



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 07:18 AM UTC

PDB ID : 7TS7 / pdb_00007ts7
Title : Structure of human neuronal nitric oxide synthase R354A/G357D mutant heme domain in complex with 4-methyl-6-(3-(methylamino)propyl)pyridine-2-amine
Authors : Li, H.; Poulos, T.L.
Deposited on : 2022-01-31
Resolution : 1.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

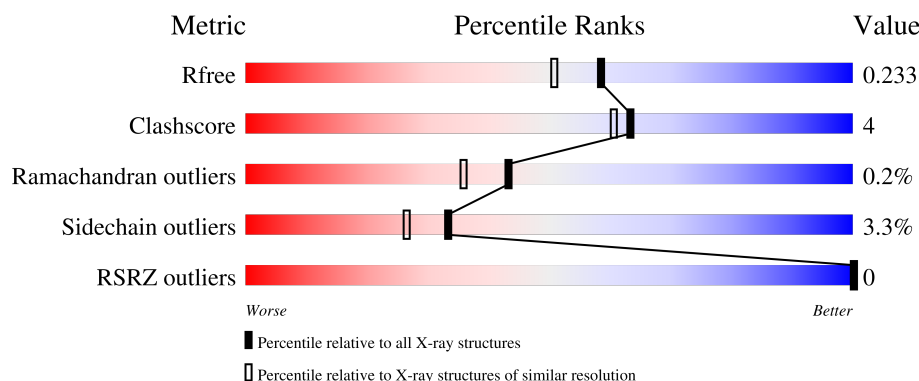
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	423	
1	B	423	
1	C	423	
1	D	423	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 15037 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, brain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	420	Total	C	N	O	S	0	3	0
			3435	2197	590	627	21			
1	B	414	Total	C	N	O	S	0	2	0
			3379	2165	575	618	21			
1	C	415	Total	C	N	O	S	0	5	0
			3399	2179	576	623	21			
1	D	418	Total	C	N	O	S	0	3	0
			3420	2188	585	626	21			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	354	ALA	ARG	engineered mutation	UNP P29475
A	357	ASP	GLY	engineered mutation	UNP P29475
A	723	LEU	-	expression tag	UNP P29475
A	724	VAL	-	expression tag	UNP P29475
B	354	ALA	ARG	engineered mutation	UNP P29475
B	357	ASP	GLY	engineered mutation	UNP P29475
B	723	LEU	-	expression tag	UNP P29475
B	724	VAL	-	expression tag	UNP P29475
C	354	ALA	ARG	engineered mutation	UNP P29475
C	357	ASP	GLY	engineered mutation	UNP P29475
C	723	LEU	-	expression tag	UNP P29475
C	724	VAL	-	expression tag	UNP P29475
D	354	ALA	ARG	engineered mutation	UNP P29475
D	357	ASP	GLY	engineered mutation	UNP P29475
D	723	LEU	-	expression tag	UNP P29475
D	724	VAL	-	expression tag	UNP P29475

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



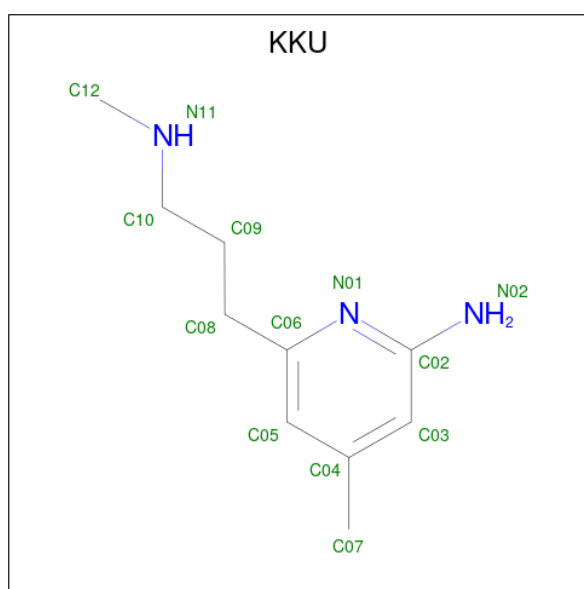
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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



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

- Molecule 4 is 4-methyl-6-[3-(methylamino)propyl]pyridin-2-amine (CCD ID: K KU) (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 GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

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

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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	271	Total O 271 271	0	0
7	B	284	Total O 284 284	0	0

Continued on next page...

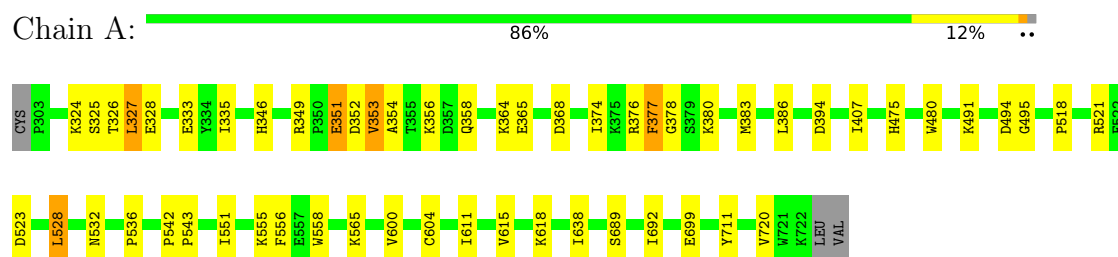
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	277	Total 277	O 277	0	0
7	D	248	Total 248	O 248	0	0

3 Residue-property plots

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, brain



I684	E668	R672	S689	G690	S691	I692	F696	E699	T706	Y711	T718	H719	V720	W721	K722	LEU	VAL
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	52.29Å 118.37Å 164.91Å 90.00° 90.10° 90.00°	Depositor
Resolution (Å)	39.20 – 1.90 39.20 – 1.90	Depositor EDS
% Data completeness (in resolution range)	96.4 (39.20-1.90) 97.0 (39.20-1.90)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.19 (at 1.89Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.190 , 0.238 0.183 , 0.233	Depositor DCC
R_{free} test set	7763 reflections (3.89%)	wwPDB-VP
Wilson B-factor (Å ²)	34.0	Xtriage
Anisotropy	0.442	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 38.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.440 for h,-k,-l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	15037	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% 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, H4B, KKK, HEM, GOL

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	0.32	0/3543	0.54	0/4808
1	B	0.33	0/3480	0.51	0/4721
1	C	0.33	0/3510	0.52	0/4763
1	D	0.33	0/3527	0.50	0/4787
All	All	0.33	0/14060	0.52	0/19079

There are no bond length outliers.

There are no bond angle outliers.

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	3435	0	3348	31	0
1	B	3379	0	3295	21	0
1	C	3399	0	3321	31	0
1	D	3420	0	3328	22	0
2	A	43	0	30	3	0
2	B	43	0	30	4	0
2	C	43	0	30	4	0
2	D	43	0	30	3	0
3	A	17	0	15	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	17	0	15	0	0
3	C	17	0	15	1	0
3	D	17	0	15	0	0
4	A	13	0	0	0	0
4	B	13	0	0	1	0
4	C	13	0	0	2	0
4	D	13	0	0	0	0
5	A	6	0	8	1	0
5	B	6	0	8	0	0
5	C	12	0	16	1	0
5	D	6	0	8	0	0
6	A	1	0	0	0	0
6	D	1	0	0	0	0
7	A	271	0	0	4	0
7	B	284	0	0	3	0
7	C	277	0	0	5	0
7	D	248	0	0	0	0
All	All	15037	0	13512	110	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 4.

