Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:02 AM GMT

PDB ID	:	3NOS
Title	:	HUMAN ENDOTHELIAL NITRIC OXIDE SYNTHASE WITH ARGININE SUBSTRATE
Authors	:	Fischmann, T.O.; Weber, P.C.
Deposited on	:	1999-02-03
Resolution	:	2.40 Å(reported)

The following versions of software and data (see references ⓘ) 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
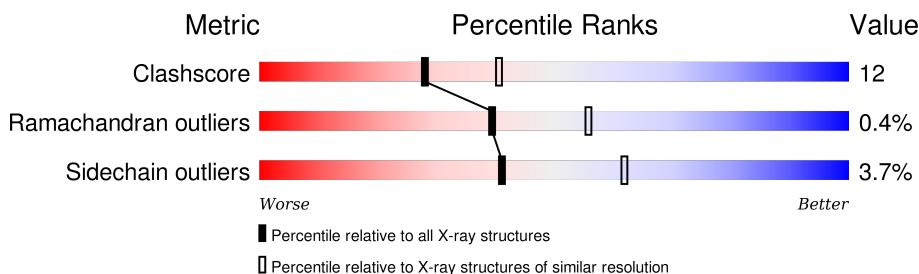
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.40 Å.
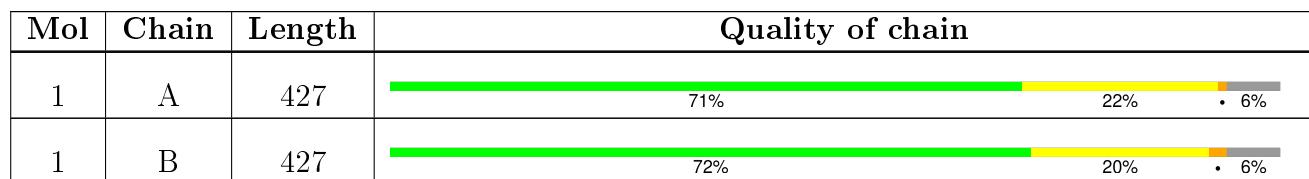
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

Metric	Percentile Ranks	Value
Clashscore		12
Ramachandran outliers		0.4%
Sidechain outliers		3.7%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)

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	427	71% 22% • 6%
1	B	427	72% 20% • 6%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7042 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.
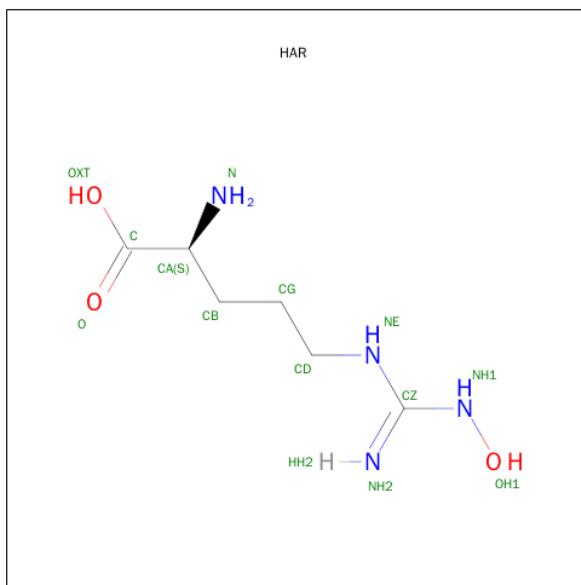
- Molecule 1 is a protein called ENDOTHELIAL NITRIC-OXIDE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	400	Total 3198	C 2037	N 566	O 579	S 16	0	0	0
1	B	400	Total 3198	C 2037	N 566	O 579	S 16	0	0	0

