



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 08:06 AM EDT

PDB ID : 3NLU / pdb_00003nlu
Title : Structure of endothelial nitric oxide synthase heme domain complexed with N 1-{(3'R,4'R)-4'-[(6"-amino-4"-methylpyridin-2"-yl)methyl]pyrrolidin-3'-yl}-N 2-(3'-fluorophenethyl)ethane-1,2-diamine tetrahydrochloride
Authors : Xue, F.; Li, H.; Fang, J.; Delker, S.L.; Poulos, T.L.; Silverman, R.B.
Deposited on : 2010-06-21
Resolution : 2.65 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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

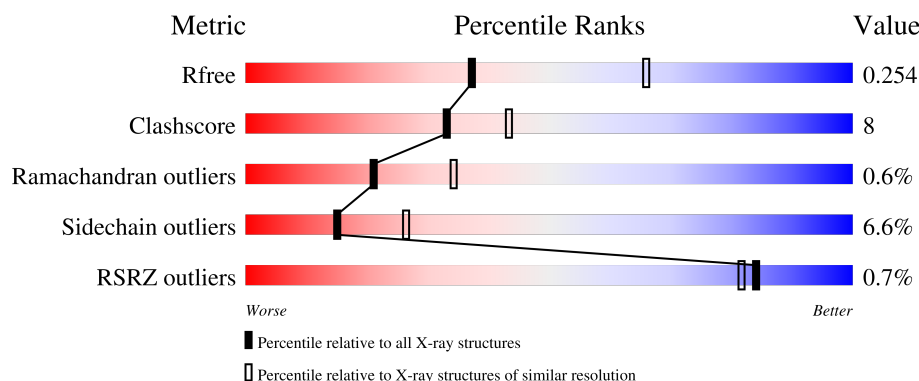
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	% 76% 14% • 9%
1	B	444	70% 19% • 9%

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	3XB	B	800	-	-	X	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 6759 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.

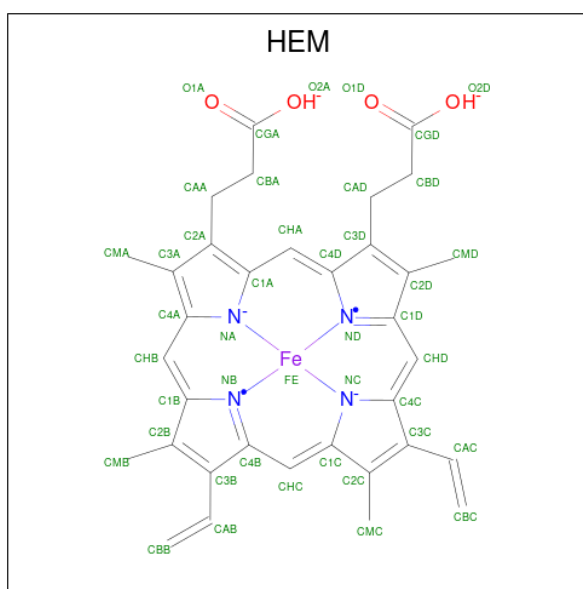
- Molecule 1 is a protein called Nitric oxide synthase, endothelial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	405	Total	C	N	O	S	0	1	0
			3229	2052	569	592	16			
1	B	403	Total	C	N	O	S	0	1	0
			3218	2045	567	590	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	ARG	CYS	SEE REMARK 999	UNP P29473
B	100	ARG	CYS	SEE REMARK 999	UNP P29473

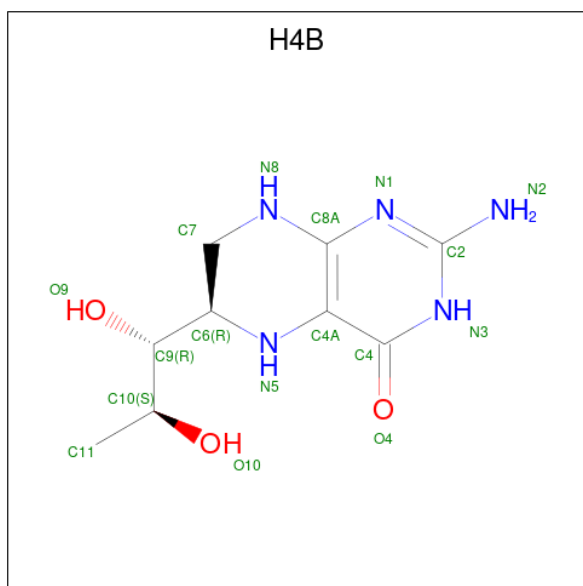
- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Continued from previous page...

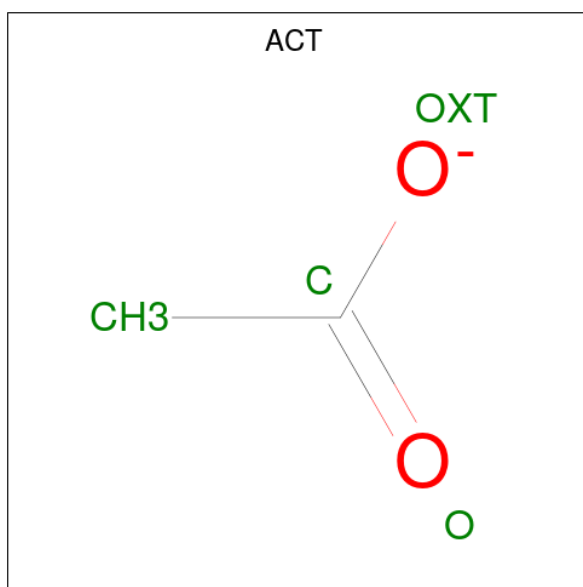
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



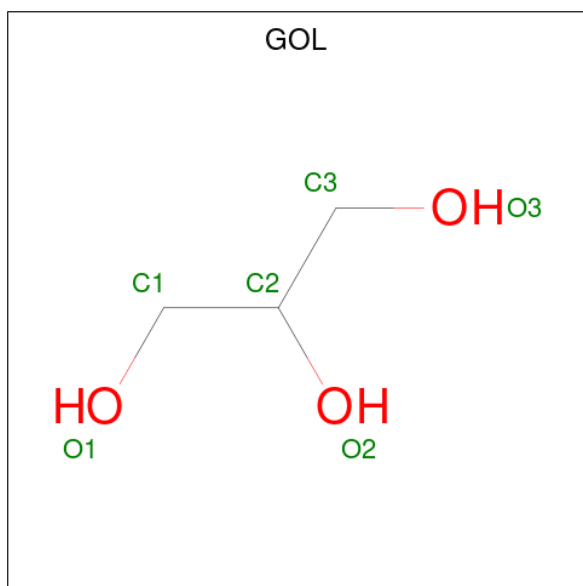
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



