



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 07:23 pm GMT

PDB ID : 3OFT  
Title : Crystal Structure of Cytochrome P450 CYP101C1  
Authors : Zhou, W.; Ma, M.; Bell, S.G.; Yang, W.; Hao, Y.; Rees, N.H.; Bartlam, M.;  
Wong, L.-L.; Rao, Z.  
Deposited on : 2010-08-16  
Resolution : 1.90 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

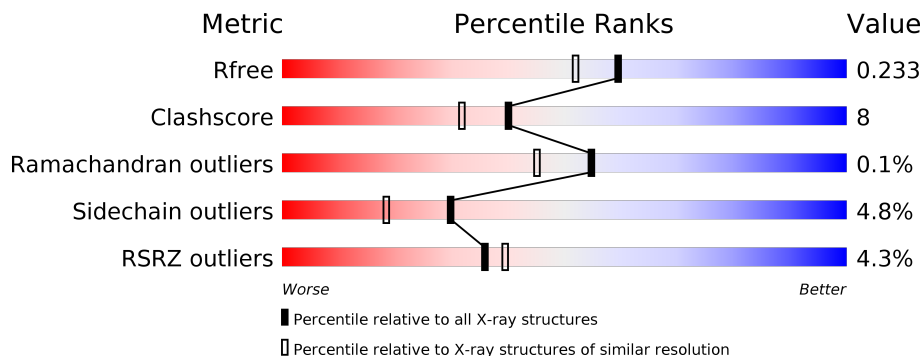
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	5047 (1.90-1.90)
Clashscore	112137	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (1.90-1.90)
RSRZ outliers	101464	5100 (1.90-1.90)

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	396	<div> <div>3%</div> <div> <div></div> <div>84%</div> <div>13%</div> <div>.</div> </div> </div>
1	B	396	<div> <div>%</div> <div> <div></div> <div>85%</div> <div>12%</div> <div>..</div> </div> </div>
1	C	396	<div> <div>9%</div> <div> <div></div> <div>81%</div> <div>15%</div> <div>..</div> </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
3	HX2	B	397	-	-	-	X

## 2 Entry composition [i](#)

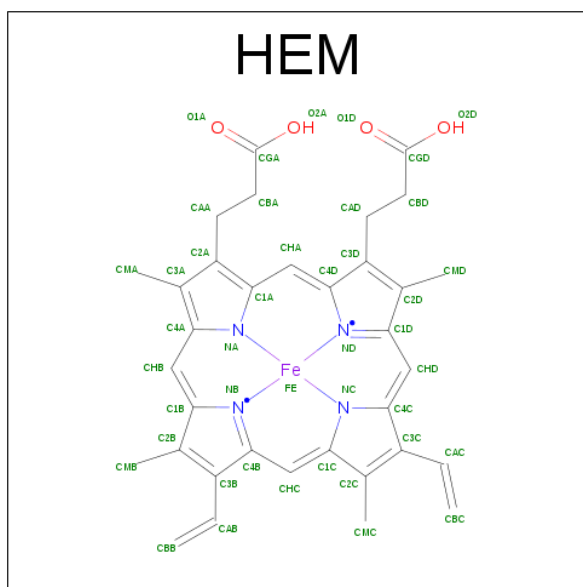
There are 4 unique types of molecules in this entry. The entry contains 10470 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

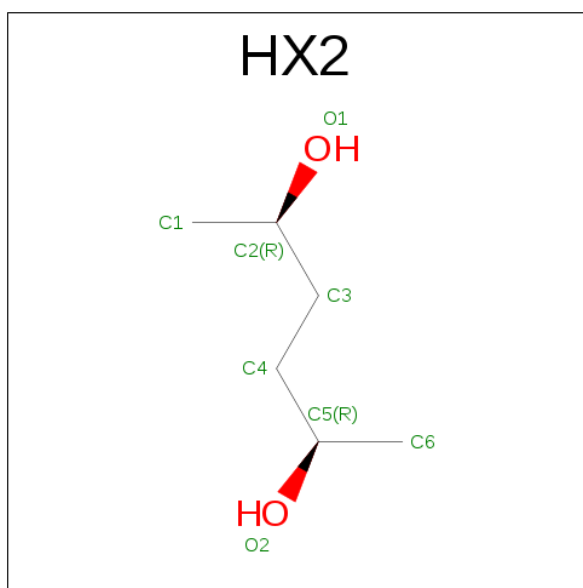
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	396	Total	C	N	O	S	0	0	0
			3068	1950	552	547	19			
1	B	393	Total	C	N	O	S	0	0	0
			3049	1939	549	542	19			
1	C	390	Total	C	N	O	S	0	0	0
			3025	1926	543	537	19			

