



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 03:13 AM EDT

PDB ID : 6NG4
Title : Structure of human neuronal nitric oxide synthase R354A/G357D mutant heme domain in complex with (R)-6-(3-fluoro-5-(2-(pyrrolidin-2-yl)ethyl)phenethyl)-4-methylpyridin-2-amine
Authors : Li, H.; Poulos, T.L.
Deposited on : 2018-12-21
Resolution : 1.78 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
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)	:	2.36.2

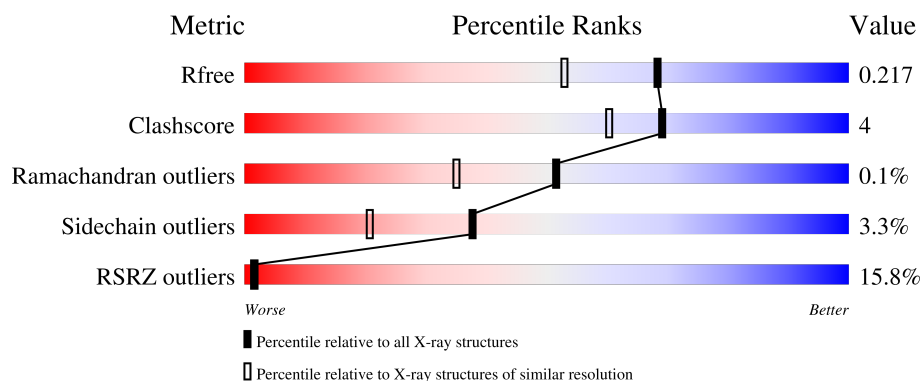
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.78 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	9185 (1.80-1.76)
Clashscore	141614	10184 (1.80-1.76)
Ramachandran outliers	138981	10051 (1.80-1.76)
Sidechain outliers	138945	10050 (1.80-1.76)
RSRZ outliers	127900	9032 (1.80-1.76)

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	421	
1	B	421	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 7539 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	414	Total	C	N	O	S	0	4	0
			3391	2171	578	619	23			
1	B	410	Total	C	N	O	S	0	2	0
			3349	2145	571	612	21			

There are 4 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
B	354	ALA	ARG	engineered mutation	UNP P29475
B	357	ASP	GLY	engineered mutation	UNP P29475

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



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

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

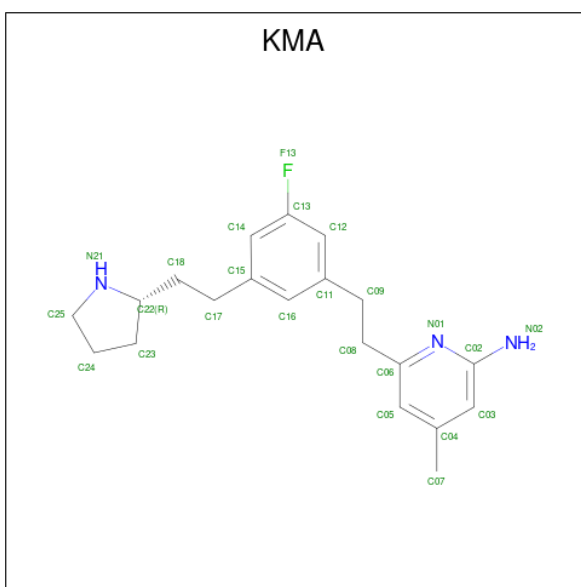


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

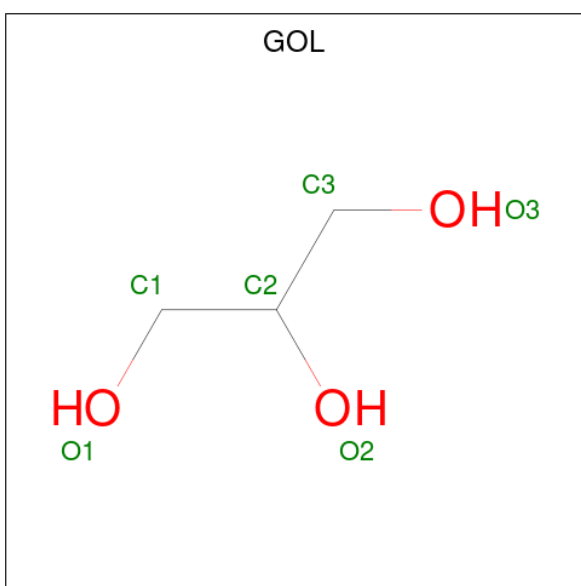
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		

- Molecule 5 is 6-[2-(3-fluoro-5-{2-[(2R)-pyrrolidin-2-yl]ethyl}phenyl)ethyl]-4-methylpyridin-2-amine (three-letter code: KMA) (formula: $C_{20}H_{26}FN_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	F	N	0	0
			24	20	1	3		
5	B	1	Total	C	F	N	0	0
			24	20	1	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	A	1	Total	C	O	0	0
			6	3	3		

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

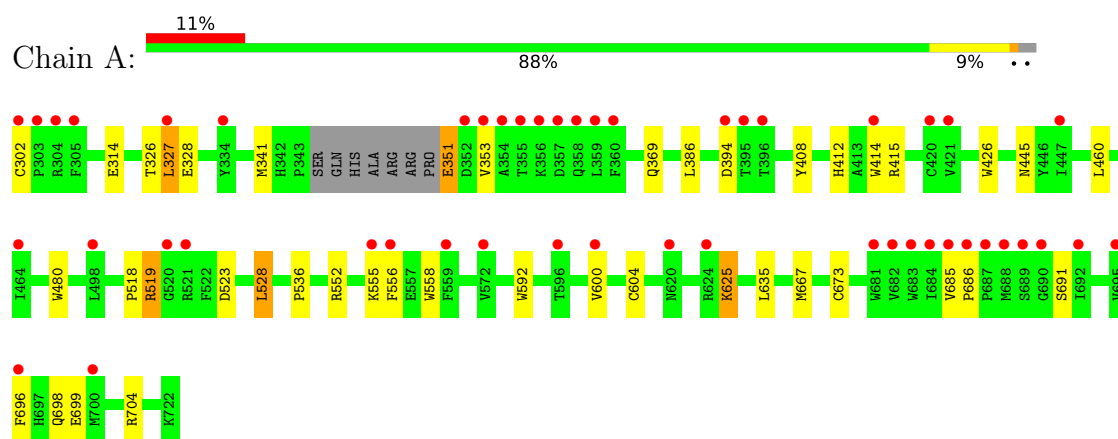
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	356	Total	O	0	0
			356	356		
7	B	256	Total	O	0	0
			256	256		

