



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 04:14 am GMT

PDB ID : 1MPW  
Title : Molecular Recognition in (+)- $\alpha$ -Pinene Oxidation by Cytochrome P450cam  
Authors : Bell, S.G.; Chen, X.; Sowden, R.J.; Xu, F.; Willams, J.N.; Wong, L.-L.; Rao, Z.  
Deposited on : 2002-09-13  
Resolution : 2.34 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

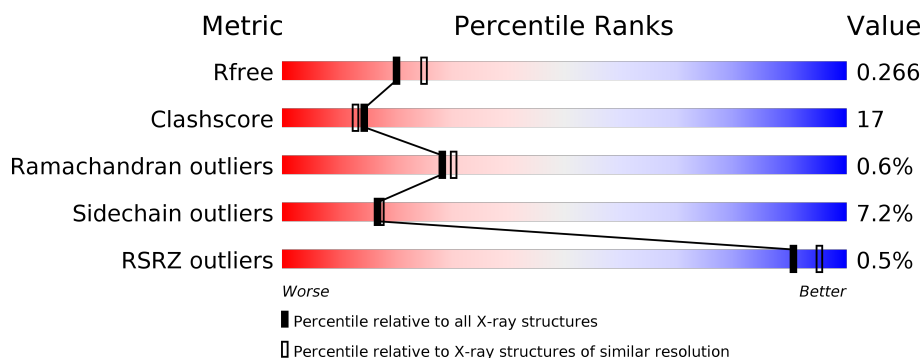
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.34 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))
$R_{free}$	100719	1570 (2.36-2.32)
Clashscore	112137	1673 (2.36-2.32)
Ramachandran outliers	110173	1654 (2.36-2.32)
Sidechain outliers	110143	1655 (2.36-2.32)
RSRZ outliers	101464	1576 (2.36-2.32)

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	414	
1	B	414	

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	TMH	A	1450	-	-	X	X
4	TMH	B	450	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6635 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 P450CAM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	405	Total	C	N	O	S	0	0	0
			3210	2036	561	596	17			
1	B	405	Total	C	N	O	S	0	0	0
			3210	2036	561	596	17			

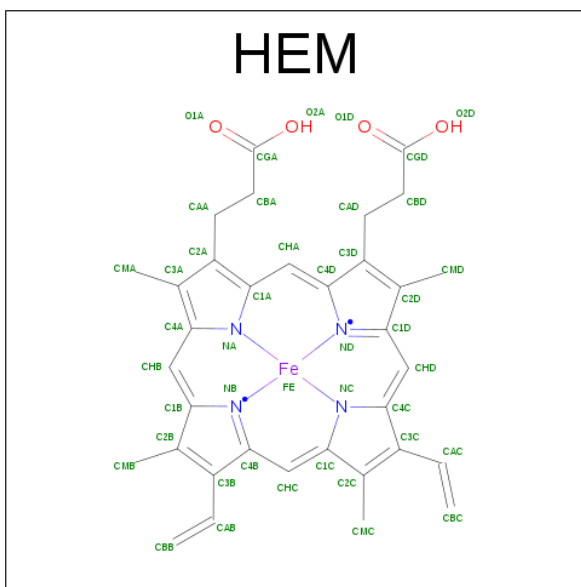
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	87	TRP	PHE	ENGINEERED	UNP P00183
A	96	PHE	TYR	ENGINEERED	UNP P00183
A	247	LEU	VAL	ENGINEERED	UNP P00183
A	334	ALA	CYS	ENGINEERED	UNP P00183
B	87	TRP	PHE	ENGINEERED	UNP P00183
B	96	PHE	TYR	ENGINEERED	UNP P00183
B	247	LEU	VAL	ENGINEERED	UNP P00183
B	334	ALA	CYS	ENGINEERED	UNP P00183

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

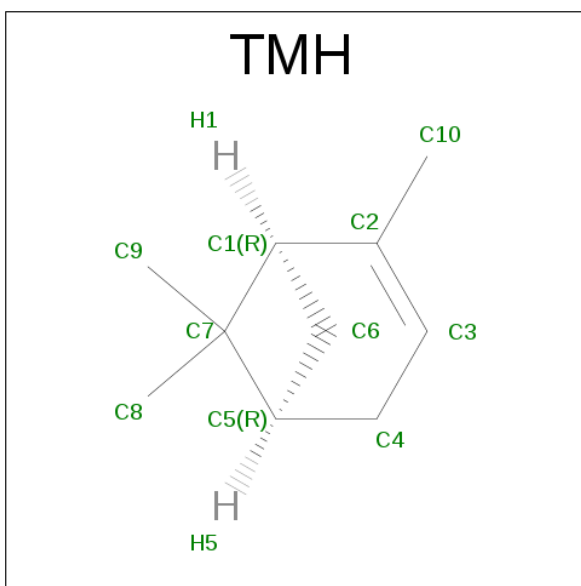
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	K	0	0
			1	1		
2	A	1	Total	K	0	0
			1	1		

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).



