



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 12:00 PM GMT

PDB ID : 2J1M  
Title : P450 BM3 HEME DOMAIN IN COMPLEX WITH DMSO  
Authors : Kuper, J.; Tuck-Seng, W.; Roccatano, D.; Wilmanns, M.; Schwaneberg, U.  
Deposited on : 2006-08-14  
Resolution : 1.70 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>

---

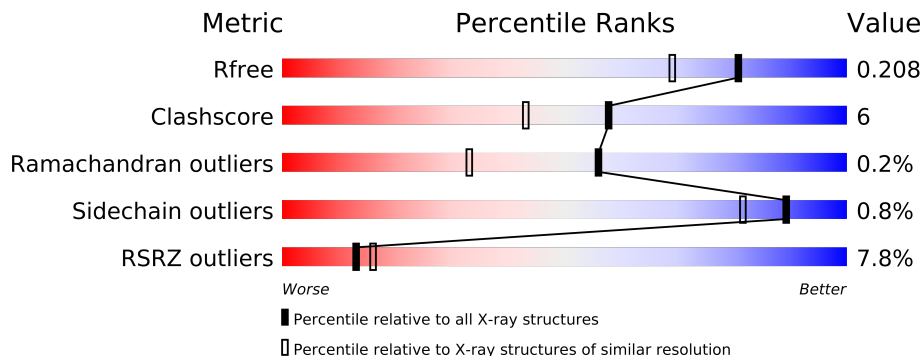
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.70 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	2456 (1.70-1.70)
Clashscore	79885	2929 (1.70-1.70)
Ramachandran outliers	78287	2878 (1.70-1.70)
Sidechain outliers	78261	2878 (1.70-1.70)
RSRZ outliers	66119	2456 (1.70-1.70)

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	455	
1	B	455	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	ZN	A	1459	-	X
3	ZN	B	1458	-	X
4	DMS	A	1463	-	X

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 8441 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 102.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	454	Total	C	N	O	S	0	4	0
			3682	2354	622	688	18			
1	B	454	Total	C	N	O	S	0	4	0
			3695	2360	627	690	18			

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

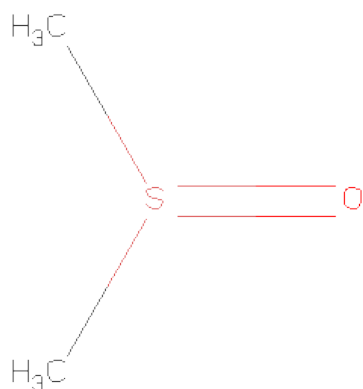


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Zn	0	0
			2	2		
3	A	5	Total	Zn	0	0
			5	5		

- Molecule 4 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C<sub>2</sub>H<sub>6</sub>OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	B	1	Total	C	O	S	0	0
			4	2	1	1		
4	B	1	Total	C	O	S	0	0
			4	2	1	1		

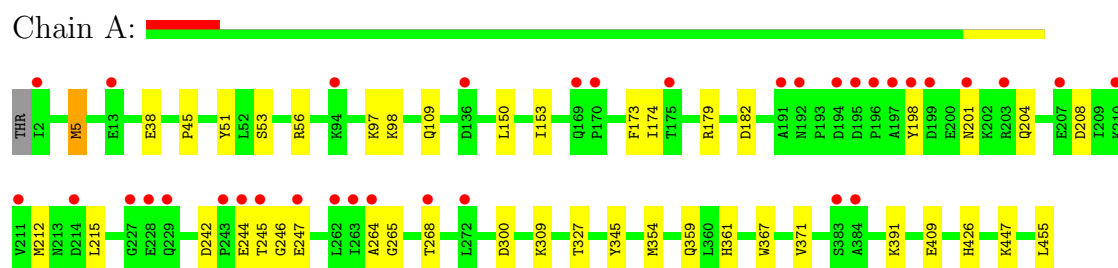
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	505	Total	O	0	0
			505	505		
5	B	450	Total	O	0	0
			450	450		