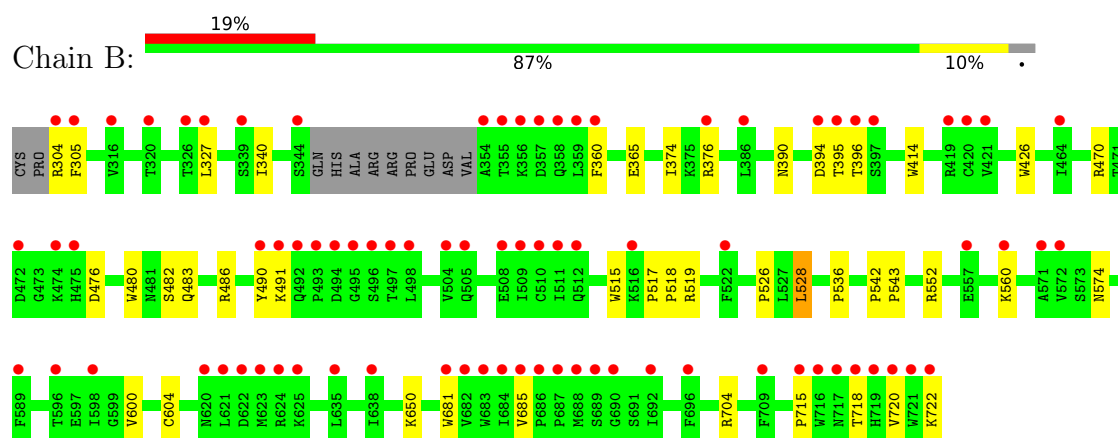
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Nitric oxide synthase, brain



- Molecule 1: Nitric oxide synthase, brain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	52.39Å 121.63Å 164.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.85 – 1.78 39.69 – 1.78	Depositor EDS
% Data completeness (in resolution range)	98.3 (38.85-1.78) 98.6 (39.69-1.78)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.03 (at 1.77Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.178 , 0.215 0.180 , 0.217	Depositor DCC
R_{free} test set	4957 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	37.6	Xtriage
Anisotropy	0.503	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 54.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	7539	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.19% 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: KMA, HEM, ZN, GOL, H4B

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	0/3499	0.52	0/4746
1	B	0.34	0/3450	0.48	0/4679
All	All	0.36	0/6949	0.50	0/9425

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	3391	0	3306	27	0
1	B	3349	0	3262	19	0
2	A	43	0	30	2	0
2	B	43	0	30	2	0
3	A	17	0	15	1	0
3	B	17	0	15	0	0
4	A	1	0	0	0	0
5	A	24	0	0	0	0
5	B	24	0	0	1	0
6	A	12	0	16	1	0
6	B	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	356	0	0	3	0
7	B	256	0	0	1	0
All	All	7539	0	6682	50	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 (50) 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:A:667:MET:HE1	1:A:698:GLN:HG2	1.63	0.79
1:B:528:LEU:HD22	1:B:536:PRO:HB2	1.66	0.77
2:B:801:HEM:HBB2	2:B:801:HEM:HHC	1.70	0.74
1:A:528:LEU:HD22	1:A:536:PRO:HB2	1.69	0.73
1:B:374:ILE:HD12	1:B:376:ARG:HG3	1.75	0.69
2:A:801:HEM:HMC2	2:A:801:HEM:HBC2	1.77	0.66
1:A:519[B]:ARG:NH1	7:A:902:HOH:O	2.30	0.64
2:A:801:HEM:HBB2	2:A:801:HEM:HHC	1.81	0.63
5:B:803:KMA:N21	7:B:902:HOH:O	2.32	0.58
1:B:327:LEU:HB2	1:B:704:ARG:NH1	2.25	0.52
1:A:415:ARG:HH12	6:A:806:GOL:H11	1.76	0.51
1:A:327:LEU:HB2	1:A:704:ARG:HH11	1.77	0.50
1:A:326:THR:OG1	1:A:327:LEU:N	2.44	0.50
1:B:600:VAL:O	1:B:604:CYS:HB2	2.12	0.49
1:A:327:LEU:HB2	1:A:704:ARG:NH1	2.27	0.49
1:B:305:PHE:H	1:B:305:PHE:HD1	1.62	0.48
1:A:600:VAL:HG22	1:A:635:LEU:HD11	1.94	0.48
1:B:470:ARG:NH2	1:B:476:ASP:OD2	2.39	0.47
1:A:480:TRP:HB2	1:A:528:LEU:HB3	1.97	0.47
1:A:327:LEU:HB2	1:A:704:ARG:HD3	1.97	0.46
1:B:490:TYR:CE1	1:B:519:ARG:HA	2.50	0.46
1:A:351:GLU:N	7:A:912:HOH:O	2.48	0.46
1:A:600:VAL:O	1:A:604:CYS:HB2	2.15	0.45
1:A:518:PRO:HG2	1:A:523:ASP:CG	2.37	0.45
1:A:341:MET:HE2	3:A:802:H4B:H9	1.98	0.45
1:A:408:TYR:CE1	1:A:412:HIS:CE1	3.05	0.45
1:B:327:LEU:HB2	1:B:704:ARG:HH11	1.81	0.44
1:B:483:GLN:OE1	1:B:486:ARG:HD2	2.17	0.44
1:A:667:MET:HE1	1:A:698:GLN:CG	2.43	0.44
1:A:691:SER:HA	1:A:696:PHE:CG	2.52	0.44
1:B:482:SER:HA	1:B:574:ASN:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:685:VAL:HA	1:A:686:PRO:HD3	1.89	0.43
1:A:699:GLU:HB3	1:B:340:ILE:HD13	2.00	0.43
1:B:327:LEU:HD13	1:B:327:LEU:HA	1.83	0.43
1:A:369:GLN:HG2	1:A:408:TYR:OH	2.18	0.43
1:A:625:LYS:HB2	1:A:625:LYS:HE3	1.71	0.43
1:B:480:TRP:CE2	1:B:715:PRO:HB2	2.54	0.43
1:B:515:TRP:CE2	1:B:526:PRO:HD3	2.54	0.43
1:A:555:LYS:HD3	1:A:555:LYS:HA	1.79	0.43
1:A:445:ASN:ND2	7:A:904:HOH:O	2.38	0.43
1:B:542:PRO:HA	1:B:543:PRO:HD3	1.82	0.42
1:B:360:PHE:CE1	1:B:390:ASN:HB2	2.55	0.42
1:B:517:PRO:HA	1:B:518:PRO:HD3	1.95	0.42
1:A:556:PHE:HB3	1:A:558:TRP:CE2	2.56	0.41
1:A:414:TRP:CE3	1:A:426:TRP:HA	2.55	0.41
1:B:414:TRP:CE3	1:B:426:TRP:HA	2.56	0.40
1:B:681:TRP:CE2	1:B:685:VAL:HG21	2.56	0.40
1:A:327:LEU:HD12	1:A:328:GLU:H	1.86	0.40
1:A:460:LEU:HD12	1:A:592:TRP:HB3	2.03	0.40
2:B:801:HEM:HBB2	2:B:801:HEM:CHC	2.44	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	414/421 (98%)	407 (98%)	6 (1%)	1 (0%)	47	32
1	B	408/421 (97%)	400 (98%)	8 (2%)	0	100	100
All	All	822/842 (98%)	807 (98%)	14 (2%)	1 (0%)	51	35