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

- Molecule 4 is (+)-ALPHA-PINENE (three-letter code: TMH) (formula: C<sub>10</sub>H<sub>16</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	C	0	0
			10	10		
4	A	1	Total	C	0	0
			10	10		

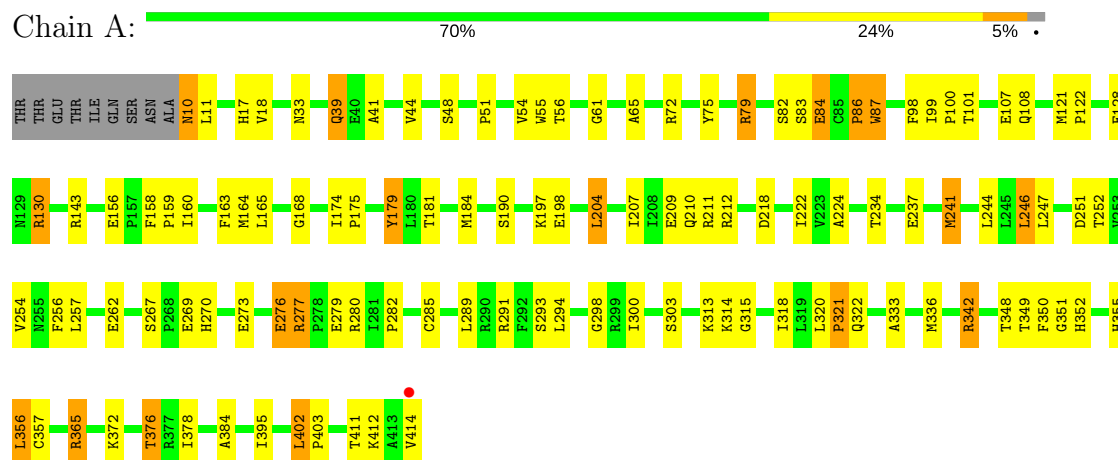
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	66	Total 66	O 66	0	0
5	B	41	Total 41	O 41	0	0

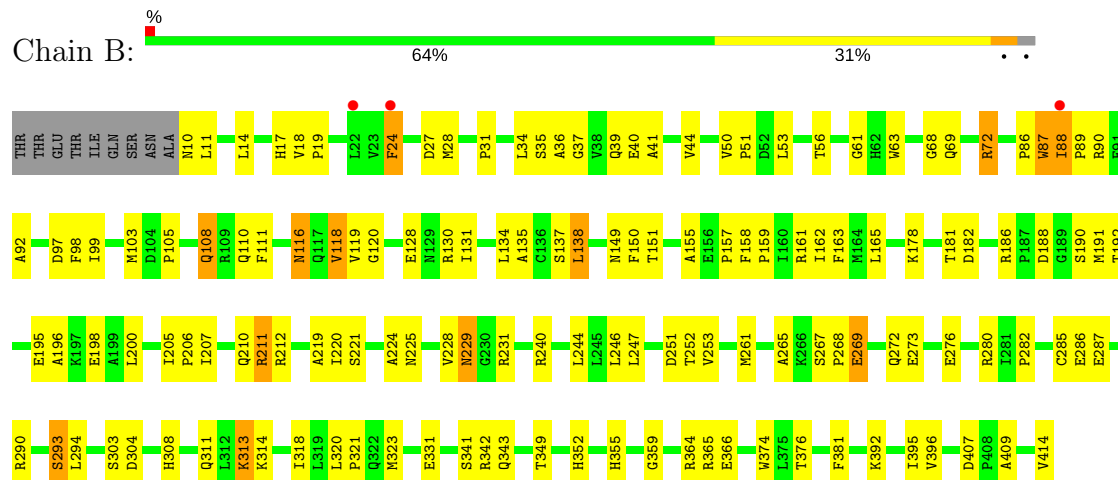
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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 P450CAM



#### • Molecule 1: CYTOCHROME P450CAM



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.90Å 62.52Å 95.70Å 90.00° 90.28° 90.00°	Depositor
Resolution (Å)	41.28 – 2.34 41.28 – 2.34	Depositor EDS
% Data completeness (in resolution range)	94.7 (41.28-2.34) 94.7 (41.28-2.34)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.27 (at 2.34Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.204 , 0.269 0.202 , 0.266	Depositor DCC
$R_{free}$ test set	3186 reflections (11.09%)	DCC
Wilson B-factor (Å <sup>2</sup> )	20.7	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 35.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	6635	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.07% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: TMH, HEM, K

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	0.73	1/3290 (0.0%)	0.83	1/4470 (0.0%)
1	B	0.71	0/3290	0.84	2/4470 (0.0%)
All	All	0.72	1/6580 (0.0%)	0.84	3/8940 (0.0%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	GLU	CG-CD	5.47	1.60	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	72	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	B	407	ASP	CB-CG-OD2	5.05	122.84	118.30
1	B	72	ARG	NE-CZ-NH1	-5.03	117.78	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	179	TYR	Sidechain

## 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	3210	0	3159	86	0
1	B	3210	0	3159	134	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	43	0	30	3	0
3	B	43	0	30	2	0
4	A	10	0	16	7	0
4	B	10	0	16	5	0
5	A	66	0	0	2	0
5	B	41	0	0	2	0
All	All	6635	0	6410	223	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 17.

