



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:17 PM UTC

PDB ID : 1I83 / pdb_00001i83
Title : BOVINE ENDOTHELIAL NITRIC OXIDE SYNTHASE HEME DOMAIN
COMPLEXED WITH N1,N14-BIS((S-METHYL)ISOTHIOUREIDO)TETR
ADECANE (H4B FREE)
Authors : Raman, C.S.; Li, H.; Martasek, P.; Babu, B.R.; Griffith, O.W.; Masters, B.S.S.;
Poulos, T.L.
Deposited on : 2001-03-12
Resolution : 2.00 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](#) ①) 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

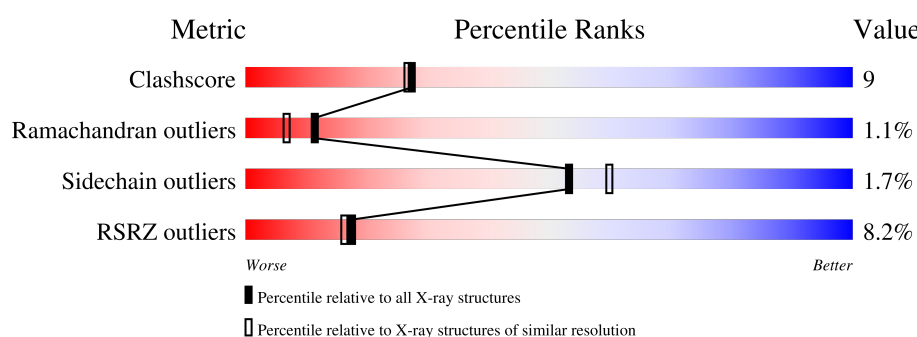
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	444	
1	B	444	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	GOL	B	2890	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 7231 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.

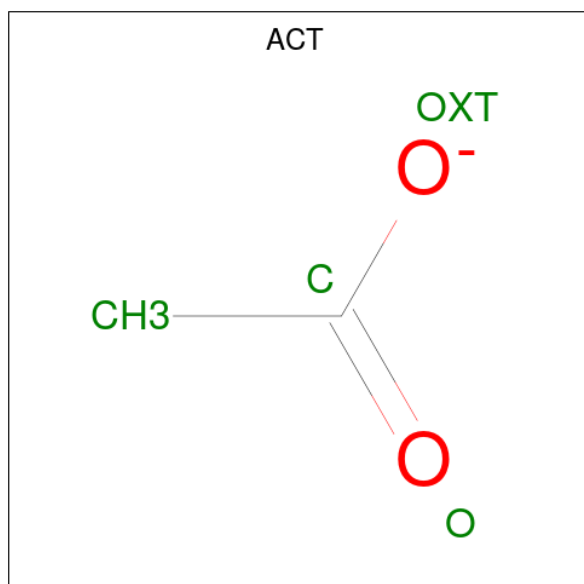
- Molecule 1 is a protein called NITRIC OXIDE SYNTHASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	416	Total	As	C	N	O	S	0	0	0
			3305	1	2101	584	603	16			
1	B	414	Total	As	C	N	O	S	0	0	0
			3294	1	2094	582	601	16			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	ARG	CYS	conflict	UNP P29473
A	384	CAS	CYS	modified residue	UNP P29473
B	100	ARG	CYS	conflict	UNP P29473
B	384	CAS	CYS	modified residue	UNP P29473

- Molecule 2 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).

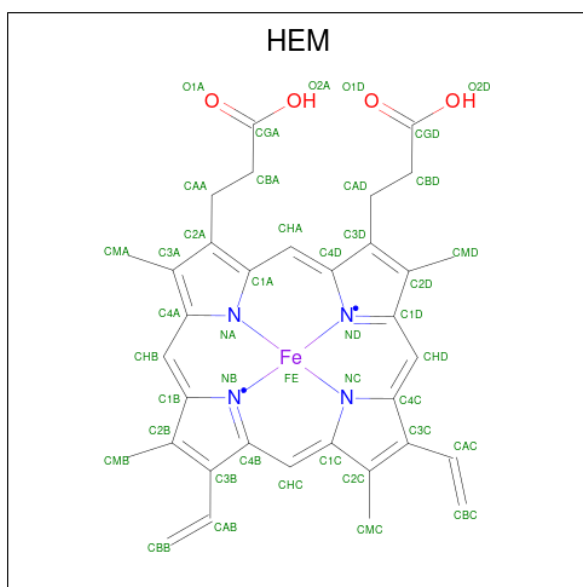


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

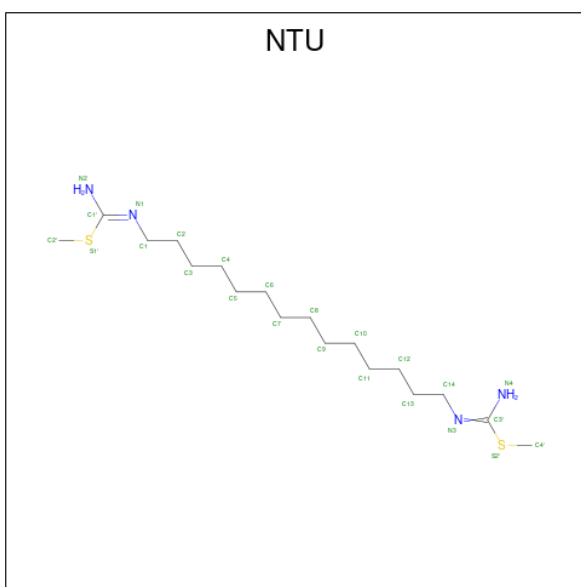
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).



