



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:03 PM UTC

PDB ID : 7DVO / pdb_00007dvo
Title : Structure of Reaction Intermediate of Cytochrome P450 NO Reductase (P450nor) Determined by XFEL
Authors : Nomura, T.; Kimura, T.; Kanematsu, Y.; Yamashita, K.; Hirata, K.; Ueno, G.; Murakami, H.; Hisano, T.; Yamagiwa, R.; Takeda, H.; Gopalasingam, C.; Yuki, K.; Kousaka, R.; Yanagasawa, S.; Shoji, O.; Kumasaka, T.; Takano, Y.; Ago, H.; Yamamoto, M.; Sugimoto, H.; Tosha, T.; Kubo, M.; Shiro, Y.
Deposited on : 2021-01-14
Resolution : 1.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

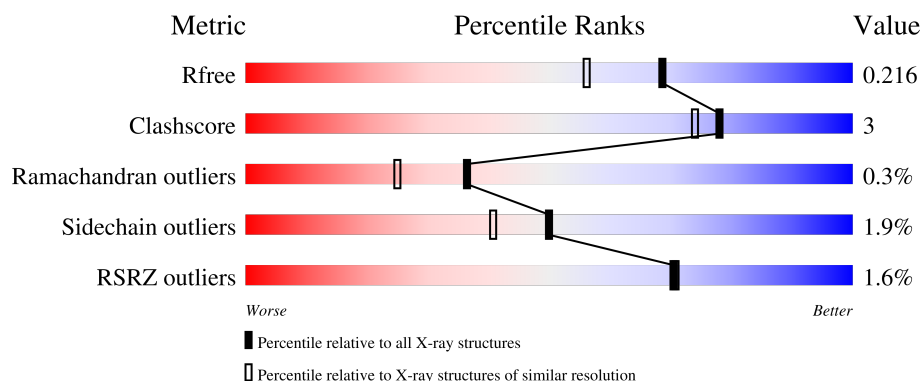
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

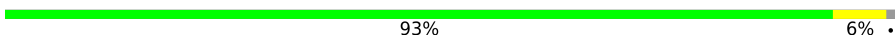
The reported resolution of this entry is 1.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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

Mol	Chain	Length	Quality of chain
1	A	403	 93% 6% .
1	B	403	 3% 90% 7% ..

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6969 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 NADP nitrous oxide-forming nitric oxide reductase.

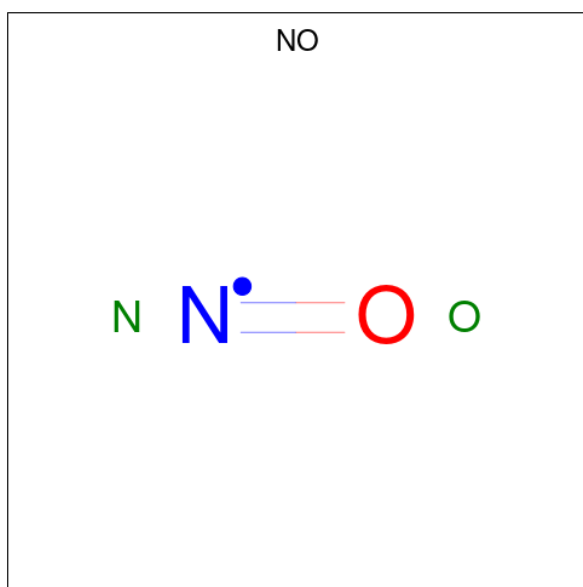
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	399	Total	C	N	O	S	0	6	0
			3133	1993	537	589	14			
1	B	399	Total	C	N	O	S	0	2	0
			3108	1977	530	587	14			

- 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	C	Fe	N	O	0	1
			48	34	2	8	4		
2	B	1	Total	C	Fe	N	O	0	1
			48	34	2	8	4		

- Molecule 3 is NITRIC OXIDE (CCD ID: NO) (formula: NO) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	N	O	0	1
			2	1	1		
3	B	1	Total	N	O	0	1
			2	1	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

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

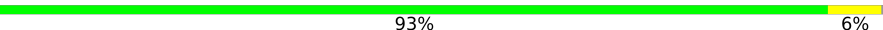
- Molecule 5 is water.

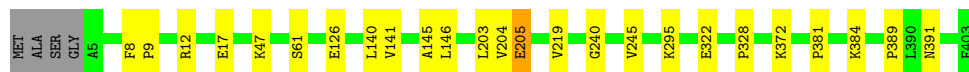
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	303	Total	O	0	3
			303	303		
5	B	289	Total	O	0	2
			289	289		

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.

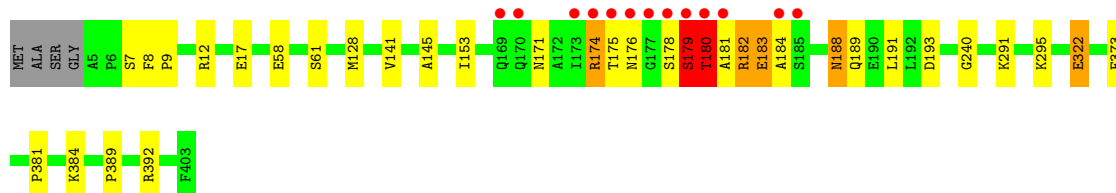
- Molecule 1: NADP nitrous oxide-forming nitric oxide reductase

Chain A:  93% 6% .



- Molecule 1: NADP nitrous oxide-forming nitric oxide reductase

Chain B:  3% 90% 7% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.27Å 101.61Å 73.19Å 90.00° 92.71° 90.00°	Depositor
Resolution (Å)	19.78 – 1.80 19.78 – 1.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.78-1.80) 99.9 (19.78-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 1.80Å)	Xtriage
Refinement program	PHENIX 1.18.2	Depositor
R, R_{free}	0.173 , 0.219 0.173 , 0.216	Depositor DCC
R_{free} test set	3678 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	22.8	Xtriage
Anisotropy	0.461	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 54.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.084 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6969	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, HEM, NO

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	0.29	0/3218	0.46	0/4371
1	B	0.28	0/3181	0.48	0/4323
All	All	0.28	0/6399	0.47	0/8694

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

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	3133	0	3166	13	0
1	B	3108	0	3127	21	0
2	A	48	0	0	0	0
2	B	48	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	18	0	24	0	0
4	B	18	0	24	0	0
5	A	303	0	0	0	0
5	B	289	0	0	3	0
All	All	6969	0	6341	34	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 3.

