



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:27 AM GMT

PDB ID : 3LXH  
Title : Crystal Structure of Cytochrome P450 CYP101D1  
Authors : Yang, W.; Bell, S.G.; Wang, H.; Bartlam, M.; Wong, L.L.; Rao, Z.  
Deposited on : 2010-02-25  
Resolution : 2.20 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

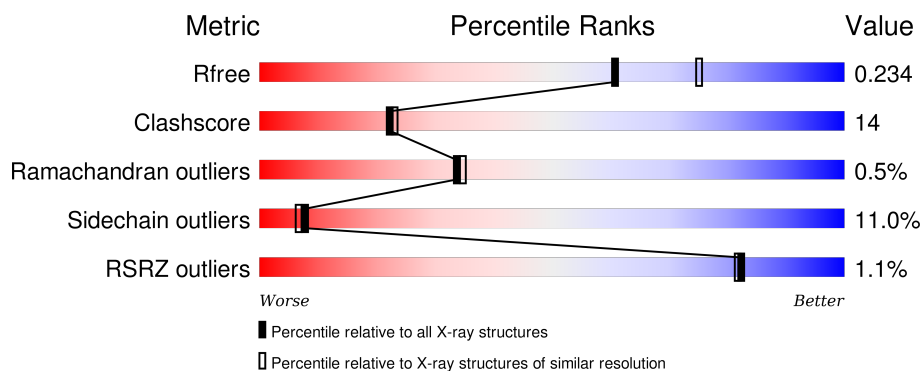
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*



The reported resolution of this entry is 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	421	 75% 16% 5% . .
1	B	421	 2% 70% 18% 6% . .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	DIO	A	423	-	-	-	X

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7040 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 Cytochrome P450.

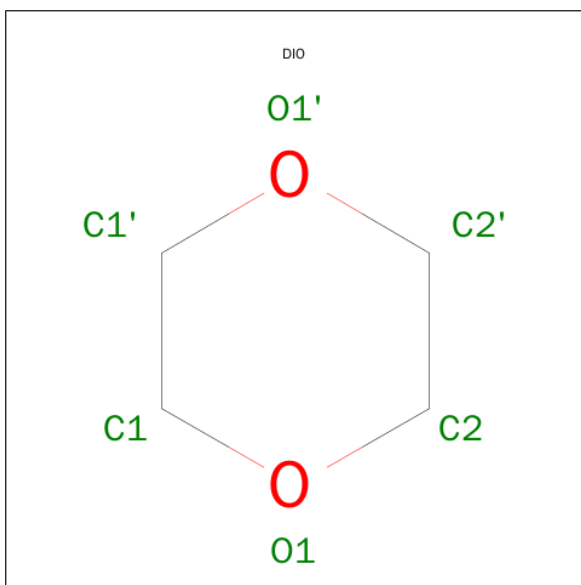
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	408	Total	C	N	O	S	0	0	0
			3240	2060	577	590	13			
1	B	405	Total	C	N	O	S	0	0	0
			3213	2044	571	585	13			

- 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 1,4-DIETHYLENE DIOXIDE (three-letter code: DIO) (formula:  $C_4H_8O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	4	2		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	A	1	Total	O	P	0	0
			5	4	1		
4	A	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		

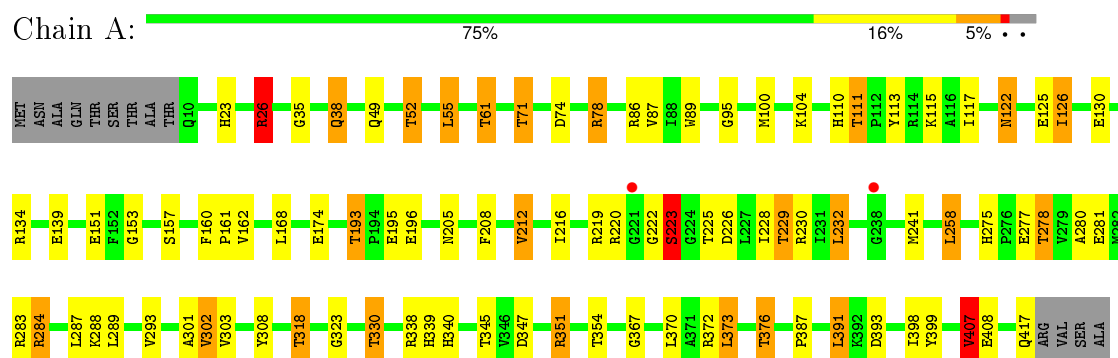
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	263	Total	O	0	0
			263	263		
5	B	202	Total	O	0	0
			202	202		

