



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:24 PM GMT

PDB ID : 1FGJ  
Title : X-RAY STRUCTURE OF HYDROXYLAMINE OXIDOREDUCTASE  
Authors : Tanaka, N.; Igarashi, N.; Moriyama, H.  
Deposited on : 1997-03-03  
Resolution : 2.80 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7 (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

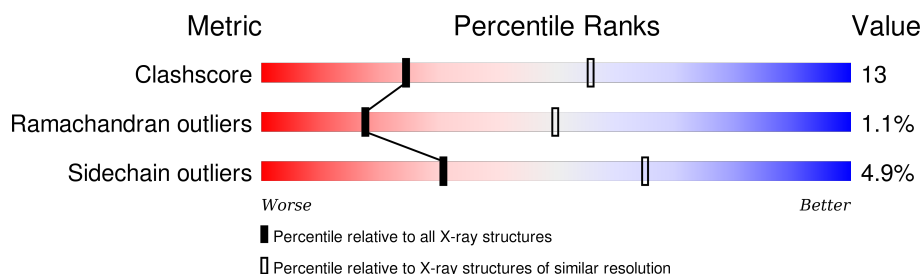
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)

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  $\geq 3$ , 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  $\leq 5\%$ . 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	546	 64% 26% • 9%
1	B	546	 64% 24% • 9%

## 2 Entry composition [i](#)

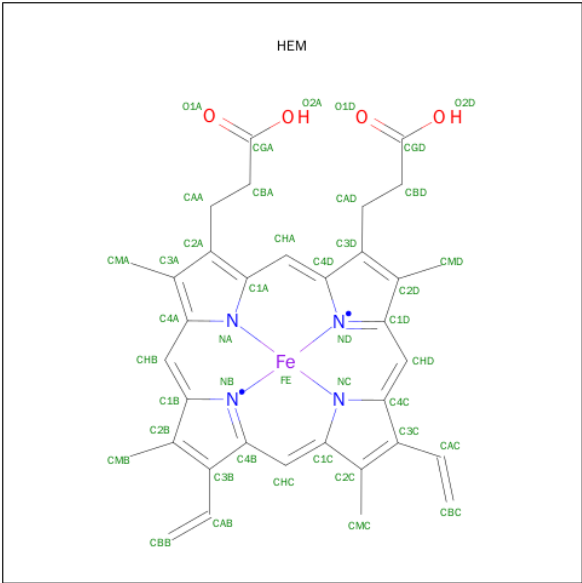
There are 3 unique types of molecules in this entry. The entry contains 8648 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 HYDROXYLAMINE OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	499	Total	C	N	O	S	0	0	0
			3980	2474	706	768	32			
1	B	499	Total	C	N	O	S	0	0	0
			3980	2474	706	768	32			

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



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

Continued on next page...

[illegible]

- 
- ORTEP diagram of the HEC molecule. The structure shows a central iron atom (Fe) coordinated by four nitrogen atoms (NA, ND, NC, NB) in a porphyrin-like ring. The ring is substituted with various side chains, including carboxylic acid groups (O1A, O2A, O1D, O2D) and other functional groups (C1A, C2A, C3A, C4A, C1B, C2B, C3B, C4B, C1C, C2C, C3C, C4C, C1D, C2D, C3D, C4D). Thermal ellipsoids are drawn at the 50% probability level.

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



*Continued from previous page...*

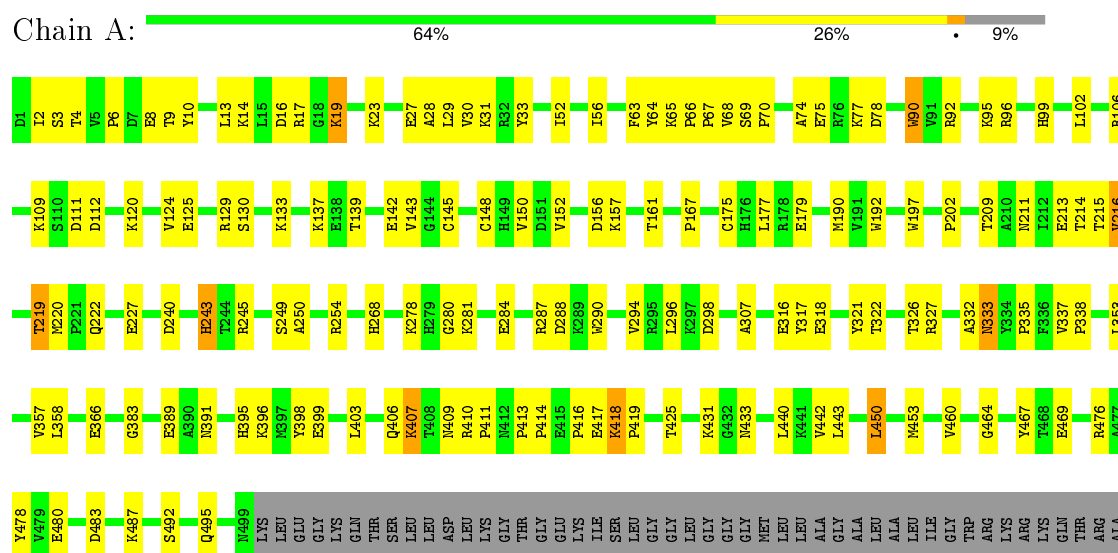
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

### 3 Residue-property plots

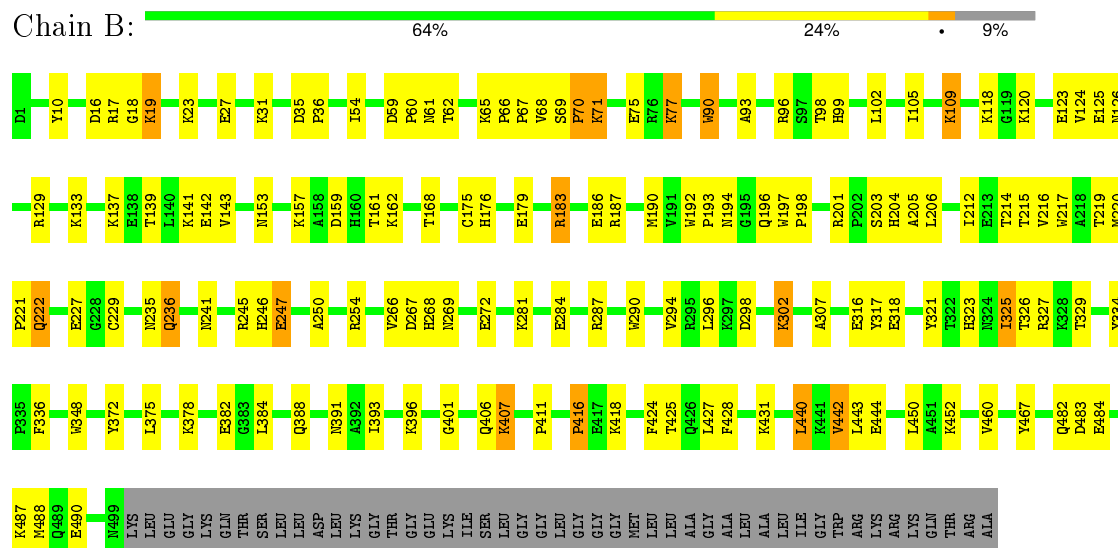
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: HYDROXYLAMINE OXIDOREDUCTASE



#### • Molecule 1: HYDROXYLAMINE OXIDOREDUCTASE



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.20 Å 96.20 Å 265.70 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 2.80	Depositor
% Data completeness (in resolution range)	99.2 (8.00-2.80)	Depositor
$R_{merge}$	0.79	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.230 , 0.309	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8648	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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, HEC

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	0/4083	0.63	0/5534
1	B	0.38	0/4083	0.61	0/5534
All	All	0.38	0/8166	0.62	0/11068

There are no bond length outliers.