All (34) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:ARG:NH1	5:B:601:HOH:O	2.23	0.72
1:B:179:SER:HB3	1:B:183:GLU:HB2	1.74	0.70
1:B:141:VAL:HA	1:B:145:ALA:HB3	1.79	0.64
1:B:180:THR:HG22	1:B:181:ALA:N	2.18	0.58
1:B:381:PRO:HD2	1:B:384:LYS:HE2	1.89	0.55
1:B:322:GLU:H	1:B:322:GLU:CD	2.15	0.55
1:A:141:VAL:HA	1:A:145:ALA:HB3	1.89	0.54
1:B:171:ASN:HB3	5:B:830:HOH:O	2.06	0.54
1:B:184:ALA:O	1:B:188:ASN:HB2	2.08	0.54
1:B:189:GLN:NE2	1:B:193:ASP:OD1	2.39	0.54
1:B:61:SER:HB2	1:B:295:LYS:HD2	1.91	0.52
1:B:8:PHE:CG	1:B:9:PRO:HA	2.47	0.49
1:A:126:GLU:OE1	1:A:372:LYS:NZ	2.41	0.48
1:A:322:GLU:H	1:A:322:GLU:CD	2.22	0.48
1:A:381:PRO:HG2	1:A:384:LYS:HD3	1.95	0.48
1:B:58:GLU:H	1:B:58:GLU:CD	2.22	0.47
1:B:389:PRO:HG2	1:B:392:ARG:HD2	1.97	0.47
1:B:291:LYS:NZ	5:B:612:HOH:O	2.48	0.46
1:B:174:ARG:NE	1:B:188:ASN:OD1	2.32	0.46
1:A:12:ARG:HB3	1:A:17:GLU:O	2.16	0.45
1:A:61:SER:HB2	1:A:295:LYS:HD2	1.99	0.45
1:B:128:MET:HE2	1:B:373:PHE:CE2	2.51	0.45
1:A:204:VAL:HG12	1:A:205:GLU:HG2	1.98	0.45
1:B:178:SER:O	1:B:179:SER:HB2	2.18	0.44
1:B:174:ARG:HD2	1:B:191:LEU:HD12	2.00	0.43
1:B:12:ARG:HB3	1:B:17:GLU:O	2.20	0.42
1:A:322:GLU:HG3	1:A:328:PRO:HG3	2.02	0.42
1:A:8:PHE:CG	1:A:9:PRO:HA	2.54	0.41
1:A:389:PRO:HB2	1:A:391:ASN:OD1	2.20	0.41
1:A:146:LEU:HA	1:A:245:VAL:HG22	2.03	0.40
1:A:203:LEU:HD21	1:A:219:VAL:HG11	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	403/403 (100%)	396 (98%)	7 (2%)	0	100	100
1	B	399/403 (99%)	388 (97%)	9 (2%)	2 (0%)	24	14
All	All	802/806 (100%)	784 (98%)	16 (2%)	2 (0%)	36	31

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	179	SER
1	B	180	THR

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	346/342 (101%)	343 (99%)	3 (1%)	70	67
1	B	342/342 (100%)	332 (97%)	10 (3%)	37	25
All	All	688/684 (101%)	675 (98%)	13 (2%)	50	41

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	LYS
1	A	140	LEU
1	A	205	GLU
1	B	7	SER

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Mol	Chain	Res	Type
1	B	174	ARG
1	B	175	THR
1	B	176	ASN
1	B	179	SER
1	B	180	THR
1	B	182	ARG
1	B	183	GLU
1	B	188	ASN
1	B	322	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	241	ASN
1	A	264	GLN
1	A	327	ASN
1	A	334	ASN
1	B	114	GLN
1	B	127	GLN
1	B	162	ASN
1	B	201	GLN
1	B	241	ASN
1	B	264	GLN
1	B	334	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	A	503[B]	-	5,5,5	1.15	1 (20%)	5,5,5	0.88	0
2	HEM	A	501[B]	1,5	50,50,50	1.32	8 (16%)	67,82,82	1.21	9 (13%)
4	GOL	B	504	-	5,5,5	0.92	0	5,5,5	1.07	0
2	HEM	A	501[A]	3,1	50,50,50	1.35	8 (16%)	67,82,82	1.24	9 (13%)
4	GOL	A	504	-	5,5,5	1.00	0	5,5,5	0.95	0
4	GOL	B	503[B]	-	5,5,5	1.28	1 (20%)	5,5,5	0.82	0
4	GOL	B	505	-	5,5,5	0.92	0	5,5,5	0.83	0
3	NO	B	502[A]	2	0,1,1	-	-	-	-	-
2	HEM	B	501[B]	1,5	50,50,50	1.55	8 (16%)	67,82,82	1.06	7 (10%)
2	HEM	B	501[A]	3,1	50,50,50	1.54	8 (16%)	67,82,82	1.04	7 (10%)
4	GOL	A	505	-	5,5,5	0.84	0	5,5,5	0.97	0
3	NO	A	502[A]	2	0,1,1	-	-	-	-	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	503[B]	-	-	0/4/4/4	-
2	HEM	A	501[B]	1,5	-	2/14/54/54	-
4	GOL	B	504	-	-	0/4/4/4	-
2	HEM	A	501[A]	3,1	-	2/14/54/54	-
4	GOL	A	504	-	-	0/4/4/4	-
4	GOL	B	503[B]	-	-	0/4/4/4	-
4	GOL	B	505	-	-	2/4/4/4	-
2	HEM	B	501[B]	1,5	-	3/14/54/54	-
2	HEM	B	501[A]	3,1	-	3/14/54/54	-
4	GOL	A	505	-	-	2/4/4/4	-