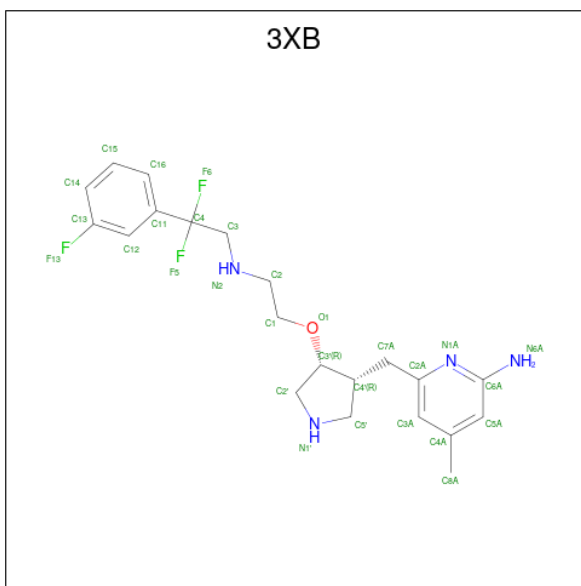
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



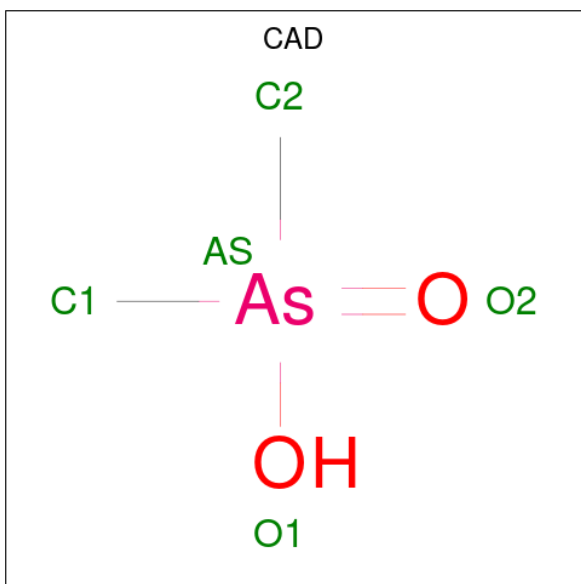
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is 6-{[(3R,4R)-4-(2-{[2,2-difluoro-2-(3-fluorophenyl)ethyl]amino}ethoxy)pyrrolid

in-3-yl)methyl}-4-methylpyridin-2-amine (CCD ID: 3XB) (formula: C₂₁H₂₇F₃N₄O).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total 29	C 21	F 3	N 4	O 1	0	0
6	B	1	Total 29	C 21	F 3	N 4	O 1	0	0

- Molecule 7 is CACODYLIC ACID (CCD ID: CAD) (formula: $\text{C}_2\text{H}_7\text{AsO}_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total 3	As 1	C 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	As	C	0	0
			3	1	2		

- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

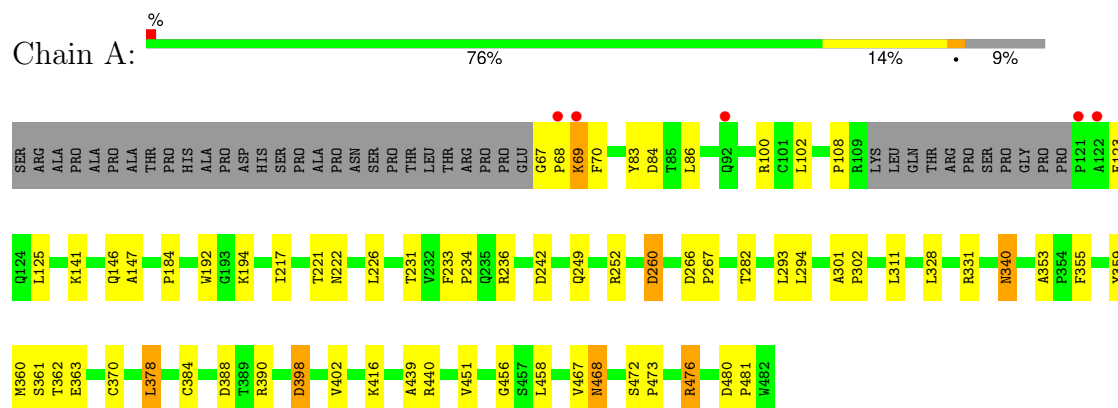
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	50	Total	O	0	0
			50	50		
9	B	61	Total	O	0	0
			61	61		

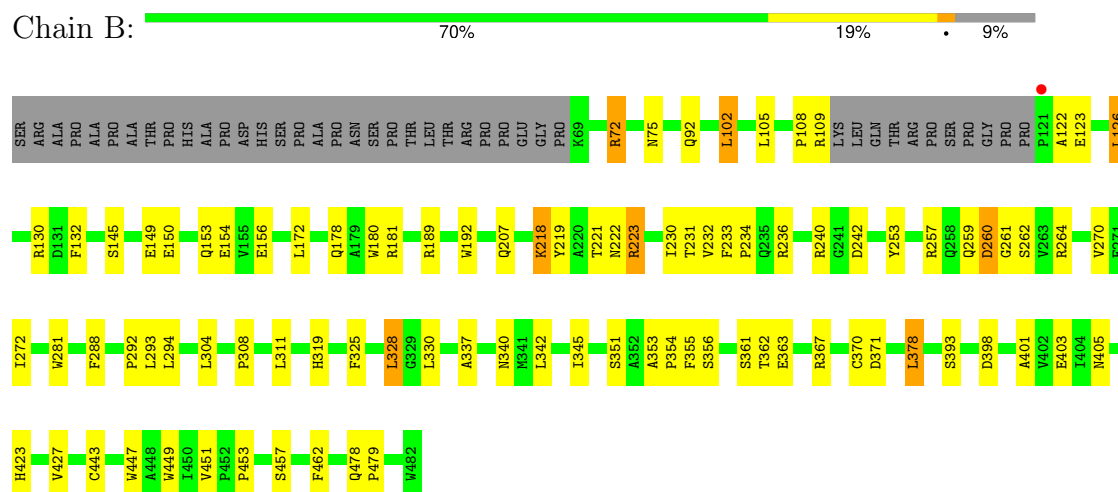
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Nitric oxide synthase, endothelial



- Molecule 1: Nitric oxide synthase, endothelial



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.98Å 107.02Å 156.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.39 – 2.65 37.39 – 2.65	Depositor EDS
% Data completeness (in resolution range)	97.3 (37.39-2.65) 97.2 (37.39-2.65)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.5.0102, CNS	Depositor
R, R_{free}	0.186 , 0.254 0.186 , 0.254	Depositor DCC
R_{free} test set	1381 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å ²)	34.9	Xtriage
Anisotropy	0.251	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 29.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6759	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ACT, 3XB, GOL, HEM, CAD, H4B, 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	0.81	0/3319	0.98	6/4520 (0.1%)
1	B	0.80	0/3307	0.98	4/4503 (0.1%)
All	All	0.80	0/6626	0.98	10/9023 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	240	ARG	N-CA-C	6.55	117.22	108.38
1	B	443	CYS	CA-C-N	-5.55	114.07	119.90
1	B	443	CYS	C-N-CA	-5.55	114.07	119.90
1	A	439	ALA	N-CA-C	5.40	118.33	111.69
1	B	361	SER	N-CA-C	5.35	117.81	111.33
1	A	100	ARG	N-CA-C	5.32	117.17	108.55
1	A	451	VAL	CA-C-N	5.20	123.40	119.66
1	A	451	VAL	C-N-CA	5.20	123.40	119.66
1	A	359	TYR	N-CA-C	5.16	117.36	110.35
1	A	192	TRP	N-CA-C	5.03	117.42	111.33

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3229	0	3133	38	0
1	B	3218	0	3122	51	0
2	A	43	0	30	8	0
2	B	43	0	30	4	0
3	A	17	0	15	1	0
3	B	17	0	15	1	0
4	A	4	0	3	0	0
5	A	6	0	8	1	0
5	B	6	0	8	1	0
6	A	29	0	27	5	0
6	B	29	0	27	9	0
7	A	3	0	0	1	0
7	B	3	0	0	0	0
8	A	1	0	0	0	0
9	A	50	0	0	0	0
9	B	61	0	0	3	0
All	All	6759	0	6418	101	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 8.