There are no bond angle outliers.

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	3980	0	3779	99	3
1	B	3980	0	3779	114	2
2	A	301	0	210	5	0
2	B	301	0	210	6	0
3	A	43	0	30	5	3
3	B	43	0	30	6	2
All	All	8648	0	8038	215	5

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 13.

All (215) 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:219:THR:HG22	1:A:416:PRO:HD2	1.51	0.92
1:B:69:SER:HB2	1:B:70:PRO:HD3	1.51	0.91
1:A:202:PRO:HB2	2:A:552:HEM:HBA1	1.54	0.89
1:B:219:THR:HG22	1:B:416:PRO:HD2	1.66	0.78
1:A:69:SER:HB2	1:A:70:PRO:HD3	1.68	0.76
1:B:284:GLU:HB2	1:B:287:ARG:HH21	1.50	0.75
1:B:204:HIS:HD1	1:B:325:ILE:HD11	1.52	0.74
1:A:215:THR:O	1:A:219:THR:HG23	1.87	0.73
1:B:215:THR:O	1:B:219:THR:HG23	1.88	0.73
1:A:216:VAL:HG13	1:A:425:THR:HG23	1.68	0.73
1:A:133:LYS:HE2	1:A:152:VAL:HB	1.70	0.73
1:A:389:GLU:HG2	1:A:478:TYR:HE2	1.53	0.73
1:A:413:PRO:HD2	1:A:419:PRO:HG3	1.71	0.73
1:A:92:ARG:O	1:A:96:ARG:HG2	1.90	0.71
1:B:290:TRP:HH2	1:B:307:ALA:HB3	1.56	0.70
1:A:407:LYS:H	1:A:407:LYS:HD3	1.57	0.69
1:B:407:LYS:N	1:B:407:LYS:HD3	2.07	0.69
1:A:75:GLU:HG3	1:A:157:LYS:HG2	1.74	0.69
1:B:90:TRP:HA	1:B:90:TRP:CE3	2.28	0.68
1:A:403:LEU:H	1:A:406:GLN:HE21	1.43	0.66
1:B:235:ASN:HD21	1:B:241:ASN:HB2	1.60	0.66
1:B:69:SER:HB2	1:B:70:PRO:CD	2.25	0.65
1:A:333:ASN:O	1:A:335:PRO:HD3	1.97	0.65
1:B:284:GLU:HB2	1:B:287:ARG:NH2	2.10	0.65
1:B:216:VAL:HG11	1:B:428:PHE:HB2	1.79	0.65
1:A:418:LYS:N	1:A:418:LYS:HD3	2.12	0.64
1:A:403:LEU:H	1:A:406:GLN:NE2	1.94	0.64
1:B:378:LYS:O	1:B:382:GLU:HG3	1.98	0.63
1:A:464:GLY:O	1:A:469:GLU:HB2	1.99	0.63
1:A:411:PRO:HG2	1:A:431:LYS:HG3	1.81	0.63
1:B:393:ILE:O	1:B:396:LYS:HG2	1.99	0.63
1:B:216:VAL:HG21	1:B:424:PHE:HD2	1.64	0.63
1:B:68:VAL:HA	1:B:161:THR:HG22	1.82	0.62
1:B:90:TRP:HA	1:B:90:TRP:HE3	1.62	0.62
1:B:65:LYS:HD2	1:B:66:PRO:HD2	1.83	0.61
1:A:202:PRO:HB2	2:A:552:HEM:CBA	2.28	0.60
1:B:190:MET:HE1	1:B:329:THR:HB	1.83	0.60
1:A:220:MET:HE2	1:A:222:GLN:HB2	1.83	0.59
1:A:396:LYS:HD3	1:A:399:GLU:HB2	1.84	0.59
1:B:192:TRP:CD1	1:B:197:TRP:HB2	2.38	0.59
1:A:90:TRP:CE3	1:A:90:TRP:HA	2.38	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:TRP:CH2	1:B:307:ALA:HB3	2.37	0.58
1:B:483:ASP:OD1	1:B:487:LYS:HE2	2.03	0.58
1:B:16:ASP:HB3	1:B:19:LYS:HB3	1.84	0.58
3:B:550:HEC:HAD2	2:B:552:HEM:HAD2	1.85	0.58
1:B:384:LEU:O	1:B:388:GLN:HG3	2.04	0.57
1:A:9:THR:O	1:A:13:LEU:HD23	2.03	0.57
1:B:194:ASN:HD22	1:B:196:GLN:HE22	1.51	0.57
1:B:229:CYS:HA	3:B:550:HEC:HMC3	1.86	0.57
1:B:129:ARG:HH11	1:B:129:ARG:HG2	1.69	0.57
1:B:183:ARG:NH2	1:B:236:GLN:HA	2.19	0.56
1:B:205:ALA:O	1:B:236:GLN:HB2	2.05	0.56
1:B:418:LYS:HB3	1:B:418:LYS:NZ	2.20	0.56
1:B:187:ARG:HG2	1:B:206:LEU:HD21	1.87	0.56
1:A:250:ALA:O	1:A:254:ARG:HG3	2.05	0.56
1:A:409:ASN:O	1:A:433:ASN:HB2	2.05	0.55
1:B:124:VAL:HG13	1:B:175:CYS:HB3	1.88	0.55
1:B:77:LYS:H	1:B:77:LYS:CE	2.20	0.55
1:B:99:HIS:HB3	1:B:143:VAL:HB	1.89	0.55
1:B:229:CYS:SG	3:B:550:HEC:HHC	2.47	0.55
1:A:190:MET:HB2	1:A:326:THR:HB	1.88	0.55
3:B:550:HEC:HBB3	3:B:550:HEC:HMB1	1.89	0.54
1:B:176:HIS:HB3	1:B:179:GLU:HG2	1.90	0.54
1:B:298:ASP:HB3	1:B:302:LYS:HG2	1.89	0.54
1:B:267:ASP:HB2	1:B:334:TYR:HE1	1.72	0.54
1:B:317:TYR:CE2	1:B:318:GLU:HG2	2.43	0.53
1:A:13:LEU:HD12	1:A:28:ALA:HB1	1.91	0.53
1:B:317:TYR:CD2	1:B:318:GLU:HG2	2.44	0.53
1:A:353:LEU:O	1:A:357:VAL:HG23	2.08	0.53