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501[B]	HEM	FE-NC	4.37	2.09	1.95
2	B	501[A]	HEM	FE-NB	4.28	2.08	1.94
2	B	501[A]	HEM	FE-NC	4.27	2.09	1.95
2	B	501[B]	HEM	FE-NB	4.09	2.07	1.94
2	A	501[A]	HEM	FE-NB	3.46	2.05	1.94
2	A	501[A]	HEM	FE-NC	3.29	2.06	1.95
2	A	501[B]	HEM	FE-NC	3.25	2.05	1.95
2	B	501[A]	HEM	CAC-C3C	3.19	1.55	1.47
2	B	501[B]	HEM	CAC-C3C	3.19	1.55	1.47
2	B	501[A]	HEM	CMB-C2B	2.97	1.56	1.50
2	B	501[B]	HEM	CMB-C2B	2.97	1.56	1.50
2	A	501[B]	HEM	FE-NB	2.91	2.03	1.94
2	A	501[A]	HEM	CAC-C3C	2.90	1.55	1.47
2	A	501[B]	HEM	CAC-C3C	2.90	1.55	1.47
2	A	501[A]	HEM	CMB-C2B	2.84	1.56	1.50
2	A	501[B]	HEM	CMB-C2B	2.84	1.56	1.50
2	B	501[A]	HEM	CMA-C3A	2.82	1.56	1.50
2	B	501[B]	HEM	CMA-C3A	2.82	1.56	1.50
2	B	501[A]	HEM	CAB-C3B	2.67	1.54	1.47
2	B	501[B]	HEM	CAB-C3B	2.67	1.54	1.47
2	A	501[A]	HEM	CAB-C3B	2.50	1.54	1.47
2	A	501[B]	HEM	CAB-C3B	2.50	1.54	1.47
2	A	501[A]	HEM	CAD-C3D	2.43	1.57	1.51
2	A	501[B]	HEM	CAD-C3D	2.43	1.57	1.51
2	A	501[A]	HEM	CMA-C3A	2.23	1.55	1.50
2	A	501[B]	HEM	CMA-C3A	2.23	1.55	1.50
2	B	501[A]	HEM	CMD-C2D	2.16	1.55	1.50
2	B	501[B]	HEM	CMD-C2D	2.16	1.55	1.50
4	A	503[B]	GOL	C1-C2	2.16	1.60	1.51
4	B	503[B]	GOL	C3-C2	2.11	1.59	1.51
2	A	501[A]	HEM	CMD-C2D	2.05	1.55	1.50
2	A	501[B]	HEM	CMD-C2D	2.05	1.55	1.50
2	B	501[A]	HEM	CAA-C2A	2.02	1.56	1.51
2	B	501[B]	HEM	CAA-C2A	2.02	1.56	1.51

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501[B]	HEM	C1B-NB-C4B	2.73	108.44	105.21
2	A	501[A]	HEM	CBA-CAA-C2A	-2.67	105.14	112.53
2	A	501[B]	HEM	CBA-CAA-C2A	-2.67	105.14	112.53
2	B	501[B]	HEM	C3B-C4B-NB	-2.56	107.63	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501[A]	HEM	C3B-C4B-NB	-2.55	107.63	109.47
2	A	501[A]	HEM	C4B-C3B-C2B	2.50	109.58	107.28
2	A	501[B]	HEM	C4B-C3B-C2B	2.50	109.58	107.28
2	B	501[B]	HEM	CHC-C4B-NB	2.42	127.03	124.42
2	A	501[A]	HEM	O2D-CGD-CBD	2.41	121.60	114.00
2	A	501[B]	HEM	O2D-CGD-CBD	2.41	121.60	114.00
2	B	501[A]	HEM	C1B-NB-C4B	2.39	108.04	105.21
2	B	501[A]	HEM	C3B-C4B-NB	-2.37	107.77	109.47
2	A	501[B]	HEM	C3B-C4B-NB	-2.31	107.81	109.47
2	B	501[A]	HEM	CBA-CAA-C2A	-2.30	106.17	112.53
2	B	501[B]	HEM	CBA-CAA-C2A	-2.30	106.17	112.53
2	B	501[A]	HEM	CHC-C4B-NB	2.29	126.89	124.42
2	A	501[A]	HEM	CHC-C4B-NB	2.24	126.84	124.42
2	A	501[A]	HEM	O1D-CGD-CBD	-2.23	116.03	123.09
2	A	501[B]	HEM	O1D-CGD-CBD	-2.23	116.03	123.09
2	A	501[A]	HEM	CMC-C2C-C1C	-2.19	120.87	124.73
2	A	501[B]	HEM	CMC-C2C-C1C	-2.19	120.87	124.73
2	A	501[A]	HEM	CHD-C1D-ND	2.18	126.77	124.42
2	B	501[A]	HEM	CHD-C1D-ND	2.18	126.77	124.42
2	A	501[B]	HEM	CHD-C1D-ND	2.13	126.71	124.42
2	A	501[A]	HEM	C1D-C2D-C3D	2.12	109.21	106.98
2	A	501[B]	HEM	C1D-C2D-C3D	2.12	109.21	106.98
2	B	501[B]	HEM	CHD-C1D-ND	2.11	126.70	124.42
2	A	501[B]	HEM	CHC-C4B-NB	2.08	126.66	124.42
2	B	501[A]	HEM	O2D-CGD-CBD	2.07	120.53	114.00
2	B	501[B]	HEM	O2D-CGD-CBD	2.07	120.53	114.00
2	B	501[A]	HEM	C4B-C3B-C2B	2.01	109.13	107.28
2	B	501[B]	HEM	C4B-C3B-C2B	2.01	109.13	107.28

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	505	GOL	O1-C1-C2-C3
4	A	505	GOL	O1-C1-C2-O2
4	A	505	GOL	O1-C1-C2-C3
4	B	505	GOL	O1-C1-C2-O2
2	A	501[A]	HEM	CAA-CBA-CGA-O1A
2	A	501[B]	HEM	CAA-CBA-CGA-O1A
2	B	501[A]	HEM	CAA-CBA-CGA-O1A
2	B	501[B]	HEM	CAA-CBA-CGA-O1A
2	A	501[A]	HEM	CAA-CBA-CGA-O2A