All (223) 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:273:GLU:HG3	1:A:280:ARG:HH21	1.24	0.98
1:A:277:ARG:HH11	1:A:277:ARG:HG2	1.31	0.94
1:B:163:PHE:HE2	1:B:246:LEU:HD23	1.34	0.93
1:B:69:GLN:HE21	1:B:308:HIS:HE1	1.22	0.86
1:A:333:ALA:O	1:A:342:ARG:NH2	2.12	0.83
1:A:128:GLU:OE2	1:A:365:ARG:HD3	1.82	0.80
1:B:69:GLN:NE2	1:B:308:HIS:HE1	1.80	0.79
1:A:101:THR:OG1	1:A:244:LEU:HD21	1.82	0.79
1:B:158:PHE:HB3	1:B:159:PRO:HD3	1.65	0.79
1:B:287:GLU:OE2	1:B:342:ARG:NH1	2.16	0.78
1:A:273:GLU:HG3	1:A:280:ARG:NH2	1.99	0.78
1:B:268:PRO:HD2	1:B:269:GLU:OE2	1.84	0.77
1:B:88:ILE:HG22	1:B:89:PRO:HD3	1.68	0.75
1:A:247:LEU:HG	4:A:1450:TMH:H42	1.70	0.74
1:A:273:GLU:CG	1:A:280:ARG:HH21	2.00	0.72
1:B:252:THR:HG21	4:B:450:TMH:H3	1.73	0.71
1:B:414:VAL:HG12	1:B:414:VAL:O	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:ARG:HH11	1:A:79:ARG:HG3	1.58	0.69
1:A:107:GLU:H	1:A:107:GLU:CD	1.96	0.69
1:B:69:GLN:HE21	1:B:308:HIS:CE1	2.09	0.69
1:B:163:PHE:CE2	1:B:246:LEU:HD23	2.24	0.68
1:B:228:VAL:O	1:B:229:ASN:HB3	1.94	0.68
1:B:252:THR:CG2	4:B:450:TMH:H3	2.24	0.68
1:B:181:THR:HG23	1:B:247:LEU:HD12	1.75	0.67
1:B:88:ILE:HG22	1:B:89:PRO:CD	2.24	0.67
1:B:97:ASP:O	1:B:240:ARG:HD2	1.95	0.66
1:A:277:ARG:HG2	1:A:277:ARG:NH1	2.06	0.65
1:A:33:ASN:HB3	1:A:41:ALA:HA	1.78	0.65
1:B:303:SER:HA	1:B:314:LYS:HB2	1.78	0.65
1:B:191:MET:CE	1:B:196:ALA:HA	2.27	0.64
1:B:273:GLU:HG2	1:B:280:ARG:NH1	2.12	0.64
1:A:244:LEU:HD11	4:A:1450:TMH:H41	1.79	0.64
1:B:165:LEU:C	1:B:165:LEU:HD23	2.18	0.64
3:A:417:HEM:HBA1	4:A:1450:TMH:H92	1.80	0.63
1:B:157:PRO:O	1:B:161:ARG:HG3	1.99	0.62
1:A:277:ARG:HD2	1:A:279:GLU:OE2	1.99	0.62
1:B:191:MET:HE2	1:B:196:ALA:N	2.14	0.62
1:B:200:LEU:HD11	1:B:246:LEU:HD12	1.83	0.61
1:B:228:VAL:O	1:B:228:VAL:HG23	2.00	0.61
1:A:269:GLU:HB2	5:A:1493:HOH:O	2.00	0.61
1:A:156:GLU:HA	1:A:254:VAL:HG22	1.82	0.61
1:B:88:ILE:CG2	1:B:89:PRO:N	2.64	0.60
1:B:88:ILE:O	1:B:90:ARG:N	2.35	0.60
1:B:293:SER:HB3	1:B:323:MET:HA	1.84	0.60
1:B:191:MET:HE1	1:B:196:ALA:HA	1.83	0.59
1:B:269:GLU:CD	1:B:269:GLU:H	2.06	0.58
1:B:87:TRP:CZ2	1:B:395:ILE:HG21	2.39	0.57
1:B:130:ARG:NH1	1:B:165:LEU:CD1	2.67	0.57
1:B:376:THR:HG22	1:B:414:VAL:HG21	1.86	0.57
1:A:218:ASP:O	1:A:222:ILE:HG12	2.05	0.57
1:B:110:GLN:NE2	1:B:229:ASN:HA	2.19	0.56
3:A:417:HEM:ND	4:A:1450:TMH:H103	2.20	0.56
1:B:98:PHE:HB3	1:B:244:LEU:HB2	1.86	0.56
1:A:39:GLN:NE2	1:A:39:GLN:H	2.03	0.56
1:A:303:SER:HA	1:A:314:LYS:HB2	1.87	0.56
1:A:41:ALA:O	1:A:44:VAL:HG22	2.05	0.56