- 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		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is (2R,5R)-HEXANE-2,5-DIOL (three-letter code: HX2) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	C	1	Total	C	O	0	0
			8	6	2		

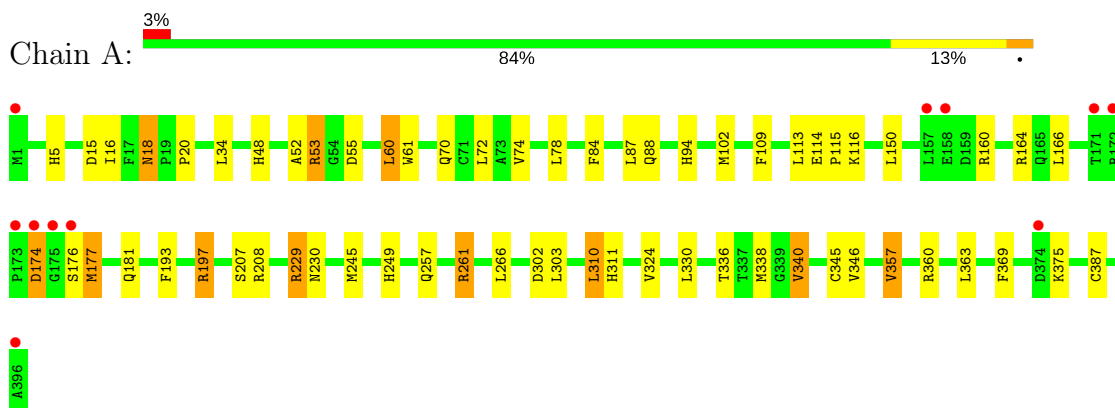
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	437	Total	O	0	0
			437	437		
4	B	431	Total	O	0	0
			431	431		
4	C	307	Total	O	0	0
			307	307		

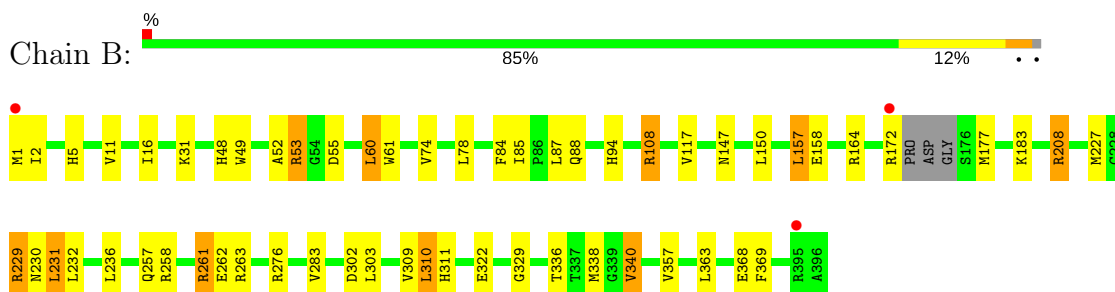
### 3 Residue-property plots

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.

