



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 11:51 pm BST

PDB ID : 4KCP
Title : Structure of bovine endothelial nitric oxide synthase heme domain in complex with N-(4-(2-((3-(thiophene-2-carboximidamido)benzyl)amino)ethyl)phenyl)thiophene-2-carboximidamide
Authors : Chreifi, G.; Li, H.; Poulos, T.L.
Deposited on : 2013-04-24
Resolution : 2.07 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 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 : 2.11
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) : 2.11

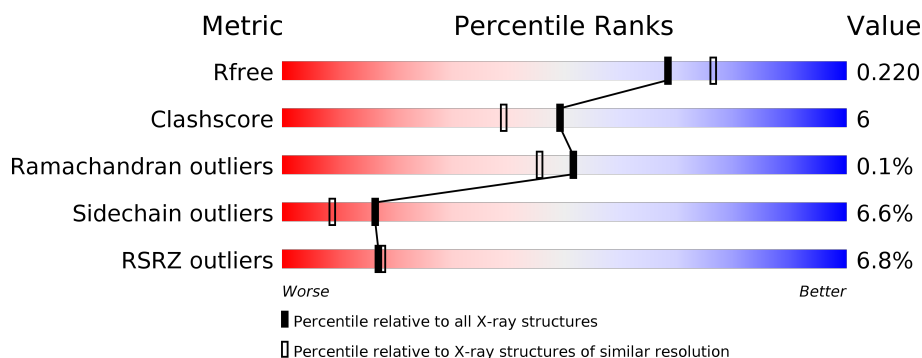
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.07 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	2684 (2.08-2.04)
Clashscore	141614	2801 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)
RSRZ outliers	127900	2646 (2.08-2.04)

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 on 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	443	<div> <div>5%</div> <div> <div></div> <div>78%</div> <div>11%</div> <div>•</div> <div>9%</div> </div> </div>
1	B	443	<div> <div>7%</div> <div> <div></div> <div>75%</div> <div>14%</div> <div>•</div> <div>9%</div> </div> </div>

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 6967 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.

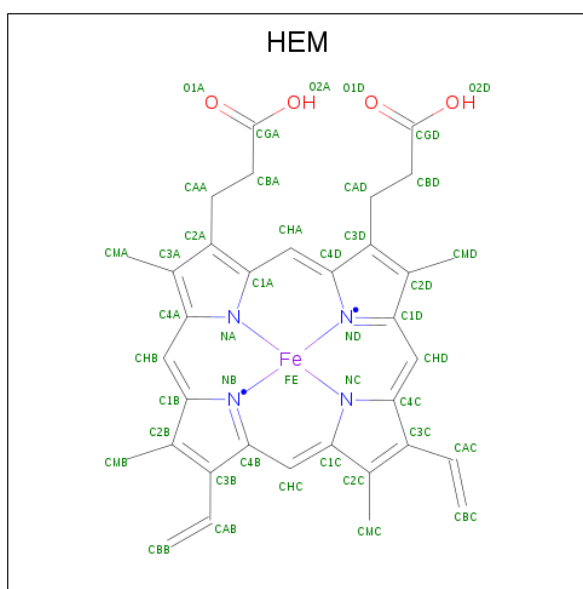
- Molecule 1 is a protein called Nitric oxide synthase, endothelial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	405	Total	As	C	N	O	S	0	0	0
			3223	1	2049	568	589	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: $C_{34}H_{32}FeN_4O_4$).



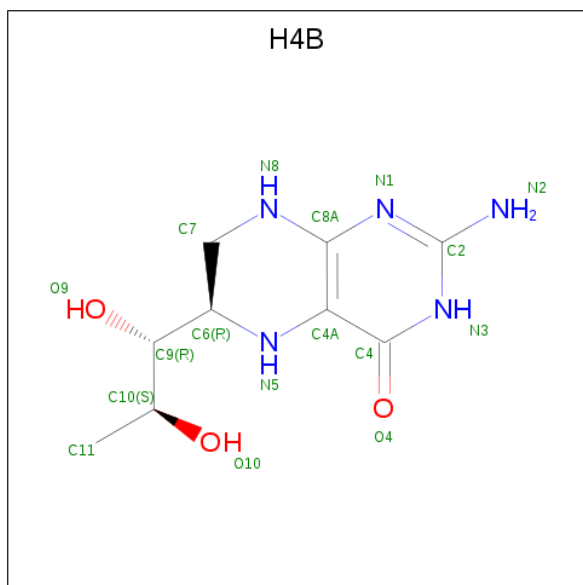
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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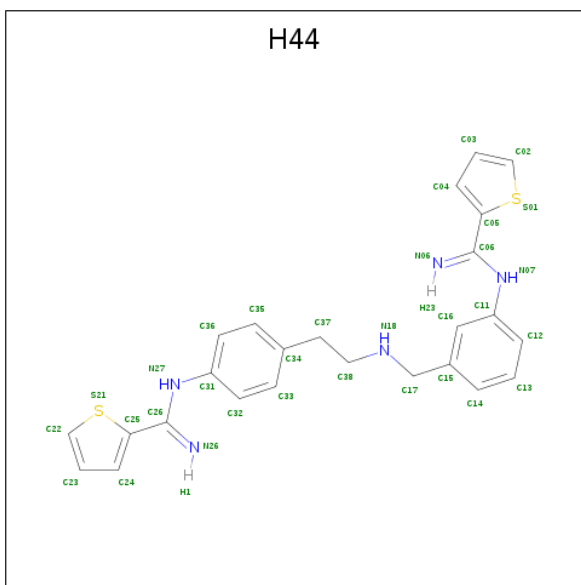
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



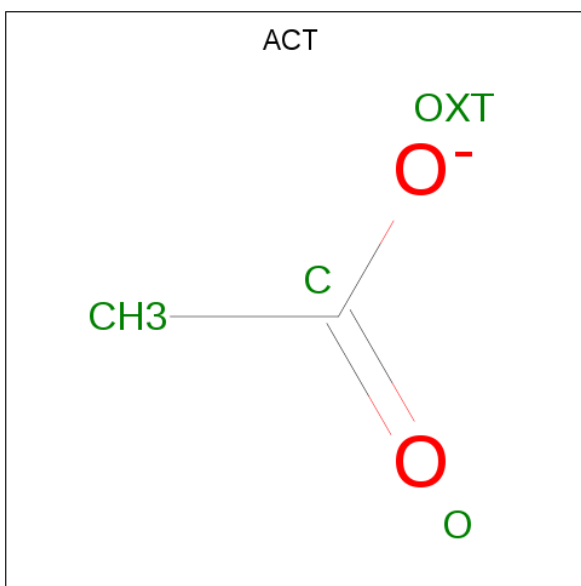
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 4 is N-(4-{2-[(3-{[(E)-imino(thiophen-2-yl)methyl]amino}benzyl)amino]ethyl}phenyl)thiophene-2-carboximidamide (three-letter code: H44) (formula: $C_{25}H_{25}N_5S_2$).