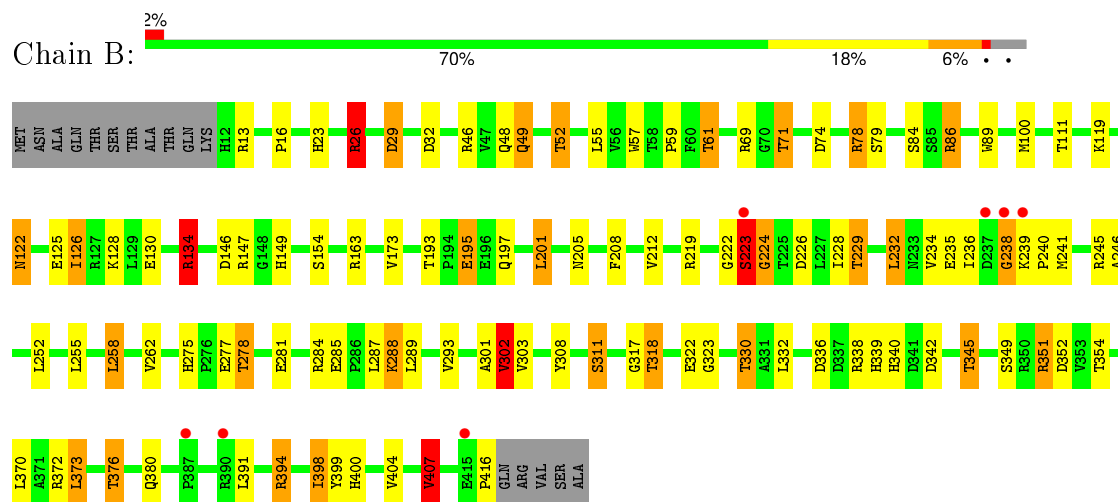
### 3 Residue-property plots [i](#)

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.

#### • Molecule 1: Cytochrome P450



#### • Molecule 1: Cytochrome P450



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	150.90Å 150.90Å 195.32Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.40 – 2.20 49.39 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.5 (49.40-2.20) 98.5 (49.39-2.20)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.73 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.5.0044	Depositor
R, $R_{free}$	0.200 , 0.240 0.196 , 0.234	Depositor DCC
$R_{free}$ test set	3332 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	31.7	Xtriage
Anisotropy	0.391	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 43.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 65971 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7040	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.21% 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, PO4, DIO

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	0.79	0/3322	0.91	10/4514 (0.2%)
1	B	0.74	0/3295	0.90	12/4479 (0.3%)
All	All	0.76	0/6617	0.91	22/8993 (0.2%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	78	ARG	NE-CZ-NH2	-12.21	114.20	120.30
1	B	78	ARG	NE-CZ-NH1	9.04	124.82	120.30
1	B	26	ARG	NE-CZ-NH1	8.53	124.56	120.30
1	B	26	ARG	NE-CZ-NH2	-8.45	116.07	120.30
1	A	407	VAL	CB-CA-C	-7.72	96.73	111.40
1	B	201	LEU	CA-CB-CG	6.94	131.27	115.30
1	B	407	VAL	CB-CA-C	-6.75	98.58	111.40
1	A	26	ARG	NE-CZ-NH2	-6.65	116.97	120.30
1	A	302	VAL	CG1-CB-CG2	6.51	121.32	110.90
1	B	134	ARG	NE-CZ-NH2	-6.45	117.08	120.30
1	A	134	ARG	NE-CZ-NH2	-6.15	117.23	120.30
1	A	78	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	A	391	LEU	CA-CB-CG	5.98	129.06	115.30
1	A	26	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	B	302	VAL	CG1-CB-CG2	5.54	119.76	110.90
1	A	219	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	B	134	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	B	352	ASP	CB-CG-OD1	5.24	123.02	118.30
1	B	78	ARG	CG-CD-NE	-5.16	100.97	111.80
1	A	347	ASP	CB-CG-OD2	5.07	122.87	118.30
1	A	55	LEU	CA-CB-CG	5.06	126.93	115.30
1	B	29	ASP	CB-CG-OD2	-5.05	113.75	118.30

