Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:40 PM GMT

PDB ID	:	1LGA
Title	:	CRYSTALLOGRAPHIC REFINEMENT OF LIGNIN PEROXIDASE AT 2 ANGSTROMS
Authors	:	Poulos, T.L.; Edwards, S.L.; Wariishi, H.; Gold, M.H.
Deposited on	:	1992-12-08
Resolution	:	2.03 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

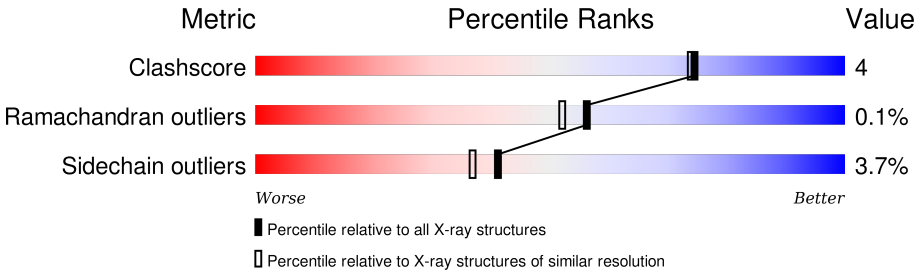
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.03 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	102246	9060 (2.04-2.00)
Ramachandran outliers	100387	8952 (2.04-2.00)
Sidechain outliers	100360	8951 (2.04-2.00)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	343	88% 11%
1	B	343	86% 12%

2 Entry composition

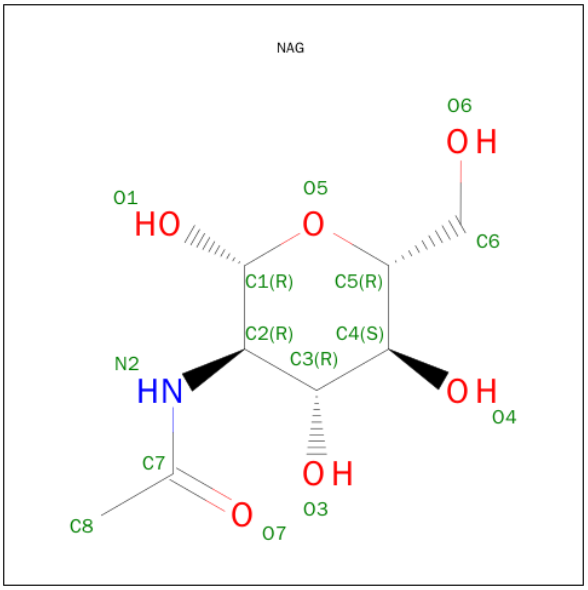
There are 5 unique types of molecules in this entry. The entry contains 5693 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 LIGNIN PEROXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	343	Total	C	N	O	S	0	0	0
			2556	1615	428	497	16			
1	B	341	Total	C	N	O	S	0	0	0
			2545	1609	426	494	16			

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

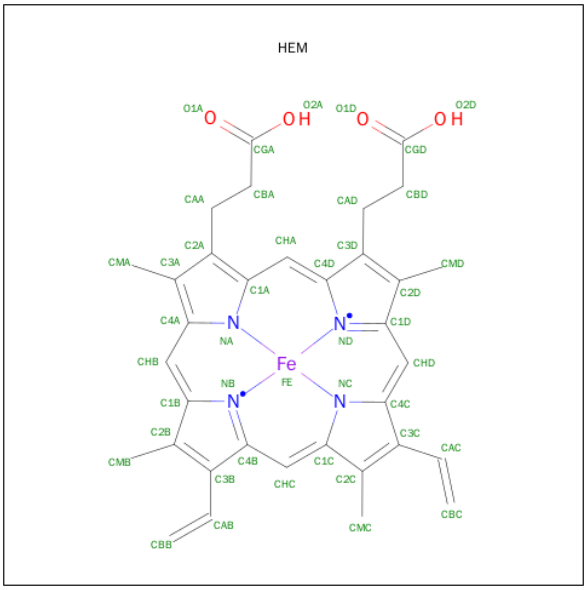


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	2	Total Ca 2 2	0	0
3	A	2	Total Ca 2 2	0	0

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	230	Total O 230 230	0	0
5	B	244	Total O 244 244	0	0