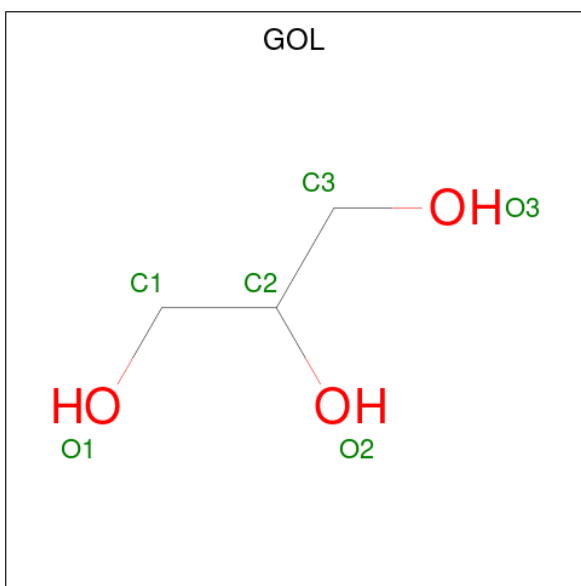
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 5 is N1,N14-BIS((S-METHYL)ISOTHIOUREIDO)TETRADECANE (CCD ID: NTU) (formula: C₁₈H₃₈N₄S₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total 9	C 6	N 2	S 1	0	0
5	B	1	Total 9	C 6	N 2	S 1	0	0

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).



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

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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	257	Total	O	0	0
			257	257		
7	B	240	Total	O	0	0
			240	240		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.39Å 106.65Å 156.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.08 – 2.00 44.08 – 2.00	Depositor EDS
% Data completeness (in resolution range)	86.1 (44.08-2.00) 87.7 (44.08-2.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.77 (at 1.91Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.213 , 0.248 0.211 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	30.2	Xtriage
Anisotropy	0.512	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 44.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7231	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% 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: NTU, HEM, CAS, GOL, ACT, ZN

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	0.39	0/3390	0.91	6/4620 (0.1%)
1	B	0.37	0/3378	0.92	9/4603 (0.2%)
All	All	0.38	0/6768	0.91	15/9223 (0.2%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	360	MET	N-CA-C	-9.13	94.36	109.24
1	B	360	MET	N-CA-C	-8.76	94.96	109.24
1	B	243	PHE	N-CA-C	-7.22	97.47	109.46
1	B	335	LEU	N-CA-C	6.83	120.99	108.69
1	A	243	PHE	N-CA-C	-6.80	98.94	109.76
1	A	361	SER	N-CA-C	6.24	119.74	111.75
1	B	451	VAL	CA-C-N	6.12	124.13	119.66
1	B	451	VAL	C-N-CA	6.12	124.13	119.66
1	B	361	SER	N-CA-C	5.63	118.96	111.75
1	B	297	ALA	N-CA-C	-5.48	103.02	110.36
1	A	226	LEU	N-CA-C	5.45	117.32	110.24
1	B	245	ILE	N-CA-C	-5.06	99.89	107.37
1	B	312	VAL	N-CA-C	5.04	113.86	106.55
1	A	470	ILE	N-CA-C	5.04	115.35	107.99
1	A	192	TRP	N-CA-C	5.00	117.38	111.33

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	3305	0	3215	63	0
1	B	3294	0	3205	57	0
2	A	8	0	6	0	0
2	B	4	0	3	0	0
3	A	1	0	0	0	0
4	A	43	0	30	0	0
4	B	43	0	30	2	0
5	A	9	0	11	1	0
5	B	9	0	11	0	0
6	A	12	0	16	2	0
6	B	6	0	8	4	0
7	A	257	0	0	1	0
7	B	240	0	0	1	0
All	All	7231	0	6535	121	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 9.

