



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:12 PM GMT

PDB ID : 1SMI  
Title : A single mutation of P450 BM3 induces the conformational rearrangement seen upon substrate-binding in wild-type enzyme  
Authors : Joyce, M.G.; Girvan, H.M.; Munro, A.W.; Leys, D.  
Deposited on : 2004-03-09  
Resolution : 2.00 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

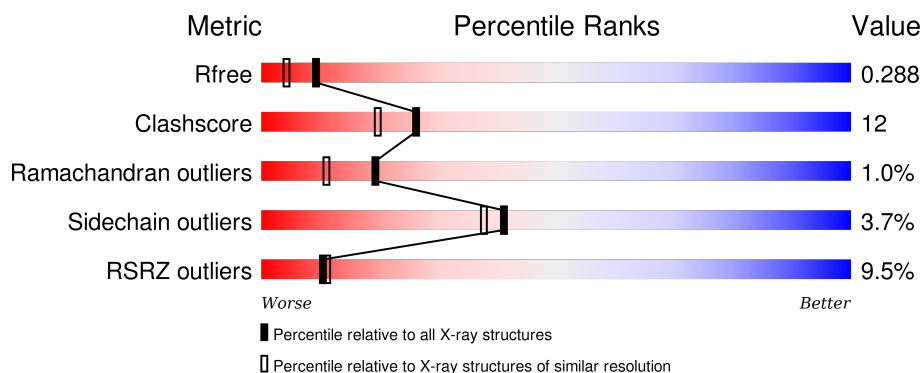
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	471	
1	B	471	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7702 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.

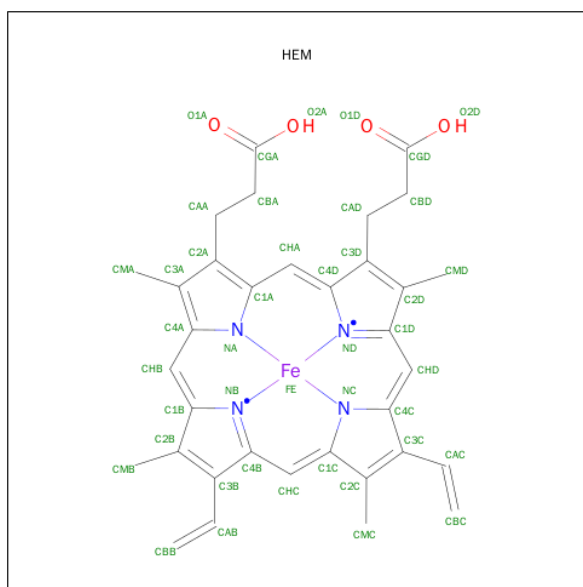
- Molecule 1 is a protein called Bifunctional P-450:NADPH-P450 reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	439	Total	C	N	O	S	0	0	0
			3500	2244	593	646	17			
1	B	455	Total	C	N	O	S	0	0	0
			3624	2310	616	681	17			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	264	GLU	ALA	ENGINEERED	UNP P14779
B	264	GLU	ALA	ENGINEERED	UNP P14779

- 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		

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

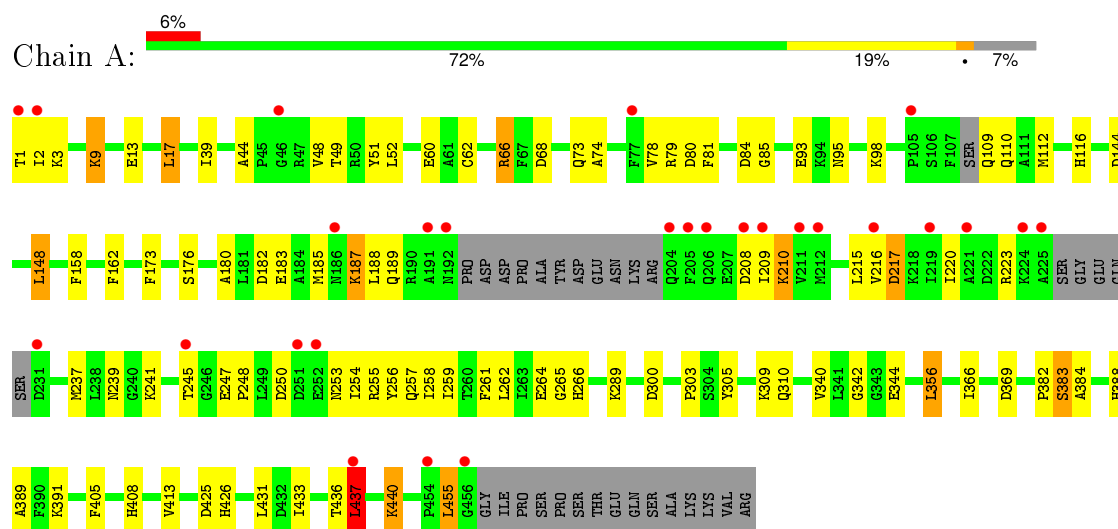
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	292	Total	O	0	0
			292	292		
3	B	200	Total	O	0	0
			200	200		