All (110) 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:C:327:LEU:HB3	1:C:704:ARG:HD3	1.55	0.88
1:C:613:GLU:HG3	1:C:623:MET:HE1	1.56	0.86
1:A:378:GLY:HA2	1:A:383:MET:HE2	1.60	0.84
1:A:711:TYR:OH	2:A:801:HEM:O1D	1.97	0.83
1:A:528:LEU:HD22	1:A:536:PRO:HB2	1.61	0.83
1:D:711:TYR:OH	2:D:802:HEM:O1D	1.98	0.79
1:D:528:LEU:HD22	1:D:536:PRO:HB2	1.65	0.78
1:C:528:LEU:HD22	1:C:536:PRO:HB2	1.64	0.78
1:B:528:LEU:HD22	1:B:536:PRO:HB2	1.64	0.77
2:A:801:HEM:HMC2	2:A:801:HEM:HBC2	1.69	0.74
2:D:802:HEM:HMC2	2:D:802:HEM:HBC2	1.72	0.70
2:B:801:HEM:HBB2	2:B:801:HEM:HHB	1.74	0.69
1:B:327:LEU:HB3	1:B:704:ARG:HD3	1.76	0.68
1:C:578:GLU:OE2	7:C:901:HOH:O	2.12	0.67
1:D:664:ILE:O	1:D:668[B]:GLU:HG2	1.94	0.67
2:B:801:HEM:HMC2	2:B:801:HEM:HBC2	1.75	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:711:TYR:OH	2:C:801:HEM:O1D	2.10	0.67
1:C:341:MET:HE2	3:C:802:H4B:H9	1.78	0.65
2:C:801:HEM:HBC2	2:C:801:HEM:HMC2	1.79	0.64
1:C:430:GLN:HA	5:C:805:GOL:H31	1.78	0.64
2:A:801:HEM:HBB2	2:A:801:HEM:HHC	1.80	0.64
2:D:802:HEM:HBB2	2:D:802:HEM:HHC	1.82	0.62
1:B:565:LYS:NZ	7:B:907:HOH:O	2.33	0.62
1:A:377:PHE:N	7:A:904:HOH:O	2.32	0.62
1:C:470:ARG:NH2	7:C:903:HOH:O	2.34	0.61
1:A:328:GLU:H	1:A:346:HIS:HD2	1.49	0.60
1:A:356:LYS:HE3	1:D:672:ARG:O	2.01	0.60
1:A:518:PRO:HG2	1:A:523:ASP:CG	2.26	0.60
1:C:723:LEU:HD12	1:C:724:VAL:H	1.66	0.60
1:D:348:ARG:NH1	1:D:365:GLU:OE2	2.28	0.59
1:A:689:SER:HB3	1:A:692:ILE:HD11	1.85	0.58
1:B:711:TYR:OH	2:B:801:HEM:O1D	2.17	0.58
1:A:407:ILE:HG21	5:A:804:GOL:H31	1.85	0.57
2:C:801:HEM:HHC	2:C:801:HEM:HBB2	1.85	0.57
1:A:374:ILE:HG13	1:A:376:ARG:HG2	1.86	0.57
1:C:723:LEU:HG	1:C:724:VAL:HG22	1.90	0.55
1:D:349:ARG:NH2	1:D:352:ASP:O	2.39	0.54
1:B:547:LEU:HD21	1:B:651:VAL:HG22	1.88	0.54
1:D:600:VAL:O	1:D:604:CYS:HB2	2.08	0.54
1:A:600:VAL:O	1:A:604:CYS:HB2	2.08	0.53
1:B:668:GLU:O	1:B:672:ARG:HG2	2.09	0.53
1:D:327:LEU:HD21	1:D:348:ARG:HG2	1.89	0.53
1:B:414:TRP:CE3	1:B:426:TRP:HA	2.45	0.52
1:C:598:ILE:HA	1:C:602:ASP:HB2	1.91	0.52
1:C:414:TRP:CE3	1:C:426:TRP:HA	2.45	0.52
1:C:340:ILE:HD13	1:D:699:GLU:HB3	1.92	0.52
1:B:480:TRP:CE2	1:B:715:PRO:HB2	2.45	0.51
1:D:689:SER:HB3	1:D:692:ILE:HD11	1.91	0.51
1:A:376:ARG:HB3	7:A:904:HOH:O	2.10	0.51
2:B:801:HEM:O2A	4:B:803:KKU:N11	2.43	0.51
1:C:483:GLN:HB2	1:C:486:ARG:HG3	1.92	0.51
1:B:334:TYR:OH	1:D:376:ARG:NH1	2.44	0.50
1:C:327:LEU:HD13	1:C:328:GLU:N	2.26	0.50
1:B:600:VAL:O	1:B:604:CYS:HB2	2.12	0.50
1:A:615:VAL:HG21	1:A:638:ILE:HD11	1.95	0.49
1:B:598:ILE:HA	1:B:602:ASP:HB2	1.95	0.48
1:B:411:LYS:NZ	7:B:910:HOH:O	2.45	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:483:GLN:HB2	1:D:486:ARG:HG3	1.96	0.47
1:A:349:ARG:NH2	1:A:352:ASP:O	2.45	0.47
1:B:327:LEU:HD13	1:B:328:GLU:N	2.30	0.47
1:C:600:VAL:O	1:C:604:CYS:HB2	2.14	0.47
1:A:699:GLU:HB3	1:B:340:ILE:HD13	1.96	0.46
1:B:480:TRP:HB2	1:B:528:LEU:HB3	1.97	0.46
1:B:556:PHE:HB3	1:B:558:TRP:CE2	2.49	0.46
1:C:668:GLU:O	1:C:672:ARG:HD2	2.16	0.46
1:A:611:ILE:HA	7:A:968:HOH:O	2.15	0.46
2:C:801:HEM:O2A	4:C:803:KKU:N11	2.49	0.45
1:A:349:ARG:HH22	1:A:354:ALA:H	1.64	0.45
1:D:691:SER:HA	1:D:696:PHE:CG	2.51	0.45
1:A:364:LYS:NZ	1:A:368:ASP:OD2	2.48	0.45
1:A:494:ASP:OD2	1:A:495:GLY:N	2.50	0.45
1:D:598:ILE:HA	1:D:602:ASP:HB2	1.98	0.45
1:C:334:TYR:C	1:C:335:ILE:HG13	2.41	0.45
1:C:452:LYS:NZ	7:C:912:HOH:O	2.49	0.45
1:A:555:LYS:HD3	1:A:555:LYS:HA	1.71	0.44
1:B:664:ILE:O	1:B:668:GLU:HG3	2.17	0.44
1:A:480:TRP:HB2	1:A:528:LEU:HB3	2.00	0.44
1:A:346:HIS:CE1	1:D:376:ARG:HA	2.53	0.44
1:D:490:TYR:CE1	1:D:519:ARG:HA	2.53	0.44
1:C:594:MET:HA	1:C:654:VAL:O	2.18	0.44
1:B:706:THR:HA	1:B:707:PRO:C	2.43	0.43
1:C:327:LEU:HD11	7:C:1163:HOH:O	2.18	0.43
1:C:419:ARG:HD3	1:C:683:TRP:CD2	2.54	0.43
1:D:668[A]:GLU:OE2	1:D:672:ARG:NH2	2.52	0.43
1:A:354:ALA:HB1	1:A:358:GLN:HB2	2.00	0.42
1:C:679:ALA:HB3	1:C:700:MET:HB3	2.01	0.42
1:C:553:HIS:CG	1:C:554:PRO:HD2	2.55	0.42
1:A:475:HIS:HB3	1:A:532:ASN:OD1	2.19	0.42
1:A:327:LEU:HD12	1:A:346:HIS:O	2.20	0.42
1:C:706[A]:THR:HA	1:C:707:PRO:C	2.45	0.42
1:D:469:GLN:HB3	1:D:584:PHE:CE2	2.55	0.42
1:C:691:SER:HA	1:C:696:PHE:CG	2.54	0.42
1:A:521:ARG:NE	7:A:907:HOH:O	2.38	0.42
1:C:452:LYS:NZ	7:C:916:HOH:O	2.52	0.41
1:B:327:LEU:HD12	1:B:704:ARG:HD3	2.02	0.41
1:C:556:PHE:HB3	1:C:558:TRP:CE2	2.54	0.41
1:D:480:TRP:HB2	1:D:528:LEU:HB3	2.01	0.41
1:B:519:ARG:NH1	7:B:922:HOH:O	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:348:ARG:NH1	1:D:706:THR:HG21	2.36	0.41
1:A:556:PHE:HB3	1:A:558:TRP:CE2	2.56	0.41
1:B:681:TRP:CZ2	1:B:685:VAL:HG21	2.55	0.41
1:D:615:VAL:HG21	1:D:638:ILE:HD11	2.03	0.41
1:A:380:LYS:HB2	1:A:380:LYS:HE2	1.83	0.40
1:C:328:GLU:H	1:C:328:GLU:HG2	1.50	0.40
1:C:597:GLU:OE2	4:C:803:KKU:N02	2.54	0.40
1:C:681:TRP:CZ2	1:C:685:VAL:HG21	2.57	0.40
1:D:414:TRP:CE3	1:D:426:TRP:HA	2.56	0.40
1:A:542:PRO:HA	1:A:543:PRO:HD3	1.93	0.40
1:A:356:LYS:HE2	1:A:394:ASP:OD2	2.21	0.40
1:A:551:ILE:HG12	1:A:565:LYS:HA	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	421/423 (100%)	404 (96%)	14 (3%)	3 (1%)	18	10
1	B	412/423 (97%)	402 (98%)	10 (2%)	0	100	100
1	C	416/423 (98%)	407 (98%)	9 (2%)	0	100	100
1	D	419/423 (99%)	406 (97%)	13 (3%)	0	100	100
All	All	1668/1692 (99%)	1619 (97%)	46 (3%)	3 (0%)	43	36

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	351	GLU
1	A	377	PHE
1	A	353	VAL

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	378/378 (100%)	364 (96%)	14 (4%)	30	22
1	B	372/378 (98%)	362 (97%)	10 (3%)	39	34
1	C	376/378 (100%)	365 (97%)	11 (3%)	37	31
1	D	376/378 (100%)	362 (96%)	14 (4%)	30	22
All	All	1502/1512 (99%)	1453 (97%)	49 (3%)	33	26

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	324	LYS
1	A	325	SER
1	A	326	THR
1	A	327	LEU
1	A	333	GLU
1	A	335	ILE
1	A	351	GLU
1	A	353	VAL
1	A	365	GLU
1	A	386	LEU
1	A	491	LYS
1	A	528	LEU
1	A	618	LYS
1	A	720	VAL
1	B	314	GLU
1	B	324	LYS
1	B	326	THR
1	B	327	LEU
1	B	365	GLU
1	B	505	GLN
1	B	516	LYS
1	B	528	LEU
1	B	625	LYS
1	B	724	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	326	THR
1	C	328	GLU
1	C	351	GLU
1	C	386	LEU
1	C	394	ASP
1	C	528	LEU
1	C	557	GLU
1	C	607	SER
1	C	672	ARG
1	C	722	LYS
1	C	724	VAL
1	D	305	PHE
1	D	325	SER
1	D	326	THR
1	D	349	ARG
1	D	353	VAL
1	D	380	LYS
1	D	383	MET
1	D	384	GLU
1	D	528	LEU
1	D	607	SER
1	D	614	GLU
1	D	718	THR
1	D	720	VAL
1	D	722	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	346	HIS
1	A	412	HIS
1	B	412	HIS
1	C	412	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 2 are monoatomic - leaving 17 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	GOL	C	805	-	5,5,5	0.42	0	5,5,5	0.45	0
3	H4B	B	802	-	17,18,18	0.89	1 (5%)	14,26,26	1.52	4 (28%)
5	GOL	A	804	-	5,5,5	0.25	0	5,5,5	0.84	0
4	KKU	C	803	-	13,13,13	0.40	0	15,16,16	1.71	3 (20%)
5	GOL	C	804	-	5,5,5	0.38	0	5,5,5	0.26	0
4	KKU	D	804	-	13,13,13	0.42	0	15,16,16	1.59	2 (13%)
4	KKU	B	803	-	13,13,13	0.40	0	15,16,16	1.75	3 (20%)
2	HEM	C	801	1	50,50,50	1.45	7 (14%)	67,82,82	1.37	5 (7%)
5	GOL	B	804	-	5,5,5	0.36	0	5,5,5	0.33	0
3	H4B	A	802	-	17,18,18	0.83	1 (5%)	14,26,26	1.86	4 (28%)
5	GOL	D	805	-	5,5,5	0.46	0	5,5,5	0.14	0
3	H4B	C	802	-	17,18,18	0.85	1 (5%)	14,26,26	1.94	5 (35%)
2	HEM	D	802	1	50,50,50	1.69	10 (20%)	67,82,82	1.36	7 (10%)
4	KKU	A	803	-	13,13,13	0.42	0	15,16,16	1.95	2 (13%)
3	H4B	D	803	-	17,18,18	0.85	1 (5%)	14,26,26	1.89	5 (35%)
2	HEM	A	801	1	50,50,50	1.66	9 (18%)	67,82,82	1.28	6 (8%)
2	HEM	B	801	1	50,50,50	1.52	9 (18%)	67,82,82	1.21	4 (5%)

