



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:26 AM GMT

PDB ID : 2D3Q  
Title : Crystal Structure of a Decolorizing Peroxidase (DyP) That Catalyses the Biological Oxidation of Anthraquinone Derivatives  
Authors : Sato, T.; Sugano, Y.; Shoda, M.  
Deposited on : 2005-09-30  
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.

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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) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

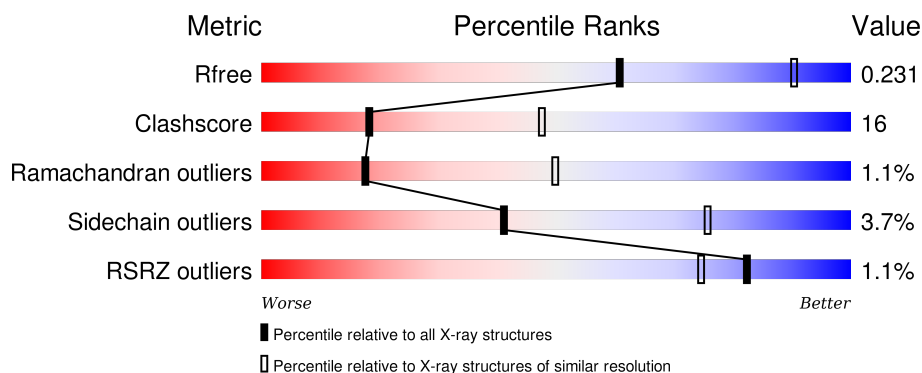
# 1 Overall quality at a glance

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))
$R_{free}$	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (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.

Mol	Chain	Length	Quality of chain
1	A	442	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%; text-align: center;">%</div> <div style="position: absolute; top: 10px; left: 0; width: 100%; text-align: center;">71% 26% ..</div> </div> </div>
1	B	442	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%; text-align: center;">%</div> <div style="position: absolute; top: 10px; left: 0; width: 100%; text-align: center;">71% 26% ..</div> </div> </div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6773 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 Decolorizing Peroxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	439	Total	C	N	O	S	0	0	0
			3338	2116	563	654	5			
1	B	439	Total	C	N	O	S	0	0	0
			3338	2116	563	654	5			

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

- Molecule 3 is water.

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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	136.21Å 136.21Å 363.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 2.80 24.77 – 2.25	Depositor EDS
% Data completeness (in resolution range)	(Not available) (25.00-2.80) 89.3 (24.77-2.25)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.24 (at 2.26Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.234 , 0.267 0.231 , 0.231	Depositor DCC
$R_{free}$ test set	4860 reflections (11.42%)	DCC
Wilson B-factor (Å <sup>2</sup> )	40.6	Xtriage
Anisotropy	0.760	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 49.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.53$ , $\langle L^2 \rangle = 0.36$	Xtriage
Outliers	5 of 84888 reflections (0.006%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6773	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	0.41	0/3425	0.66	0/4672
1	B	0.39	0/3425	0.65	0/4672
All	All	0.40	0/6850	0.65	0/9344

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	3338	0	3191	106	1
1	B	3338	0	3191	100	0
2	A	43	0	30	1	0
2	B	43	0	30	0	0
3	A	5	0	0	0	0
3	B	6	0	0	0	0
All	All	6773	0	6442	206	1

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 16.