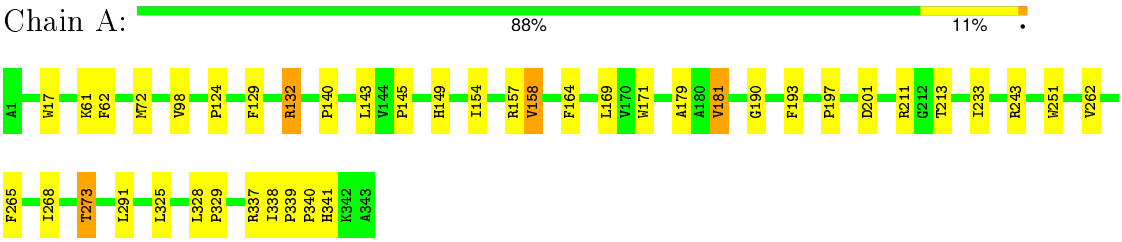
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

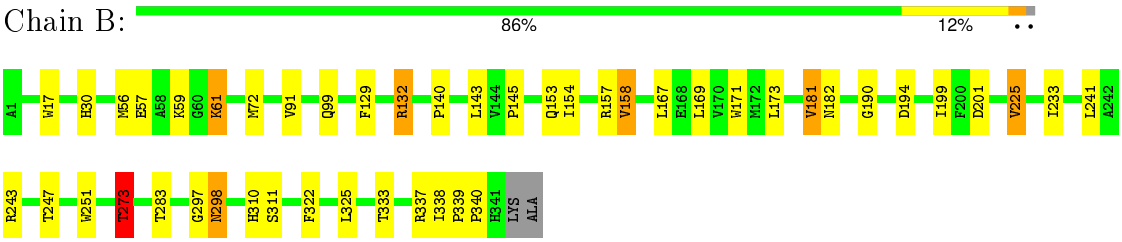
- Molecule 1: LIGNIN PEROXIDASE

Chain A:



- Molecule 1: LIGNIN PEROXIDASE

Chain B:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	44.70Å 77.50Å 100.00Å 90.00° 101.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.03	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.03)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.150 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5693	wwPDB-VP
Average B, all atoms (Å^2)	13.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, CA, NAG

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	0/2626	1.42	22/3578 (0.6%)
1	B	0.83	0/2615	1.47	25/3564 (0.7%)
All	All	0.82	0/5241	1.45	47/7142 (0.7%)

There are no bond length outliers.

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	132	ARG	NE-CZ-NH2	-25.26	107.67	120.30
1	B	132	ARG	NE-CZ-NH1	19.31	129.96	120.30
1	A	132	ARG	NE-CZ-NH2	-18.21	111.20	120.30
1	A	132	ARG	NE-CZ-NH1	17.40	129.00	120.30
1	B	337	ARG	NE-CZ-NH1	10.15	125.38	120.30
1	A	243	ARG	NE-CZ-NH2	-9.89	115.35	120.30
1	A	201	ASP	CB-CG-OD1	9.50	126.85	118.30
1	B	201	ASP	CB-CG-OD1	9.39	126.75	118.30
1	A	243	ARG	NE-CZ-NH1	9.16	124.88	120.30
1	A	17	TRP	CD1-CG-CD2	9.03	113.52	106.30
1	B	243	ARG	NE-CZ-NH1	8.01	124.31	120.30
1	A	17	TRP	CE2-CD2-CG	-7.71	101.13	107.30
1	B	251	TRP	CD1-CG-CD2	7.53	112.32	106.30
1	B	171	TRP	CD1-CG-CD2	7.47	112.28	106.30
1	B	17	TRP	CD1-CG-CD2	7.28	112.13	106.30
1	A	251	TRP	CD1-CG-CD2	7.25	112.10	106.30
1	A	157	ARG	NE-CZ-NH1	7.03	123.81	120.30
1	B	17	TRP	CE2-CD2-CG	-6.84	101.83	107.30
1	B	171	TRP	CE2-CD2-CG	-6.83	101.84	107.30
1	A	337	ARG	NE-CZ-NH1	6.75	123.67	120.30
1	A	273	THR	N-CA-CB	-6.71	97.55	110.30
1	A	171	TRP	CD1-CG-CD2	6.53	111.53	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	251	TRP	CE2-CD2-CG	-6.51	102.09	107.30
1	B	337	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	B	17	TRP	CG-CD2-CE3	6.32	139.59	133.90
1	B	132	ARG	CB-CG-CD	6.30	127.98	111.60
1	A	171	TRP	CE2-CD2-CG	-6.28	102.28	107.30
1	B	297	GLY	CA-C-N	-6.22	103.52	117.20
1	B	132	ARG	CG-CD-NE	-6.08	99.02	111.80
1	A	251	TRP	CE2-CD2-CG	-6.07	102.45	107.30
1	B	17	TRP	CB-CG-CD1	-5.96	119.25	127.00
1	B	132	ARG	CD-NE-CZ	5.94	131.91	123.60
1	B	194	ASP	CB-CG-OD1	5.93	123.63	118.30
1	A	132	ARG	CG-CD-NE	-5.81	99.60	111.80
1	A	17	TRP	CG-CD2-CE3	5.80	139.12	133.90
1	A	17	TRP	CG-CD1-NE1	-5.71	104.39	110.10
1	A	158	VAL	N-CA-CB	-5.51	99.37	111.50
1	A	251	TRP	CG-CD1-NE1	-5.47	104.63	110.10
1	A	17	TRP	CB-CG-CD1	-5.45	119.91	127.00
1	B	225	VAL	N-CA-CB	-5.43	99.55	111.50
1	B	273	THR	N-CA-CB	-5.33	100.18	110.30
1	A	132	ARG	CB-CG-CD	5.32	125.44	111.60
1	B	56	MET	CA-CB-CG	-5.24	104.40	113.30
1	B	158	VAL	N-CA-CB	-5.23	100.00	111.50
1	B	298	ASN	N-CA-C	-5.20	96.97	111.00
1	A	273	THR	OG1-CB-CG2	5.19	121.94	110.00
1	B	251	TRP	CG-CD1-NE1	-5.04	105.06	110.10