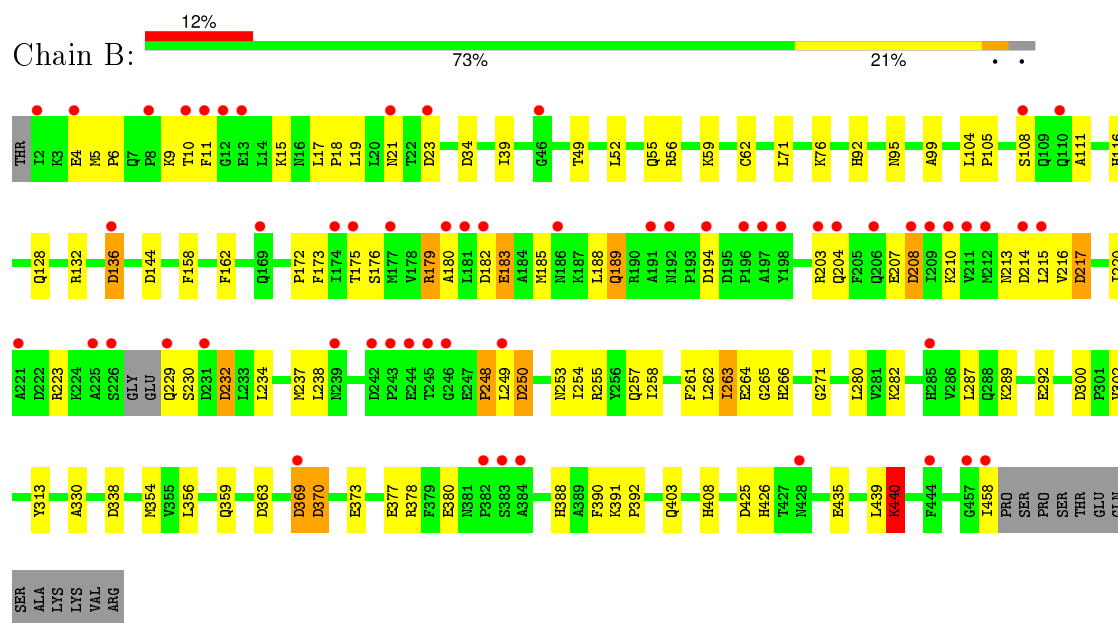
### 3 Residue-property plots

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: Bifunctional P-450:NADPH-P450 reductase



- Molecule 1: Bifunctional P-450:NADPH-P450 reductase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.21Å 118.93Å 146.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.92 – 2.00 14.92 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (14.92-2.00) 94.1 (14.92-2.00)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.55 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.1	Depositor
R, $R_{free}$	0.224 , 0.288 0.224 , 0.288	Depositor DCC
$R_{free}$ test set	3440 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.9	Xtriage
Anisotropy	0.012	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 65.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 68450 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7702	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% 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

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	0.88	2/3579 (0.1%)	0.96	11/4839 (0.2%)
1	B	0.74	0/3708	0.90	14/5018 (0.3%)
All	All	0.81	2/7287 (0.0%)	0.93	25/9857 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	440	LYS	CE-NZ	5.88	1.63	1.49
1	A	405	PHE	CE1-CZ	5.84	1.48	1.37

