



# Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 01:28 AM GMT

PDB ID : 1F4T  
Title : THERMOPHILIC P450: CYP119 FROM SULFOLOBUS SOLFACTARICUS  
WITH 4-PHENYLMIDAZOLE BOUND  
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T.L.  
Deposited on : 2000-06-09  
Resolution : 1.93 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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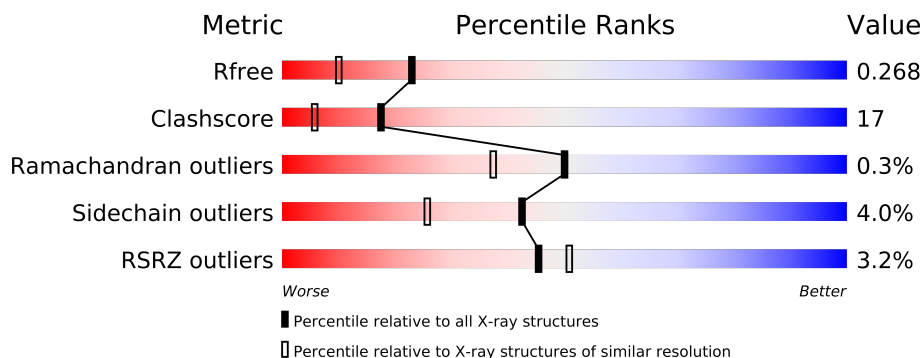
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.93 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	2024 (1.96-1.92)
Clashscore	79885	2281 (1.96-1.92)
Ramachandran outliers	78287	2255 (1.96-1.92)
Sidechain outliers	78261	2255 (1.96-1.92)
RSRZ outliers	66119	2024 (1.96-1.92)

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	368	
1	B	368	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6774 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.

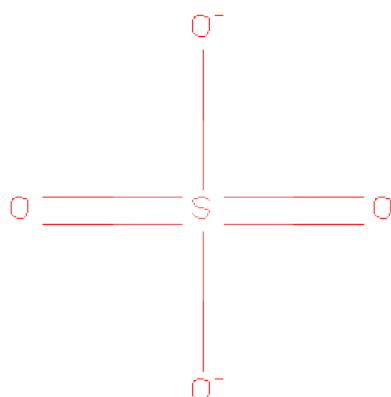
- Molecule 1 is a protein called CYTOCHROME P450 119.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	367	Total	C	N	O	S	0	0	0
			3018	1932	519	561	6			
1	B	367	Total	C	N	O	S	0	0	0
			3018	1932	519	561	6			

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

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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



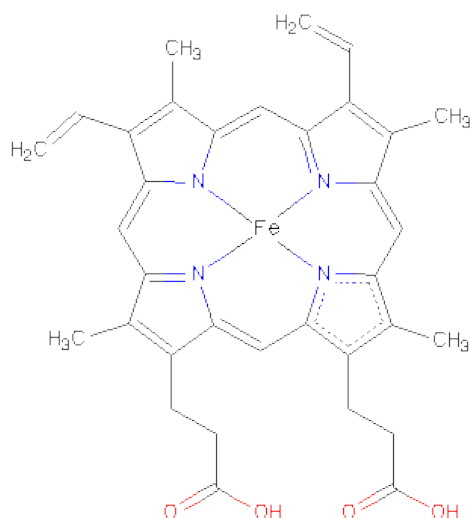
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		

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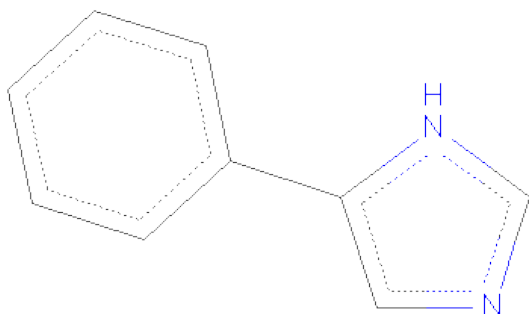
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



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

- Molecule 5 is 4-PHENYL-1H-IMIDAZOLE (three-letter code: PIM) (formula:  $C_9H_8N_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	N	0	0
			11	9	2		
5	B	1	Total	C	N	0	0
			11	9	2		

- Molecule 6 is water.