All (121) 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:119:PRO:HG3	1:A:238:PRO:HB3	1.31	1.11
1:A:99:ARG:HB2	1:A:99:ARG:HH11	1.26	0.98
1:B:112:GLN:HG3	1:B:113:THR:H	1.34	0.91
1:A:115:PRO:HD3	1:A:479:PRO:HG2	1.52	0.91
1:B:114:ARG:HA	1:B:114:ARG:HH11	1.44	0.83
6:A:2880:GOL:H32	6:B:2890:GOL:O1	1.86	0.75
1:A:270:VAL:O	1:A:274:GLU:HG3	1.92	0.69
1:B:114:ARG:HD3	1:B:115:PRO:HD2	1.75	0.68
1:A:146:GLN:O	1:A:150:GLU:HG3	1.94	0.67
1:A:115:PRO:O	1:A:117:PRO:HD3	1.96	0.66
1:A:115:PRO:HD3	1:A:479:PRO:CG	2.26	0.64
1:B:113:THR:HG21	1:B:342:LEU:HD13	1.80	0.63
1:B:370:CYS:SG	1:B:378:LEU:HD13	2.40	0.62
1:A:152:LEU:O	1:A:156:GLU:HG3	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:GLN:HG3	1:B:113:THR:N	2.11	0.61
1:B:366:THR:O	1:B:370:CYS:HB2	2.00	0.61
1:B:367:ARG:HH12	6:B:2890:GOL:H31	1.65	0.61
1:B:114:ARG:HH11	1:B:115:PRO:HD3	1.64	0.60
1:B:378:LEU:HB2	7:B:2902:HOH:O	2.01	0.59
1:B:320:PRO:HG3	1:B:410:HIS:CG	2.38	0.59
1:A:115:PRO:C	1:A:117:PRO:HD3	2.27	0.59
1:A:285:ASN:HD22	1:A:285:ASN:C	2.09	0.59
1:B:167:LEU:HG	1:B:348:LEU:HD12	1.85	0.58
1:A:119:PRO:HG3	1:A:238:PRO:CB	2.21	0.58
1:A:111:LEU:HD12	1:A:111:LEU:H	1.69	0.58
1:B:108:PRO:HB3	1:B:111:LEU:HB2	1.85	0.57
1:A:378:LEU:HB2	7:A:2881:HOH:O	2.03	0.57
1:A:99:ARG:HH11	1:A:99:ARG:CB	2.08	0.57
1:A:77:GLU:HG3	1:B:372:PRO:HG2	1.87	0.56
1:B:110:LYS:C	1:B:112:GLN:H	2.13	0.56
1:B:281:TRP:HB2	1:B:304:LEU:HD21	1.87	0.56
1:B:367:ARG:NH1	6:B:2890:GOL:H31	2.21	0.56
1:B:114:ARG:NH1	1:B:115:PRO:HD3	2.22	0.55
1:A:472:SER:HA	1:A:473:PRO:C	2.33	0.54
1:A:94:GLY:O	1:A:110:LYS:HE2	2.08	0.54
1:A:108:PRO:O	1:A:110:LYS:N	2.41	0.53
1:B:381:VAL:HG21	1:B:404:ILE:HD11	1.90	0.53
1:B:252:ARG:HB2	1:B:291:LEU:HD12	1.91	0.53
1:B:455:SER:HB3	1:B:458:LEU:HD12	1.90	0.53
1:A:109:ARG:O	1:A:110:LYS:HD2	2.09	0.52
1:A:158:GLU:HG2	1:A:165:TYR:HA	1.91	0.52
1:A:218:LYS:HG2	1:A:311:LEU:HD22	1.92	0.52
1:A:111:LEU:O	1:A:112:GLN:C	2.53	0.51
1:A:99:ARG:HB2	1:A:99:ARG:NH1	2.10	0.51
1:A:340:ASN:H	1:A:340:ASN:HD22	1.59	0.51
1:A:115:PRO:CD	1:A:479:PRO:HG2	2.35	0.51
1:A:77:GLU:HG3	1:B:372:PRO:CG	2.41	0.51
1:B:116:SER:O	1:B:238:PRO:HA	2.11	0.51
1:A:463:HIS:HA	6:A:2880:GOL:H11	1.93	0.50
1:A:126:LEU:HD11	1:A:156:GLU:HA	1.91	0.50
1:B:472:SER:HA	1:B:473:PRO:C	2.36	0.50
1:A:455:SER:HB3	1:A:458:LEU:HD12	1.92	0.50
1:B:114:ARG:HA	1:B:114:ARG:NH1	2.19	0.50
1:A:111:LEU:HG	1:A:470:ILE:HD13	1.94	0.50
1:B:324:TRP:HB2	1:B:384:CAS:CE2	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:ARG:HD3	1:B:115:PRO:CD	2.41	0.49
1:A:285:ASN:C	1:A:285:ASN:ND2	2.68	0.49
1:A:114:ARG:HD2	1:A:479:PRO:CG	2.42	0.49
1:A:366:THR:HG21	1:A:454:ILE:HG23	1.95	0.49
1:A:462:PHE:CZ	6:B:2890:GOL:H11	2.47	0.49
1:B:218:LYS:HE3	1:B:311:LEU:HD11	1.95	0.49
1:A:168:ARG:HB2	1:A:171:GLU:HG3	1.94	0.48
1:A:155:VAL:O	1:A:159:VAL:HG23	2.14	0.48
1:B:111:LEU:HD12	1:B:111:LEU:N	2.29	0.48
1:B:340:ASN:HD22	1:B:340:ASN:H	1.61	0.47
1:A:370:CYS:SG	1:A:378:LEU:HD13	2.54	0.47
1:A:360:MET:HE3	1:A:362:THR:OG1	2.15	0.47
1:B:117:PRO:HA	1:B:239:GLY:H	1.80	0.47
1:B:214:CYS:O	1:B:218:LYS:HG3	2.16	0.46
1:B:219:TYR:CD1	1:B:219:TYR:C	2.93	0.46
1:B:113:THR:HG21	1:B:342:LEU:CD1	2.46	0.46
1:A:154:GLU:OE2	1:A:168:ARG:NH2	2.44	0.46
4:B:500:HEM:HMC1	4:B:500:HEM:HBC2	1.97	0.46
1:B:220:ALA:O	1:B:226:LEU:HA	2.17	0.45
1:A:281:TRP:HB2	1:A:304:LEU:HD21	1.97	0.45
1:B:110:LYS:O	1:B:112:GLN:N	2.49	0.45
1:B:384:CAS:CE1	1:B:384:CAS:HA	2.46	0.45
1:A:322:LEU:HD13	1:A:324:TRP:CZ2	2.51	0.45
1:A:149:GLU:O	1:A:153:GLN:HG3	2.17	0.44
1:A:114:ARG:HD2	1:A:479:PRO:HG3	1.99	0.44
1:B:146:GLN:O	1:B:150:GLU:HG3	2.17	0.44
1:A:319:HIS:CG	1:A:320:PRO:HD2	2.52	0.44
1:B:258:GLN:O	1:B:259:GLN:C	2.59	0.44
1:A:114:ARG:HA	1:A:479:PRO:HG2	2.00	0.44
1:B:471:LEU:O	1:B:474:ALA:HB2	2.17	0.44
1:A:336:PRO:HG2	5:A:840:NTU:H2'2	1.99	0.44
1:A:117:PRO:O	1:A:118:GLY:C	2.60	0.43
1:B:244:ARG:NH2	1:B:481:PRO:HD3	2.33	0.43
1:B:116:SER:N	1:B:117:PRO:CD	2.81	0.43
1:B:129:ALA:O	1:B:133:ILE:HG12	2.18	0.43
1:B:180:TRP:CE3	1:B:192:TRP:HA	2.54	0.43
1:B:340:ASN:HD22	1:B:340:ASN:N	2.15	0.43
1:B:342:LEU:C	1:B:342:LEU:HD23	2.44	0.43
1:B:281:TRP:O	1:B:283:PRO:HD3	2.19	0.43
1:A:340:ASN:HD22	1:A:340:ASN:N	2.16	0.43
1:A:109:ARG:HA	1:A:109:ARG:HD3	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:VAL:HB	1:A:355:PHE:CZ	2.55	0.42
1:B:388:ASP:OD1	1:B:390:ARG:HB2	2.19	0.42
1:A:244:ARG:NH2	1:A:481:PRO:HD3	2.35	0.42
1:A:366:THR:O	1:A:370:CYS:HB2	2.20	0.42
1:A:113:THR:HG21	1:A:342:LEU:HD22	2.02	0.42
1:B:423:HIS:O	1:B:427:VAL:HG23	2.20	0.42
1:A:234:PRO:HB2	1:A:243:PHE:CE1	2.54	0.42
1:B:111:LEU:HD12	1:B:111:LEU:H	1.84	0.41
1:A:113:THR:CG2	1:A:476:ARG:HD2	2.50	0.41
1:A:343:LEU:HB3	1:A:350:PHE:HB2	2.02	0.41
1:B:182:ASN:O	1:B:184:PRO:HD3	2.21	0.41
1:A:114:ARG:HD2	1:A:479:PRO:HG2	2.02	0.41
1:A:274:GLU:O	1:A:278:GLN:HG3	2.20	0.41
1:B:149:GLU:O	1:B:153:GLN:HG3	2.21	0.41
1:B:117:PRO:HA	1:B:239:GLY:HA2	2.03	0.41
1:B:216:HIS:CD2	1:B:216:HIS:C	2.98	0.41
1:B:71:PRO:HG2	1:B:84:ASP:HB3	2.03	0.41
1:B:322:LEU:HD13	1:B:324:TRP:CZ2	2.55	0.41
1:A:167:LEU:HG	1:A:348:LEU:HD12	2.03	0.41
1:A:238:PRO:C	1:A:240:ARG:H	2.29	0.40
1:B:231:THR:O	1:B:353:ALA:HA	2.21	0.40
1:A:336:PRO:HB3	1:A:359:TYR:CZ	2.57	0.40
1:A:264:ARG:HH11	1:A:264:ARG:HG3	1.86	0.40
1:A:342:LEU:C	1:A:342:LEU:HD23	2.46	0.40
4:B:500:HEM:HBC2	4:B:500:HEM:CMC	2.51	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	413/444 (93%)	391 (95%)	18 (4%)	4 (1%)	12 8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	411/444 (93%)	382 (93%)	24 (6%)	5 (1%)	10	6
All	All	824/888 (93%)	773 (94%)	42 (5%)	9 (1%)	11	7