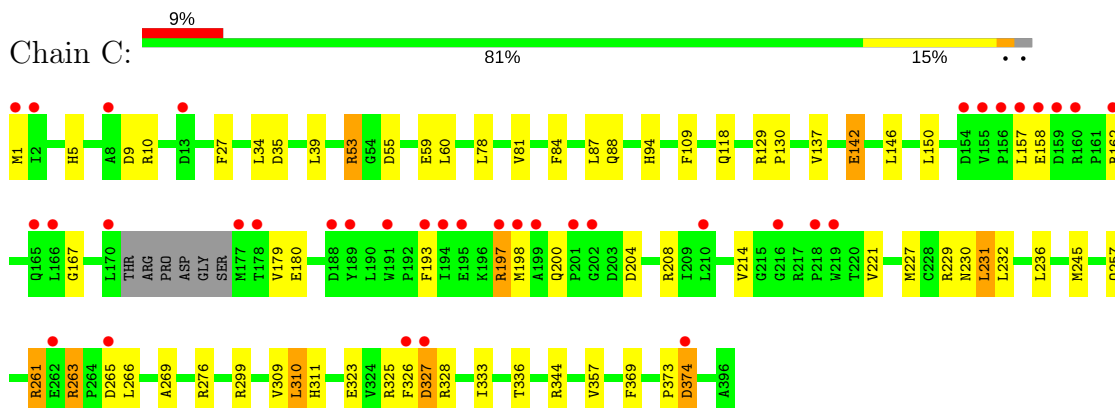
#### • Molecule 1: Cytochrome P450



#### • Molecule 1: Cytochrome P450



#### • Molecule 1: Cytochrome P450



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.99Å 150.15Å 68.45Å 90.00° 99.89° 90.00°	Depositor
Resolution (Å)	50.00 – 1.90 40.34 – 1.90	Depositor EDS
% Data completeness (in resolution range)	95.0 (50.00-1.90) 99.1 (40.34-1.90)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.43 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, $R_{free}$	0.174 , 0.232 0.174 , 0.233	Depositor DCC
$R_{free}$ test set	4494 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	16.9	Xtriage
Anisotropy	0.232	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 49.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10470	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 3.98% 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: HEM, HX2

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	0.77	1/3140 (0.0%)	0.94	12/4269 (0.3%)
1	B	0.78	0/3119	0.96	11/4238 (0.3%)
1	C	0.69	0/3095	0.76	6/4206 (0.1%)
All	All	0.75	1/9354 (0.0%)	0.89	29/12713 (0.2%)

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	B	0	1
1	C	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	387	CYS	CB-SG	-5.28	1.73	1.81

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	261	ARG	NE-CZ-NH2	-18.05	111.28	120.30
1	A	261	ARG	NE-CZ-NH2	-17.95	111.32	120.30
1	B	261	ARG	NE-CZ-NH1	16.85	128.73	120.30
1	A	261	ARG	NE-CZ-NH1	16.40	128.50	120.30
1	B	53	ARG	NE-CZ-NH2	-12.38	114.11	120.30
1	B	53	ARG	NE-CZ-NH1	11.35	125.97	120.30
1	A	229	ARG	NE-CZ-NH1	9.62	125.11	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	229	ARG	NE-CZ-NH2	-9.04	115.78	120.30
1	A	197	ARG	NE-CZ-NH1	8.58	124.59	120.30
1	A	197	ARG	NE-CZ-NH2	-8.36	116.12	120.30
1	B	229	ARG	NE-CZ-NH1	8.28	124.44	120.30
1	A	53	ARG	NE-CZ-NH2	-7.58	116.51	120.30
1	C	53	ARG	NE-CZ-NH2	-7.55	116.52	120.30
1	A	229	ARG	NE-CZ-NH2	-7.44	116.58	120.30
1	B	276	ARG	NE-CZ-NH1	7.10	123.85	120.30
1	C	261	ARG	NE-CZ-NH1	6.78	123.69	120.30
1	A	53	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	C	276	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	C	53	ARG	NE-CZ-NH1	6.09	123.34	120.30
1	B	261	ARG	CD-NE-CZ	6.04	132.06	123.60
1	C	261	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	A	261	ARG	CD-NE-CZ	5.82	131.75	123.60
1	B	60	LEU	CB-CG-CD1	5.74	120.76	111.00
1	C	276	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	B	276	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	B	338	MET	CG-SD-CE	-5.23	91.84	100.20
1	A	60	LEU	CB-CG-CD1	5.15	119.75	111.00
1	A	15	ASP	CB-CG-OD2	5.11	122.90	118.30
1	A	357	VAL	CG1-CB-CG2	5.10	119.06	110.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	329	GLY	Peptide
1	C	327	ASP	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	3068	0	3088	46	0
1	B	3049	0	3073	47	0
1	C	3025	0	3048	57	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	43	0	30	2	0
2	B	43	0	30	3	0
2	C	43	0	30	2	0
3	A	8	0	14	0	0
3	B	8	0	14	5	0
3	C	8	0	14	0	0
4	A	437	0	0	13	0
4	B	431	0	0	9	0
4	C	307	0	0	8	0
All	All	10470	0	9341	154	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 8.