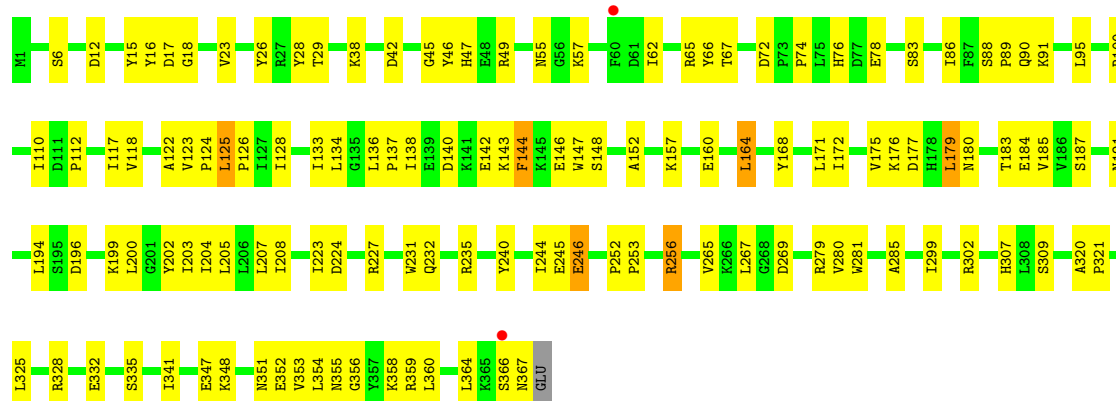
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	363	Total	O	0	0
			363	363		
6	B	256	Total	O	0	0
			256	256		

### 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.

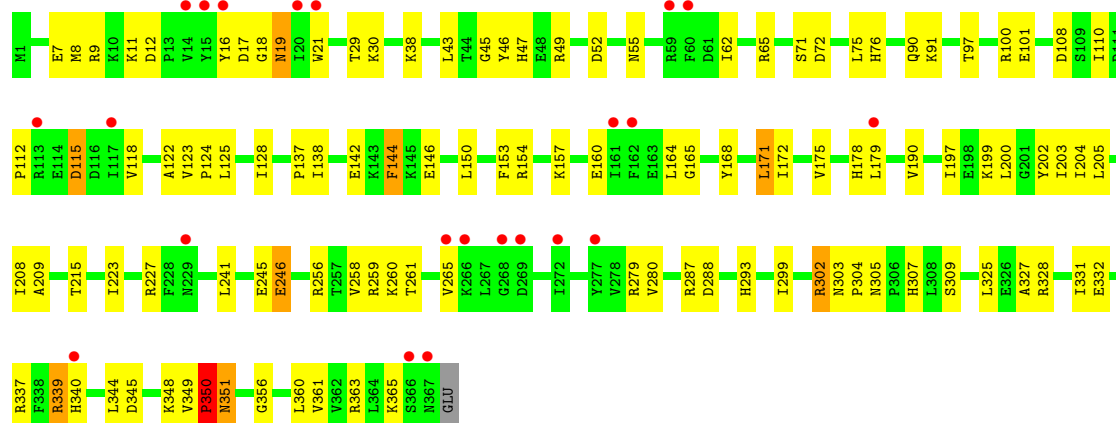
#### • Molecule 1: CYTOCHROME P450 119

Chain A: 



#### • Molecule 1: CYTOCHROME P450 119

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.96Å 114.60Å 185.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.40 – 1.93 44.39 – 1.92	Depositor EDS
% Data completeness (in resolution range)	93.5 (44.40-1.93) 92.8 (44.39-1.92)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.72 (at 1.92Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.225 , 0.274 0.222 , 0.268	Depositor DCC
$R_{free}$ test set	2913 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	30.6	Xtriage
Anisotropy	0.438	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 42.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 62351 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6774	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.28% 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, ZN, SO4, PIM

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	0.33	0/3082	0.60	0/4165
1	B	0.33	0/3082	0.56	0/4165
All	All	0.33	0/6164	0.58	0/8330

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	3018	0	3047	107	0
1	B	3018	0	3047	109	0
2	A	1	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	2	0
4	A	43	0	30	1	0
4	B	43	0	30	2	0
5	A	11	0	8	0	0
5	B	11	0	8	0	0
6	A	363	0	0	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	256	0	0	16	0
All	All	6774	0	6170	215	0

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 17.

