WORLDWIDE PDB

PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Sep 10, 2023 – 02:57 PM EDT

PDB ID	:	4JSM
Title	:	Structure of bovine endothelial nitric oxide synthase heme domain in complex with 6-(((5-(((3-fluorophenethyl)amino)methyl)pyridin-3-yl)oxy)methyl)-4-m ethylpyridin-2-amine
Authors	:	Li, H.; Poulos, T.L.
Deposited on	:	2013-03-22
Resolution	:	2.25 Å(reported)

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

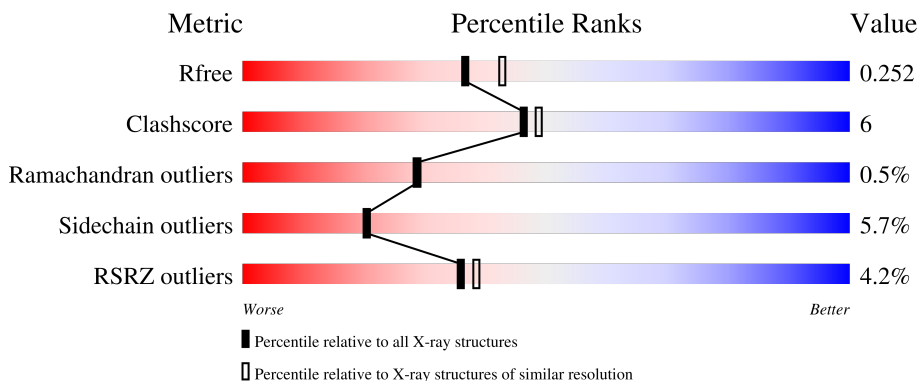|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	Percentile Ranks	Value
Rfree		0.252
Clashscore		6
Ramachandran outliers		0.5%
Sidechain outliers		5.7%
RSRZ outliers		4.2%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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 <=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	443	5% / 77% / 13% / 8%
1	B	443	3% / 74% / 16% / 9%

2 Entry composition ⓘ

There are 8 unique types of molecules in this entry. The entry contains 6900 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	406	Total	As	C	N	O	S	0	0	0
			3232	1	2055	570	590	16			
1	B	405	Total	As	C	N	O	S	0	0	0
			3229	1	2054	569	589	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	ARG	CYS	conflict	UNP P29473
B	100	ARG	CYS	conflict	UNP P29473

- 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	C	Fe	N	O	0	0
			43	34	1	4	4		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
2	B	1	43	34	1	4	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
			Total	C	N	O		
3	A	1	17	9	5	3	0	0
3	B	1	17	9	5	3	0	0

- Molecule 4 is 6-({[5-({[2-(3-fluorophenyl)ethyl]amino}methyl)pyridin-3-yl]oxy}methyl)-4-methylpyridin-2-amine (three-letter code: QJ7) (formula: $C_{21}H_{23}FN_4O$).

QJ7
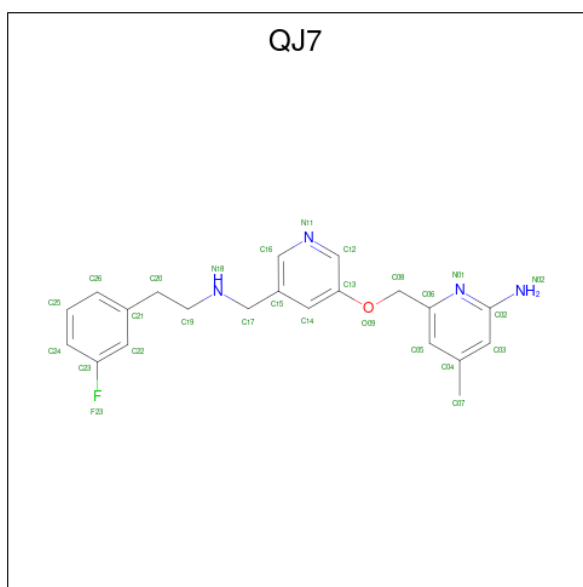
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	0	0
			27	21	1	4	1		
4	B	1	Total	C	F	N	O	0	0
			27	21	1	4	1		

• Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).