All (154) 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:C:55:ASP:O	1:C:59:GLU:HG3	1.50	1.09
1:A:53:ARG:HD2	1:A:55:ASP:OD1	1.55	1.06
1:B:283:VAL:HG12	3:B:397:HX2:H6B	1.06	1.05
1:B:283:VAL:HG12	3:B:397:HX2:C6	1.88	1.03
1:A:261:ARG:HD3	1:A:363:LEU:O	1.62	0.99
1:C:53:ARG:HD2	1:C:55:ASP:OD1	1.64	0.96
1:B:53:ARG:HD2	1:B:55:ASP:OD1	1.65	0.94
1:C:257:GLN:HE21	1:C:261:ARG:HH22	1.11	0.92
1:C:257:GLN:HE21	1:C:261:ARG:NH2	1.65	0.92
1:B:108:ARG:HD3	4:B:874:HOH:O	1.70	0.89
1:A:257:GLN:HE21	1:A:261:ARG:HH22	1.21	0.88
1:C:245:MET:HE3	4:C:481:HOH:O	1.73	0.87
1:B:257:GLN:HE21	1:B:261:ARG:HH22	1.19	0.86
1:A:245:MET:HE3	4:A:596:HOH:O	1.77	0.84
1:C:78:LEU:HD12	1:C:179:VAL:HG21	1.59	0.83
1:A:208:ARG:HD3	4:A:895:HOH:O	1.76	0.82
1:C:257:GLN:NE2	1:C:261:ARG:HH22	1.76	0.82
1:C:55:ASP:O	1:C:59:GLU:CG	2.28	0.81
1:C:5:HIS:CD2	1:C:299:ARG:HD3	2.19	0.77
1:C:84:PHE:HE1	1:C:229:ARG:HG2	1.50	0.77
1:C:137:VAL:O	1:C:142:GLU:HG2	1.86	0.74
1:C:78:LEU:CD1	1:C:179:VAL:HG21	2.18	0.74
1:B:257:GLN:HE21	1:B:261:ARG:NH2	1.85	0.74
1:A:257:GLN:HE21	1:A:261:ARG:NH2	1.86	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:PHE:CE1	1:C:229:ARG:HG2	2.24	0.73
1:B:147:ASN:OD1	1:B:164:ARG:HD3	1.89	0.72
1:C:326:PHE:O	1:C:326:PHE:CG	2.43	0.71
1:C:257:GLN:NE2	1:C:261:ARG:NH2	2.38	0.69
1:A:245:MET:CE	4:A:596:HOH:O	2.39	0.68
1:B:257:GLN:NE2	1:B:261:ARG:HH22	1.92	0.68
1:A:193:PHE:HA	1:A:197:ARG:HH21	1.58	0.68
1:A:174:ASP:OD1	1:A:174:ASP:N	2.29	0.66
3:B:397:HX2:H6A	4:B:519:HOH:O	1.95	0.66
1:B:261:ARG:HD3	1:B:363:LEU:O	1.95	0.66
1:C:373:PRO:O	1:C:374:ASP:OD1	2.12	0.66
1:A:197:ARG:HG2	1:A:207:SER:OG	1.97	0.65
1:B:283:VAL:CG1	3:B:397:HX2:H6B	2.02	0.64
1:A:53:ARG:CD	1:A:55:ASP:OD1	2.40	0.64
1:A:16:ILE:HD11	1:A:74:VAL:HG21	1.80	0.64
1:B:117:VAL:HG12	1:B:357:VAL:HG21	1.80	0.63
1:C:323:GLU:OE1	1:C:325:ARG:NH1	2.30	0.63
1:A:360:ARG:NE	4:A:571:HOH:O	2.31	0.63
1:B:5:HIS:HE1	1:B:302:ASP:OD1	1.81	0.62
1:A:257:GLN:NE2	1:A:261:ARG:HH22	1.94	0.61
1:C:257:GLN:HE22	1:C:369:PHE:H	1.48	0.61
1:B:257:GLN:HE22	1:B:369:PHE:H	1.48	0.61
1:A:5:HIS:HE1	1:A:302:ASP:OD1	1.83	0.61
1:A:84:PHE:H	1:A:88:GLN:NE2	1.99	0.60
1:B:208:ARG:HG2	1:B:208:ARG:HH11	1.67	0.60
1:B:227:MET:SD	1:B:231:LEU:HD22	2.42	0.59
1:C:87:LEU:HB2	1:C:230:ASN:HD21	1.66	0.59
1:C:197:ARG:HD3	1:C:204:ASP:OD1	2.02	0.59
