



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:52 AM 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 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

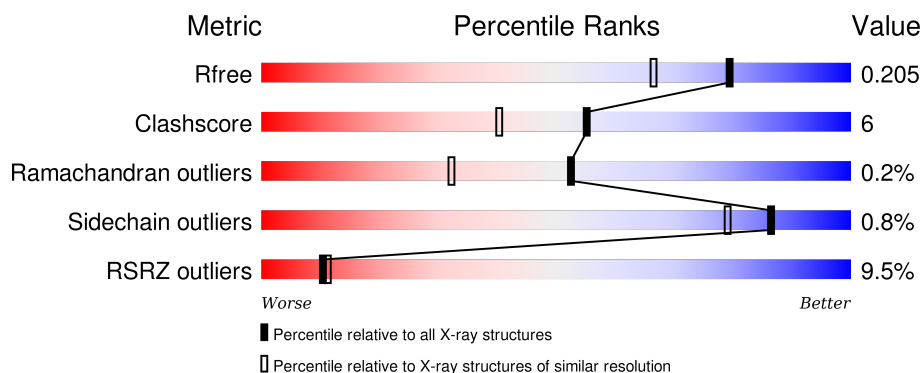
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	91344	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (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. 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	455	<div> <div>9%</div> <div>90%</div> <div>9%</div> </div>
1	B	455	<div> <div>9%</div> <div>90%</div> <div>9%</div> </div>

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
4	DMS	A	1462	-	-	X	-
4	DMS	B	1459	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8441 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 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:  $C_{34}H_{32}FeN_4O_4$ ).

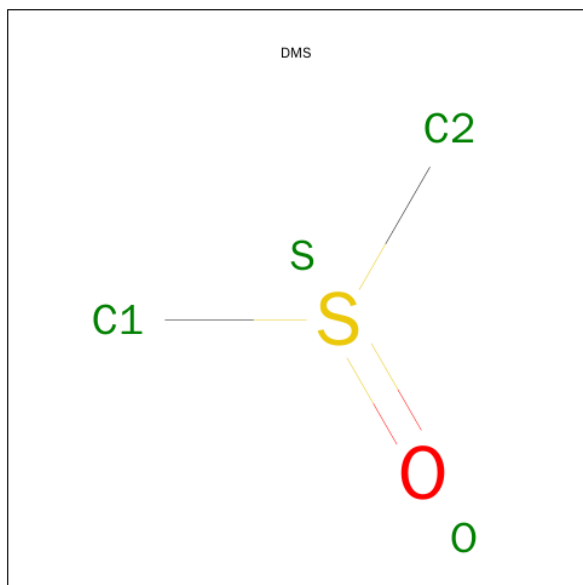


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- 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		

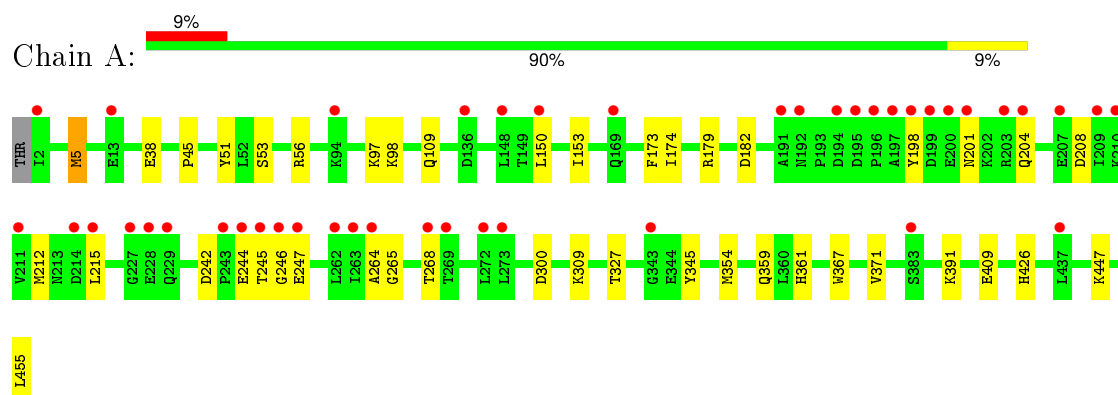
- Molecule 5 is water.