All (206) 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:B:192:VAL:HB	1:B:196:ILE:HD12	1.41	1.02
1:B:14:ASP:H	1:B:68:ASN:HD21	1.15	0.91
1:B:241:ALA:HB2	1:B:246:ASN:HA	1.57	0.85
1:B:325:PHE:HA	1:B:365:ASN:O	1.81	0.81
1:A:33:ASP:OD2	1:A:36:SER:HB2	1.82	0.79
1:B:31:VAL:H	1:B:118:HIS:HD2	1.30	0.78
1:A:50:THR:HG22	1:A:67:VAL:H	1.49	0.78
1:A:338:THR:CG2	1:A:343:LEU:HG	2.17	0.75
1:B:182:GLU:CD	1:B:183:THR:H	1.90	0.75
1:A:227:VAL:HB	1:A:228:PRO:HD3	1.70	0.72
1:A:393:ILE:HG22	1:A:394:ILE:HG23	1.72	0.71
1:A:14:ASP:H	1:A:68:ASN:HD21	1.39	0.69
1:A:339:SER:OG	1:A:342:GLU:HG3	1.92	0.69
1:B:31:VAL:H	1:B:118:HIS:CD2	2.10	0.68
1:A:338:THR:HG21	1:A:343:LEU:HG	1.76	0.67
1:B:64:LEU:HD13	1:B:130:PHE:CE1	2.31	0.66
1:A:300:GLU:OE1	1:A:404:GLY:HA3	1.94	0.66
1:A:157:ARG:HH12	1:A:161:GLN:HE21	1.40	0.66
1:A:318:LEU:HD23	1:A:318:LEU:N	2.11	0.65
1:A:241:ALA:HB2	1:A:246:ASN:HA	1.78	0.65
1:A:97:ASP:CG	1:A:368:ARG:HH12	2.01	0.64
1:B:14:ASP:H	1:B:68:ASN:ND2	1.93	0.64
1:A:50:THR:CG2	1:A:67:VAL:H	2.10	0.64
1:A:360:GLN:HE21	1:A:367:PHE:H	1.45	0.64
1:B:295:ASP:OD1	1:B:302:ARG:HD3	1.97	0.64
1:A:139:SER:HB3	1:A:148:GLN:OE1	1.97	0.63
1:B:150:GLN:HG3	1:B:151:ALA:N	2.13	0.63
1:A:136:ASP:O	1:A:140:SER:HB2	1.99	0.63
1:B:221:ARG:HD2	1:B:367:PHE:CZ	2.33	0.63
1:B:31:VAL:N	1:B:118:HIS:HD2	1.95	0.63
1:B:186:PHE:CE1	1:B:285:PRO:HB2	2.33	0.63
1:B:11:ILE:HD13	1:B:214:ASP:HB3	1.81	0.63
1:A:164:HIS:HD2	1:A:168:GLY:O	1.82	0.63
1:A:60:SER:HB2	1:A:61:GLN:HE22	1.65	0.62
1:B:94:GLN:NE2	1:B:221:ARG:HH11	1.98	0.62
1:A:314:PRO:HG2	1:A:318:LEU:CD2	2.29	0.61
1:B:241:ALA:CB	1:B:246:ASN:HA	2.31	0.61
1:A:157:ARG:NH1	1:A:161:GLN:HE21	1.99	0.61
1:B:243:SER:HB2	1:B:275:THR:HG21	1.83	0.61
1:A:241:ALA:HA	1:A:247:LEU:HG	1.83	0.60
1:A:318:LEU:H	1:A:318:LEU:HD23	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:ASN:ND2	1:A:432:SER:HB2	2.16	0.60
1:A:315:ARG:O	1:A:318:LEU:HD23	2.02	0.60
1:B:248:THR:HG23	1:B:251:GLU:OE1	2.01	0.59
1:A:338:THR:HG22	1:A:343:LEU:HG	1.84	0.59
1:B:108:TRP:CE3	1:B:424:GLY:HA2	2.37	0.59
1:B:11:ILE:CD1	1:B:214:ASP:HB3	2.32	0.59
1:A:94:GLN:NE2	1:A:221:ARG:HH11	2.00	0.59
1:B:73:ASN:O	1:B:77:GLN:HG2	2.02	0.59
1:A:182:GLU:OE2	1:A:182:GLU:N	2.37	0.58