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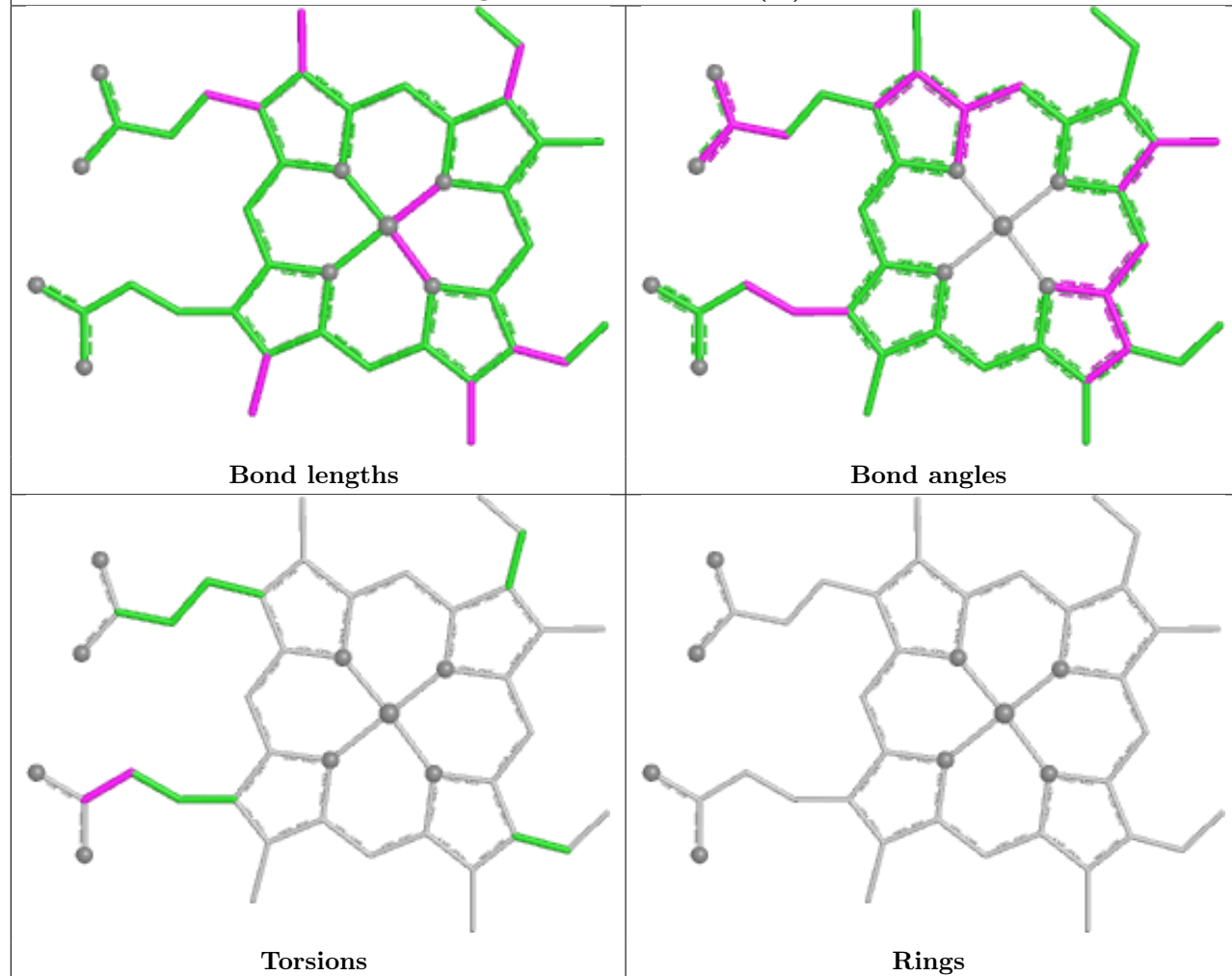
Mol	Chain	Res	Type	Atoms
2	A	501[B]	HEM	CAA-CBA-CGA-O2A
2	B	501[A]	HEM	CAA-CBA-CGA-O2A
2	B	501[B]	HEM	CAA-CBA-CGA-O2A
2	B	501[A]	HEM	CAD-CBD-CGD-O2D
2	B	501[B]	HEM	CAD-CBD-CGD-O2D

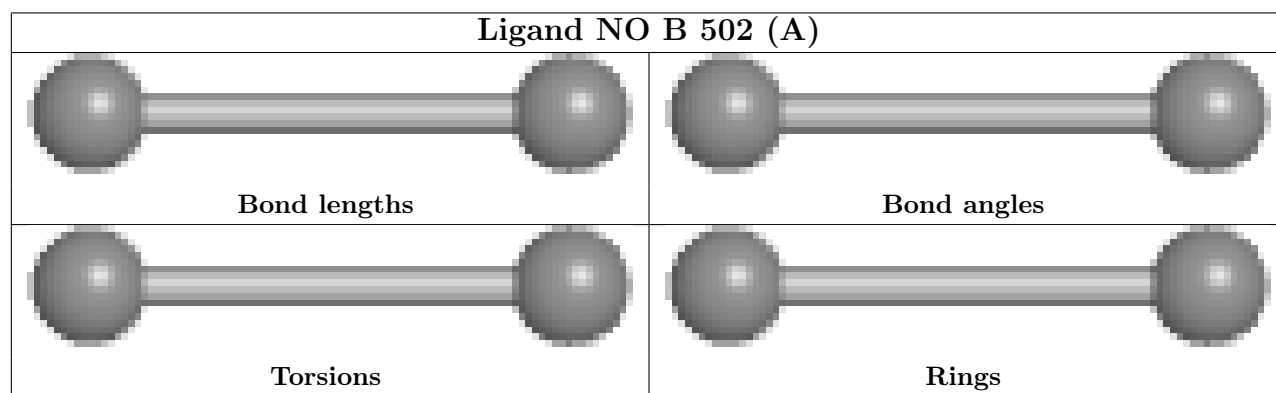
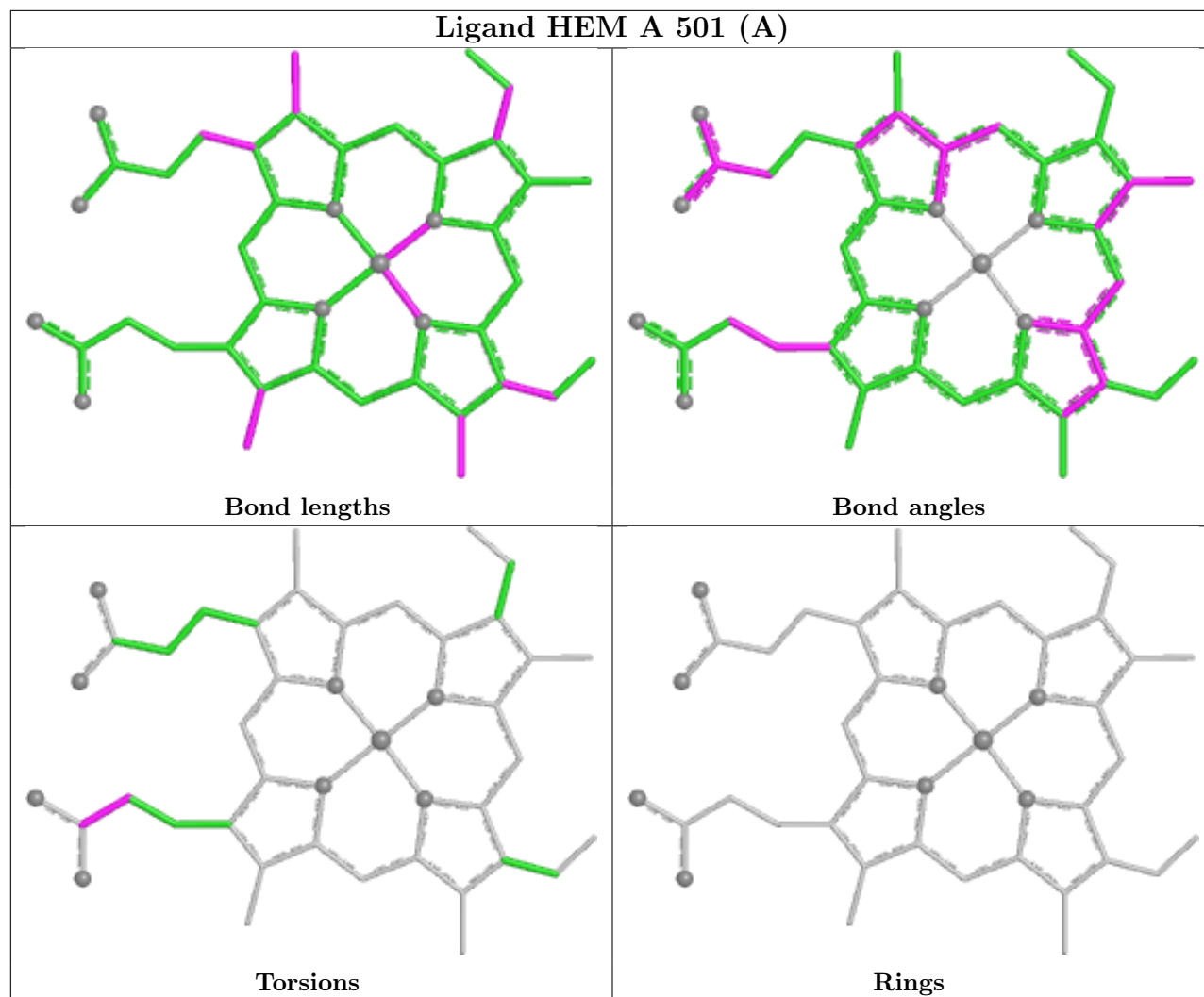
There are no ring outliers.