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

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $\text{C}_2\text{H}_3\text{O}_2$).



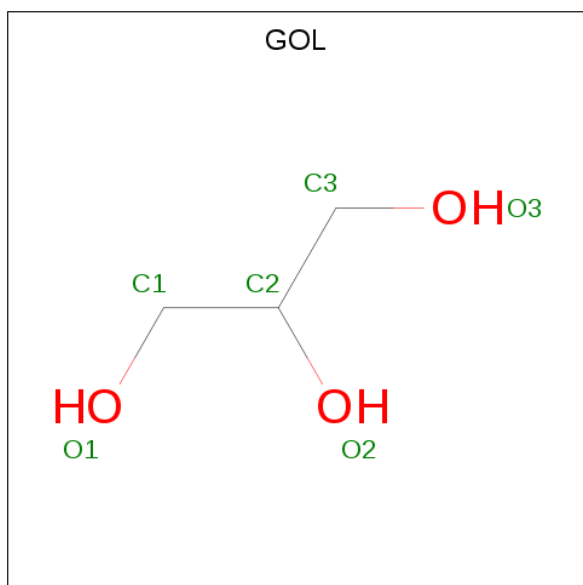
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0

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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 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	B	1	Total	C	O	0	0
			6	3	3		

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

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

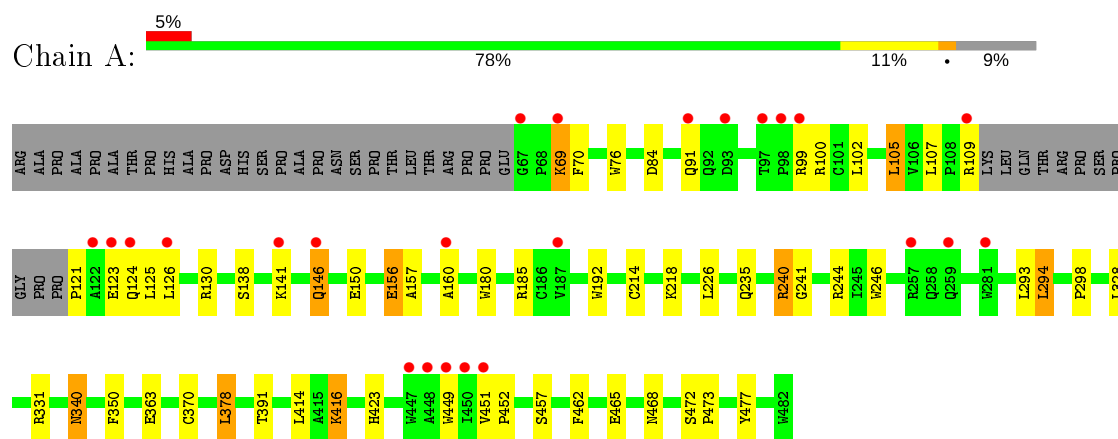
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	151	Total	O	0	0
			151	151		
8	B	151	Total	O	0	0
			151	151		

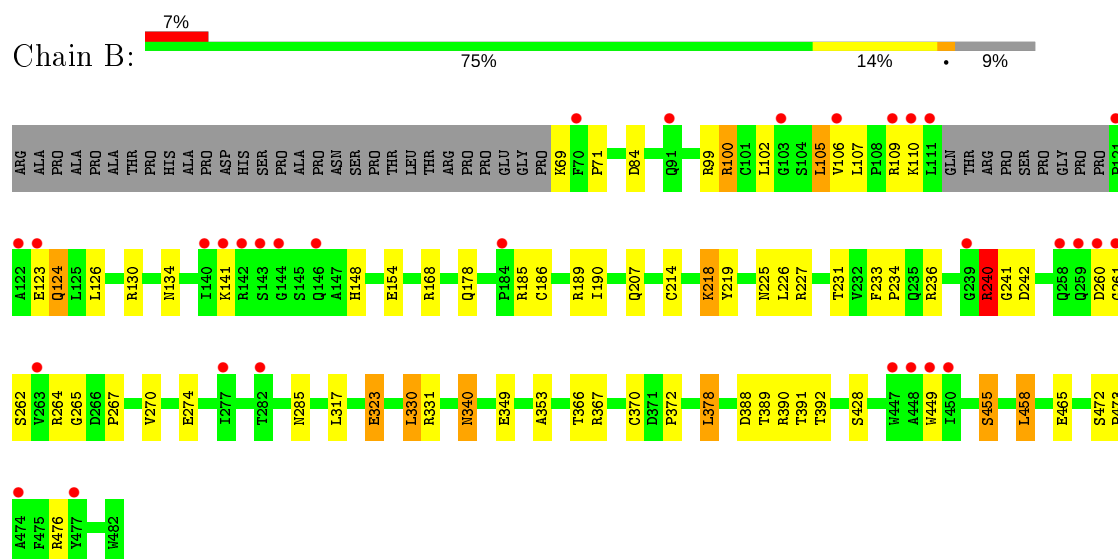
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.69Å 106.22Å 156.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.95 – 2.07 46.91 – 2.07	Depositor EDS
% Data completeness (in resolution range)	99.2 (46.95-2.07) 99.0 (46.91-2.07)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 2.07Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.166 , 0.213 0.174 , 0.220	Depositor DCC
R_{free} test set	2962 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	37.8	Xtriage
Anisotropy	0.394	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 51.2	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	0.97	EDS
Total number of atoms	6967	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% 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, ZN, H4B, CAS, H44, ACT, HEM

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	0.97	1/3303 (0.0%)	0.96	6/4497 (0.1%)
1	B	1.00	3/3308 (0.1%)	0.98	7/4502 (0.2%)
All	All	0.99	4/6611 (0.1%)	0.97	13/8999 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	455	SER	CB-OG	6.45	1.50	1.42
1	A	363	GLU	CD-OE1	6.41	1.32	1.25
1	B	349	GLU	CD-OE2	-6.11	1.19	1.25
1	B	428	SER	CB-OG	5.33	1.49	1.42