1:A:90:PHE:HB3	1:A:91:PRO:HD3	1.86	0.58
1:B:192:VAL:HB	1:B:196:ILE:CD1	2.27	0.58
1:B:241:ALA:O	1:B:408:LEU:HD12	2.04	0.57
1:A:314:PRO:HB2	1:A:317:ASP:HB2	1.86	0.57
1:A:74:THR:HG21	1:A:115:THR:HB	1.86	0.56
1:A:360:GLN:NE2	1:A:367:PHE:H	2.02	0.56
1:B:196:ILE:HD11	1:B:323:ASP:HB3	1.87	0.56
1:A:50:THR:HG21	1:A:66:PHE:HA	1.86	0.56
1:A:21:LYS:HE2	1:A:126:ASP:OD2	2.06	0.56
1:A:405:LEU:HB2	1:A:414:PHE:CE2	2.41	0.55
1:B:65:ALA:HB3	1:B:134:PHE:CE1	2.42	0.55
1:A:170:LEU:HD23	1:A:173:ILE:HD11	1.89	0.55
1:A:50:THR:HG21	1:A:66:PHE:HB3	1.89	0.54
1:A:314:PRO:HG2	1:A:318:LEU:HD22	1.87	0.54
1:B:193:PRO:HB2	1:B:202:ASP:O	2.07	0.54
1:A:15:ILE:HD13	1:A:216:SER:HB3	1.89	0.54
1:B:437:THR:HA	1:B:441:ALA:HB3	1.90	0.54
1:A:50:THR:HG21	1:A:66:PHE:CA	2.37	0.54
1:A:41:LEU:HD23	1:A:441:ALA:HB2	1.89	0.53
1:A:97:ASP:OD2	1:A:368:ARG:NH1	2.40	0.53
1:B:170:LEU:HD23	1:B:173:ILE:HD11	1.91	0.53
1:A:368:ARG:HH11	1:A:368:ARG:HG3	1.74	0.53
1:A:13:GLY:HA3	1:A:55:LEU:HD12	1.91	0.53
1:A:157:ARG:HH12	1:A:161:GLN:NE2	2.07	0.52
1:A:373:ASN:N	1:A:373:ASN:HD22	2.06	0.52
1:A:380:PHE:HA	1:A:381:PRO:C	2.30	0.52
1:B:227:VAL:HB	1:B:228:PRO:HD3	1.91	0.52
1:B:225:GLN:HG3	1:B:353:GLY:HA2	1.92	0.52
1:B:90:PHE:HB3	1:B:91:PRO:HD3	1.92	0.52
1:B:164:HIS:HD2	1:B:168:GLY:O	1.93	0.52
1:A:34:ALA:O	1:A:38:LYS:HG3	2.10	0.51
1:B:111:PRO:HG2	1:B:117:ILE:HD11	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:GLN:HE21	1:B:353:GLY:C	2.13	0.51
1:B:22:GLN:C	1:B:23:LYS:HD3	2.30	0.51
1:A:101:LEU:HA	1:A:372:ILE:HD11	1.93	0.51
1:B:360:GLN:NE2	1:B:367:PHE:H	2.09	0.50
1:B:168:GLY:O	1:B:265:LYS:HB3	2.11	0.50
1:B:107:GLN:HA	1:B:107:GLN:OE1	2.11	0.50
1:B:150:GLN:HG3	1:B:151:ALA:H	1.77	0.50
1:B:368:ARG:HG2	1:B:372:ILE:HD12	1.92	0.50
1:A:50:THR:HG21	1:A:66:PHE:CB	2.42	0.50
1:B:420:VAL:C	1:B:421:ILE:HD12	2.31	0.50
1:A:340:ASP:O	1:A:344:ALA:HB3	2.12	0.50
1:A:314:PRO:HG2	1:A:318:LEU:HD21	1.94	0.49
1:B:328:MET:O	1:B:358:GLU:HA	2.13	0.49
1:A:21:LYS:HD3	1:A:66:PHE:CE2	2.47	0.49
1:A:358:GLU:OE1	1:A:367:PHE:HB2	2.12	0.49
1:A:315:ARG:O	1:A:318:LEU:CD2	2.60	0.49
1:B:197:ILE:HD12	1:B:328:MET:HG2	1.93	0.49
1:A:94:GLN:HE22	1:A:221:ARG:HD2	1.78	0.49
1:B:404:GLY:HA2	1:B:410:GLN:HA	1.93	0.49
1:A:248:THR:HG23	1:A:251:GLU:OE1	2.12	0.49