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is N-OMEGA-HYDROXY-L-ARGININE (three-letter code: HAR) (formula: $C_6H_{14}N_4O_3$).
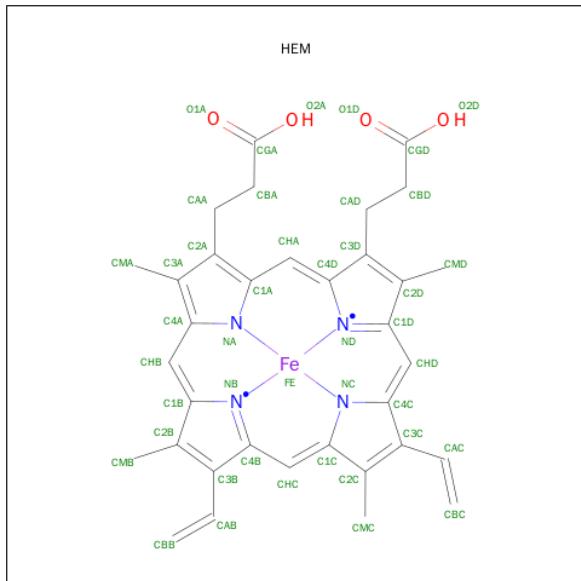
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 13	C 6	N 4	O 3	0	0

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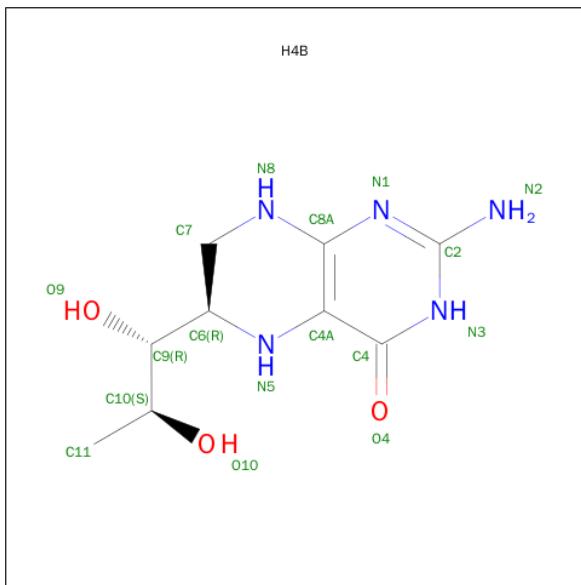
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			13	6	4	3		

- 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	0	0
			43	34	1	4	4		
4	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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

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

• Molecule 6 is water.
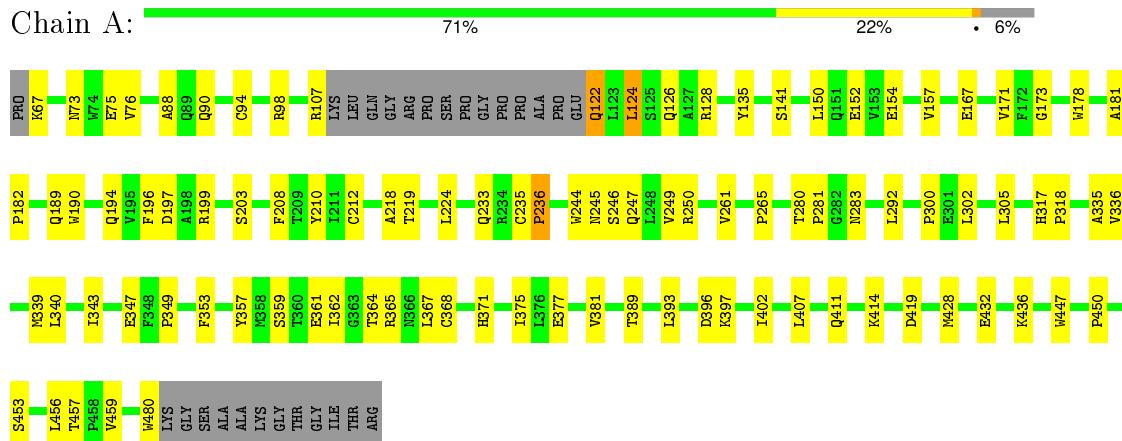
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	253	Total 253	O 253	0	0
6	B	246	Total 246	O 246	0	0