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	3240	0	3215	72	0
1	B	3213	0	3186	106	0
2	A	43	0	30	2	0
2	B	43	0	30	4	0
3	A	6	0	8	1	0
4	A	20	0	0	1	0
4	B	10	0	0	1	0
5	A	263	0	0	14	0
5	B	202	0	0	21	0
All	All	7040	0	6469	180	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 14.

All (180) 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:351:ARG:HG2	1:B:351:ARG:HH11	1.12	1.14
1:B:222:GLY:HA3	1:B:223:SER:HB2	1.37	1.05
1:A:226:ASP:OD2	1:A:229:THR:HG23	1.65	0.95
1:A:71:THR:HG22	1:A:339:HIS:CE1	2.05	0.92
1:A:71:THR:HG22	1:A:339:HIS:HE1	1.37	0.90
1:A:338:ARG:O	1:B:71:THR:HG21	1.72	0.90
1:B:351:ARG:HH11	1:B:351:ARG:CG	1.84	0.88
1:B:222:GLY:CA	1:B:223:SER:HB2	2.05	0.87
1:A:278:THR:HG21	5:A:532:HOH:O	1.75	0.86
1:A:301:ALA:HB1	1:A:330:THR:CG2	2.05	0.85
1:B:49:GLN:HB2	1:B:52:THR:HG22	1.59	0.85
1:B:193:THR:HG23	5:B:542:HOH:O	1.77	0.84
1:B:226:ASP:OD2	1:B:229:THR:HG23	1.77	0.84
1:A:71:THR:HG21	5:B:491:HOH:O	1.77	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:GLN:HB2	1:A:52:THR:HG22	1.60	0.82
1:A:303:VAL:O	1:A:330:THR:HB	1.78	0.82
1:B:351:ARG:HG2	1:B:351:ARG:NH1	1.88	0.82
1:B:71:THR:HG22	1:B:339:HIS:CE1	2.15	0.82
1:B:339:HIS:HD2	5:B:553:HOH:O	1.64	0.80
1:A:330:THR:HG21	5:A:546:HOH:O	1.82	0.79
1:B:398:ILE:HD11	1:B:400:HIS:CE1	2.17	0.79
1:A:74:ASP:O	1:A:78:ARG:HG3	1.83	0.78
1:A:281:GLU:OE1	1:A:288:LYS:NZ	2.17	0.78
1:B:303:VAL:O	1:B:330:THR:HB	1.84	0.78
1:A:139:GLU:OE1	5:A:576:HOH:O	2.04	0.76
1:A:226:ASP:OD2	1:A:229:THR:CG2	2.33	0.75
1:B:330:THR:HG21	5:B:469:HOH:O	1.85	0.75
1:B:49:GLN:HB2	1:B:52:THR:CG2	2.17	0.74
1:B:13:ARG:HG3	1:B:59:PRO:HB2	1.70	0.73
1:B:372:ARG:O	1:B:376:THR:HG23	1.90	0.71
1:A:301:ALA:HB1	1:A:330:THR:HG22	1.72	0.71
1:A:74:ASP:OD2	1:A:78:ARG:HD2	1.91	0.70
1:B:301:ALA:HB1	1:B:330:THR:CG2	2.22	0.70
1:B:340:HIS:HE1	1:B:354:THR:O	1.74	0.70
1:B:49:GLN:H	1:B:52:THR:CG2	2.03	0.69
1:A:220:ARG:NH2	1:A:241:MET:O	2.22	0.69
1:B:278:THR:HG21	5:B:513:HOH:O	1.91	0.69
2:B:422:HEM:HBB2	2:B:422:HEM:HMB1	1.75	0.69
1:A:301:ALA:HB1	1:A:330:THR:HG23	1.76	0.68
1:B:49:GLN:CB	1:B:52:THR:HG22	2.23	0.68