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	2556	0	2411	21	0
1	B	2545	0	2405	19	0
2	A	14	0	13	0	0
2	B	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	43	0	30	1	0
4	B	43	0	30	1	0
5	A	230	0	0	1	0
5	B	244	0	0	2	0
All	All	5693	0	4902	40	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 4.

All (40) 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:181:VAL:HG21	1:A:233:ILE:HD13	1.75	0.68
1:A:158:VAL:HG13	1:A:164:PHE:HB2	1.86	0.58
1:A:265:PHE:HA	1:A:268:ILE:HG22	1.88	0.56
1:B:132:ARG:NH1	1:B:273:THR:HG23	2.25	0.51
1:B:145:PRO:HB3	1:B:154:ILE:HD12	1.92	0.51
1:A:140:PRO:HG2	1:A:143:LEU:HD11	1.93	0.51
1:B:310:HIS:HE1	1:B:322:PHE:O	1.94	0.50
1:B:273:THR:HG21	5:B:473:HOH:O	2.13	0.49
1:A:145:PRO:HB3	1:A:154:ILE:HD12	1.93	0.49
1:B:129:PHE:O	1:B:132:ARG:NH2	2.45	0.49
1:B:181:VAL:HG21	1:B:233:ILE:HD13	1.95	0.49
1:B:182:ASN:ND2	1:B:340:PRO:HB3	2.28	0.48
1:A:149:HIS:HB2	1:A:154:ILE:HD11	1.94	0.48
1:A:181:VAL:CG2	1:A:233:ILE:HD13	2.44	0.48
1:B:72:MET:HG3	1:B:91:VAL:HG13	1.95	0.48
1:A:190:GLY:HA3	1:A:338:ILE:O	2.15	0.46
1:A:154:ILE:HG21	4:A:396:HEM:HBB1	1.97	0.46
1:B:190:GLY:HA3	1:B:338:ILE:O	2.17	0.45
1:A:129:PHE:O	1:A:132:ARG:NH2	2.50	0.44
1:B:339:PRO:HA	1:B:340:PRO:HD2	1.82	0.44
1:B:241:LEU:HD22	1:B:247:THR:HG21	1.99	0.44
1:B:140:PRO:HG2	1:B:143:LEU:HD11	2.00	0.43
1:A:179:ALA:HB3	1:A:193:PHE:HD2	1.84	0.43
1:A:197:PRO:HG3	1:A:338:ILE:HD11	2.01	0.43
1:A:211:ARG:NH1	1:A:213:THR:HG22	2.34	0.43
1:A:339:PRO:HA	1:A:340:PRO:HD2	1.85	0.42
1:A:72:MET:SD	1:A:98:VAL:HG21	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:338:ILE:HA	1:B:339:PRO:HD2	1.85	0.42
1:B:199:ILE:HG21	1:B:199:ILE:HD13	1.87	0.42
1:A:145:PRO:HB3	1:A:154:ILE:CD1	2.50	0.41
1:B:173:LEU:HD23	1:B:173:LEU:HA	1.92	0.41
1:A:124:PRO:HB3	1:A:262:VAL:HG13	2.01	0.41
1:B:129:PHE:HA	1:B:283:THR:O	2.20	0.41
1:B:57:GLU:HA	1:B:61:LYS:O	2.20	0.41
1:B:167:LEU:HD23	5:B:439:HOH:O	2.21	0.41
1:A:273:THR:HG21	5:A:485:HOH:O	2.21	0.41
1:B:181:VAL:HB	4:B:396:HEM:HAA2	2.03	0.40
1:A:268:ILE:HD12	1:A:268:ILE:HA	1.93	0.40
1:A:328:LEU:HA	1:A:329:PRO:HD3	1.84	0.40
1:A:61:LYS:HD3	1:A:61:LYS:H	1.85	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	341/343 (99%)	331 (97%)	9 (3%)	1 (0%)	46 40
1	B	339/343 (99%)	331 (98%)	8 (2%)	0	100 100
All	All	680/686 (99%)	662 (97%)	17 (2%)	1 (0%)	56 52