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	259	GLN
1	A	109	ARG
1	A	112	GLN
1	A	117	PRO
1	B	111	LEU
1	B	115	PRO
1	A	239	GLY
1	B	262	SER
1	B	121	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	353/376 (94%)	347 (98%)	6 (2%)	53	60
1	B	352/376 (94%)	346 (98%)	6 (2%)	53	60
All	All	705/752 (94%)	693 (98%)	12 (2%)	53	60

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	ARG
1	A	285	ASN
1	A	328	LEU
1	A	340	ASN
1	A	378	LEU
1	A	414	LEU
1	B	89	GLN

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Mol	Chain	Res	Type
1	B	99	ARG
1	B	114	ARG
1	B	257	ARG
1	B	340	ASN
1	B	378	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	GLN
1	A	124	GLN
1	A	128	GLN
1	A	153	GLN
1	A	191	GLN
1	A	278	GLN
1	A	285	ASN
1	A	340	ASN
1	A	376	ASN
1	A	405	ASN
1	A	410	HIS
1	A	413	GLN
1	A	468	ASN
1	A	478	GLN
1	B	89	GLN
1	B	112	GLN
1	B	153	GLN
1	B	191	GLN
1	B	222	ASN
1	B	225	ASN
1	B	258	GLN
1	B	278	GLN
1	B	340	ASN
1	B	478	GLN

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	3.03	2 (40%)	1,9,11	0.81	0
1	CAS	B	384	1	5,8,9	3.26	2 (40%)	1,9,11	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
1	CAS	A	384	1	-	0/0/7/9	-
1	CAS	B	384	1	-	0/0/7/9	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	384	CAS	AS-CE2	-5.16	1.82	1.96
1	B	384	CAS	AS-CE1	-4.98	1.82	1.96
1	A	384	CAS	AS-CE1	-4.86	1.83	1.96
1	A	384	CAS	AS-CE2	-4.61	1.83	1.96

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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$
4	HEM	B	500	1	50,50,50	1.10	2 (4%)	67,82,82	1.06	2 (2%)
2	ACT	A	1850	-	3,3,3	0.93	0	3,3,3	0.80	0
6	GOL	B	2890	-	5,5,5	0.26	0	5,5,5	0.27	0
2	ACT	B	2860	-	3,3,3	0.93	0	3,3,3	0.82	0
6	GOL	A	1890	-	5,5,5	0.22	0	5,5,5	0.21	0
5	NTU	B	840	-	8,8,23	1.67	2 (25%)	6,8,24	3.44	3 (50%)
6	GOL	A	2880	-	5,5,5	0.25	0	5,5,5	0.24	0
2	ACT	A	1860	-	3,3,3	0.97	0	3,3,3	0.75	0
4	HEM	A	500	1	50,50,50	1.07	2 (4%)	67,82,82	1.06	2 (2%)
5	NTU	A	840	-	8,8,23	1.97	2 (25%)	6,8,24	3.44	3 (50%)

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	HEM	B	500	1	-	2/14/54/54	-
6	GOL	B	2890	-	-	0/4/4/4	-
6	GOL	A	1890	-	-	0/4/4/4	-
5	NTU	B	840	-	-	3/5/7/23	-
6	GOL	A	2880	-	-	0/4/4/4	-
4	HEM	A	500	1	-	2/14/54/54	-
5	NTU	A	840	-	-	1/5/7/23	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	840	NTU	C1'-S1'	4.65	1.80	1.75
5	B	840	NTU	C1'-S1'	3.60	1.79	1.75
4	A	500	HEM	CAB-C3B	-3.37	1.38	1.47
5	B	840	NTU	C1'-N1	2.56	1.36	1.28
5	A	840	NTU	C1'-N1	2.46	1.36	1.28
4	B	500	HEM	CAB-C3B	-2.32	1.41	1.47
4	A	500	HEM	CAC-C3C	-2.17	1.41	1.47
4	B	500	HEM	CHB-C1B	2.05	1.42	1.38

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	840	NTU	C1-N1-C1'	6.75	129.14	117.92
5	A	840	NTU	C1-N1-C1'	6.36	128.50	117.92
5	A	840	NTU	C2'-S1'-C1'	4.79	108.83	103.10
5	B	840	NTU	C2'-S1'-C1'	4.39	108.35	103.10
4	A	500	HEM	C3B-C4B-NB	2.82	111.49	109.47
5	A	840	NTU	C2-C1-N1	2.58	115.24	110.67
4	B	500	HEM	CMA-C3A-C4A	2.43	129.11	125.42
4	A	500	HEM	C2B-C1B-NB	2.18	112.35	109.84
5	B	840	NTU	C2-C1-N1	2.11	114.42	110.67
4	B	500	HEM	C3B-C4B-NB	2.10	110.98	109.47

There are no chirality outliers.