3 Residue-property plots (i)
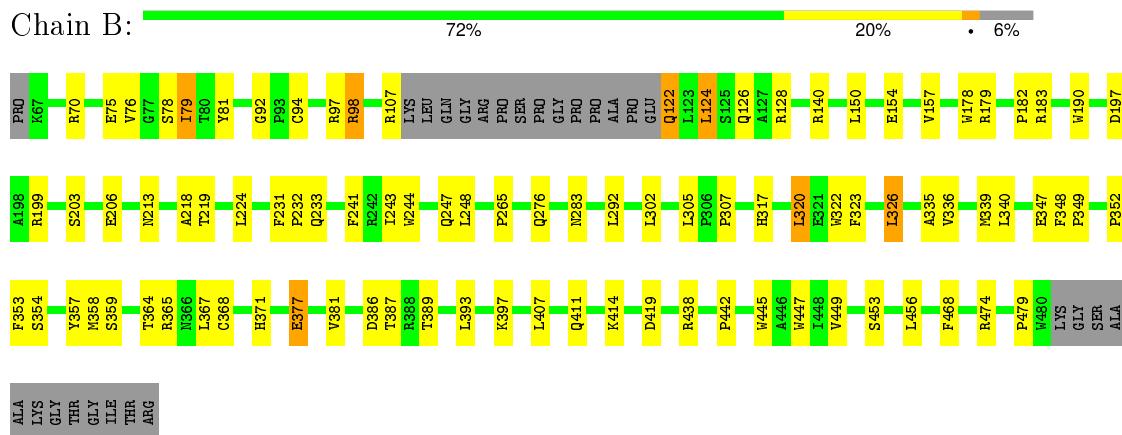
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: ENDOTHELIAL NITRIC-OXIDE SYNTHASE

- Molecule 1: ENDOTHELIAL NITRIC-OXIDE SYNTHASE

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 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	68.86Å 93.26Å 156.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.40	Depositor
% Data completeness (in resolution range)	90.0 (8.00-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.193 , 0.308	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7042	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

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: HEM, ZN, HAR, H4B

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	0.50	0/3289	0.68	0/4481
1	B	0.49	0/3289	0.69	0/4481
All	All	0.49	0/6578	0.69	0/8962

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	135	TYR	Sidechain
1	A	210	TYR	Sidechain

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	3198	0	3106	75	0
1	B	3198	0	3106	75	0
2	A	1	0	0	0	0
3	A	13	0	12	2	0
3	B	13	0	12	2	0
4	A	43	0	30	11	0
4	B	43	0	30	8	0
5	A	17	0	15	2	0
5	B	17	0	15	2	0
6	A	253	0	0	7	0
6	B	246	0	0	6	0
All	All	7042	0	6326	150	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 12.