All (215) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:6:SER:HB3	6:A:760:HOH:O	1.65	0.97
1:A:47:HIS:HE1	1:A:72:ASP:H	1.18	0.91
1:B:256:ARG:HH11	1:B:279:ARG:HD2	1.39	0.86
1:A:223:ILE:O	1:A:227:ARG:HG3	1.81	0.80
1:A:62:ILE:HD12	1:A:164:LEU:HD13	1.63	0.80
1:A:47:HIS:CE1	1:A:72:ASP:H	2.00	0.79
1:B:71:SER:HB2	1:B:75:LEU:HD12	1.65	0.79
1:A:38:LYS:HD3	1:A:265:VAL:HG12	1.65	0.79
1:A:200:LEU:O	1:A:204:ILE:HG12	1.83	0.79
1:A:142:GLU:O	1:A:146:GLU:HG3	1.85	0.77
1:B:287:ARG:NH1	6:B:660:HOH:O	2.18	0.77
1:A:348:LYS:NZ	1:A:355:ASN:HD22	1.82	0.77
1:A:49:ARG:HD2	1:A:66:TYR:OH	1.86	0.76
1:B:344:LEU:HB2	1:B:361:VAL:HG23	1.67	0.75
1:B:43:LEU:HD21	1:B:260:LYS:HB2	1.69	0.74
1:B:7:GLU:HG3	1:B:11:LYS:NZ	2.03	0.74
1:A:246:GLU:HG3	1:A:299:ILE:O	1.89	0.72
1:A:196:ASP:O	1:A:200:LEU:HD13	1.89	0.71
1:B:246:GLU:HG3	1:B:299:ILE:O	1.89	0.71
1:B:47:HIS:CE1	1:B:72:ASP:H	2.09	0.70
1:B:47:HIS:HE1	1:B:72:ASP:H	1.40	0.70
1:A:235:ARG:HH11	1:A:335:SER:HB2	1.55	0.70
1:A:207:LEU:HD23	1:A:207:LEU:O	1.91	0.70
1:A:29:THR:HG23	1:A:280:VAL:CG1	2.21	0.70
1:B:171:LEU:HD21	1:B:208:ILE:HD11	1.73	0.69
1:B:204:ILE:HG23	1:B:208:ILE:HD12	1.75	0.68
1:A:62:ILE:CD1	1:A:164:LEU:HD13	2.24	0.68
1:A:267:LEU:HD21	6:A:689:HOH:O	1.92	0.68
1:A:223:ILE:HG22	1:A:227:ARG:HD2	1.76	0.67
1:A:348:LYS:HZ1	1:A:355:ASN:HD22	1.43	0.67
1:B:100:ARG:NH1	6:B:548:HOH:O	2.27	0.67
1:B:90:GLN:HB2	6:B:575:HOH:O	1.94	0.66
1:A:224:ASP:HA	1:A:227:ARG:HD3	1.77	0.66
1:A:74:PRO:O	1:A:78:GLU:HG3	1.95	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:345:ASP:O	1:B:361:VAL:HG22	1.96	0.66
1:B:256:ARG:NH1	1:B:279:ARG:HD2	2.10	0.66
1:A:207:LEU:HD22	1:A:208:ILE:HG13	1.78	0.65
1:A:144:PHE:CZ	1:A:207:LEU:HD21	2.31	0.65
1:A:140:ASP:OD2	1:A:143:LYS:HE2	1.97	0.64
1:B:52:ASP:HA	1:B:55:ASN:ND2	2.13	0.64
1:B:29:THR:HG23	1:B:280:VAL:CG1	2.28	0.64
1:A:348:LYS:NZ	1:A:355:ASN:ND2	2.46	0.63
1:A:45:GLY:O	1:A:49:ARG:HG2	1.99	0.62
1:A:23:VAL:HG11	6:A:689:HOH:O	2.00	0.62
1:B:302:ARG:HG2	1:B:305:ASN:ND2	2.14	0.61
1:A:133:ILE:O	1:A:183:THR:HG21	2.00	0.61
1:B:307:HIS:HD2	1:B:309:SER:H	1.49	0.61
1:B:29:THR:HG23	1:B:280:VAL:HG13	1.83	0.61
1:B:339:ARG:NE	1:B:340:HIS:H	1.99	0.60
1:B:223:ILE:HG22	1:B:227:ARG:CD	2.31	0.60
1:A:76:HIS:HD2	6:A:693:HOH:O	1.85	0.59
1:A:352:GLU:HB3	6:A:772:HOH:O	2.01	0.59
1:B:123:VAL:HB	1:B:124:PRO:HD3	1.83	0.59