1:B:131:ILE:HG12	1:B:162:ILE:HD13	1.87	0.56
1:A:181:THR:CG2	1:A:251:ASP:HB2	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:ILE:HG13	1:B:240:ARG:HB3	1.88	0.56
1:B:205:ILE:HB	1:B:206:PRO:HD3	1.89	0.55
1:A:322:GLN:HB3	1:A:348:THR:O	2.06	0.55
1:B:88:ILE:O	1:B:89:PRO:C	2.42	0.55
1:A:18:VAL:HG11	1:A:55:TRP:CG	2.42	0.55
1:B:294:LEU:HD23	1:B:294:LEU:H	1.72	0.55
1:B:72:ARG:HH11	1:B:72:ARG:HG3	1.71	0.55
1:B:253:VAL:HG11	1:B:366:GLU:OE1	2.07	0.55
1:A:349:THR:HG23	5:A:1472:HOH:O	2.07	0.55
1:A:51:PRO:HG2	1:A:54:VAL:HG12	1.90	0.54
1:A:234:THR:HG23	1:A:237:GLU:OE2	2.06	0.54
1:A:291:ARG:CZ	1:A:336:MET:CE	2.85	0.54
1:B:105:PRO:HG3	1:B:108:GLN:NE2	2.23	0.54
1:B:191:MET:HE2	1:B:196:ALA:CA	2.37	0.53
1:A:121:MET:HB3	1:A:122:PRO:HD3	1.90	0.53
1:A:244:LEU:CD1	4:A:1450:TMH:H41	2.36	0.53
1:B:134:LEU:HG	1:B:138:LEU:HD22	1.90	0.53
1:B:290:ARG:NH2	1:B:342:ARG:NH1	2.57	0.53
1:B:244:LEU:HD11	4:B:450:TMH:H62	1.91	0.53
1:A:86:PRO:HA	1:A:298:GLY:O	2.08	0.53
1:A:276:GLU:O	1:A:277:ARG:HD3	2.08	0.52
1:B:294:LEU:N	1:B:294:LEU:HD23	2.24	0.52
1:B:188:ASP:OD1	1:B:190:SER:CB	2.58	0.52
1:A:212:ARG:NH2	1:A:224:ALA:O	2.43	0.52
1:B:68:GLY:HA3	1:B:331:GLU:OE2	2.10	0.52
1:B:28:MET:CE	1:B:395:ILE:HD13	2.41	0.51
1:B:376:THR:CG2	1:B:414:VAL:HG21	2.40	0.51
1:B:396:VAL:CG2	4:B:450:TMH:H103	2.40	0.51
1:B:150:PHE:CE2	1:B:155:ALA:HB2	2.45	0.51
1:A:294:LEU:H	1:A:294:LEU:HD23	1.75	0.51
1:B:323:MET:HG2	1:B:323:MET:O	2.10	0.51
1:B:228:VAL:O	1:B:228:VAL:CG2	2.59	0.51
1:A:17:HIS:CD2	1:A:313:LYS:HG2	2.46	0.50
1:A:378:ILE:HG22	1:A:378:ILE:O	2.11	0.50
1:B:188:ASP:OD1	1:B:190:SER:HB2	2.12	0.50
1:B:228:VAL:O	1:B:229:ASN:CB	2.60	0.50
1:A:158:PHE:HB3	1:A:159:PRO:CD	2.42	0.50
1:B:205:ILE:CB	1:B:206:PRO:HD3	2.42	0.50
1:A:212:ARG:HG3	1:A:224:ALA:HB1	1.93	0.49
1:B:396:VAL:HG21	4:B:450:TMH:H103	1.93	0.49
1:B:192:THR:OG1	1:B:195:GLU:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:PRO:HD2	1:A:244:LEU:HD23	1.93	0.49
1:A:291:ARG:CZ	1:A:336:MET:HE3	2.42	0.49
1:B:228:VAL:O	1:B:231:ARG:HG3	2.12	0.49
1:B:273:GLU:CG	1:B:280:ARG:HH12	2.25	0.49
1:B:34:LEU:O	1:B:36:ALA:N	2.45	0.49
1:B:11:LEU:N	1:B:11:LEU:HD22	2.27	0.48
1:B:72:ARG:NH1	1:B:72:ARG:HG3	2.28	0.48
1:B:37:GLY:HA3	1:B:40:GLU:OE2	2.13	0.48
1:B:17:HIS:O	1:B:19:PRO:HD3	2.13	0.48
1:B:318:ILE:O	1:B:318:ILE:HG23	2.13	0.48
1:B:186:ARG:HD2	1:B:392:LYS:HB3	1.96	0.48
1:B:244:LEU:O	1:B:244:LEU:HG	2.13	0.48
1:B:304:ASP:N	1:B:314:LYS:HB2	2.28	0.48
1:A:291:ARG:CZ	1:A:336:MET:HE1	2.43	0.48