All (101) 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)
2:B:500:HEM:HBA2	6:B:800:3XB:H3	1.30	1.07
1:B:363[A]:GLU:OE1	6:B:800:3XB:H16	1.56	1.04
1:A:476:ARG:HH11	1:A:476:ARG:HG3	1.36	0.90
1:A:360:MET:HE3	1:A:362:THR:OG1	1.80	0.79
1:A:360:MET:CE	1:A:362:THR:OG1	2.34	0.76
2:A:500:HEM:HBB2	2:A:500:HEM:HHC	1.70	0.74
2:B:500:HEM:CBA	6:B:800:3XB:H3	2.15	0.73
6:B:800:3XB:H2	6:B:800:3XB:F6	1.81	0.71
2:B:500:HEM:HBA2	6:B:800:3XB:C3	2.17	0.70
1:B:126:LEU:O	1:B:130:ARG:HG3	1.92	0.69
1:A:476:ARG:HH11	1:A:476:ARG:CG	2.05	0.68
1:B:281:TRP:HB2	1:B:304:LEU:HD21	1.77	0.66
2:A:500:HEM:HHC	2:A:500:HEM:CBB	2.28	0.63
1:B:223:ARG:HB2	1:B:223:ARG:HH11	1.64	0.62
1:B:423:HIS:O	1:B:427:VAL:HG23	2.01	0.61
1:A:472:SER:HA	1:A:473:PRO:C	2.26	0.61
1:B:325:PHE:HA	1:B:328:LEU:HD12	1.81	0.61
1:A:363[A]:GLU:OE1	6:A:800:3XB:H16	2.02	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:PRO:HD2	1:B:311:LEU:HD12	1.83	0.59
1:B:236:ARG:HD2	1:B:242:ASP:OD1	2.02	0.58
6:B:800:3XB:F6	6:B:800:3XB:C2	2.41	0.58
1:A:146:GLN:NE2	1:A:147:ALA:H	2.01	0.58
1:B:457:SER:HA	1:B:462:PHE:CG	2.41	0.56
1:A:69:LYS:O	1:A:69:LYS:HD3	2.07	0.55
1:A:476:ARG:HG3	1:A:476:ARG:NH1	2.16	0.55
2:A:500:HEM:HBA1	6:A:800:3XB:H3	1.88	0.55
1:A:355:PHE:CD1	2:A:500:HEM:HAC	2.42	0.54
1:B:218:LYS:C	1:B:218:LYS:HD3	2.34	0.53
1:B:172:LEU:HD11	1:B:232:VAL:HG11	1.90	0.52
3:A:600:H4B:O4	5:A:880:GOL:O2	2.28	0.52
1:A:384:CYS:CB	7:A:950:CAD:AS	3.18	0.51
1:A:217:ILE:O	1:A:221:THR:OG1	2.26	0.51
1:A:458:LEU:HD21	1:B:401:ALA:HB2	1.92	0.51
1:A:388:ASP:OD1	1:A:390:ARG:HB2	2.11	0.51
1:B:367:ARG:O	1:B:371:ASP:HB2	2.11	0.51
1:B:342:LEU:C	1:B:342:LEU:HD23	2.37	0.50
1:B:378:LEU:HB2	9:B:1040:HOH:O	2.12	0.50
1:A:370:CYS:SG	1:A:378:LEU:HD13	2.52	0.50
2:A:500:HEM:HBB2	2:A:500:HEM:CHC	2.35	0.50
1:B:236:ARG:HD2	1:B:242:ASP:CG	2.36	0.50
1:B:180:TRP:CE3	1:B:192:TRP:HA	2.47	0.50
1:B:236:ARG:HD3	1:B:351:SER:HB3	1.94	0.50
1:B:218:LYS:HD3	1:B:219:TYR:N	2.28	0.49
1:A:398:ASP:O	1:A:402:VAL:HG23	2.13	0.49
1:B:449:TRP:HA	3:B:600:H4B:N1	2.28	0.49
1:B:478:GLN:HB2	1:B:479:PRO:HD2	1.95	0.48
1:A:184:PRO:CB	1:A:468:ASN:HD21	2.26	0.48
1:A:233:PHE:HB3	1:A:234:PRO:CD	2.43	0.48
1:B:272:ILE:HG22	9:B:1034:HOH:O	2.13	0.48
1:B:370:CYS:SG	1:B:378:LEU:HD13	2.54	0.48
1:B:231:THR:O	1:B:353:ALA:HA	2.13	0.47
1:A:184:PRO:HB3	1:A:468:ASN:ND2	2.30	0.47
1:A:458:LEU:HD21	1:B:401:ALA:CB	2.45	0.47
1:B:230:ILE:HG13	1:B:354:PRO:O	2.15	0.47
2:A:500:HEM:C4B	6:A:800:3XB:H14	2.50	0.47
1:B:132:PHE:CE1	1:B:345:ILE:HG23	2.50	0.47
1:B:150:GLU:O	1:B:154:GLU:HG3	2.15	0.47
1:A:260:ASP:N	1:A:260:ASP:OD1	2.48	0.47
1:B:447:TRP:CZ2	1:B:451:VAL:HG21	2.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:447:TRP:CE2	1:B:451:VAL:HG21	2.51	0.46
1:B:233:PHE:HB3	1:B:234:PRO:CD	2.46	0.46
1:A:70:PHE:HB3	1:A:84:ASP:O	2.16	0.46
1:B:362:THR:HA	1:B:405:ASN:HD21	1.81	0.45
1:A:249:GLN:HB2	1:A:252:ARG:HG3	1.97	0.45
1:A:467:VAL:HG13	1:B:102:LEU:CD1	2.47	0.45
1:A:249:GLN:HB2	1:A:252:ARG:CG	2.47	0.45
1:A:340:ASN:H	1:A:340:ASN:HD22	1.65	0.44
1:A:184:PRO:HB3	1:A:468:ASN:HD21	1.83	0.44
6:A:800:3XB:F5	6:A:800:3XB:H2A	2.07	0.44
1:A:221:THR:O	1:A:222:ASN:C	2.59	0.44
1:B:363[B]:GLU:OE1	6:B:800:3XB:F6	2.26	0.44
1:B:319:HIS:NE2	1:B:403:GLU:OE1	2.47	0.43
1:A:355:PHE:CG	2:A:500:HEM:HAC	2.53	0.43
1:A:86:LEU:HD13	1:A:440:ARG:HB3	1.99	0.43
1:A:355:PHE:CD1	2:A:500:HEM:CAC	3.02	0.43
1:B:453:PRO:HD3	9:B:1038:HOH:O	2.18	0.43
1:B:189:ARG:O	1:B:192:TRP:HD1	2.02	0.42
1:B:337:ALA:HB2	1:B:356:SER:HB3	2.02	0.42
1:B:122:ALA:O	1:B:126:LEU:HB2	2.20	0.42
1:B:337:ALA:CB	1:B:356:SER:HB3	2.49	0.42
1:A:301:ALA:HB1	1:A:302:PRO:HD2	2.02	0.42
1:B:221:THR:O	1:B:222:ASN:C	2.62	0.42
1:B:233:PHE:HB3	1:B:234:PRO:HD2	2.00	0.42
1:B:355:PHE:CD1	2:B:500:HEM:HAC	2.55	0.42
1:A:266:ASP:HA	1:A:267:PRO:HD3	1.88	0.42
1:B:259:GLN:C	1:B:261:GLY:H	2.28	0.42
1:B:75:ASN:OD1	1:B:75:ASN:C	2.63	0.42
1:A:231:THR:O	1:A:353:ALA:HA	2.20	0.42
5:B:880:GOL:H11	6:B:800:3XB:H5'A	2.02	0.42
1:B:281:TRP:CD1	1:B:292:PRO:HG3	2.54	0.42
1:A:67:GLY:HA3	1:A:83:TYR:CZ	2.55	0.41
1:B:72:ARG:HG2	1:B:72:ARG:HH11	1.85	0.41
6:A:800:3XB:H3AA	6:A:800:3XB:H4'	1.87	0.41
1:B:178:GLN:HE22	1:B:181:ARG:HH11	1.67	0.41
1:B:231:THR:O	1:B:354:PRO:HD2	2.20	0.41
1:B:253:TYR:CD2	1:B:288:PHE:HD1	2.38	0.41
6:B:800:3XB:H2	6:B:800:3XB:F5	2.09	0.41
1:A:141:LYS:HA	1:A:141:LYS:HD3	1.91	0.41
1:B:145:SER:O	1:B:149:GLU:HG2	2.20	0.41
1:A:236:ARG:HG2	1:A:242:ASP:OD1	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:480:ASP:HA	1:A:481:PRO:HD3	1.82	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	402/444 (90%)	380 (94%)	19 (5%)	3 (1%)	18	30
1	B	400/444 (90%)	382 (96%)	16 (4%)	2 (0%)	24	39
All	All	802/888 (90%)	762 (95%)	35 (4%)	5 (1%)	21	34

