



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:26 AM UTC

PDB ID : 9MWP / pdb_00009mwp
Title : Structure of human endothelial nitric oxide synthase heme domain bound with N-(4-(2-((3-(furan-3-carboximidamido)benzyl)amino)ethyl)phenyl)furan-3-carboximidamide
Authors : Li, H.; Poulos, T.L.
Deposited on : 2025-01-17
Resolution : 1.86 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

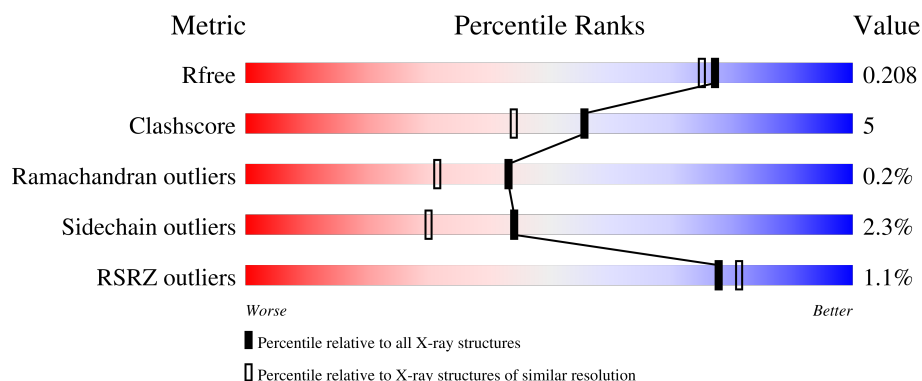
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.86 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	441	 2% 83% 9% • 8%
1	B	441	 85% 6% • 8%

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 7534 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 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	407	Total	C	N	O	S	0	2	0
			3255	2073	575	591	16			
1	B	405	Total	C	N	O	S	0	3	0
			3246	2068	572	590	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	298	GLU	ASP	variant	UNP P29474
B	298	GLU	ASP	variant	UNP P29474

- 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	0
			43	34	1	4	4		

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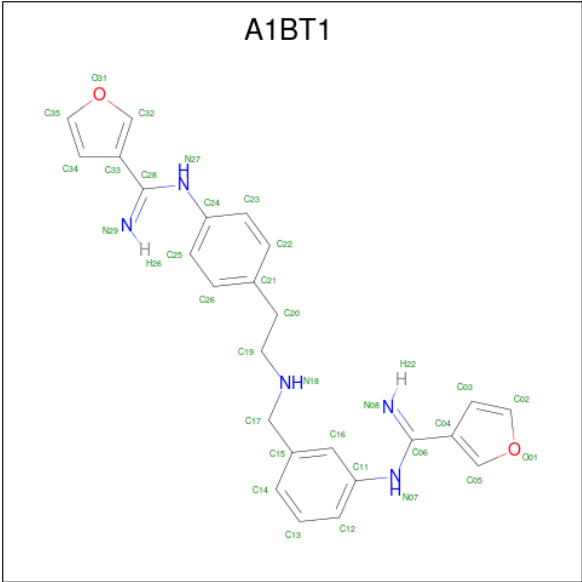
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



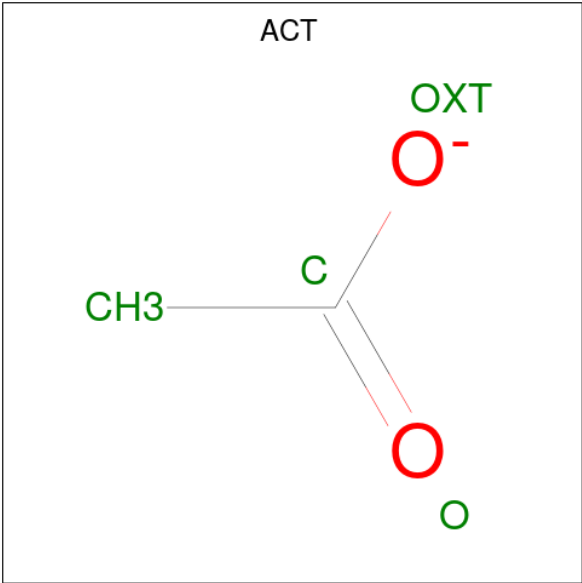
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 4 is N-[3-({[2-(4-{{(E)-(furan-3-yl)(imino)methyl}amino}phenyl)ethyl]amino}methyl)phenyl]furan-3-carboximidamide (CCD ID: A1BT1) (formula: $C_{25}H_{25}N_5O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			32	25	5	2		
4	B	1	Total	C	N	O	0	0
			32	25	5	2		

- Molecule 5 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



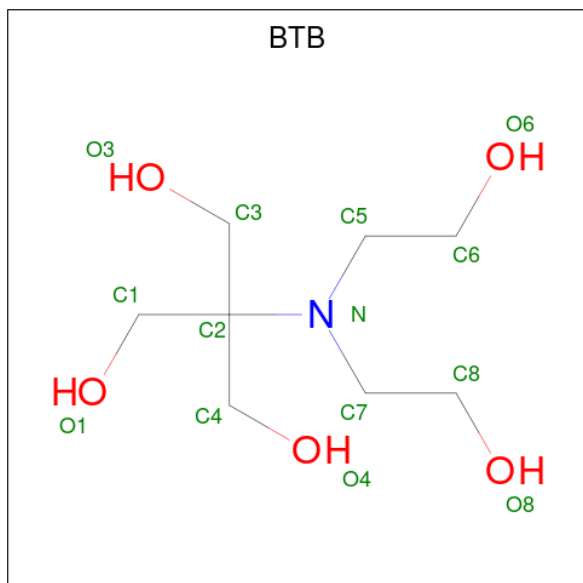
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		

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

- Molecule 6 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (CCD ID: BTB) (formula: $C_8H_{19}NO_5$).