No monomer is involved in short contacts.

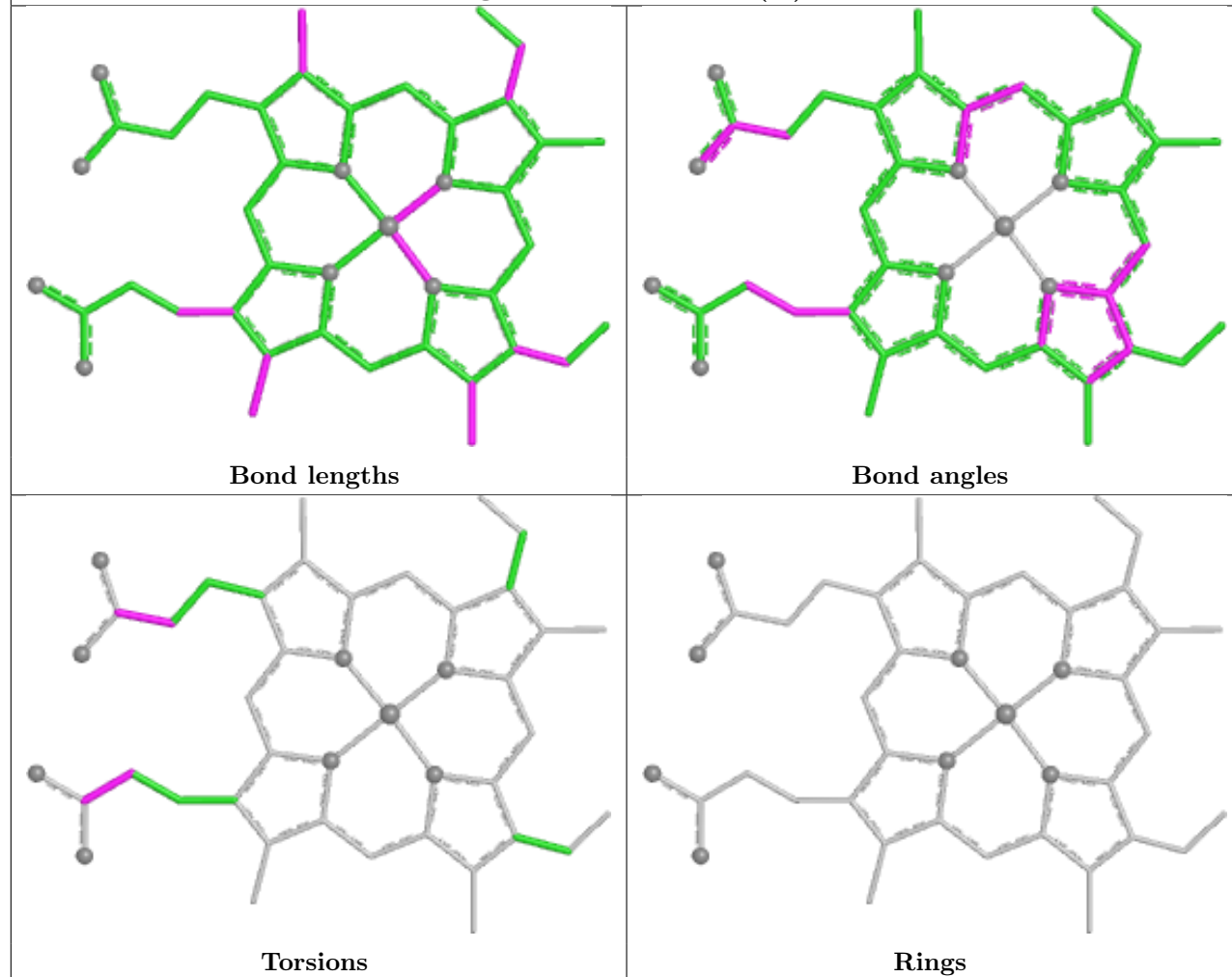
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