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	GOL	C	805	-	-	4/4/4/4	-
3	H4B	B	802	-	-	0/8/17/17	0/2/2/2
5	GOL	A	804	-	-	1/4/4/4	-
4	KKU	C	803	-	-	2/5/5/5	0/1/1/1
5	GOL	C	804	-	-	0/4/4/4	-
4	KKU	D	804	-	-	1/5/5/5	0/1/1/1
4	KKU	B	803	-	-	2/5/5/5	0/1/1/1
2	HEM	C	801	1	-	0/14/54/54	-
5	GOL	B	804	-	-	2/4/4/4	-
3	H4B	A	802	-	-	3/8/17/17	0/2/2/2
5	GOL	D	805	-	-	2/4/4/4	-
3	H4B	C	802	-	-	0/8/17/17	0/2/2/2
2	HEM	D	802	1	-	2/14/54/54	-
4	KKU	A	803	-	-	1/5/5/5	0/1/1/1
3	H4B	D	803	-	-	3/8/17/17	0/2/2/2
2	HEM	A	801	1	-	2/14/54/54	-
2	HEM	B	801	1	-	1/14/54/54	-

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	HEM	FE-NA	5.81	2.14	1.95
2	D	802	HEM	FE-NC	5.01	2.11	1.95
2	D	802	HEM	FE-NA	4.73	2.10	1.95
2	B	801	HEM	FE-NA	4.52	2.10	1.95
2	C	801	HEM	FE-NA	4.39	2.09	1.95
2	C	801	HEM	FE-NC	4.18	2.09	1.95
2	A	801	HEM	FE-NC	4.13	2.08	1.95
2	B	801	HEM	FE-NC	3.91	2.08	1.95
2	D	802	HEM	FE-NB	3.85	2.06	1.94
2	A	801	HEM	FE-NB	3.29	2.05	1.94
2	D	802	HEM	CAB-C3B	3.19	1.55	1.47
2	B	801	HEM	FE-NB	3.13	2.04	1.94
2	A	801	HEM	CAC-C3C	3.02	1.55	1.47
2	B	801	HEM	CAB-C3B	3.00	1.55	1.47
2	A	801	HEM	CAB-C3B	2.99	1.55	1.47
2	D	802	HEM	FE-ND	2.99	2.04	1.94
2	C	801	HEM	CAC-C3C	2.94	1.55	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	801	HEM	CAB-C3B	2.93	1.55	1.47
2	B	801	HEM	CAC-C3C	2.83	1.54	1.47
2	D	802	HEM	CAC-C3C	2.66	1.54	1.47
2	A	801	HEM	CMA-C3A	2.59	1.56	1.50
2	D	802	HEM	CMC-C2C	2.53	1.56	1.50
2	D	802	HEM	CMB-C2B	2.53	1.56	1.50
2	C	801	HEM	FE-ND	2.46	2.02	1.94
2	B	801	HEM	CMB-C2B	2.34	1.55	1.50
2	B	801	HEM	FE-ND	2.30	2.02	1.94
3	D	803	H4B	C4-N3	-2.29	1.34	1.38
2	A	801	HEM	CMC-C2C	2.21	1.55	1.50
2	C	801	HEM	CMB-C2B	2.21	1.55	1.50
2	A	801	HEM	CMB-C2B	2.19	1.55	1.50
2	D	802	HEM	CMA-C3A	2.19	1.55	1.50
3	B	802	H4B	C4-N3	-2.17	1.34	1.38
2	A	801	HEM	CMD-C2D	2.14	1.55	1.50
2	B	801	HEM	CMC-C2C	2.12	1.55	1.50
2	B	801	HEM	CMA-C3A	2.10	1.55	1.50
3	A	802	H4B	C4-N3	-2.07	1.35	1.38
2	D	802	HEM	CMD-C2D	2.05	1.55	1.50
2	C	801	HEM	FE-NB	2.04	2.01	1.94
3	C	802	H4B	C4-N3	-2.01	1.35	1.38

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	803	KKU	C02-N01-C06	5.80	122.41	118.07
2	C	801	HEM	CBA-CAA-C2A	-5.12	98.37	112.53
4	B	803	KKU	C02-N01-C06	5.01	121.82	118.07
4	C	803	KKU	C02-N01-C06	5.00	121.81	118.07
2	B	801	HEM	CBA-CAA-C2A	-4.83	99.19	112.53
2	D	802	HEM	CBA-CAA-C2A	-4.36	100.47	112.53
3	D	803	H4B	C2-N1-C8A	4.05	120.50	113.36
4	D	804	KKU	C02-N01-C06	4.04	121.09	118.07
3	A	802	H4B	C2-N1-C8A	4.00	120.41	113.36
3	C	802	H4B	C2-N1-C8A	3.57	119.65	113.36
2	A	801	HEM	CBA-CAA-C2A	-3.55	102.73	112.53
2	C	801	HEM	C2A-C1A-NA	-3.28	106.51	110.15
2	A	801	HEM	CBD-CAD-C3D	-3.23	103.61	112.53
3	C	802	H4B	O4-C4-C4A	-3.18	119.58	127.26
2	D	802	HEM	C3B-C4B-NB	-3.00	107.31	109.47
3	D	803	H4B	C4A-C4-N3	2.99	120.33	112.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	802	H4B	C2-N1-C8A	2.98	118.63	113.36
2	D	802	HEM	CBD-CAD-C3D	-2.90	104.50	112.53
4	B	803	KKU	C05-C06-N01	-2.90	119.43	122.73
3	A	802	H4B	C4A-C4-N3	2.85	119.97	112.13
3	D	803	H4B	C2-N3-C4	-2.83	119.97	125.11
2	A	801	HEM	C3B-C2B-C1B	2.81	108.52	106.41
2	A	801	HEM	C3B-C4B-NB	-2.80	107.46	109.47
3	C	802	H4B	C4A-C4-N3	2.76	119.71	112.13
3	A	802	H4B	C2-N3-C4	-2.73	120.16	125.11
3	A	802	H4B	O4-C4-C4A	-2.73	120.68	127.26
3	C	802	H4B	C11-C10-C9	-2.71	108.80	112.11
2	D	802	HEM	C2A-C1A-NA	-2.70	107.16	110.15
2	B	801	HEM	C2A-C1A-NA	-2.68	107.18	110.15
2	C	801	HEM	CBD-CAD-C3D	-2.59	105.37	112.53
3	C	802	H4B	C2-N3-C4	-2.54	120.50	125.11
2	A	801	HEM	C2A-C1A-NA	-2.50	107.38	110.15
4	B	803	KKU	C08-C06-N01	2.46	119.78	116.06
4	D	804	KKU	C10-C09-C08	-2.40	108.59	113.10
3	B	802	H4B	C2-N3-C4	-2.40	120.75	125.11
4	C	803	KKU	C10-C09-C08	-2.37	108.66	113.10
2	C	801	HEM	C3D-C4D-ND	-2.36	107.58	110.17
3	B	802	H4B	O4-C4-C4A	-2.35	121.59	127.26
3	B	802	H4B	C4A-C4-N3	2.31	118.47	112.13
3	D	803	H4B	O4-C4-C4A	-2.25	121.84	127.26
2	D	802	HEM	C4C-NC-C1C	2.23	109.46	105.82
2	D	802	HEM	C4D-ND-C1D	2.18	107.79	105.21
2	D	802	HEM	C3B-C2B-C1B	2.17	108.04	106.41
4	A	803	KKU	C05-C06-N01	-2.17	120.26	122.73
2	C	801	HEM	CHD-C1D-ND	2.16	126.75	124.42
2	B	801	HEM	CHD-C1D-ND	2.15	126.74	124.42
2	B	801	HEM	CBD-CAD-C3D	-2.05	106.86	112.53
3	D	803	H4B	C4-C4A-N5	2.04	121.84	116.27
2	A	801	HEM	C4C-NC-C1C	2.01	109.10	105.82
4	C	803	KKU	C05-C06-N01	-2.01	120.44	122.73

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	803	KKU	C09-C10-N11-C12
4	C	803	KKU	C09-C10-N11-C12
5	B	804	GOL	O1-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	D	805	GOL	O1-C1-C2-C3
4	D	804	KKU	C08-C09-C10-N11
2	A	801	HEM	C2A-CAA-CBA-CGA
4	B	803	KKU	C08-C09-C10-N11
5	A	804	GOL	C1-C2-C3-O3
5	C	805	GOL	O1-C1-C2-C3
5	C	805	GOL	C1-C2-C3-O3
4	A	803	KKU	C08-C09-C10-N11
4	C	803	KKU	C08-C09-C10-N11
5	D	805	GOL	O1-C1-C2-O2
2	D	802	HEM	C4B-C3B-CAB-CBB
5	B	804	GOL	O1-C1-C2-O2
2	D	802	HEM	C2A-CAA-CBA-CGA
5	C	805	GOL	O1-C1-C2-O2
5	C	805	GOL	O2-C2-C3-O3
2	A	801	HEM	C4B-C3B-CAB-CBB
2	B	801	HEM	C4B-C3B-CAB-CBB
3	A	802	H4B	C7-C6-C9-C10
3	D	803	H4B	C7-C6-C9-C10
3	D	803	H4B	C7-C6-C9-O9
3	A	802	H4B	C7-C6-C9-O9
3	A	802	H4B	N5-C6-C9-O9
3	D	803	H4B	N5-C6-C9-O9