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	456	GLY
1	B	108	PRO
1	A	108	PRO
1	A	68	PRO
1	B	260	ASP

5.3.2 Protein sidechains [i](#)

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.

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	345/377 (92%)	325 (94%)	20 (6%)	18	31
1	B	344/377 (91%)	319 (93%)	25 (7%)	13	22
All	All	689/754 (91%)	644 (94%)	45 (6%)	15	27

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

Mol	Chain	Res	Type
1	A	69	LYS
1	A	102	LEU
1	A	123	GLU
1	A	125	LEU
1	A	194	LYS
1	A	226	LEU
1	A	260	ASP
1	A	282	THR
1	A	293	LEU
1	A	294	LEU
1	A	311	LEU
1	A	328	LEU
1	A	331	ARG
1	A	340	ASN
1	A	361	SER
1	A	378	LEU
1	A	398	ASP
1	A	416	LYS
1	A	468	ASN
1	A	476	ARG
1	B	72	ARG
1	B	92	GLN
1	B	102	LEU
1	B	105	LEU
1	B	109	ARG
1	B	123	GLU
1	B	126	LEU
1	B	153	GLN
1	B	156	GLU
1	B	207	GLN
1	B	218	LYS
1	B	223	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	257	ARG
1	B	260	ASP
1	B	262	SER
1	B	264	ARG
1	B	270	VAL
1	B	293	LEU
1	B	294	LEU
1	B	328	LEU
1	B	330	LEU
1	B	340	ASN
1	B	378	LEU
1	B	393	SER
1	B	398	ASP

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

Mol	Chain	Res	Type
1	A	124	GLN
1	A	146	GLN
1	A	166	HIS
1	A	196	GLN
1	A	340	ASN
1	A	376	ASN
1	A	435	ASN
1	A	468	ASN
1	B	128	GLN
1	B	178	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 ⓘ

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 12 ligands modelled in this entry, 1 is monoatomic - leaving 11 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	3XB	B	800	-	29,31,31	0.82	2 (6%)	32,43,43	1.49	4 (12%)
2	HEM	A	500	1	50,50,50	1.72	6 (12%)	67,82,82	1.32	6 (8%)
3	H4B	A	600	-	17,18,18	0.86	0	14,26,26	2.12	6 (42%)
7	CAD	B	950	1	0,2,4	-	-	0,1,6	-	-
5	GOL	B	880	-	5,5,5	0.35	0	5,5,5	0.96	0
6	3XB	A	800	-	29,31,31	0.85	2 (6%)	32,43,43	1.60	7 (21%)
4	ACT	A	860	-	3,3,3	0.97	0	3,3,3	0.39	0
7	CAD	A	950	1	0,2,4	-	-	0,1,6	-	-
2	HEM	B	500	1	50,50,50	1.84	6 (12%)	67,82,82	1.15	3 (4%)
3	H4B	B	600	-	17,18,18	0.83	0	14,26,26	2.09	7 (50%)
5	GOL	A	880	-	5,5,5	0.48	0	5,5,5	0.32	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
6	3XB	B	800	-	-	4/18/29/29	0/3/3/3
2	HEM	A	500	1	-	3/14/54/54	-
3	H4B	A	600	-	-	0/8/17/17	0/2/2/2
2	HEM	B	500	1	-	6/14/54/54	-
5	GOL	B	880	-	-	1/4/4/4	-
6	3XB	A	800	-	-	4/18/29/29	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	A	880	-	-	2/4/4/4	-
3	H4B	B	600	-	-	0/8/17/17	0/2/2/2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	HEM	C3D-C2D	8.06	1.54	1.36
2	A	500	HEM	C3D-C2D	6.68	1.51	1.36
2	B	500	HEM	FE-ND	5.33	2.11	1.94
2	A	500	HEM	FE-NA	4.35	2.09	1.95
2	A	500	HEM	CMA-C3A	3.36	1.57	1.50
2	A	500	HEM	FE-NB	2.92	2.03	1.94
2	B	500	HEM	CAB-C3B	2.86	1.55	1.47
2	A	500	HEM	CAB-C3B	2.56	1.54	1.47
6	A	800	3XB	F5-C4	-2.40	1.32	1.37
6	B	800	3XB	F5-C4	-2.37	1.32	1.37
2	B	500	HEM	C2A-C3A	-2.37	1.32	1.38
2	B	500	HEM	CAC-C3C	2.36	1.53	1.47
2	B	500	HEM	CMB-C2B	2.30	1.55	1.50
2	A	500	HEM	CAC-C3C	2.26	1.53	1.47
6	B	800	3XB	F6-C4	-2.20	1.32	1.37
6	A	800	3XB	F6-C4	-2.04	1.33	1.37