1:B:102:LEU:HD23	1:B:142:GLU:HA	1.90	0.53
1:B:198:PRO:HB2	1:B:201:ARG:HG3	1.91	0.53
1:B:302:LYS:HB3	1:B:302:LYS:NZ	2.22	0.53
1:A:96:ARG:NH2	1:B:109:LYS:HD2	2.24	0.52
1:A:407:LYS:N	1:A:407:LYS:HD3	2.22	0.52
1:B:125:GLU:O	1:B:129:ARG:HG3	2.09	0.52
1:A:2:ILE:O	1:A:4:THR:N	2.42	0.52
1:A:391:ASN:HA	1:A:442:VAL:HG21	1.90	0.52
1:B:220:MET:O	1:B:220:MET:HG3	2.10	0.52
1:A:92:ARG:HA	1:A:95:LYS:NZ	2.25	0.52
1:A:64:TYR:OH	1:A:67:PRO:HD3	2.09	0.51
1:A:483:ASP:OD1	1:A:487:LYS:HE2	2.10	0.51
1:A:492:SER:O	1:A:495:GLN:HB3	2.09	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:LYS:HE2	1:B:139:THR:HG21	1.93	0.51
1:A:211:ASN:ND2	3:A:550:HEC:HMB3	2.26	0.51
1:B:159:ASP:OD2	1:B:162:LYS:HG2	2.11	0.51
1:A:75:GLU:CG	1:A:157:LYS:HG2	2.40	0.51
1:A:66:PRO:HB2	1:A:161:THR:O	2.11	0.51
1:B:93:ALA:HB1	1:B:246:HIS:O	2.11	0.51
1:A:69:SER:HB2	1:A:70:PRO:CD	2.38	0.51
1:B:109:LYS:HE2	1:B:109:LYS:HA	1.93	0.50
1:A:90:TRP:HE3	1:A:90:TRP:HA	1.74	0.50
1:A:148:CYS:O	1:A:167:PRO:HG3	2.11	0.50
1:A:192:TRP:CH2	1:A:332:ALA:HB2	2.47	0.50
1:A:68:VAL:HA	1:A:161:THR:HG22	1.92	0.50
1:A:294:VAL:CG1	1:A:298:ASP:HB2	2.41	0.50
1:A:6:PRO:HB2	1:A:8:GLU:HG2	1.93	0.50
1:B:193:PRO:HD3	1:B:348:TRP:CE2	2.47	0.50
1:B:187:ARG:HG2	1:B:206:LEU:CD2	2.42	0.50
1:B:246:HIS:O	1:B:247:GLU:HB2	2.11	0.50
3:A:550:HEC:HMB1	3:A:550:HEC:HBB3	1.94	0.49
1:A:120:LYS:O	1:A:124:VAL:HG23	2.12	0.49
1:A:16:ASP:HB3	1:A:19:LYS:HE3	1.94	0.49
1:A:383:GLY:HA3	1:A:453:MET:SD	2.53	0.49
1:B:216:VAL:HG21	1:B:424:PHE:CD2	2.47	0.49
1:A:214:THR:HG21	3:A:550:HEC:HMB2	1.94	0.49
1:A:13:LEU:O	1:A:14:LYS:HB2	2.12	0.48
1:B:334:TYR:HB3	1:B:336:PHE:CE1	2.48	0.48
1:B:75:GLU:CG	1:B:157:LYS:HB3	2.43	0.48
1:B:54:ILE:CG2	1:B:227:GLU:HG2	2.43	0.48
1:A:357:VAL:HG11	1:A:366:GLU:HG3	1.94	0.48
1:B:71:LYS:N	1:B:71:LYS:HD3	2.28	0.48
1:B:27:GLU:O	1:B:31:LYS:HG2	2.14	0.48
1:B:216:VAL:HG22	1:B:425:THR:OG1	2.13	0.48
1:B:391:ASN:HA	1:B:442:VAL:HG21	1.95	0.48
1:A:357:VAL:CG1	1:A:366:GLU:HG3	2.44	0.48
1:B:59:ASP:OD2	1:B:62:THR:HB	2.14	0.48
1:B:294:VAL:CG1	1:B:298:ASP:HB2	2.44	0.48
1:B:123:GLU:O	1:B:126:ASN:HB3	2.13	0.48
1:B:60:PRO:HG2	1:B:168:THR:CG2	2.44	0.47
1:B:212:ILE:HG22	1:B:217:TRP:CZ3	2.50	0.47
1:A:476:ARG:O	1:A:480:GLU:HG3	2.14	0.47
1:A:296:LEU:HD23	1:A:321:TYR:HD2	1.79	0.47
1:A:197:TRP:CZ3	3:A:550:HEC:HBA1	2.50	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:ALA:HB1	1:A:78:ASP:HB2	1.97	0.47
1:A:335:PRO:HB2	1:A:450:LEU:HD11	1.96	0.47
1:B:120:LYS:HE2	2:B:551:HEM:HAA1	1.95	0.47
1:B:23:LYS:O	1:B:27:GLU:HG3	2.14	0.47
1:A:28:ALA:O	1:A:31:LYS:HB3	2.14	0.47
1:B:250:ALA:O	1:B:254:ARG:HG3	2.15	0.47
1:B:67:PRO:C	1:B:69:SER:H	2.16	0.46
1:A:179:GLU:HG2	2:A:551:HEM:C4A	2.49	0.46
1:B:75:GLU:HG2	1:B:157:LYS:HB3	1.98	0.46
1:A:52:ILE:HD11	1:A:227:GLU:HG2	1.97	0.46
1:A:99:HIS:HB3	1:A:143:VAL:HB	1.97	0.46
1:B:204:HIS:ND1	1:B:325:ILE:HD11	2.25	0.46
1:B:105:ILE:HG22	1:B:118:LYS:HA	1.98	0.46
1:A:316:GLU:HB2	1:A:321:TYR:CE2	2.50	0.46
1:A:10:TYR:CG	1:A:17:ARG:HG2	2.51	0.46
1:A:109:LYS:HE2	1:A:111:ASP:OD1	2.16	0.46
1:A:23:LYS:O	1:A:27:GLU:HG3	2.15	0.46
1:B:269:ASN:HB2	1:B:272:GLU:HB2	1.98	0.46
1:B:266:VAL:O	1:B:452:LYS:HG3	2.16	0.45
3:B:550:HEC:O1A	3:B:550:HEC:HMA3	2.16	0.45
1:B:219:THR:HG22	1:B:416:PRO:CD	2.42	0.45
1:A:240:ASP:OD2	1:A:245:ARG:NH1	2.49	0.45