1:B:394:ARG:CZ	5:B:501:HOH:O	2.43	0.67
1:A:288:LYS:HD2	5:A:598:HOH:O	1.95	0.66
1:A:113:TYR:HE2	1:A:241:MET:HE3	1.60	0.66
1:A:288:LYS:CD	5:A:598:HOH:O	2.44	0.66
1:B:126:ILE:HD12	1:B:373:LEU:HD12	1.79	0.65
1:B:281:GLU:OE1	5:B:591:HOH:O	2.13	0.65
1:B:222:GLY:CA	1:B:223:SER:CB	2.71	0.65
1:B:372:ARG:O	1:B:376:THR:CG2	2.45	0.65
1:B:275:HIS:HB3	1:B:278:THR:HG23	1.78	0.65
1:A:283:ARG:NH2	5:A:592:HOH:O	2.30	0.65
1:A:340:HIS:HE1	1:A:354:THR:O	1.80	0.64
1:A:280:ALA:O	1:A:284:ARG:HG2	1.99	0.63
1:B:74:ASP:O	1:B:78:ARG:HG3	1.98	0.63
1:A:110:HIS:HE1	2:A:422:HEM:O2D	1.82	0.63
2:B:422:HEM:HBB2	2:B:422:HEM:CMB	2.28	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:LYS:HG3	1:B:234:VAL:HG21	1.80	0.62
1:B:61:THR:HG23	5:B:534:HOH:O	1.99	0.62
1:B:293:VAL:HG21	1:B:376:THR:HB	1.81	0.62
1:B:394:ARG:NH1	1:B:394:ARG:HB2	2.15	0.62
1:B:49:GLN:H	1:B:52:THR:HG21	1.66	0.61
3:A:423:DIO:H21	5:A:463:HOH:O	2.01	0.60
1:B:71:THR:HG22	1:B:339:HIS:HE1	1.64	0.60
1:B:235:GLU:HB3	1:B:239:LYS:H	1.65	0.60
1:B:23:HIS:O	1:B:26:ARG:NH2	2.34	0.60
1:A:49:GLN:H	1:A:52:THR:CG2	2.16	0.59
1:B:122:ASN:ND2	1:B:125:GLU:H	2.01	0.59
1:A:351:ARG:O	1:A:351:ARG:HD3	2.02	0.58
1:B:134:ARG:NH2	1:B:380:GLN:OE1	2.34	0.58
5:A:656:HOH:O	1:B:338:ARG:HD3	2.02	0.58
1:B:301:ALA:HB1	1:B:330:THR:HG22	1.84	0.58
1:B:416:PRO:O	5:B:496:HOH:O	2.17	0.58
1:B:197:GLN:NE2	5:B:610:HOH:O	2.28	0.57
1:B:275:HIS:HB3	1:B:278:THR:CG2	2.35	0.56
1:A:122:ASN:ND2	1:A:125:GLU:H	2.04	0.56
1:A:275:HIS:HB3	1:A:278:THR:HG23	1.85	0.56
1:B:399:TYR:CD2	1:B:407:VAL:HG13	2.40	0.56
1:A:126:ILE:HD13	1:A:370:LEU:HA	1.87	0.56
1:A:399:TYR:CD2	1:A:407:VAL:HG13	2.41	0.56
1:B:318:THR:HG21	5:B:441:HOH:O	2.05	0.55
1:A:160:PHE:HB3	1:A:161:PRO:HD3	1.87	0.55
1:B:130:GLU:OE2	1:B:134:ARG:NH1	2.39	0.55
1:A:372:ARG:O	1:A:376:THR:CG2	2.54	0.55
1:B:57:TRP:CZ3	1:B:59:PRO:HA	2.41	0.55
5:A:550:HOH:O	1:B:71:THR:HB	2.07	0.54
1:A:38:GLN:HG3	5:A:602:HOH:O	2.06	0.54
1:B:340:HIS:CE1	1:B:354:THR:O	2.59	0.54
1:A:216:ILE:O	1:A:220:ARG:HG3	2.08	0.54
1:B:394:ARG:HH11	1:B:394:ARG:HB2	1.72	0.54