All (8) torsion outliers are listed below:

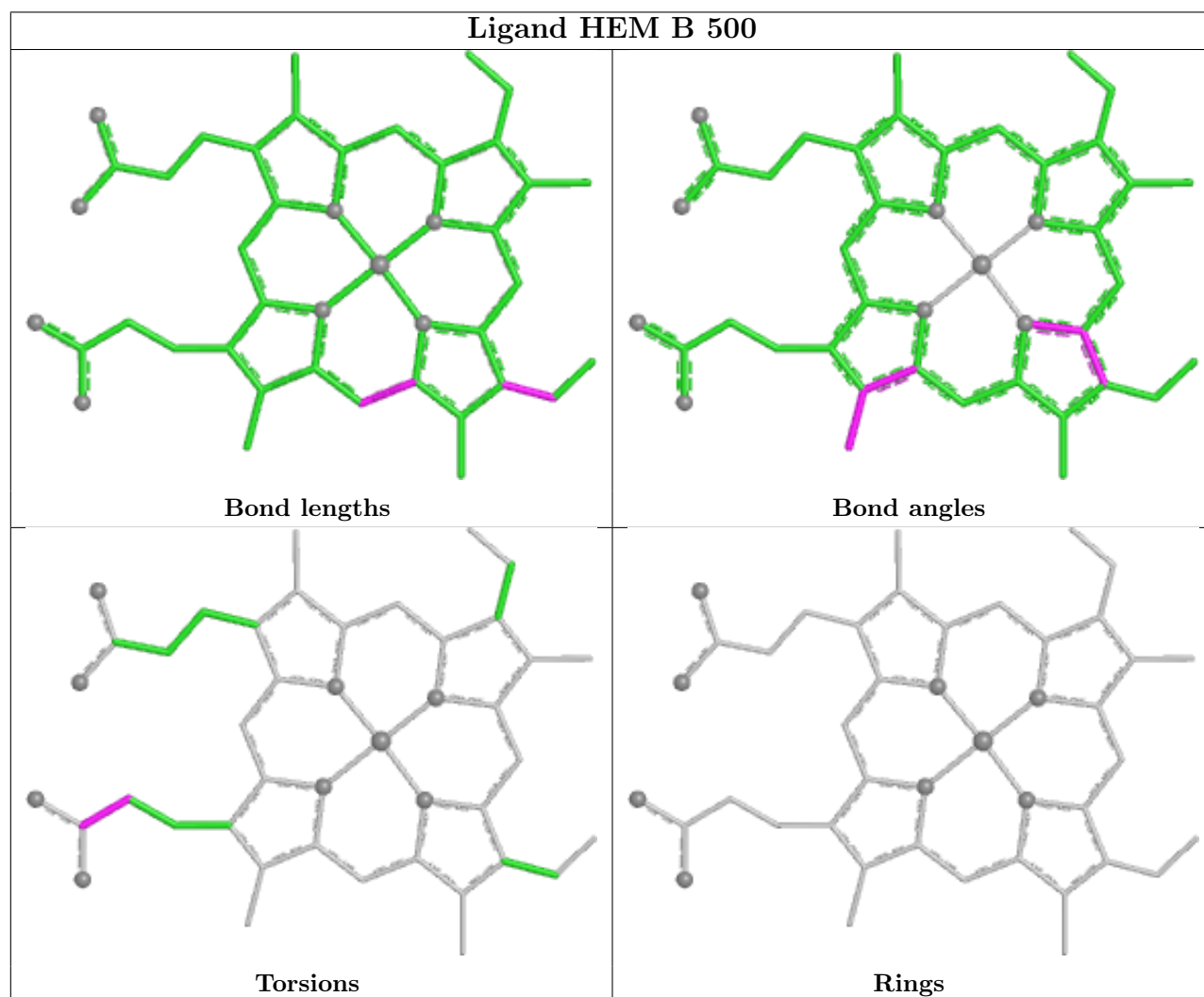
Mol	Chain	Res	Type	Atoms
5	A	840	NTU	N2-C1'-S1'-C2'
5	B	840	NTU	N1-C1-C2-C3
5	B	840	NTU	C1-C2-C3-C4
5	B	840	NTU	N2-C1'-S1'-C2'
4	A	500	HEM	CAA-CBA-CGA-O2A
4	A	500	HEM	CAA-CBA-CGA-O1A
4	B	500	HEM	CAA-CBA-CGA-O2A
4	B	500	HEM	CAA-CBA-CGA-O1A