2:B:417:HEM:HBB2	2:B:417:HEM:HMB1	1.86	0.58
1:B:94:HIS:HE1	2:B:417:HEM:O2D	1.86	0.58
1:A:109:PHE:CZ	1:A:113:LEU:HD11	2.39	0.57
1:A:257:GLN:HE22	1:A:369:PHE:H	1.51	0.57
1:A:84:PHE:HE1	1:A:229:ARG:HG2	1.69	0.57
1:B:52:ALA:HA	1:B:310:LEU:HD23	1.85	0.57
1:A:94:HIS:HE1	2:A:417:HEM:O2D	1.88	0.56
1:A:48:HIS:HE1	4:A:413:HOH:O	1.88	0.56
1:C:53:ARG:CD	1:C:55:ASP:OD1	2.48	0.55
1:A:94:HIS:HD2	4:A:476:HOH:O	1.88	0.55
1:A:102:MET:HG2	1:A:346:VAL:HG12	1.87	0.55
1:B:258:ARG:NH1	1:B:368:GLU:OE2	2.39	0.55
1:C:94:HIS:HE1	2:C:417:HEM:O2D	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:PHE:HE1	1:B:229:ARG:HG2	1.72	0.55
1:B:311:HIS:CD2	1:B:336:THR:OG1	2.60	0.54
1:C:162:ARG:HB2	4:C:575:HOH:O	2.07	0.54
1:A:18:ASN:ND2	4:A:450:HOH:O	2.40	0.54
1:B:262:GLU:HG3	4:C:600:HOH:O	2.08	0.54
1:B:5:HIS:HD2	4:B:621:HOH:O	1.91	0.54
1:C:94:HIS:HD2	4:C:502:HOH:O	1.91	0.53
1:B:48:HIS:HE1	4:B:438:HOH:O	1.91	0.52
2:B:417:HEM:CMB	2:B:417:HEM:HBB2	2.39	0.52
1:C:311:HIS:HE1	4:C:438:HOH:O	1.91	0.52
1:B:61:TRP:CG	1:B:340:VAL:HG13	2.45	0.52
1:A:5:HIS:H	1:A:5:HIS:CD2	2.27	0.52
1:C:309:VAL:HG13	1:C:310:LEU:HD13	1.91	0.52
1:B:16:ILE:HD11	1:B:74:VAL:HG21	1.91	0.51
1:C:269:ALA:HB1	1:C:326:PHE:CG	2.44	0.51
2:A:417:HEM:HBB2	2:A:417:HEM:HMB1	1.92	0.51
1:B:157:LEU:HD12	1:C:200:GLN:NE2	2.25	0.51
1:B:157:LEU:HD12	1:C:200:GLN:HE22	1.76	0.51
1:B:5:HIS:CD2	4:B:621:HOH:O	2.63	0.51
1:B:336:THR:HG23	1:B:340:VAL:HG12	1.92	0.51
1:C:344:ARG:NH2	4:C:494:HOH:O	2.35	0.51
1:C:193:PHE:HB3	1:C:197:ARG:HE	1.76	0.50
1:B:84:PHE:H	1:B:88:GLN:NE2	2.10	0.50
1:C:118:GLN:HA	1:C:357:VAL:HG13	1.94	0.50
1:B:53:ARG:CD	1:B:55:ASP:OD1	2.51	0.50
1:C:118:GLN:HA	1:C:357:VAL:CG1	2.42	0.50
1:C:129:ARG:N	1:C:130:PRO:CD	2.75	0.49
1:A:109:PHE:CE2	1:A:113:LEU:HD11	2.47	0.49
1:B:2:ILE:HD13	1:B:11:VAL:HG21	1.95	0.49
1:C:232:LEU:O	1:C:236:LEU:HG	2.12	0.49
1:C:269:ALA:HB1	1:C:326:PHE:CD1	2.48	0.49
1:C:5:HIS:CG	1:C:299:ARG:HD3	2.47	0.49
1:B:311:HIS:HD2	1:B:336:THR:OG1	1.96	0.49
1:B:87:LEU:HB2	1:B:230:ASN:HD21	1.77	0.48
1:A:116:LYS:NZ	4:A:1004:HOH:O	2.47	0.48
1:B:31:LYS:HE2	1:B:322:GLU:OE1	2.14	0.48
1:B:87:LEU:H	1:B:230:ASN:ND2	2.12	0.47
1:A:102:MET:SD	4:A:702:HOH:O	2.61	0.47
1:C:326:PHE:O	1:C:327:ASP:C	2.51	0.47
1:B:48:HIS:HD2	1:B:49:TRP:O	1.98	0.46