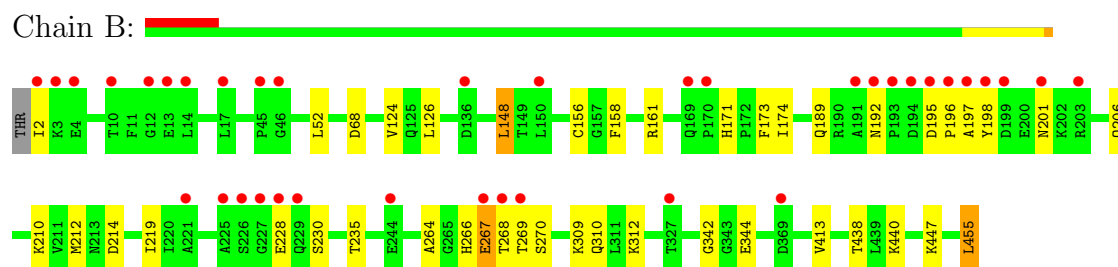
### 3 Residue-property plots

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 102



#### • Molecule 1: CYTOCHROME P450 102



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.77Å 86.85Å 159.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.04 – 1.70 33.62 – 1.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (36.04-1.70) 99.9 (33.62-1.70)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.11 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.169 , 0.199 0.181 , 0.208	Depositor DCC
$R_{free}$ test set	6339 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	20.4	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 52.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 125040 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8441	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% 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, DMS

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	0.80	0/3779	0.75	1/5107 (0.0%)
1	B	0.74	1/3784 (0.0%)	0.73	4/5114 (0.1%)
All	All	0.77	1/7563 (0.0%)	0.74	5/10221 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	156	CYS	CB-SG	-6.71	1.70	1.82

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	300	ASP	CB-CG-OD1	6.29	123.96	118.30
1	B	68	ASP	CB-CG-OD1	6.28	123.95	118.30
1	B	161	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	B	455	LEU	CA-CB-CG	5.84	128.73	115.30
1	B	148	LEU	CA-CB-CG	5.65	128.29	115.30

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	3682	0	3662	45	0
1	B	3695	0	3663	46	0
2	A	43	0	30	0	0
2	B	43	0	30	5	0
3	A	5	0	0	0	0
3	B	2	0	0	0	0
4	A	8	0	12	12	0
4	B	8	0	12	9	0
5	A	505	0	0	6	0
5	B	450	0	0	8	0
All	All	8441	0	7409	94	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 6.

All (94) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:268[A]:THR:HG21	4:A:1462:DMS:C1	1.65	1.25
1:A:268[A]:THR:CG2	4:A:1462:DMS:H12	1.76	1.15
1:A:268[A]:THR:HG21	4:A:1462:DMS:H12	1.22	1.13
1:A:268[A]:THR:HG21	4:A:1462:DMS:H11	1.51	0.89
1:B:266[B]:HIS:O	1:B:268[B]:THR:N	2.05	0.89
1:A:268[A]:THR:CG2	4:A:1462:DMS:C1	2.39	0.88
1:A:179:ARG:HD2	1:A:208:ASP:OD2	1.74	0.86
1:A:361:HIS:HE1	1:A:391:LYS:H	1.23	0.84
1:A:268[B]:THR:OG1	4:A:1462:DMS:H12	1.85	0.77
1:A:198:TYR:HA	1:A:201:ASN:HD22	1.50	0.75
1:B:206:GLN:O	1:B:210:LYS:HD3	1.88	0.74
1:B:264:ALA:HA	4:B:1459:DMS:H12	1.70	0.74
1:B:230:SER:O	1:B:235:THR:OG1	2.03	0.74
1:B:264:ALA:O	1:B:268[A]:THR:HG22	1.90	0.72
1:A:264:ALA:CB	4:A:1462:DMS:H13	2.20	0.71
1:A:245:THR:HG21	5:A:2300:HOH:O	1.90	0.71
1:B:266[B]:HIS:C	5:B:2274:HOH:O	2.28	0.71
1:B:171:HIS:HD2	1:B:173:PHE:H	1.37	0.70
1:A:268[A]:THR:HG23	4:A:1462:DMS:H12	1.70	0.69
1:A:409[A]:GLU:OE1	5:A:2438:HOH:O	2.12	0.67
1:B:440:LYS:HB3	5:B:2275:HOH:O	1.94	0.66
1:B:266[B]:HIS:HE1	5:B:2273:HOH:O	1.77	0.65
1:A:109:GLN:HE22	1:A:309:LYS:HZ2	1.45	0.65
1:B:214:ASP:OD1	5:B:2243:HOH:O	2.14	0.65
1:A:45:PRO:O	5:A:2076:HOH:O	2.13	0.64
4:A:1463:DMS:H23	5:A:2191:HOH:O	1.98	0.63

