



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 02:54 PM 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 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/ValidationPDFNotes.html>

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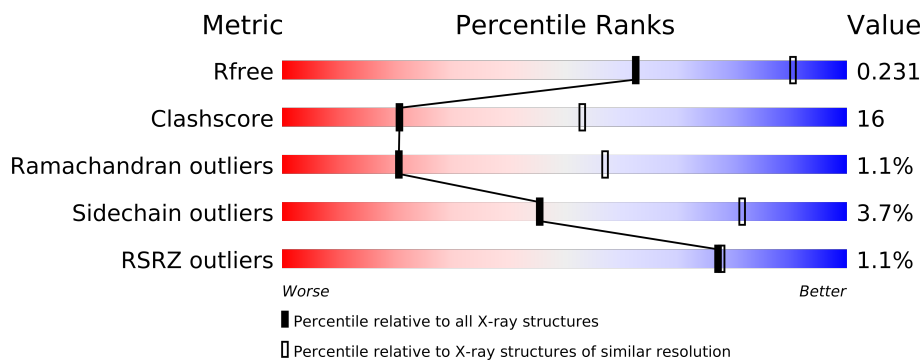
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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))
$R_{free}$	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	442	
1	B	442	

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 6773 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

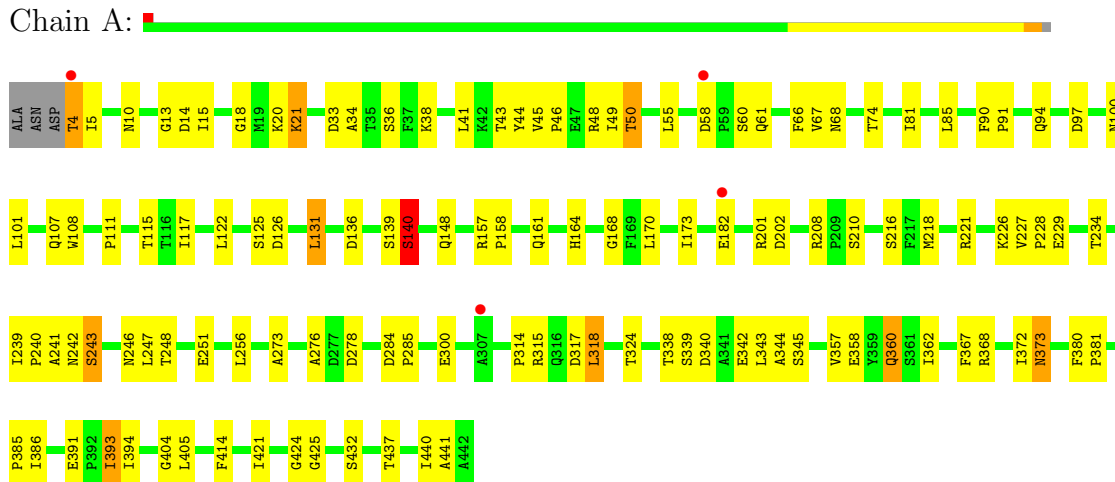
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	5	Total 5	O 5	0	0
3	B	6	Total 6	O 6	0	0