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

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 8 is GADOLINIUM ATOM (CCD ID: GD) (formula: Gd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Gd	0	0
			1	1		
8	B	1	Total	Gd	0	0
			1	1		

- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

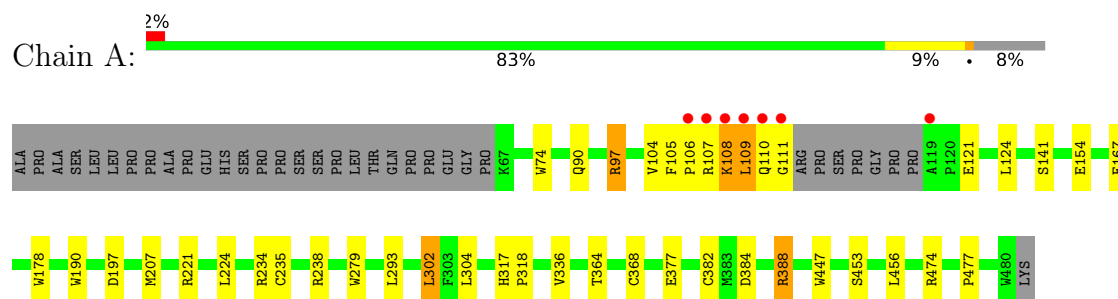
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	328	Total 328	O 328	0	0
10	B	402	Total 402	O 402	0	0

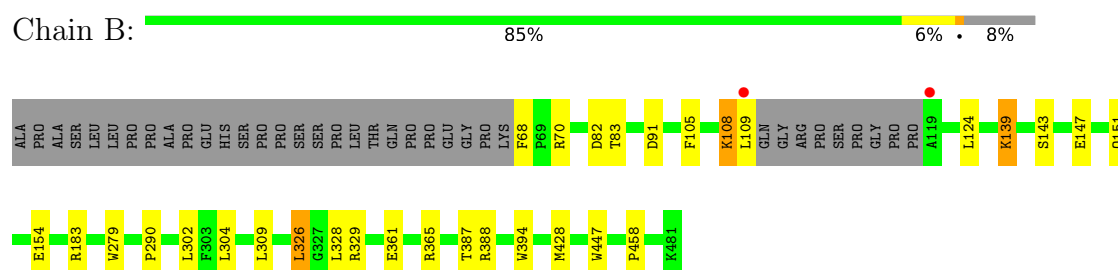
3 Residue-property plots [i](#)

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 3



- Molecule 1: Nitric oxide synthase 3



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	61.62Å 109.41Å 152.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.14 – 1.86 46.14 – 1.86	Depositor EDS
% Data completeness (in resolution range)	95.8 (46.14-1.86) 98.0 (46.14-1.86)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 1.86Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, R_{free}	0.179 , 0.214 0.174 , 0.208	Depositor DCC
R_{free} test set	4289 reflections (3.63%)	wwPDB-VP
Wilson B-factor (Å ²)	30.2	Xtriage
Anisotropy	0.388	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 44.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7534	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% 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: ACT, GD, H4B, ZN, HEM, A1BT1, BTB, 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	0.28	0/3353	0.50	0/4567
1	B	0.31	0/3347	0.51	0/4558
All	All	0.30	0/6700	0.51	0/9125

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	3255	0	3169	30	0
1	B	3246	0	3163	21	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	1	0
4	A	32	0	0	1	0
4	B	32	0	0	1	0
5	A	8	0	6	0	0
5	B	8	0	6	0	0
6	A	42	0	56	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	28	0	34	2	0
7	A	12	0	16	2	0
7	B	18	0	24	2	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
9	A	1	0	0	0	0
10	A	328	0	0	2	0
10	B	402	0	0	3	0
All	All	7534	0	6564	63	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 5.

All (63) 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:110:GLN:HE21	1:A:111:GLY:H	1.30	0.80
6:A:508:BTB:O4	6:A:508:BTB:O3	1.97	0.78
1:A:110:GLN:OE1	1:A:474:ARG:NH2	2.17	0.76
1:A:279:TRP:HB2	1:A:302:LEU:HD11	1.69	0.74
7:A:510:GOL:H31	10:A:859:HOH:O	1.94	0.67
1:B:279:TRP:HB2	1:B:302:LEU:HD21	1.80	0.64
2:A:501:HEM:HMC2	2:A:501:HEM:HBC2	1.80	0.63
2:A:501:HEM:HBB2	2:A:501:HEM:HHC	1.79	0.63
1:A:97:ARG:NH1	1:B:91:ASP:OD1	2.33	0.62
1:B:365:ARG:NH2	7:B:509:GOL:H12	2.15	0.61
1:B:124:LEU:HD21	1:B:154:GLU:HA	1.83	0.60
2:B:501:HEM:HBC2	2:B:501:HEM:HMC2	1.85	0.59
1:A:110:GLN:HE21	1:A:111:GLY:N	2.00	0.59
1:A:105:PHE:O	1:A:107:ARG:N	2.31	0.58
1:A:74:TRP:HB3	7:B:509:GOL:H2	1.85	0.58
1:B:290:PRO:HB3	1:B:304:LEU:HD23	1.86	0.55
1:A:377:GLU:OE1	6:A:507:BTB:H42	2.06	0.55
1:B:143:SER:O	1:B:147:GLU:HG2	2.09	0.53
2:B:501:HEM:HHC	2:B:501:HEM:HBB2	1.91	0.53
1:A:105:PHE:C	1:A:107:ARG:H	2.16	0.53
1:A:110:GLN:HB3	1:A:477:PRO:HD3	1.90	0.52
1:A:110:GLN:CD	1:A:234:ARG:HH12	2.17	0.52
1:B:447:TRP:HA	3:B:502:H4B:N1	2.25	0.52
1:A:447:TRP:HA	3:A:502:H4B:N1	2.25	0.51
6:A:507:BTB:O4	6:A:507:BTB:O3	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:510:GOL:O3	10:A:601:HOH:O	2.14	0.51
6:A:507:BTB:O4	6:A:507:BTB:O1	2.27	0.51
1:B:108:LYS:O	1:B:109:LEU:HB2	2.11	0.50
1:B:151:GLN:NE2	10:B:610:HOH:O	2.45	0.50
1:A:167:GLU:OE1	6:A:508:BTB:H41	2.13	0.48
1:A:453:SER:HB3	1:A:456:LEU:HD12	1.95	0.48
1:B:428:MET:HG3	1:B:458:PRO:HB2	1.95	0.48
1:A:364:THR:O	1:A:368:CYS:HB2	2.14	0.47
1:B:68:PHE:CD2	1:B:83:THR:HA	2.50	0.47
1:B:326:LEU:HB3	1:B:328:LEU:HG	1.97	0.47
1:A:235:CYS:SG	1:A:238:ARG:HD2	2.56	0.46
1:A:97:ARG:HA	1:A:97:ARG:HD2	1.53	0.46
1:A:107:ARG:NH2	1:B:70:ARG:H	2.13	0.45
1:B:139:LYS:N	1:B:139:LYS:HD3	2.31	0.45
1:B:82:ASP:OD2	10:B:601:HOH:O	2.21	0.45
1:A:382:CYS:O	6:A:506:BTB:H52	2.17	0.45
1:B:105:PHE:CD1	1:B:109:LEU:HD11	2.51	0.45
6:A:508:BTB:H11	6:A:508:BTB:H72	1.84	0.44
1:A:388:ARG:HG2	6:A:507:BTB:H81	1.99	0.44
1:B:70:ARG:NE	10:B:614:HOH:O	2.48	0.44
1:A:207:MET:HG2	1:A:293:LEU:HD13	1.99	0.44
6:B:507:BTB:H72	6:B:507:BTB:H11	1.61	0.44
1:A:384:ASP:OD2	6:A:506:BTB:O3	2.35	0.44
1:A:317:HIS:CG	1:A:318:PRO:HD2	2.53	0.43
1:A:104:VAL:O	1:A:106:PRO:HD3	2.18	0.43
1:B:183:ARG:HD3	1:B:447:TRP:CD2	2.54	0.42
6:B:507:BTB:H51	6:B:507:BTB:H32	1.63	0.42
6:A:506:BTB:O8	6:A:506:BTB:H41	2.20	0.41
6:A:507:BTB:H11	6:A:507:BTB:H51	1.65	0.41
1:A:336:VAL:HG21	4:A:503:A1BT1:C14	2.50	0.41
1:B:361:GLU:OE1	4:B:503:A1BT1:N07	2.54	0.41
1:A:178:TRP:CE3	1:A:190:TRP:HA	2.56	0.41
1:B:309:LEU:HD12	1:B:309:LEU:HA	1.94	0.41
1:A:124:LEU:HD21	1:A:154:GLU:HA	2.03	0.41
1:A:167:GLU:OE2	6:A:508:BTB:H32	2.22	0.40
1:A:382:CYS:HA	6:A:506:BTB:C1	2.51	0.40
1:A:197:ASP:HB3	6:A:508:BTB:H62	2.04	0.40
1:B:387:THR:HA	1:B:394:TRP:CD1	2.56	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	405/441 (92%)	394 (97%)	9 (2%)	2 (0%)	24	13
1	B	404/441 (92%)	399 (99%)	5 (1%)	0	100	100
All	All	809/882 (92%)	793 (98%)	14 (2%)	2 (0%)	43	31