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	HEM	C4D-ND-C1D	4.53	110.57	105.21
3	A	600	H4B	C2-N1-C8A	4.53	121.36	113.36
3	B	600	H4B	C2-N1-C8A	4.45	121.22	113.36
2	A	500	HEM	C4D-ND-C1D	4.29	110.29	105.21
6	B	800	3XB	C6A-N1A-C2A	4.02	121.08	118.07
6	A	800	3XB	C6A-N1A-C2A	4.02	121.08	118.07
2	A	500	HEM	CBD-CAD-C3D	-3.72	102.24	112.53
2	B	500	HEM	CBA-CAA-C2A	-3.62	102.52	112.53
6	B	800	3XB	C5'-N1'-C2'	3.40	113.89	105.45
6	A	800	3XB	C5'-N1'-C2'	3.34	113.76	105.45
6	A	800	3XB	C2-N2-C3	3.21	119.84	113.35
3	A	600	H4B	C4A-C4-N3	3.17	120.82	112.13
6	B	800	3XB	C2-N2-C3	2.99	119.40	113.35
3	B	600	H4B	O4-C4-C4A	-2.88	120.32	127.26
3	A	600	H4B	O4-C4-C4A	-2.81	120.49	127.26
3	B	600	H4B	C4A-C4-N3	2.72	119.60	112.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	600	H4B	C4-C4A-N5	2.65	123.51	116.27
3	A	600	H4B	N3-C2-N1	-2.60	118.56	123.32
2	A	500	HEM	CBA-CAA-C2A	-2.59	105.36	112.53
6	B	800	3XB	C16-C11-C4	2.42	122.16	120.08
3	B	600	H4B	C11-C10-C9	-2.36	109.22	112.11
6	A	800	3XB	C7A-C2A-N1A	2.33	119.42	116.57
2	A	500	HEM	CHA-C4D-ND	2.30	127.22	124.37
3	B	600	H4B	C2-N3-C4	-2.29	120.96	125.11
2	A	500	HEM	C4C-C3C-C2C	2.21	108.73	106.81
2	A	500	HEM	CAD-C3D-C4D	2.16	128.47	124.70
3	A	600	H4B	C2-N3-C4	-2.15	121.20	125.11
6	A	800	3XB	C8A-C4A-C3A	-2.13	118.04	120.92
3	B	600	H4B	C4-C4A-N5	2.13	122.06	116.27
2	B	500	HEM	C1D-C2D-C3D	-2.12	104.75	106.98
6	A	800	3XB	C2'-C3'-C4'	2.08	106.29	103.22
6	A	800	3XB	C14-C13-C12	-2.08	120.48	123.23
3	B	600	H4B	O10-C10-C9	2.01	113.11	109.77

There are no chirality outliers.

All (20) torsion outliers are listed below:

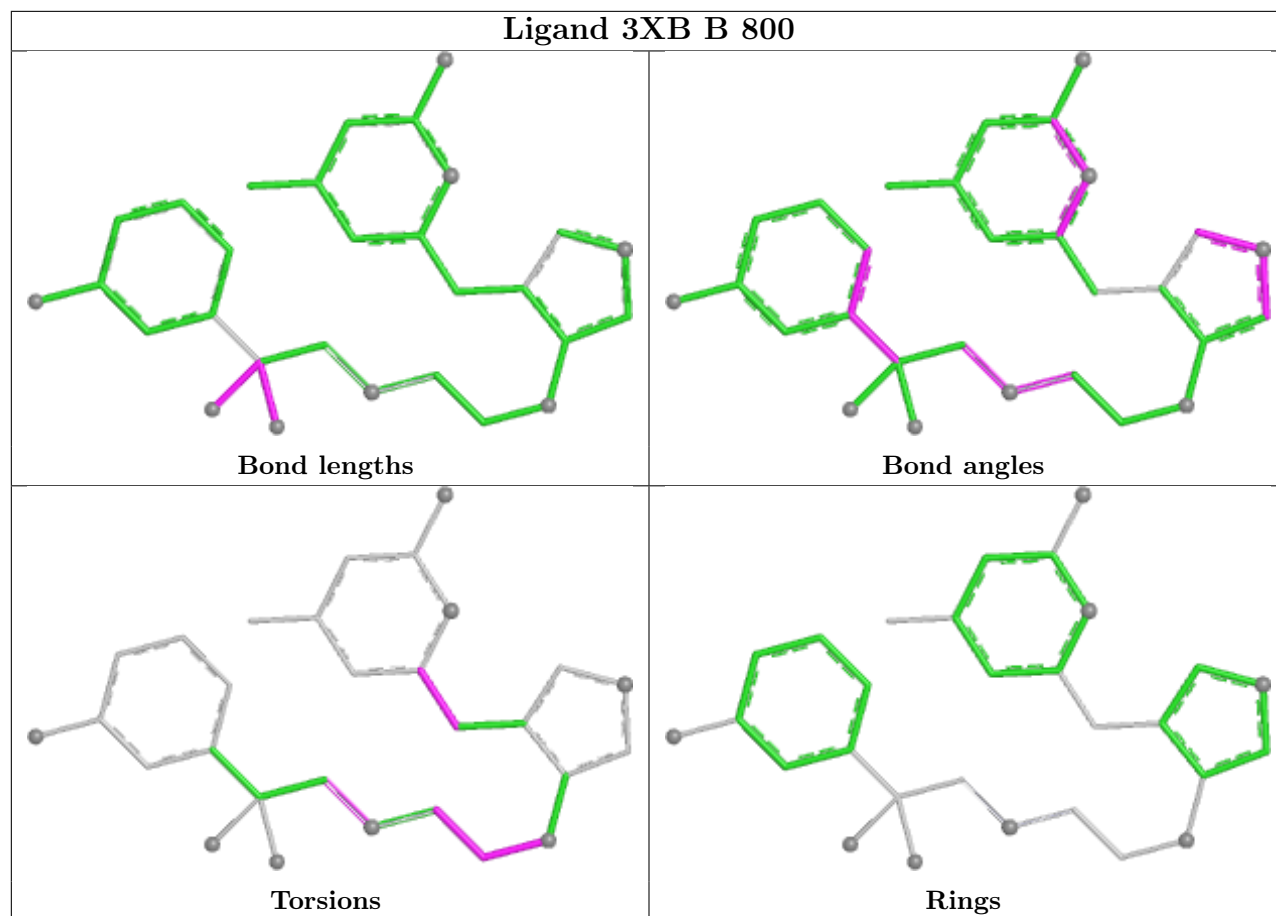
Mol	Chain	Res	Type	Atoms
5	A	880	GOL	C1-C2-C3-O3
6	A	800	3XB	C4-C3-N2-C2
6	B	800	3XB	C4-C3-N2-C2
6	A	800	3XB	N1A-C2A-C7A-C4'
6	B	800	3XB	O1-C1-C2-N2
2	A	500	HEM	C2C-C3C-CAC-CBC
2	B	500	HEM	C2C-C3C-CAC-CBC
5	B	880	GOL	C1-C2-C3-O3
5	A	880	GOL	O2-C2-C3-O3
6	B	800	3XB	N1A-C2A-C7A-C4'
6	B	800	3XB	C2-C1-O1-C3'
2	B	500	HEM	CAA-CBA-CGA-O1A
2	A	500	HEM	C2A-CAA-CBA-CGA
2	B	500	HEM	C3D-CAD-CBD-CGD
2	B	500	HEM	CAA-CBA-CGA-O2A
6	A	800	3XB	C3A-C2A-C7A-C4'
6	A	800	3XB	C16-C11-C4-F6
2	B	500	HEM	C4D-C3D-CAD-CBD
2	A	500	HEM	C4C-C3C-CAC-CBC
2	B	500	HEM	C4C-C3C-CAC-CBC