### 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.

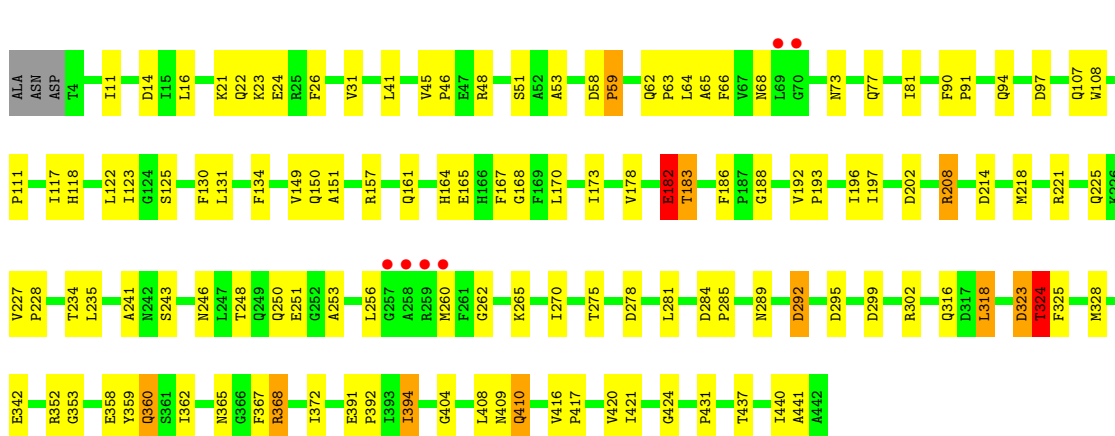
#### • Molecule 1: Decolorizing Peroxidase

Chain A:



#### • Molecule 1: Decolorizing Peroxidase

Chain B:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	136.21 Å   136.21 Å   363.60 Å 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 2.26 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.234   ,   0.267 0.231   ,   0.231	Depositor DCC
$R_{free}$ test set	4865 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 , 48.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.53$ , $\langle L^2 \rangle = 0.36$	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.

## 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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 16.

All (206) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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
1:A:10:ASN:ND2	1:A:432:SER:HB2	2.16	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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	Distance(Å)	Clash(Å)
1:A:278:ASP:OD1	1:A:278:ASP:OD1[10.665]	2.13	0.07

## 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	437/442 (99%)	390 (89%)	43 (10%)	4 (1%)	25	63
1	B	437/442 (99%)	400 (92%)	31 (7%)	6 (1%)	16	49
All	All	874/884 (99%)	790 (90%)	74 (8%)	10 (1%)	21	57

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%)	43	80
1	B	355/357 (99%)	343 (97%)	12 (3%)	49	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	710/714 (99%)	684 (96%)	26 (4%)	45 81

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

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Mol	Chain	Res	Type
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 chains 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	49,50,50	3.03	20 (40%)	46,82,82	9.70	32 (69%)
2	HEM	B	446	1	49,50,50	3.43	22 (44%)	46,82,82	8.49	31 (67%)

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	-	0/14/114/114	0/0/8/8
2	HEM	B	446	1	-	0/14/114/114	0/0/8/8