1:A:372:ARG:O	1:A:376:THR:HG22	2.07	0.54
1:B:163:ARG:HD3	1:B:173:VAL:HG21	1.90	0.53
1:A:49:GLN:H	1:A:52:THR:HG21	1.73	0.53
4:A:425:PO4:O3	1:B:78:ARG:NH2	2.40	0.53
1:B:238:GLY:O	1:B:239:LYS:HB2	2.08	0.53
1:A:193:THR:CG2	1:A:196:GLU:H	2.21	0.53
1:B:46:ARG:HD3	5:B:619:HOH:O	2.09	0.53
1:B:302:VAL:HG13	1:B:404:VAL:HG13	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:THR:HG21	5:A:516:HOH:O	2.10	0.52
1:B:49:GLN:N	1:B:52:THR:CG2	2.73	0.51
1:B:126:ILE:HD13	1:B:370:LEU:HA	1.93	0.51
1:B:228:ILE:O	1:B:232:LEU:HB2	2.11	0.50
1:A:49:GLN:HB2	1:A:52:THR:CG2	2.38	0.50
1:A:35:GLY:O	1:A:38:GLN:HG2	2.12	0.50
1:A:61:THR:CG2	5:A:481:HOH:O	2.60	0.49
1:B:208:PHE:O	1:B:212:VAL:HB	2.12	0.49
1:A:399:TYR:CE2	1:A:407:VAL:HG13	2.47	0.49
1:B:241:MET:CE	1:B:246:ALA:HA	2.43	0.49
1:A:174:GLU:CD	1:A:174:GLU:H	2.16	0.49
1:B:193:THR:HG22	1:B:195:GLU:N	2.27	0.49
1:A:208:PHE:O	1:A:212:VAL:HB	2.12	0.49
1:B:340:HIS:HD2	5:B:532:HOH:O	1.96	0.48
1:B:332:LEU:O	1:B:336:ASP:HB2	2.13	0.48
1:A:111:THR:O	1:A:115:LYS:HG2	2.14	0.48
1:B:71:THR:HG23	5:B:468:HOH:O	2.13	0.48
1:B:301:ALA:HB1	1:B:330:THR:HG23	1.95	0.48
1:A:338:ARG:O	1:B:71:THR:CG2	2.51	0.48
1:A:293:VAL:HG21	1:A:376:THR:HB	1.96	0.48
1:A:318:THR:HG21	5:A:471:HOH:O	2.14	0.48
1:A:162:VAL:HA	1:A:258:LEU:HD12	1.95	0.48
1:B:61:THR:CG2	5:B:534:HOH:O	2.57	0.48
1:A:61:THR:HG23	5:A:481:HOH:O	2.14	0.48
1:B:128:LYS:NZ	5:B:452:HOH:O	2.47	0.48
1:A:113:TYR:O	1:A:117:ILE:HG12	2.14	0.47
1:A:193:THR:HG22	1:A:196:GLU:H	1.80	0.47
1:B:241:MET:HE2	1:B:246:ALA:HB2	1.97	0.47
1:B:284:ARG:HG3	5:B:596:HOH:O	2.14	0.47
1:B:339:HIS:HE1	5:B:468:HOH:O	1.97	0.47
1:B:49:GLN:CB	1:B:52:THR:CG2	2.89	0.47
1:A:225:THR:O	1:A:230:ARG:NH2	2.45	0.47
1:B:48:GLN:HE22	1:B:336:ASP:HA	1.80	0.47
1:A:23:HIS:O	1:A:26:ARG:NH2	2.47	0.47
1:B:29:ASP:OD2	1:B:32:ASP:HB3	2.15	0.46
1:B:119:LYS:HG3	1:B:234:VAL:CG2	2.44	0.46
1:B:239:LYS:HG3	1:B:240:PRO:HD2	1.98	0.46
1:B:285:GLU:HB2	1:B:288:LYS:HB2	1.96	0.46
1:B:146:ASP:O	1:B:416:PRO:HB3	2.16	0.45
1:A:222:GLY:HA3	1:A:223:SER:HB2	1.98	0.45