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	369	ASP	CB-CG-OD2	8.58	126.02	118.30
1	A	144	ASP	CB-CG-OD2	7.15	124.73	118.30
1	B	370	ASP	CB-CG-OD2	6.95	124.56	118.30
1	B	250	ASP	CB-CG-OD2	6.82	124.44	118.30
1	A	80	ASP	CB-CG-OD2	6.60	124.24	118.30
1	B	232	ASP	CB-CG-OD2	5.88	123.59	118.30
1	A	455	LEU	CA-CB-CG	5.87	128.81	115.30
1	B	217	ASP	CB-CG-OD2	5.77	123.50	118.30
1	B	144	ASP	CB-CG-OD2	5.74	123.47	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	300	ASP	CB-CG-OD2	5.64	123.38	118.30
1	B	363	ASP	CB-CG-OD2	5.59	123.33	118.30
1	B	34	ASP	CB-CG-OD2	5.58	123.32	118.30
1	A	217	ASP	CB-CG-OD2	5.48	123.23	118.30
1	B	440	LYS	CD-CE-NZ	5.37	124.04	111.70
1	A	66	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	B	194	ASP	CB-CG-OD2	5.33	123.09	118.30
1	B	300	ASP	CB-CG-OD2	5.28	123.05	118.30
1	B	369	ASP	CB-CG-OD2	5.27	123.04	118.30
1	A	425	ASP	CB-CG-OD1	5.20	122.98	118.30
1	B	208	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	68	ASP	CB-CG-OD1	5.20	122.98	118.30
1	B	182	ASP	CB-CG-OD2	5.14	122.92	118.30
1	A	437	LEU	C-N-CA	5.13	134.54	121.70
1	B	338	ASP	CB-CG-OD2	5.09	122.88	118.30
1	A	182	ASP	CB-CG-OD2	5.08	122.88	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	437	LEU	Peptide

## 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	3500	0	3448	67	0
1	B	3624	0	3530	103	0
2	A	43	0	30	3	0
2	B	43	0	30	2	0
3	A	292	0	0	10	0
3	B	200	0	0	18	0
All	All	7702	0	7038	175	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 12.