All (150) 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:152:GLU:HG2	6:A:1224:HOH:O	1.59	1.00
1:B:339:MET:HE1	4:B:1010:HEM:HBD2	1.54	0.89
4:A:510:HEM:HBC2	4:A:510:HEM:HMC2	1.58	0.85
1:A:428:MET:HE3	1:A:459:VAL:HG12	1.59	0.81
1:A:339:MET:HE1	4:A:510:HEM:HBD2	1.71	0.72
1:B:124:LEU:HD22	1:B:157:VAL:HG11	1.72	0.71
1:B:70:ARG:HD2	1:B:79:ILE:HD12	1.73	0.69
1:A:197:ASP:OD1	1:A:199:ARG:HD3	1.92	0.69
1:A:219:THR:HA	1:A:224:LEU:HD23	1.74	0.68
1:B:197:ASP:OD1	1:B:199:ARG:HD3	1.93	0.68
1:B:323:PHE:O	1:B:326:LEU:HB2	1.93	0.67
1:B:339:MET:HE3	1:B:353:PHE:HZ	1.60	0.67
4:B:1010:HEM:HBC2	4:B:1010:HEM:HMC2	1.76	0.66
1:A:428:MET:HE3	1:A:459:VAL:CG1	2.26	0.66
1:A:124:LEU:HD22	1:A:157:VAL:HG11	1.76	0.66
1:A:339:MET:HE3	1:A:353:PHE:HZ	1.61	0.65
1:A:244:TRP:HB2	1:A:292:LEU:HB3	1.80	0.64
1:B:213:ASN:HB3	6:B:1248:HOH:O	1.98	0.63
1:A:361:GLU:OE1	3:A:512:HAR:HB3	2.01	0.60
1:B:231:PHE:HB3	1:B:232:PRO:CD	2.33	0.59
1:B:124:LEU:O	1:B:128:ARG:HG3	2.02	0.58
1:A:292:LEU:HD13	1:A:302:LEU:HD23	1.86	0.58
1:A:336:VAL:HG11	1:A:339:MET:HE2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:SER:OG	1:B:206:GLU:HG3	2.03	0.58
1:B:244:TRP:HB2	1:B:292:LEU:HB3	1.86	0.58
1:A:428:MET:CE	1:A:459:VAL:HG12	2.32	0.58
1:B:243:ILE:HD12	1:B:352:PRO:HG3	1.85	0.58
1:A:219:THR:HA	1:A:224:LEU:CD2	2.34	0.57
1:A:189:GLN:HB3	6:A:1099:HOH:O	2.04	0.57
1:B:393:LEU:O	1:B:397:LYS:HG3	2.05	0.56
1:B:183:ARG:HD3	1:B:447:TRP:CD2	2.41	0.56
1:A:124:LEU:O	1:A:128:ARG:HG3	2.06	0.56
1:A:339:MET:CE	1:A:353:PHE:HZ	2.19	0.55
1:A:173:GLY:HA3	1:A:343:ILE:HD13	1.88	0.55
1:B:357:TYR:HE1	3:B:1012:HAR:O	1.89	0.55
1:B:359:SER:OG	1:B:419:ASP:HA	2.06	0.55
1:A:178:TRP:CZ2	4:A:510:HEM:HBB2	2.42	0.55
1:A:94:CYS:HB3	1:B:94:CYS:HB3	1.88	0.55
1:A:371:HIS:HD2	1:B:75:GLU:O	1.89	0.55
1:A:292:LEU:HD13	1:A:302:LEU:CD2	2.36	0.55
1:B:76:VAL:HG23	1:B:78:SER:H	1.73	0.54
4:A:510:HEM:CHA	4:A:510:HEM:HBA1	2.38	0.54
1:B:231:PHE:HB3	1:B:232:PRO:HD2	1.89	0.54
1:B:365:ARG:HH12	5:B:1011:H4B:C4	2.21	0.54
1:A:393:LEU:O	1:A:397:LYS:HG3	2.07	0.54
1:A:371:HIS:CD2	1:B:75:GLU:O	2.61	0.54
1:B:414:LYS:HE2	6:B:1189:HOH:O	2.08	0.53
1:B:453:SER:HB3	1:B:456:LEU:HD12	1.91	0.53
1:A:357:TYR:CD2	1:A:362:ILE:HD11	2.43	0.53
1:A:218:ALA:O	1:A:224:LEU:HA	2.08	0.52
1:B:218:ALA:O	1:B:224:LEU:HA	2.10	0.52