1:B:38:LYS:HD3	1:B:265:VAL:HG11	1.84	0.59
1:A:194:LEU:O	1:A:199:LYS:HE3	2.03	0.59
1:B:245:GLU:OE1	1:B:307:HIS:HE1	1.87	0.58
1:B:142:GLU:O	1:B:146:GLU:HG3	2.03	0.58
1:B:138:ILE:HG23	1:B:144:PHE:HD1	1.68	0.58
1:B:303:ASN:ND2	1:B:304:PRO:HA	2.19	0.57
1:A:240:TYR:O	1:A:244:ILE:HG12	2.03	0.57
1:B:138:ILE:HA	1:B:144:PHE:CE1	2.40	0.57
1:B:7:GLU:HG3	1:B:11:LYS:HZ2	1.68	0.57
1:B:241:LEU:HD13	1:B:328:ARG:NH1	2.20	0.57
1:B:339:ARG:HE	1:B:339:ARG:HA	1.69	0.57
1:B:76:HIS:HE1	4:B:410:HEM:O2D	1.88	0.57
1:B:49:ARG:CZ	6:B:638:HOH:O	2.53	0.57
1:B:197:ILE:HG12	6:B:438:HOH:O	2.05	0.56
1:B:223:ILE:HD11	1:B:360:LEU:HG	1.86	0.56
1:B:246:GLU:CG	1:B:299:ILE:O	2.53	0.56
1:B:52:ASP:HA	1:B:55:ASN:HD21	1.71	0.56
1:A:176:LYS:HA	1:A:179:LEU:CD2	2.36	0.56
1:A:148:SER:HA	1:A:208:ILE:HG23	1.87	0.56
1:A:256:ARG:HB3	1:A:281:TRP:HA	1.88	0.56
1:B:350:PRO:O	1:B:351:ASN:O	2.25	0.55
1:B:43:LEU:CD2	1:B:260:LYS:HB2	2.35	0.55
1:A:245:GLU:OE1	1:A:307:HIS:HE1	1.89	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:150:LEU:HD13	3:B:369:SO4:O4	2.07	0.55
1:B:49:ARG:NH1	1:B:65:ARG:HH12	2.05	0.55
1:A:348:LYS:HZ1	1:A:355:ASN:ND2	2.04	0.54
1:B:9:ARG:HD2	6:B:460:HOH:O	2.06	0.54
1:A:12:ASP:HB3	1:A:15:TYR:HB2	1.90	0.54
1:A:351:ASN:OD1	1:A:353:VAL:HG12	2.08	0.54
1:B:122:ALA:HB1	1:B:215:THR:HG23	1.89	0.54
1:B:349:VAL:HG13	1:B:350:PRO:HD2	1.90	0.54
1:A:90:GLN:CD	1:A:90:GLN:H	2.12	0.54
1:A:95:LEU:HD11	1:A:133:ILE:HG12	1.90	0.53
1:A:347:GLU:OE1	1:A:359:ARG:NH1	2.40	0.53
1:B:157:LYS:HD3	1:B:160:GLU:OE2	2.08	0.53
1:B:345:ASP:H	1:B:361:VAL:CG2	2.22	0.53
1:A:67:THR:HB	1:A:205:LEU:HD22	1.91	0.53
1:A:144:PHE:HZ	1:A:207:LEU:HD21	1.73	0.53
1:B:205:LEU:HD21	4:B:410:HEM:HMD3	1.91	0.53
1:A:172:ILE:HG23	1:A:200:LEU:HD23	1.91	0.52
1:A:148:SER:HA	1:A:208:ILE:CG2	2.40	0.52
1:B:241:LEU:HD13	1:B:328:ARG:HH11	1.74	0.52
1:A:28:TYR:HB3	6:A:689:HOH:O	2.09	0.52
1:B:223:ILE:HG22	1:B:227:ARG:HD3	1.90	0.52
1:A:123:VAL:HB	1:A:124:PRO:HD3	1.91	0.52
1:B:128:ILE:HA	1:B:138:ILE:HD11	1.93	0.51
1:B:223:ILE:HG22	1:B:227:ARG:HD2	1.91	0.51
1:A:140:ASP:CG	1:A:143:LYS:HG3	2.31	0.51
1:A:246:GLU:CG	1:A:299:ILE:O	2.59	0.51
1:A:76:HIS:HE1	4:A:410:HEM:O2D	1.94	0.51
1:B:110:ILE:O	1:B:112:PRO:HD3	2.11	0.51
1:A:26:TYR:HA	1:A:285:ALA:HB1	1.94	0.50
1:A:38:LYS:HB3	1:A:265:VAL:HG11	1.94	0.50
1:A:118:VAL:HA	1:A:122:ALA:HB3	1.94	0.50