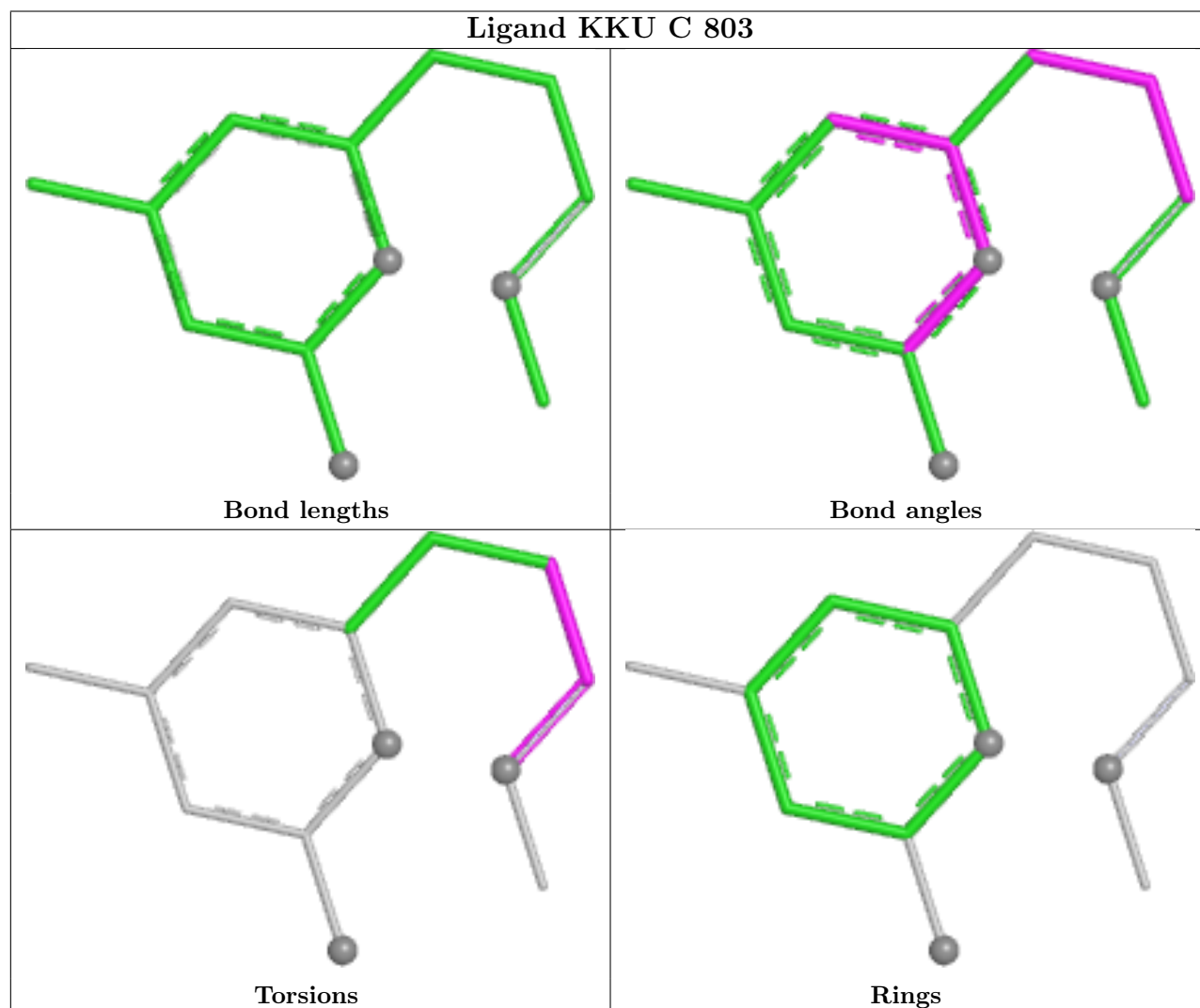
There are no ring outliers.

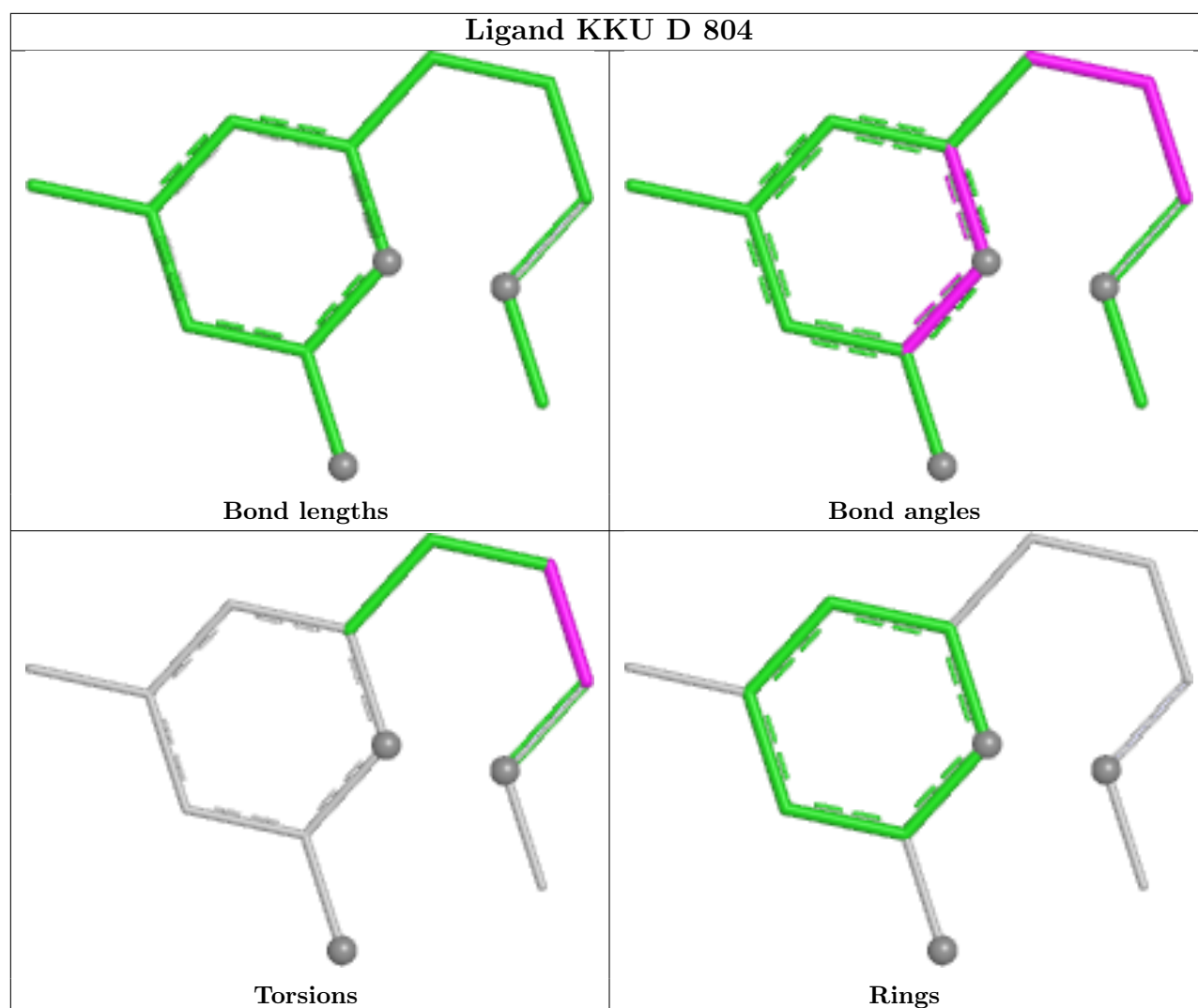
9 monomers are involved in 18 short contacts:

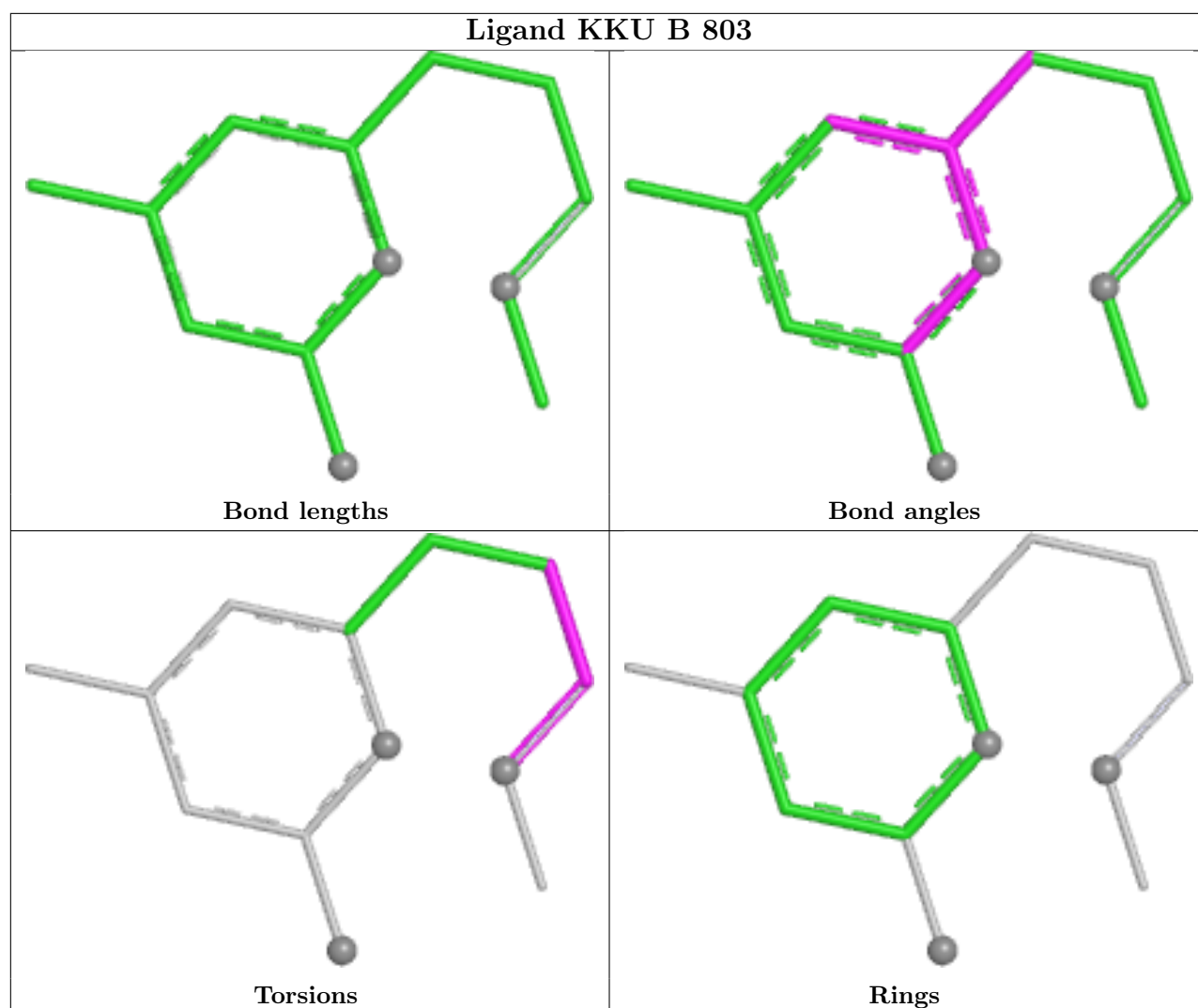
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	805	GOL	1	0
5	A	804	GOL	1	0
4	C	803	KKU	2	0
4	B	803	KKU	1	0
2	C	801	HEM	4	0
3	C	802	H4B	1	0
2	D	802	HEM	3	0
2	A	801	HEM	3	0
2	B	801	HEM	4	0