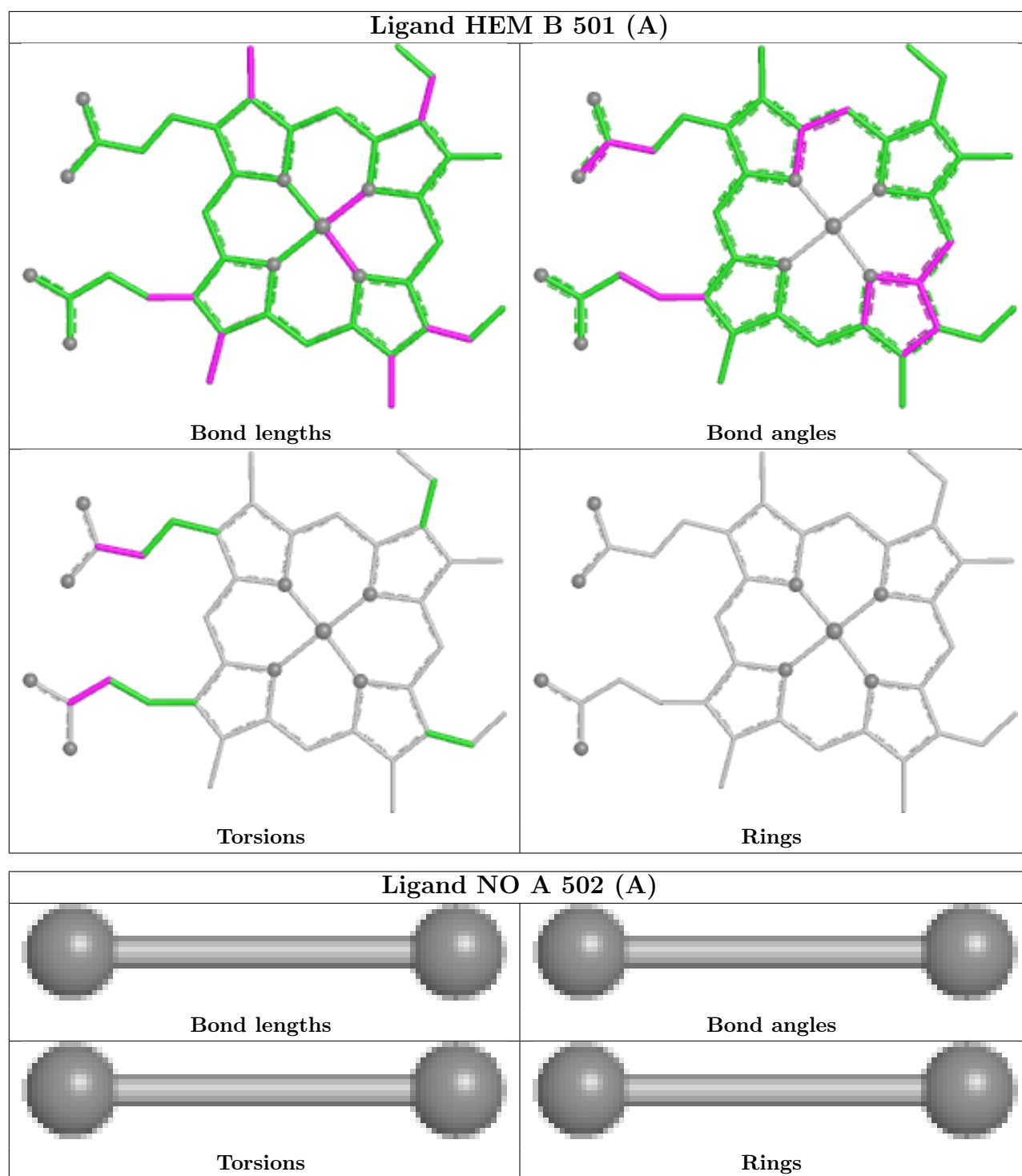
Ligand HEM A 501 (B)





Ligand HEM B 501 (B)





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	399/403 (99%)	-0.56	0 100 100	12, 23, 39, 62	6 (1%)
1	B	399/403 (99%)	-0.30	13 (3%) 49 49	13, 25, 55, 78	2 (0%)
All	All	798/806 (99%)	-0.43	13 (1%) 70 71	12, 24, 45, 78	8 (1%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	180	THR	4.5
1	B	177	GLY	4.1
1	B	175	THR	3.9
1	B	179	SER	3.5
1	B	184	ALA	3.3
1	B	178	SER	2.8
1	B	170	GLN	2.6
1	B	173	ILE	2.6
1	B	169	GLN	2.4
1	B	181	ALA	2.4
1	B	174	ARG	2.3
1	B	185	SER	2.2
1	B	176	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 oligosaccharides in this entry.

6.4 Ligands

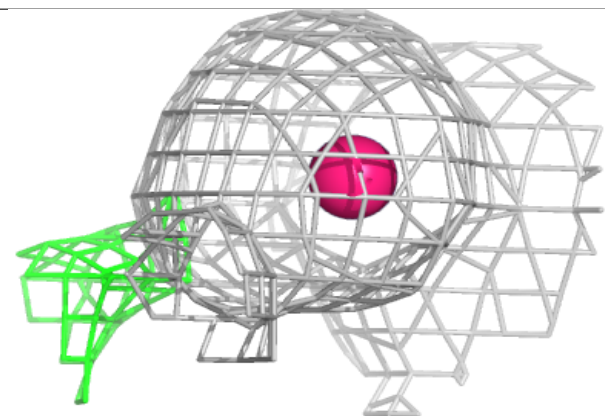
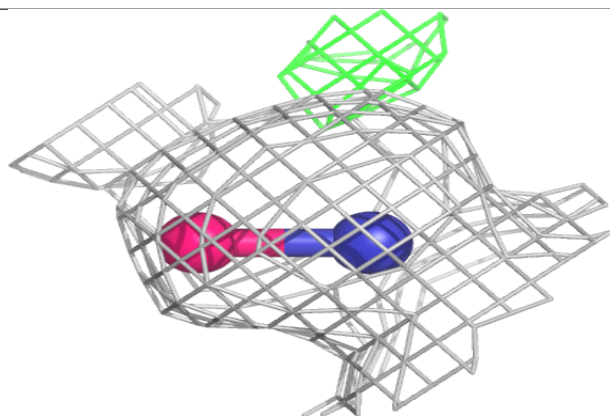
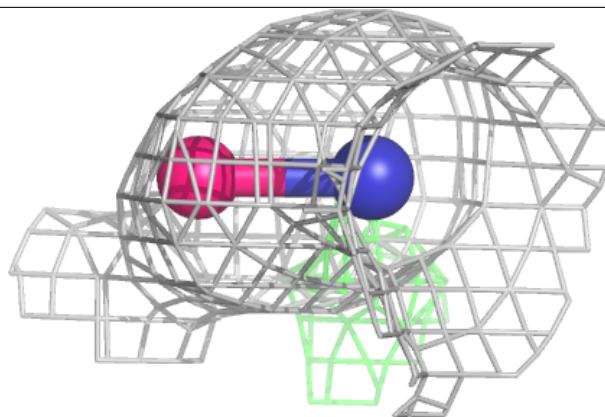
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	B	505	6/6	0.75	0.14	32,35,43,55	0
4	GOL	B	503[B]	6/6	0.82	0.25	18,22,24,29	6
4	GOL	A	505	6/6	0.84	0.10	30,38,43,43	0
4	GOL	A	503[B]	6/6	0.85	0.17	12,17,22,22	6
4	GOL	B	504	6/6	0.90	0.10	28,36,39,43	0
3	NO	B	502[A]	2/2	0.91	0.14	20,20,20,22	2
3	NO	A	502[A]	2/2	0.92	0.14	16,16,16,20	2
4	GOL	A	504	6/6	0.94	0.09	24,33,37,40	0
2	HEM	B	501[A]	43/43	0.96	0.05	16,19,23,32	5
2	HEM	B	501[B]	43/43	0.96	0.05	16,19,23,32	5
2	HEM	A	501[A]	43/43	0.97	0.05	13,17,20,25	5
2	HEM	A	501[B]	43/43	0.97	0.05	13,17,20,25	5