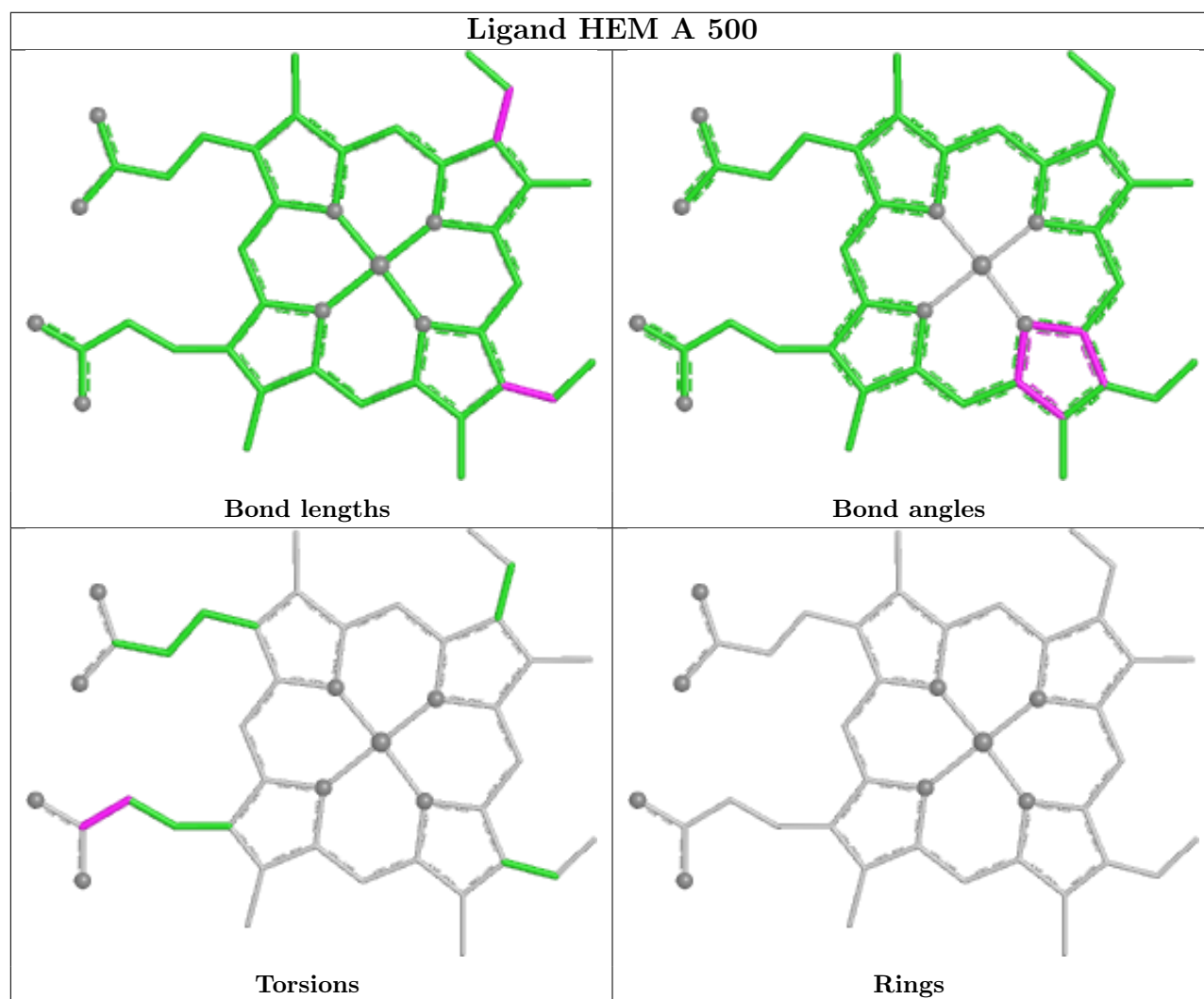
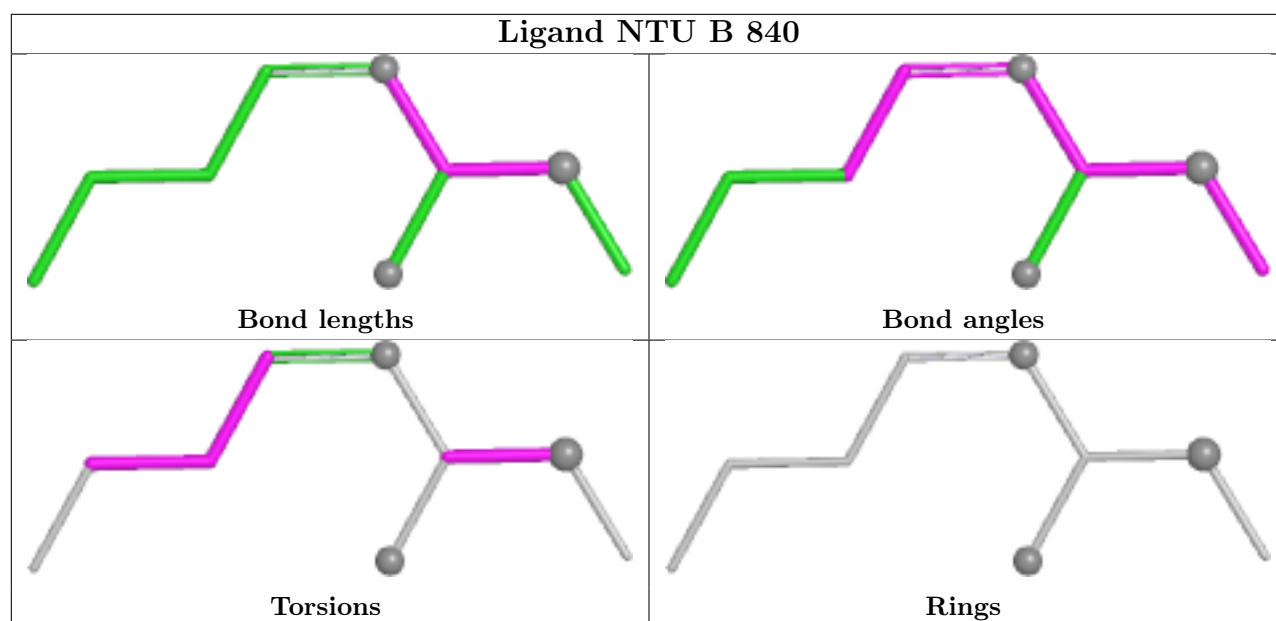
There are no ring outliers.