1:B:140:ARG:NH2	6:B:1240:HOH:O	2.42	0.52
1:A:67:LYS:HG2	1:B:98:ARG:HH21	1.74	0.52
1:A:88:ALA:O	1:B:97:ARG:NH1	2.43	0.51
4:A:510:HEM:HHA	4:A:510:HEM:HBA1	1.92	0.51
1:B:122:GLN:O	1:B:126:GLN:HG3	2.11	0.51
1:B:317:HIS:CE1	1:B:320:LEU:HD22	2.46	0.50
1:A:453:SER:HB3	1:A:456:LEU:HD12	1.93	0.50
1:A:432:GLU:O	1:A:436:LYS:HE2	2.12	0.50
1:A:245:ASN:HB3	6:A:1193:HOH:O	2.12	0.50
1:A:407:LEU:O	1:A:411:GLN:HG3	2.12	0.50
1:B:265:PRO:HB2	1:B:371:HIS:O	2.12	0.50
1:B:320:LEU:HG	1:B:322:TRP:CZ2	2.47	0.49
1:B:407:LEU:O	1:B:411:GLN:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:474:ARG:HD2	6:B:1038:HOH:O	2.12	0.49
1:A:122:GLN:O	1:A:126:GLN:HG3	2.12	0.49
1:B:447:TRP:CZ3	4:B:1010:HEM:HBA2	2.47	0.49
1:A:94:CYS:CB	1:B:94:CYS:HB3	2.42	0.49
1:B:386:ASP:OD2	1:B:389:THR:HG22	2.13	0.49
4:A:510:HEM:HHC	4:A:510:HEM:CBB	2.44	0.48
1:A:340:LEU:HD21	1:A:347:GLU:HG2	1.95	0.48
1:B:150:LEU:O	1:B:154:GLU:HG3	2.13	0.48
1:B:232:PRO:HG2	1:B:241:PHE:CE2	2.48	0.48
1:B:243:ILE:CD1	1:B:352:PRO:HG3	2.43	0.48
1:B:377:GLU:O	1:B:381:VAL:HG23	2.13	0.48
1:A:94:CYS:HB3	1:B:94:CYS:CB	2.44	0.47
1:B:339:MET:CE	4:B:1010:HEM:HMD1	2.45	0.47
1:B:340:LEU:HD11	1:B:347:GLU:HB3	1.95	0.47
1:B:445:TRP:O	1:B:449:VAL:HG23	2.15	0.47
1:A:189:GLN:NE2	6:A:1126:HOH:O	2.47	0.47
1:B:364:THR:O	1:B:368:CYS:HB2	2.16	0.46
1:A:208:PHE:CZ	1:A:212:CYS:SG	3.08	0.46
1:A:150:LEU:O	1:A:154:GLU:HG3	2.15	0.46
1:B:183:ARG:HD3	1:B:447:TRP:CE2	2.51	0.46
1:A:90:GLN:HG2	1:B:97:ARG:HB2	1.97	0.46
1:A:246:SER:OG	1:A:250:ARG:HD2	2.16	0.46
1:A:377:GLU:O	1:A:381:VAL:HG23	2.16	0.46
1:B:178:TRP:CE3	1:B:190:TRP:HA	2.51	0.45
1:A:357:TYR:HE1	3:A:512:HAR:OXT	1.99	0.45
1:A:359:SER:OG	1:A:419:ASP:HA	2.16	0.45
1:B:339:MET:CE	1:B:353:PHE:HZ	2.27	0.45
4:A:510:HEM:HHC	4:A:510:HEM:HBB2	1.99	0.45
1:B:447:TRP:CE3	4:B:1010:HEM:HBA2	2.52	0.45
3:B:1012:HAR:HG2	4:B:1010:HEM:O1A	2.17	0.45
1:B:124:LEU:HA	1:B:124:LEU:HD13	1.76	0.44
1:B:339:MET:HE1	4:B:1010:HEM:HMD1	1.99	0.44
1:A:339:MET:HE3	1:A:353:PHE:CZ	2.47	0.44
1:B:124:LEU:HD11	1:B:154:GLU:HG2	2.00	0.44
1:B:178:TRP:HZ2	4:B:1010:HEM:HBB2	1.80	0.44
1:B:365:ARG:HG3	6:B:1131:HOH:O	2.18	0.44
1:B:292:LEU:HD13	1:B:302:LEU:CD2	2.47	0.44
1:A:375:ILE:HD11	1:A:402:ILE:HD13	1.99	0.44
1:B:70:ARG:HG3	1:B:81:TYR:CZ	2.53	0.44