1:A:160:ARG:O	1:A:164:ARG:HB2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:MET:HA	1:A:181:GLN:OE1	2.14	0.46
3:B:397:HX2:H6A	4:B:518:HOH:O	2.15	0.46
1:B:208:ARG:CG	1:B:208:ARG:HH11	2.28	0.46
1:A:176:SER:O	1:A:177:MET:C	2.53	0.46
1:C:146:LEU:HD21	1:C:167:GLY:HA3	1.98	0.46
1:C:263:ARG:HG3	1:C:265:ASP:OD1	2.16	0.46
1:B:16:ILE:HD11	1:B:74:VAL:CG2	2.45	0.45
1:A:87:LEU:HB2	1:A:230:ASN:HD21	1.82	0.45
1:C:59:GLU:HG2	4:C:448:HOH:O	2.16	0.45
1:C:84:PHE:H	1:C:88:GLN:NE2	2.15	0.45
1:C:87:LEU:H	1:C:230:ASN:ND2	2.15	0.45
1:C:227:MET:SD	1:C:231:LEU:HD22	2.56	0.45
1:C:81:VAL:HG21	1:C:179:VAL:HG22	1.98	0.44
1:A:311:HIS:CD2	1:A:336:THR:OG1	2.70	0.44
1:C:81:VAL:HG21	1:C:179:VAL:CG2	2.48	0.44
1:A:336:THR:O	1:A:336:THR:HG22	2.17	0.44
1:A:109:PHE:CE2	1:A:208:ARG:NH2	2.86	0.44
1:A:61:TRP:HB3	1:A:340:VAL:HG13	2.00	0.44
1:B:309:VAL:HG13	1:B:310:LEU:HD13	1.97	0.44
1:C:311:HIS:CD2	1:C:336:THR:OG1	2.71	0.44
1:C:326:PHE:C	1:C:328:ARG:N	2.71	0.43
1:C:336:THR:HG22	1:C:336:THR:O	2.18	0.43
2:C:417:HEM:HMB2	2:C:417:HEM:HBB2	1.99	0.43
1:A:48:HIS:CE1	4:A:413:HOH:O	2.67	0.43
1:C:27:PHE:HE2	1:C:245:MET:CE	2.30	0.43
1:B:5:HIS:CD2	1:B:5:HIS:H	2.37	0.43
1:C:109:PHE:HB3	4:C:692:HOH:O	2.18	0.43
1:A:52:ALA:HA	1:A:310:LEU:HD23	2.00	0.43
1:C:311:HIS:HD2	1:C:336:THR:OG1	2.02	0.43
1:B:85:ILE:C	1:B:230:ASN:HD22	2.22	0.42
1:C:326:PHE:CD2	1:C:326:PHE:O	2.72	0.42
1:A:375:LYS:NZ	4:A:430:HOH:O	2.52	0.42
1:B:61:TRP:HB3	1:B:340:VAL:HG13	2.01	0.42
1:A:5:HIS:CD2	4:A:463:HOH:O	2.72	0.42
1:A:72:LEU:HD23	1:A:78:LEU:HD22	2.01	0.42
1:C:193:PHE:O	1:C:197:ARG:HB2	2.20	0.42
1:C:198:MET:CE	1:C:221:VAL:HG22	2.49	0.42
1:B:1:MET:HA	4:B:1098:HOH:O	2.18	0.42
1:C:27:PHE:CE2	1:C:245:MET:CE	3.02	0.42
1:B:158:GLU:HB2	4:B:996:HOH:O	2.19	0.42
1:A:114:GLU:HB3	1:A:115:PRO:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:PHE:CZ	1:A:208:ARG:NH2	2.87	0.41
1:A:249:HIS:CE1	1:A:324:VAL:HG21	2.56	0.41
1:B:232:LEU:O	1:B:236:LEU:HG	2.20	0.41
1:C:10:ARG:HD2	1:C:39:LEU:O	2.20	0.41
1:A:20:PRO:HD3	4:A:583:HOH:O	2.21	0.40
1:A:338:MET:HE3	1:A:345:CYS:CB	2.51	0.40
1:B:311:HIS:HE1	4:B:1056:HOH:O	2.03	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	394/396 (100%)	382 (97%)	11 (3%)	1 (0%)	44	34
1	B	389/396 (98%)	379 (97%)	10 (3%)	0	100	100
1	C	386/396 (98%)	371 (96%)	15 (4%)	0	100	100
All	All	1169/1188 (98%)	1132 (97%)	36 (3%)	1 (0%)	55	45