1:B:391:GLU:OE1	1:B:394:ILE:HD13	2.12	0.48
1:A:218:MET:HG3	1:A:357:VAL:HG13	1.94	0.48
1:A:21:LYS:HD3	1:A:66:PHE:HE2	1.78	0.48
1:B:108:TRP:CD2	1:B:424:GLY:HA2	2.48	0.48
1:A:45:VAL:HA	1:A:49:ILE:HG12	1.95	0.48
1:A:314:PRO:CG	1:A:318:LEU:HD22	2.44	0.48
1:B:165:GLU:CD	1:B:167:PHE:H	2.17	0.48
1:B:196:ILE:HD11	1:B:323:ASP:CB	2.44	0.48
1:B:221:ARG:CD	1:B:367:PHE:CZ	2.97	0.48
1:A:242:ASN:O	1:A:243:SER:C	2.51	0.48
1:B:182:GLU:CG	1:B:183:THR:H	2.26	0.47
1:B:362:ILE:HG21	1:B:365:ASN:ND2	2.29	0.47
1:B:150:GLN:CG	1:B:151:ALA:N	2.77	0.47
1:A:44:TYR:CE1	1:A:48:ARG:HG3	2.49	0.47
1:B:182:GLU:O	1:B:183:THR:HG22	2.14	0.47
1:B:262:GLY:O	1:B:270:ILE:HG12	2.15	0.47
1:B:208:ARG:HG3	1:B:208:ARG:HH11	1.79	0.47
1:A:108:TRP:CE3	1:A:424:GLY:HA2	2.50	0.47
1:A:241:ALA:CB	1:A:246:ASN:HA	2.44	0.46
1:B:161:GLN:O	1:B:164:HIS:HB2	2.15	0.46
1:A:100:ASN:O	1:A:372:ILE:HD12	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:431:PRO:HG2	1:B:440:ILE:CD1	2.46	0.46
1:B:157:ARG:HD3	1:B:164:HIS:O	2.15	0.46
1:B:262:GLY:HA2	1:B:270:ILE:HD11	1.97	0.46
1:A:125:SER:HB3	1:A:131:LEU:HD13	1.97	0.46
1:B:14:ASP:HB3	1:B:68:ASN:HD22	1.81	0.46
1:B:117:ILE:HD13	1:B:149:VAL:HG21	1.97	0.46
1:A:45:VAL:HB	1:A:46:PRO:CD	2.46	0.46
1:A:81:ILE:N	1:A:81:ILE:HD12	2.30	0.46
1:B:26:PHE:O	1:B:151:ALA:HA	2.16	0.46
1:B:421:ILE:N	1:B:421:ILE:HD12	2.31	0.46
1:A:67:VAL:HA	1:A:122:LEU:O	2.16	0.46
1:B:278:ASP:O	1:B:281:LEU:HB3	2.16	0.45
1:B:81:ILE:HD12	1:B:81:ILE:N	2.30	0.45
1:B:165:GLU:OE2	1:B:167:PHE:HB2	2.16	0.45
1:A:226:LYS:HE3	1:A:421:ILE:HD12	1.99	0.45
1:B:48:ARG:HH11	1:B:48:ARG:HG2	1.82	0.45
1:A:122:LEU:HD21	1:A:218:MET:CE	2.47	0.45
1:B:284:ASP:HA	1:B:285:PRO:HD2	1.83	0.44
1:A:60:SER:HB2	1:A:61:GLN:NE2	2.29	0.44
1:A:38:LYS:HB3	1:A:441:ALA:HA	1.99	0.44
1:B:16:LEU:HD11	1:B:178:VAL:HG21	1.98	0.44
1:B:292:ASP:O	1:B:316:GLN:HB2	2.17	0.44
1:A:60:SER:CB	1:A:61:GLN:HE22	2.30	0.44
1:A:101:LEU:HA	1:A:372:ILE:CD1	2.48	0.44
1:A:85:LEU:HD12	1:A:90:PHE:CE2	2.53	0.44
1:B:234:THR:HA	1:B:256:LEU:HD23	1.98	0.44
1:A:318:LEU:CD2	1:A:318:LEU:N	2.79	0.44
1:A:440:ILE:HD12	1:A:440:ILE:N	2.32	0.44
1:B:41:LEU:O	1:B:45:VAL:HG23	2.18	0.44
1:A:437:THR:HA	1:A:441:ALA:HB3	2.00	0.43
1:B:431:PRO:HG2	1:B:440:ILE:HD11	2.00	0.43