ACT

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

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

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

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	127	Total 127	O 127	0	0
8	B	117	Total 117	O 117	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.
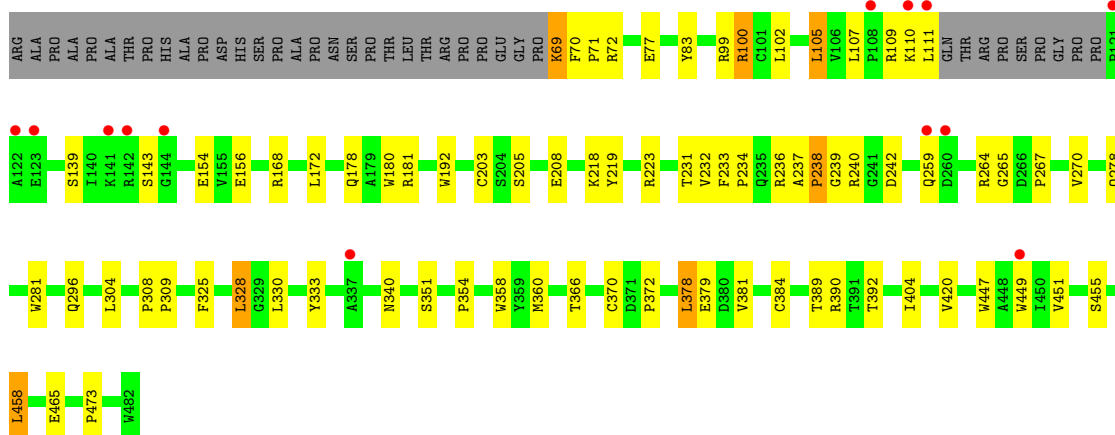
• Molecule 1: Nitric oxide synthase, endothelial
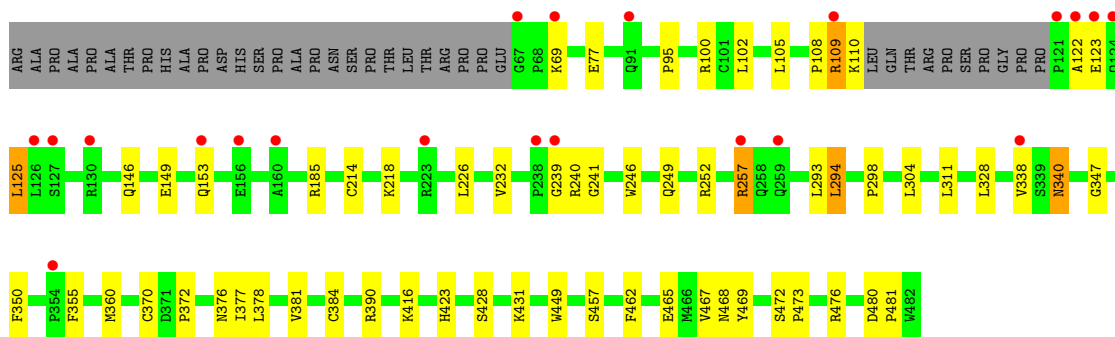
• Molecule 1: Nitric oxide synthase, endothelial

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	58.28Å 106.44Å 157.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.13 – 2.25 39.30 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.5 (38.13-2.25) 99.5 (39.30-2.25)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$<I/\sigma(I)>$ [1]	2.25 (at 2.24Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.187 , 0.244 0.200 , 0.252	Depositor DCC
R_{free} test set	2334 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	39.8	Xtriage
Anisotropy	0.603	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 43.5	EDS
L-test for twinning[2]	$<|L|> = 0.49, <L^2> = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6900	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $<|L|>$, $<L^2>$ 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: ACT, QJ7, HEM, GOL, H4B, ZN, CAS

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	0.76	1/3312 (0.0%)	0.76	1/4508 (0.0%)
1	B	0.78	2/3308 (0.1%)	0.77	0/4502
All	All	0.77	3/6620 (0.0%)	0.77	1/9010 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	333	TYR	CD2-CE2	6.76	1.49	1.39
1	B	203	CYS	CB-SG	-6.71	1.70	1.82
1	A	428	SER	CB-OG	5.11	1.48	1.42

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	304	LEU	CA-CB-CG	5.03	126.88	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	239	GLY	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3232	0	3140	39	0
1	B	3229	0	3141	44	0
2	A	43	0	30	2	0
2	B	43	0	30	3	0
3	A	17	0	15	1	0
3	B	17	0	15	1	0
4	A	27	0	23	2	0
4	B	27	0	23	1	0
5	A	4	0	3	0	0
5	B	4	0	3	0	0
6	A	6	0	8	0	0
6	B	6	0	8	1	0
7	A	1	0	0	0	0
8	A	127	0	0	5	0
8	B	117	0	0	3	0
All	All	6900	0	6439	82	0

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

The worst 5 of 82 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:384:CAS:SG	1:B:384:CAS:AS	2.51	1.29
1:A:384:CAS:SG	1:A:384:CAS:AS	2.53	1.26
1:B:236:ARG:HD3	1:B:351:SER:HB3	1.67	0.74
1:A:257:ARG:HG3	1:A:257:ARG:HH11	1.58	0.68
1:B:236:ARG:HD2	1:B:242:ASP:OD1	1.94	0.67

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	401/443 (90%)	387 (96%)	12 (3%)	2 (0%)	29	29
1	B	400/443 (90%)	384 (96%)	14 (4%)	2 (0%)	29	29
All	All	801/886 (90%)	771 (96%)	26 (3%)	4 (0%)	29	29

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	109	ARG
1	A	122	ALA
1	B	328	LEU
1	B	238	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	344/375 (92%)	326 (95%)	18 (5%)	23	24
1	B	344/375 (92%)	323 (94%)	21 (6%)	18	18
All	All	688/750 (92%)	649 (94%)	39 (6%)	20	20

5 of 39 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	240	ARG
1	B	378	LEU

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Mol	Chain	Res	Type
1	B	264	ARG
1	B	296	GLN
1	B	389	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	222	ASN
1	B	225	ASN
1	B	405	ASN
1	B	340	ASN
1	A	376	ASN