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	240	ARG	NE-CZ-NH2	-8.71	115.94	120.30
1	A	331	ARG	NE-CZ-NH1	8.30	124.45	120.30
1	B	240	ARG	NE-CZ-NH1	7.93	124.26	120.30
1	B	367	ARG	NE-CZ-NH2	-6.92	116.84	120.30
1	B	185	ARG	NE-CZ-NH1	6.43	123.52	120.30
1	B	367	ARG	NE-CZ-NH1	6.35	123.48	120.30
1	B	189	ARG	NE-CZ-NH1	-6.16	117.22	120.30
1	A	240	ARG	NE-CZ-NH1	5.87	123.24	120.30
1	A	414	LEU	CA-CB-CG	5.72	128.45	115.30
1	A	240	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	A	244	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	B	227	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	A	331	ARG	NE-CZ-NH2	-5.00	117.80	120.30

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	3223	0	3127	36	0
1	B	3229	0	3141	36	0
2	A	43	0	30	1	0
2	B	43	0	30	4	0
3	A	17	0	15	1	0
3	B	17	0	15	1	0
4	A	32	0	23	3	0
4	B	32	0	23	3	0
5	A	8	0	6	0	0
5	B	8	0	6	0	0
6	A	6	0	8	0	0
6	B	6	0	8	0	0
7	A	1	0	0	0	0
8	A	151	0	0	2	0
8	B	151	0	0	2	0
All	All	6967	0	6432	77	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.

All (77) 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:240:ARG:HD3	1:A:298:PRO:HB3	1.60	0.83
1:A:240:ARG:HD3	1:A:298:PRO:CB	2.15	0.75
1:B:270:VAL:O	1:B:274:GLU:HG3	1.87	0.74
1:A:146:GLN:O	1:A:150:GLU:HG3	1.88	0.74
1:A:214:CYS:SG	8:A:730:HOH:O	2.50	0.70
1:A:126:LEU:HD23	1:A:130:ARG:NH2	2.10	0.66
1:B:107:LEU:HD21	4:B:503:H44:H5	1.64	0.63
1:A:138:SER:O	1:A:141:LYS:HE3	1.99	0.63
1:A:126:LEU:HD21	1:A:156:GLU:HB3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:LYS:HD3	1:B:219:TYR:N	2.14	0.62
1:B:340:ASN:HD22	1:B:340:ASN:H	1.49	0.61
1:B:265:GLY:O	1:B:267:PRO:HD3	2.01	0.61
1:B:236:ARG:HD2	1:B:242:ASP:OD1	2.00	0.60
1:B:455:SER:O	1:B:458:LEU:HB2	2.02	0.59
2:B:501:HEM:HBC2	2:B:501:HEM:HMC1	1.85	0.59
1:A:76:TRP:CZ2	1:B:106:VAL:HB	2.37	0.59
1:B:233:PHE:HB3	1:B:234:PRO:CD	2.33	0.58
2:B:501:HEM:HBC2	2:B:501:HEM:CMC	2.33	0.58
1:A:465:GLU:OE1	1:B:105:LEU:HD13	2.04	0.57
1:A:240:ARG:HD2	1:A:241:GLY:O	2.04	0.57
1:A:449:TRP:HA	3:A:502:H4B:N1	2.20	0.57
1:A:126:LEU:HD11	1:A:156:GLU:HA	1.85	0.57
1:B:370:CYS:SG	1:B:378:LEU:HD13	2.46	0.56
4:A:503:H44:N26	4:A:503:H44:H6	2.22	0.55
1:B:260:ASP:O	1:B:262:SER:N	2.38	0.55
1:B:366:THR:O	1:B:370:CYS:HB2	2.08	0.54
1:B:154:GLU:OE1	1:B:168:ARG:NH2	2.42	0.52
4:B:503:H44:N26	4:B:503:H44:H6	2.25	0.51
1:A:240:ARG:CD	1:A:298:PRO:HB3	2.38	0.51
1:A:340:ASN:HD22	1:A:340:ASN:H	1.58	0.50
2:B:501:HEM:HBB2	2:B:501:HEM:HHC	1.93	0.50
1:B:455:SER:HB3	1:B:458:LEU:HD22	1.94	0.50
1:A:378:LEU:HB2	8:A:625:HOH:O	2.11	0.49
1:B:340:ASN:N	1:B:340:ASN:HD22	2.07	0.49
1:B:323:GLU:CD	1:B:323:GLU:H	2.16	0.49
1:A:246:TRP:HB2	1:A:294:LEU:HB3	1.95	0.49
1:B:388:ASP:CG	1:B:390:ARG:HH21	2.17	0.48
1:B:476:ARG:NH1	8:B:694:HOH:O	2.47	0.48
1:A:70:PHE:HB3	1:A:84:ASP:O	2.14	0.48
1:A:370:CYS:SG	1:A:378:LEU:HD13	2.53	0.47
1:A:69:LYS:CE	1:A:69:LYS:HA	2.43	0.47
1:A:69:LYS:HE2	1:A:69:LYS:HA	1.97	0.47
1:B:240:ARG:HD2	1:B:241:GLY:O	2.15	0.47
1:A:126:LEU:HD23	1:A:130:ARG:HH21	1.80	0.47
4:A:503:H44:C12	4:A:503:H44:C05	2.92	0.47
1:A:105:LEU:HD22	1:B:465:GLU:HB3	1.96	0.47
4:B:503:H44:C05	4:B:503:H44:C12	2.93	0.46
1:A:105:LEU:N	1:A:105:LEU:HD23	2.31	0.45
1:A:214:CYS:O	1:A:218:LYS:HG3	2.17	0.45
1:B:264:ARG:NE	1:B:285:ASN:O	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:CYS:HB2	2:B:501:HEM:ND	2.33	0.44
1:B:99:ARG:HG2	1:B:100:ARG:HD2	1.99	0.44
1:A:185:ARG:NH1	1:A:477:TYR:OH	2.51	0.43
1:B:472:SER:HA	1:B:473:PRO:C	2.39	0.43
4:A:503:H44:H2O	4:A:503:H44:C05	2.49	0.43
1:B:449:TRP:HA	3:B:502:H4B:N1	2.32	0.43
2:A:501:HEM:HBB2	2:A:501:HEM:HHC	2.01	0.43
1:A:423:HIS:HB2	1:B:392:THR:HB	2.00	0.43
1:A:157:ALA:O	1:A:160:ALA:HB3	2.19	0.43
1:A:235:GLN:HB3	1:A:350:PHE:CE1	2.54	0.42
1:A:451:VAL:HA	1:A:452:PRO:HD3	1.91	0.42
1:A:121:PRO:O	1:A:124:GLN:N	2.53	0.41
1:A:457:SER:HA	1:A:462:PHE:CG	2.55	0.41
1:B:134:ASN:OD1	1:B:148:HIS:NE2	2.51	0.41
1:A:180:TRP:CE3	1:A:192:TRP:HA	2.55	0.41
1:B:126:LEU:O	1:B:130:ARG:HG3	2.20	0.41
1:B:236:ARG:CD	1:B:242:ASP:OD1	2.67	0.41
1:A:472:SER:HA	1:A:473:PRO:C	2.40	0.41
1:B:317:LEU:HD12	1:B:330:LEU:HB3	2.02	0.41
1:B:123:GLU:HG2	1:B:124:GLN:N	2.36	0.41
1:B:71:PRO:HG2	1:B:84:ASP:HB3	2.02	0.41
1:A:121:PRO:HB2	1:A:124:GLN:HB3	2.03	0.41
1:A:146:GLN:CD	1:A:150:GLU:OE2	2.59	0.41
1:B:214:CYS:SG	8:B:733:HOH:O	2.45	0.41
1:A:416:LYS:HA	1:A:416:LYS:HE3	2.03	0.40
1:B:231:THR:O	1:B:353:ALA:HA	2.22	0.40
1:B:340:ASN:ND2	1:B:340:ASN:H	2.17	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	400/443 (90%)	388 (97%)	12 (3%)	0	100	100
1	B	400/443 (90%)	388 (97%)	11 (3%)	1 (0%)	41	32
All	All	800/886 (90%)	776 (97%)	23 (3%)	1 (0%)	51	45