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
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	374/376 (100%)	361 (96%)	13 (4%)	36	19
1	B	368/376 (98%)	355 (96%)	13 (4%)	36	19
All	All	742/752 (99%)	716 (96%)	26 (4%)	38	19

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	302	CYS
1	A	314	GLU
1	A	327	LEU
1	A	351	GLU
1	A	386	LEU
1	A	394	ASP
1	A	519[A]	ARG
1	A	519[B]	ARG
1	A	528	LEU
1	A	552	ARG
1	A	625	LYS
1	A	673[A]	CYS
1	A	673[B]	CYS
1	B	304	ARG
1	B	365	GLU
1	B	394	ASP
1	B	395	THR
1	B	396	THR
1	B	491	LYS
1	B	528	LEU
1	B	552	ARG
1	B	560	LYS
1	B	650	LYS

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Mol	Chain	Res	Type
1	B	718	THR
1	B	720	VAL
1	B	722	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 1 is monoatomic - leaving 9 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	KMA	B	803	-	25,26,26	0.43	0	32,35,35	2.07	10 (31%)
2	HEM	B	801	1	41,50,50	1.88	9 (21%)	45,82,82	2.06	11 (24%)
3	H4B	B	802	-	16,18,18	0.88	0	11,26,26	2.67	5 (45%)
6	GOL	A	806	-	5,5,5	0.37	0	5,5,5	0.26	0
2	HEM	A	801	1	41,50,50	1.79	6 (14%)	45,82,82	1.86	10 (22%)
5	KMA	A	804	-	25,26,26	0.41	0	32,35,35	1.67	6 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	H4B	A	802	-	16,18,18	0.78	0	11,26,26	2.60	6 (54%)
6	GOL	B	804	-	5,5,5	0.36	0	5,5,5	0.16	0
6	GOL	A	805	-	5,5,5	0.38	0	5,5,5	0.33	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	KMA	B	803	-	-	3/10/17/17	0/3/3/3
2	HEM	B	801	1	-	1/12/54/54	-
3	H4B	B	802	-	-	0/8/17/17	0/2/2/2
6	GOL	A	806	-	-	3/4/4/4	-
2	HEM	A	801	1	-	1/12/54/54	-
5	KMA	A	804	-	-	2/10/17/17	0/3/3/3
3	H4B	A	802	-	-	0/8/17/17	0/2/2/2
6	GOL	B	804	-	-	2/4/4/4	-
6	GOL	A	805	-	-	4/4/4/4	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	HEM	C3D-C2D	7.34	1.52	1.36
2	A	801	HEM	C3D-C2D	7.04	1.51	1.36
2	A	801	HEM	C3C-C2C	-3.83	1.35	1.40
2	B	801	HEM	C3C-CAC	3.57	1.55	1.47
2	B	801	HEM	C3C-C2C	-3.54	1.35	1.40
2	B	801	HEM	CAB-C3B	2.95	1.55	1.47
2	A	801	HEM	C3C-CAC	2.94	1.53	1.47
2	A	801	HEM	CAB-C3B	2.88	1.55	1.47
2	B	801	HEM	CMD-C2D	2.22	1.55	1.50
2	B	801	HEM	FE-NB	2.16	2.07	1.96
2	B	801	HEM	C3B-C2B	-2.13	1.33	1.37
2	B	801	HEM	CMB-C2B	2.08	1.55	1.50
2	A	801	HEM	CMC-C2C	2.04	1.56	1.51
2	B	801	HEM	FE-ND	2.04	2.06	1.96
2	A	801	HEM	FE-ND	2.01	2.06	1.96

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	HEM	CBA-CAA-C2A	-6.66	101.25	112.62
2	A	801	HEM	CBA-CAA-C2A	-6.44	101.63	112.62
5	A	804	KMA	C09-C08-C06	-6.17	99.16	112.99
5	B	803	KMA	C09-C08-C06	-6.10	99.31	112.99
2	B	801	HEM	C4D-ND-C1D	5.84	111.10	105.07
3	B	802	H4B	C8A-C4A-C4	5.44	119.40	114.57
5	B	803	KMA	C02-N01-C06	5.17	122.02	118.10
3	A	802	H4B	C8A-C4A-C4	4.65	118.70	114.57
2	B	801	HEM	C4B-CHC-C1C	4.65	128.69	122.56
2	A	801	HEM	C4D-ND-C1D	4.64	109.87	105.07
3	A	802	H4B	C4-C4A-N5	3.83	122.33	119.12
5	A	804	KMA	C02-N01-C06	3.75	120.94	118.10
3	B	802	H4B	C2-N3-C4	3.63	121.70	115.93
5	B	803	KMA	C05-C06-N01	-3.47	119.22	122.90
2	A	801	HEM	CBD-CAD-C3D	-3.32	103.39	112.63
3	A	802	H4B	C2-N3-C4	3.29	121.15	115.93
5	B	803	KMA	C14-C13-C12	-3.28	119.38	123.52
3	B	802	H4B	N1-C2-N3	-3.12	120.53	125.42
3	A	802	H4B	N1-C2-N3	-3.04	120.66	125.42
2	A	801	HEM	C3B-C2B-C1B	3.00	108.71	106.49
2	A	801	HEM	C4B-CHC-C1C	2.90	126.39	122.56
2	B	801	HEM	CMA-C3A-C4A	-2.83	124.11	128.46
2	B	801	HEM	C3B-C2B-C1B	2.77	108.54	106.49
3	B	802	H4B	C4-C4A-N5	2.67	121.36	119.12
5	A	804	KMA	C14-C13-C12	-2.63	120.20	123.52
2	B	801	HEM	CAD-C3D-C4D	2.60	129.20	124.66
2	B	801	HEM	CMD-C2D-C1D	2.52	128.88	125.04
2	A	801	HEM	CMC-C2C-C3C	2.49	129.34	124.68
2	B	801	HEM	CBD-CAD-C3D	-2.46	105.80	112.63
3	A	802	H4B	C2-N1-C8A	2.45	120.04	114.54
3	B	802	H4B	C2-N1-C8A	2.43	119.99	114.54
5	B	803	KMA	C09-C11-C12	-2.39	116.62	120.54
5	B	803	KMA	C08-C06-N01	2.37	119.49	115.95
5	B	803	KMA	C11-C12-C13	2.35	120.95	118.81
3	A	802	H4B	N2-C2-N3	2.35	120.90	117.25
2	A	801	HEM	CMA-C3A-C4A	-2.30	124.92	128.46
2	A	801	HEM	CAD-C3D-C4D	2.30	128.67	124.66
2	A	801	HEM	C1B-NB-C4B	2.28	107.43	105.07
2	A	801	HEM	CHD-C1D-ND	2.24	126.87	124.43
5	A	804	KMA	C05-C06-N01	-2.21	120.55	122.90
2	B	801	HEM	CHA-C4D-ND	2.21	127.11	124.38
5	B	803	KMA	C17-C15-C14	-2.18	116.97	120.54
2	B	801	HEM	CHC-C4B-NB	2.09	126.70	124.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	804	KMA	C08-C06-N01	2.08	119.05	115.95
5	B	803	KMA	C09-C11-C16	2.07	123.94	120.54
5	A	804	KMA	F13-C13-C14	2.03	121.16	118.25
2	B	801	HEM	CHD-C1D-ND	2.03	126.64	124.43
5	B	803	KMA	F13-C13-C12	2.03	121.15	118.25