1:A:351:ARG:HD2	1:B:317:GLY:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:MET:HE1	1:B:246:ALA:HA	1.99	0.45
1:A:340:HIS:CE1	1:A:354:THR:O	2.66	0.45
1:B:351:ARG:NH1	1:B:351:ARG:CG	2.55	0.45
1:B:219:ARG:HG2	1:B:229:THR:HG22	1.99	0.45
1:B:258:LEU:O	1:B:262:VAL:HG23	2.16	0.45
1:A:289:LEU:HD23	1:A:289:LEU:C	2.37	0.45
1:B:193:THR:HG22	1:B:195:GLU:H	1.82	0.44
1:B:52:THR:HB	4:B:424:PO4:O1	2.17	0.44
1:A:367:GLY:HA3	2:A:422:HEM:C3C	2.53	0.44
1:B:86:ARG:CD	5:B:587:HOH:O	2.65	0.44
1:A:38:GLN:H	1:A:38:GLN:HG2	1.66	0.44
1:A:228:ILE:O	1:A:232:LEU:HB2	2.17	0.44
1:B:100:MET:HB3	1:B:252:LEU:HB2	2.00	0.44
1:A:87:VAL:HG13	1:A:95:GLY:HA3	1.99	0.44
1:A:100:MET:O	1:A:104:LYS:HG2	2.18	0.43
1:A:113:TYR:CE2	1:A:241:MET:HE3	2.46	0.43
1:A:49:GLN:N	1:A:52:THR:CG2	2.82	0.43
1:B:16:PRO:HA	1:B:57:TRP:CH2	2.53	0.43
1:B:86:ARG:HD3	5:B:587:HOH:O	2.19	0.43
1:B:226:ASP:CG	1:B:229:THR:HG23	2.38	0.43
1:B:308:TYR:CZ	1:B:323:GLY:HA2	2.53	0.43
1:B:398:ILE:HD11	1:B:400:HIS:NE2	2.33	0.42
1:B:311:SER:HA	1:B:322:GLU:HB2	2.01	0.42
1:A:153:GLY:HA2	1:A:157:SER:OG	2.19	0.42
1:B:342:ASP:HB3	1:B:345:THR:HG23	2.02	0.42
2:B:422:HEM:CBB	2:B:422:HEM:HMB1	2.47	0.42
2:B:422:HEM:HHB	2:B:422:HEM:CBH	2.49	0.41
1:B:147:ARG:HG2	1:B:149:HIS:CE1	2.55	0.41
1:B:223:SER:HB3	1:B:224:GLY:CA	2.50	0.41
1:B:84:SER:OG	1:B:86:ARG:HB3	2.19	0.41
1:A:372:ARG:O	1:A:376:THR:HG23	2.19	0.41
1:B:241:MET:HE2	1:B:246:ALA:CA	2.50	0.41
1:B:284:ARG:HD2	5:B:596:HOH:O	2.20	0.41
1:B:49:GLN:N	1:B:52:THR:HG23	2.36	0.41
1:A:168:LEU:HD11	1:A:230:ARG:HH12	1.86	0.41
1:A:308:TYR:CZ	1:A:323:GLY:HA2	2.56	0.41
1:A:387:PRO:HG3	1:A:417:GLN:NE2	2.35	0.41
1:B:71:THR:HG22	1:B:339:HIS:NE2	2.33	0.41
1:B:69:ARG:HA	1:B:69:ARG:HD3	1.87	0.41
1:A:130:GLU:HA	1:A:373:LEU:HD11	2.02	0.41
1:B:236:ILE:HG13	1:B:241:MET:HG2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:288:LYS:HE3	1:B:288:LYS:HA	2.03	0.40
1:B:289:LEU:HD23	1:B:289:LEU:C	2.41	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	406/421 (96%)	387 (95%)	18 (4%)	1 (0%)	52	59
1	B	403/421 (96%)	384 (95%)	16 (4%)	3 (1%)	26	25
All	All	809/842 (96%)	771 (95%)	34 (4%)	4 (0%)	34	35