1:A:99:ILE:O	1:A:241:MET:HA	2.14	0.48
1:B:103:MET:O	1:B:355:HIS:CE1	2.67	0.48
1:B:191:MET:HE2	1:B:196:ALA:HA	1.96	0.48
1:B:365:ARG:HD3	5:B:1455:HOH:O	2.13	0.48
1:B:151:THR:HA	1:B:155:ALA:HB3	1.96	0.48
1:B:56:THR:O	1:B:61:GLY:HA2	2.14	0.48
1:A:39:GLN:HE21	1:A:39:GLN:H	1.60	0.48
1:B:88:ILE:HG22	1:B:89:PRO:N	2.27	0.48
1:A:160:ILE:O	1:A:164:MET:HG2	2.14	0.48
1:B:135:ALA:HB2	1:B:158:PHE:CE1	2.49	0.48
1:B:303:SER:CA	1:B:314:LYS:HB2	2.43	0.47
1:A:294:LEU:N	1:A:294:LEU:HD23	2.28	0.47
1:A:56:THR:O	1:A:61:GLY:HA2	2.14	0.47
1:B:150:PHE:CE1	1:B:261:MET:HG2	2.50	0.47
1:B:31:PRO:HB2	1:B:41:ALA:HB1	1.95	0.47
3:B:417:HEM:HMB1	3:B:417:HEM:HBB2	1.95	0.47
1:B:212:ARG:HA	1:B:225:ASN:HD21	1.80	0.47
1:B:318:ILE:HD13	1:B:320:LEU:HD21	1.95	0.47
1:B:72:ARG:HD3	1:B:352:HIS:CE1	2.50	0.47
1:B:14:LEU:HD11	1:B:18:VAL:HG11	1.96	0.47
1:A:267:SER:HB2	1:A:270:HIS:HB2	1.96	0.46
1:A:282:PRO:O	1:A:285:CYS:HB3	2.15	0.46
1:B:212:ARG:HG3	1:B:224:ALA:HB1	1.98	0.46
1:A:322:GLN:HG2	1:A:351:GLY:HA2	1.97	0.46
1:B:261:MET:HE2	1:B:374:TRP:CD2	2.51	0.46
1:A:168:GLY:O	1:A:211:ARG:NH2	2.48	0.46
1:B:69:GLN:NE2	1:B:308:HIS:CE1	2.71	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:TYR:HB3	1:A:352:HIS:O	2.16	0.46
1:B:313:LYS:HG3	1:B:314:LYS:N	2.30	0.46
1:B:89:PRO:O	1:B:92:ALA:N	2.48	0.46
1:B:272:GLN:O	1:B:276:GLU:HG3	2.16	0.45
1:A:101:THR:HG21	4:A:1450:TMH:H91	1.98	0.45
1:A:87:TRP:CH2	1:A:395:ILE:HG21	2.51	0.45
1:B:118:VAL:HG22	5:B:1433:HOH:O	2.17	0.45
1:A:79:ARG:NH1	1:A:79:ARG:HG3	2.29	0.45
1:A:83:SER:O	1:A:86:PRO:HD3	2.16	0.45
1:B:87:TRP:CH2	1:B:395:ILE:HG21	2.51	0.45
1:A:355:HIS:HD1	3:A:417:HEM:CGD	2.30	0.45
1:A:181:THR:HG21	1:A:251:ASP:HB2	1.99	0.45
1:A:384:ALA:HB3	1:A:403:PRO:HB2	1.99	0.45
1:B:88:ILE:HD12	1:B:88:ILE:HA	1.75	0.45
1:A:262:GLU:CA	1:A:402:LEU:HD11	2.47	0.45
1:A:384:ALA:CB	1:A:403:PRO:HB2	2.47	0.45
1:B:273:GLU:CG	1:B:280:ARG:NH1	2.78	0.45
1:B:63:TRP:HB2	1:B:318:ILE:HG13	1.99	0.45
1:A:350:PHE:HB3	1:A:357:CYS:HB3	1.99	0.44
1:B:293:SER:CB	1:B:323:MET:HA	2.46	0.44
1:B:303:SER:HA	1:B:314:LYS:CG	2.47	0.44
1:B:14:LEU:HD11	1:B:18:VAL:CG1	2.48	0.44
1:A:184:MET:CE	1:A:197:LYS:HB2	2.48	0.44
1:B:287:GLU:CD	1:B:342:ARG:HH11	2.21	0.44
1:B:290:ARG:NH2	1:B:342:ARG:HH12	2.15	0.44
1:B:303:SER:O	1:B:304:ASP:C	2.56	0.44
1:B:99:ILE:HG21	1:B:111:PHE:CD2	2.53	0.44
1:A:174:ILE:HB	1:A:175:PRO:HD3	2.00	0.43
1:B:178:LYS:HE3	1:B:182:ASP:OD1	2.19	0.43
1:B:116:ASN:ND2	1:B:120:GLY:HA3	2.33	0.43
1:B:24:PHE:C	1:B:24:PHE:CD2	2.91	0.43