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	803	KMA	C17-C18-C22-C23
5	B	803	KMA	C17-C18-C22-N21
6	A	805	GOL	O1-C1-C2-C3
6	A	805	GOL	C1-C2-C3-O3
6	B	804	GOL	O1-C1-C2-C3
6	B	804	GOL	O1-C1-C2-O2
6	A	805	GOL	O1-C1-C2-O2
6	A	805	GOL	O2-C2-C3-O3
2	A	801	HEM	C4B-C3B-CAB-CBB
2	B	801	HEM	C4B-C3B-CAB-CBB
6	A	806	GOL	O1-C1-C2-O2
6	A	806	GOL	O2-C2-C3-O3
6	A	806	GOL	O1-C1-C2-C3
5	A	804	KMA	C08-C09-C11-C16
5	A	804	KMA	C08-C09-C11-C12
5	B	803	KMA	C08-C09-C11-C16

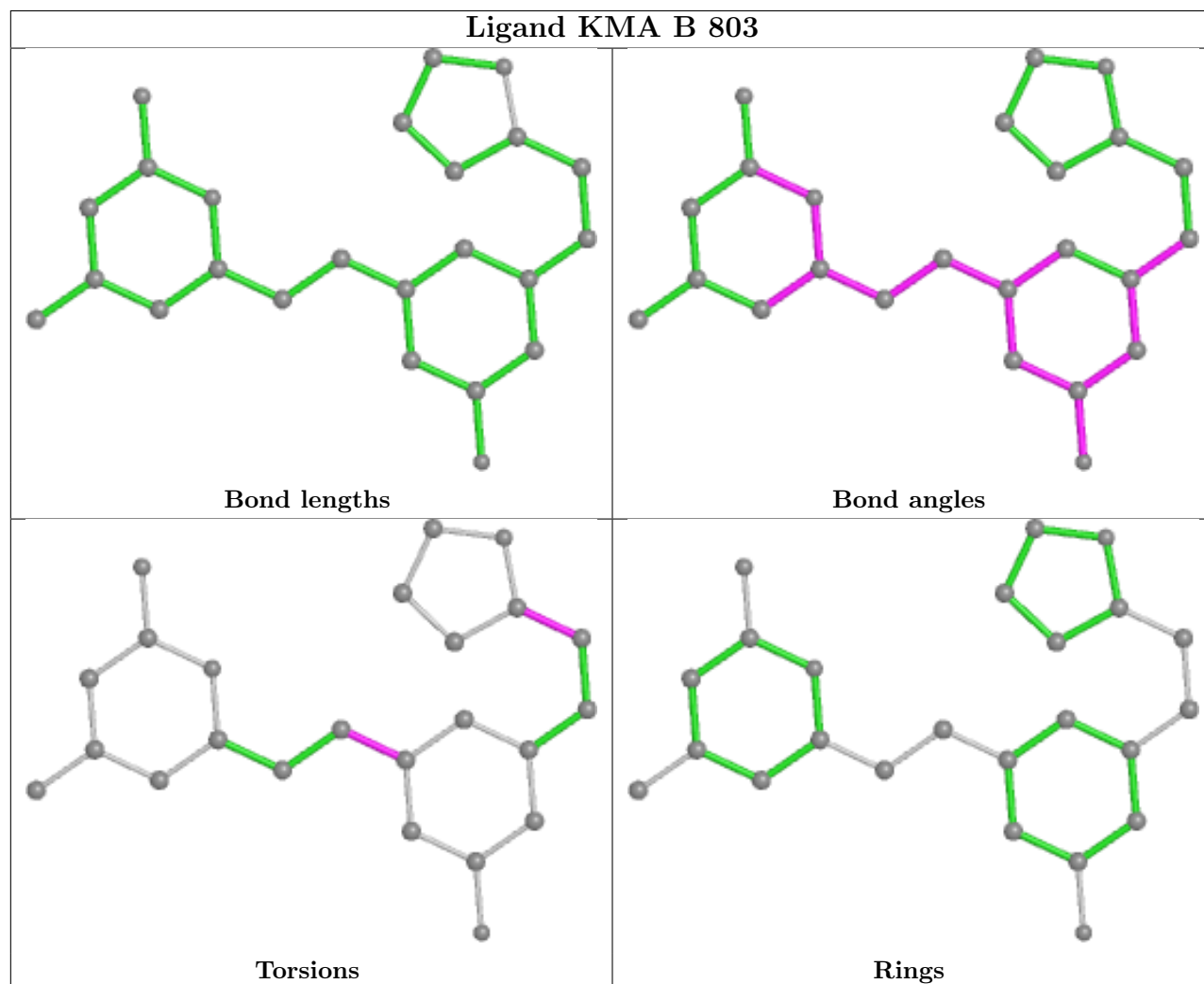
There are no ring outliers.