1:A:234:THR:HA	1:A:256:LEU:HD23	1.99	0.43
1:B:14:ASP:CB	1:B:68:ASN:ND2	2.80	0.43
1:A:385:PRO:O	1:A:386:ILE:HD13	2.18	0.43
1:A:94:GLN:NE2	1:A:425:GLY:HA3	2.33	0.43
1:B:262:GLY:HA2	1:B:270:ILE:CD1	2.48	0.43
1:B:21:LYS:HA	1:B:21:LYS:HD3	1.80	0.43
1:B:45:VAL:N	1:B:46:PRO:HD2	2.34	0.43
1:B:318:LEU:HD12	1:B:318:LEU:HA	1.82	0.43
1:B:235:LEU:HA	1:B:253:ALA:HB2	2.01	0.43
1:A:182:GLU:CG	1:A:182:GLU:O	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:ARG:HA	1:A:201:ARG:HD3	1.86	0.42
1:A:368:ARG:HG3	1:A:368:ARG:NH1	2.34	0.42
1:B:342:GLU:OE2	1:B:352:ARG:NH2	2.52	0.42
1:B:188:GLY:HA3	1:B:289:ASN:O	2.19	0.42
1:B:196:ILE:HD13	1:B:323:ASP:O	2.19	0.42
1:A:229:GLU:OE1	1:A:229:GLU:N	2.47	0.42
1:B:62:GLN:HA	1:B:63:PRO:HD3	1.94	0.42
1:A:440:ILE:N	1:A:440:ILE:CD1	2.82	0.42
1:B:416:VAL:HG12	1:B:417:PRO:O	2.18	0.42
1:A:273:ALA:HB1	1:A:276:ALA:O	2.20	0.42
1:A:394:ILE:HD13	2:A:446:HEM:C2C	2.54	0.42
1:A:58:ASP:OD1	1:A:60:SER:HB2	2.20	0.42
1:A:111:PRO:HG2	1:A:117:ILE:HD11	2.01	0.42
1:B:391:GLU:HA	1:B:392:PRO:HD2	1.88	0.42
1:A:284:ASP:HA	1:A:285:PRO:HD2	1.88	0.42
1:A:208:ARG:NH2	1:A:362:ILE:HG12	2.34	0.42
1:A:248:THR:OG1	1:A:251:GLU:HG3	2.20	0.42
1:B:416:VAL:HA	1:B:417:PRO:HD3	1.92	0.41
1:A:343:LEU:C	1:A:345:SER:H	2.23	0.41
1:A:61:GLN:N	1:A:61:GLN:NE2	2.68	0.41
1:B:58:ASP:HA	1:B:59:PRO:HD3	1.98	0.41
1:A:18:GLY:O	1:A:20:LYS:HG3	2.20	0.41
1:B:208:ARG:N	1:B:208:ARG:HD2	2.35	0.41
1:A:131:LEU:HD12	1:A:131:LEU:HA	1.88	0.41
1:B:256:LEU:O	1:B:260:MET:HG3	2.20	0.41
1:B:324:THR:O	1:B:325:PHE:CB	2.68	0.41
1:B:51:SER:OG	1:B:53:ALA:HB3	2.20	0.41
1:A:50:THR:CG2	1:A:67:VAL:N	2.82	0.41
1:A:100:ASN:O	1:A:372:ILE:CD1	2.69	0.41
1:A:339:SER:HG	1:A:342:GLU:HG3	1.84	0.41
1:A:182:GLU:O	1:A:182:GLU:HG2	2.21	0.41
1:B:122:LEU:HD11	1:B:218:MET:HE1	2.03	0.41
1:B:21:LYS:HE2	1:B:66:PHE:CE2	2.56	0.40
1:B:218:MET:HB2	1:B:359:TYR:CE1	2.56	0.40
1:B:182:GLU:O	1:B:183:THR:O	2.39	0.40
1:B:97:ASP:OD2	1:B:368:ARG:HD2	2.22	0.40
1:A:4:THR:O	1:A:4:THR:OG1	2.39	0.40
1:B:24:GLU:HA	1:B:123:ILE:O	2.22	0.40
1:B:324:THR:O	1:B:325:PHE:HB2	2.22	0.40
1:A:239:ILE:HA	1:A:240:PRO:HD3	1.93	0.40
1:A:158:PRO:O	1:A:161:GLN:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:LYS:HB3	1:B:125:SER:O	2.21	0.40