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	177	MET

### 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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	321/321 (100%)	308 (96%)	13 (4%)	36	25
1	B	319/321 (99%)	305 (96%)	14 (4%)	33	22
1	C	316/321 (98%)	297 (94%)	19 (6%)	22	11
All	All	956/963 (99%)	910 (95%)	46 (5%)	30	18

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	34	LEU
1	A	60	LEU
1	A	70	GLN
1	A	150	LEU
1	A	166	LEU
1	A	174	ASP
1	A	266	LEU
1	A	303	LEU
1	A	310	LEU
1	A	330	LEU
1	A	340	VAL
1	A	357	VAL
1	B	60	LEU
1	B	78	LEU
1	B	108	ARG
1	B	150	LEU
1	B	157	LEU
1	B	172	ARG
1	B	177	MET
1	B	183	LYS
1	B	208	ARG
1	B	231	LEU
1	B	263	ARG
1	B	303	LEU
1	B	310	LEU
1	B	340	VAL
1	C	1	MET
1	C	9	ASP
1	C	34	LEU
1	C	35	ASP
1	C	60	LEU
1	C	142	GLU
1	C	150	LEU

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Mol	Chain	Res	Type
1	C	157	LEU
1	C	158	GLU
1	C	180	GLU
1	C	197	ARG
1	C	208	ARG
1	C	214	VAL
1	C	231	LEU
1	C	263	ARG
1	C	266	LEU
1	C	310	LEU
1	C	333	ILE
1	C	374	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	HIS
1	A	18	ASN
1	A	48	HIS
1	A	70	GLN
1	A	88	GLN
1	A	94	HIS
1	A	230	ASN
1	A	257	GLN
1	A	311	HIS
1	B	5	HIS
1	B	48	HIS
1	B	70	GLN
1	B	88	GLN
1	B	94	HIS
1	B	184	GLN
1	B	230	ASN
1	B	257	GLN
1	B	311	HIS
1	C	5	HIS
1	C	48	HIS
1	C	88	GLN
1	C	94	HIS
1	C	230	ASN
1	C	257	GLN
1	C	311	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 ⓘ

6 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	$\# Z  > 2$
3	HX2	A	397	-	7,7,7	0.48	0	8,8,8	0.36	0
2	HEM	A	417	1,4	28,50,50	2.17	9 (32%)	17,82,82	2.17	7 (41%)
3	HX2	B	397	-	7,7,7	0.30	0	8,8,8	1.47	1 (12%)
2	HEM	B	417	1,4	28,50,50	2.03	9 (32%)	17,82,82	2.10	7 (41%)
3	HX2	C	397	-	7,7,7	0.33	0	8,8,8	0.69	0
2	HEM	C	417	1,4	28,50,50	2.11	10 (35%)	17,82,82	2.13	5 (29%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HX2	A	397	-	-	0/5/5/5	0/0/0/0
2	HEM	A	417	1,4	-	0/6/54/54	0/0/8/8
3	HX2	B	397	-	-	0/5/5/5	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	B	417	1,4	-	0/6/54/54	0/0/8/8
3	HX2	C	397	-	-	0/5/5/5	0/0/0/0
2	HEM	C	417	1,4	-	0/6/54/54	0/0/8/8

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	417	HEM	C3B-C2B	-4.52	1.34	1.40
2	B	417	HEM	C3C-C2C	-3.95	1.35	1.40
2	A	417	HEM	C3B-C2B	-3.87	1.35	1.40
2	B	417	HEM	C3B-C2B	-3.22	1.36	1.40
2	A	417	HEM	C3C-C2C	-2.74	1.36	1.40
2	C	417	HEM	C3C-C2C	-2.40	1.37	1.40
2	C	417	HEM	CMA-C3A	2.06	1.55	1.51
2	B	417	HEM	CMD-C2D	2.10	1.55	1.51
2	C	417	HEM	CMB-C2B	2.16	1.56	1.51
2	C	417	HEM	CMD-C2D	2.22	1.56	1.51
2	B	417	HEM	C4D-ND	2.29	1.39	1.36
2	B	417	HEM	CMC-C2C	2.31	1.56	1.51
2	A	417	HEM	CMC-C2C	2.39	1.56	1.51
2	A	417	HEM	CAA-C2A	2.41	1.56	1.52
2	C	417	HEM	C4D-ND	2.59	1.39	1.36
2	B	417	HEM	C3B-CAB	2.84	1.53	1.47
2	A	417	HEM	CMD-C2D	2.86	1.57	1.51
2	A	417	HEM	C3B-CAB	2.88	1.53	1.47
2	C	417	HEM	CMC-C2C	2.99	1.58	1.51
2	C	417	HEM	C3B-CAB	3.31	1.54	1.47
2	A	417	HEM	C4D-ND	3.47	1.40	1.36
2	B	417	HEM	C1B-NB	3.54	1.40	1.36
2	C	417	HEM	C3C-CAC	3.62	1.54	1.47
2	A	417	HEM	C3C-CAC	3.79	1.55	1.47
2	B	417	HEM	C3C-CAC	3.91	1.55	1.47
2	B	417	HEM	C3D-C2D	4.45	1.50	1.37
2	A	417	HEM	C3D-C2D	4.90	1.52	1.37
2	C	417	HEM	C3D-C2D	5.26	1.53	1.37