1:B:141:LYS:HG3	1:B:142:GLU:HG2	1.97	0.45
1:A:96:ARG:NH2	1:B:109:LYS:HE3	2.31	0.45
1:B:407:LYS:HD3	1:B:407:LYS:H	1.79	0.45
1:A:243:HIS:HB3	1:A:249:SER:O	2.17	0.45
1:B:18:GLY:O	1:B:19:LYS:HB2	2.17	0.45
1:B:214:THR:HG21	3:B:550:HEC:HMB2	1.98	0.45
1:A:317:TYR:CD2	1:A:318:GLU:HG2	2.52	0.45
1:B:179:GLU:HG3	2:B:551:HEM:CHB	2.47	0.45
1:A:414:PRO:O	1:A:417:GLU:HB3	2.17	0.45
1:B:190:MET:HB2	1:B:326:THR:HB	2.00	0.44
1:A:280:GLY:O	1:A:284:GLU:HG3	2.18	0.44
1:B:294:VAL:HG13	1:B:298:ASP:HB2	2.00	0.44
1:A:245:ARG:HD3	2:A:548:HEM:C4D	2.52	0.44
1:B:17:ARG:HH11	1:B:17:ARG:HG3	1.83	0.44
1:A:296:LEU:HD23	1:A:321:TYR:CD2	2.53	0.44
1:B:222:GLN:CD	1:B:222:GLN:H	2.21	0.44
1:A:278:LYS:HA	1:A:278:LYS:HD3	1.77	0.44
1:B:401:GLY:HA2	1:B:406:GLN:NE2	2.33	0.43
1:B:133:LYS:O	1:B:153:ASN:ND2	2.51	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:484:GLU:O	1:B:488:MET:HG3	2.17	0.43
1:B:10:TYR:CE2	1:B:17:ARG:NH1	2.86	0.43
1:A:214:THR:CB	3:A:550:HEC:HMB2	2.49	0.43
1:B:98:THR:HG23	1:B:105:ILE:HD11	2.01	0.43
1:B:372:TYR:OH	1:B:460:VAL:HA	2.19	0.43
1:A:124:VAL:HG13	1:A:175:CYS:HB3	2.00	0.43
1:B:411:PRO:HG2	1:B:431:LYS:HG2	2.01	0.43
1:B:16:ASP:HB3	1:B:19:LYS:CB	2.49	0.43
1:A:395:HIS:O	1:A:398:TYR:HB3	2.19	0.43
1:A:95:LYS:HB3	1:A:96:ARG:NH1	2.33	0.43
1:B:77:LYS:H	1:B:77:LYS:HE3	1.84	0.43
1:B:71:LYS:HB2	1:B:71:LYS:HE2	1.87	0.42
1:B:440:LEU:HD22	1:B:444:GLU:HG3	2.01	0.42
1:A:406:GLN:HA	1:A:410:ARG:CD	2.49	0.42
1:A:296:LEU:HB3	1:A:321:TYR:CD2	2.54	0.42
1:A:332:ALA:O	1:A:333:ASN:HB3	2.20	0.42
1:A:290:TRP:HH2	1:A:307:ALA:HB3	1.84	0.42
1:A:209:THR:O	1:A:213:GLU:HG2	2.20	0.42
1:A:133:LYS:CE	1:A:152:VAL:HB	2.46	0.42
1:A:56:ILE:HA	1:A:63:PHE:HB2	2.01	0.42
1:B:317:TYR:CD2	1:B:327:ARG:NH1	2.87	0.42
1:B:220:MET:HA	1:B:221:PRO:HD2	1.90	0.41
1:B:245:ARG:HD2	1:B:246:HIS:CE1	2.55	0.41
1:B:54:ILE:HG21	1:B:227:GLU:HG2	2.02	0.41
1:A:30:VAL:HA	1:A:33:TYR:HB3	2.02	0.41
1:B:281:LYS:HA	1:B:281:LYS:HD3	1.83	0.41
1:B:192:TRP:NE1	1:B:197:TRP:HB2	2.35	0.41
1:A:281:LYS:HD3	1:A:281:LYS:HA	1.81	0.41
1:B:424:PHE:O	1:B:427:LEU:HB2	2.21	0.41
1:A:16:ASP:HB3	1:A:19:LYS:HB3	2.01	0.41
1:A:335:PRO:HD2	1:A:450:LEU:HD13	2.02	0.41
1:A:337:VAL:HA	1:A:338:PRO:HD3	1.93	0.41
1:B:67:PRO:C	1:B:69:SER:N	2.74	0.41
1:A:109:LYS:O	1:A:112:ASP:HB3	2.21	0.41
1:B:203:SER:O	2:B:552:HEM:HBD2	2.21	0.41
1:B:375:LEU:HD23	1:B:375:LEU:C	2.41	0.41
1:B:325:ILE:H	1:B:325:ILE:HD13	1.86	0.41
1:B:302:LYS:HB3	1:B:302:LYS:HZ2	1.86	0.41
1:A:74:ALA:HB1	1:A:78:ASP:CB	2.51	0.41
1:A:102:LEU:HD12	1:A:142:GLU:HA	2.01	0.41
1:A:106:ARG:NH2	1:A:139:THR:HB	2.36	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:GLU:OE1	1:B:203:SER:HB2	2.20	0.41
1:A:67:PRO:HG3	2:A:547:HEM:HBA2	2.03	0.41
1:A:95:LYS:HD2	1:A:96:ARG:HH12	1.86	0.40
1:A:125:GLU:O	1:A:129:ARG:HG3	2.21	0.40
1:B:235:ASN:ND2	1:B:241:ASN:HB2	2.34	0.40
2:B:552:HEM:HAA2	2:B:552:HEM:HHA	1.95	0.40
1:B:99:HIS:CD2	2:B:549:HEM:ND	2.89	0.40
1:B:316:GLU:HB2	1:B:321:TYR:CE2	2.56	0.40
1:A:406:GLN:HA	1:A:410:ARG:HD2	2.04	0.40
1:B:35:ASP:HA	1:B:36:PRO:HD3	1.96	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:467:TYR:OH	3:A:550:HEC:C4B[2_655]	1.48	0.72
1:A:467:TYR:CE1	3:A:550:HEC:CHC[2_655]	1.79	0.41
1:B:467:TYR:CE1	3:B:550:HEC:CHC[3_665]	1.95	0.25
1:A:467:TYR:OH	3:A:550:HEC:C3B[2_655]	2.00	0.20
1:B:467:TYR:OH	3:B:550:HEC:C4B[3_665]	2.11	0.09