All (175) 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:437:LEU:HA	3:A:576:HOH:O	1.33	1.23
1:B:179:ARG:NH1	1:B:180:ALA:HB2	1.59	1.16
1:B:173:PHE:HA	3:B:663:HOH:O	1.49	1.07
1:B:263:ILE:HG22	3:B:530:HOH:O	1.55	1.06
1:B:108:SER:O	1:B:111:ALA:HB3	1.58	1.04
1:B:172:PRO:HA	3:B:548:HOH:O	1.62	0.99
1:B:179:ARG:HD2	1:B:180:ALA:N	1.82	0.93
1:B:179:ARG:HD2	1:B:180:ALA:CA	2.00	0.90
1:B:271:GLY:CA	1:B:440:LYS:HE3	2.03	0.87
1:B:21:ASN:HB3	3:B:608:HOH:O	1.74	0.86
1:B:179:ARG:CZ	1:B:208:ASP:HB3	2.08	0.82
1:B:248:PRO:HD3	3:B:586:HOH:O	1.78	0.81
1:B:179:ARG:HD2	1:B:180:ALA:HA	1.61	0.80
1:B:179:ARG:CZ	1:B:180:ALA:HB2	2.12	0.79
1:A:180:ALA:HB2	3:A:759:HOH:O	1.85	0.77
1:A:162:PHE:HE1	1:A:215:LEU:HD11	1.51	0.75
1:B:179:ARG:CD	1:B:180:ALA:N	2.50	0.75
1:B:158:PHE:CE1	1:B:258:ILE:HG12	2.21	0.74
1:B:17:LEU:HD11	1:B:189:GLN:HA	1.69	0.74
1:B:56:ARG:HA	1:B:59:LYS:HE2	1.68	0.74
1:B:216:VAL:O	1:B:220:ILE:HD12	1.89	0.73
1:B:271:GLY:N	1:B:440:LYS:HE3	2.05	0.72
1:B:176:SER:C	1:B:179:ARG:HH21	1.93	0.72
1:B:55:GLN:O	1:B:59:LYS:HG2	1.88	0.72
1:B:108:SER:O	1:B:111:ALA:CB	2.37	0.72
1:B:116:HIS:HD2	1:B:408:HIS:NE2	1.89	0.69
1:B:330:ALA:HB1	1:B:354:MET:HE3	1.75	0.68
1:A:210:LYS:HA	1:A:210:LYS:HE2	1.76	0.67
1:B:11:PHE:CD1	1:B:18:PRO:HD2	2.31	0.66
1:B:11:PHE:HE1	1:B:19:LEU:HG	1.60	0.66
1:B:185:MET:HA	1:B:188:LEU:HD12	1.77	0.66
1:B:207:GLU:O	1:B:210:LYS:HB2	1.94	0.66
2:B:472:HEM:HBC2	2:B:472:HEM:HMC2	1.78	0.66
1:B:179:ARG:NH2	1:B:208:ASP:HB3	2.09	0.66
1:A:210:LYS:CE	1:A:210:LYS:HA	2.26	0.66
1:B:435:GLU:HG2	1:B:439:LEU:CD2	2.27	0.65
2:A:472:HEM:HMC2	2:A:472:HEM:HBC2	1.78	0.65
1:B:207:GLU:HG3	3:B:615:HOH:O	1.97	0.64
1:A:253:ASN:O	1:A:256:TYR:HB2	1.97	0.64
1:B:214:ASP:O	1:B:217:ASP:HB2	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:GLY:HA2	1:A:257:GLN:NE2	2.12	0.64
1:A:436:THR:O	1:A:437:LEU:C	2.37	0.63
1:B:92:HIS:HB3	3:B:634:HOH:O	1.98	0.62
1:B:11:PHE:CE1	1:B:19:LEU:HG	2.34	0.62
1:B:173:PHE:CA	3:B:663:HOH:O	2.22	0.61
1:A:241:LYS:HG3	1:A:248:PRO:HB3	1.82	0.61
1:B:229:GLN:HA	3:B:662:HOH:O	2.00	0.60
1:B:173:PHE:CD1	1:B:215:LEU:HD11	2.37	0.60
1:B:330:ALA:HB1	1:B:354:MET:CE	2.31	0.59
1:A:162:PHE:CE1	1:A:215:LEU:HD11	2.35	0.59
1:B:261:PHE:O	1:B:265:GLY:N	2.34	0.59
1:A:255:ARG:O	1:A:259:ILE:HD12	2.04	0.57
1:B:263:ILE:CG2	3:B:530:HOH:O	2.32	0.57
1:B:179:ARG:HH11	1:B:180:ALA:HB2	1.60	0.57
1:A:66:ARG:NH2	1:A:340:VAL:O	2.37	0.57
1:A:223:ARG:HB3	3:A:722:HOH:O	2.05	0.57
1:B:234:LEU:HD13	1:B:258:ILE:HD11	1.88	0.56
1:A:216:VAL:HG21	1:A:259:ILE:CG1	2.35	0.56
1:B:204:GLN:NE2	1:B:207:GLU:OE2	2.40	0.55