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	109	LEU
1	A	108	LYS

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	347/374 (93%)	336 (97%)	11 (3%)	34	19
1	B	347/374 (93%)	342 (99%)	5 (1%)	59	49
All	All	694/748 (93%)	678 (98%)	16 (2%)	44	30

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	GLN
1	A	97	ARG
1	A	108	LYS
1	A	109	LEU

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Mol	Chain	Res	Type
1	A	121	GLU
1	A	141	SER
1	A	221	ARG
1	A	224	LEU
1	A	302	LEU
1	A	304	LEU
1	A	388	ARG
1	B	108	LYS
1	B	139	LYS
1	B	326	LEU
1	B	329	ARG
1	B	388	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	GLN
1	A	126	GLN
1	B	90	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 23 ligands modelled in this entry, 3 are monoatomic - leaving 20 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	ACT	B	504	-	3,3,3	0.79	0	3,3,3	0.79	0
7	GOL	B	508	-	5,5,5	0.32	0	5,5,5	0.35	0
4	A1BT1	A	503	-	35,35,35	1.70	5 (14%)	39,46,46	1.39	7 (17%)
6	BTB	A	507	-	13,13,13	0.51	0	7,16,16	1.08	1 (14%)
5	ACT	A	505	-	3,3,3	0.88	0	3,3,3	0.49	0
2	HEM	A	501	1	50,50,50	1.68	7 (14%)	67,82,82	1.26	6 (8%)
3	H4B	B	502	-	17,18,18	0.95	1 (5%)	14,26,26	1.66	3 (21%)
7	GOL	B	510	-	5,5,5	0.38	0	5,5,5	0.30	0
7	GOL	A	509	-	5,5,5	0.36	0	5,5,5	0.62	0
6	BTB	A	506	8	13,13,13	0.42	0	7,16,16	1.21	1 (14%)
4	A1BT1	B	503	-	35,35,35	1.44	6 (17%)	39,46,46	1.78	9 (23%)
6	BTB	B	507	-	13,13,13	0.43	0	7,16,16	1.40	0
2	HEM	B	501	1	50,50,50	1.53	8 (16%)	67,82,82	1.20	5 (7%)
5	ACT	A	504	-	3,3,3	0.82	0	3,3,3	0.74	0
5	ACT	B	505	-	3,3,3	0.80	0	3,3,3	0.66	0
3	H4B	A	502	-	17,18,18	1.06	1 (5%)	14,26,26	2.11	5 (35%)
6	BTB	B	506	8	13,13,13	0.40	0	7,16,16	0.69	0
7	GOL	B	509	-	5,5,5	0.48	0	5,5,5	0.87	0
7	GOL	A	510	-	5,5,5	0.38	0	5,5,5	0.65	0
6	BTB	A	508	-	13,13,13	0.44	0	7,16,16	0.53	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
7	GOL	B	508	-	-	2/4/4/4	-
7	GOL	B	510	-	-	2/4/4/4	-
6	BTB	B	507	-	-	6/21/21/21	-
4	A1BT1	A	503	-	-	2/15/23/23	0/4/4/4
3	H4B	A	502	-	-	0/8/17/17	0/2/2/2
7	GOL	A	509	-	-	2/4/4/4	-
6	BTB	B	506	8	-	0/21/21/21	-
2	HEM	B	501	1	-	1/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GOL	B	509	-	-	3/4/4/4	-
7	GOL	A	510	-	-	0/4/4/4	-
6	BTB	A	506	8	-	13/21/21/21	-
6	BTB	A	507	-	-	8/21/21/21	-
6	BTB	A	508	-	-	11/21/21/21	-
2	HEM	A	501	1	-	1/14/54/54	-
4	A1BT1	B	503	-	-	3/15/23/23	0/4/4/4
3	H4B	B	502	-	-	0/8/17/17	0/2/2/2