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	261	GLY

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	343/375 (92%)	322 (94%)	21 (6%)	18	10
1	B	344/375 (92%)	320 (93%)	24 (7%)	15	7
All	All	687/750 (92%)	642 (93%)	45 (7%)	16	9

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	LYS
1	A	91	GLN
1	A	99	ARG
1	A	100	ARG
1	A	102	LEU
1	A	105	LEU
1	A	107	LEU
1	A	109	ARG
1	A	123	GLU
1	A	125	LEU
1	A	146	GLN
1	A	156	GLU
1	A	226	LEU
1	A	293	LEU
1	A	294	LEU

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Mol	Chain	Res	Type
1	A	328	LEU
1	A	340	ASN
1	A	378	LEU
1	A	391	THR
1	A	416	LYS
1	A	468	ASN
1	B	69	LYS
1	B	100	ARG
1	B	102	LEU
1	B	105	LEU
1	B	109	ARG
1	B	110	LYS
1	B	124	GLN
1	B	141	LYS
1	B	178	GLN
1	B	190	ILE
1	B	207	GLN
1	B	218	LYS
1	B	225	ASN
1	B	226	LEU
1	B	240	ARG
1	B	323	GLU
1	B	330	LEU
1	B	331	ARG
1	B	340	ASN
1	B	372	PRO
1	B	378	LEU
1	B	389	THR
1	B	391	THR
1	B	458	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	A	146	GLN
1	A	153	GLN
1	A	166	HIS
1	A	191	GLN
1	A	340	ASN
1	A	376	ASN
1	A	413	GLN

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Mol	Chain	Res	Type
1	A	468	ASN
1	B	191	GLN
1	B	222	ASN
1	B	225	ASN
1	B	340	ASN
1	B	376	ASN
1	B	405	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	0.96	0	1,9,11	0.73	0
1	CAS	B	384	1	5,8,9	1.48	2 (40%)	1,9,11	0.12	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	-
1	CAS	B	384	1	-	0/0/7/9	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	384	CAS	AS-CE2	2.11	2.01	1.96
1	B	384	CAS	AS-CE1	2.05	2.01	1.96

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 1 is monoatomic - leaving 12 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	$\# Z > 2$
6	GOL	B	506	-	5,5,5	0.45	0	5,5,5	0.87	0
5	ACT	B	505	-	1,3,3	4.90	1 (100%)	0,3,3	0.00	-
4	H44	A	503	-	35,35,35	1.58	4 (11%)	29,46,46	1.81	7 (24%)
4	H44	B	503	-	35,35,35	1.41	3 (8%)	29,46,46	1.60	5 (17%)
3	H4B	B	502	-	16,18,18	1.14	1 (6%)	11,26,26	2.34	5 (45%)
5	ACT	B	504	-	1,3,3	0.04	0	0,3,3	0.00	-
3	H4B	A	502	-	16,18,18	1.60	3 (18%)	11,26,26	3.04	7 (63%)
2	HEM	B	501	1	27,50,50	1.18	3 (11%)	17,82,82	1.48	4 (23%)
6	GOL	A	506	-	5,5,5	0.66	0	5,5,5	0.62	0
5	ACT	A	505	-	1,3,3	0.83	0	0,3,3	0.00	-
2	HEM	A	501	1	27,50,50	1.41	5 (18%)	17,82,82	2.12	9 (52%)
5	ACT	A	504	-	1,3,3	0.63	0	0,3,3	0.00	-

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	B	502	-	-	0/8/17/17	0/2/2/2
4	H44	A	503	-	-	3/15/23/23	0/4/4/4
4	H44	B	503	-	-	2/15/23/23	0/4/4/4
6	GOL	B	506	-	-	0/4/4/4	-
3	H4B	A	502	-	-	0/8/17/17	0/2/2/2
2	HEM	B	501	1	-	0/6/54/54	-
6	GOL	A	506	-	-	1/4/4/4	-
2	HEM	A	501	1	-	0/6/54/54	-

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	503	H44	C25-C26	5.26	1.52	1.45
5	B	505	ACT	CH3-C	4.90	1.55	1.48
4	B	503	H44	C25-C26	4.65	1.52	1.45
3	A	502	H4B	C4-C4A	-4.04	1.36	1.41
2	A	501	HEM	C4D-C3D	3.77	1.51	1.42
4	A	503	H44	C05-C06	3.32	1.50	1.45
2	A	501	HEM	C3B-C2B	-3.27	1.35	1.40
4	A	503	H44	C06-N07	-2.90	1.33	1.39
4	B	503	H44	C06-N07	-2.89	1.33	1.39
2	B	501	HEM	C3B-C2B	-2.78	1.36	1.40
3	A	502	H4B	C4-N3	2.61	1.37	1.33
2	A	501	HEM	C4B-NB	-2.49	1.31	1.36
2	B	501	HEM	C3C-C2C	-2.42	1.37	1.40
2	A	501	HEM	C4A-NA	2.22	1.40	1.36
4	A	503	H44	C25-S21	2.16	1.74	1.72
4	B	503	H44	C05-C06	2.11	1.48	1.45
2	A	501	HEM	C1A-NA	2.11	1.40	1.36
2	B	501	HEM	CAD-C3D	2.07	1.55	1.52
3	B	502	H4B	C7-C6	2.04	1.54	1.52
3	A	502	H4B	C7-N8	2.02	1.48	1.44