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

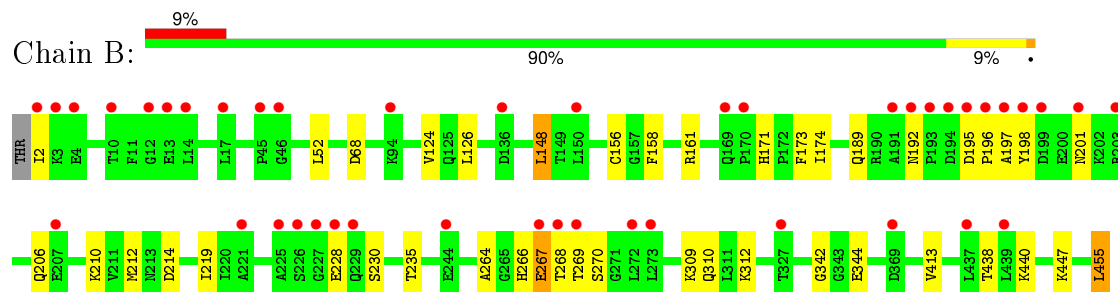
### 3 Residue-property plots

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 0.179 , 0.205	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> )	0.37 , 51.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	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.

<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, 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 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	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

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 6.

All (94) 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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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%)	26	9
All	All	912/910 (100%)	884 (97%)	25 (3%)	3 (0%)	52	26

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%)	92	88
1	B	402/399 (101%)	398 (99%)	4 (1%)	82	72
All	All	804/798 (101%)	798 (99%)	6 (1%)	86	82

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

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Mol	Chain	Res	Type
1	A	189	GLN
1	A	201	ASN
1	A	204	GLN
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 [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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	30,50,50	1.99	6 (20%)	24,82,82	2.37	9 (37%)
4	DMS	A	1462	2	3,3,3	2.58	1 (33%)	3,3,3	1.21	1 (33%)
4	DMS	A	1463	-	3,3,3	2.47	1 (33%)	3,3,3	0.80	0
2	HEM	B	1456	1,4	30,50,50	1.90	5 (16%)	24,82,82	2.42	10 (41%)
4	DMS	B	1459	2	3,3,3	2.60	1 (33%)	3,3,3	1.01	0
4	DMS	B	1460	-	3,3,3	2.52	1 (33%)	3,3,3	0.42	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	-	0/10/54/54	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	-	0/10/54/54	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 (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1456	HEM	C3B-C4B	-5.99	1.46	1.51
2	B	1456	HEM	C3D-C4D	-5.41	1.44	1.51
2	B	1456	HEM	C3B-C4B	-4.96	1.47	1.51
2	A	1456	HEM	C3D-C4D	-4.94	1.45	1.51
2	A	1456	HEM	C2C-C1C	-3.82	1.45	1.52
2	B	1456	HEM	C2C-C1C	-3.69	1.45	1.52
2	B	1456	HEM	FE-NC	2.03	2.03	1.95
2	A	1456	HEM	FE-NC	2.06	2.04	1.95
2	A	1456	HEM	C3C-CAC	2.09	1.55	1.51
2	A	1456	HEM	CAA-C2A	2.73	1.56	1.52
2	B	1456	HEM	CAA-C2A	2.92	1.57	1.52
4	A	1463	DMS	O-S	4.15	1.78	1.50
4	B	1460	DMS	O-S	4.23	1.79	1.50
4	A	1462	DMS	O-S	4.41	1.80	1.50
4	B	1459	DMS	O-S	4.44	1.80	1.50

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1456	HEM	C3B-CAB-CBB	-3.52	119.06	124.46
2	B	1456	HEM	CBA-CAA-C2A	-3.07	107.02	112.53
2	A	1456	HEM	CMA-C3A-C4A	-3.05	123.32	128.36
2	A	1456	HEM	CBD-CAD-C3D	-2.98	104.89	113.55
2	A	1456	HEM	CBA-CAA-C2A	-2.71	107.67	112.53
2	B	1456	HEM	CBD-CAD-C3D	-2.28	106.91	113.55
2	B	1456	HEM	C3C-CAC-CBC	-2.09	121.26	124.46
4	A	1462	DMS	O-S-C2	-2.03	95.48	106.64
2	A	1456	HEM	C2D-C3D-C4D	2.21	105.25	101.50
2	A	1456	HEM	CMD-C2D-C3D	2.41	125.00	114.35
2	B	1456	HEM	CMD-C2D-C3D	2.59	125.81	114.35
2	B	1456	HEM	C2D-C3D-C4D	3.01	106.60	101.50
2	B	1456	HEM	CMC-C2C-C3C	4.14	126.86	116.53
2	A	1456	HEM	CAD-C3D-C2D	4.28	125.52	113.22
2	B	1456	HEM	CAD-C3D-C2D	4.29	125.56	113.22
2	B	1456	HEM	CAD-C3D-C4D	4.35	127.82	112.47
2	A	1456	HEM	CMC-C2C-C3C	4.72	128.32	116.53
2	B	1456	HEM	CMB-C2B-C3B	4.73	128.33	116.53
2	A	1456	HEM	CAD-C3D-C4D	4.75	129.23	112.47
2	A	1456	HEM	CMB-C2B-C3B	4.76	128.42	116.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1462	DMS	11	0
4	A	1463	DMS	1	0
2	B	1456	HEM	5	0
4	B	1459	DMS	9	0