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	FE-NA	5.90	2.14	1.95
4	A	503	A1BT1	C04-C06	5.87	1.50	1.46
2	A	501	HEM	FE-NB	5.55	2.12	1.94
2	B	501	HEM	FE-NB	4.73	2.09	1.94
4	A	503	A1BT1	C33-C28	4.67	1.49	1.46
4	B	503	A1BT1	C33-C28	4.39	1.49	1.46
2	B	501	HEM	FE-ND	4.07	2.07	1.94
4	B	503	A1BT1	C04-C06	3.24	1.48	1.46
2	A	501	HEM	FE-NC	3.23	2.05	1.95
2	B	501	HEM	CAC-C3C	2.97	1.55	1.47
2	B	501	HEM	CAB-C3B	2.97	1.55	1.47
4	A	503	A1BT1	C24-N27	-2.95	1.35	1.41
2	B	501	HEM	FE-NC	2.94	2.04	1.95
2	A	501	HEM	CAB-C3B	2.94	1.55	1.47
2	A	501	HEM	CAC-C3C	2.81	1.54	1.47
4	B	503	A1BT1	C24-N27	-2.75	1.36	1.41
2	B	501	HEM	FE-NA	2.72	2.04	1.95
4	A	503	A1BT1	C28-N27	-2.62	1.33	1.38
4	B	503	A1BT1	C11-N07	-2.54	1.36	1.41
4	B	503	A1BT1	C28-N27	-2.43	1.34	1.38
2	B	501	HEM	CMD-C2D	2.27	1.55	1.50
3	A	502	H4B	C4-N3	-2.20	1.34	1.38
2	A	501	HEM	CMC-C2C	2.12	1.55	1.50
2	A	501	HEM	CMB-C2B	2.09	1.55	1.50
3	B	502	H4B	C4-N3	-2.08	1.35	1.38
4	A	503	A1BT1	C11-N07	-2.07	1.37	1.41
2	B	501	HEM	CMC-C2C	2.05	1.55	1.50
4	B	503	A1BT1	C06-N07	-2.04	1.34	1.38

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	503	A1BT1	C03-C04-C05	4.65	109.03	105.59
3	A	502	H4B	C2-N1-C8A	4.51	121.33	113.36
4	B	503	A1BT1	O01-C05-C04	-4.00	107.33	110.81
3	A	502	H4B	C11-C10-C9	-3.75	107.52	112.11
2	A	501	HEM	CBA-CAA-C2A	-3.60	102.57	112.53
3	B	502	H4B	C2-N1-C8A	3.37	119.31	113.36
4	A	503	A1BT1	O31-C32-C33	-3.36	107.89	110.81
4	B	503	A1BT1	O31-C32-C33	-3.34	107.90	110.81
4	B	503	A1BT1	C17-C15-C14	-3.20	114.41	120.94
2	B	501	HEM	CBA-CAA-C2A	-3.15	103.81	112.53
4	B	503	A1BT1	C34-C33-C32	3.15	107.92	105.59
4	A	503	A1BT1	C34-C33-C32	2.95	107.77	105.59
4	B	503	A1BT1	C15-C17-N18	-2.92	103.61	112.79
2	A	501	HEM	C3B-C2B-C1B	2.90	108.59	106.41
4	A	503	A1BT1	O01-C05-C04	-2.84	108.34	110.81
6	A	506	BTB	O3-C3-C2	2.79	117.95	111.40
4	B	503	A1BT1	C24-N27-C28	-2.71	122.17	128.41
3	A	502	H4B	C4A-C4-N3	2.58	119.22	112.13
3	B	502	H4B	O4-C4-C4A	-2.52	121.18	127.26
4	A	503	A1BT1	C03-C04-C05	2.51	107.45	105.59
4	A	503	A1BT1	C24-N27-C28	-2.34	123.03	128.41
2	B	501	HEM	C3B-C4B-NB	-2.34	107.79	109.47
4	B	503	A1BT1	C13-C12-C11	2.32	122.41	119.73
2	B	501	HEM	C1B-NB-C4B	2.31	107.94	105.21
4	B	503	A1BT1	C14-C15-C16	2.28	121.70	118.55
2	A	501	HEM	C2A-C1A-NA	-2.24	107.66	110.15
3	A	502	H4B	O4-C4-C4A	-2.23	121.88	127.26
4	A	503	A1BT1	C04-C06-N07	2.23	123.15	116.61
2	A	501	HEM	CHB-C1B-NB	2.23	127.12	124.37
6	A	507	BTB	O3-C3-C2	-2.23	106.17	111.40
2	B	501	HEM	C3B-C2B-C1B	2.21	108.07	106.41
2	A	501	HEM	C3B-C4B-NB	-2.20	107.89	109.47
3	B	502	H4B	C4A-C4-N3	2.16	118.06	112.13
2	A	501	HEM	C1B-NB-C4B	2.16	107.76	105.21
4	A	503	A1BT1	C17-C15-C14	-2.10	116.66	120.94
2	B	501	HEM	CHC-C1C-NC	2.06	126.69	124.45
3	A	502	H4B	N3-C2-N1	-2.03	119.60	123.32