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	H4B	N2-C2-N3	5.37	125.61	117.25
2	A	501	HEM	CAA-CBA-CGA	4.69	120.54	112.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	H4B	C4-C4A-C8A	4.35	118.43	114.57
3	A	502	H4B	C4-C4A-N5	4.33	122.75	119.12
4	A	503	H44	C03-C02-S01	-4.17	109.60	112.98
3	B	502	H4B	C4-C4A-C8A	4.10	118.21	114.57
4	A	503	H44	C17-C15-C14	-4.09	112.43	120.91
4	B	503	H44	C17-N18-C38	4.01	127.14	113.41
4	B	503	H44	C17-C15-C14	-3.79	113.05	120.91
3	B	502	H4B	N2-C2-N3	3.71	123.02	117.25
4	B	503	H44	C23-C22-S21	-3.44	110.19	112.98
4	A	503	H44	C23-C22-S21	-3.37	110.25	112.98
2	B	501	HEM	CAA-CBA-CGA	3.33	118.26	112.67
4	A	503	H44	C12-C11-C16	-3.30	115.74	119.65
2	B	501	HEM	CBA-CAA-C2A	-3.14	106.70	112.49
3	A	502	H4B	C4-N3-C2	3.11	120.86	115.93
3	B	502	H4B	C2-N1-C8A	3.09	121.47	114.54
4	A	503	H44	C17-C15-C16	3.08	127.29	120.64
3	B	502	H4B	N3-C2-N1	-3.02	120.67	125.42
4	B	503	H44	C17-C15-C16	2.91	126.92	120.64
4	B	503	H44	C03-C02-S01	-2.86	110.66	112.98
3	A	502	H4B	N3-C2-N1	-2.78	121.06	125.42
2	B	501	HEM	CBD-CAD-C3D	2.63	117.32	112.48
4	A	503	H44	C17-N18-C38	2.55	122.13	113.41
2	A	501	HEM	CMC-C2C-C3C	2.53	129.42	124.68
3	A	502	H4B	N2-C2-N1	-2.52	113.33	117.25
3	B	502	H4B	C4-C4A-N5	2.36	121.10	119.12
2	A	501	HEM	C1D-C2D-C3D	-2.28	105.41	107.00
2	A	501	HEM	CBD-CAD-C3D	2.24	116.61	112.48
2	A	501	HEM	CAD-CBD-CGD	2.24	116.43	112.67
2	A	501	HEM	CMB-C2B-C3B	2.21	128.81	124.68
2	A	501	HEM	CMD-C2D-C3D	2.16	129.01	124.94
4	A	503	H44	C13-C12-C11	2.16	122.30	119.72
2	A	501	HEM	CMA-C3A-C2A	-2.13	120.92	124.94
3	A	502	H4B	C4A-C4-N3	-2.11	118.01	124.01
2	B	501	HEM	C4A-C3A-C2A	2.10	108.46	107.00
2	A	501	HEM	CMA-C3A-C4A	2.06	131.63	128.46

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	503	H44	C15-C17-N18-C38
4	B	503	H44	C15-C17-N18-C38

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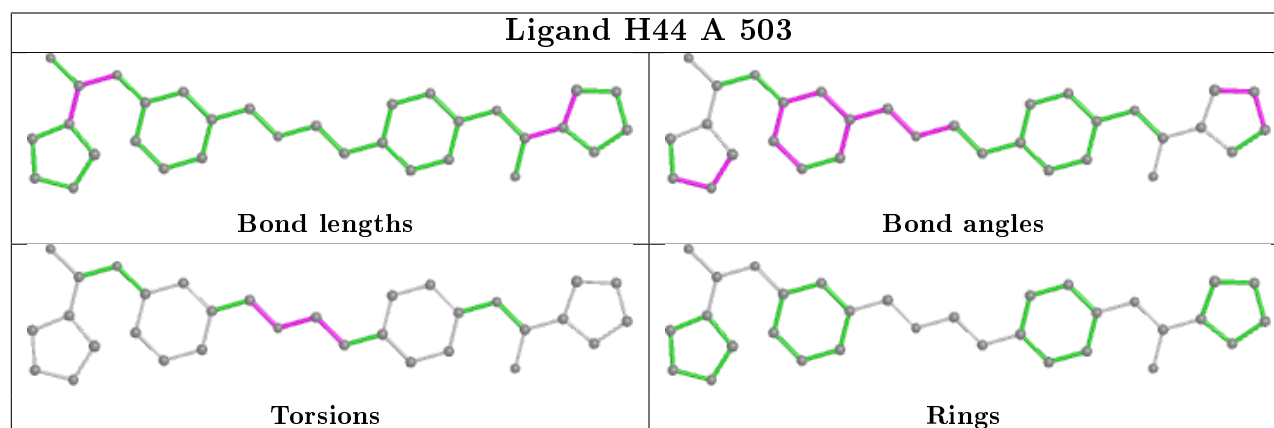
Mol	Chain	Res	Type	Atoms
4	B	503	H44	C37-C38-N18-C17
4	A	503	H44	C37-C38-N18-C17
4	A	503	H44	C34-C37-C38-N18
6	A	506	GOL	O1-C1-C2-C3