1:A:262:GLU:HA	1:A:402:LEU:HD11	2.01	0.43
1:B:303:SER:HA	1:B:314:LYS:CB	2.46	0.43
1:B:89:PRO:HD2	1:B:92:ALA:HB3	2.01	0.43
1:B:265:ALA:HB2	1:B:381:PHE:HE1	1.83	0.43
1:B:181:THR:HG21	1:B:251:ASP:HB2	2.01	0.43
1:B:294:LEU:N	1:B:294:LEU:CD2	2.82	0.43
1:A:163:PHE:CE2	1:A:246:LEU:HD13	2.53	0.42
1:B:290:ARG:HH21	1:B:342:ARG:NH1	2.18	0.42
1:B:108:GLN:HB3	1:B:108:GLN:HE21	1.61	0.42
1:B:50:VAL:HA	1:B:51:PRO:HD3	1.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:LEU:HA	1:A:257:LEU:HD23	1.85	0.42
1:B:359:GLY:HA3	3:B:417:HEM:C3C	2.54	0.42
1:B:130:ARG:NH1	1:B:165:LEU:HD11	2.34	0.42
1:B:118:VAL:HG22	1:B:219:ALA:HA	2.02	0.42
1:A:204:LEU:O	1:A:207:ILE:N	2.46	0.42
1:A:130:ARG:HE	1:A:130:ARG:HB3	1.34	0.42
1:A:98:PHE:HB3	1:A:244:LEU:HB2	2.01	0.42
1:B:28:MET:HE1	1:B:395:ILE:HD13	2.02	0.42
1:B:211:ARG:HG2	1:B:221:SER:OG	2.18	0.41
1:B:28:MET:HE2	1:B:395:ILE:HD13	2.01	0.41
1:A:10:ASN:N	1:A:10:ASN:OD1	2.52	0.41
1:A:56:THR:HG23	1:A:56:THR:O	2.20	0.41
1:A:289:LEU:HA	1:A:289:LEU:HD23	1.89	0.41
1:B:34:LEU:HD12	1:B:34:LEU:HA	1.73	0.41
1:A:101:THR:OG1	1:A:244:LEU:CD2	2.62	0.41
1:B:188:ASP:OD1	1:B:190:SER:HB3	2.20	0.41
1:A:252:THR:HG21	4:A:1450:TMH:H102	2.03	0.41
1:A:179:TYR:HH	1:A:190:SER:HG	1.66	0.41
1:A:279:GLU:OE1	1:A:279:GLU:N	2.39	0.41
1:B:105:PRO:HG3	1:B:108:GLN:HE22	1.84	0.41
1:B:341:SER:O	1:B:342:ARG:C	2.59	0.41
1:A:277:ARG:CG	1:A:277:ARG:NH1	2.77	0.41
1:B:63:TRP:CB	1:B:318:ILE:HG13	2.51	0.41
1:B:72:ARG:HH12	1:B:331:GLU:CD	2.18	0.41
1:B:286:GLU:OE1	1:B:364:ARG:NH1	2.53	0.41
1:A:267:SER:CB	1:A:270:HIS:HB2	2.50	0.41
1:A:372:LYS:O	1:A:376:THR:HB	2.20	0.41
1:A:65:ALA:HB3	1:A:320:LEU:HD23	2.02	0.41
1:B:41:ALA:O	1:B:44:VAL:HG22	2.21	0.41
1:A:82:SER:OG	1:A:84:GLU:HB2	2.21	0.41
1:B:10:ASN:C	1:B:11:LEU:HD22	2.41	0.41
1:B:118:VAL:HG12	1:B:119:VAL:HG13	2.03	0.41
1:A:300:ILE:HD11	1:A:315:GLY:HA2	2.03	0.40
1:B:293:SER:OG	1:B:349:THR:OG1	2.35	0.40
1:B:251:ASP:OD1	1:B:251:ASP:O	2.39	0.40
1:A:321:PRO:O	1:A:322:GLN:C	2.59	0.40
1:B:207:ILE:HA	1:B:210:GLN:HG2	2.03	0.40
1:B:27:ASP:C	1:B:27:ASP:OD1	2.60	0.40
1:A:256:PHE:CZ	1:A:289:LEU:HD23	2.57	0.40
1:A:318:ILE:HG23	1:A:318:ILE:O	2.21	0.40
1:A:143:ARG:HD2	1:A:411:THR:HB	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:LEU:HA	1:A:356:LEU:HD12	1.85	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	403/414 (97%)	381 (94%)	20 (5%)	2 (0%)	32	35
1	B	403/414 (97%)	362 (90%)	38 (9%)	3 (1%)	25	26
All	All	806/828 (97%)	743 (92%)	58 (7%)	5 (1%)	28	30