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:171:HIS:CD2	1:B:173:PHE:H	2.16	0.63
1:A:173:PHE:CE1	1:A:212:MET:HA	2.34	0.62
1:A:268[B]:THR:OG1	4:A:1462:DMS:C1	2.48	0.62
1:B:266[B]:HIS:CD2	1:B:267[B]:GLU:H	2.18	0.62
1:B:268[A]:THR:HG21	2:B:1456:HEM:C4B	2.35	0.61
1:A:179:ARG:HD3	1:A:204:GLN:CG	2.34	0.58
1:A:268[B]:THR:HG22	1:A:327:THR:HG23	1.85	0.58
1:A:361:HIS:CE1	1:A:391:LYS:H	2.14	0.57
1:B:264:ALA:CA	4:B:1459:DMS:H12	2.35	0.56
1:B:264:ALA:CB	4:B:1459:DMS:H12	2.35	0.56
1:A:179:ARG:HD3	1:A:204:GLN:HG3	1.88	0.56
1:A:5:MET:HE2	1:A:345:TYR:CD1	2.40	0.56
1:A:268[A]:THR:CG2	4:A:1462:DMS:H11	2.26	0.56
1:B:268[B]:THR:OG1	4:B:1459:DMS:H11	2.06	0.55
1:B:266[A]:HIS:C	5:B:2274:HOH:O	2.44	0.54
1:A:150:LEU:CD2	1:A:174:ILE:CD1	2.86	0.54
1:B:268[B]:THR:HG22	1:B:438:THR:HB	1.89	0.54
1:A:182:ASP:HB3	5:A:2251:HOH:O	2.08	0.53
1:B:124:VAL:HG13	1:B:455:LEU:HD13	1.91	0.52
2:B:1456:HEM:HBC2	2:B:1456:HEM:HMC1	1.91	0.52
1:B:266[B]:HIS:CD2	1:B:267[B]:GLU:N	2.77	0.52
1:B:158:PHE:CE2	1:B:219:ILE:HD13	2.46	0.51
1:A:5:MET:CE	1:A:345:TYR:CD1	2.94	0.51
1:A:264:ALA:HB1	4:A:1462:DMS:H13	1.93	0.50
1:B:309:LYS:O	1:B:312:LYS:HE3	2.10	0.50
1:B:171:HIS:HD2	1:B:173:PHE:N	2.08	0.50
1:B:440:LYS:CB	5:B:2275:HOH:O	2.58	0.50
1:A:367:TRP:HB2	1:A:371:VAL:HG12	1.94	0.50
1:A:215:LEU:HA	5:A:2278:HOH:O	2.13	0.49
1:B:268[A]:THR:HG23	2:B:1456:HEM:HAB	1.92	0.49
1:B:268[A]:THR:HG21	2:B:1456:HEM:CHC	2.42	0.49
1:B:447:LYS:NZ	5:B:2438:HOH:O	2.45	0.49
1:A:150:LEU:HD21	1:A:174:ILE:HD11	1.95	0.49
1:B:268[A]:THR:HG21	4:B:1459:DMS:H13	1.96	0.47
1:B:266[B]:HIS:CG	1:B:267[B]:GLU:H	2.32	0.47
1:A:268[B]:THR:CG2	1:A:327:THR:HG23	2.45	0.47
2:B:1456:HEM:CMC	2:B:1456:HEM:HBC2	2.44	0.47
1:B:264:ALA:CB	4:B:1459:DMS:C1	2.93	0.46
1:B:173:PHE:HD2	1:B:174:ILE:HD13	1.81	0.46
1:A:150:LEU:HD21	1:A:174:ILE:CD1	2.44	0.46
1:B:268[A]:THR:HG23	1:B:269:THR:N	2.31	0.46
1:B:173:PHE:CE1	1:B:212:MET:HA	2.51	0.46