## 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	497/546 (91%)	455 (92%)	35 (7%)	7 (1%)	14	42
1	B	497/546 (91%)	450 (90%)	43 (9%)	4 (1%)	24	58
All	All	994/1092 (91%)	905 (91%)	78 (8%)	11 (1%)	17	50

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	327	ARG
1	B	247	GLU
1	B	268	HIS
1	A	150	VAL
1	A	333	ASN
1	B	19	LYS
1	A	19	LYS
1	A	268	HIS
1	B	70	PRO
1	A	460	VAL

### 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	427/460 (93%)	407 (95%)	20 (5%)	32	67
1	B	427/460 (93%)	405 (95%)	22 (5%)	29	62
All	All	854/920 (93%)	812 (95%)	42 (5%)	31	65

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LEU
1	A	65	LYS
1	A	90	TRP
1	A	130	SER
1	A	137	LYS
1	A	145	CYS
1	A	156	ASP
1	A	177	LEU
1	A	216	VAL
1	A	219	THR
1	A	243	HIS
1	A	287	ARG
1	A	288	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	322	THR
1	A	358	LEU
1	A	407	LYS
1	A	418	LYS
1	A	440	LEU
1	A	443	LEU
1	A	450	LEU
1	B	61	ASN
1	B	71	LYS
1	B	77	LYS
1	B	90	TRP
1	B	96	ARG
1	B	109	LYS
1	B	137	LYS
1	B	183	ARG
1	B	222	GLN
1	B	236	GLN
1	B	296	LEU
1	B	302	LYS
1	B	323	HIS
1	B	325	ILE
1	B	407	LYS
1	B	416	PRO
1	B	440	LEU
1	B	442	VAL
1	B	443	LEU
1	B	450	LEU
1	B	482	GLN
1	B	490	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	127	ASN
1	A	211	ASN
1	A	233	HIS
1	A	241	ASN
1	A	270	ASN
1	A	333	ASN
1	A	362	GLN
1	A	406	GLN
1	A	448	ASN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	449	ASN
1	A	461	ASN
1	A	482	GLN
1	B	38	HIS
1	B	127	ASN
1	B	153	ASN
1	B	194	ASN
1	B	211	ASN
1	B	235	ASN
1	B	241	ASN
1	B	270	ASN
1	B	333	ASN
1	B	391	ASN
1	B	448	ASN
1	B	461	ASN
1	B	482	GLN
1	B	499	ASN

### 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](#)

16 ligands 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
2	HEM	A	547	1	30,50,50	2.73	9 (30%)	24,82,82	2.48	7 (29%)
2	HEM	A	548	1	30,50,50	2.47	7 (23%)	24,82,82	2.81	10 (41%)
2	HEM	A	549	1	30,50,50	2.69	10 (33%)	24,82,82	2.69	9 (37%)
3	HEC	A	550	1	24,50,50	1.69	5 (20%)	19,82,82	2.39	7 (36%)
2	HEM	A	551	1	30,50,50	2.29	8 (26%)	24,82,82	2.53	8 (33%)
2	HEM	A	552	1	30,50,50	2.45	11 (36%)	24,82,82	2.63	9 (37%)
2	HEM	A	553	1	30,50,50	2.58	7 (23%)	24,82,82	3.08	9 (37%)
2	HEM	A	554	1	30,50,50	2.21	10 (33%)	24,82,82	2.72	10 (41%)
2	HEM	B	547	1	30,50,50	2.81	8 (26%)	24,82,82	2.44	7 (29%)
2	HEM	B	548	1	30,50,50	2.54	8 (26%)	24,82,82	3.18	9 (37%)
2	HEM	B	549	1	30,50,50	2.40	12 (40%)	24,82,82	2.59	9 (37%)
3	HEC	B	550	1	24,50,50	2.06	4 (16%)	19,82,82	1.85	7 (36%)
2	HEM	B	551	1	30,50,50	2.61	10 (33%)	24,82,82	2.58	8 (33%)
2	HEM	B	552	1	30,50,50	2.43	9 (30%)	24,82,82	2.96	12 (50%)
2	HEM	B	553	1	30,50,50	2.71	9 (30%)	24,82,82	2.40	9 (37%)
2	HEM	B	554	1	30,50,50	2.26	7 (23%)	24,82,82	2.83	9 (37%)

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
2	HEM	A	547	1	-	0/10/54/54	0/0/8/8
2	HEM	A	548	1	-	0/10/54/54	0/0/8/8
2	HEM	A	549	1	-	0/10/54/54	0/0/8/8
3	HEC	A	550	1	-	0/6/54/54	0/0/8/8
2	HEM	A	551	1	-	0/10/54/54	0/0/8/8
2	HEM	A	552	1	-	0/10/54/54	0/0/8/8
2	HEM	A	553	1	-	0/10/54/54	0/0/8/8
2	HEM	A	554	1	-	0/10/54/54	0/0/8/8
2	HEM	B	547	1	-	0/10/54/54	0/0/8/8
2	HEM	B	548	1	-	0/10/54/54	0/0/8/8
2	HEM	B	549	1	-	0/10/54/54	0/0/8/8
3	HEC	B	550	1	-	0/6/54/54	0/0/8/8
2	HEM	B	551	1	-	0/10/54/54	0/0/8/8
2	HEM	B	552	1	-	0/10/54/54	0/0/8/8
2	HEM	B	553	1	-	0/10/54/54	0/0/8/8
2	HEM	B	554	1	-	0/10/54/54	0/0/8/8