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	223	SER
1	A	223	SER
1	B	238	GLY
1	B	224	GLY

### 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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	346/356 (97%)	310 (90%)	36 (10%)	9	8
1	B	343/356 (96%)	303 (88%)	40 (12%)	7	5
All	All	689/712 (97%)	613 (89%)	76 (11%)	8	7

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	ARG
1	A	38	GLN
1	A	52	THR
1	A	55	LEU
1	A	61	THR
1	A	71	THR
1	A	86	ARG
1	A	89	TRP
1	A	111	THR
1	A	122	ASN
1	A	126	ILE
1	A	151	GLU
1	A	193	THR
1	A	195	GLU
1	A	205	ASN
1	A	212	VAL
1	A	223	SER
1	A	229	THR
1	A	232	LEU
1	A	258	LEU
1	A	277	GLU
1	A	278	THR
1	A	284	ARG
1	A	287	LEU
1	A	302	VAL
1	A	318	THR
1	A	330	THR
1	A	345	THR
1	A	351	ARG
1	A	373	LEU
1	A	376	THR
1	A	391	LEU

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Mol	Chain	Res	Type
1	A	393	ASP
1	A	398	ILE
1	A	407	VAL
1	A	408	GLU
1	B	26	ARG
1	B	49	GLN
1	B	52	THR
1	B	55	LEU
1	B	61	THR
1	B	71	THR
1	B	79	SER
1	B	86	ARG
1	B	89	TRP
1	B	111	THR
1	B	122	ASN
1	B	126	ILE
1	B	134	ARG
1	B	154	SER
1	B	195	GLU
1	B	201	LEU
1	B	205	ASN
1	B	223	SER
1	B	229	THR
1	B	232	LEU
1	B	245	ARG
1	B	255	LEU
1	B	258	LEU
1	B	277	GLU
1	B	278	THR
1	B	287	LEU
1	B	288	LYS
1	B	302	VAL
1	B	311	SER
1	B	318	THR
1	B	330	THR
1	B	345	THR
1	B	349	SER
1	B	351	ARG
1	B	373	LEU
1	B	376	THR
1	B	391	LEU
1	B	394	ARG

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Mol	Chain	Res	Type
1	B	398	ILE
1	B	407	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	A	49	GLN
1	A	110	HIS
1	A	122	ASN
1	A	197	GLN
1	A	290	GLN
1	A	339	HIS
1	A	340	HIS
1	A	360	GLN
1	A	417	GLN
1	B	48	GLN
1	B	122	ASN
1	B	149	HIS
1	B	197	GLN
1	B	339	HIS
1	B	340	HIS
1	B	360	GLN

### 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 ⓘ

9 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	422	1,5	30,50,50	2.56	6 (20%)	24,82,82	2.14	8 (33%)
3	DIO	A	423	-	6,6,6	0.55	0	6,6,6	1.16	1 (16%)
4	PO4	A	424	-	4,4,4	0.43	0	6,6,6	0.26	0
4	PO4	A	425	-	4,4,4	0.40	0	6,6,6	0.31	0
4	PO4	A	426	-	4,4,4	0.32	0	6,6,6	0.30	0
4	PO4	A	427	-	4,4,4	0.36	0	6,6,6	0.31	0
2	HEM	B	422	1,5	30,50,50	2.53	7 (23%)	24,82,82	2.58	10 (41%)
4	PO4	B	423	-	4,4,4	0.34	0	6,6,6	0.28	0
4	PO4	B	424	-	4,4,4	0.49	0	6,6,6	0.27	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
2	HEM	A	422	1,5	-	0/10/54/54	0/0/8/8
3	DIO	A	423	-	-	0/0/6/6	0/1/1/1
4	PO4	A	424	-	-	0/0/0/0	0/0/0/0
4	PO4	A	425	-	-	0/0/0/0	0/0/0/0
4	PO4	A	426	-	-	0/0/0/0	0/0/0/0
4	PO4	A	427	-	-	0/0/0/0	0/0/0/0
2	HEM	B	422	1,5	-	0/10/54/54	0/0/8/8
4	PO4	B	423	-	-	0/0/0/0	0/0/0/0
4	PO4	B	424	-	-	0/0/0/0	0/0/0/0