1:A:237:MET:HE1	1:A:257:GLN:HB2	1.88	0.55
1:A:261:PHE:O	1:A:265:GLY:HA3	2.05	0.55
1:B:179:ARG:CZ	1:B:208:ASP:CB	2.84	0.55
1:B:426:HIS:HE1	3:B:577:HOH:O	1.89	0.55
1:B:213:ASN:HB3	1:B:255:ARG:HH21	1.72	0.55
1:B:377:GLU:O	1:B:380:GLU:HB2	2.07	0.55
1:B:238:LEU:HD23	1:B:254:ILE:HD13	1.87	0.54
1:A:289:LYS:NZ	3:A:684:HOH:O	2.33	0.54
1:A:51:TYR:HD2	1:A:356:LEU:HD13	1.71	0.54
1:A:237:MET:CE	1:A:257:GLN:HB2	2.37	0.54
1:B:176:SER:O	1:B:179:ARG:NE	2.41	0.53
1:A:74:ALA:O	1:A:78:VAL:HG23	2.08	0.53
1:A:183:GLU:HA	3:A:694:HOH:O	2.08	0.53
1:B:204:GLN:NE2	1:B:208:ASP:OD1	2.42	0.53
1:A:382:PRO:C	1:A:384:ALA:H	2.11	0.52
1:B:179:ARG:NH1	1:B:180:ALA:CB	2.53	0.52
1:B:249:LEU:HD22	1:B:253:ASN:OD1	2.09	0.52
1:B:261:PHE:O	1:B:265:GLY:HA3	2.10	0.52
1:B:282:LYS:NZ	1:B:425:ASP:OD2	2.40	0.51
1:B:158:PHE:HE1	1:B:258:ILE:HG12	1.73	0.51
1:B:390:PHE:CZ	1:B:392:PRO:HG3	2.45	0.51
1:A:116:HIS:HE1	1:A:303:PRO:O	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:472:HEM:CMC	2:A:472:HEM:HBC2	2.40	0.51
1:A:62:CYS:SG	1:A:391:LYS:HE2	2.51	0.51
1:B:280:LEU:HB3	1:B:287:LEU:HD13	1.93	0.51
1:B:262:LEU:O	1:B:266:HIS:HD2	1.95	0.50
1:A:73:GLN:HB2	1:A:188:LEU:HD21	1.94	0.50
1:A:245:THR:OG1	1:A:247:GLU:HG2	2.11	0.50
1:B:173:PHE:HD1	1:B:215:LEU:HD21	1.77	0.49
1:B:264:GLU:HB3	3:B:496:HOH:O	2.12	0.49
1:B:289:LYS:HD2	1:B:313:TYR:CZ	2.47	0.49
1:B:176:SER:C	1:B:179:ARG:NH2	2.64	0.49
1:A:3:LYS:HD2	1:A:344:GLU:OE1	2.13	0.49
1:B:62:CYS:SG	1:B:391:LYS:HE2	2.52	0.49
1:A:216:VAL:HG21	1:A:259:ILE:HG13	1.93	0.49
1:B:39:ILE:HD12	1:B:52:LEU:CD2	2.43	0.49
1:A:426:HIS:CD2	1:A:426:HIS:H	2.31	0.49
1:A:237:MET:HE2	1:A:254:ILE:HG23	1.94	0.49
1:A:310:GLN:HG2	3:A:560:HOH:O	2.12	0.48
1:B:271:GLY:HA2	1:B:440:LYS:HE3	1.93	0.48
1:B:216:VAL:HG12	1:B:220:ILE:HD11	1.96	0.48
1:A:158:PHE:CE1	1:A:258:ILE:HD12	2.49	0.48
1:B:391:LYS:HA	3:B:524:HOH:O	2.12	0.48
1:B:223:ARG:NH2	1:B:232:ASP:OD2	2.30	0.48
1:A:17:LEU:HD12	1:A:17:LEU:O	2.13	0.48
1:A:81:PHE:HB3	1:A:209:ILE:HG12	1.96	0.48
1:A:431:LEU:HD21	1:A:433:ILE:HD11	1.96	0.47
1:A:208:ASP:HB2	3:A:759:HOH:O	2.13	0.47
1:B:220:ILE:HG23	3:B:570:HOH:O	2.14	0.47
1:B:216:VAL:HG12	1:B:220:ILE:CD1	2.45	0.47
2:B:472:HEM:HBC2	2:B:472:HEM:CMC	2.43	0.47
1:A:98:LYS:HE3	1:A:247:GLU:HG3	1.97	0.47
1:A:17:LEU:HD22	1:A:44:ALA:HB1	1.96	0.47
1:B:179:ARG:O	1:B:183:GLU:N	2.35	0.46
1:A:109:GLN:HA	1:A:112:MET:HB2	1.98	0.46
1:B:179:ARG:HD2	1:B:179:ARG:C	2.37	0.45
1:A:9:LYS:HB2	1:A:9:LYS:HE2	1.73	0.45
1:B:261:PHE:O	1:B:265:GLY:CA	2.65	0.45
1:B:99:ALA:HB2	1:B:249:LEU:HD21	1.99	0.45
1:A:220:ILE:HA	3:A:722:HOH:O	2.16	0.45
1:B:391:LYS:N	1:B:392:PRO:CD	2.80	0.45