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	#$|Z| > 2$
1	CAS	A	384	1	5,8,9	1.32	0	1,9,11	0.53	0
1	CAS	B	384	1	5,8,9	1.22	0	1,9,11	0.23	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
1	CAS	A	384	1	-	0/0/7/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CAS	B	384	1	-	0/0/7/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	384	CAS	2	0
1	B	384	CAS	2	0

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
3	H4B	A	502	-	16,18,18	1.14	2 (12%)	11,26,26	3.19	7 (63%)
3	H4B	B	502	-	16,18,18	1.05	1 (6%)	11,26,26	3.06	7 (63%)
4	QJ7	B	505	-	29,29,29	0.91	3 (10%)	37,38,38	1.75	8 (21%)
5	ACT	B	503	-	3,3,3	0.83	0	3,3,3	0.48	0
5	ACT	A	504	-	3,3,3	0.83	0	3,3,3	0.44	0
4	QJ7	A	503	-	29,29,29	0.88	0	37,38,38	1.60	8 (21%)
2	HEM	B	501	1	41,50,50	2.03	7 (17%)	45,82,82	1.75	9 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	GOL	B	504	-	5,5,5	0.65	0	5,5,5	1.64	2 (40%)
6	GOL	A	505	-	5,5,5	0.55	0	5,5,5	1.15	0
2	HEM	A	501	1	41,50,50	1.82	6 (14%)	45,82,82	1.46	8 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	H4B	A	502	-	-	0/8/17/17	0/2/2/2
3	H4B	B	502	-	-	0/8/17/17	0/2/2/2
4	QJ7	B	505	-	-	1/12/12/12	0/3/3/3
4	QJ7	A	503	-	-	0/12/12/12	0/3/3/3
2	HEM	B	501	1	-	2/12/54/54	-
6	GOL	B	504	-	-	1/4/4/4	-
6	GOL	A	505	-	-	1/4/4/4	-
2	HEM	A	501	1	-	2/12/54/54	-

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	HEM	C3D-C2D	7.87	1.53	1.36
2	A	501	HEM	C3D-C2D	6.35	1.50	1.36
2	B	501	HEM	C3C-C2C	-4.88	1.33	1.40
2	B	501	HEM	C3C-CAC	3.64	1.55	1.47
2	A	501	HEM	C3C-C2C	-3.43	1.35	1.40

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(º)	Ideal(º)
3	A	502	H4B	C8A-C4A-C4	6.37	120.23	114.57
4	B	505	QJ7	C02-N01-C06	5.28	122.10	118.10
3	B	502	H4B	C4-C4A-N5	5.11	123.41	119.12
2	B	501	HEM	CBA-CAA-C2A	-5.02	104.05	112.62
3	A	502	H4B	C2-N3-C4	4.62	123.27	115.93