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	35	SER
1	B	409	ALA
1	A	48	SER
1	B	321	PRO
1	A	321	PRO

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	349/357 (98%)	324 (93%)	25 (7%)	17	17
1	B	349/357 (98%)	324 (93%)	25 (7%)	17	17
All	All	698/714 (98%)	648 (93%)	50 (7%)	17	17

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	11	LEU
1	A	39	GLN
1	A	79	ARG
1	A	84	GLU
1	A	86	PRO
1	A	87	TRP
1	A	108	GLN
1	A	130	ARG
1	A	165	LEU
1	A	204	LEU
1	A	209	GLU
1	A	210	GLN
1	A	241	MET
1	A	246	LEU
1	A	276	GLU
1	A	277	ARG
1	A	293	SER
1	A	342	ARG
1	A	356	LEU
1	A	365	ARG
1	A	376	THR
1	A	402	LEU
1	A	412	LYS
1	A	414	VAL
1	B	24	PHE
1	B	39	GLN
1	B	53	LEU
1	B	86	PRO
1	B	87	TRP
1	B	88	ILE
1	B	108	GLN

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Mol	Chain	Res	Type
1	B	116	ASN
1	B	118	VAL
1	B	128	GLU
1	B	137	SER
1	B	138	LEU
1	B	149	ASN
1	B	198	GLU
1	B	211	ARG
1	B	220	ILE
1	B	229	ASN
1	B	267	SER
1	B	269	GLU
1	B	282	PRO
1	B	285	CYS
1	B	293	SER
1	B	311	GLN
1	B	313	LYS
1	B	343	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	46	GLN
1	A	108	GLN
1	A	110	GLN
1	A	129	ASN
1	A	132	GLN
1	A	213	GLN
1	A	225	ASN
1	A	270	HIS
1	A	272	GLN
1	B	39	GLN
1	B	46	GLN
1	B	59	ASN
1	B	69	GLN
1	B	108	GLN
1	B	110	GLN
1	B	116	ASN
1	B	132	GLN
1	B	149	ASN
1	B	225	ASN

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Mol	Chain	Res	Type
1	B	229	ASN
1	B	308	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 ⓘ

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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$
4	TMH	A	1450	-	11,11,11	2.79	7 (63%)	18,18,18	5.57	8 (44%)
3	HEM	A	417	1	28,50,50	2.70	11 (39%)	17,82,82	2.32	7 (41%)
3	HEM	B	417	1	28,50,50	2.49	11 (39%)	17,82,82	2.17	7 (41%)
4	TMH	B	450	-	11,11,11	2.84	7 (63%)	18,18,18	5.15	7 (38%)

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
4	TMH	A	1450	-	-	0/0/25/25	0/0/2/2
3	HEM	A	417	1	-	0/6/54/54	0/0/8/8
3	HEM	B	417	1	-	0/6/54/54	0/0/8/8
4	TMH	B	450	-	-	0/0/25/25	0/0/2/2

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	417	HEM	C3B-C2B	-6.32	1.32	1.40
3	A	417	HEM	C3B-C2B	-5.40	1.33	1.40
3	B	417	HEM	C3C-C2C	-5.08	1.33	1.40
4	A	1450	TMH	C10-C2	-3.33	1.44	1.50
4	B	450	TMH	C10-C2	-2.95	1.45	1.50
3	A	417	HEM	C3C-C2C	-2.92	1.36	1.40
3	A	417	HEM	C4C-NC	-2.02	1.34	1.36
3	A	417	HEM	C4A-NA	2.07	1.40	1.36
3	B	417	HEM	CMC-C2C	2.10	1.56	1.51
3	B	417	HEM	C4B-NB	2.26	1.41	1.36
4	A	1450	TMH	C3-C2	2.34	1.37	1.32
3	B	417	HEM	CMD-C2D	2.38	1.56	1.51
4	A	1450	TMH	C4-C3	2.48	1.55	1.50
3	A	417	HEM	C4B-NB	2.48	1.41	1.36
4	B	450	TMH	C4-C3	2.59	1.55	1.50
3	B	417	HEM	C4A-NA	2.63	1.41	1.36
3	B	417	HEM	C1C-NC	2.66	1.39	1.36
3	B	417	HEM	CAD-C3D	2.67	1.57	1.52
3	A	417	HEM	CMD-C2D	2.96	1.57	1.51
4	A	1450	TMH	C6-C1	3.06	1.63	1.55
4	A	1450	TMH	C6-C5	3.08	1.64	1.54
4	B	450	TMH	C6-C5	3.17	1.64	1.54
4	B	450	TMH	C3-C2	3.28	1.39	1.32
3	B	417	HEM	CAA-C2A	3.36	1.57	1.52
3	A	417	HEM	CMC-C2C	3.60	1.59	1.51
3	A	417	HEM	CAA-C2A	3.66	1.58	1.52
4	B	450	TMH	C4-C5	3.75	1.60	1.52
4	B	450	TMH	C6-C1	3.80	1.65	1.55
4	A	1450	TMH	C4-C5	3.95	1.61	1.52
4	B	450	TMH	C1-C2	4.64	1.59	1.52
3	A	417	HEM	C1C-NC	4.73	1.42	1.36
3	A	417	HEM	C3B-CAB	4.80	1.57	1.47
3	B	417	HEM	C3B-CAB	4.85	1.57	1.47
3	B	417	HEM	C3C-CAC	4.87	1.57	1.47
4	A	1450	TMH	C1-C2	5.03	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	417	HEM	C3C-CAC	7.36	1.62	1.47

