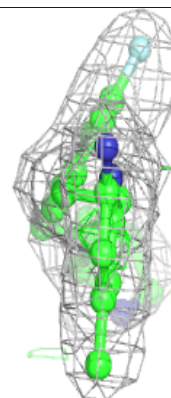
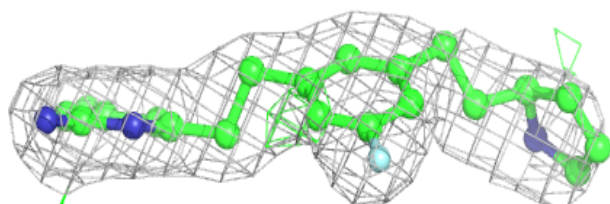
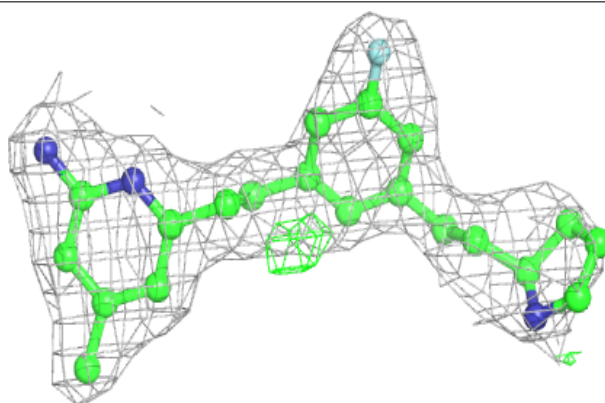


**Electron density around KL4 C 502:**

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

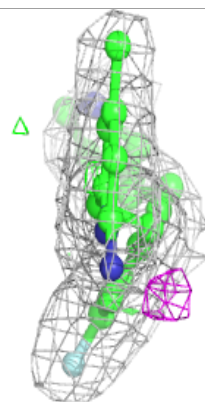
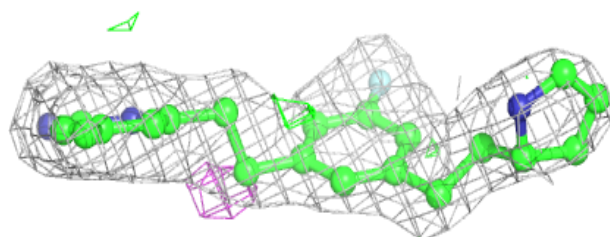
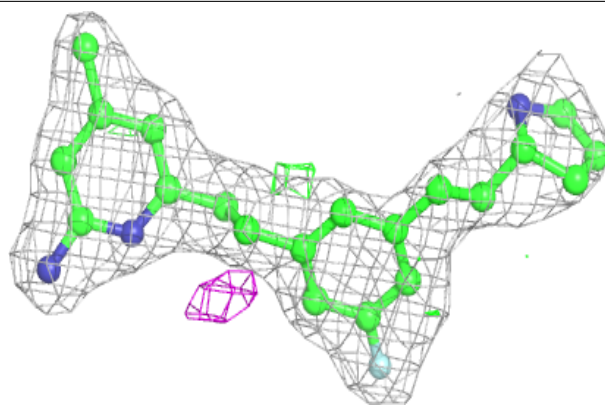
**Electron density around KL4 B 803:**

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

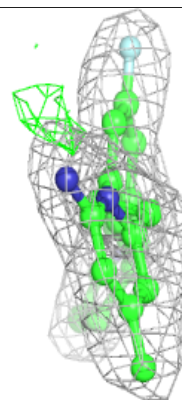
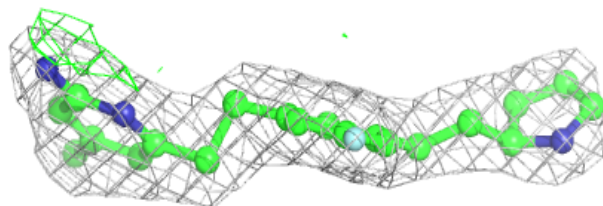
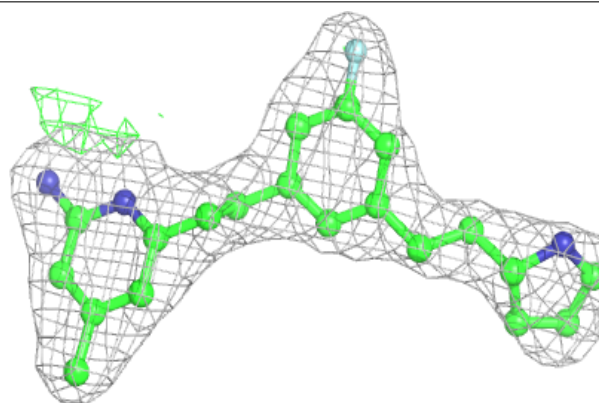