There are no chirality outliers.
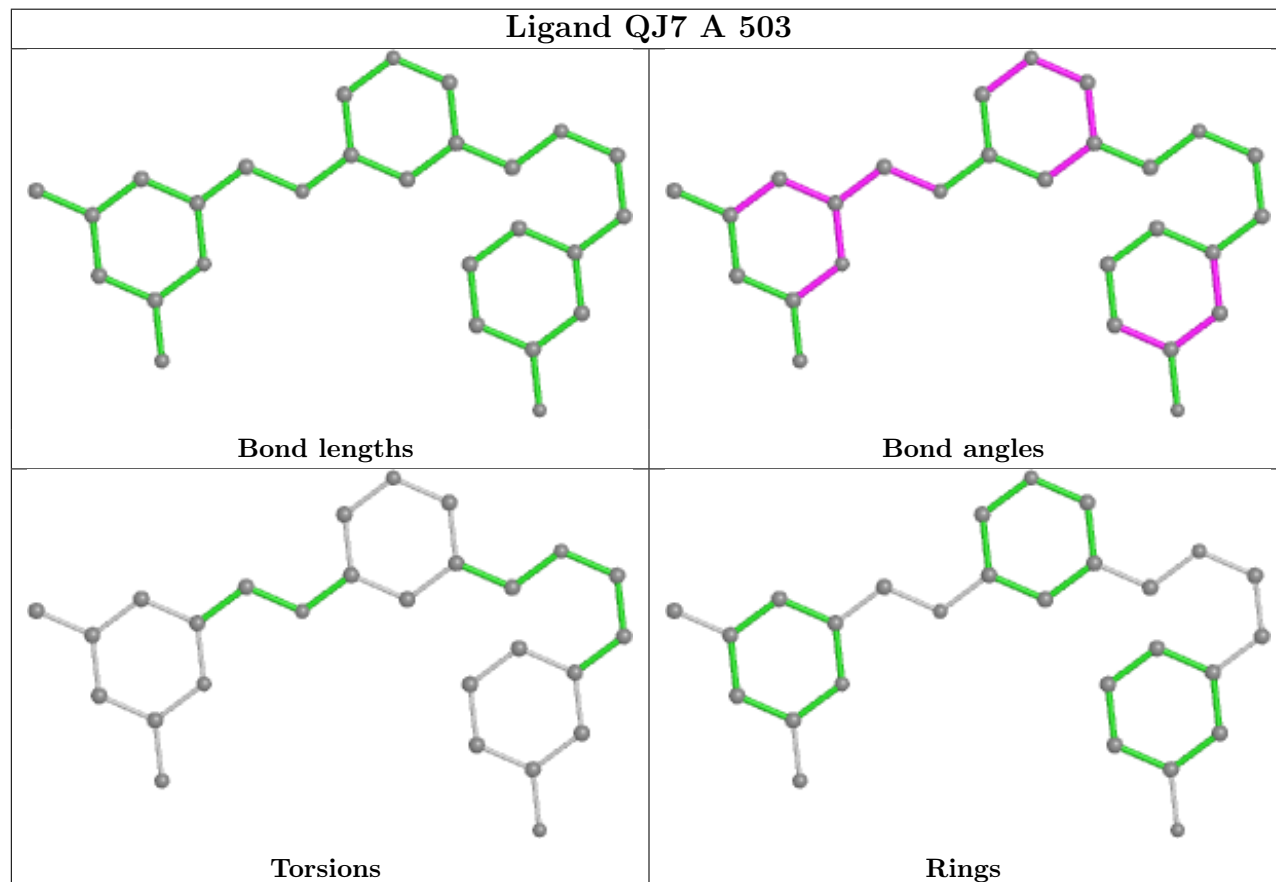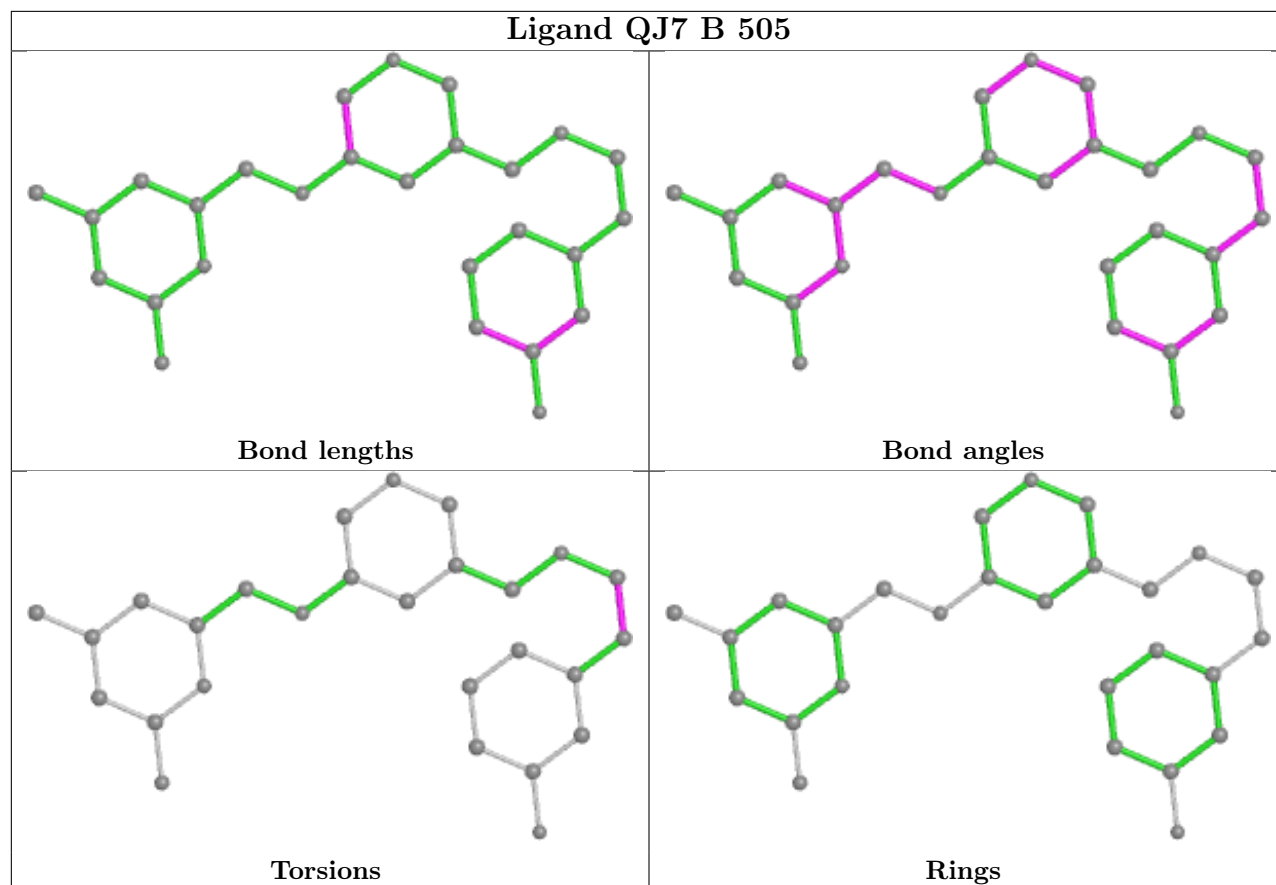
5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	505	QJ7	N18-C19-C20-C21
2	B	501	HEM	C2B-C3B-CAB-CBB
2	B	501	HEM	C4B-C3B-CAB-CBB
6	B	504	GOL	C1-C2-C3-O3
2	A	501	HEM	CAA-CBA-CGA-O2A

There are no ring outliers.