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	506	BTB	O1-C1-C2-C3
6	A	506	BTB	O1-C1-C2-C4
6	A	506	BTB	O1-C1-C2-N
6	A	506	BTB	C1-C2-C4-O4
6	A	506	BTB	C3-C2-C4-O4
6	A	506	BTB	N-C2-C4-O4
6	A	506	BTB	C1-C2-N-C5
6	A	506	BTB	C1-C2-N-C7
6	A	506	BTB	C3-C2-N-C5
6	A	506	BTB	C3-C2-N-C7
6	A	506	BTB	C4-C2-N-C5
6	A	507	BTB	C1-C2-N-C5
6	A	507	BTB	C1-C2-N-C7
6	A	507	BTB	C3-C2-N-C5
6	A	507	BTB	C3-C2-N-C7
6	A	507	BTB	C4-C2-N-C7
6	A	508	BTB	C1-C2-C3-O3
6	A	508	BTB	C4-C2-C3-O3
6	A	508	BTB	N-C2-C3-O3
6	A	508	BTB	C1-C2-C4-O4
6	A	508	BTB	N-C2-C4-O4
6	A	508	BTB	C6-C5-N-C7
7	A	509	GOL	O1-C1-C2-C3
7	B	510	GOL	O1-C1-C2-C3
6	A	506	BTB	N-C7-C8-O8
7	B	509	GOL	O1-C1-C2-C3
7	B	509	GOL	C1-C2-C3-O3
4	B	503	A1BT1	C20-C19-N18-C17
7	A	509	GOL	O1-C1-C2-O2
7	B	509	GOL	O2-C2-C3-O3
6	A	508	BTB	N-C7-C8-O8
6	B	507	BTB	N-C5-C6-O6
6	B	507	BTB	N-C7-C8-O8
6	A	508	BTB	N-C5-C6-O6
6	A	507	BTB	N-C7-C8-O8
4	A	503	A1BT1	C23-C24-N27-C28
4	A	503	A1BT1	C25-C24-N27-C28
7	B	510	GOL	O1-C1-C2-O2
6	A	506	BTB	C4-C2-N-C7
6	A	507	BTB	C4-C2-N-C5
6	A	508	BTB	C1-C2-N-C7
6	B	507	BTB	C1-C2-N-C5
7	B	508	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
6	A	507	BTB	N-C5-C6-O6
7	B	508	GOL	O1-C1-C2-O2
4	B	503	A1BT1	C25-C24-N27-C28
4	B	503	A1BT1	C23-C24-N27-C28
2	A	501	HEM	C4B-C3B-CAB-CBB
2	B	501	HEM	C4B-C3B-CAB-CBB
6	A	508	BTB	C1-C2-N-C5
6	A	508	BTB	C3-C2-N-C5
6	B	507	BTB	C1-C2-N-C7
6	B	507	BTB	C3-C2-N-C5
6	B	507	BTB	C4-C2-N-C5

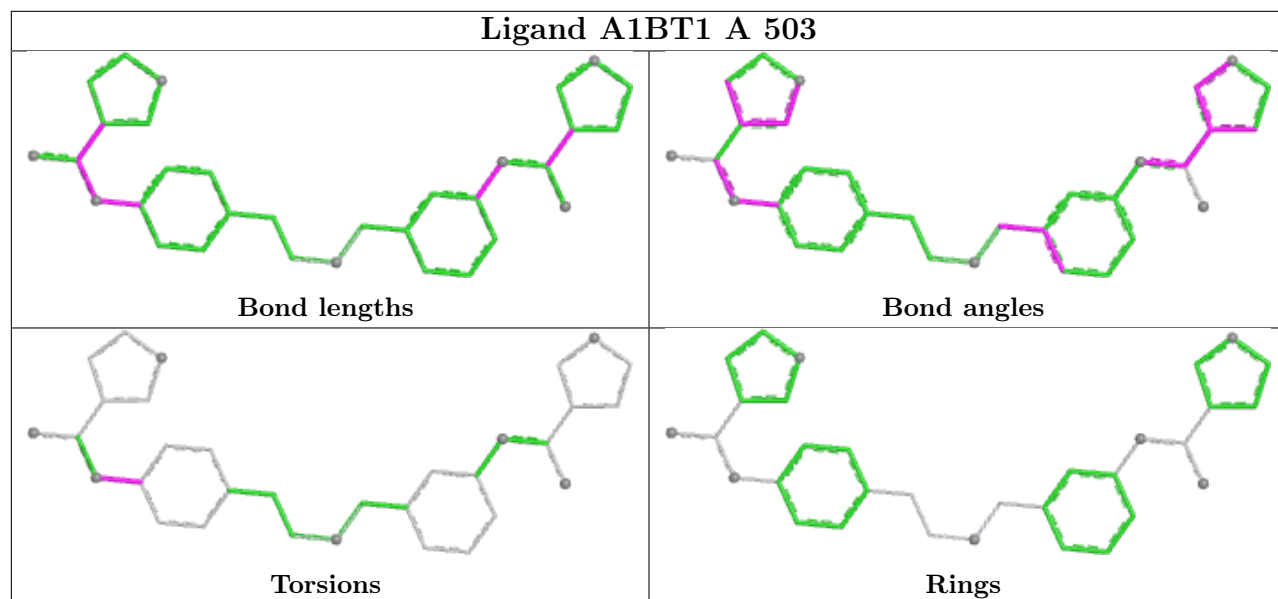
There are no ring outliers.

12 monomers are involved in 28 short contacts:

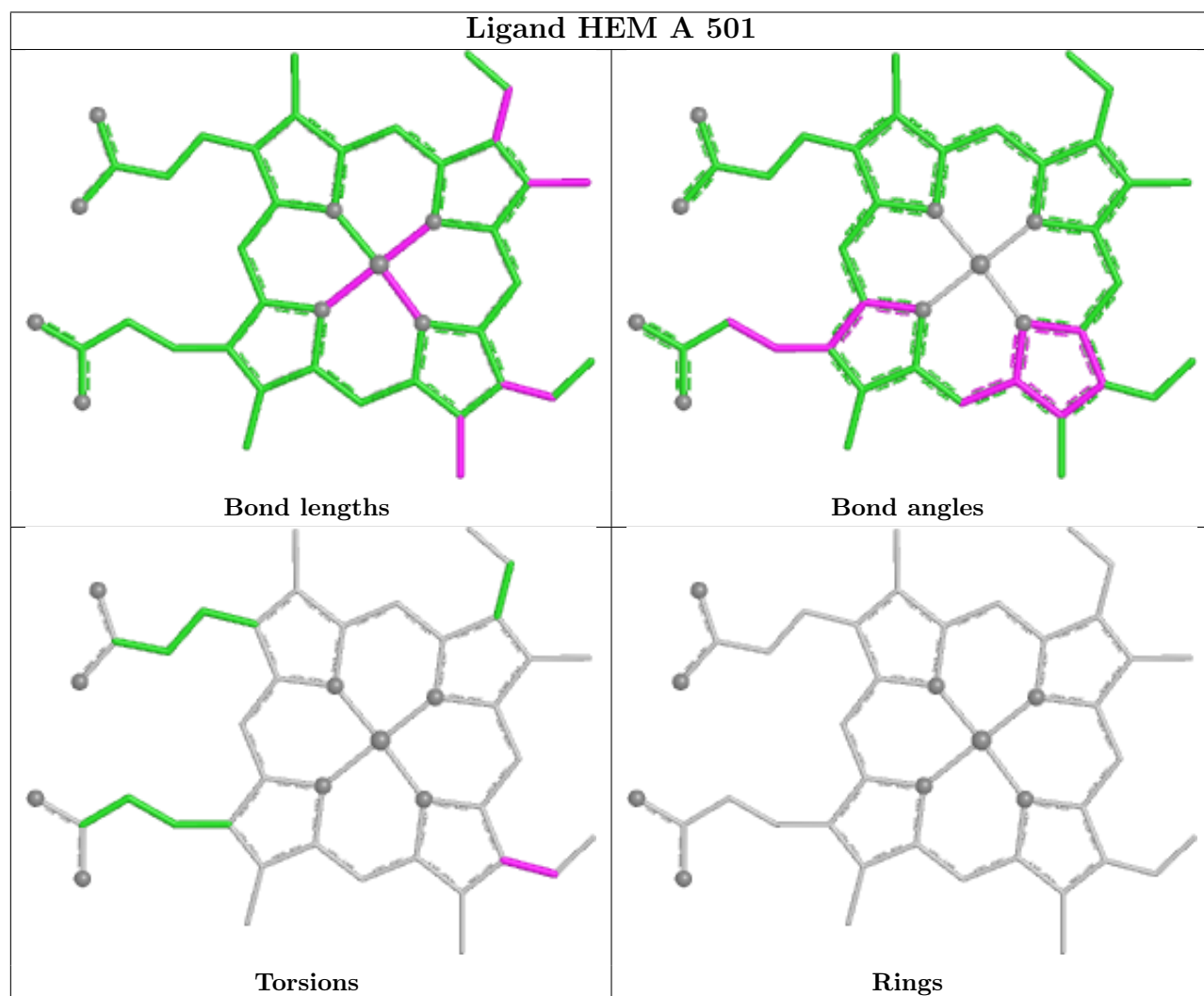
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	503	A1BT1	1	0
6	A	507	BTB	5	0
2	A	501	HEM	2	0
3	B	502	H4B	1	0
6	A	506	BTB	4	0
4	B	503	A1BT1	1	0
6	B	507	BTB	2	0
2	B	501	HEM	2	0
3	A	502	H4B	1	0
7	B	509	GOL	2	0
7	A	510	GOL	2	0
6	A	508	BTB	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