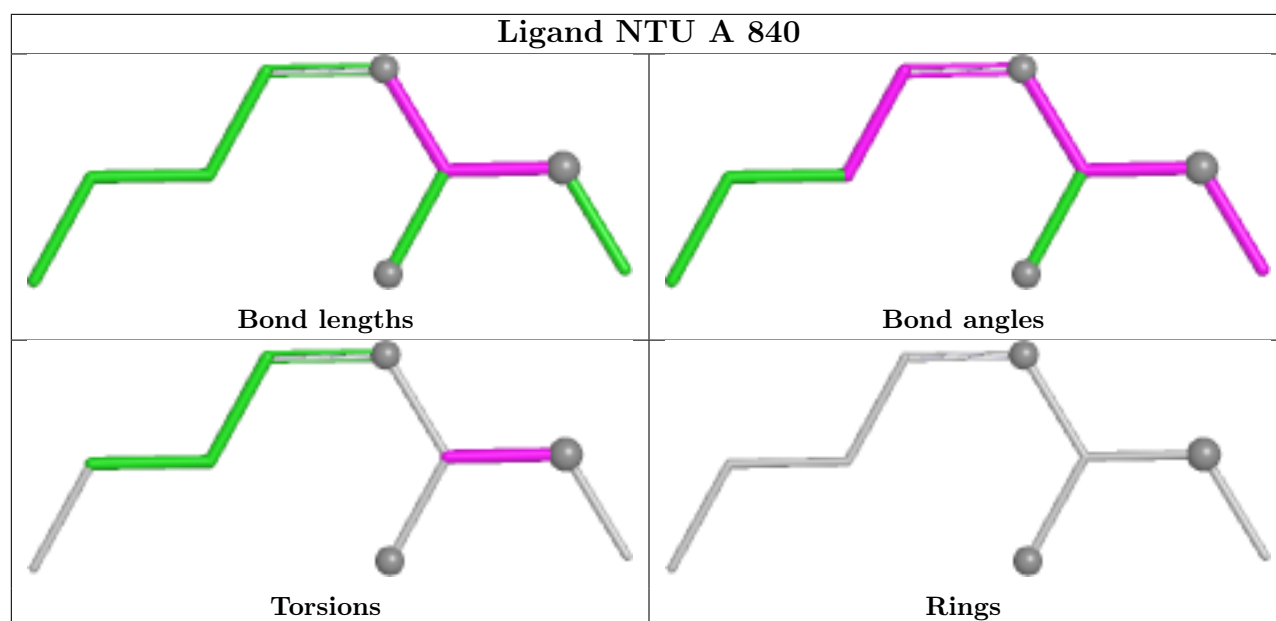
4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	500	HEM	2	0
6	B	2890	GOL	4	0
6	A	2880	GOL	2	0
5	A	840	NTU	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	415/444 (93%)	0.66	28 (6%) 24 22	26, 37, 68, 100	0
1	B	413/444 (93%)	0.79	40 (9%) 13 12	27, 41, 74, 100	0
All	All	828/888 (93%)	0.72	68 (8%) 17 16	26, 39, 71, 100	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	113	THR	10.1
1	A	115	PRO	6.2
1	A	111	LEU	5.4
1	B	113	THR	5.3
1	A	118	GLY	5.0
1	A	117	PRO	4.9
1	A	109	ARG	4.8
1	B	120	PRO	4.7
1	B	118	GLY	4.2
1	B	121	PRO	4.1
1	B	144	GLY	4.0
1	B	117	PRO	3.9
1	A	110	LYS	3.9
1	A	239	GLY	3.8
1	A	114	ARG	3.7
1	B	111	LEU	3.7
1	A	112	GLN	3.7
1	B	261	GLY	3.6
1	B	116	SER	3.6
1	A	108	PRO	3.6
1	B	115	PRO	3.5
1	B	262	SER	3.4
1	A	122	ALA	3.4
1	B	258	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	119	PRO	3.0
1	A	121	PRO	3.0
1	A	120	PRO	2.9
1	B	112	GLN	2.9
1	B	259	GLN	2.8
1	B	119	PRO	2.8
1	B	391	THR	2.8
1	B	482	TRP	2.7
1	B	304	LEU	2.6
1	B	110	LYS	2.5
1	A	130	ARG	2.5
1	B	389	THR	2.5
1	B	390	ARG	2.5
1	A	241	GLY	2.4
1	A	160	ALA	2.4
1	B	97	THR	2.4
1	B	277	ILE	2.4
1	B	143	SER	2.3
1	B	323	GLU	2.3
1	A	258	GLN	2.3
1	A	482	TRP	2.3
1	B	145	SER	2.3
1	A	123	GLU	2.2
1	A	116	SER	2.2
1	B	263	VAL	2.2
1	A	261	GLY	2.2
1	B	326	ALA	2.2
1	B	203	CYS	2.2
1	B	71	PRO	2.2
1	B	327	ALA	2.2
1	B	260	ASP	2.2
1	B	108	PRO	2.1
1	A	157	ALA	2.1
1	B	122	ALA	2.1
1	B	90	SER	2.1
1	A	190	ILE	2.1
1	B	147	ALA	2.1
1	A	96	CYS	2.1
1	A	236	ARG	2.1
1	B	276	CYS	2.0
1	B	278	GLN	2.0
1	B	70	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	237	ALA	2.0
1	B	130	ARG	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(Å ²)	Q<0.9
1	CAS	B	384	9/10	0.93	0.15	52,53,61,63	0
1	CAS	A	384	9/10	0.96	0.10	35,37,51,58	0

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.

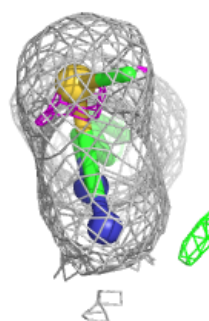
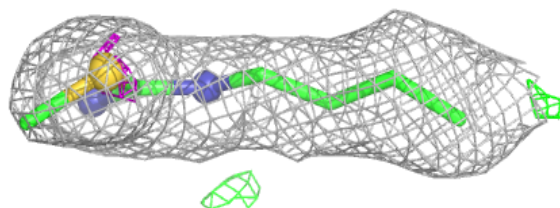
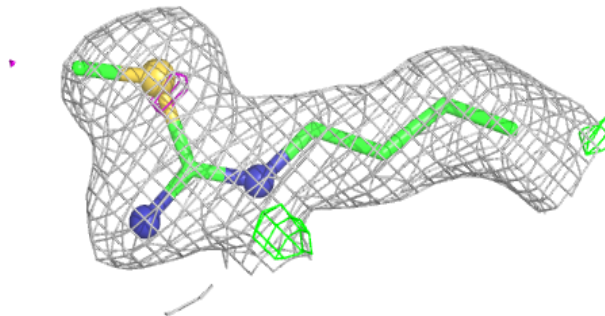
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	GOL	A	2880	6/6	0.78	0.15	56,58,59,59	0
6	GOL	A	1890	6/6	0.87	0.14	56,57,57,59	0
5	NTU	A	840	9/24	0.88	0.14	41,44,45,47	0
6	GOL	B	2890	6/6	0.88	0.13	51,53,54,57	0
2	ACT	A	1860	4/4	0.90	0.09	40,41,42,44	0
2	ACT	B	2860	4/4	0.91	0.11	44,46,47,48	0
2	ACT	A	1850	4/4	0.91	0.12	46,47,48,49	0
5	NTU	B	840	9/24	0.91	0.13	41,43,47,48	0
4	HEM	B	500	43/43	0.96	0.08	24,28,44,55	0
4	HEM	A	500	43/43	0.96	0.09	22,29,45,52	0
3	ZN	A	900	1/1	0.99	0.06	36,36,36,36	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.