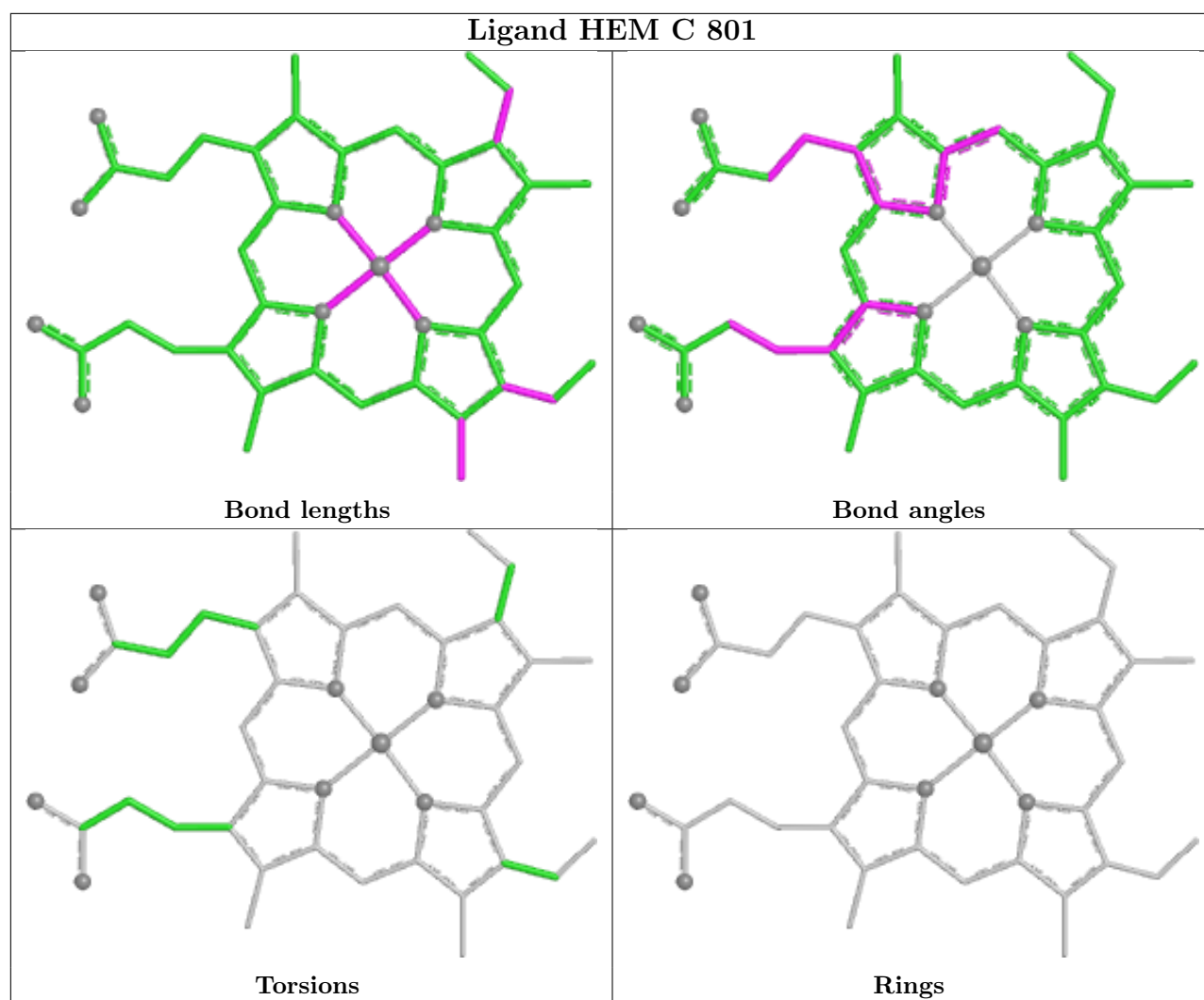
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

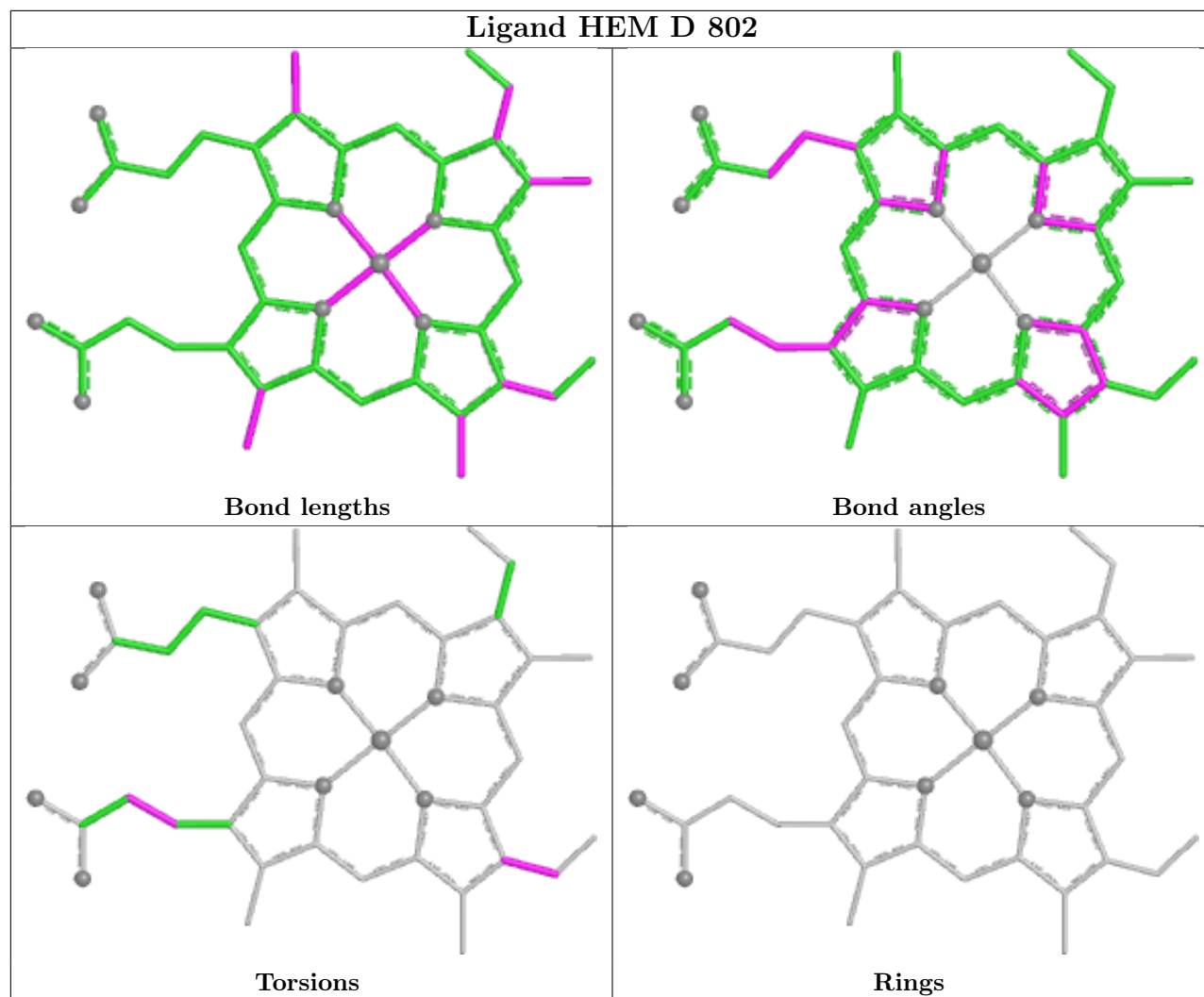
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