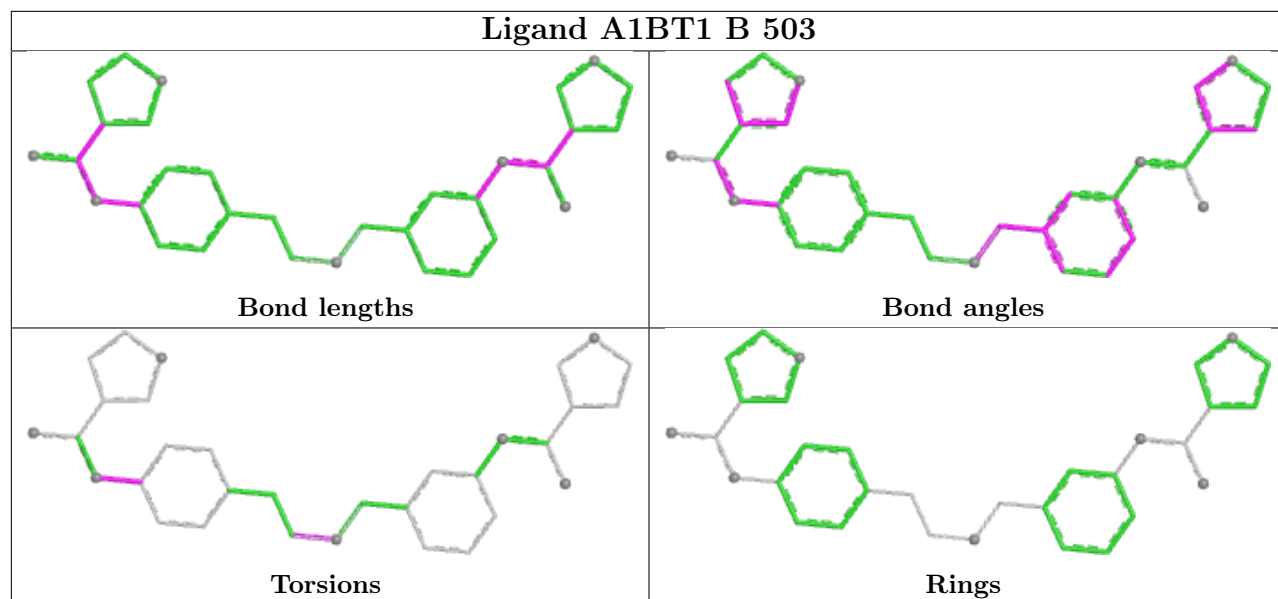
Ligand A1BT1 A 503



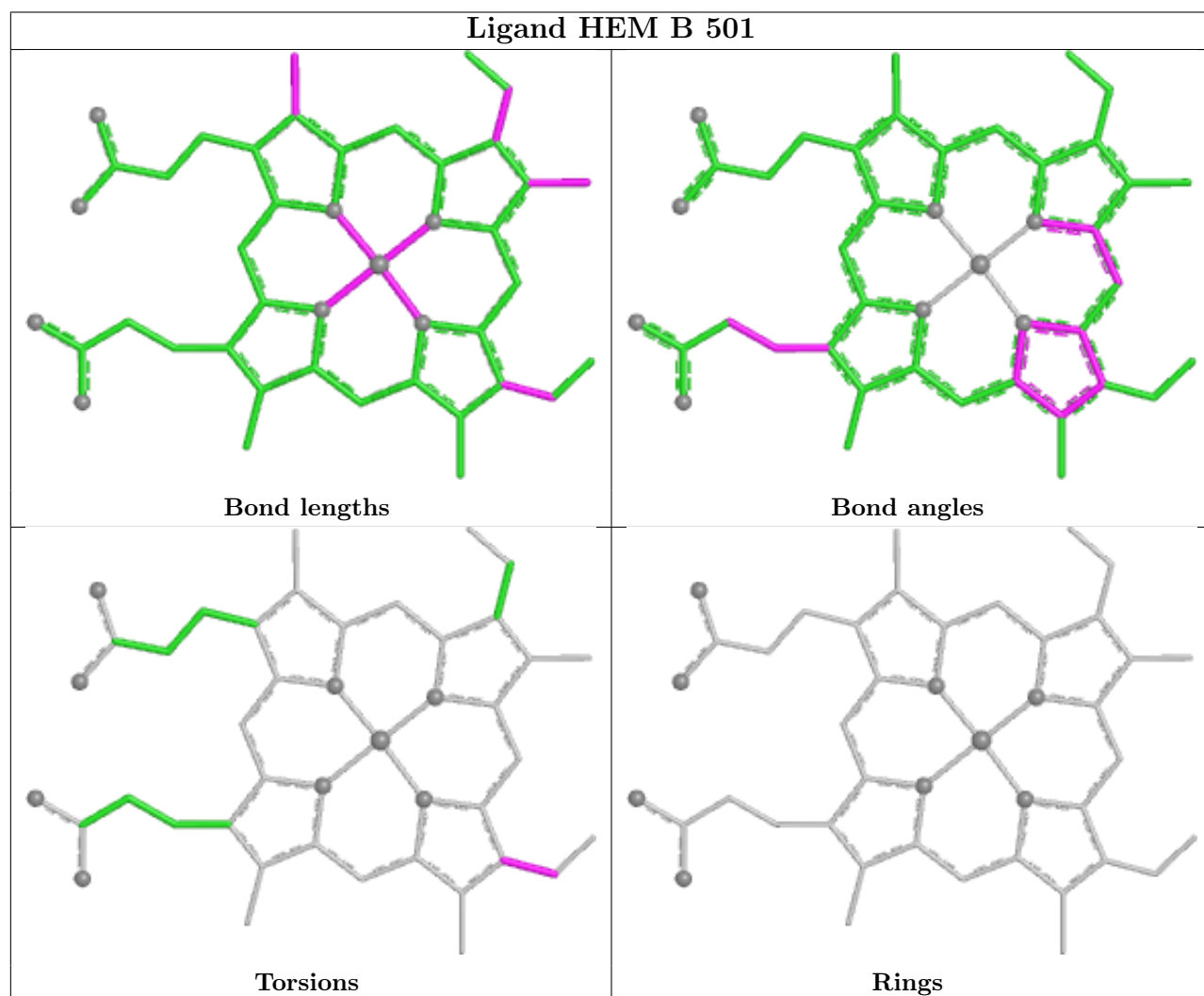
Ligand HEM A 501



Ligand A1BT1 B 503



Ligand HEM B 501



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	407/441 (92%)	-0.19	7 (1%) 69 73	19, 35, 66, 103	2 (0%)
1	B	405/441 (91%)	-0.32	2 (0%) 87 90	20, 31, 59, 91	3 (0%)
All	All	812/882 (92%)	-0.25	9 (1%) 78 81	19, 33, 63, 103	5 (0%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	109	LEU	3.9
1	B	119	ALA	3.7
1	A	109	LEU	3.6
1	A	119	ALA	3.3
1	A	110	GLN	3.2
1	A	111	GLY	3.1
1	A	107	ARG	3.0
1	A	108	LYS	2.6
1	A	106	PRO	2.6

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,

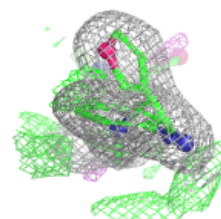
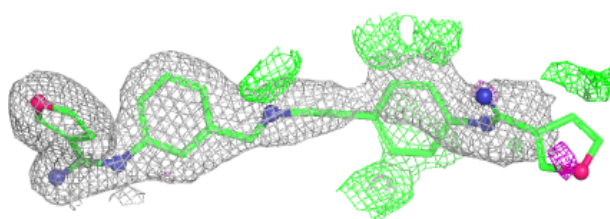
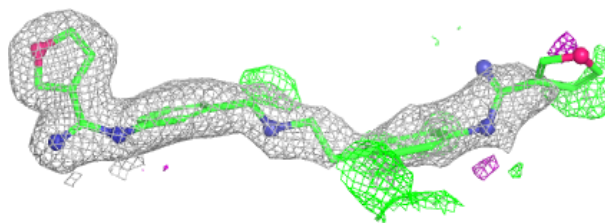
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	GOL	B	510	6/6	0.55	0.14	73,74,77,79	0
7	GOL	A	509	6/6	0.62	0.15	66,75,79,82	0
7	GOL	B	508	6/6	0.67	0.16	68,73,79,83	0
7	GOL	B	509	6/6	0.75	0.20	46,58,62,68	0