**Electron density around KL4 D 502:**

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

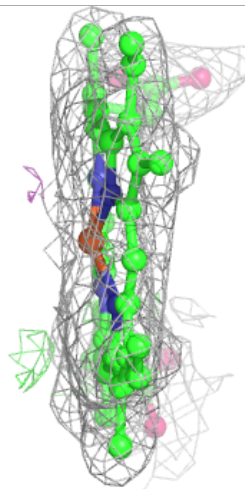
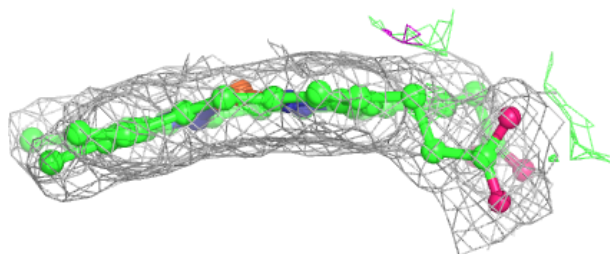
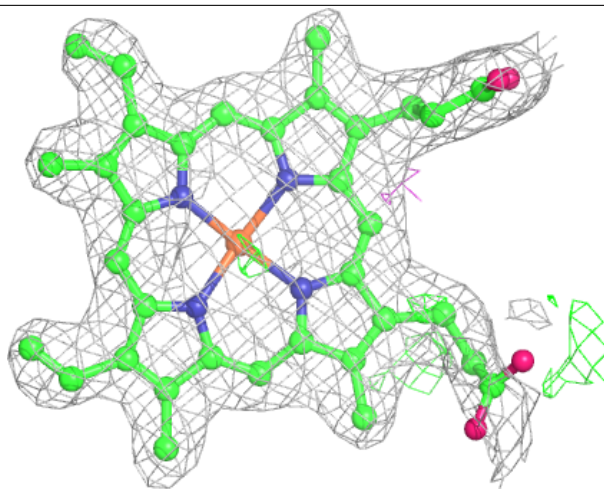
**Electron density around KL4 C 511:**

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



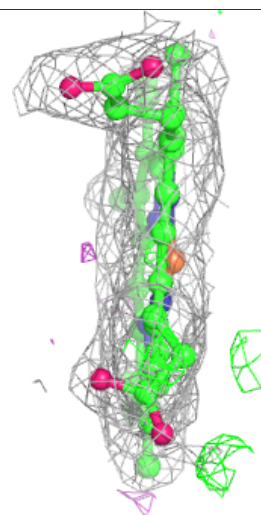
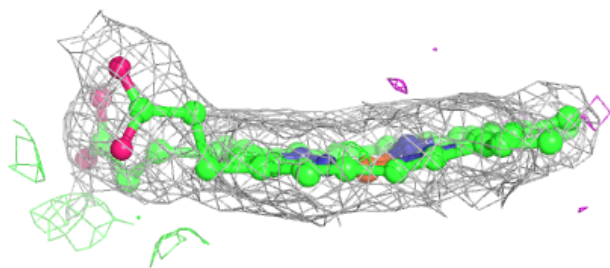
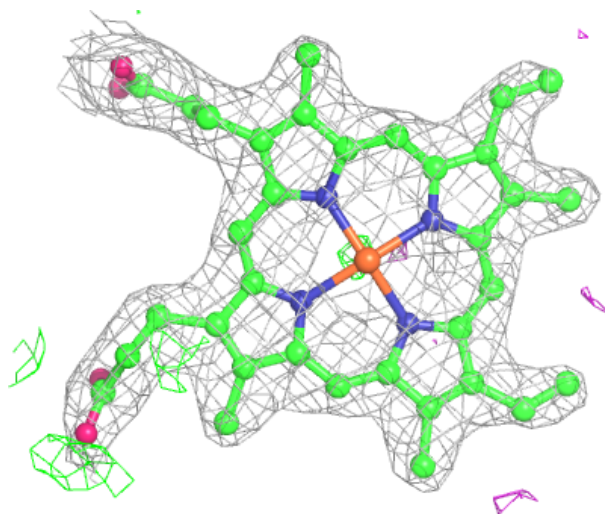
**Electron density around HEM C 501:**