1:A:244:TRP:CH2	1:A:480:TRP:HB3	2.52	0.44
1:B:233:GLN:HB3	1:B:348:PHE:CE2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:TRP:CE3	1:A:190:TRP:HA	2.53	0.44
1:B:447:TRP:HA	5:B:1011:H4B:N1	2.32	0.43
1:A:450:PRO:HG3	1:A:457:THR:HG21	2.00	0.43
1:B:335:ALA:HA	1:B:354:SER:HB3	1.99	0.43
1:A:411:GLN:O	1:A:414:LYS:HD2	2.18	0.43
1:A:364:THR:O	1:A:368:CYS:HB2	2.18	0.43
4:A:510:HEM:HBC2	4:A:510:HEM:CMC	2.40	0.43
1:B:339:MET:HE3	1:B:353:PHE:CZ	2.46	0.43
1:A:67:LYS:CG	1:B:98:ARG:HH21	2.30	0.43
1:A:167:GLU:O	1:A:171:VAL:HG23	2.19	0.43
4:A:510:HEM:HHA	4:A:510:HEM:CBA	2.49	0.43
1:B:276:GLN:O	1:B:276:GLN:HG2	2.19	0.43
1:A:244:TRP:CZ2	1:A:300:PRO:HG2	2.54	0.43
1:A:247:GLN:HA	1:A:335:ALA:O	2.18	0.43
1:B:219:THR:HA	1:B:224:LEU:HD22	2.01	0.42
1:B:122:GLN:NE2	6:B:1137:HOH:O	2.52	0.42
1:A:447:TRP:HA	5:A:511:H4B:N1	2.34	0.42
1:A:233:GLN:HG2	6:A:1058:HOH:O	2.19	0.42
1:A:339:MET:CE	4:A:510:HEM:HMD1	2.50	0.42
1:A:124:LEU:HD13	1:A:124:LEU:HA	1.73	0.42
1:B:248:LEU:HD12	1:B:335:ALA:CB	2.49	0.42
1:B:336:VAL:HG11	1:B:339:MET:HE2	2.01	0.42
1:A:414:LYS:HD2	1:A:414:LYS:N	2.33	0.42
1:A:244:TRP:CZ3	1:A:480:TRP:HB3	2.54	0.42
1:A:141:SER:HB3	6:A:1223:HOH:O	2.19	0.41
1:B:347:GLU:O	1:B:349:PRO:HD3	2.20	0.41
1:B:247:GLN:HA	1:B:335:ALA:O	2.20	0.41
1:A:280:THR:HA	1:A:281:PRO:HD2	1.90	0.41
1:A:178:TRP:CH2	4:A:510:HEM:HMC1	2.55	0.41
1:A:365:ARG:HH12	5:A:511:H4B:C4	2.33	0.41
1:B:179:ARG:CZ	1:B:438:ARG:HD2	2.50	0.41
1:A:203:SER:HB2	6:A:1064:HOH:O	2.21	0.41
1:A:347:GLU:O	1:A:349:PRO:HD3	2.20	0.41
1:B:182:PRO:HA	1:B:442:PRO:O	2.20	0.41
1:A:261:VAL:HG11	1:A:265:PRO:HA	2.03	0.41
1:A:194:GLN:HG3	1:A:196:PHE:CE1	2.56	0.41
1:B:292:LEU:HD13	1:B:302:LEU:HD23	2.03	0.40
1:B:244:TRP:CD1	1:B:479:PRO:HG3	2.56	0.40
1:B:92:GLY:HA2	1:B:468:PHE:HE2	1.86	0.40
1:A:432:GLU:HG2	1:A:436:LYS:HE2	2.03	0.40
1:A:124:LEU:HD11	1:A:154:GLU:HG2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:HIS:CG	1:A:318:PRO:HD2	2.56	0.40
1:A:397:LYS:HE2	1:A:397:LYS:HB3	1.92	0.40
1:A:73:ASN:OD1	1:A:76:VAL:HG13	2.22	0.40
1:A:181:ALA:HA	1:A:182:PRO:HD3	1.96	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	396/427 (93%)	377 (95%)	17 (4%)	2 (0%)	34	48
1	B	396/427 (93%)	380 (96%)	15 (4%)	1 (0%)	46	63
All	All	792/854 (93%)	757 (96%)	32 (4%)	3 (0%)	39	56