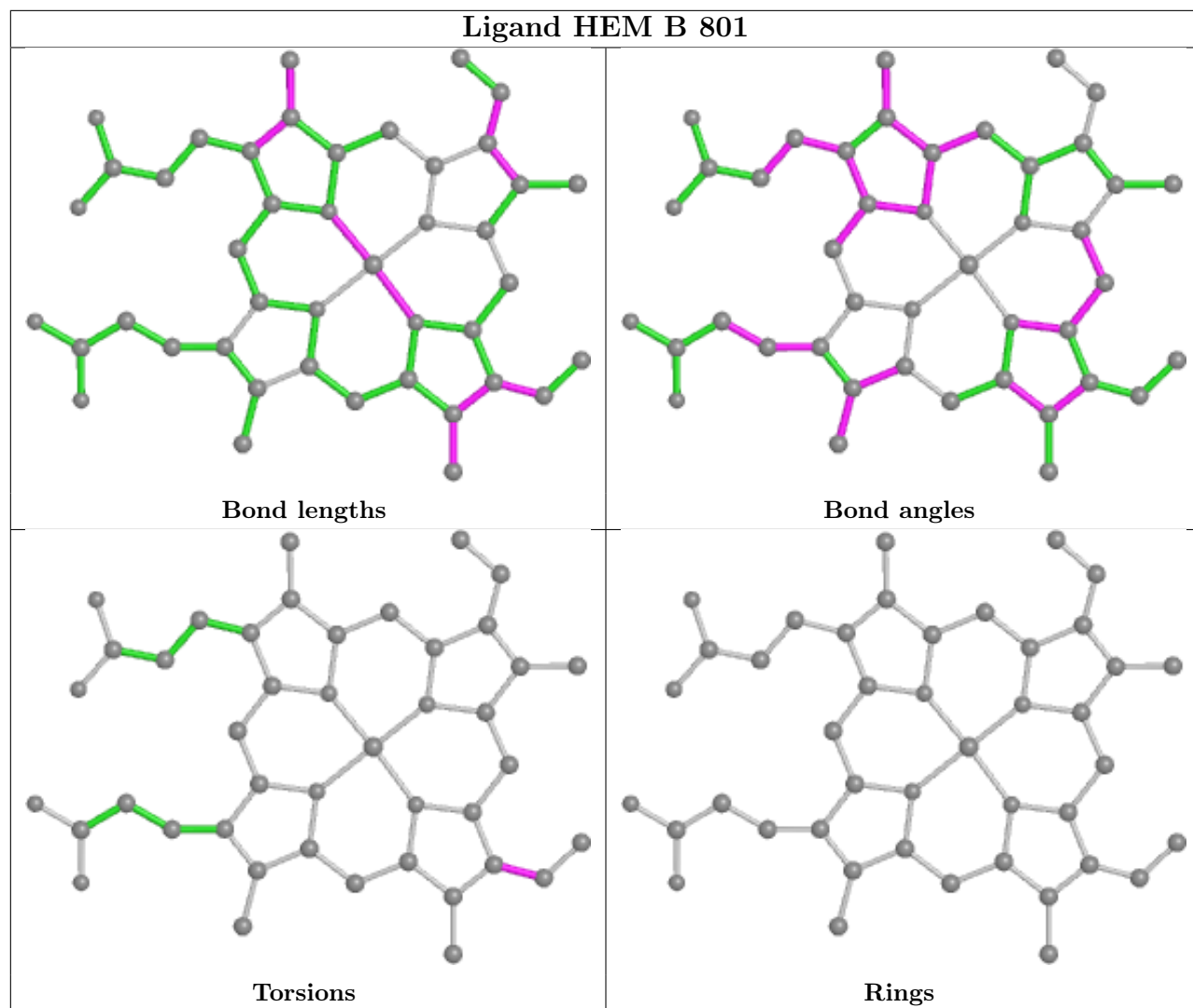
5 monomers are involved in 7 short contacts:

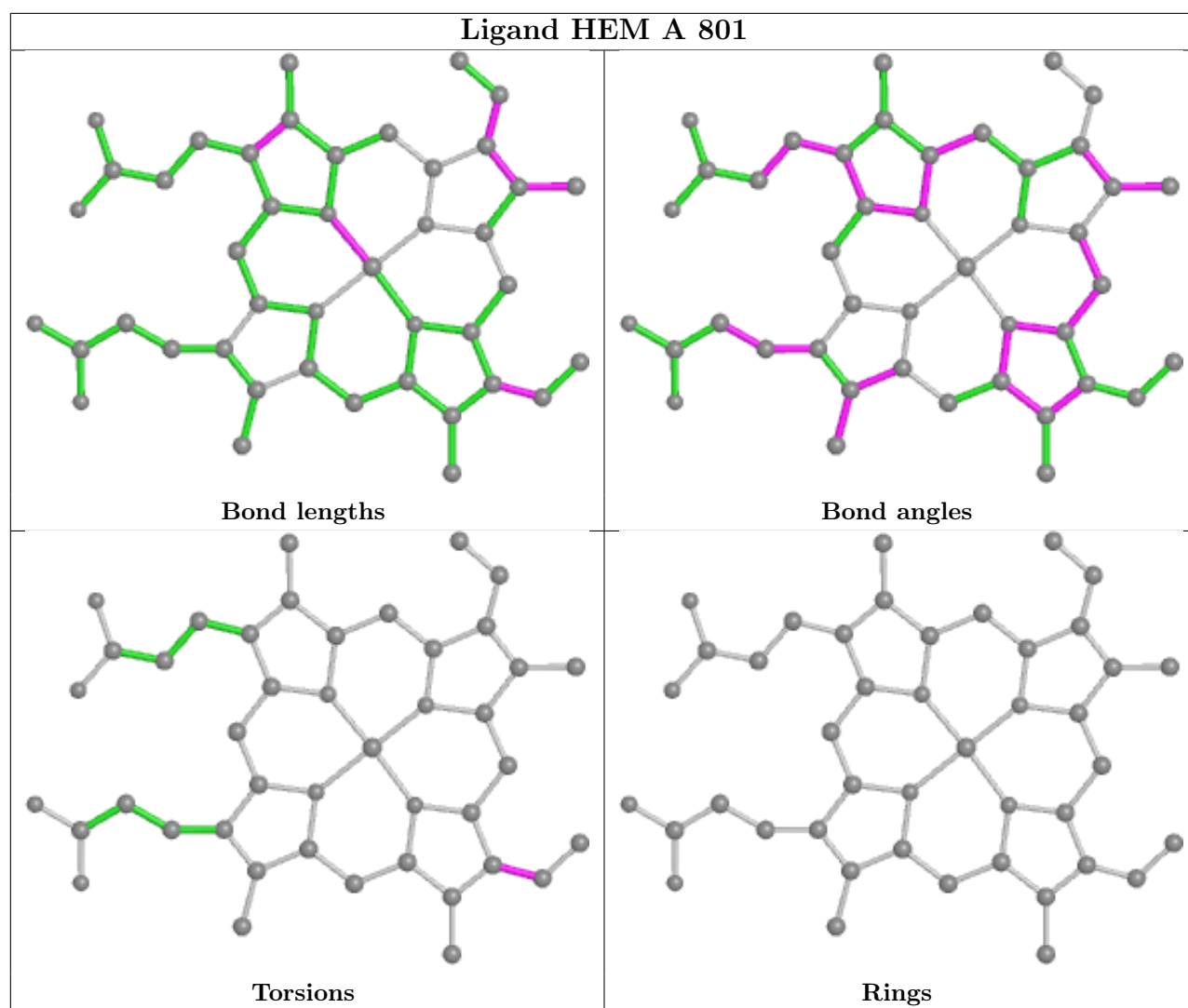
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	803	KMA	1	0
2	B	801	HEM	2	0
6	A	806	GOL	1	0
2	A	801	HEM	2	0
3	A	802	H4B	1	0