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



**Electron density around HEM A 501:**

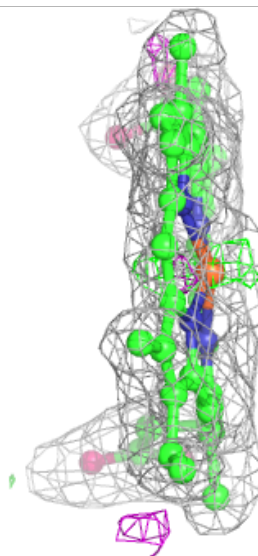
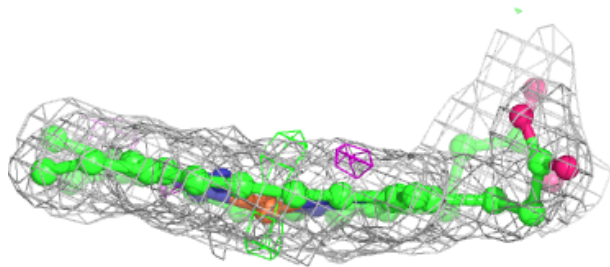
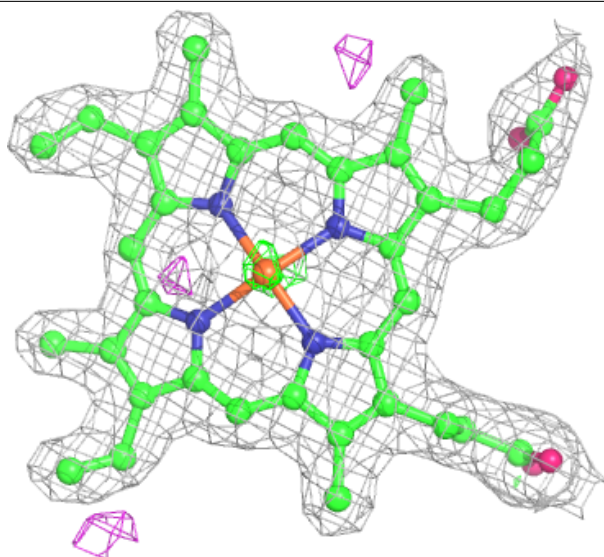
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

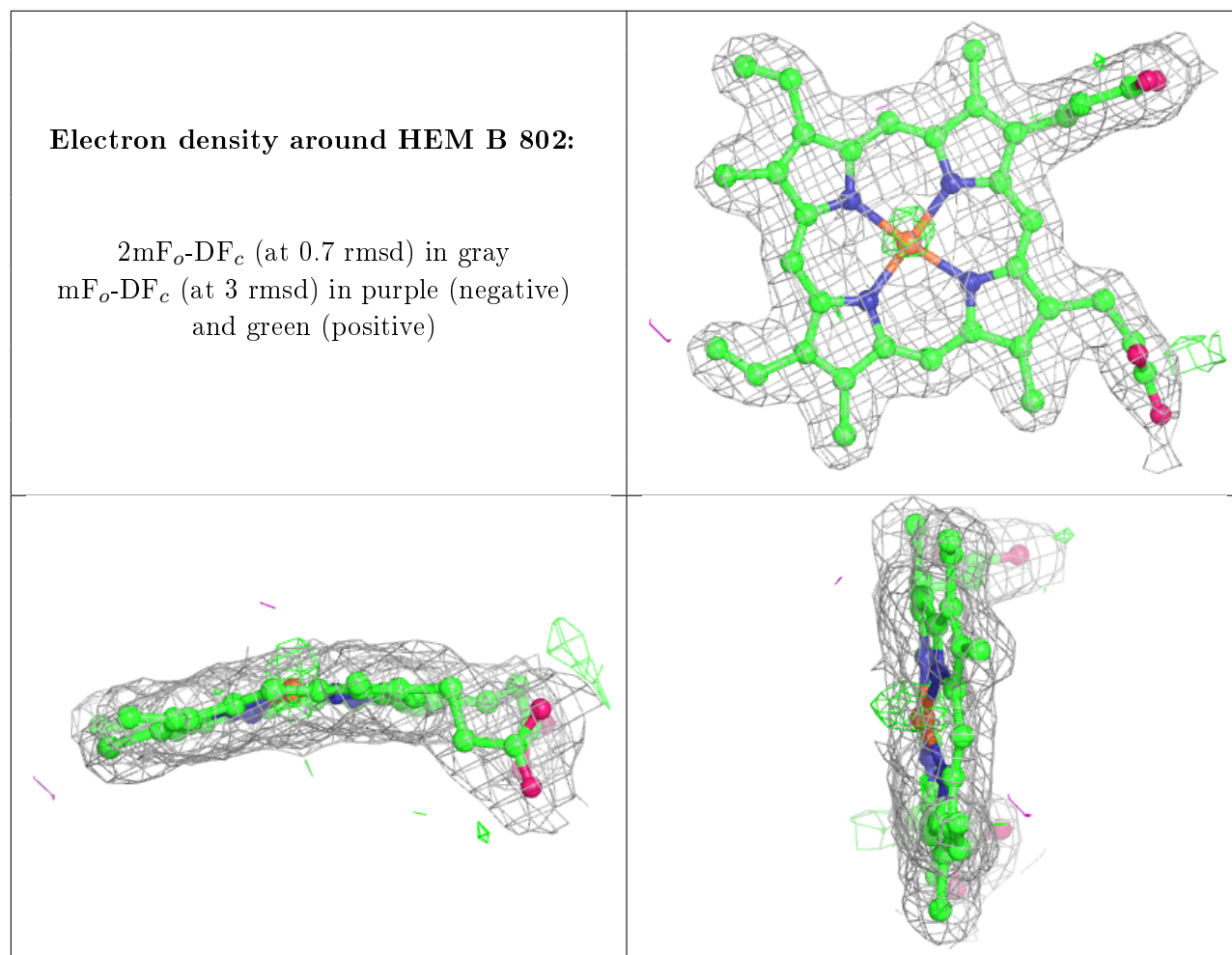




**Electron density around HEM D 501:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.