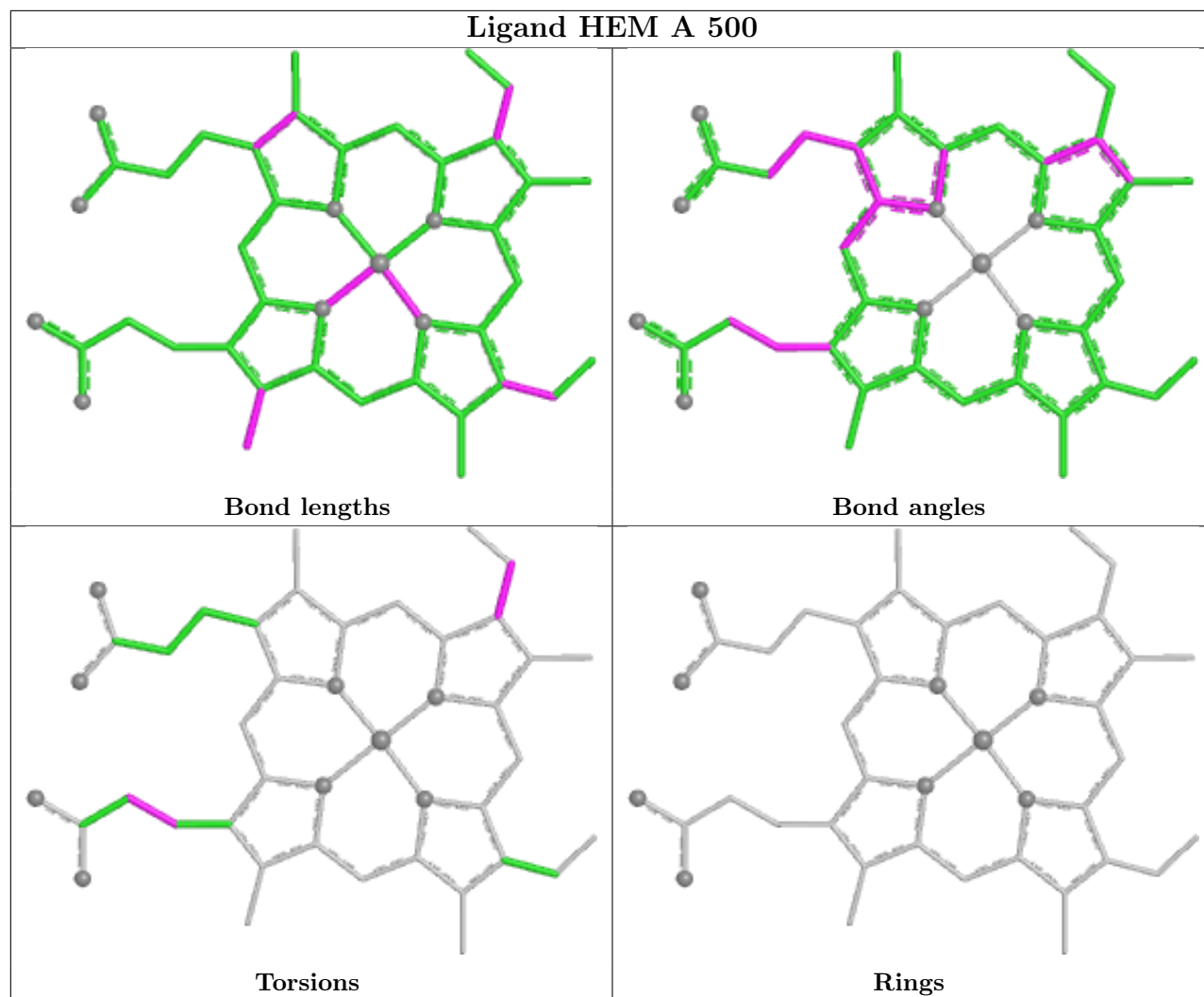
There are no ring outliers.

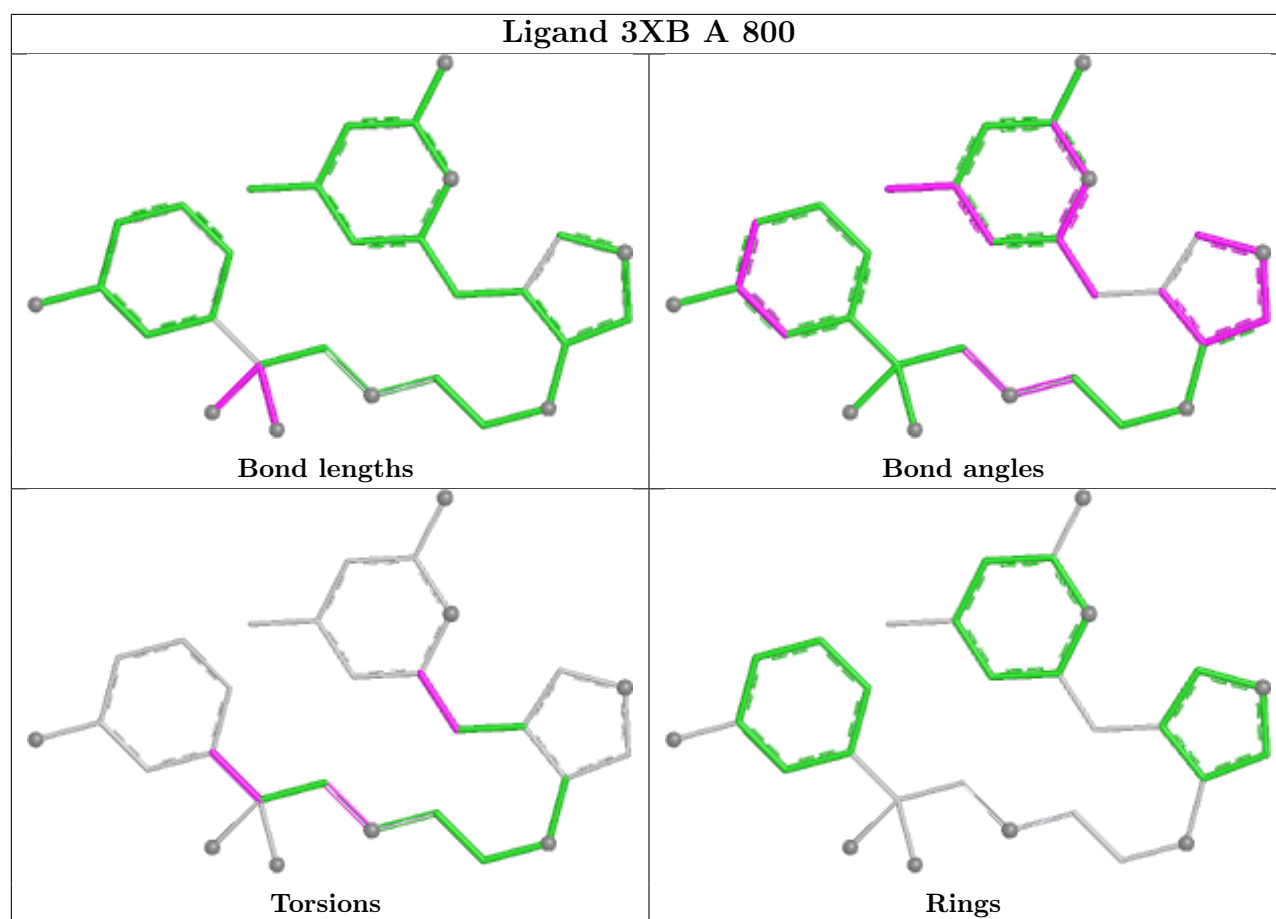
9 monomers are involved in 24 short contacts:

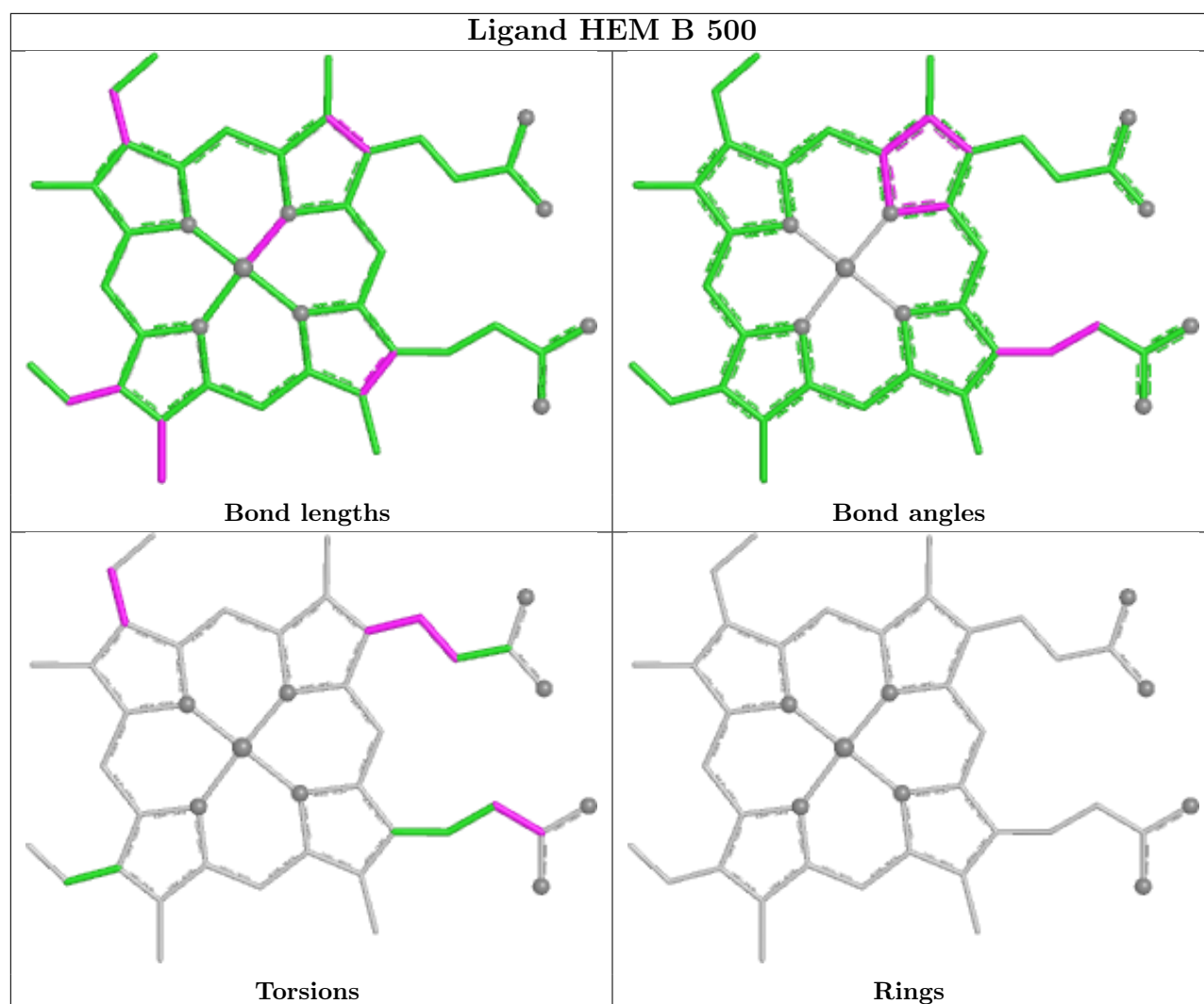
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	800	3XB	9	0
2	A	500	HEM	8	0
3	A	600	H4B	1	0
5	B	880	GOL	1	0
6	A	800	3XB	5	0
7	A	950	CAD	1	0
2	B	500	HEM	4	0
3	B	600	H4B	1	0
5	A	880	GOL	1	0

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 [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	405/444 (91%)	-0.48	5 (1%) 76 72	8, 30, 55, 73	1 (0%)
1	B	403/444 (90%)	-0.45	1 (0%) 91 90	10, 32, 55, 75	1 (0%)
All	All	808/888 (90%)	-0.47	6 (0%) 84 82	8, 31, 56, 75	2 (0%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	121	PRO	3.2
1	A	122	ALA	2.4
1	A	69	LYS	2.3
1	B	121	PRO	2.2
1	A	68	PRO	2.1
1	A	92	GLN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