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	283	ASN
1	B	283	ASN
1	A	236	PRO

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	340/359 (95%)	328 (96%)	12 (4%)	43	64
1	B	340/359 (95%)	327 (96%)	13 (4%)	40	60
All	All	680/718 (95%)	655 (96%)	25 (4%)	41	62

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	GLU
1	A	98	ARG
1	A	107	ARG
1	A	122	GLN
1	A	124	LEU
1	A	235	CYS
1	A	236	PRO
1	A	249	VAL
1	A	305	LEU
1	A	367	LEU
1	A	389	THR
1	A	396	ASP
1	B	79	ILE
1	B	98	ARG
1	B	107	ARG
1	B	122	GLN
1	B	124	LEU
1	B	305	LEU
1	B	307	PRO
1	B	320	LEU
1	B	326	LEU
1	B	358	MET
1	B	367	LEU
1	B	377	GLU
1	B	387	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	371	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 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	510	1	30,50,50	2.99	10 (33%)	24,82,82	3.07	12 (50%)
5	H4B	A	511	-	13,18,18	1.85	3 (23%)	11,26,26	4.50	7 (63%)
3	HAR	A	512	-	5,12,12	0.58	0	3,14,14	0.48	0
4	HEM	B	1010	1	30,50,50	2.92	11 (36%)	24,82,82	3.11	11 (45%)
5	H4B	B	1011	-	13,18,18	1.94	3 (23%)	11,26,26	4.37	7 (63%)
3	HAR	B	1012	-	5,12,12	0.44	0	3,14,14	0.19	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
4	HEM	A	510	1	-	0/10/54/54	0/0/8/8
5	H4B	A	511	-	-	0/8/17/17	0/2/2/2
3	HAR	A	512	-	-	0/5/13/13	0/0/0/0
4	HEM	B	1010	1	-	0/10/54/54	0/0/8/8
5	H4B	B	1011	-	-	0/8/17/17	0/2/2/2
3	HAR	B	1012	-	-	0/5/13/13	0/0/0/0

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1010	HEM	C3B-C4B	-8.54	1.44	1.51
4	A	510	HEM	C3B-C4B	-6.72	1.45	1.51
4	B	1010	HEM	C2D-C3D	-6.64	1.34	1.54
4	A	510	HEM	C2D-C3D	-6.61	1.34	1.54
4	A	510	HEM	C3D-C4D	-6.25	1.43	1.51
4	B	1010	HEM	C3D-C4D	-5.19	1.44	1.51
4	A	510	HEM	C2D-C1D	-2.80	1.42	1.51
4	A	510	HEM	C2C-C1C	-2.54	1.47	1.52
4	B	1010	HEM	C2B-C1B	-2.50	1.43	1.51
4	B	1010	HEM	C2C-C1C	-2.38	1.48	1.52
4	B	1010	HEM	C2D-C1D	-2.35	1.44	1.51
4	A	510	HEM	CAD-C3D	-2.10	1.49	1.54
5	B	1011	H4B	C6-N5	2.12	1.50	1.45
5	B	1011	H4B	C8A-N1	2.20	1.38	1.34
5	A	511	H4B	C4A-C8A	2.27	1.46	1.41
4	B	1010	HEM	FE-NB	2.28	2.09	1.97
4	B	1010	HEM	C3C-CAC	2.32	1.55	1.51
5	A	511	H4B	C6-N5	2.42	1.50	1.45
4	B	1010	HEM	CBB-CAB	4.23	1.53	1.29
4	B	1010	HEM	CBC-CAC	4.31	1.54	1.29
4	A	510	HEM	CBB-CAB	4.35	1.54	1.29
4	A	510	HEM	CBC-CAC	4.41	1.54	1.29
4	A	510	HEM	FE-NB	4.64	2.22	1.97
5	A	511	H4B	C4-N3	5.07	1.42	1.33
4	B	1010	HEM	FE-NC	5.15	2.16	1.95
5	B	1011	H4B	C4-N3	5.43	1.43	1.33
4	A	510	HEM	FE-NC	6.60	2.21	1.95