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1450	TMH	C6-C1-C2	-9.72	99.54	107.05
4	B	450	TMH	C6-C1-C2	-7.59	101.19	107.05
4	A	1450	TMH	C4-C3-C2	-5.58	116.45	124.84
4	B	450	TMH	C1-C6-C5	-5.08	78.07	86.95
4	B	450	TMH	C4-C3-C2	-4.94	117.41	124.84
4	A	1450	TMH	C1-C6-C5	-4.90	78.38	86.95
4	A	1450	TMH	C6-C5-C4	-4.72	103.23	108.95
4	B	450	TMH	C6-C5-C4	-4.30	103.73	108.95
3	A	417	HEM	CMA-C3A-C4A	-4.09	122.18	128.46
3	B	417	HEM	CMA-C3A-C4A	-3.04	123.79	128.46
3	A	417	HEM	CMD-C2D-C1D	-3.02	123.83	128.46
3	B	417	HEM	CMD-C2D-C1D	-2.60	124.47	128.46
4	B	450	TMH	C1-C2-C3	-2.22	116.78	121.46
4	A	1450	TMH	C1-C2-C3	-2.12	116.99	121.46
3	B	417	HEM	CMD-C2D-C3D	2.03	128.76	124.94
4	A	1450	TMH	C9-C7-C1	2.20	123.20	114.97
3	B	417	HEM	CMA-C3A-C2A	2.53	129.71	124.94
3	A	417	HEM	CMD-C2D-C3D	2.74	130.12	124.94
3	A	417	HEM	CMA-C3A-C2A	2.89	130.40	124.94
3	B	417	HEM	CBA-CAA-C2A	3.15	118.51	112.48
3	A	417	HEM	CBA-CAA-C2A	3.26	118.71	112.48
3	B	417	HEM	CMB-C2B-C3B	3.44	131.27	124.89
3	A	417	HEM	CMB-C2B-C3B	3.53	131.44	124.89
3	A	417	HEM	CBD-CAD-C3D	4.27	120.62	112.47
3	B	417	HEM	CBD-CAD-C3D	4.81	121.64	112.47
4	A	1450	TMH	C4-C5-C7	9.04	121.40	111.03
4	B	450	TMH	C4-C5-C7	10.28	122.81	111.03
4	B	450	TMH	C7-C1-C2	15.06	121.29	109.53
4	A	1450	TMH	C7-C1-C2	16.96	122.78	109.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1450	TMH	7	0
3	A	417	HEM	3	0
3	B	417	HEM	2	0
4	B	450	TMH	5	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	405/414 (97%)	-0.36	1 (0%) 94 97	6, 17, 31, 43	0
1	B	405/414 (97%)	-0.16	3 (0%) 87 92	12, 22, 37, 44	0
All	All	810/828 (97%)	-0.26	4 (0%) 90 95	6, 20, 35, 44	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	24	PHE	3.1
1	B	88	ILE	3.0
1	A	414	VAL	2.4
1	B	22	LEU	2.1

### 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( $\text{\AA}^2$ )	Q<0.9
4	TMH	B	450	10/10	0.84	0.21	7.03	30,31,32,32	0
4	TMH	A	1450	10/10	0.85	0.23	4.40	33,33,36,36	0
3	HEM	B	417	43/43	0.97	0.13	0.34	11,15,20,22	0
3	HEM	A	417	43/43	0.98	0.11	-0.23	2,8,14,19	0
2	K	A	418	1/1	0.97	0.11	-0.54	22,22,22,22	0
2	K	B	1418	1/1	0.97	0.07	-1.19	24,24,24,24	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.