1:A:3:LYS:CD	1:A:344:GLU:OE1	2.64	0.45
1:B:388:HIS:HD2	1:B:391:LYS:NZ	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:LEU:HD21	1:A:413:VAL:HG21	1.98	0.44
1:B:217:ASP:OD1	1:B:255:ARG:NH1	2.50	0.44
1:A:254:ILE:O	1:A:258:ILE:HG12	2.17	0.44
1:B:162:PHE:HE1	1:B:215:LEU:HD13	1.82	0.44
1:A:185:MET:O	1:A:188:LEU:HB2	2.18	0.44
1:A:180:ALA:CB	3:A:759:HOH:O	2.56	0.44
1:B:216:VAL:O	1:B:220:ILE:CD1	2.62	0.44
1:A:366:ILE:HG21	1:A:389:ALA:HB1	2.00	0.44
1:A:183:GLU:O	1:A:187:LYS:HB2	2.18	0.43
1:B:179:ARG:NE	1:B:208:ASP:HB3	2.32	0.43
1:A:388:HIS:HD2	1:A:391:LYS:NZ	2.15	0.43
1:A:79:ARG:NH2	1:A:93:GLU:OE2	2.40	0.43
1:A:84:ASP:OD2	1:A:95:ASN:OD1	2.36	0.43
1:A:1:THR:HB	1:A:2:ILE:H	1.65	0.43
1:A:60:GLU:OE2	1:A:342:GLY:HA2	2.18	0.43
1:B:403:GLN:NE2	3:B:529:HOH:O	2.47	0.43
1:B:370:ASP:HB2	1:B:373:GLU:OE1	2.18	0.43
1:B:257:GLN:O	1:B:261:PHE:CD1	2.72	0.43
1:B:237:MET:HB3	1:B:254:ILE:HG12	2.01	0.43
1:A:162:PHE:HE1	1:A:215:LEU:CD1	2.27	0.43
1:A:39:ILE:HD12	1:A:52:LEU:HD21	2.00	0.43
2:A:472:HEM:CMB	2:A:472:HEM:HBB2	2.49	0.43
1:A:262:LEU:O	1:A:266:HIS:ND1	2.50	0.43
1:A:116:HIS:HD2	1:A:408:HIS:NE2	2.17	0.42
1:A:305:TYR:O	1:A:309:LYS:HG2	2.19	0.42
1:B:271:GLY:HA2	1:B:440:LYS:HG3	2.02	0.42
1:B:253:ASN:O	1:B:257:GLN:HG2	2.20	0.42
1:B:257:GLN:O	1:B:261:PHE:HD1	2.02	0.42
1:B:237:MET:SD	1:B:254:ILE:HG23	2.59	0.42
1:B:71:LEU:O	1:B:76:LYS:HE3	2.20	0.42
1:A:239:ASN:HB2	3:A:688:HOH:O	2.20	0.42
1:B:175:THR:HB	3:B:548:HOH:O	2.19	0.42
1:B:213:ASN:O	1:B:255:ARG:NH2	2.52	0.42
1:A:237:MET:O	1:A:254:ILE:HD11	2.20	0.42
1:A:73:GLN:CB	1:A:188:LEU:HD21	2.50	0.42
1:B:458:ILE:HG23	3:B:650:HOH:O	2.20	0.42
1:A:257:GLN:O	1:A:261:PHE:HD1	2.03	0.41
1:B:302:VAL:HG23	3:B:508:HOH:O	2.19	0.41
1:B:5:MET:HA	1:B:6:PRO:HD3	1.80	0.41
1:B:179:ARG:CD	1:B:179:ARG:C	2.88	0.41
1:B:95:ASN:HA	1:B:95:ASN:HD22	1.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:SER:HB3	1:B:179:ARG:HH21	1.86	0.41
1:B:356:LEU:HD23	1:B:359:GLN:HG3	2.01	0.41
1:A:342:GLY:O	1:A:344:GLU:HG3	2.21	0.41
1:B:5:MET:HB2	1:B:5:MET:HE3	2.01	0.41
1:B:128:GLN:O	1:B:132:ARG:HG3	2.21	0.41
1:A:388:HIS:HD2	1:A:391:LYS:HZ2	1.68	0.41
1:A:217:ASP:OD1	1:A:255:ARG:NH1	2.46	0.40
1:B:439:LEU:O	1:B:440:LYS:NZ	2.46	0.40
1:A:173:PHE:HB2	1:A:215:LEU:HD13	2.03	0.40
1:B:104:LEU:N	1:B:105:PRO:HD2	2.36	0.40
1:A:183:GLU:O	1:A:187:LYS:NZ	2.55	0.40
1:B:10:THR:HA	1:B:15:LYS:O	2.21	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	431/471 (92%)	412 (96%)	17 (4%)	2 (0%)	34	26
1	B	451/471 (96%)	419 (93%)	25 (6%)	7 (2%)	12	5
All	All	882/942 (94%)	831 (94%)	42 (5%)	9 (1%)	19	11