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1010	HEM	C3B-CAB-CBB	-7.18	113.45	124.46
4	A	510	HEM	C3B-CAB-CBB	-6.11	115.08	124.46
4	A	510	HEM	C3C-CAC-CBC	-5.88	115.43	124.46
4	B	1010	HEM	C3C-CAC-CBC	-5.39	116.19	124.46
5	B	1011	H4B	N3-C2-N1	-3.70	119.47	125.53
5	A	511	H4B	N3-C2-N1	-3.57	119.68	125.53
4	A	510	HEM	CAA-C2A-C1A	-3.36	123.36	127.01
5	A	511	H4B	C8A-C4A-N5	-3.32	114.66	118.85
4	B	1010	HEM	CBD-CAD-C3D	-3.32	103.89	113.55
4	A	510	HEM	CBD-CAD-C3D	-3.23	104.16	113.55
5	B	1011	H4B	C8A-C4A-N5	-2.86	115.25	118.85
4	B	1010	HEM	CAA-C2A-C1A	-2.67	124.11	127.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	510	HEM	CMA-C3A-C4A	-2.40	124.39	128.36
5	B	1011	H4B	N2-C2-N3	2.26	120.94	117.20
5	A	511	H4B	N2-C2-N3	2.41	121.19	117.20
4	B	1010	HEM	C3B-C4B-CHC	2.52	126.72	123.16
4	A	510	HEM	C3B-C4B-CHC	2.82	127.14	123.16
4	B	1010	HEM	CMD-C2D-C3D	2.98	127.55	114.35
4	A	510	HEM	CMD-C2D-C3D	3.11	128.10	114.35
5	B	1011	H4B	C2-N1-C8A	3.52	122.45	114.54
4	A	510	HEM	C2D-C3D-C4D	3.58	107.57	101.50
5	A	511	H4B	C2-N1-C8A	3.60	122.62	114.54
4	B	1010	HEM	C2D-C3D-C4D	3.78	107.91	101.50
4	B	1010	HEM	CAD-C3D-C4D	3.90	126.22	112.47
4	A	510	HEM	CAD-C3D-C4D	4.05	126.74	112.47
4	A	510	HEM	CAD-C3D-C2D	4.33	125.68	113.22
4	B	1010	HEM	CAD-C3D-C2D	4.40	125.85	113.22
4	A	510	HEM	CMB-C2B-C3B	4.84	128.62	116.53
4	B	1010	HEM	CMB-C2B-C3B	5.26	129.67	116.53
4	B	1010	HEM	CMC-C2C-C3C	5.29	129.74	116.53
4	A	510	HEM	CMC-C2C-C3C	5.49	130.23	116.53
5	B	1011	H4B	C4-N3-C2	5.67	123.80	115.94
5	B	1011	H4B	C4A-C8A-N8	5.71	125.16	118.43
5	A	511	H4B	C4-N3-C2	5.83	124.03	115.94
5	A	511	H4B	C4A-C8A-N8	6.35	125.91	118.43
5	A	511	H4B	C4-C4A-C8A	9.94	123.56	114.56
5	B	1011	H4B	C4-C4A-C8A	9.99	123.61	114.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	510	HEM	11	0
5	A	511	H4B	2	0
3	A	512	HAR	2	0
4	B	1010	HEM	8	0
5	B	1011	H4B	2	0
3	B	1012	HAR	2	0

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)

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

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

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

6.3 Carbohydrates (i)

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

6.4 Ligands (i)

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

6.5 Other polymers (i)

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