7 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	H4B	1	0
3	B	502	H4B	1	0
4	B	505	QJ7	1	0
4	A	503	QJ7	2	0
2	B	501	HEM	3	0
6	B	504	GOL	1	0
2	A	501	HEM	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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 QJ7 B 505

Bond lengths

Bond angles

Torsions

Rings

Ligand QJ7 A 503

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM B 501

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM A 501

Bond lengths

Bond angles

Torsions

Rings
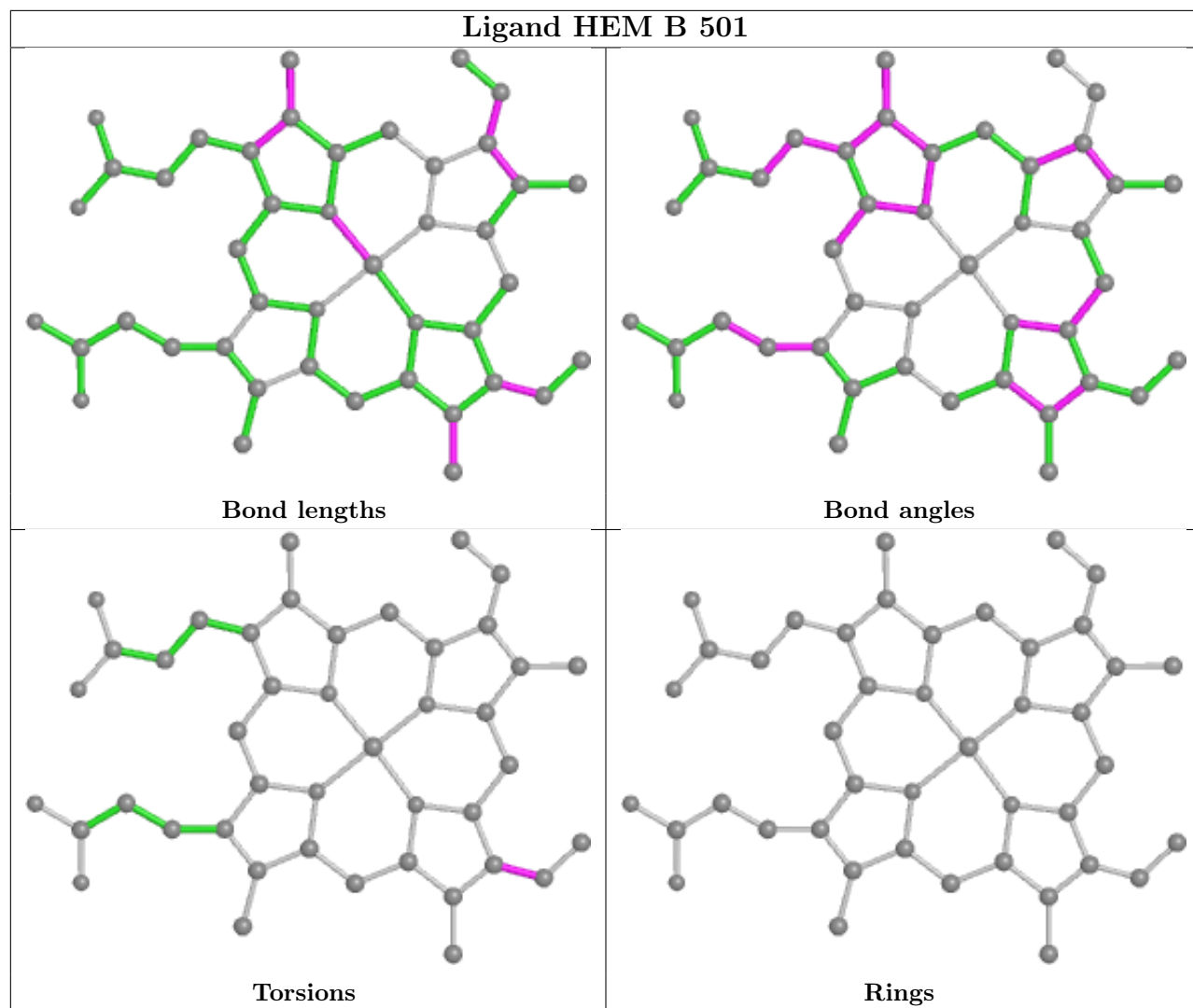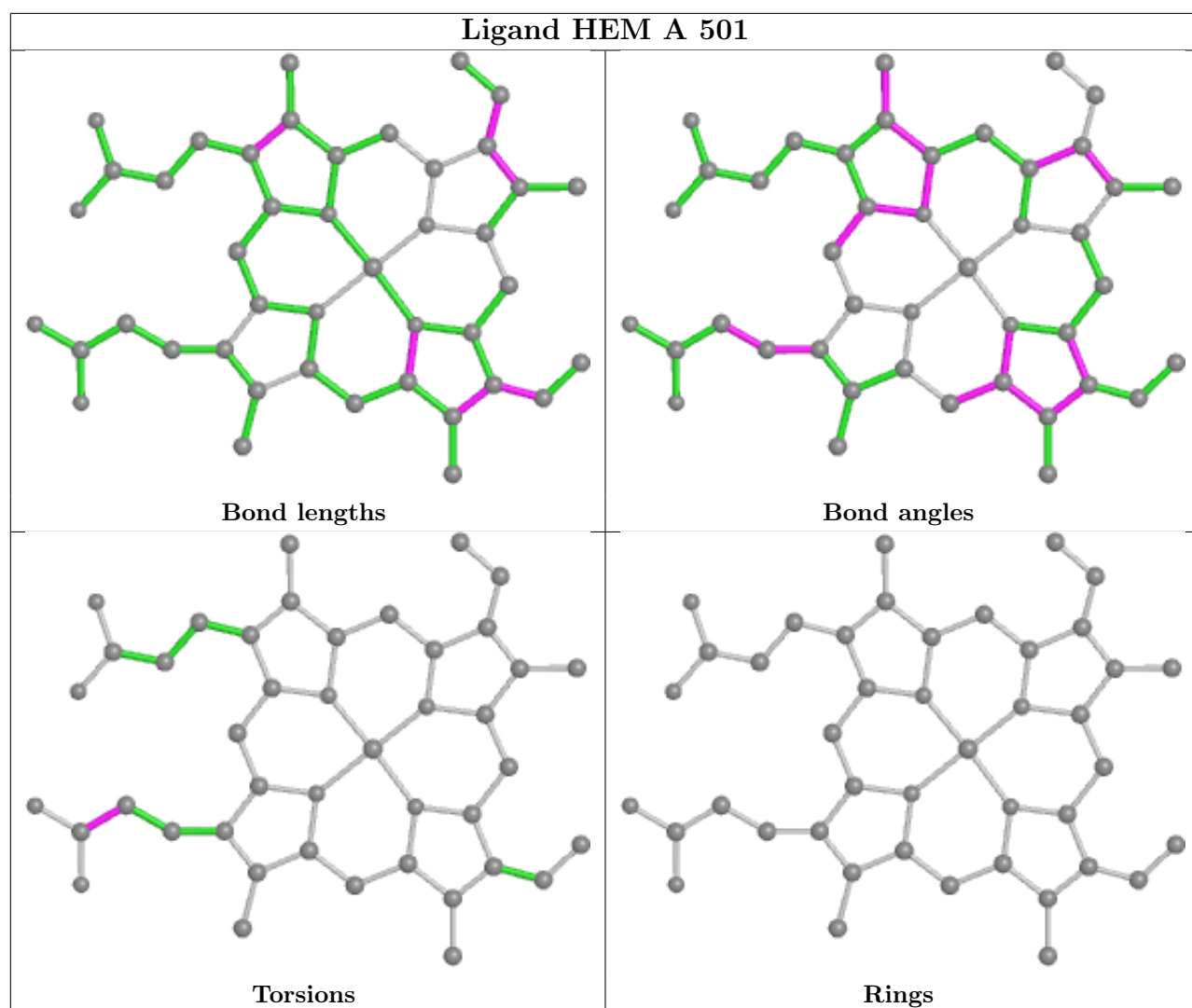
5.7 Other polymers ⓘ