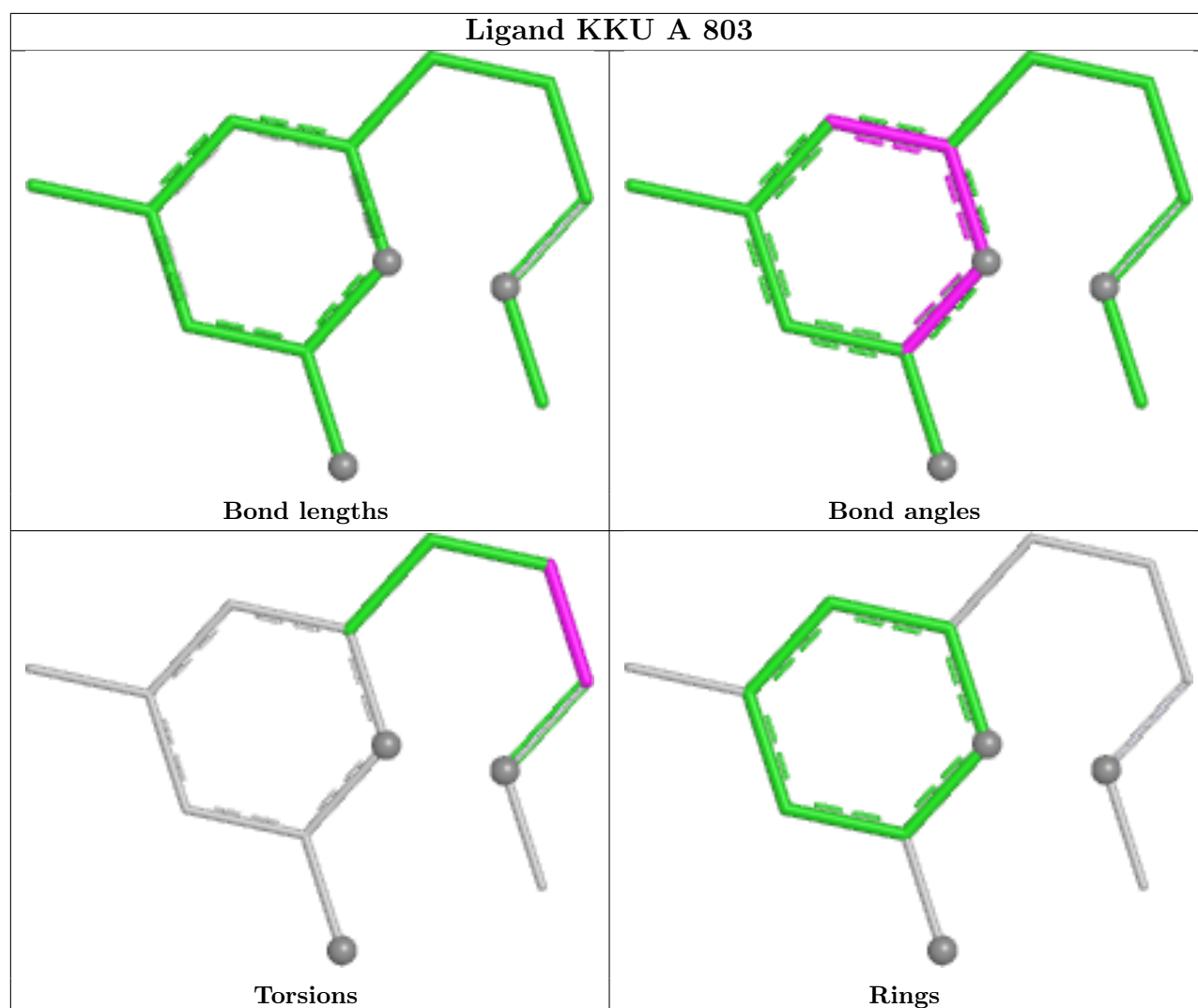


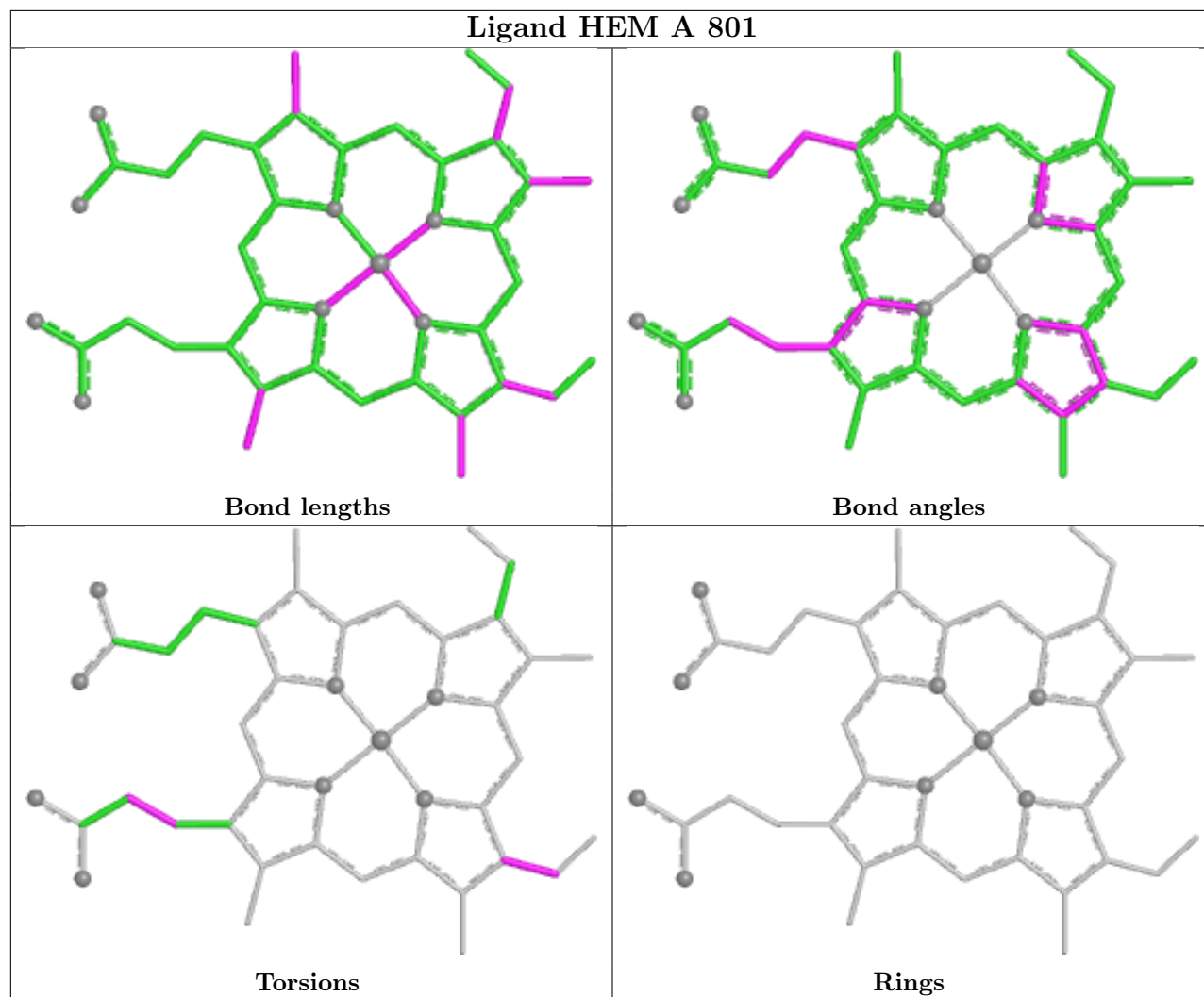


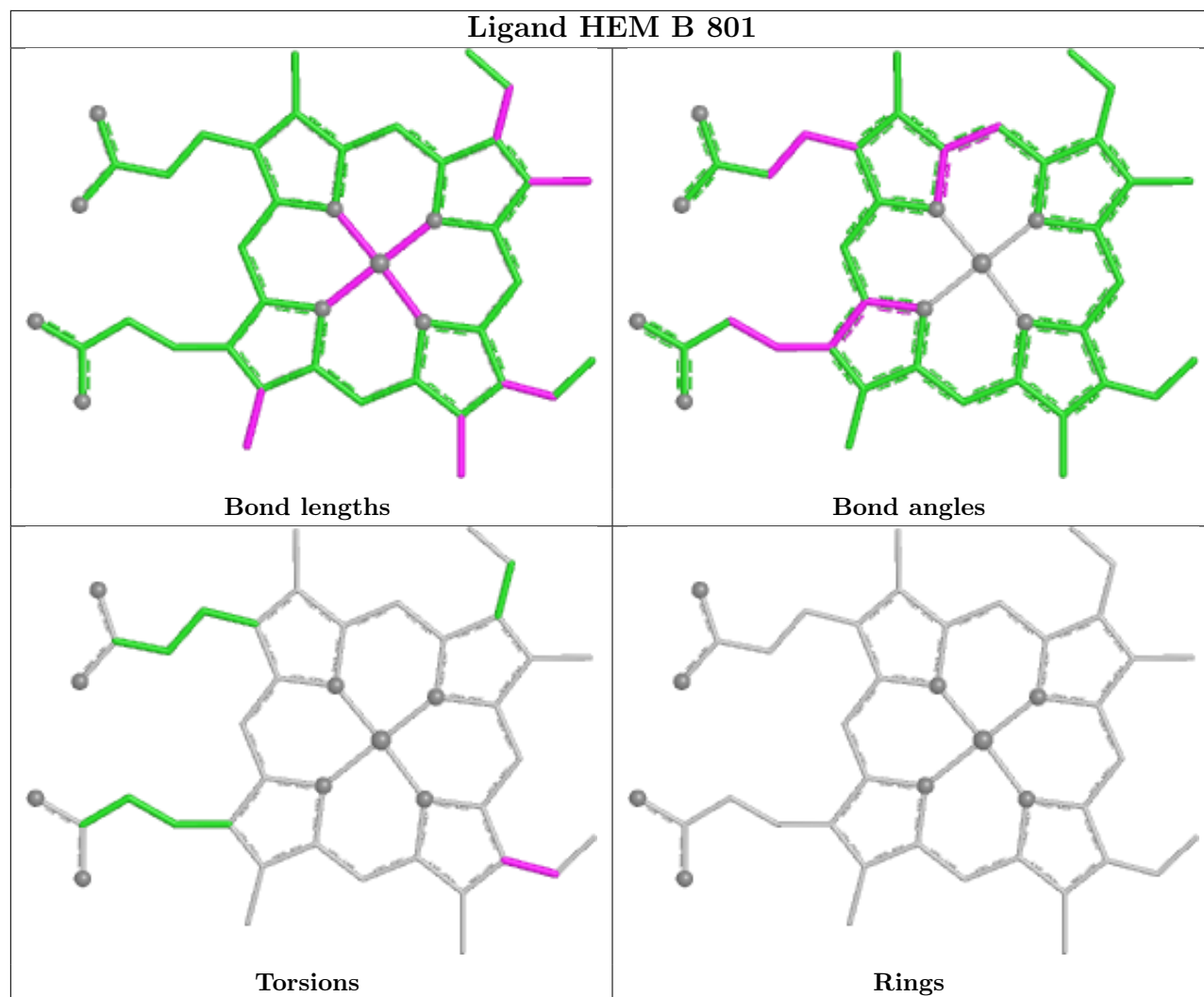












5.7 Other polymers [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	420/423 (99%)	-1.31	0 100 100	19, 43, 82, 137	3 (0%)
1	B	414/423 (97%)	-1.38	0 100 100	20, 39, 71, 108	2 (0%)
1	C	415/423 (98%)	-1.39	0 100 100	18, 40, 72, 117	5 (1%)
1	D	418/423 (98%)	-1.32	0 100 100	21, 43, 79, 136	3 (0%)
All	All	1667/1692 (98%)	-1.35	0 100 100	18, 41, 77, 137	13 (0%)