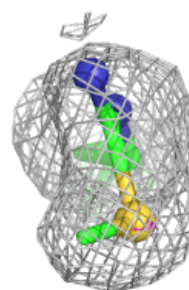
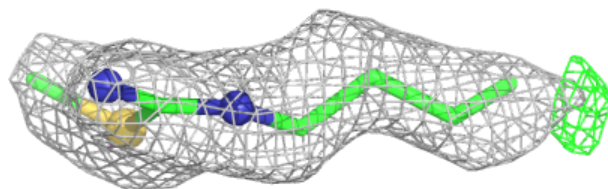
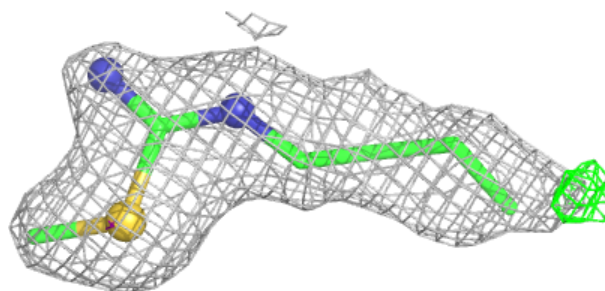
Electron density around NTU A 840:

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



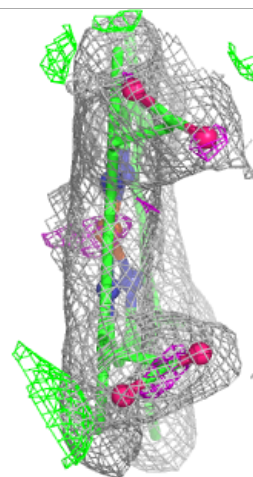
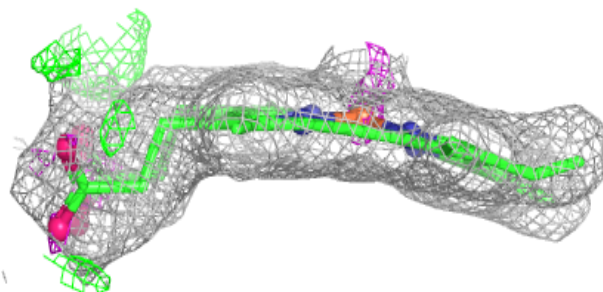
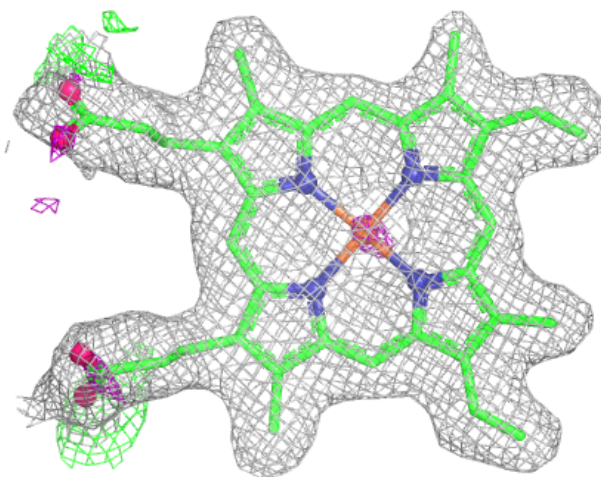
Electron density around NTU B 840:

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



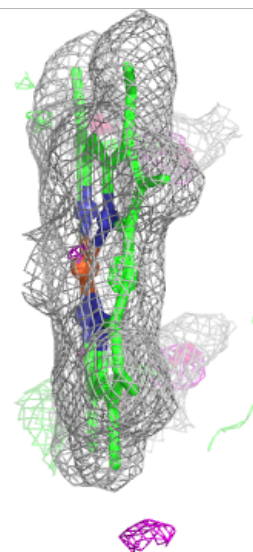
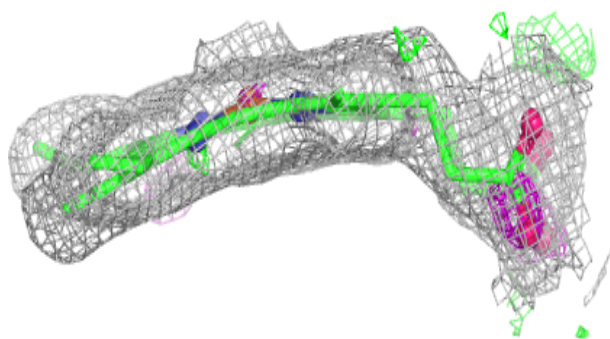
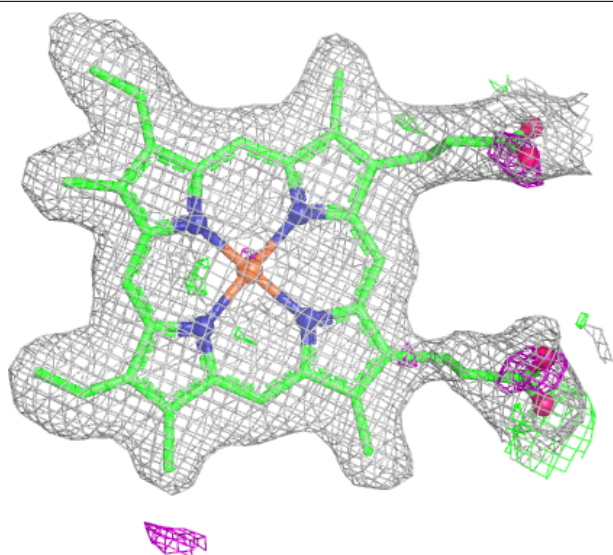
Electron density around HEM B 500:

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



Electron density around HEM A 500:

$2mF_o-DF_c$ (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.