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	422	HEM	C3B-C4B	-10.49	1.42	1.51
2	A	422	HEM	C3B-C4B	-9.78	1.43	1.51
2	A	422	HEM	C3D-C4D	-5.86	1.44	1.51
2	B	422	HEM	C3D-C4D	-5.27	1.44	1.51
2	A	422	HEM	C2C-C1C	-4.27	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	422	HEM	C2C-C1C	-3.15	1.46	1.52
2	B	422	HEM	C2D-C1D	-2.30	1.44	1.51
2	A	422	HEM	C2D-C1D	-2.24	1.44	1.51
2	B	422	HEM	C2B-C1B	-2.23	1.44	1.51
2	A	422	HEM	C2B-C1B	-2.05	1.45	1.51
2	B	422	HEM	C3B-CAB	2.09	1.55	1.51
2	A	422	HEM	CAA-C2A	2.29	1.55	1.52
2	B	422	HEM	FE-NC	4.00	2.11	1.95

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	422	HEM	C3C-CAC-CBC	-4.56	117.46	124.46
2	A	422	HEM	C3C-CAC-CBC	-3.25	119.47	124.46
2	B	422	HEM	CMA-C3A-C4A	-3.18	123.10	128.36
2	B	422	HEM	CAA-C2A-C1A	-2.95	123.81	127.01
2	B	422	HEM	C3B-CAB-CBB	-2.20	121.08	124.46
2	B	422	HEM	CAA-CBA-CGA	-2.20	108.72	112.75
2	A	422	HEM	CMA-C3A-C4A	-2.07	124.93	128.36
2	B	422	HEM	CMD-C2D-C3D	2.06	123.44	114.35
3	A	423	DIO	C2'-O1'-C1'	2.60	118.65	109.89
2	A	422	HEM	C2D-C3D-C4D	2.60	105.91	101.50
2	A	422	HEM	CMD-C2D-C3D	2.74	126.46	114.35
2	A	422	HEM	CMC-C2C-C3C	3.29	124.74	116.53
2	B	422	HEM	CMB-C2B-C3B	3.46	125.18	116.53
2	A	422	HEM	CMB-C2B-C3B	3.84	126.11	116.53
2	A	422	HEM	CAD-C3D-C2D	3.89	124.40	113.22
2	B	422	HEM	CAD-C3D-C2D	4.10	125.00	113.22
2	A	422	HEM	CAD-C3D-C4D	4.88	129.67	112.47
2	B	422	HEM	CMC-C2C-C3C	4.99	129.00	116.53
2	B	422	HEM	CAD-C3D-C4D	5.00	130.09	112.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	422	HEM	2	0
3	A	423	DIO	1	0
4	A	425	PO4	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	422	HEM	4	0
4	B	424	PO4	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	408/421 (96%)	-0.54	2 (0%) 91 91	19, 30, 45, 56	0
1	B	405/421 (96%)	-0.31	7 (1%) 73 72	22, 35, 52, 60	0
All	All	813/842 (96%)	-0.42	9 (1%) 82 82	19, 32, 50, 60	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	238	GLY	3.2
1	B	239	LYS	3.1
1	A	238	GLY	2.6
1	B	390	ARG	2.4
1	B	237	ASP	2.4
1	B	387	PRO	2.2
1	B	415	GLU	2.2
1	A	221	GLY	2.2
1	B	223	SER	2.0

### 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(Å <sup>2</sup> )	Q<0.9
3	DIO	A	423	6/6	0.91	0.17	2.29	52,54,55,56	0
2	HEM	A	422	43/43	0.99	0.12	0.98	15,20,26,28	0
4	PO4	B	424	5/5	0.97	0.12	0.39	55,56,57,58	0
2	HEM	B	422	43/43	0.98	0.12	0.23	21,24,29,32	0
4	PO4	A	424	5/5	0.99	0.09	-0.90	32,33,34,38	0
4	PO4	A	425	5/5	0.97	0.09	-0.90	35,36,40,41	0
4	PO4	A	427	5/5	0.94	0.13	-	49,49,51,51	0
4	PO4	A	426	5/5	0.97	0.14	-	34,37,39,40	0
4	PO4	B	423	5/5	0.98	0.10	-	46,46,49,49	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.