1:B:363:ARG:NH2	6:B:667:HOH:O	2.43	0.50
1:B:38:LYS:HD3	1:B:265:VAL:CG1	2.42	0.50
1:B:327:ALA:O	1:B:331:ILE:HG12	2.12	0.50
1:A:341:ILE:HA	1:A:364:LEU:HD23	1.93	0.49
1:B:16:TYR:HB2	1:B:21:TRP:CZ3	2.47	0.49
1:B:150:LEU:HD11	1:B:154:ARG:HE	1.76	0.49
1:B:30:LYS:NZ	6:B:648:HOH:O	2.41	0.49
1:A:117:ILE:HD11	1:A:360:LEU:HD22	1.93	0.49
1:A:100:ARG:NH1	6:A:697:HOH:O	2.45	0.49
1:A:152:ALA:HB1	1:A:354:LEU:HD11	1.93	0.49
1:B:49:ARG:NH1	1:B:65:ARG:NH1	2.61	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:256:ARG:NH1	6:B:661:HOH:O	2.45	0.48
1:A:235:ARG:HG2	1:A:240:TYR:OH	2.13	0.48
1:B:223:ILE:CG2	1:B:227:ARG:HD2	2.43	0.48
1:B:223:ILE:HG12	1:B:360:LEU:HD11	1.93	0.48
1:A:125:LEU:HB3	1:A:126:PRO:HD3	1.95	0.48
1:A:49:ARG:HA	6:A:437:HOH:O	2.13	0.48
1:A:136:LEU:CD1	1:A:207:LEU:HD12	2.44	0.48
1:A:199:LYS:O	1:A:203:ILE:HG12	2.13	0.48
1:A:89:PRO:HD2	1:A:90:GLN:HE22	1.79	0.48
1:B:303:ASN:HD22	1:B:304:PRO:HA	1.78	0.48
1:A:42:ASP:OD1	1:A:47:HIS:HB2	2.14	0.48
1:B:165:GLY:HA3	3:B:369:SO4:O1	2.13	0.48
1:B:118:VAL:HA	1:B:122:ALA:HB3	1.95	0.48
1:B:16:TYR:HB2	1:B:21:TRP:CE3	2.49	0.48
1:A:136:LEU:HD13	1:A:207:LEU:HD12	1.95	0.48
1:A:83:SER:O	1:A:86:ILE:HG22	2.14	0.48
1:A:62:ILE:HB	1:A:65:ARG:HG3	1.96	0.47
1:A:88:SER:OG	1:A:91:LYS:HG3	2.14	0.47
1:B:17:ASP:OD1	1:B:19:ASN:HB3	2.13	0.47
1:B:38:LYS:O	1:B:261:THR:HA	2.14	0.47
1:B:178:HIS:HB3	6:B:577:HOH:O	2.14	0.47
1:A:175:VAL:O	1:A:179:LEU:HD13	2.15	0.47
1:B:16:TYR:CZ	1:B:18:GLY:HA2	2.50	0.47
1:B:246:GLU:HA	1:B:246:GLU:OE1	2.15	0.47
1:A:366:SER:O	1:A:367:ASN:HB2	2.15	0.47
1:A:86:ILE:HG13	1:A:185:VAL:HG21	1.96	0.47
1:B:45:GLY:HA2	6:B:419:HOH:O	2.15	0.47
1:A:307:HIS:HD2	1:A:309:SER:H	1.61	0.47
1:A:110:ILE:O	1:A:112:PRO:HD3	2.15	0.47
1:A:90:GLN:NE2	1:A:90:GLN:H	2.12	0.46
1:A:328:ARG:HD3	1:A:332:GLU:OE2	2.15	0.46
1:A:175:VAL:O	1:A:179:LEU:HD22	2.16	0.46
1:B:256:ARG:HH11	1:B:279:ARG:CD	2.20	0.46
1:A:320:ALA:HB3	1:A:321:PRO:HD3	1.98	0.46
1:A:147:TRP:HB3	1:A:208:ILE:HD13	1.97	0.46
1:B:227:ARG:HG2	6:B:518:HOH:O	2.16	0.46
1:A:328:ARG:O	1:A:332:GLU:HB2	2.15	0.46
1:B:138:ILE:HG12	1:B:144:PHE:CE1	2.51	0.45
1:A:55:ASN:OD1	1:A:57:LYS:HG3	2.17	0.45
1:B:179:LEU:HG	1:B:190:VAL:CG2	2.47	0.45
1:B:150:LEU:O	1:B:153:PHE:HB3	2.16	0.45
1:B:258:VAL:HG12	1:B:259:ARG:N	2.31	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:90:GLN:HG2	1:B:91:LYS:N	2.32	0.45