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	446	HEM	C3D-C4D	10.52	1.47	1.44
2	B	446	HEM	C3D-C4D	9.89	1.47	1.44
2	B	446	HEM	FE-NC	8.45	2.29	1.97
2	B	446	HEM	C2D-C1D	8.33	1.46	1.44
2	B	446	HEM	FE-NA	7.78	2.26	1.92
2	A	446	HEM	C2D-C1D	6.12	1.46	1.44
2	B	446	HEM	C2B-C1B	5.43	1.45	1.44
2	B	446	HEM	C3C-C2C	-5.30	1.34	1.43
2	A	446	HEM	FE-NB	5.09	2.16	1.97
2	A	446	HEM	C3C-C2C	-5.01	1.35	1.43
2	A	446	HEM	C3D-C2D	-4.73	1.35	1.43
2	A	446	HEM	CBC-CAC	4.72	1.56	1.28
2	B	446	HEM	C4A-C3A	4.68	1.46	1.40
2	A	446	HEM	C4A-C3A	4.67	1.46	1.40
2	B	446	HEM	CBC-CAC	4.62	1.55	1.28
2	B	446	HEM	C3D-C2D	-4.50	1.35	1.43
2	A	446	HEM	CBB-CAB	4.47	1.54	1.28
2	B	446	HEM	CBB-CAB	4.41	1.54	1.28
2	A	446	HEM	C3B-C2B	-4.23	1.36	1.43
2	A	446	HEM	FE-NA	4.17	2.10	1.92
2	A	446	HEM	C2B-C1B	4.04	1.45	1.44
2	B	446	HEM	C3C-CAC	3.96	1.52	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	446	HEM	C3C-CAC	3.95	1.52	1.40
2	B	446	HEM	CBD-CGD	-3.75	1.40	1.50
2	B	446	HEM	C3B-C2B	-3.74	1.37	1.43
2	A	446	HEM	CHA-C4D	3.56	1.40	1.35
2	A	446	HEM	CBD-CGD	-3.49	1.41	1.50
2	B	446	HEM	CBA-CGA	-3.36	1.41	1.50
2	B	446	HEM	C3B-CAB	3.25	1.50	1.40
2	A	446	HEM	CBA-CGA	-3.15	1.42	1.50
2	B	446	HEM	CHA-C4D	3.14	1.40	1.35
2	A	446	HEM	C3B-CAB	2.94	1.49	1.40
2	B	446	HEM	CHB-C1B	2.86	1.39	1.35
2	A	446	HEM	O1A-CGA	2.75	1.32	1.22
2	B	446	HEM	FE-NB	2.74	2.07	1.97
2	A	446	HEM	FE-ND	2.69	2.07	1.97
2	A	446	HEM	CAD-CBD	2.61	1.59	1.52
2	B	446	HEM	FE-ND	2.60	2.07	1.97
2	B	446	HEM	O1A-CGA	2.59	1.31	1.22
2	B	446	HEM	CAD-CBD	2.55	1.59	1.52
2	A	446	HEM	FE-NC	2.22	2.06	1.97
2	B	446	HEM	C1C-NC	2.06	1.40	1.38