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	250	ASP
1	A	110	GLN
1	A	383	SER
1	B	4	GLU
1	B	263	ILE
1	B	9	LYS

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Mol	Chain	Res	Type
1	B	378	ARG
1	B	136	ASP
1	B	248	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	374/413 (91%)	357 (96%)	17 (4%)	34	29
1	B	387/413 (94%)	376 (97%)	11 (3%)	51	50
All	All	761/826 (92%)	733 (96%)	28 (4%)	41	38

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LYS
1	A	13	GLU
1	A	17	LEU
1	A	48	VAL
1	A	49	THR
1	A	148	LEU
1	A	176	SER
1	A	187	LYS
1	A	189	GLN
1	A	210	LYS
1	A	250	ASP
1	A	264	GLU
1	A	356	LEU
1	A	383	SER
1	A	437	LEU
1	A	440	LYS
1	A	455	LEU
1	B	23	ASP
1	B	49	THR
1	B	136	ASP

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Mol	Chain	Res	Type
1	B	179	ARG
1	B	183	GLU
1	B	189	GLN
1	B	203	ARG
1	B	230	SER
1	B	292	GLU
1	B	369	ASP
1	B	440	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	95	ASN
1	A	116	HIS
1	A	189	GLN
1	A	388	HIS
1	A	403	GLN
1	A	426	HIS
1	B	95	ASN
1	B	116	HIS
1	B	204	GLN
1	B	388	HIS
1	B	403	GLN
1	B	426	HIS

### 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

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	HEM	A	472	1	30,50,50	2.19	9 (30%)	24,82,82	2.58	11 (45%)
2	HEM	B	472	1,3	30,50,50	2.40	8 (26%)	24,82,82	2.65	13 (54%)

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	472	1	-	0/10/54/54	0/0/8/8
2	HEM	B	472	1,3	-	0/10/54/54	0/0/8/8

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	472	HEM	C3D-C4D	-7.44	1.42	1.51
2	B	472	HEM	C3B-C4B	-7.32	1.45	1.51
2	A	472	HEM	C3B-C4B	-5.73	1.46	1.51
2	A	472	HEM	C2C-C1C	-4.00	1.45	1.52
2	A	472	HEM	C3D-C4D	-3.61	1.46	1.51
2	B	472	HEM	C2C-C1C	-3.31	1.46	1.52
2	B	472	HEM	C2D-C1D	-2.41	1.44	1.51
2	A	472	HEM	CMB-C2B	2.03	1.57	1.53
2	B	472	HEM	C3B-CAB	2.20	1.55	1.51
2	B	472	HEM	CAA-C2A	2.33	1.56	1.52
2	B	472	HEM	CMA-C3A	2.36	1.56	1.51
2	A	472	HEM	C3C-CAC	2.62	1.56	1.51
2	A	472	HEM	FE-ND	2.91	2.12	1.97
2	A	472	HEM	FE-NB	2.98	2.13	1.97
2	B	472	HEM	FE-NC	3.53	2.09	1.95
2	A	472	HEM	C1C-NC	3.74	1.40	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	472	HEM	C4C-NC	4.55	1.41	1.36