## 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%)	0.41	43 (9%) 10 11	16, 23, 49, 68	0
1	B	454/455 (99%)	0.46	43 (9%) 10 11	18, 25, 55, 89	0
All	All	908/910 (99%)	0.44	86 (9%) 10 11	16, 24, 51, 89	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	227	GLY	8.4
1	B	2	ILE	7.9
1	B	191	ALA	6.7
1	A	2	ILE	5.7
1	A	197	ALA	5.4
1	B	13	GLU	5.3
1	B	192	ASN	5.2
1	A	227	GLY	5.1
1	A	229	GLN	5.0
1	A	203	ARG	4.7
1	B	193	PRO	4.7
1	B	196	PRO	4.7
1	A	211	VAL	4.6
1	B	198	TYR	4.5
1	B	45	PRO	4.2
1	A	194	ASP	4.1
1	B	268[A]	THR	4.1
1	A	196	PRO	4.1
1	B	195	ASP	4.0
1	A	198	TYR	3.8
1	B	46	GLY	3.8
1	B	14	LEU	3.7
1	A	245	THR	3.7
1	B	194	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	225	ALA	3.5
1	A	263	ILE	3.5
1	A	262	LEU	3.4
1	A	207	GLU	3.4
1	B	136	ASP	3.4
1	A	268[A]	THR	3.3
1	B	3	LYS	3.2
1	B	221	ALA	3.2
1	B	226	SER	3.2
1	A	192	ASN	3.1
1	B	267[A]	GLU	3.1
1	B	17	LEU	3.1
1	A	243	PRO	3.0
1	A	264	ALA	3.0
1	A	191	ALA	3.0
1	A	244	GLU	2.9
1	A	136	ASP	2.9
1	B	369	ASP	2.9
1	A	214	ASP	2.9
1	B	4	GLU	2.8
1	B	10	THR	2.8
1	B	199	ASP	2.8
1	A	169	GLN	2.8
1	A	201	ASN	2.7
1	A	272	LEU	2.7
1	B	244	GLU	2.7
1	B	229	GLN	2.6
1	B	201	ASN	2.6
1	B	197	ALA	2.6
1	A	195	ASP	2.6
1	A	228	GLU	2.6
1	A	246	GLY	2.5
1	B	12	GLY	2.5
1	B	327	THR	2.4
1	A	343	GLY	2.4
1	A	215	LEU	2.4
1	A	269	THR	2.4
1	A	204	GLN	2.4
1	A	273	LEU	2.4
1	B	203	ARG	2.4
1	B	169	GLN	2.4
1	A	210	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	247	GLU	2.2
1	A	437	LEU	2.2
1	A	209	ILE	2.2
1	B	272	LEU	2.2
1	B	439	LEU	2.2
1	B	228	GLU	2.2
1	B	170	PRO	2.2
1	B	150	LEU	2.2
1	B	269	THR	2.2
1	A	199	ASP	2.2
1	A	383	SER	2.1
1	A	148	LEU	2.1
1	A	13	GLU	2.1
1	A	94	LYS	2.1
1	A	200	GLU	2.1
1	B	94	LYS	2.1
1	B	273	LEU	2.1
1	B	437	LEU	2.1
1	B	207	GLU	2.1
1	A	150	LEU	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
4	DMS	A	1463	4/4	0.97	0.17	1.84	33,43,43,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	DMS	B	1460	4/4	0.97	0.13	0.90	41,45,49,49	0
4	DMS	A	1462	4/4	0.95	0.21	0.26	25,26,34,36	0
2	HEM	B	1456	43/43	0.98	0.08	-0.83	14,18,22,32	0
2	HEM	A	1456	43/43	0.99	0.09	-0.89	14,17,23,29	0
4	DMS	B	1459	4/4	0.98	0.10	-0.94	25,25,28,31	0
3	ZN	B	1457	1/1	0.99	0.03	-	23,23,23,23	0
3	ZN	A	1461	1/1	0.65	0.08	-	98,98,98,98	0
3	ZN	A	1457	1/1	0.99	0.08	-	34,34,34,34	0
3	ZN	B	1458	1/1	0.89	0.18	-	58,58,58,58	0
3	ZN	A	1460	1/1	0.97	0.11	-	57,57,57,57	0
3	ZN	A	1458	1/1	0.97	0.10	-	45,45,45,45	0
3	ZN	A	1459	1/1	0.94	0.21	-	71,71,71,71	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.