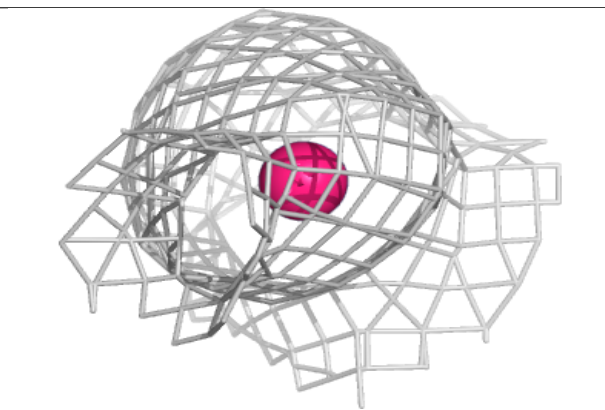
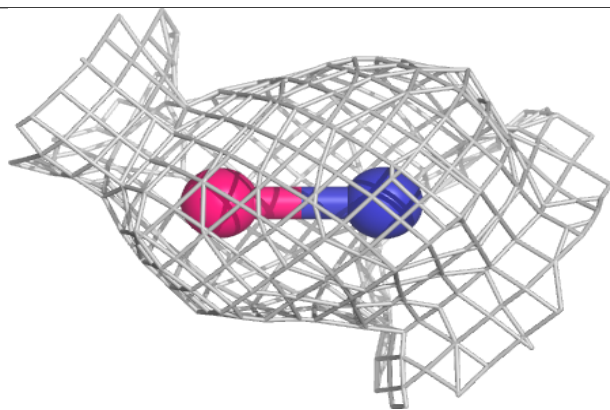
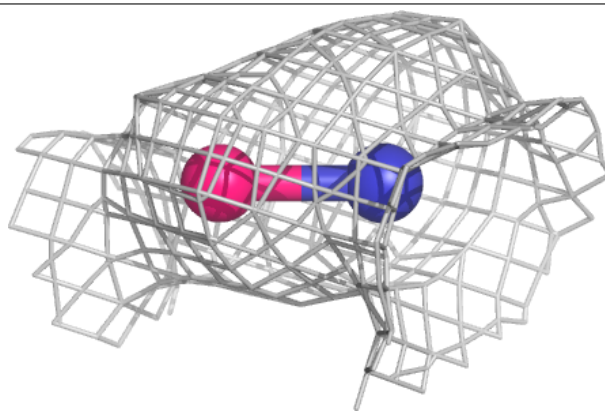
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NO B 502 (A):

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

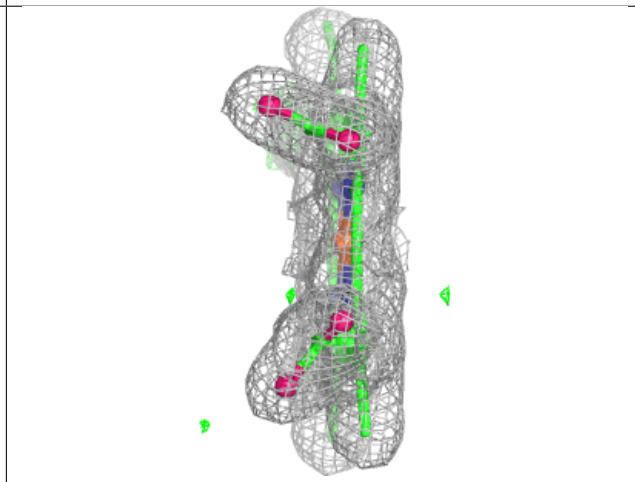
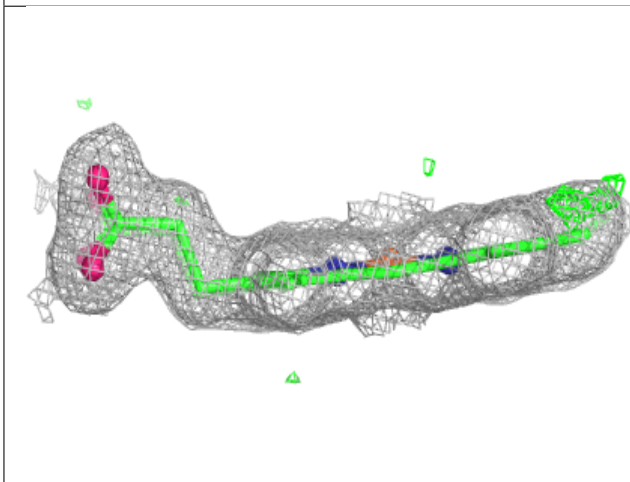
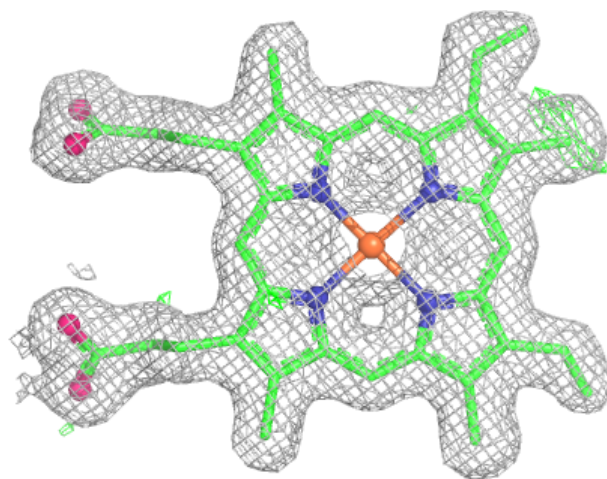
**Electron density around NO A 502 (A):**