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	446	HEM	CHC-C4B-NB	-23.67	104.92	124.58
2	A	446	HEM	CHB-C1B-NB	-22.98	92.73	124.31
2	B	446	HEM	C1A-CHA-C4D	22.95	157.67	127.47
2	A	446	HEM	CHC-C1C-NC	-20.71	106.74	124.73
2	B	446	HEM	CHD-C1D-ND	-18.72	109.03	124.58
2	A	446	HEM	C1A-CHA-C4D	18.52	151.84	127.47
2	B	446	HEM	C4A-CHB-C1B	18.16	151.37	127.47
2	A	446	HEM	CHD-C1D-ND	-17.98	109.65	124.58
2	A	446	HEM	CHB-C4A-NA	-17.83	94.80	124.58
2	A	446	HEM	C4A-CHB-C1B	16.25	148.85	127.47
2	B	446	HEM	CHD-C4C-NC	-15.69	111.10	124.73
2	B	446	HEM	O2A-CGA-O1A	14.70	160.70	123.30
2	A	446	HEM	CHD-C4C-NC	-14.59	112.05	124.73
2	B	446	HEM	CHA-C4D-ND	-13.78	105.37	124.31
2	A	446	HEM	CHA-C1A-NA	-12.84	103.13	124.58
2	B	446	HEM	CHC-C4B-NB	-12.47	114.22	124.58
2	A	446	HEM	CMA-C3A-C4A	-11.47	110.97	128.62
2	B	446	HEM	CHB-C1B-NB	-11.13	109.01	124.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	446	HEM	C3A-C4A-CHB	11.12	147.08	126.00
2	A	446	HEM	O2A-CGA-O1A	11.08	151.47	123.30
2	B	446	HEM	CHB-C4A-NA	-10.94	106.30	124.58
2	A	446	HEM	CHA-C4D-ND	-10.51	109.86	124.31
2	A	446	HEM	C4B-CHC-C1C	10.49	154.18	126.57
2	B	446	HEM	C1D-CHD-C4C	10.48	154.16	126.57
2	B	446	HEM	O2A-CGA-CBA	-10.22	78.10	114.22
2	B	446	HEM	CMA-C3A-C4A	-10.11	113.06	128.62
2	B	446	HEM	C4C-NC-C1C	10.06	115.99	105.53
2	A	446	HEM	CMA-C3A-C2A	9.45	142.76	124.94
2	A	446	HEM	C1D-CHD-C4C	9.08	150.48	126.57
2	B	446	HEM	C3A-C4A-CHB	8.96	143.00	126.00
2	A	446	HEM	C2A-C1A-CHA	8.91	142.91	126.00
2	B	446	HEM	O2D-CGD-O1D	-8.82	100.85	123.30
2	B	446	HEM	C1B-NB-C4B	-7.73	97.25	105.16
2	A	446	HEM	O2A-CGA-CBA	-7.51	87.66	114.22
2	B	446	HEM	CHA-C1A-NA	-7.27	112.43	124.58
2	B	446	HEM	CMA-C3A-C2A	7.22	138.56	124.94
2	B	446	HEM	C4B-CHC-C1C	7.19	145.50	126.57
2	B	446	HEM	C2A-C1A-CHA	7.13	139.53	126.00
2	B	446	HEM	O2D-CGD-CBD	6.60	137.55	114.22
2	A	446	HEM	C4C-NC-C1C	-6.43	98.85	105.53
2	B	446	HEM	C4D-ND-C1D	-6.16	98.86	105.16
2	B	446	HEM	CHC-C1C-NC	-6.02	119.50	124.73
2	A	446	HEM	CAD-C3D-C2D	5.60	139.71	127.25
2	A	446	HEM	CAA-CBA-CGA	5.35	130.66	113.47
2	A	446	HEM	C3A-C4A-NA	4.95	113.15	109.41
2	A	446	HEM	C3B-C4B-NB	-4.67	110.66	114.00
2	A	446	HEM	C2D-C1D-ND	-4.61	107.49	112.93
2	A	446	HEM	CMC-C2C-C3C	4.25	136.18	126.16
2	A	446	HEM	C4D-ND-C1D	-4.08	100.98	105.16
2	B	446	HEM	CMC-C2C-C3C	4.00	135.59	126.16
2	B	446	HEM	CAD-CBD-CGD	-3.86	101.45	113.48
2	A	446	HEM	C4A-C3A-C2A	-3.53	104.54	107.00
2	A	446	HEM	CMB-C2B-C3B	3.29	133.92	126.16
2	B	446	HEM	C3B-C4B-NB	-3.26	111.67	114.00
2	B	446	HEM	CBD-CAD-C3D	-3.20	107.39	114.37
2	B	446	HEM	CMB-C2B-C3B	3.17	133.63	126.16
2	B	446	HEM	CAD-C3D-C2D	2.94	133.81	127.25
2	A	446	HEM	C4A-NA-C1A	-2.94	102.89	106.76
2	B	446	HEM	C3A-C4A-NA	-2.93	107.20	109.41
2	A	446	HEM	O1D-CGD-CBD	-2.88	113.11	123.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	446	HEM	CAA-CBA-CGA	2.78	122.39	113.47
2	A	446	HEM	O2D-CGD-CBD	2.77	124.02	114.22
2	A	446	HEM	C1B-NB-C4B	-2.70	102.40	105.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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 ⓘ

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%)	-0.55	4 (0%) 81 81	41, 57, 78, 90	0
1	B	439/442 (99%)	-0.57	6 (1%) 72 72	38, 59, 77, 90	0
All	All	878/884 (99%)	-0.56	10 (1%) 77 78	38, 58, 77, 90	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	70	GLY	3.2
1	A	4	THR	3.2
1	B	258	ALA	3.0
1	B	257	GLY	2.9
1	A	307	ALA	2.9
1	B	260	MET	2.4
1	A	182	GLU	2.4
1	B	69	LEU	2.2
1	A	58	ASP	2.1
1	B	259	ARG	2.1

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands

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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	HEM	B	446	43/43	0.16	0.11	45,53,60,61	0
2	HEM	A	446	43/43	0.15	-0.18	37,44,57,65	0

## 6.5 Other polymers

There are no such residues in this entry.