1:A:177:ASP:HB3	1:B:137:PRO:HG3	1.98	0.45
1:A:134:LEU:O	1:A:183:THR:HG22	2.17	0.45
1:B:171:LEU:HD11	1:B:208:ILE:CD1	2.47	0.45
1:A:207:LEU:HD22	1:A:208:ILE:CG1	2.47	0.44
1:B:328:ARG:O	1:B:332:GLU:HG3	2.17	0.44
1:B:199:LYS:O	1:B:203:ILE:HG12	2.17	0.44
1:A:348:LYS:HD2	1:A:356:GLY:O	2.18	0.44
1:B:293:HIS:HD2	6:B:626:HOH:O	2.00	0.44
1:A:347:GLU:OE2	1:A:358:LYS:HD3	2.18	0.44
1:A:136:LEU:HA	1:A:137:PRO:HD3	1.72	0.44
1:B:348:LYS:HE3	1:B:356:GLY:O	2.18	0.44
1:B:179:LEU:HG	1:B:190:VAL:HG21	1.98	0.44
1:A:176:LYS:HA	1:A:179:LEU:HD22	2.00	0.43
1:A:15:TYR:CE1	1:A:17:ASP:HB3	2.53	0.43
1:A:175:VAL:HG21	1:A:204:ILE:CD1	2.47	0.43
1:B:49:ARG:NE	6:B:638:HOH:O	2.51	0.43
1:B:287:ARG:CZ	6:B:660:HOH:O	2.63	0.43
1:A:183:THR:OG1	1:A:184:GLU:N	2.51	0.43
1:B:340:HIS:HB2	1:B:365:LYS:HG3	2.00	0.43
1:B:138:ILE:HA	1:B:144:PHE:HE1	1.82	0.43
1:B:62:ILE:CD1	1:B:164:LEU:HD13	2.49	0.43
1:A:16:TYR:CE2	1:A:18:GLY:HA2	2.54	0.43
1:B:62:ILE:HB	1:B:65:ARG:HG3	2.01	0.43
1:B:227:ARG:NH1	6:B:656:HOH:O	2.49	0.43
1:A:231:TRP:N	6:A:755:HOH:O	2.52	0.43
1:B:108:ASP:OD2	1:B:337:ARG:NH1	2.52	0.43
1:B:205:LEU:O	1:B:209:ALA:HB3	2.19	0.42
1:A:207:LEU:HD23	1:A:207:LEU:C	2.39	0.42
1:A:29:THR:HG23	1:A:280:VAL:HG12	1.98	0.42
1:B:246:GLU:HG3	1:B:299:ILE:C	2.40	0.42
1:B:62:ILE:HD13	1:B:164:LEU:HD13	2.01	0.42
1:A:232:GLN:NE2	6:A:564:HOH:O	2.41	0.42
1:B:97:THR:O	1:B:101:GLU:HG3	2.20	0.42
1:A:176:LYS:HE3	1:A:200:LEU:HD21	2.02	0.42
1:B:345:ASP:H	1:B:361:VAL:HG23	1.83	0.42
1:A:180:ASN:ND2	6:A:659:HOH:O	2.53	0.42
1:B:172:ILE:HG23	1:B:200:LEU:HD21	2.01	0.42
1:A:187:SER:O	1:A:191:ASN:ND2	2.53	0.41
1:B:9:ARG:HD3	1:B:288:ASP:HA	2.02	0.41
1:B:8:MET:O	1:B:12:ASP:C	2.58	0.41
1:A:175:VAL:CG1	1:A:179:LEU:HD11	2.51	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:348:LYS:HE3	1:A:348:LYS:HB3	1.85	0.41
1:B:115:ASP:O	1:B:361:VAL:HA	2.21	0.41
1:A:246:GLU:HA	1:A:246:GLU:OE1	2.21	0.41
1:B:223:ILE:HD11	1:B:360:LEU:CG	2.51	0.41
1:A:128:ILE:HA	1:A:138:ILE:HD11	2.03	0.41
1:B:7:GLU:HG2	1:B:11:LYS:HD3	2.03	0.41
1:B:171:LEU:O	1:B:175:VAL:HG23	2.20	0.41
1:B:349:VAL:CG1	1:B:350:PRO:HD2	2.51	0.41
1:B:179:LEU:HD11	1:B:203:ILE:HG13	2.03	0.41
1:A:157:LYS:HD3	1:A:160:GLU:OE2	2.21	0.40
1:A:246:GLU:HG3	1:A:299:ILE:C	2.42	0.40
1:A:38:LYS:HD3	1:A:265:VAL:CG1	2.44	0.40
1:A:252:PRO:HA	1:A:253:PRO:HD3	1.85	0.40