All (1) 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:278:ASP:OD1	1:A:278:ASP:OD1[10_665]	2.13	0.07

## 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	437/442 (99%)	390 (89%)	43 (10%)	4 (1%)	21	55
1	B	437/442 (99%)	400 (92%)	31 (7%)	6 (1%)	14	42
All	All	874/884 (99%)	790 (90%)	74 (8%)	10 (1%)	17	50

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	B	182	GLU
1	B	183	THR
1	A	140	SER
1	A	324	THR
1	A	243	SER
1	B	323	ASP
1	B	324	THR
1	B	292	ASP
1	B	59	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	355/357 (99%)	341 (96%)	14 (4%)	39	74
1	B	355/357 (99%)	343 (97%)	12 (3%)	44	78
All	All	710/714 (99%)	684 (96%)	26 (4%)	41	76

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	THR
1	A	21	LYS
1	A	43	THR
1	A	50	THR
1	A	107	GLN
1	A	131	LEU
1	A	140	SER
1	A	202	ASP
1	A	210	SER
1	A	318	LEU
1	A	360	GLN
1	A	373	ASN
1	A	391	GLU
1	A	393	ILE
1	B	131	LEU
1	B	182	GLU
1	B	208	ARG
1	B	250	GLN
1	B	299	ASP
1	B	318	LEU
1	B	324	THR
1	B	360	GLN
1	B	368	ARG
1	B	394	ILE
1	B	409	ASN
1	B	410	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	GLN
1	A	68	ASN
1	A	94	GLN
1	A	107	GLN
1	A	127	GLN
1	A	133	GLN
1	A	161	GLN
1	A	164	HIS
1	A	225	GLN
1	A	316	GLN
1	A	326	HIS
1	A	360	GLN
1	A	371	GLN
1	A	373	ASN
1	B	68	ASN
1	B	94	GLN
1	B	118	HIS
1	B	127	GLN
1	B	148	GLN
1	B	164	HIS
1	B	225	GLN
1	B	231	ASN
1	B	326	HIS
1	B	360	GLN
1	B	365	ASN
1	B	373	ASN
1	B	409	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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

2 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	446	1	30,50,50	2.66	9 (30%)	24,82,82	7.80	18 (75%)
2	HEM	B	446	1	30,50,50	2.95	8 (26%)	24,82,82	6.77	19 (79%)

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	446	1	-	0/10/54/54	0/0/8/8
2	HEM	B	446	1	-	0/10/54/54	0/0/8/8

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	446	HEM	C3B-C4B	-6.50	1.46	1.51
2	A	446	HEM	C2D-C3D	-6.34	1.35	1.54
2	B	446	HEM	C2D-C3D	-6.21	1.35	1.54
2	B	446	HEM	C3B-C4B	-6.17	1.46	1.51
2	B	446	HEM	C2C-C1C	-3.98	1.45	1.52
2	A	446	HEM	C2C-C1C	-3.80	1.45	1.52
2	B	446	HEM	C3D-C4D	-3.55	1.47	1.51
2	A	446	HEM	C3D-C4D	-3.43	1.47	1.51
2	A	446	HEM	FE-NC	2.62	2.06	1.95
2	A	446	HEM	FE-NB	3.56	2.16	1.97
2	A	446	HEM	C1C-NC	3.92	1.40	1.36
2	B	446	HEM	C1C-NC	3.99	1.40	1.36
2	B	446	HEM	CBB-CAB	4.38	1.54	1.29
2	A	446	HEM	CBB-CAB	4.44	1.54	1.29
2	B	446	HEM	CBC-CAC	4.59	1.55	1.29
2	A	446	HEM	CBC-CAC	4.69	1.56	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	446	HEM	FE-NC	8.65	2.29	1.95