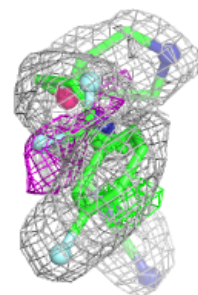
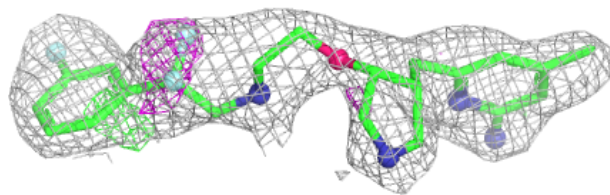
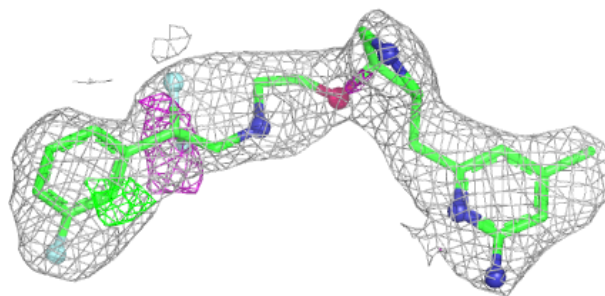
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	GOL	B	880	6/6	0.85	0.18	51,54,55,57	0
5	GOL	A	880	6/6	0.86	0.12	46,50,52,53	0
6	3XB	B	800	29/29	0.86	0.15	43,49,52,57	0
6	3XB	A	800	29/29	0.89	0.14	44,54,56,56	0
4	ACT	A	860	4/4	0.92	0.09	34,34,35,36	0
3	H4B	B	600	17/17	0.96	0.06	27,30,32,32	0
3	H4B	A	600	17/17	0.97	0.05	23,26,30,31	0
7	CAD	A	950	3/5	0.97	0.10	59,59,59,60	0
7	CAD	B	950	3/5	0.97	0.11	59,59,60,61	0
2	HEM	B	500	43/43	0.98	0.05	13,21,33,36	0
2	HEM	A	500	43/43	0.98	0.06	15,21,32,35	0
8	ZN	A	900	1/1	1.00	0.01	25,25,25,25	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.

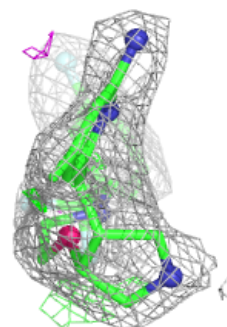
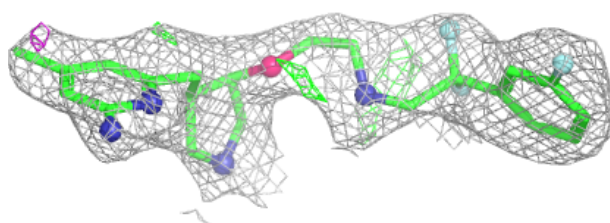
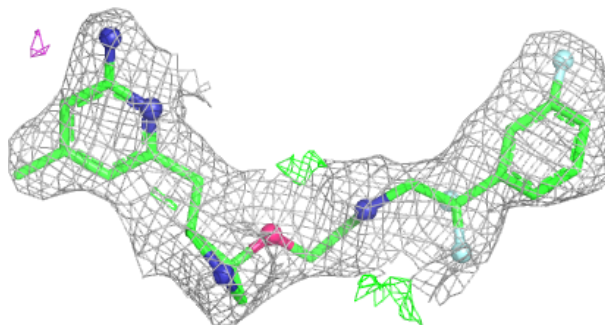
Electron density around 3XB B 800:

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



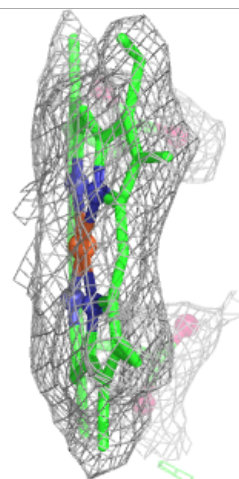
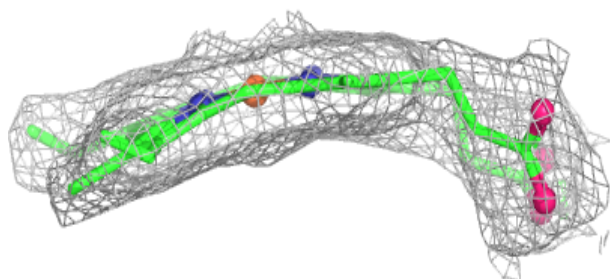
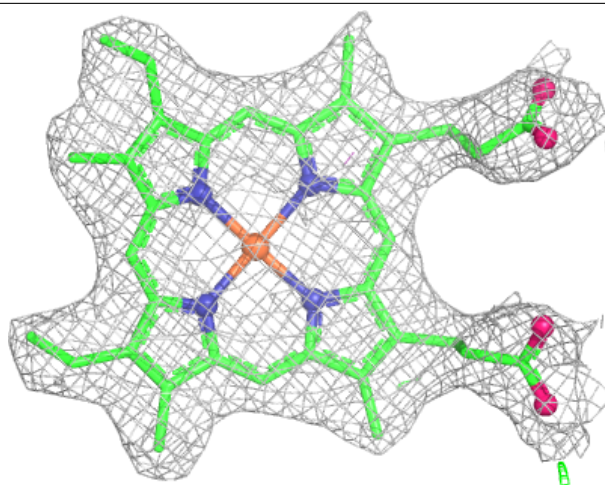
Electron density around 3XB A 800:

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



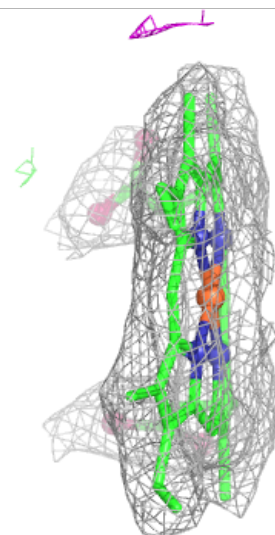
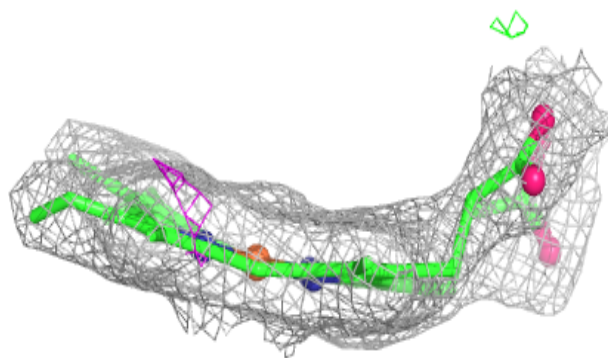
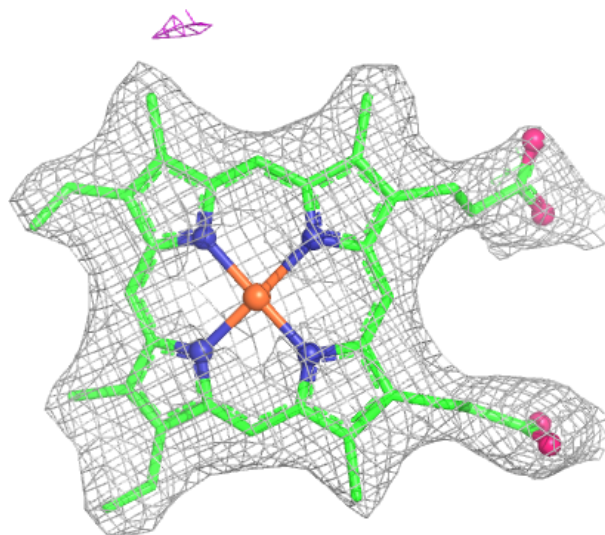
Electron density around HEM B 500:

$2mF_o-DF_c$ (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.