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



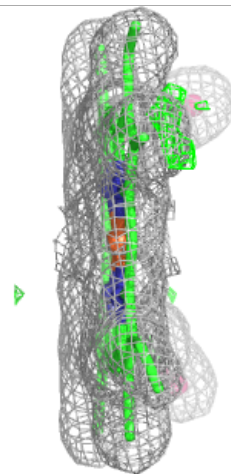
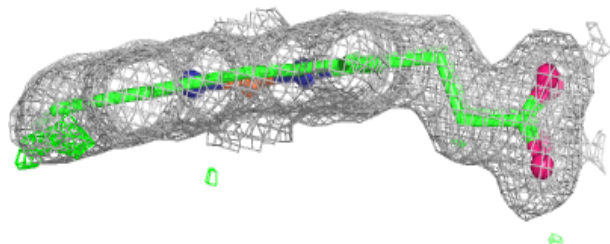
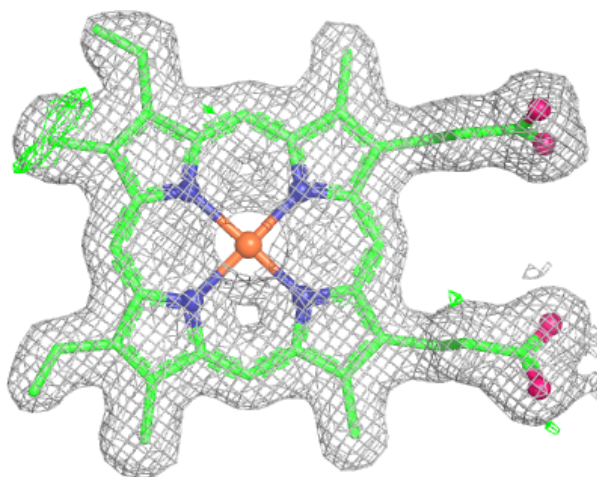
Electron density around HEM B 501 (A):

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



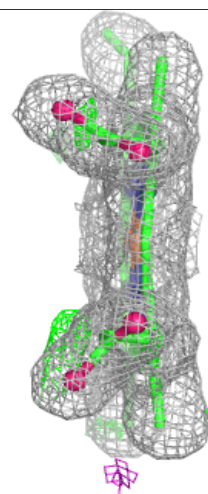
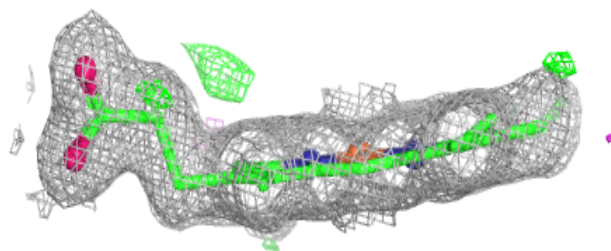
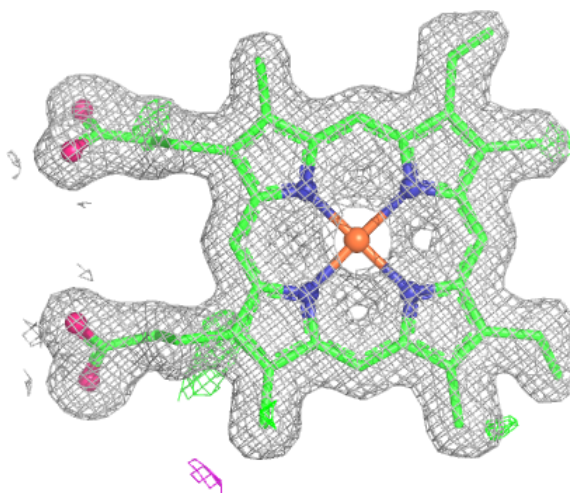
Electron density around HEM B 501 (B):

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



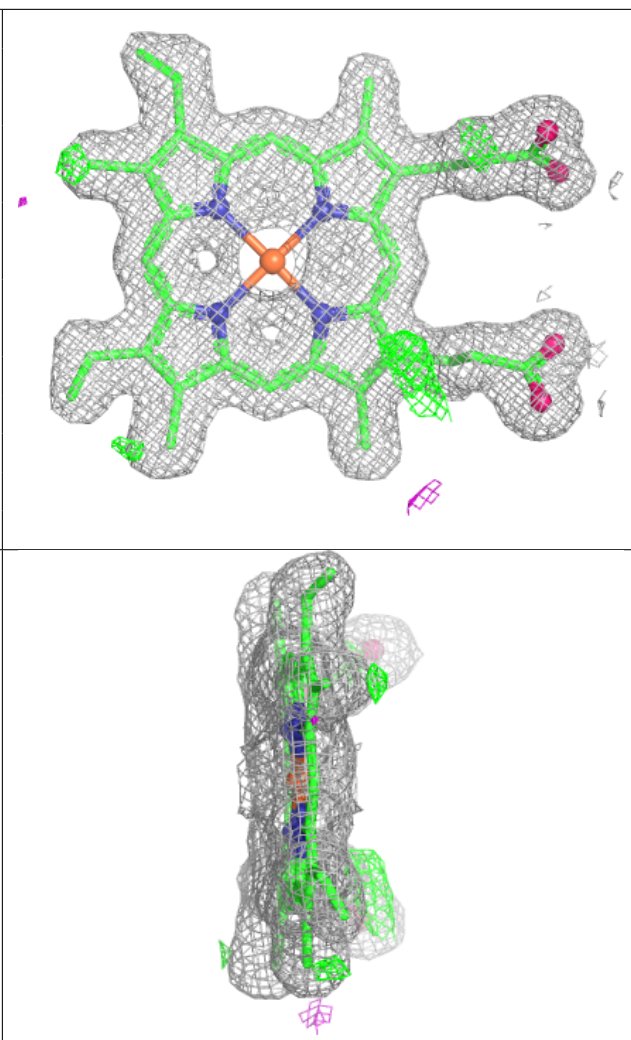
Electron density around HEM A 501 (A):

$2mF_o-DF_c$ (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 (B):

$2mF_o-DF_c$ (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.