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:268[A]:THR:CG2	1:B:269:THR:N	2.78	0.46
1:A:426:HIS:HB3	1:A:447:LYS:HE2	1.99	0.45
1:A:109:GLN:NE2	1:A:309:LYS:HZ2	2.14	0.45
1:A:426:HIS:CB	1:A:447:LYS:HE2	2.46	0.45
1:B:126:LEU:C	1:B:126:LEU:HD13	2.37	0.45
1:B:148:LEU:HD11	1:B:413:VAL:HG21	1.99	0.45
1:A:97:LYS:HE3	1:A:244:GLU:OE2	2.16	0.44
1:B:342:GLY:O	1:B:344:GLU:HG3	2.18	0.44
1:A:109:GLN:HE22	1:A:309:LYS:NZ	2.11	0.44
1:A:150:LEU:CD2	1:A:174:ILE:HD11	2.47	0.44
1:B:264:ALA:HB1	4:B:1459:DMS:H13	2.00	0.44
1:A:242:ASP:O	1:A:246:GLY:N	2.47	0.44
1:A:268[B]:THR:HG22	1:A:327:THR:CG2	2.47	0.44
1:B:2:ILE:HG13	5:B:2002:HOH:O	2.19	0.43
1:A:51:TYR:CE2	1:A:354:MET:HG2	2.54	0.43
1:B:264:ALA:HA	4:B:1459:DMS:C1	2.44	0.42
1:B:310:GLN:HA	1:B:312:LYS:HE3	2.00	0.42
1:B:195:ASP:O	1:B:197:ALA:N	2.53	0.42
1:A:98:LYS:HE3	1:A:247:GLU:HB2	2.02	0.41
1:B:266[B]:HIS:CG	1:B:267[B]:GLU:N	2.88	0.41
1:B:267[B]:GLU:HA	1:B:270:SER:OG	2.20	0.41
1:A:53:SER:HB3	1:A:359:GLN:HB3	2.02	0.40
1:B:198:TYR:HA	1:B:201:ASN:HD22	1.86	0.40
1:B:264:ALA:HB1	4:B:1459:DMS:C1	2.52	0.40
1:A:153:ILE:HG21	1:A:265:GLY:HA3	2.02	0.40
1:A:38:GLU:OE2	1:A:56:ARG:NH1	2.54	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	456/455 (100%)	443 (97%)	13 (3%)	0	100	100
1	B	456/455 (100%)	441 (97%)	12 (3%)	3 (1%)	30	10

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	912/910 (100%)	884 (97%)	25 (3%)	3 (0%)	56 27

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	267[A]	GLU
1	B	267[B]	GLU
1	B	196	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	402/399 (101%)	400 (100%)	2 (0%)	94 89
1	B	402/399 (101%)	398 (99%)	4 (1%)	85 76
All	All	804/798 (101%)	798 (99%)	6 (1%)	89 85

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	MET
1	A	455	LEU
1	B	52	LEU
1	B	189	GLN
1	B	192	ASN
1	B	228	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	GLN
1	A	128	GLN
1	A	189	GLN
1	A	201	ASN
1	A	204	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	206	GLN
1	A	361	HIS
1	A	395	ASN
1	A	404	GLN
1	A	426	HIS
1	B	21	ASN
1	B	159	ASN
1	B	171	HIS
1	B	201	ASN
1	B	319	ASN
1	B	403	GLN

### 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 13 ligands modelled in this entry, 7 are 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$
2	HEM	A	1456	1,4	49,50,50	2.41	14 (28%)	46,82,82	2.19	15 (32%)
4	DMS	A	1462	2	3,3,3	2.62	1 (33%)	3,3,3	1.20	1 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	DMS	A	1463	-	3,3,3	2.52	1 (33%)	3,3,3	0.75	0
2	HEM	B	1456	1,4	49,50,50	2.85	13 (26%)	46,82,82	2.00	7 (15%)
4	DMS	B	1459	2	3,3,3	2.65	1 (33%)	3,3,3	0.98	0
4	DMS	B	1460	-	3,3,3	2.56	1 (33%)	3,3,3	0.38	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	1456	1,4	-	0/14/114/114	0/0/8/8
4	DMS	A	1462	2	-	0/0/0/0	0/0/0/0
4	DMS	A	1463	-	-	0/0/0/0	0/0/0/0
2	HEM	B	1456	1,4	-	0/14/114/114	0/0/8/8
4	DMS	B	1459	2	-	0/0/0/0	0/0/0/0
4	DMS	B	1460	-	-	0/0/0/0	0/0/0/0