All (134) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	553	HEM	C3B-C4B	-9.89	1.43	1.51
2	B	547	HEM	C3B-C4B	-8.41	1.44	1.51
2	B	548	HEM	C3B-C4B	-8.37	1.44	1.51
2	A	547	HEM	C3B-C4B	-8.11	1.44	1.51
2	A	548	HEM	C3B-C4B	-7.33	1.45	1.51
2	A	553	HEM	C3D-C4D	-7.31	1.42	1.51
2	A	547	HEM	C2D-C3D	-7.19	1.32	1.54
2	A	549	HEM	C3B-C4B	-7.15	1.45	1.51
2	B	551	HEM	C3B-C4B	-7.08	1.45	1.51
2	A	552	HEM	C2D-C3D	-6.91	1.33	1.54
2	B	552	HEM	C3B-C4B	-6.89	1.45	1.51
3	B	550	HEC	C3B-C2B	-6.67	1.33	1.40
2	A	554	HEM	C2D-C3D	-6.63	1.34	1.54
2	A	553	HEM	C2D-C3D	-6.55	1.34	1.54
2	B	547	HEM	C2D-C3D	-6.54	1.34	1.54
2	B	553	HEM	C2D-C3D	-6.39	1.35	1.54
2	B	551	HEM	C2D-C3D	-6.32	1.35	1.54
2	B	552	HEM	C2D-C3D	-6.30	1.35	1.54
2	B	548	HEM	C2D-C3D	-6.28	1.35	1.54
2	A	549	HEM	C2D-C3D	-6.08	1.36	1.54
2	B	549	HEM	C2D-C3D	-6.06	1.36	1.54
2	A	553	HEM	C3B-C4B	-6.04	1.46	1.51
2	B	554	HEM	C3B-C4B	-5.98	1.46	1.51
2	A	549	HEM	C3D-C4D	-5.83	1.44	1.51
2	B	554	HEM	C2D-C3D	-5.81	1.37	1.54
2	B	547	HEM	C3D-C4D	-5.75	1.44	1.51
2	A	551	HEM	C2D-C3D	-5.72	1.37	1.54
2	A	548	HEM	C2D-C3D	-5.70	1.37	1.54
2	A	551	HEM	C3B-C4B	-5.56	1.46	1.51
2	B	549	HEM	C3B-C4B	-5.38	1.47	1.51
2	A	552	HEM	C3B-C4B	-5.35	1.47	1.51
2	B	551	HEM	C3D-C4D	-5.05	1.45	1.51
2	A	547	HEM	C3D-C4D	-4.87	1.45	1.51
2	B	552	HEM	C2C-C1C	-4.50	1.44	1.52
2	A	551	HEM	C3D-C4D	-4.50	1.45	1.51
3	A	550	HEC	C3C-C2C	-4.46	1.36	1.40
3	B	550	HEC	C3C-C2C	-4.45	1.36	1.40
2	B	554	HEM	C2C-C1C	-4.32	1.44	1.52
2	A	547	HEM	C2C-C1C	-4.16	1.44	1.52
2	A	548	HEM	C2C-C1C	-4.08	1.44	1.52
2	B	547	HEM	C2C-C1C	-4.05	1.44	1.52
2	A	548	HEM	C3D-C4D	-4.03	1.46	1.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	554	HEM	C2C-C1C	-3.84	1.45	1.52
2	B	548	HEM	C2C-C1C	-3.84	1.45	1.52
2	B	551	HEM	C2C-C1C	-3.81	1.45	1.52
2	A	554	HEM	C3B-C4B	-3.78	1.48	1.51
2	A	553	HEM	C2C-C1C	-3.57	1.45	1.52
2	B	548	HEM	C3D-C4D	-3.41	1.47	1.51
2	A	549	HEM	C2C-C1C	-3.39	1.46	1.52
2	B	554	HEM	C3D-C4D	-3.22	1.47	1.51
2	A	552	HEM	C2C-C1C	-3.11	1.46	1.52
2	B	549	HEM	C2C-C1C	-3.09	1.46	1.52
2	B	553	HEM	C2C-C1C	-3.02	1.46	1.52
2	A	547	HEM	C2B-C1B	-2.87	1.42	1.51
2	A	554	HEM	C3D-C4D	-2.81	1.48	1.51
2	B	552	HEM	C2D-C1D	-2.80	1.42	1.51
3	A	550	HEC	C3B-C2B	-2.79	1.37	1.40
2	A	549	HEM	C2B-C1B	-2.76	1.42	1.51
2	B	553	HEM	C2B-C1B	-2.73	1.42	1.51
2	B	549	HEM	C3D-C4D	-2.69	1.48	1.51
2	B	547	HEM	C2B-C1B	-2.62	1.43	1.51
2	A	552	HEM	C2D-C1D	-2.58	1.43	1.51
2	A	551	HEM	C2C-C1C	-2.57	1.47	1.52
2	B	548	HEM	C2B-C1B	-2.51	1.43	1.51
2	A	549	HEM	C2D-C1D	-2.50	1.43	1.51
2	B	553	HEM	C3D-C4D	-2.49	1.48	1.51
2	A	552	HEM	C3D-C4D	-2.36	1.48	1.51
2	B	549	HEM	C2B-C1B	-2.35	1.44	1.51
2	B	552	HEM	C2B-C1B	-2.29	1.44	1.51
2	A	547	HEM	C2D-C1D	-2.27	1.44	1.51
2	B	551	HEM	CAD-C3D	-2.27	1.49	1.54
2	B	552	HEM	C3D-C4D	-2.19	1.48	1.51
2	A	551	HEM	C2B-C1B	-2.16	1.44	1.51
2	A	552	HEM	C2B-C1B	-2.14	1.44	1.51
2	B	549	HEM	C2D-C1D	-2.10	1.45	1.51
2	A	553	HEM	C2B-C1B	-2.02	1.45	1.51
2	A	554	HEM	CHD-C4C	2.07	1.41	1.36
2	A	554	HEM	CHC-C1C	2.13	1.41	1.36
2	B	551	HEM	C4C-NC	2.13	1.38	1.36
2	B	549	HEM	CHD-C4C	2.36	1.42	1.36
2	B	551	HEM	C3B-CAB	2.44	1.55	1.51
2	B	554	HEM	C1C-NC	2.47	1.39	1.36
2	B	553	HEM	C1C-NC	2.55	1.39	1.36
2	A	554	HEM	C4C-NC	2.57	1.39	1.36

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	550	HEC	C4C-NC	2.58	1.40	1.36
2	B	553	HEM	C4C-NC	2.63	1.39	1.36
2	A	549	HEM	C4C-NC	2.70	1.39	1.36
2	B	549	HEM	C3B-CAB	2.70	1.56	1.51
2	B	552	HEM	C1C-NC	2.84	1.39	1.36
3	A	550	HEC	C4A-NA	2.86	1.40	1.36
2	A	547	HEM	C1C-NC	2.91	1.39	1.36
2	B	549	HEM	C4C-NC	2.95	1.39	1.36
2	A	554	HEM	C1C-NC	3.00	1.39	1.36
2	A	552	HEM	C3C-CAC	3.08	1.57	1.51
2	B	548	HEM	C1C-NC	3.12	1.39	1.36
3	A	550	HEC	C1C-CHC	3.16	1.48	1.39
3	B	550	HEC	C4A-NA	3.25	1.41	1.36
3	B	550	HEC	C1C-CHC	3.27	1.48	1.39
2	B	551	HEM	C1C-NC	3.45	1.40	1.36
2	A	552	HEM	C3B-CAB	3.56	1.58	1.51
2	A	551	HEM	C1C-NC	3.65	1.40	1.36
2	A	552	HEM	C1C-NC	3.72	1.40	1.36
2	A	553	HEM	CBB-CAB	3.83	1.51	1.29
2	A	547	HEM	CBC-CAC	3.88	1.51	1.29
2	A	554	HEM	CBC-CAC	3.89	1.51	1.29
2	A	553	HEM	CBC-CAC	3.90	1.51	1.29
2	B	553	HEM	CBC-CAC	3.93	1.52	1.29
2	B	548	HEM	CBC-CAC	3.93	1.52	1.29
2	A	551	HEM	CBB-CAB	3.97	1.52	1.29
2	B	552	HEM	CBC-CAC	3.97	1.52	1.29
2	A	548	HEM	CBB-CAB	3.98	1.52	1.29
2	A	548	HEM	C1C-NC	3.99	1.40	1.36
2	B	548	HEM	CBB-CAB	3.99	1.52	1.29
2	A	548	HEM	CBC-CAC	4.00	1.52	1.29
2	B	547	HEM	CBC-CAC	4.00	1.52	1.29
2	B	554	HEM	CBC-CAC	4.01	1.52	1.29
2	B	552	HEM	CBB-CAB	4.02	1.52	1.29
2	B	547	HEM	C1C-NC	4.03	1.41	1.36
2	B	551	HEM	CBB-CAB	4.04	1.52	1.29
2	A	549	HEM	CBB-CAB	4.04	1.52	1.29
2	B	549	HEM	C1C-NC	4.05	1.41	1.36
2	A	554	HEM	CBB-CAB	4.05	1.52	1.29
2	B	547	HEM	CBB-CAB	4.06	1.52	1.29
2	B	554	HEM	CBB-CAB	4.07	1.52	1.29
2	B	553	HEM	CBB-CAB	4.09	1.52	1.29
2	B	549	HEM	CBC-CAC	4.10	1.53	1.29