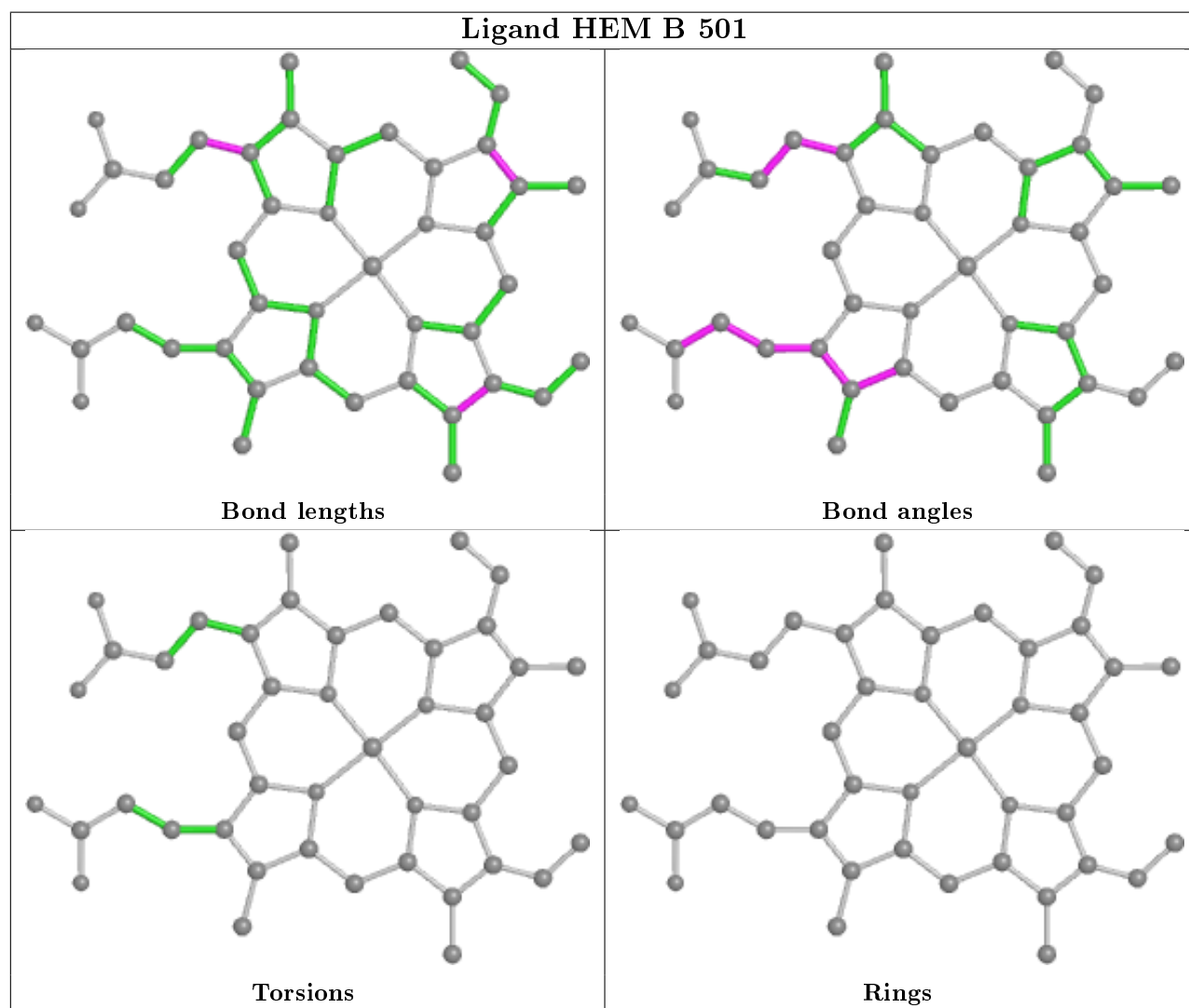
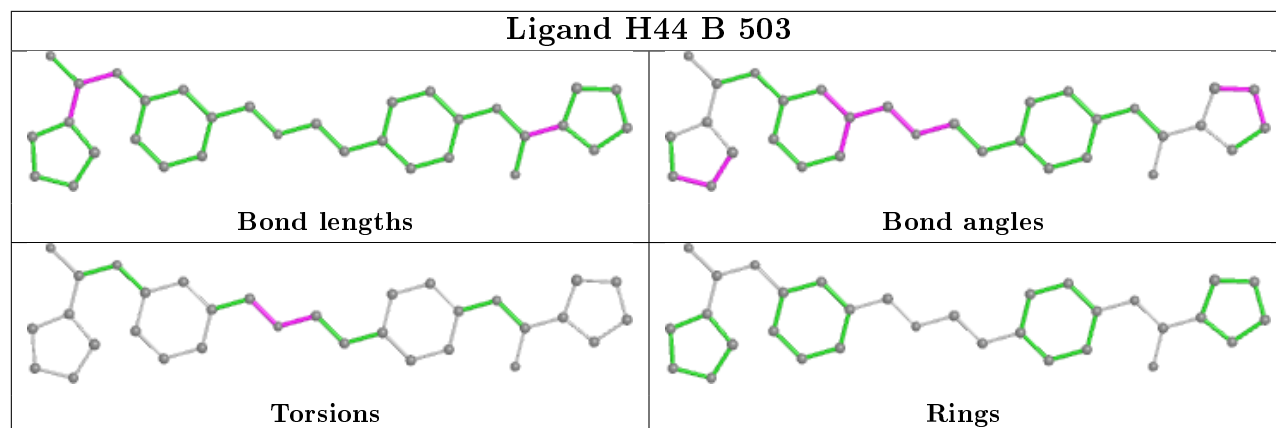
There are no ring outliers.