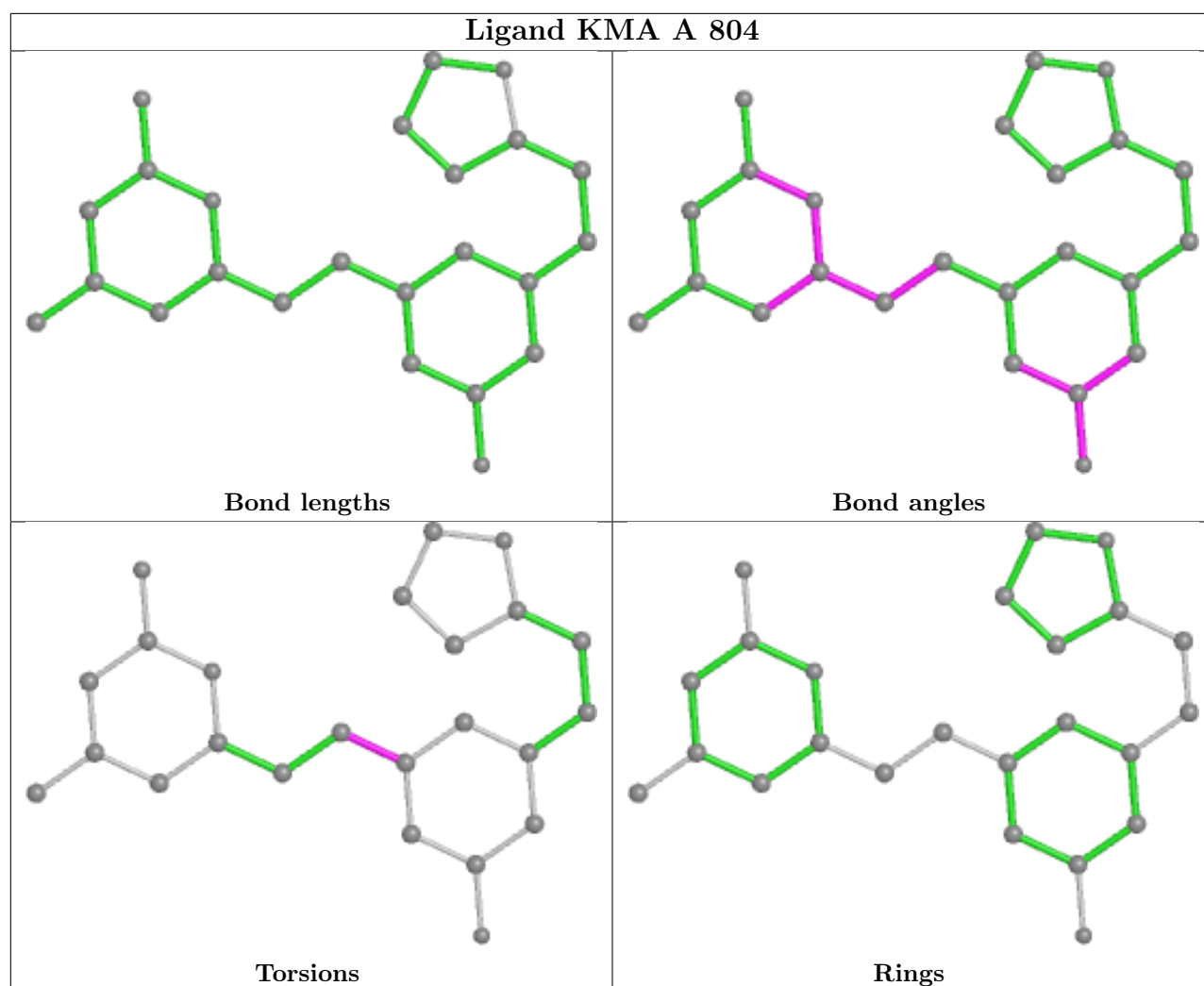
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	414/421 (98%)	0.57	48 (11%) 4 4	32, 47, 84, 146	0
1	B	410/421 (97%)	0.96	82 (20%) 1 0	35, 54, 102, 137	0
All	All	824/842 (97%)	0.76	130 (15%) 2 1	32, 50, 96, 146	0

All (130) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	721	TRP	9.4
1	B	720	VAL	7.9
1	B	326	THR	6.3
1	A	302	CYS	6.3
1	B	357	ASP	6.0
1	A	353	VAL	5.8
1	B	682	VAL	5.5
1	B	683	TRP	5.4
1	B	716	TRP	5.4
1	B	360	PHE	5.4
1	B	685	VAL	5.3
1	A	352	ASP	5.0
1	A	685	VAL	5.0
1	A	696	PHE	5.0
1	B	396	THR	4.9
1	A	682	VAL	4.8
1	A	305	PHE	4.8
1	B	624	ARG	4.8
1	A	681	TRP	4.8
1	B	493	PRO	4.6
1	A	684	ILE	4.5
1	A	692	ILE	4.4
1	B	510	CYS	4.4
1	B	305	PHE	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	686	PRO	4.3
1	B	355	THR	4.2
1	B	496	SER	4.2
1	B	504	VAL	4.1
1	B	511	ILE	4.1
1	B	681	TRP	3.9
1	B	560	LYS	3.9
1	B	684	ILE	3.9
1	B	572	VAL	3.9
1	B	722	LYS	3.9
1	B	354	ALA	3.8
1	A	686	PRO	3.7
1	A	355	THR	3.6
1	B	688	MET	3.6
1	B	719	HIS	3.6
1	B	690	GLY	3.5
1	A	304	ARG	3.5
1	B	557	GLU	3.4
1	B	344	SER	3.4
1	B	474	LYS	3.4
1	A	687	PRO	3.4
1	B	571	ALA	3.2
1	B	359	LEU	3.2
1	B	687	PRO	3.2
1	A	624	ARG	3.2
1	B	358	GLN	3.1
1	A	327	LEU	3.1
1	B	492	GLN	3.1
1	B	421	VAL	3.1
1	B	495	GLY	3.1
1	A	689	SER	3.1
1	A	356	LYS	3.1
1	B	589	PHE	3.0
1	B	717	ASN	3.0
1	B	356	LYS	3.0
1	A	620	ASN	3.0
1	B	420	CYS	3.0
1	A	395	THR	3.0
1	A	303	PRO	2.9
1	B	304	ARG	2.9
1	B	709	PHE	2.9
1	A	421	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	376	ARG	2.8
1	A	690	GLY	2.8
1	A	688	MET	2.8
1	A	683	TRP	2.8
1	B	327	LEU	2.8
1	B	508	GLU	2.7
1	B	689	SER	2.7
1	B	472	ASP	2.7
1	A	520	GLY	2.7
1	B	490	TYR	2.7
1	B	505	GLN	2.7
1	B	596	THR	2.7
1	B	718	THR	2.7
1	B	394	ASP	2.7
1	A	572	VAL	2.7
1	B	491	LYS	2.7
1	B	715	PRO	2.7
1	A	360	PHE	2.6
1	A	334	TYR	2.6
1	A	700	MET	2.6
1	A	559	PHE	2.6
1	B	509	ILE	2.6
1	B	598	ILE	2.6
1	B	498	LEU	2.6
1	B	635	LEU	2.6
1	B	497	THR	2.5
1	B	516	LYS	2.5
1	B	320	THR	2.5
1	B	621	LEU	2.5
1	A	396	THR	2.5
1	B	464	ILE	2.5
1	B	696	PHE	2.5
1	B	316	VAL	2.5
1	B	512	GLN	2.5
1	A	354	ALA	2.4
1	B	395	THR	2.4
1	B	419	ARG	2.4
1	A	357	ASP	2.4
1	B	494	ASP	2.4
1	A	358	GLN	2.4
1	A	420	CYS	2.4
1	A	556	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	386	LEU	2.3
1	B	522	PHE	2.3
1	A	521	ARG	2.2
1	A	596	THR	2.2
1	A	464	ILE	2.2
1	B	638	ILE	2.2
1	B	625	LYS	2.2
1	B	692	ILE	2.2
1	A	555	LYS	2.1
1	A	695	VAL	2.1
1	B	475	HIS	2.1
1	A	447	ILE	2.1
1	B	622	ASP	2.1
1	B	397	SER	2.1
1	B	623	MET	2.1
1	B	339	SER	2.1
1	A	359	LEU	2.1
1	A	498	LEU	2.1
1	A	394	ASP	2.0
1	A	600	VAL	2.0
1	A	414	TRP	2.0
1	B	620	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