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	472	HEM	CAA-C2A-C1A	-4.69	121.92	127.01
2	B	472	HEM	CMA-C3A-C4A	-4.51	120.90	128.36
2	A	472	HEM	C3B-CAB-CBB	-3.60	118.94	124.46
2	A	472	HEM	CBD-CAD-C3D	-3.28	103.99	113.55
2	B	472	HEM	CBA-CAA-C2A	-2.57	107.93	112.53
2	B	472	HEM	CBD-CAD-C3D	-2.56	106.11	113.55
2	A	472	HEM	C3B-C4B-NB	-2.53	106.79	111.63
2	B	472	HEM	C3C-CAC-CBC	-2.52	120.58	124.46
2	B	472	HEM	CMD-C2D-C3D	2.31	124.57	114.35
2	A	472	HEM	C2C-C1C-CHC	2.34	127.24	123.68
2	B	472	HEM	C2C-C1C-CHC	2.39	127.32	123.68
2	B	472	HEM	C2D-C3D-C4D	2.47	105.69	101.50
2	A	472	HEM	C2D-C3D-C4D	2.49	105.72	101.50
2	A	472	HEM	C1D-CHD-C4C	2.60	130.17	125.82
2	B	472	HEM	CMA-C3A-C2A	2.80	131.08	125.24
2	A	472	HEM	CAD-C3D-C4D	2.84	122.50	112.47
2	B	472	HEM	CMB-C2B-C3B	2.85	123.64	116.53
2	A	472	HEM	CMD-C2D-C3D	2.95	127.38	114.35
2	B	472	HEM	CAD-C3D-C2D	3.40	122.98	113.22
2	A	472	HEM	CMC-C2C-C3C	4.23	127.08	116.53
2	A	472	HEM	CMB-C2B-C3B	4.48	127.71	116.53
2	B	472	HEM	CMC-C2C-C3C	5.16	129.40	116.53
2	B	472	HEM	CAD-C3D-C4D	5.34	131.31	112.47
2	A	472	HEM	CAD-C3D-C2D	6.39	131.60	113.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	472	HEM	3	0
2	B	472	HEM	2	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	439/471 (93%)	0.17	27 (6%) 24 25	24, 39, 66, 76	0
1	B	455/471 (96%)	0.57	58 (12%) 5 5	32, 49, 75, 82	0
All	All	894/942 (94%)	0.38	85 (9%) 10 11	24, 44, 72, 82	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	225	ALA	9.8
1	B	458	ILE	6.8
1	B	110	GLN	5.9
1	B	211	VAL	5.3
1	A	2	ILE	5.2
1	A	205	PHE	5.2
1	B	2	ILE	5.1
1	A	1	THR	5.0
1	B	214	ASP	4.9
1	B	243	PRO	4.7
1	A	209	ILE	4.6
1	B	225	ALA	4.5
1	A	191	ALA	4.4
1	B	11	PHE	4.3
1	A	245	THR	4.3
1	B	229	GLN	4.2
1	B	231	ASP	4.0
1	B	182	ASP	4.0
1	B	204	GLN	3.9
1	B	192	ASN	3.9
1	B	180	ALA	3.7
1	B	457	GLY	3.7
1	B	203	ARG	3.7
1	A	211	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	181	LEU	3.6
1	A	204	GLN	3.4
1	B	285	HIS	3.4
1	B	194	ASP	3.4
1	B	169	GLN	3.3
1	B	23	ASP	3.3
1	A	192	ASN	3.2
1	A	46	GLY	3.1
1	B	21	ASN	3.1
1	B	209	ILE	3.1
1	B	136	ASP	3.0
1	B	244	GLU	3.0
1	B	174	ILE	2.9
1	B	212	MET	2.8
1	B	191	ALA	2.8
1	A	219	ILE	2.8
1	A	456	GLY	2.7
1	A	212	MET	2.7
1	B	382	PRO	2.7
1	B	108	SER	2.7
1	A	231	ASP	2.7
1	B	208	ASP	2.7
1	B	384	ALA	2.7
1	B	221	ALA	2.6
1	B	4	GLU	2.6
1	B	444	PHE	2.6
1	A	251	ASP	2.6
1	B	226	SER	2.6
1	B	175	THR	2.6
1	B	239	ASN	2.6
1	B	242	ASP	2.5
1	B	245	THR	2.5
1	A	206	GLN	2.5
1	A	105	PRO	2.5
1	B	369	ASP	2.5
1	B	10	THR	2.5
1	A	208	ASP	2.5
1	A	437	LEU	2.4
1	B	13	GLU	2.4
1	B	196	PRO	2.4
1	B	215	LEU	2.3
1	B	206	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	198	TYR	2.2
1	A	454	PRO	2.2
1	A	224	LYS	2.2
1	B	46	GLY	2.2
1	B	249	LEU	2.2
1	B	177	MET	2.2
1	A	221	ALA	2.2
1	A	252	GLU	2.1
1	B	383	SER	2.1
1	B	210	LYS	2.1
1	B	197	ALA	2.1
1	B	428	ASN	2.1
1	B	8	PRO	2.1
1	A	186	ASN	2.1
1	B	246	GLY	2.1
1	B	12	GLY	2.0
1	A	77	PHE	2.0
1	B	186	ASN	2.0
1	A	216	VAL	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
2	HEM	A	472	43/43	0.98	0.11	0.08	21,27,29,36	0
2	HEM	B	472	43/43	0.98	0.11	-0.05	29,34,37,41	0

## 6.5 Other polymers

There are no such residues in this entry.