There are no symmetry-related clashes.

## 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	365/368 (99%)	351 (96%)	14 (4%)	0	100	100
1	B	365/368 (99%)	344 (94%)	19 (5%)	2 (0%)	38	22
All	All	730/736 (99%)	695 (95%)	33 (4%)	2 (0%)	50	37

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	351	ASN
1	B	350	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	337/338 (100%)	323 (96%)	14 (4%)	40	23
1	B	337/338 (100%)	324 (96%)	13 (4%)	43	26
All	All	674/676 (100%)	647 (96%)	27 (4%)	42	26

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	TYR
1	A	125	LEU
1	A	144	PHE
1	A	164	LEU
1	A	168	TYR
1	A	171	LEU
1	A	179	LEU
1	A	202	TYR
1	A	246	GLU
1	A	256	ARG
1	A	269	ASP
1	A	279	ARG
1	A	302	ARG
1	A	325	LEU
1	B	19	ASN
1	B	46	TYR
1	B	115	ASP
1	B	125	LEU
1	B	144	PHE
1	B	168	TYR
1	B	171	LEU
1	B	202	TYR
1	B	246	GLU
1	B	302	ARG
1	B	325	LEU
1	B	339	ARG
1	B	350	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	ASN

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Mol	Chain	Res	Type
1	A	34	ASN
1	A	47	HIS
1	A	76	HIS
1	A	90	GLN
1	A	180	ASN
1	A	191	ASN
1	A	307	HIS
1	A	355	ASN
1	B	19	ASN
1	B	34	ASN
1	B	47	HIS
1	B	76	HIS
1	B	229	ASN
1	B	232	GLN
1	B	303	ASN
1	B	307	HIS
1	B	355	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 ⓘ

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	SO4	A	370	-	4,4,4	1.00	0	6,6,6	0.34	0
4	HEM	A	410	1,5	49,50,50	1.69	11 (22%)	46,82,82	1.21	4 (8%)
5	PIM	A	411	4	12,12,12	2.66	6 (50%)	15,15,15	1.56	2 (13%)
3	SO4	B	369	-	4,4,4	1.06	0	6,6,6	0.37	0
4	HEM	B	410	1,5	49,50,50	2.33	13 (26%)	46,82,82	1.31	6 (13%)
5	PIM	B	411	4	12,12,12	2.60	5 (41%)	15,15,15	1.56	2 (13%)

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
3	SO4	A	370	-	-	0/0/0/0	0/0/0/0
4	HEM	A	410	1,5	-	0/14/114/114	0/0/8/8
5	PIM	A	411	4	-	0/4/4/4	0/2/2/2
3	SO4	B	369	-	-	0/0/0/0	0/0/0/0
4	HEM	B	410	1,5	-	0/14/114/114	0/0/8/8
5	PIM	B	411	4	-	0/4/4/4	0/2/2/2