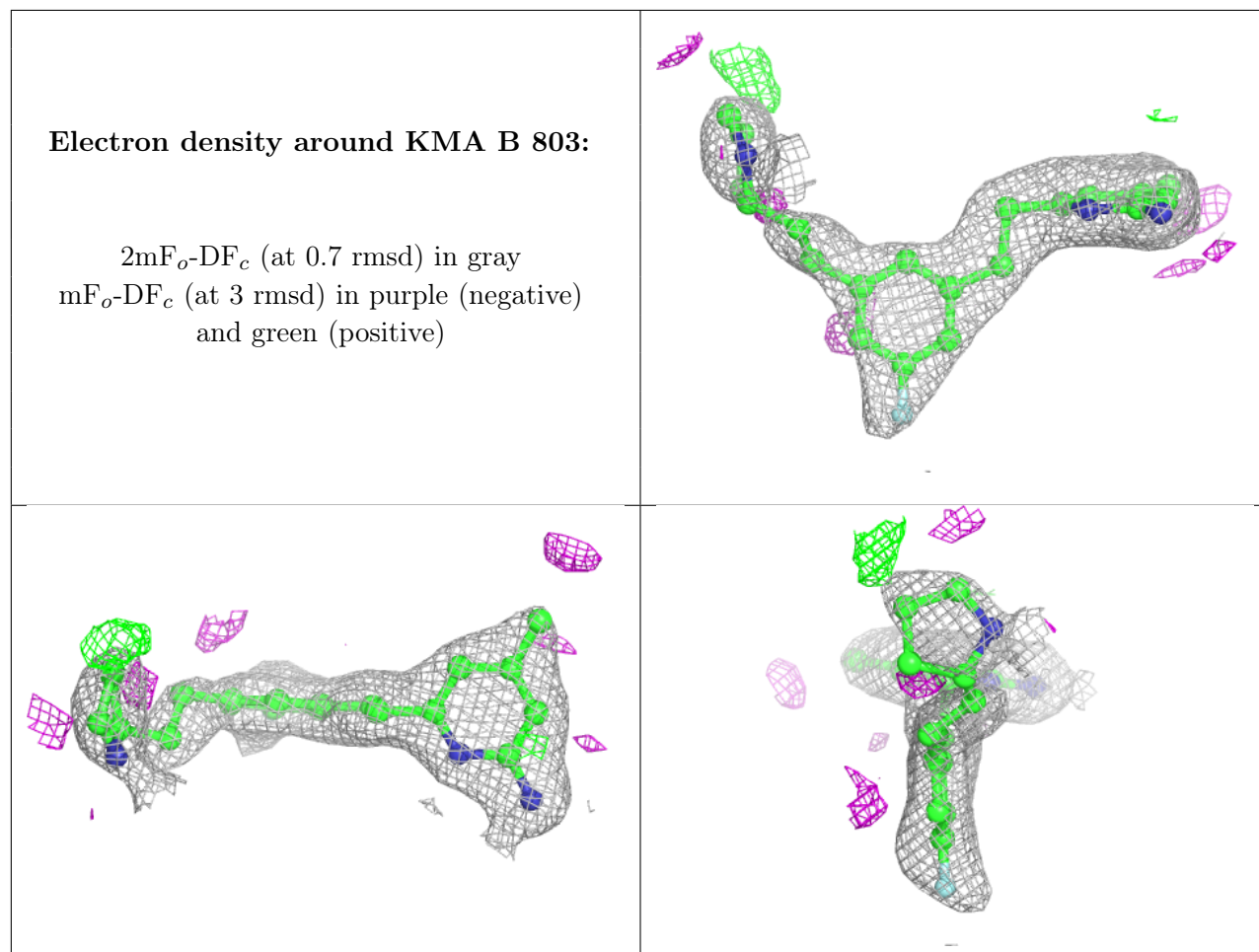
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	GOL	A	806	6/6	0.72	0.21	75,82,87,91	0