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	549	HEM	CBC-CAC	4.10	1.53	1.29
2	A	549	HEM	C1C-NC	4.11	1.41	1.36
2	A	552	HEM	CBC-CAC	4.11	1.53	1.29
2	A	551	HEM	CBC-CAC	4.13	1.53	1.29
2	B	549	HEM	CBB-CAB	4.14	1.53	1.29
2	A	547	HEM	CBB-CAB	4.17	1.53	1.29
2	A	552	HEM	CBB-CAB	4.18	1.53	1.29
2	B	551	HEM	CBC-CAC	4.26	1.53	1.29

All (139) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	548	HEM	C3C-CAC-CBC	-8.90	110.80	124.46
2	A	553	HEM	C3C-CAC-CBC	-7.91	112.32	124.46
2	A	547	HEM	C3B-CAB-CBB	-7.24	113.35	124.46
2	B	551	HEM	C3B-CAB-CBB	-7.02	113.69	124.46
2	A	551	HEM	C3B-CAB-CBB	-7.02	113.70	124.46
2	B	548	HEM	C3B-CAB-CBB	-6.72	114.15	124.46
2	B	554	HEM	C3C-CAC-CBC	-6.66	114.24	124.46
2	B	554	HEM	C3B-CAB-CBB	-6.63	114.29	124.46
2	A	549	HEM	C3B-CAB-CBB	-6.62	114.30	124.46
2	A	548	HEM	C3C-CAC-CBC	-6.29	114.81	124.46
2	A	554	HEM	C3B-CAB-CBB	-6.13	115.05	124.46
2	B	549	HEM	C3B-CAB-CBB	-6.10	115.09	124.46
2	B	547	HEM	C3B-CAB-CBB	-5.93	115.37	124.46
2	B	552	HEM	CAA-C2A-C1A	-5.75	120.76	127.01
3	A	550	HEC	CBC-CAC-C3C	-5.47	115.21	127.35
2	A	553	HEM	C3B-CAB-CBB	-5.45	116.09	124.46
2	A	552	HEM	C3B-CAB-CBB	-5.40	116.17	124.46
2	B	549	HEM	C3C-CAC-CBC	-5.35	116.25	124.46
2	B	553	HEM	C3C-CAC-CBC	-5.23	116.44	124.46
2	A	548	HEM	C3B-CAB-CBB	-5.01	116.77	124.46
2	B	552	HEM	C3B-CAB-CBB	-4.94	116.89	124.46
2	A	549	HEM	C3C-CAC-CBC	-4.71	117.24	124.46
3	B	550	HEC	CBC-CAC-C3C	-4.54	117.26	127.35
2	B	551	HEM	C3C-CAC-CBC	-4.39	117.73	124.46
2	A	554	HEM	C3C-CAC-CBC	-3.71	118.77	124.46
2	A	551	HEM	C3C-CAC-CBC	-3.31	119.38	124.46
2	A	554	HEM	CAA-C2A-C1A	-3.20	123.53	127.01
2	B	553	HEM	C3B-CAB-CBB	-3.14	119.63	124.46
3	A	550	HEC	CMB-C2B-C1B	-3.01	123.39	128.36
2	A	548	HEM	CMA-C3A-C4A	-2.95	123.48	128.36

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	552	HEM	CAA-C2A-C1A	-2.83	123.94	127.01
3	B	550	HEC	CBB-CAB-C3B	-2.82	121.08	127.35
2	B	552	HEM	C3C-CAC-CBC	-2.80	120.16	124.46
2	B	552	HEM	CMA-C3A-C4A	-2.71	123.89	128.36
2	B	554	HEM	CBA-CAA-C2A	-2.54	107.97	112.53
2	A	552	HEM	C3C-CAC-CBC	-2.53	120.58	124.46
3	A	550	HEC	CBD-CAD-C3D	-2.43	108.18	112.53
3	B	550	HEC	CMB-C2B-C1B	-2.40	124.40	128.36
3	A	550	HEC	CBB-CAB-C3B	-2.37	122.08	127.35
3	B	550	HEC	CAD-C3D-C2D	-2.08	123.07	129.00
3	B	550	HEC	CMC-C2C-C1C	-2.08	124.93	128.36
3	A	550	HEC	CAA-C2A-C1A	-2.05	124.78	127.01
3	A	550	HEC	C4B-C3B-C2B	-2.03	104.16	106.35
2	B	551	HEM	CMD-C2D-C3D	2.11	123.67	114.35
3	B	550	HEC	CBA-CAA-C2A	2.14	116.37	112.53
2	B	549	HEM	CBA-CAA-C2A	2.14	116.37	112.53
3	B	550	HEC	CBD-CAD-C3D	2.16	116.40	112.53
2	A	547	HEM	CMD-C2D-C3D	2.21	124.13	114.35
2	B	549	HEM	CBD-CAD-C3D	2.24	120.07	113.55
2	A	547	HEM	C2D-C3D-C4D	2.35	105.48	101.50
2	A	549	HEM	CBA-CAA-C2A	2.38	116.79	112.53
2	B	552	HEM	C2D-C3D-C4D	2.38	105.53	101.50
2	B	549	HEM	CMD-C2D-C3D	2.40	124.97	114.35
2	A	554	HEM	CMD-C2D-C3D	2.41	125.01	114.35
2	A	552	HEM	CMD-C2D-C3D	2.44	125.12	114.35
2	A	549	HEM	C2D-C3D-C4D	2.53	105.79	101.50
2	B	553	HEM	CMD-C2D-C3D	2.56	125.69	114.35
2	B	553	HEM	C2D-C3D-C4D	2.66	106.01	101.50
2	A	553	HEM	CMD-C2D-C3D	2.68	126.19	114.35
2	B	554	HEM	CMD-C2D-C3D	2.70	126.28	114.35
2	B	552	HEM	CMA-C3A-C2A	2.70	130.89	125.24
2	A	551	HEM	CMD-C2D-C3D	2.70	126.31	114.35
2	A	549	HEM	CMD-C2D-C3D	2.72	126.38	114.35
2	B	553	HEM	CBA-CAA-C2A	2.73	117.43	112.53
2	A	552	HEM	C2D-C3D-C4D	2.78	106.22	101.50
2	B	548	HEM	CMD-C2D-C3D	2.79	126.71	114.35
2	B	552	HEM	CMD-C2D-C3D	2.82	126.84	114.35
2	B	554	HEM	C2D-C3D-C4D	2.94	106.48	101.50
2	A	548	HEM	CMD-C2D-C3D	2.96	127.42	114.35
2	B	547	HEM	CMD-C2D-C3D	2.96	127.43	114.35
2	A	554	HEM	C2D-C3D-C4D	3.10	106.76	101.50
2	B	552	HEM	CAD-C3D-C2D	3.20	122.42	113.22