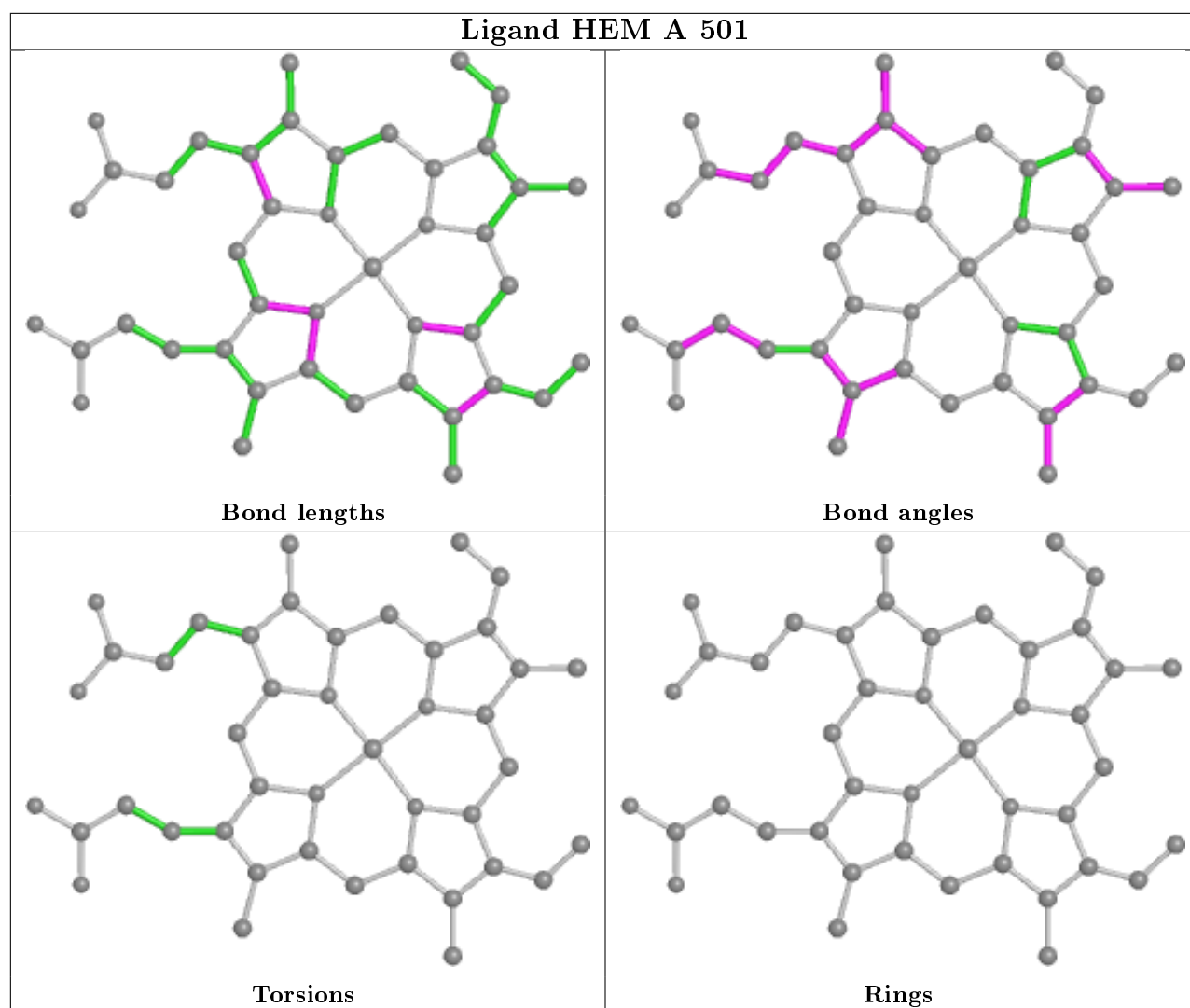
6 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	503	H44	3	0
4	B	503	H44	3	0
3	B	502	H4B	1	0
3	A	502	H4B	1	0
2	B	501	HEM	4	0
2	A	501	HEM	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	404/443 (91%)	0.25	24 (5%) 22 23	29, 41, 73, 119	0
1	B	404/443 (91%)	0.28	31 (7%) 13 13	29, 43, 74, 131	0
All	All	808/886 (91%)	0.26	55 (6%) 17 18	29, 42, 74, 131	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	110	LYS	7.8
1	B	111	LEU	6.0
1	B	259	GLN	5.0
1	B	91	GLN	4.5
1	A	123	GLU	4.2
1	A	91	GLN	4.1
1	B	146	GLN	3.8
1	A	126	LEU	3.7
1	A	67	GLY	3.7
1	A	99	ARG	3.6
1	A	450	ILE	3.5
1	B	261	GLY	3.4
1	A	69	LYS	3.3
1	A	109	ARG	3.3
1	B	142	ARG	3.2
1	B	449	TRP	3.2
1	B	140	ILE	3.1
1	A	97	THR	3.1
1	B	121	PRO	3.1
1	B	70	PHE	3.1
1	A	259	GLN	3.1
1	B	143	SER	3.0
1	B	448	ALA	3.0
1	B	260	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	448	ALA	2.8
1	B	109	ARG	2.8
1	A	146	GLN	2.7
1	B	258	GLN	2.7
1	A	160	ALA	2.7
1	A	449	TRP	2.7
1	B	122	ALA	2.7
1	A	451	VAL	2.7
1	B	447	TRP	2.6
1	A	447	TRP	2.5
1	B	141	LYS	2.5
1	B	263	VAL	2.5
1	A	187	VAL	2.4
1	A	141	LYS	2.4
1	A	257	ARG	2.4
1	B	477	TYR	2.4
1	B	277	ILE	2.3
1	A	98	PRO	2.3
1	B	450	ILE	2.3
1	B	144	GLY	2.2
1	A	281	TRP	2.2
1	B	282	THR	2.1
1	A	93	ASP	2.1
1	B	103	GLY	2.1
1	B	123	GLU	2.1
1	A	122	ALA	2.0
1	B	474	ALA	2.0
1	B	106	VAL	2.0
1	B	184	PRO	2.0
1	A	124	GLN	2.0
1	B	239	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(\AA^2)	Q<0.9
1	CAS	B	384	9/10	0.96	0.10	42,47,62,71	0
1	CAS	A	384	9/10	0.98	0.09	38,41,65,67	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

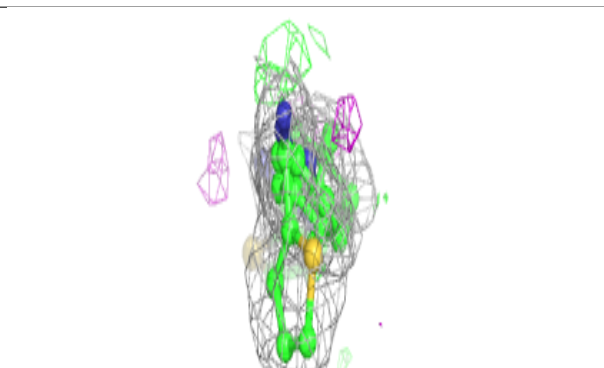
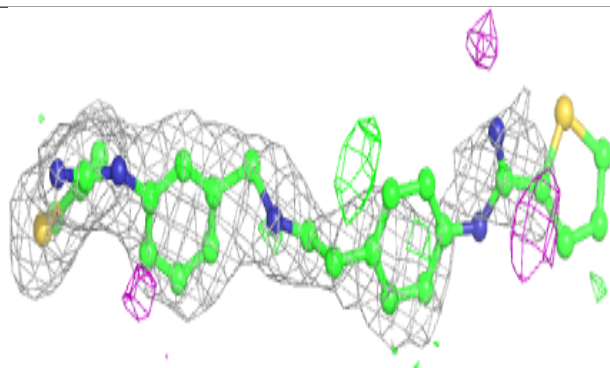
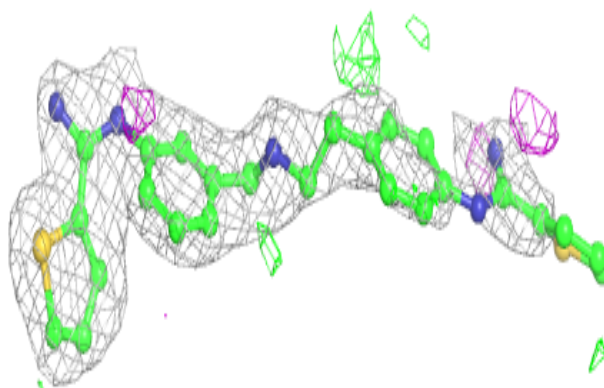
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	H44	A	503	32/32	0.92	0.23	29,55,128,147	0
6	GOL	A	506	6/6	0.93	0.21	58,64,69,71	0
6	GOL	B	506	6/6	0.94	0.26	54,69,77,82	0
4	H44	B	503	32/32	0.94	0.23	25,54,141,147	0
5	ACT	B	504	4/4	0.95	0.20	50,50,53,56	0
5	ACT	B	505	4/4	0.97	0.10	37,37,38,41	0
3	H4B	A	502	17/17	0.97	0.20	33,38,42,43	0
3	H4B	B	502	17/17	0.97	0.23	33,36,43,44	0
2	HEM	B	501	43/43	0.98	0.18	31,35,44,47	0
5	ACT	A	505	4/4	0.98	0.12	38,40,40,42	0
2	HEM	A	501	43/43	0.98	0.19	29,35,40,46	0
5	ACT	A	504	4/4	0.98	0.12	47,49,55,58	0
7	ZN	A	507	1/1	0.99	0.06	59,59,59,59	0