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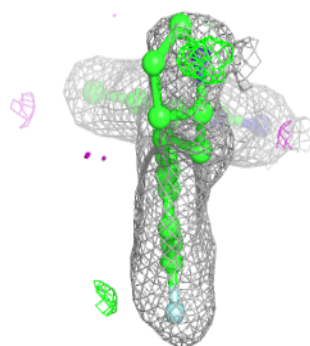
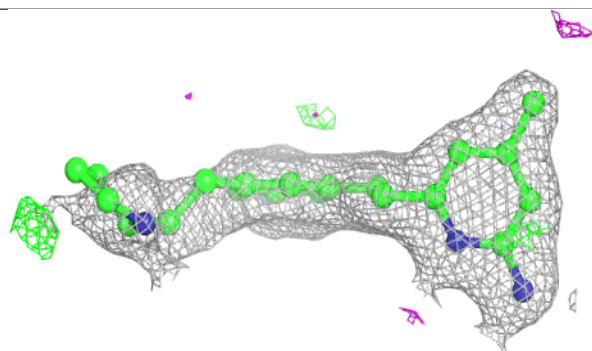
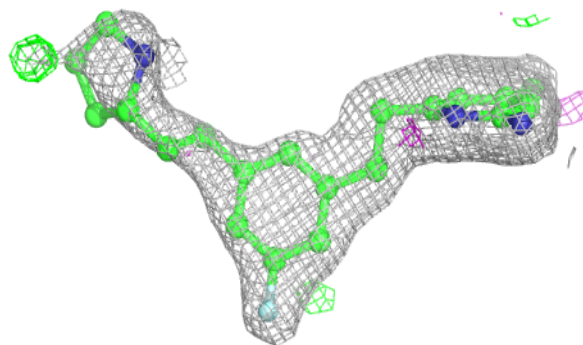
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	GOL	B	804	6/6	0.76	0.17	72,83,87,88	0
6	GOL	A	805	6/6	0.81	0.24	68,73,77,78	0
5	KMA	B	803	24/24	0.92	0.25	35,71,88,93	0
5	KMA	A	804	24/24	0.93	0.20	33,62,91,94	0
3	H4B	B	802	17/17	0.96	0.18	39,44,52,57	0
3	H4B	A	802	17/17	0.97	0.15	34,39,43,45	0
2	HEM	B	801	43/43	0.98	0.19	31,41,53,57	0
2	HEM	A	801	43/43	0.98	0.18	29,36,45,47	0
4	ZN	A	803	1/1	0.99	0.10	41,41,41,41	0

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

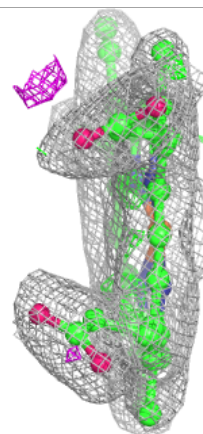
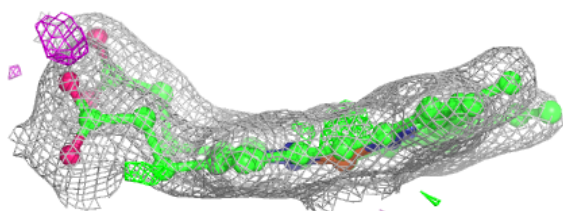
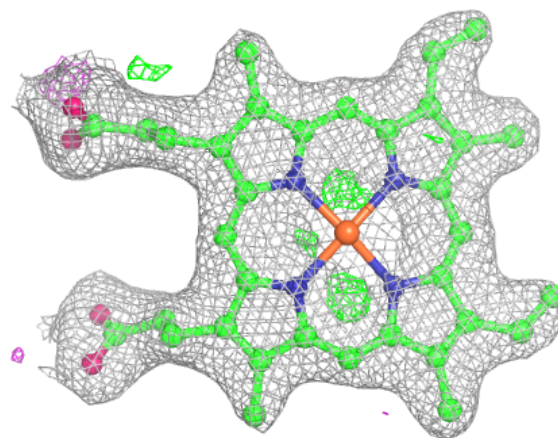


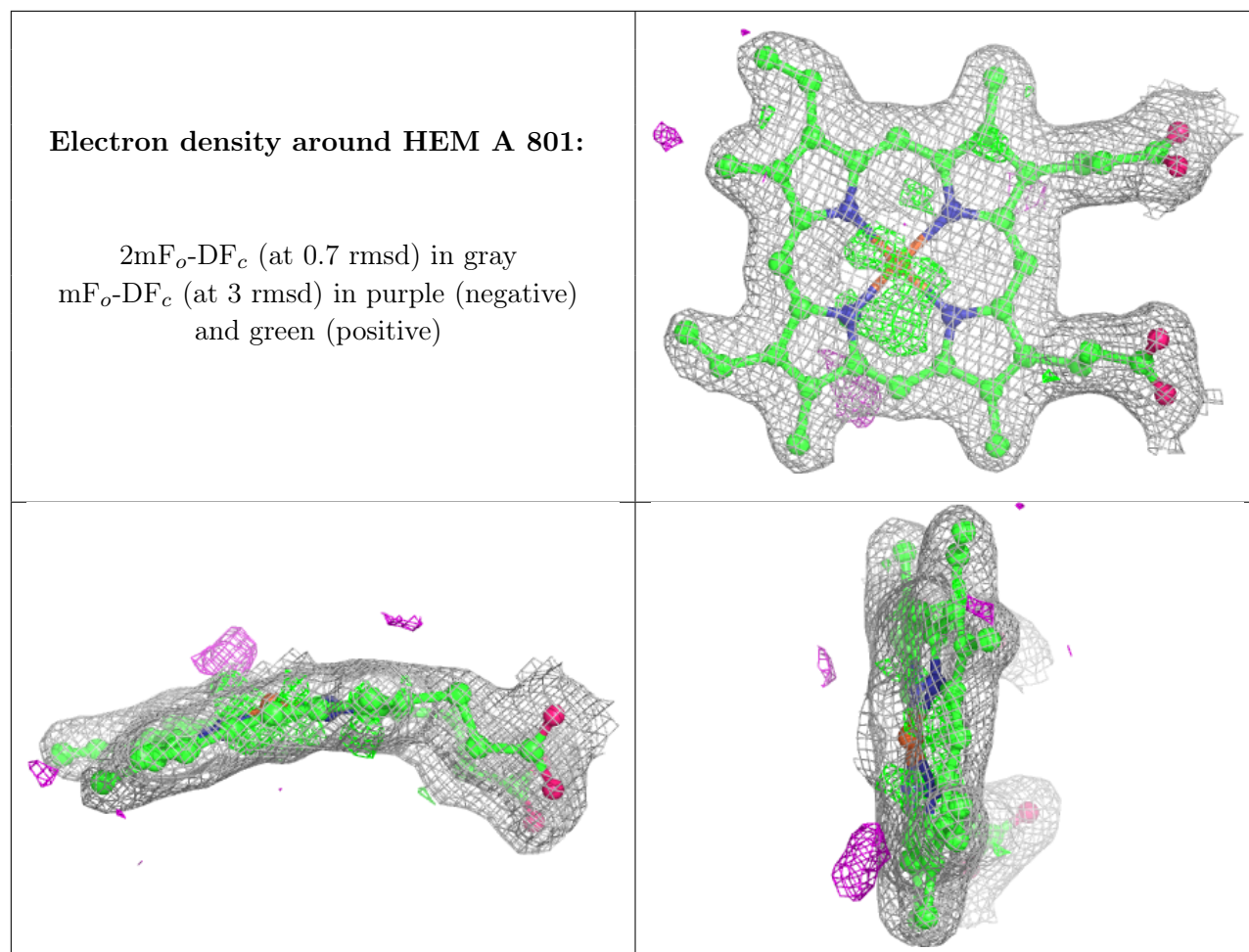
Electron density around KMA A 804:

$2mF_o-DF_c$ (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)





6.5 Other polymers [i](#)

There are no such residues in this entry.