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1456	HEM	C2B-C1B	14.02	1.48	1.44
2	A	1456	HEM	C2D-C1D	7.84	1.46	1.44
2	B	1456	HEM	C3C-C2C	-5.11	1.34	1.43
2	B	1456	HEM	C2D-C1D	5.02	1.45	1.44
2	A	1456	HEM	C3B-C2B	-4.81	1.35	1.43
2	A	1456	HEM	C2B-C1B	4.80	1.45	1.44
2	A	1456	HEM	C3C-CAC	4.71	1.55	1.40
2	B	1456	HEM	C4A-C3A	4.68	1.46	1.40
2	A	1456	HEM	C3C-C2C	-4.56	1.35	1.43
4	B	1459	DMS	O-S	4.53	1.80	1.50
2	A	1456	HEM	C3B-CAB	4.51	1.54	1.40
4	A	1462	DMS	O-S	4.50	1.80	1.50
4	B	1460	DMS	O-S	4.31	1.79	1.50
2	B	1456	HEM	C3B-CAB	4.30	1.53	1.40
2	B	1456	HEM	C3C-CAC	4.29	1.53	1.40
4	A	1463	DMS	O-S	4.23	1.78	1.50
2	A	1456	HEM	C4A-C3A	4.20	1.45	1.40
2	A	1456	HEM	FE-NA	3.42	2.07	1.92
2	A	1456	HEM	C3D-C2D	3.40	1.49	1.43
2	B	1456	HEM	C3D-C2D	3.14	1.49	1.43

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1456	HEM	C3B-C2B	-2.93	1.38	1.43
2	B	1456	HEM	CAA-C2A	2.84	1.57	1.52
2	B	1456	HEM	FE-NA	2.75	2.04	1.92
2	A	1456	HEM	C3D-C4D	2.71	1.45	1.44
2	A	1456	HEM	CAA-C2A	2.66	1.56	1.52
2	A	1456	HEM	CMC-C2C	2.58	1.55	1.47
2	B	1456	HEM	C3B-C4B	2.53	1.47	1.44
2	A	1456	HEM	CMD-C2D	2.50	1.55	1.47
2	B	1456	HEM	CMB-C2B	2.49	1.55	1.47
2	B	1456	HEM	CMC-C2C	2.33	1.54	1.47
2	A	1456	HEM	CMB-C2B	2.14	1.54	1.47

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1456	HEM	C3B-C4B-NB	-7.94	108.32	114.00
2	A	1456	HEM	C3B-C4B-NB	-7.86	108.38	114.00
2	B	1456	HEM	C4D-ND-C1D	4.98	110.26	105.16
2	A	1456	HEM	C4D-ND-C1D	4.48	109.75	105.16
2	A	1456	HEM	CBD-CAD-C3D	-4.34	104.89	114.37
2	A	1456	HEM	CMA-C3A-C4A	-3.45	123.32	128.62
2	B	1456	HEM	CHD-C1D-ND	3.44	127.44	124.58
2	B	1456	HEM	CBD-CAD-C3D	-3.42	106.91	114.37
2	B	1456	HEM	C2D-C1D-ND	-3.42	108.90	112.93
2	B	1456	HEM	CBA-CAA-C2A	-3.22	107.02	112.69
2	A	1456	HEM	C2D-C1D-ND	-3.15	109.21	112.93
2	A	1456	HEM	C1B-NB-C4B	2.92	108.15	105.16
2	B	1456	HEM	C1B-NB-C4B	2.92	108.15	105.16
2	A	1456	HEM	CBA-CAA-C2A	-2.85	107.67	112.69
2	A	1456	HEM	CHB-C1B-NB	2.73	128.05	124.31
2	A	1456	HEM	CHC-C4B-NB	2.62	126.77	124.58
2	A	1456	HEM	CAD-C3D-C4D	2.61	129.23	124.53
2	A	1456	HEM	C4C-NC-C1C	2.53	108.17	105.53
2	A	1456	HEM	C4A-CHB-C1B	-2.36	124.37	127.47
2	A	1456	HEM	CHA-C4D-ND	2.34	127.52	124.31
2	A	1456	HEM	CHC-C1C-NC	2.22	126.66	124.73
4	A	1462	DMS	O-S-C2	-2.02	95.48	106.62
2	A	1456	HEM	C4A-C3A-C2A	2.02	108.40	107.00