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	62	PHE

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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	273/274 (100%)	268 (98%)	5 (2%)	66 68
1	B	273/274 (100%)	258 (94%)	15 (6%)	27 20
All	All	546/548 (100%)	526 (96%)	20 (4%)	41 37

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	169	LEU
1	A	181	VAL
1	A	291	LEU
1	A	325	LEU
1	A	341	HIS
1	B	30	HIS
1	B	59	LYS
1	B	61	LYS
1	B	99	GLN
1	B	153	GLN
1	B	157	ARG
1	B	158	VAL
1	B	169	LEU
1	B	181	VAL
1	B	225	VAL
1	B	273	THR
1	B	298	ASN
1	B	311	SER
1	B	325	LEU
1	B	333	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	GLN
1	A	258	GLN

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Mol	Chain	Res	Type
1	A	310	HIS
1	B	33	GLN
1	B	153	GLN
1	B	310	HIS

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

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	A	396	1,5	30,50,50	3.05	10 (33%)	24,82,82	2.12	7 (29%)
2	NAG	A	397	1	14,14,15	0.92	0	15,19,21	0.83	0
4	HEM	B	396	1,5	30,50,50	3.11	9 (30%)	24,82,82	2.26	6 (25%)
2	NAG	B	397	1	14,14,15	0.88	0	15,19,21	1.27	2 (13%)

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	A	396	1,5	-	0/10/54/54	0/0/8/8
2	NAG	A	397	1	-	0/6/23/26	0/1/1/1
4	HEM	B	396	1,5	-	0/10/54/54	0/0/8/8
2	NAG	B	397	1	-	0/6/23/26	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	396	HEM	C3B-C4B	-9.20	1.43	1.51
4	A	396	HEM	C3B-C4B	-8.89	1.43	1.51
4	B	396	HEM	C2D-C3D	-6.85	1.34	1.54
4	A	396	HEM	C3D-C4D	-6.57	1.43	1.51
4	A	396	HEM	C2D-C3D	-6.42	1.35	1.54
4	B	396	HEM	C3B-CAB	-6.28	1.39	1.51
4	B	396	HEM	C3C-CAC	-5.81	1.40	1.51
4	A	396	HEM	C3C-CAC	-5.72	1.40	1.51
4	A	396	HEM	C3B-CAB	-5.62	1.40	1.51
4	B	396	HEM	C3D-C4D	-5.28	1.44	1.51
4	B	396	HEM	C2C-C1C	-4.89	1.43	1.52
4	A	396	HEM	C2C-C1C	-4.46	1.44	1.52
4	B	396	HEM	C2B-C1B	-2.16	1.44	1.51
4	A	396	HEM	C2B-C1B	-2.02	1.45	1.51
4	A	396	HEM	C4C-NC	2.13	1.38	1.36
4	B	396	HEM	CBB-CAB	2.30	1.42	1.29
4	A	396	HEM	CBC-CAC	2.30	1.42	1.29
4	A	396	HEM	CBB-CAB	2.59	1.44	1.29
4	B	396	HEM	CBC-CAC	2.87	1.45	1.29

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	397	NAG	C2-N2-C7	-2.92	119.28	123.04
2	B	397	NAG	O4-C4-C3	-2.71	104.24	110.34
4	A	396	HEM	C3C-CAC-CBC	2.04	127.59	124.46
4	B	396	HEM	CMD-C2D-C3D	3.00	127.62	114.35
4	A	396	HEM	CMD-C2D-C3D	3.32	129.05	114.35
4	A	396	HEM	CAD-C3D-C4D	3.33	124.20	112.47
4	B	396	HEM	CAD-C3D-C4D	3.68	125.44	112.47
4	B	396	HEM	CMC-C2C-C3C	3.88	126.23	116.53
4	B	396	HEM	CAD-C3D-C2D	3.89	124.41	113.22
4	A	396	HEM	CMC-C2C-C3C	4.03	126.58	116.53
4	A	396	HEM	C2D-C3D-C4D	4.06	108.38	101.50
4	A	396	HEM	CMB-C2B-C3B	4.46	127.67	116.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	396	HEM	CAD-C3D-C2D	4.88	127.26	113.22
4	B	396	HEM	C2D-C3D-C4D	4.91	109.82	101.50
4	B	396	HEM	CMB-C2B-C3B	5.61	130.52	116.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	396	HEM	1	0
4	B	396	HEM	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.