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	446	HEM	CMA-C3A-C4A	-10.51	110.97	128.36
2	B	446	HEM	CMA-C3A-C4A	-9.25	113.06	128.36
2	A	446	HEM	CHC-C4B-NB	-8.14	104.92	124.52
2	B	446	HEM	CHD-C1D-ND	-6.43	109.03	124.52
2	A	446	HEM	CHD-C1D-ND	-6.18	109.65	124.52
2	B	446	HEM	CHC-C4B-NB	-4.28	114.22	124.52
2	A	446	HEM	C2D-C3D-C4D	-3.90	94.88	101.50
2	B	446	HEM	CAD-CBD-CGD	-2.83	101.45	113.02
2	B	446	HEM	CAA-C2A-C1A	-2.36	124.44	127.01
2	B	446	HEM	CBD-CAD-C3D	-2.12	107.39	113.55
2	A	446	HEM	CAA-C2A-C1A	2.16	129.35	127.01
2	A	446	HEM	CMD-C2D-C3D	2.51	125.45	114.35
2	B	446	HEM	CMD-C2D-C3D	2.66	126.11	114.35
2	B	446	HEM	CAD-C3D-C4D	3.17	123.66	112.47
2	A	446	HEM	CAD-C3D-C4D	3.45	124.63	112.47
2	A	446	HEM	C2C-C1C-NC	4.68	118.10	110.21
2	A	446	HEM	C3C-CAC-CBC	5.01	132.13	124.46
2	B	446	HEM	CAA-CBA-CGA	5.26	122.39	112.75
2	B	446	HEM	C2C-C1C-CHC	5.41	131.91	123.68
2	B	446	HEM	CMA-C3A-C2A	6.37	138.56	125.24
2	B	446	HEM	CMB-C2B-C3B	6.85	133.63	116.53
2	A	446	HEM	CMB-C2B-C3B	6.97	133.92	116.53
2	B	446	HEM	C3B-C4B-CHC	7.15	133.22	123.16
2	B	446	HEM	CAD-C3D-C2D	7.16	133.81	113.22
2	B	446	HEM	C3B-CAB-CBB	7.28	135.63	124.46
2	A	446	HEM	C2C-C1C-CHC	7.54	135.15	123.68
2	B	446	HEM	CMC-C2C-C3C	7.64	135.59	116.53
2	A	446	HEM	CMC-C2C-C3C	7.87	136.18	116.53
2	A	446	HEM	CMA-C3A-C2A	8.38	142.76	125.24
2	A	446	HEM	CAD-C3D-C2D	9.21	139.71	113.22
2	A	446	HEM	CAA-CBA-CGA	9.78	130.66	112.75
2	B	446	HEM	C3C-CAC-CBC	11.46	142.03	124.46
2	B	446	HEM	C4B-CHC-C1C	11.77	145.50	125.82
2	A	446	HEM	C1D-CHD-C4C	14.75	150.48	125.82
2	A	446	HEM	C3B-C4B-CHC	15.09	144.41	123.16
2	B	446	HEM	C1D-CHD-C4C	16.95	154.16	125.82
2	A	446	HEM	C4B-CHC-C1C	16.96	154.18	125.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	446	HEM	1	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](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	439/442 (99%)	-0.54	5 (1%) 82 74	41, 57, 78, 90	0
1	B	439/442 (99%)	-0.56	5 (1%) 82 74	38, 59, 77, 90	0
All	All	878/884 (99%)	-0.55	10 (1%) 82 74	38, 58, 77, 90	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	4	THR	3.0
1	B	70	GLY	2.9
1	B	257	GLY	2.6
1	B	258	ALA	2.5
1	B	260	MET	2.4
1	A	307	ALA	2.4
1	A	58	ASP	2.4
1	A	182	GLU	2.3
1	B	69	LEU	2.3
1	A	409	ASN	2.3

### 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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	HEM	B	446	43/43	0.97	0.16	-0.04	45,53,60,61	0
2	HEM	A	446	43/43	0.97	0.14	-0.25	37,44,57,65	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.