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	454/455 (99%)	0.17	35 (7%) 13 17	16, 23, 49, 68	0
1	B	454/455 (99%)	0.31	37 (8%) 12 15	18, 25, 55, 89	0
All	All	908/910 (99%)	0.24	72 (7%) 13 15	16, 24, 51, 89	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2	ILE	8.0
1	B	191	ALA	6.5
1	B	227	GLY	6.3
1	A	227	GLY	5.7
1	A	229	GLN	4.9
1	B	13	GLU	4.8
1	B	193	PRO	4.5
1	A	2	ILE	4.5
1	A	197	ALA	4.4
1	B	192	ASN	4.4
1	A	196	PRO	4.2
1	B	14	LEU	4.1
1	B	268[A]	THR	4.0
1	B	225	ALA	4.0
1	A	203	ARG	3.8
1	A	194	ASP	3.7
1	B	194	ASP	3.7
1	B	221	ALA	3.6
1	A	211	VAL	3.6
1	B	196	PRO	3.5
1	B	198	TYR	3.5
1	B	45	PRO	3.5
1	B	4	GLU	3.4
1	B	195	ASP	3.4

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	136	ASP	3.3
1	B	17	LEU	3.3
1	B	226	SER	3.2
1	A	198	TYR	3.1
1	A	192	ASN	3.1
1	B	244	GLU	3.1
1	A	191	ALA	3.0
1	B	229	GLN	3.0
1	A	245	THR	2.9
1	A	228	GLU	2.9
1	A	169	GLN	2.8
1	A	207	GLU	2.7
1	B	267[A]	GLU	2.7
1	A	262	LEU	2.7
1	A	268[A]	THR	2.7
1	B	46	GLY	2.7
1	A	263	ILE	2.6
1	A	170	PRO	2.6
1	B	369	ASP	2.5
1	A	264	ALA	2.5
1	B	10	THR	2.5
1	B	228	GLU	2.4
1	A	214	ASP	2.4
1	A	243	PRO	2.4
1	B	199	ASP	2.4
1	A	272	LEU	2.4
1	A	383	SER	2.4
1	A	201	ASN	2.3
1	A	244	GLU	2.3
1	A	175	THR	2.3
1	A	210	LYS	2.3
1	B	201	ASN	2.3
1	A	94	LYS	2.3
1	B	3	LYS	2.3
1	B	12	GLY	2.2
1	B	170	PRO	2.2
1	A	195	ASP	2.2
1	A	199	ASP	2.2
1	A	136	ASP	2.1
1	B	269	THR	2.1
1	A	247	GLU	2.1
1	A	13	GLU	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	169	GLN	2.1
1	B	197	ALA	2.1
1	B	327	THR	2.1
1	B	203	ARG	2.0
1	A	384	ALA	2.0
1	B	150	LEU	2.0

## 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
3	ZN	B	1458	1/1	0.15	8.95	58,58,58,58	0
3	ZN	A	1459	1/1	0.17	2.87	71,71,71,71	0
4	DMS	A	1463	4/4	0.15	2.22	33,43,43,45	0
4	DMS	A	1462	4/4	0.22	1.01	25,26,34,36	0
4	DMS	B	1460	4/4	0.11	0.50	41,45,49,49	0
2	HEM	A	1456	43/43	0.12	-0.19	14,17,23,29	0
2	HEM	B	1456	43/43	0.11	-0.28	14,18,22,32	0
4	DMS	B	1459	4/4	0.13	-0.50	25,25,28,31	0
3	ZN	A	1460	1/1	0.08	-0.65	57,57,57,57	0
3	ZN	A	1461	1/1	0.07	-1.39	98,98,98,98	0
3	ZN	A	1458	1/1	0.07	-1.91	45,45,45,45	0
3	ZN	A	1457	1/1	0.04	-4.01	34,34,34,34	0
3	ZN	B	1457	1/1	0.04	-4.06	23,23,23,23	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.