6	BTB	A	507	14/14	0.78	0.16	68,77,87,91	0
6	BTB	A	508	14/14	0.80	0.19	57,69,81,89	0
7	GOL	A	510	6/6	0.83	0.23	55,62,68,70	0
5	ACT	B	505	4/4	0.83	0.19	36,48,52,55	0
6	BTB	B	507	14/14	0.86	0.14	50,64,79,86	0
6	BTB	A	506	14/14	0.89	0.15	32,74,82,86	0
5	ACT	A	505	4/4	0.90	0.12	37,38,45,45	0
4	A1BT1	B	503	32/32	0.91	0.16	22,49,116,121	0
4	A1BT1	A	503	32/32	0.92	0.14	23,45,106,113	0
5	ACT	A	504	4/4	0.93	0.10	42,45,50,52	0
6	BTB	B	506	14/14	0.93	0.09	27,31,38,39	0
5	ACT	B	504	4/4	0.94	0.09	35,42,42,43	0
3	H4B	A	502	17/17	0.97	0.05	20,27,34,36	0
2	HEM	A	501	43/43	0.98	0.06	20,27,36,45	0
3	H4B	B	502	17/17	0.98	0.04	21,26,35,38	0
8	GD	A	511	1/1	0.98	0.04	57,57,57,57	1
2	HEM	B	501	43/43	0.99	0.05	17,23,32,38	0
8	GD	B	511	1/1	0.99	0.03	32,32,32,32	0
9	ZN	A	512	1/1	1.00	0.01	28,28,28,28	0

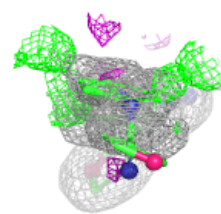
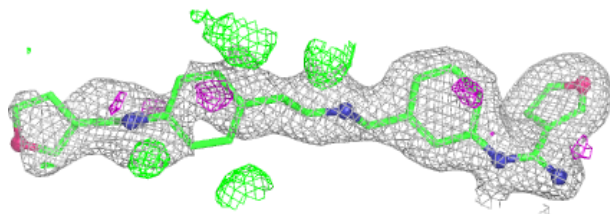
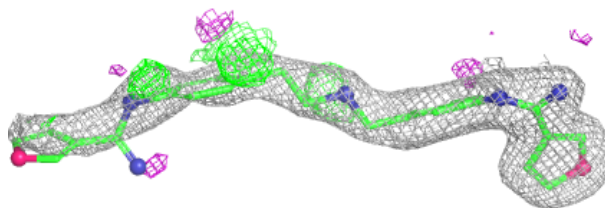
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1BT1 B 503:

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

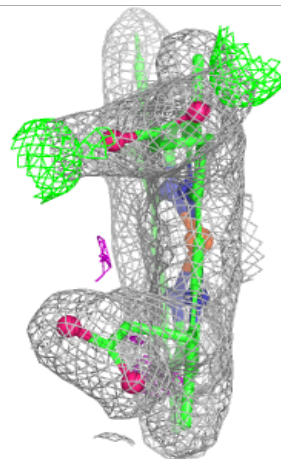
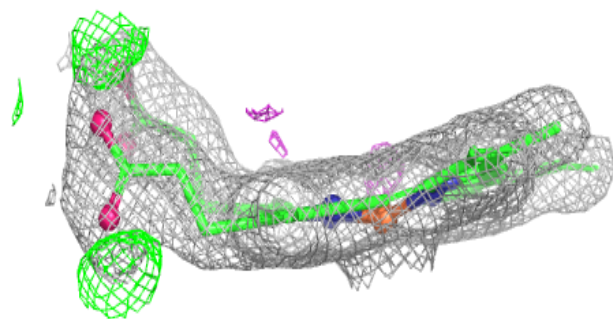
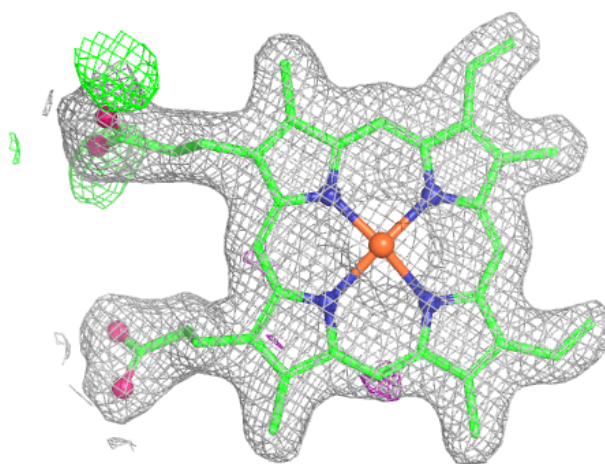
**Electron density around A1BT1 A 503:**

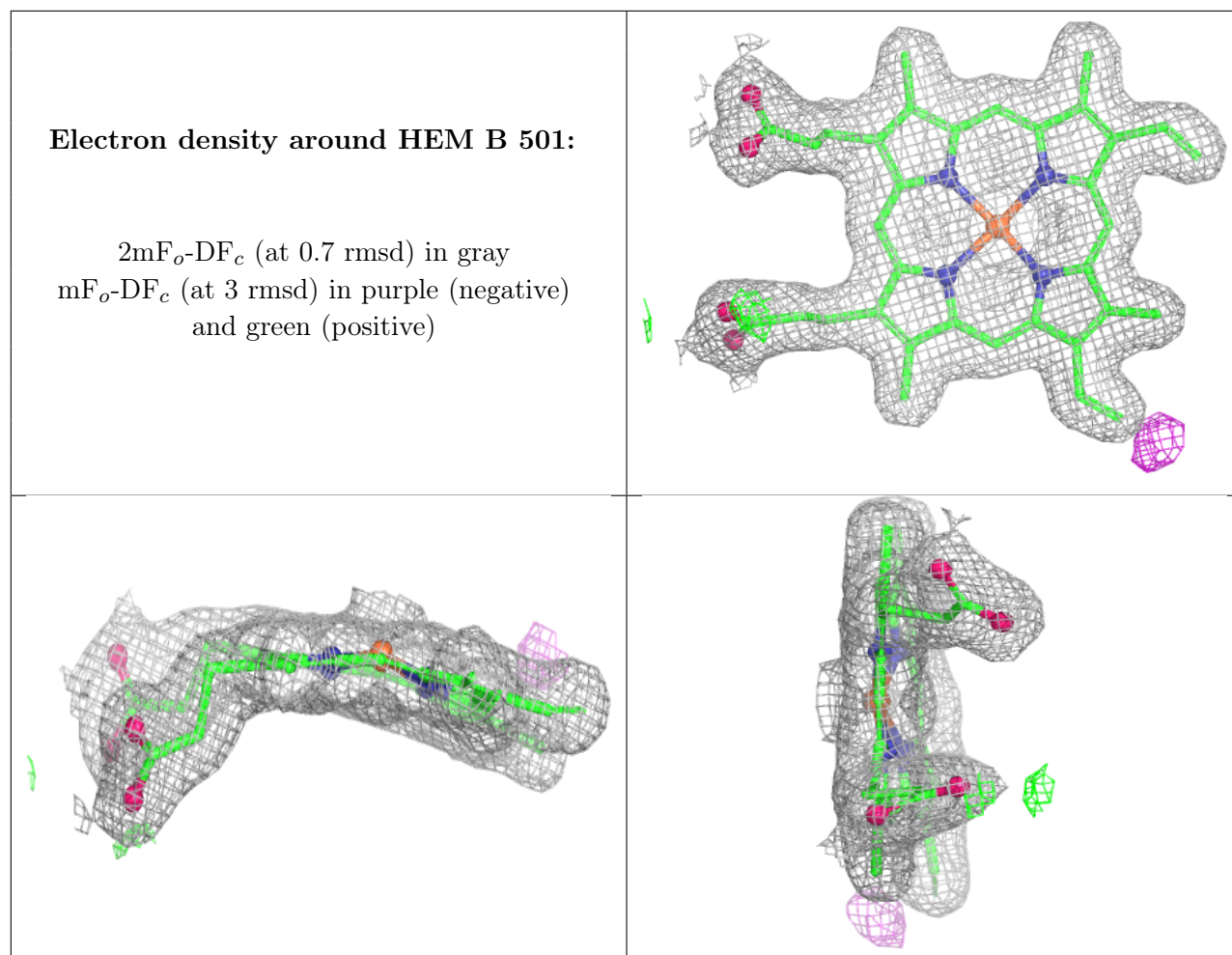
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.5 Other polymers [i](#)

There are no such residues in this entry.