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

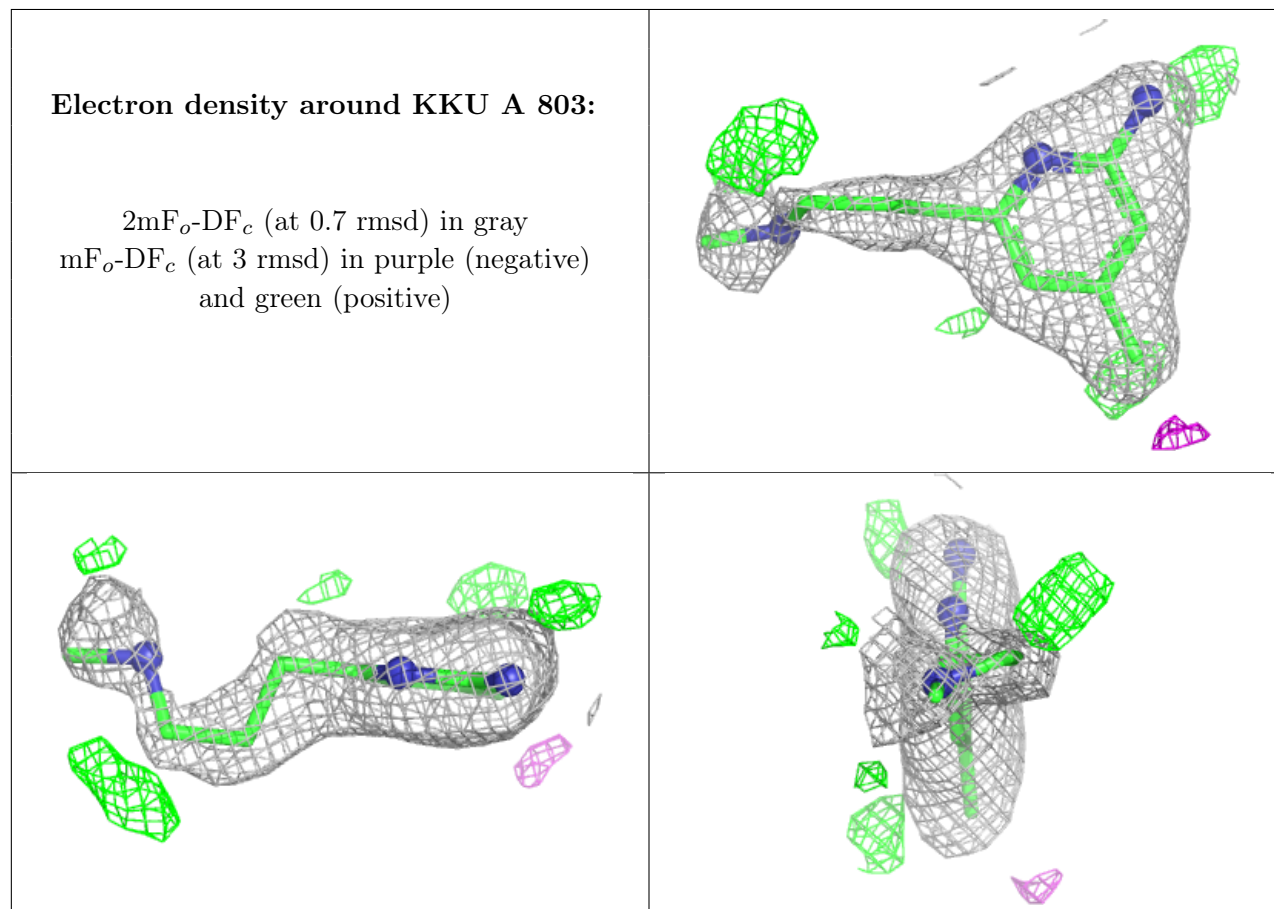
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	H4B	A	802	17/17	0.99	0.03	37,45,58,60	0
3	H4B	B	802	17/17	0.99	0.03	29,40,45,45	0
3	H4B	C	802	17/17	0.99	0.03	30,40,47,47	0
3	H4B	D	803	17/17	0.99	0.03	35,44,56,57	0

Continued on next page...

Continued from previous page...

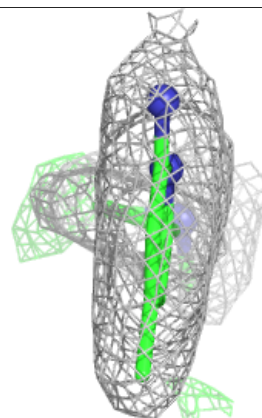
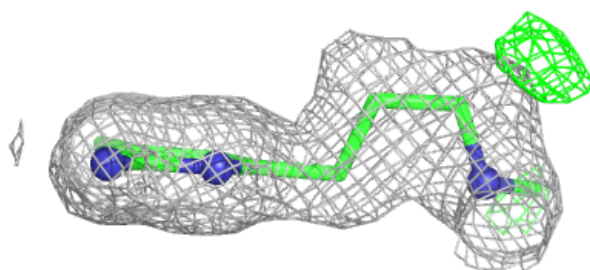
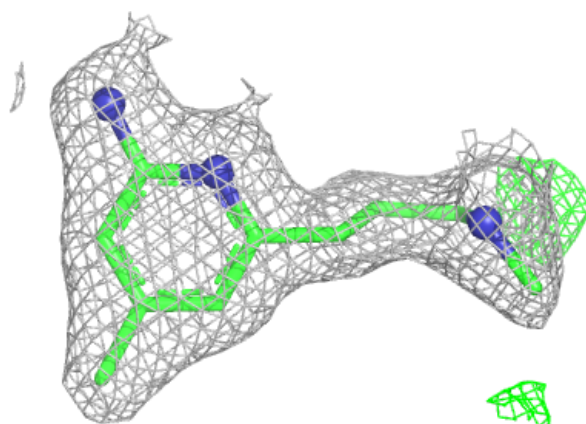
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	KKU	A	803	13/13	0.99	0.04	27,35,67,68	0
4	KKU	B	803	13/13	0.99	0.04	27,32,59,61	0
4	KKU	C	803	13/13	0.99	0.04	23,34,61,63	0
4	KKU	D	804	13/13	0.99	0.03	22,34,62,64	0
5	GOL	A	804	6/6	0.99	0.03	47,56,59,61	0
5	GOL	B	804	6/6	0.99	0.05	62,65,68,69	0
5	GOL	C	804	6/6	0.99	0.04	64,69,70,71	0
5	GOL	C	805	6/6	0.99	0.05	54,64,70,74	0
5	GOL	D	805	6/6	0.99	0.04	68,69,74,81	0
2	HEM	B	801	43/43	1.00	0.03	26,33,48,61	0
2	HEM	C	801	43/43	1.00	0.03	23,32,43,63	0
2	HEM	D	802	43/43	1.00	0.02	23,30,50,56	0
2	HEM	A	801	43/43	1.00	0.03	24,32,52,57	0
6	ZN	A	805	1/1	1.00	0.02	32,32,32,32	0
6	ZN	D	801	1/1	1.00	0.01	33,33,33,33	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.

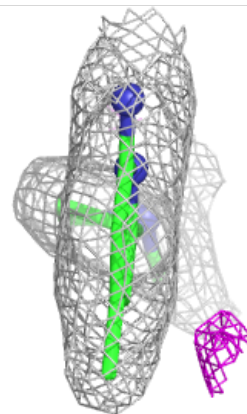
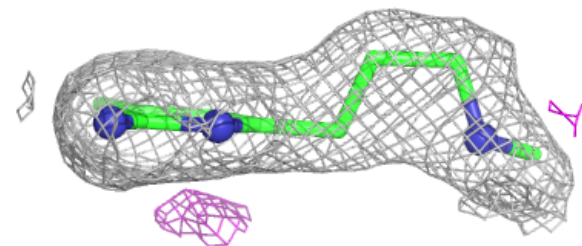
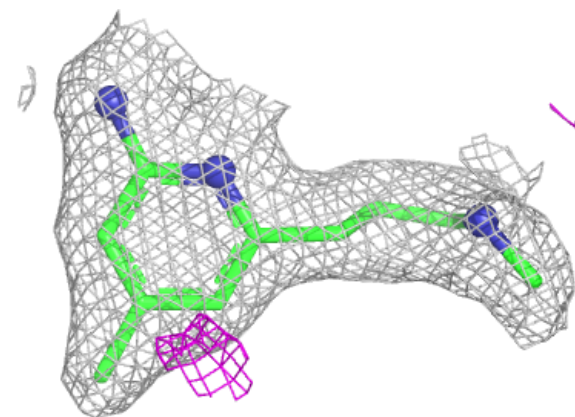


Electron density around KCU B 803:

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

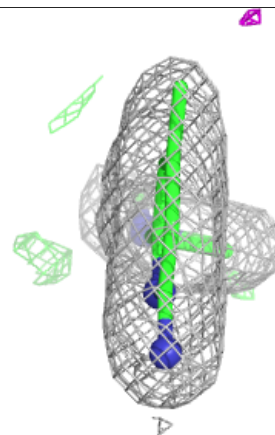
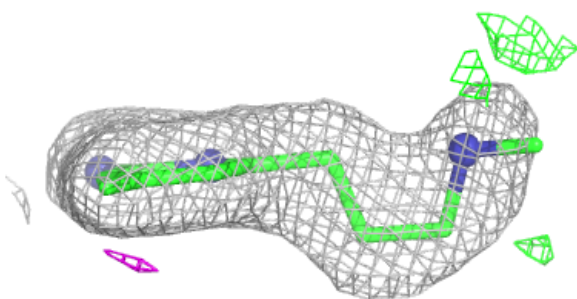
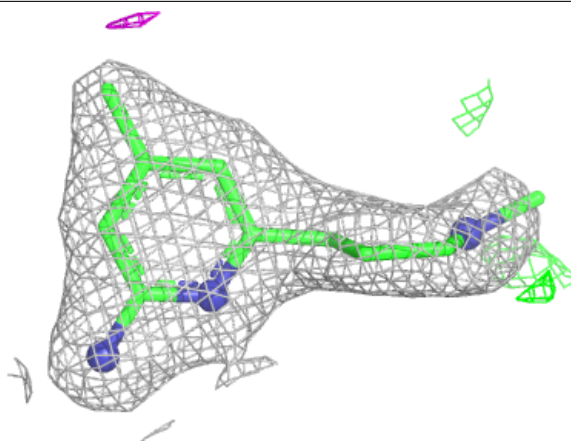
**Electron density around KCU C 803:**

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



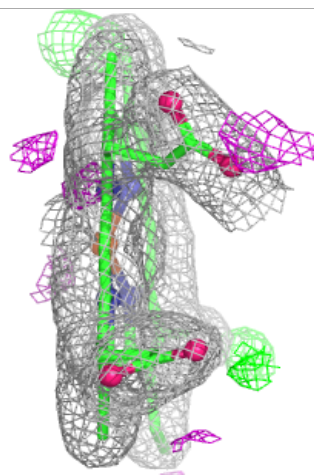
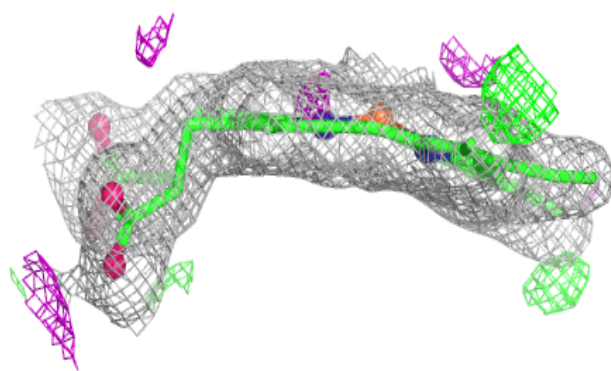
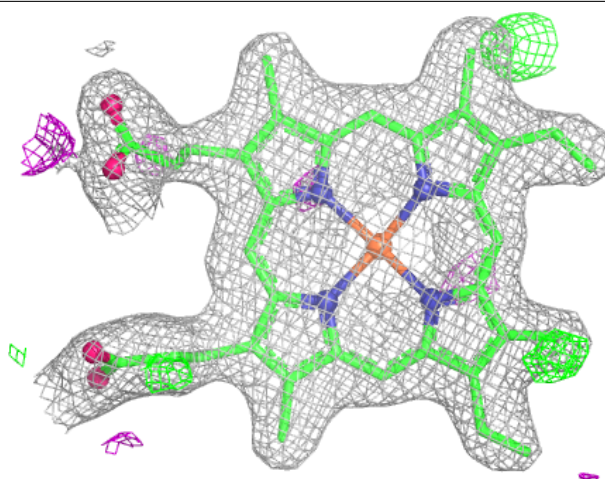
Electron density around KKV D 804:

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



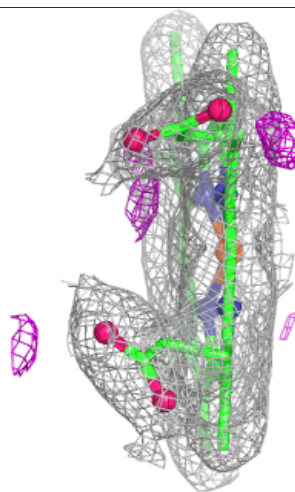
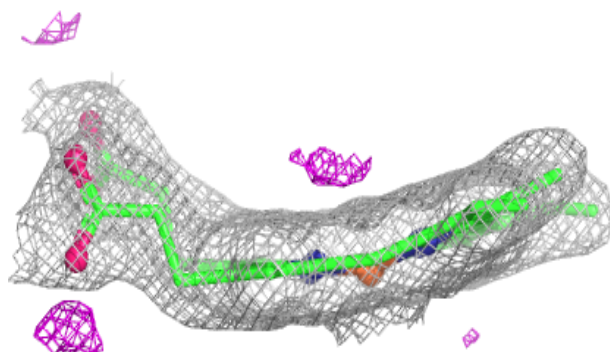
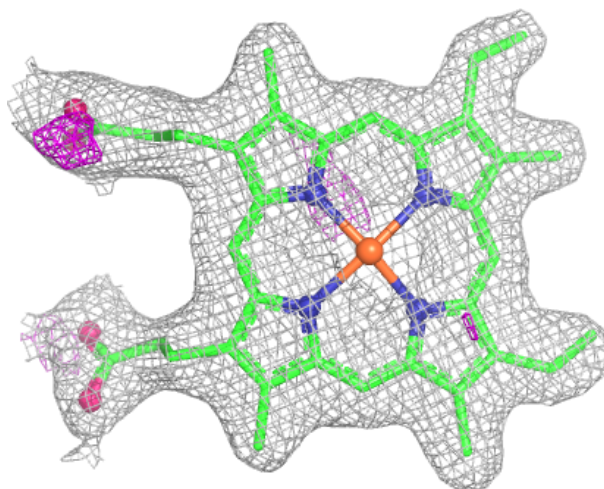
Electron density around HEM B 801:

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



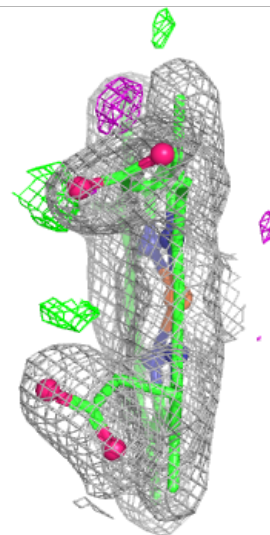
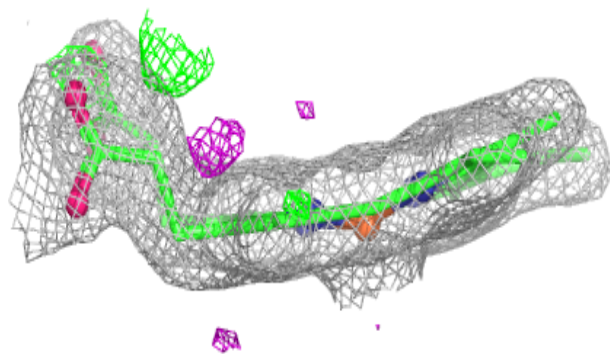
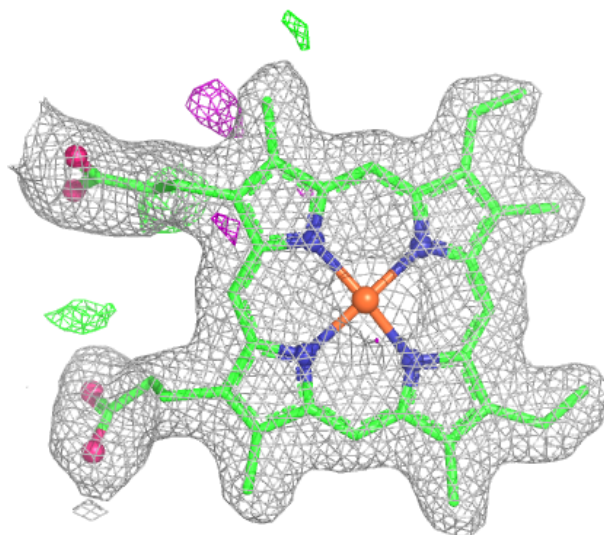
Electron density around HEM C 801:

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



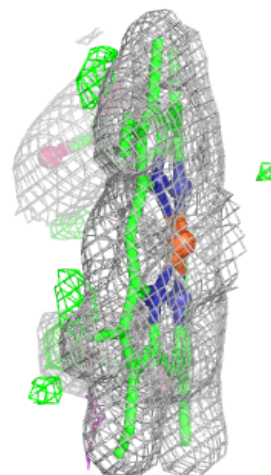
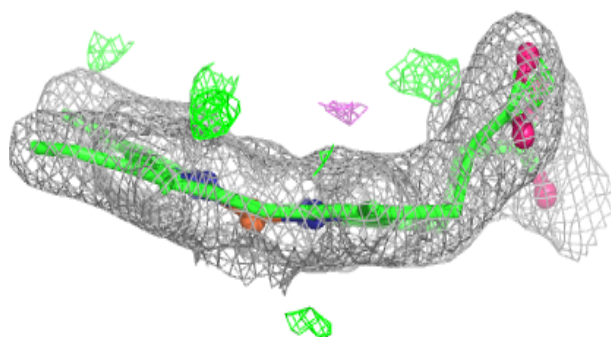
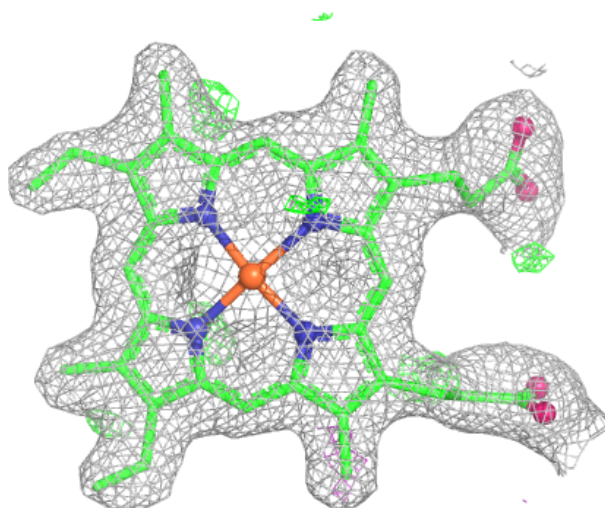
Electron density around HEM D 802:

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



Electron density around HEM A 801:

$2mF_o-DF_c$ (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.