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	549	HEM	CMC-C2C-C3C	3.31	124.79	116.53
2	B	552	HEM	CMC-C2C-C3C	3.38	124.97	116.53
2	B	551	HEM	CMB-C2B-C3B	3.38	124.97	116.53
2	A	553	HEM	C2D-C3D-C4D	3.40	107.27	101.50
2	B	553	HEM	CMC-C2C-C3C	3.44	125.12	116.53
2	B	547	HEM	CAD-C3D-C4D	3.44	124.62	112.47
2	A	553	HEM	CMC-C2C-C3C	3.59	125.50	116.53
2	B	551	HEM	CAD-C3D-C2D	3.62	123.62	113.22
2	A	548	HEM	CMB-C2B-C3B	3.62	125.58	116.53
2	A	551	HEM	CMC-C2C-C3C	3.66	125.67	116.53
2	B	549	HEM	CMB-C2B-C3B	3.68	125.71	116.53
2	B	547	HEM	C2D-C3D-C4D	3.74	107.85	101.50
2	B	548	HEM	CBA-CAA-C2A	3.78	119.30	112.53
2	A	549	HEM	CAD-C3D-C4D	3.81	125.89	112.47
2	B	548	HEM	C2D-C3D-C4D	3.85	108.02	101.50
2	A	548	HEM	C2D-C3D-C4D	3.85	108.03	101.50
2	A	551	HEM	C2D-C3D-C4D	3.87	108.06	101.50
2	B	554	HEM	CAD-C3D-C4D	3.90	126.22	112.47
2	A	554	HEM	CAD-C3D-C4D	3.90	126.23	112.47
2	A	551	HEM	CAD-C3D-C2D	3.91	124.46	113.22
2	B	548	HEM	CAD-C3D-C4D	3.95	126.39	112.47
2	B	553	HEM	CAD-C3D-C2D	3.95	124.58	113.22
2	A	553	HEM	CAD-C3D-C4D	3.97	126.48	112.47
2	A	551	HEM	CAD-C3D-C4D	3.98	126.50	112.47
2	B	551	HEM	C2D-C3D-C4D	3.98	108.25	101.50
2	A	553	HEM	CMB-C2B-C3B	3.99	126.50	116.53
2	A	547	HEM	CAD-C3D-C2D	4.06	124.88	113.22
2	A	548	HEM	CAD-C3D-C2D	4.09	124.99	113.22
2	A	548	HEM	CAD-C3D-C4D	4.11	126.96	112.47
2	A	548	HEM	CBA-CAA-C2A	4.12	119.91	112.53
2	A	554	HEM	CMB-C2B-C3B	4.13	126.85	116.53
2	A	547	HEM	CMB-C2B-C3B	4.14	126.87	116.53
2	A	552	HEM	CMC-C2C-C3C	4.15	126.90	116.53
2	B	547	HEM	CMB-C2B-C3B	4.17	126.93	116.53
2	A	549	HEM	CMC-C2C-C3C	4.17	126.95	116.53
2	A	552	HEM	CBD-CAD-C3D	4.20	125.78	113.55
2	B	554	HEM	CMB-C2B-C3B	4.21	127.03	116.53
2	B	551	HEM	CAD-C3D-C4D	4.25	127.46	112.47
2	B	548	HEM	CAD-C3D-C2D	4.29	125.55	113.22
2	A	554	HEM	CMC-C2C-C3C	4.31	127.29	116.53
2	B	551	HEM	CMC-C2C-C3C	4.32	127.31	116.53
2	B	547	HEM	CMC-C2C-C3C	4.36	127.41	116.53

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	548	HEM	CMC-C2C-C3C	4.37	127.44	116.53
2	B	548	HEM	CMB-C2B-C3B	4.37	127.44	116.53
2	B	554	HEM	CMC-C2C-C3C	4.39	127.48	116.53
2	A	551	HEM	CMB-C2B-C3B	4.40	127.51	116.53
2	A	553	HEM	CAD-C3D-C2D	4.53	126.24	113.22
2	B	548	HEM	CMC-C2C-C3C	4.53	127.84	116.53
2	A	547	HEM	CMC-C2C-C3C	4.55	127.88	116.53
2	A	554	HEM	CBA-CAA-C2A	4.56	120.70	112.53
2	B	553	HEM	CMB-C2B-C3B	4.65	128.13	116.53
2	A	554	HEM	CAD-C3D-C2D	4.67	126.66	113.22
2	B	549	HEM	CAD-C3D-C2D	4.73	126.82	113.22
2	B	549	HEM	CAD-C3D-C4D	4.76	129.28	112.47
2	B	553	HEM	CAD-C3D-C4D	4.77	129.31	112.47
2	A	547	HEM	CAD-C3D-C4D	4.81	129.45	112.47
2	B	552	HEM	CMB-C2B-C3B	4.84	128.62	116.53
2	B	554	HEM	CAD-C3D-C2D	4.85	127.16	113.22
2	A	549	HEM	CMB-C2B-C3B	4.86	128.67	116.53
2	B	547	HEM	CAD-C3D-C2D	4.98	127.53	113.22
2	A	549	HEM	CAD-C3D-C2D	5.10	127.88	113.22
2	A	552	HEM	CMB-C2B-C3B	5.22	129.56	116.53
2	B	552	HEM	CAD-C3D-C4D	5.50	131.86	112.47
2	B	552	HEM	CBA-CAA-C2A	5.81	122.95	112.53
2	A	553	HEM	CBA-CAA-C2A	6.08	123.42	112.53
2	A	552	HEM	CAD-C3D-C4D	6.32	134.75	112.47
3	A	550	HEC	CBA-CAA-C2A	6.32	123.86	112.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	547	HEM	1	0
2	A	548	HEM	1	0
3	A	550	HEC	5	3
2	A	551	HEM	1	0
2	A	552	HEM	2	0
2	B	549	HEM	1	0
3	B	550	HEC	6	2
2	B	551	HEM	2	0
2	B	552	HEM	3	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.