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	410	HEM	C2B-C1B	-8.23	1.42	1.44
4	B	410	HEM	C2D-C1D	-6.00	1.43	1.44
5	A	411	PIM	C2-N3	-5.74	1.24	1.34
5	B	411	PIM	C2-N3	-5.23	1.25	1.34
4	A	410	HEM	C3D-C2D	-4.99	1.35	1.43
4	B	410	HEM	C3D-C2D	-4.93	1.35	1.43
4	B	410	HEM	C3C-C2C	-4.86	1.35	1.43
4	B	410	HEM	C4A-C3A	4.38	1.45	1.40
4	B	410	HEM	C3B-C2B	-4.10	1.36	1.43
4	A	410	HEM	C3B-C2B	-4.06	1.36	1.43
5	B	411	PIM	C2-N1	3.88	1.40	1.34
4	B	410	HEM	CHB-C1B	3.80	1.41	1.35
5	A	411	PIM	C2-N1	3.69	1.40	1.34
5	A	411	PIM	C6-C5	3.34	1.52	1.47
5	B	411	PIM	C6-C5	3.33	1.52	1.47
4	A	410	HEM	C4A-C3A	3.21	1.44	1.40
4	A	410	HEM	C3C-C2C	-3.19	1.38	1.43
4	A	410	HEM	CHA-C4D	3.11	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	410	HEM	CHB-C1B	3.05	1.40	1.35
4	A	410	HEM	CBB-CAB	3.02	1.46	1.28
5	B	411	PIM	C8-C7	2.84	1.45	1.39
4	B	410	HEM	C3D-C4D	-2.83	1.43	1.44
5	A	411	PIM	C8-C7	2.78	1.45	1.39
4	B	410	HEM	CHA-C4D	2.74	1.39	1.35
4	B	410	HEM	C1A-NA	2.58	1.41	1.36
4	A	410	HEM	CBC-CAC	2.50	1.43	1.28
4	B	410	HEM	CBB-CAB	2.45	1.43	1.28
5	B	411	PIM	C7-C6	2.37	1.44	1.39
4	A	410	HEM	C3D-C4D	2.27	1.45	1.44
5	A	411	PIM	C7-C6	2.25	1.44	1.39
4	B	410	HEM	C4A-NA	2.19	1.40	1.36
4	B	410	HEM	CBC-CAC	2.16	1.41	1.28
4	A	410	HEM	CMC-C2C	2.14	1.54	1.47
5	A	411	PIM	C10-C11	2.10	1.43	1.39
4	A	410	HEM	CMD-C2D	2.08	1.53	1.47

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	410	HEM	C3B-C4B-NB	-3.67	111.38	114.00
5	B	411	PIM	C2-N1-C5	-3.64	106.37	108.58
4	A	410	HEM	C3B-C4B-NB	-3.46	111.52	114.00
5	A	411	PIM	C2-N1-C5	-3.39	106.52	108.58
5	A	411	PIM	C4-N3-C2	3.06	110.43	105.76
4	B	410	HEM	C1A-CHA-C4D	-2.98	123.55	127.47
5	B	411	PIM	C4-N3-C2	2.97	110.29	105.76
4	B	410	HEM	C4A-CHB-C1B	-2.89	123.67	127.47
4	A	410	HEM	C1A-CHA-C4D	-2.65	123.98	127.47
4	B	410	HEM	CAD-C3D-C4D	2.64	129.27	124.53
4	A	410	HEM	CAD-C3D-C4D	2.48	128.99	124.53
4	A	410	HEM	C3A-C4A-NA	2.36	111.20	109.41
4	B	410	HEM	C4A-NA-C1A	-2.30	103.73	106.76
4	B	410	HEM	CBD-CAD-C3D	-2.22	109.53	114.37

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	367/368 (99%)	0.19	2 (0%) 88 93	24, 36, 51, 64	0
1	B	367/368 (99%)	0.36	22 (5%) 21 25	21, 39, 65, 75	0
All	All	734/736 (99%)	0.27	24 (3%) 45 49	21, 37, 59, 75	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	162	PHE	4.6
1	B	268	GLY	3.8
1	B	15	TYR	3.4
1	B	272	ILE	3.3
1	B	161	ILE	3.2
1	B	16	TYR	3.0
1	B	266	LYS	2.9
1	B	367	ASN	2.9
1	B	229	ASN	2.8
1	B	366	SER	2.8
1	A	366	SER	2.7
1	B	20	ILE	2.7
1	B	265	VAL	2.6
1	B	269	ASP	2.5
1	B	60	PHE	2.4
1	B	277	TYR	2.4
1	B	59	ARG	2.4
1	B	179	LEU	2.4
1	B	14	VAL	2.4
1	B	117	ILE	2.3
1	B	113	ARG	2.2
1	B	21	TRP	2.2
1	A	60	PHE	2.1
1	B	340	HIS	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(Å <sup>2</sup> )	Q<0.9
4	HEM	B	410	43/43	0.11	0.50	21,23,28,28	0
3	SO4	B	369	5/5	0.18	0.38	69,69,70,70	0
3	SO4	A	370	5/5	0.14	0.26	52,52,53,53	0
4	HEM	A	410	43/43	0.12	0.12	23,25,29,32	0
5	PIM	B	411	11/11	0.12	0.07	28,30,33,34	0
5	PIM	A	411	11/11	0.09	-0.75	29,29,30,31	0
2	ZN	A	369	1/1	0.07	-2.91	37,37,37,37	0

## 6.5 Other polymers

There are no such residues in this entry.