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 ⓘ

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	405/443 (91%)	0.05	21 (5%)	27	30	26, 43, 68, 83	0
1	B	404/443 (91%)	-0.00	13 (3%)	47	50	29, 45, 71, 89	0
All	All	809/886 (91%)	0.03	34 (4%)	36	38	26, 44, 70, 89	0

The worst 5 of 34 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	259	GLN	5.0
1	A	239	GLY	4.7
1	A	259	GLN	4.1
1	B	111	LEU	3.9
1	B	110	LYS	3.8

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

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.

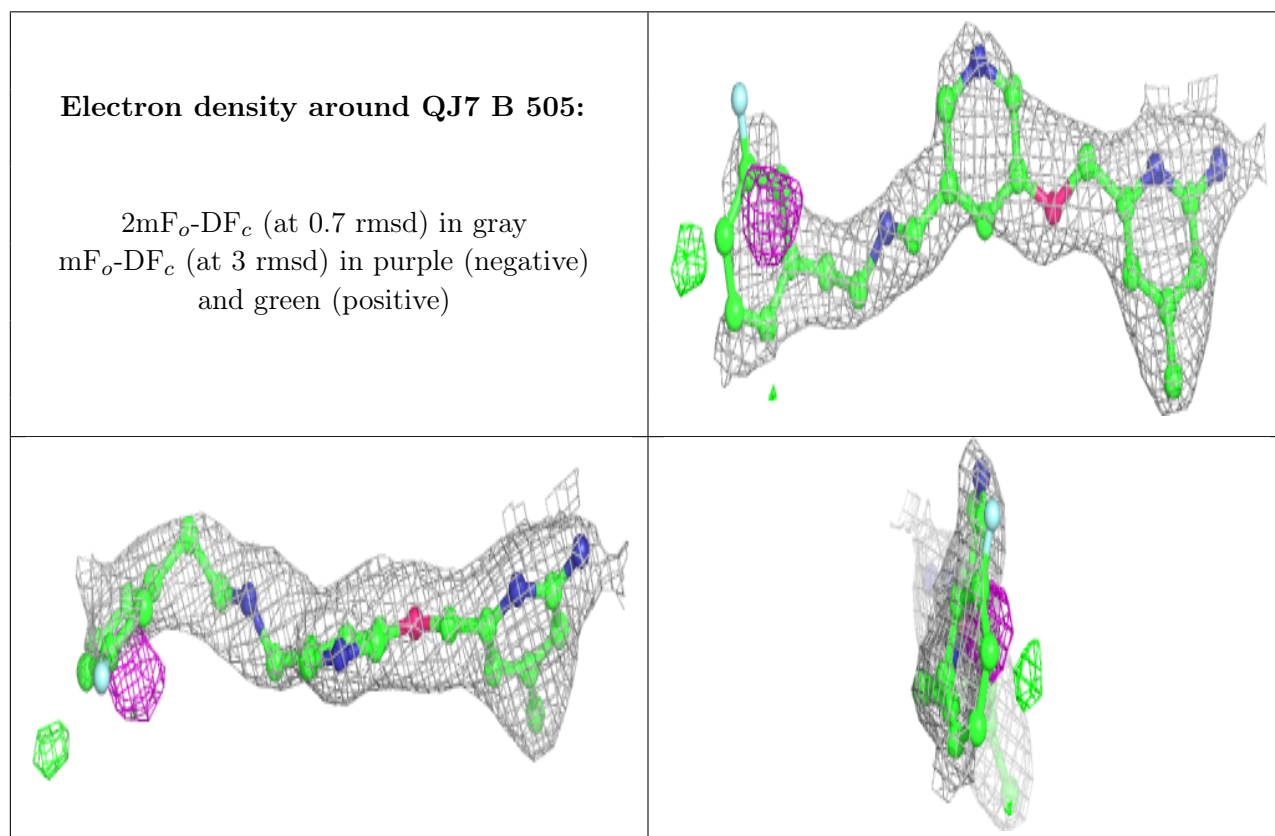| Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	CAS	A	384	9/10	0.96	0.09	43,45,73,74	0
1	CAS	B	384	9/10	0.98	0.09	52,53,75,77	0

6.3   Carbohydrates ⓘ

There are no monosaccharides 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	QJ7	B	505	27/27	0.89	0.23	35,58,79,81	0
6	GOL	A	505	6/6	0.90	0.35	62,62,64,69	0
6	GOL	B	504	6/6	0.93	0.26	50,50,52,53	0
4	QJ7	A	503	27/27	0.94	0.24	29,49,72,75	0
5	ACT	B	503	4/4	0.94	0.23	51,51,52,54	0
5	ACT	A	504	4/4	0.96	0.14	47,47,49,49	0
2	HEM	A	501	43/43	0.98	0.18	24,30,40,44	0
2	HEM	B	501	43/43	0.98	0.16	30,34,39,44	0
3	H4B	B	502	17/17	0.98	0.19	27,31,35,36	0
3	H4B	A	502	17/17	0.99	0.21	29,33,37,38	0
7	ZN	A	506	1/1	1.00	0.10	37,37,37,37	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 QJ7 B 505:

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

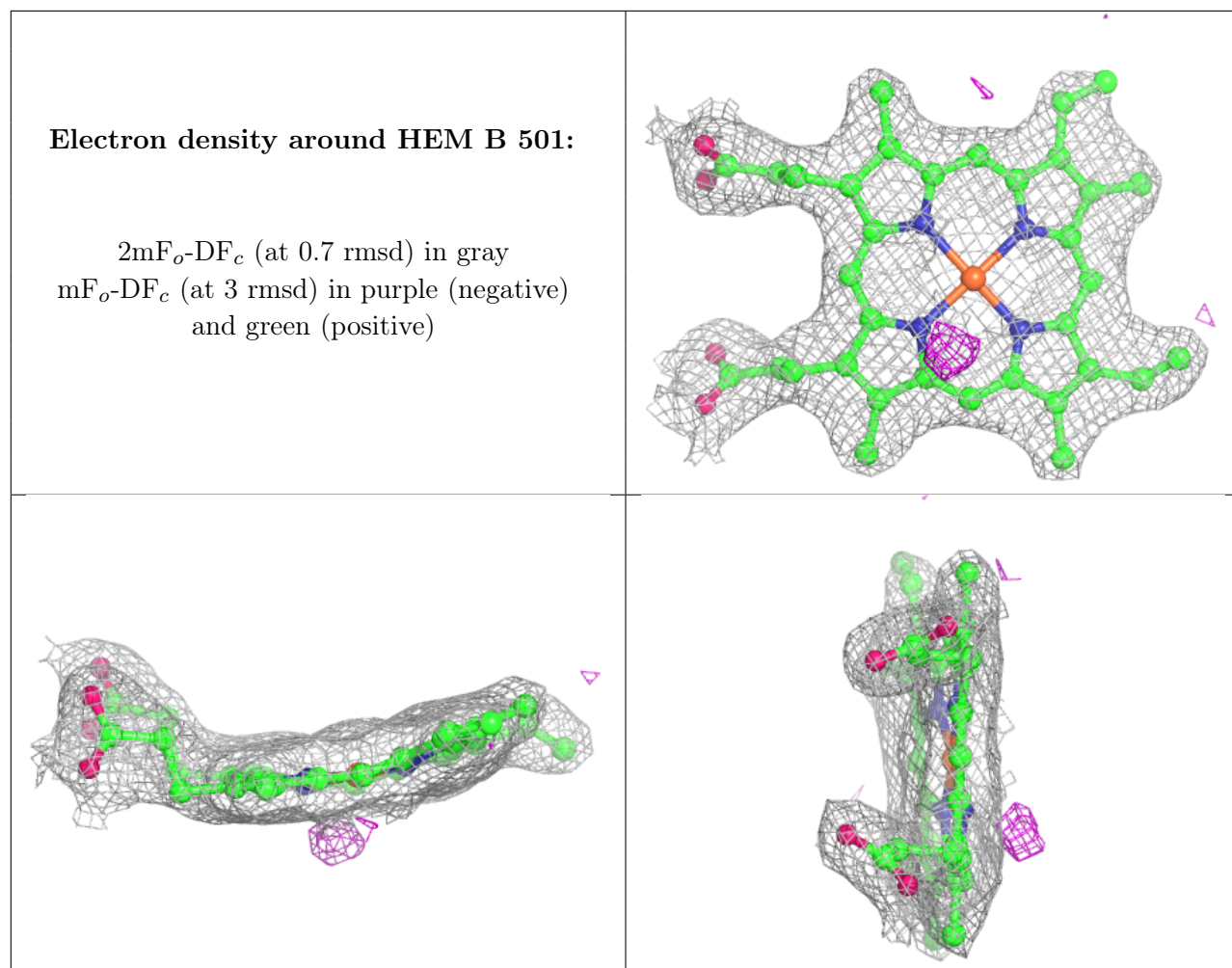**Electron density around QJ7 A 503:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
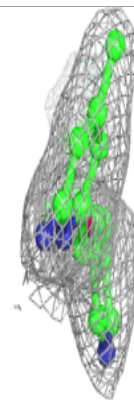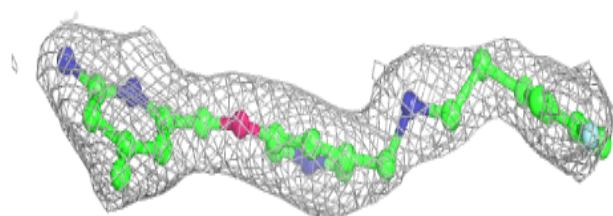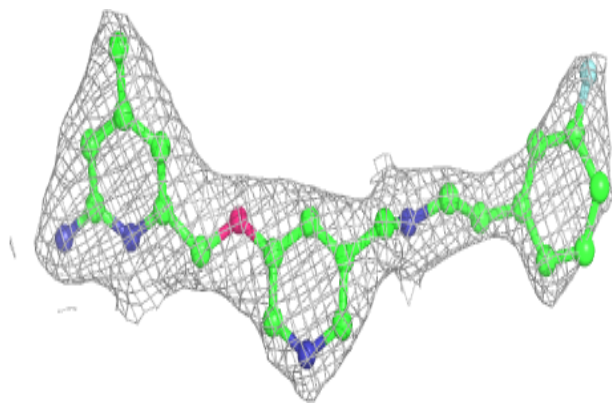
Electron density around HEM A 501:

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

Electron density around HEM B 501:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
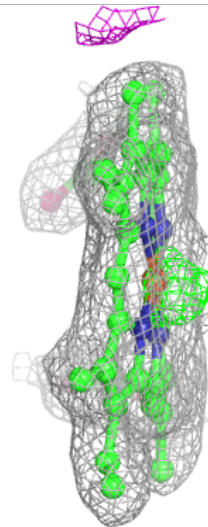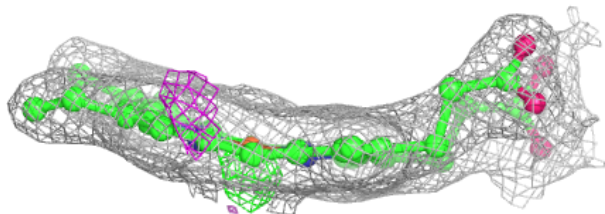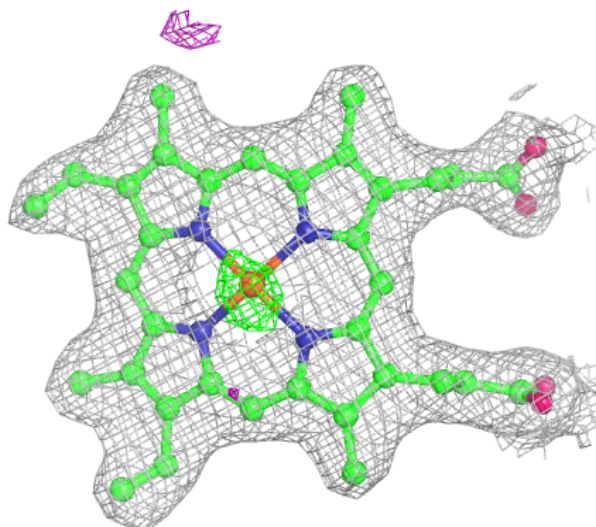
6.5 Other polymers (i)

There are no such residues in this entry.