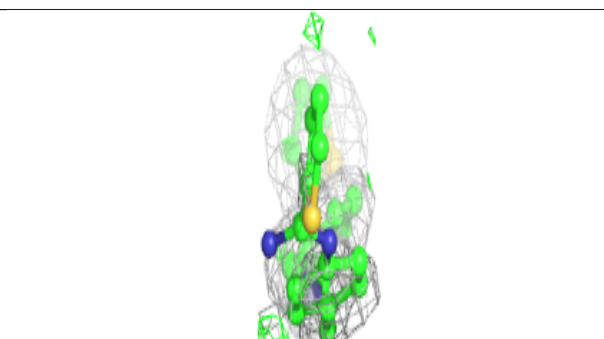
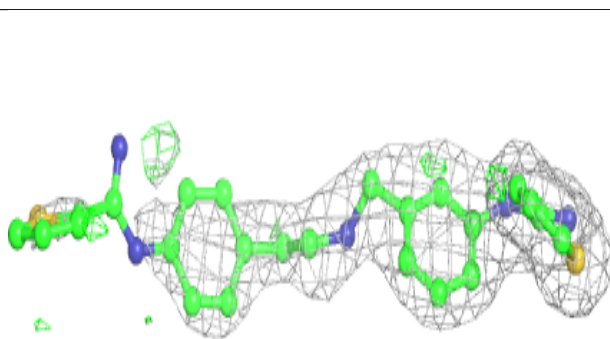
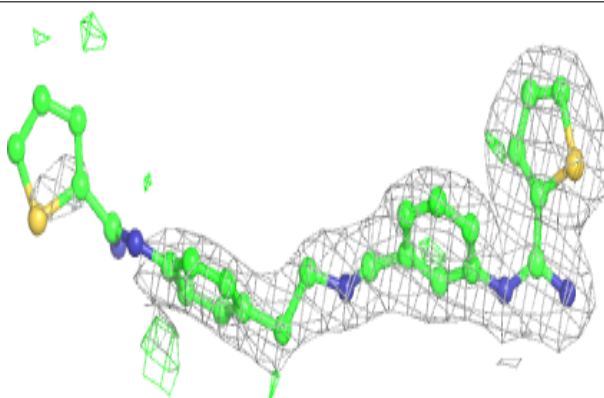
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around H44 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)

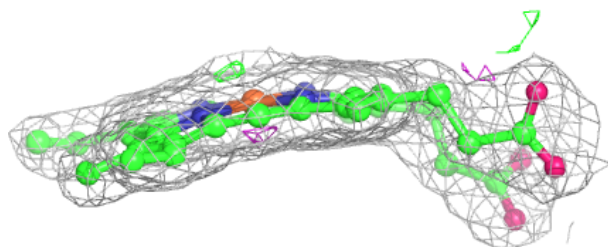
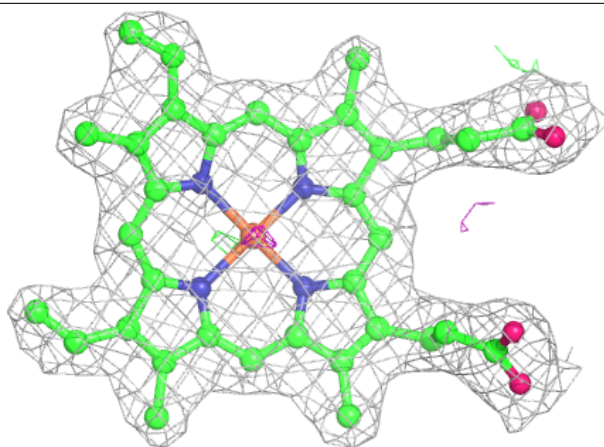
**Electron density around H44 B 503:**

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



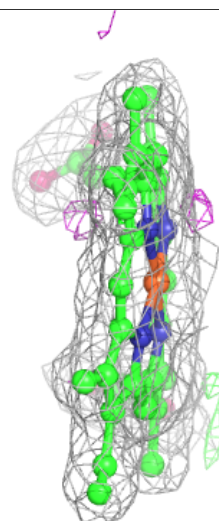
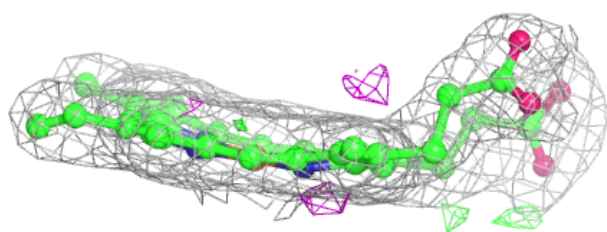
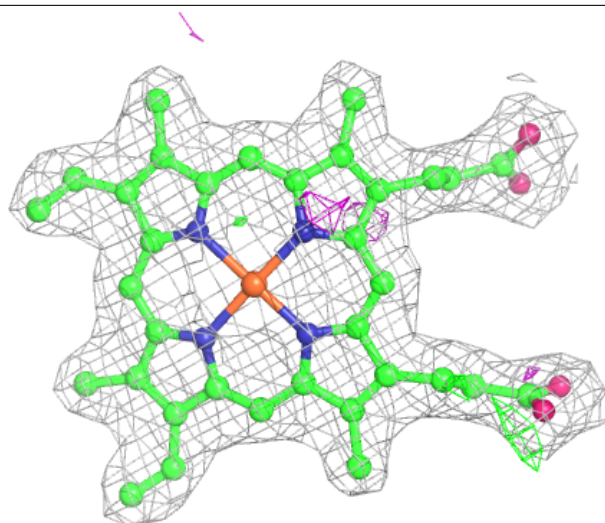
Electron density around HEM B 501:

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



Electron density around HEM 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 ⓘ

There are no such residues in this entry.