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	417	HEM	C1D-C2D-C3D	-4.13	104.13	107.00
2	A	417	HEM	CAD-CBD-CGD	-4.06	105.73	112.66
2	B	417	HEM	CMA-C3A-C4A	-3.74	122.71	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	397	HX2	C3-C4-C5	-3.54	107.83	113.01
2	A	417	HEM	CBD-CAD-C3D	-3.47	105.85	112.47
2	C	417	HEM	CBD-CAD-C3D	-3.42	105.95	112.47
2	A	417	HEM	C1D-C2D-C3D	-3.36	104.66	107.00
2	B	417	HEM	CBD-CAD-C3D	-3.10	106.55	112.47
2	C	417	HEM	CBA-CAA-C2A	-2.61	107.49	112.48
2	B	417	HEM	C1D-C2D-C3D	-2.59	105.19	107.00
2	A	417	HEM	CBA-CAA-C2A	-2.44	107.81	112.48
2	B	417	HEM	C3C-C4C-NC	-2.38	106.44	110.94
2	B	417	HEM	CBA-CAA-C2A	-2.28	108.12	112.48
2	A	417	HEM	CMB-C2B-C3B	2.46	129.45	124.89
2	A	417	HEM	CMC-C2C-C3C	2.52	129.57	124.89
2	B	417	HEM	CMA-C3A-C2A	2.68	129.99	124.94
2	C	417	HEM	CMD-C2D-C3D	2.75	130.13	124.94
2	C	417	HEM	CMC-C2C-C3C	3.12	130.69	124.89
2	A	417	HEM	C4C-C3C-C2C	3.26	109.18	106.90
2	B	417	HEM	C4C-C3C-C2C	3.46	109.32	106.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	417	HEM	2	0
3	B	397	HX2	5	0
2	B	417	HEM	3	0
2	C	417	HEM	2	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	396/396 (100%)	-0.25	11 (2%) 53 57	7, 15, 32, 59	0
1	B	393/396 (99%)	-0.31	3 (0%) 86 87	6, 15, 33, 54	0
1	C	390/396 (98%)	0.27	37 (9%) 9 10	9, 23, 55, 62	0
All	All	1179/1188 (99%)	-0.10	51 (4%) 36 39	6, 17, 43, 62	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	176	SER	5.1
1	A	157	LEU	4.7
1	C	216	GLY	4.6
1	C	202	GLY	4.3
1	C	157	LEU	4.3
1	C	326	PHE	4.2
1	C	1	MET	4.1
1	C	194	ILE	4.0
1	B	172	ARG	4.0
1	C	165	GLN	3.9
1	C	327	ASP	3.8
1	C	191	TRP	3.8
1	C	166	LEU	3.8
1	A	173	PRO	3.6
1	A	172	ARG	3.5
1	C	155	VAL	3.4
1	C	2	ILE	3.4
1	C	198	MET	3.3
1	C	158	GLU	3.3
1	C	193	PHE	3.2
1	C	199	ALA	3.2
1	C	197	ARG	3.2
1	A	174	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	13	ASP	3.1
1	A	396	ALA	3.0
1	C	201	PRO	2.9
1	A	171	THR	2.9
1	C	195	GLU	2.8
1	C	177	MET	2.8
1	C	162	ARG	2.7
1	C	8	ALA	2.6
1	A	374	ASP	2.6
1	C	156	PRO	2.6
1	C	189	TYR	2.6
1	C	178	THR	2.5
1	C	160	ARG	2.4
1	A	175	GLY	2.4
1	C	159	ASP	2.3
1	C	265	ASP	2.3
1	C	262	GLU	2.3
1	C	170	LEU	2.3
1	A	158	GLU	2.3
1	C	210	LEU	2.2
1	A	1	MET	2.2
1	C	188	ASP	2.2
1	C	218	PRO	2.2
1	C	374	ASP	2.2
1	B	1	MET	2.1
1	C	219	TRP	2.0
1	C	154	ASP	2.0
1	B	395	ARG	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
3	HX2	B	397	8/8	0.90	0.13	2.14	15,21,25,29	0
3	HX2	A	397	8/8	0.94	0.12	1.65	16,17,24,24	0
2	HEM	B	417	43/43	0.98	0.10	1.21	4,7,11,21	0
3	HX2	C	397	8/8	0.94	0.10	0.75	16,23,24,25	0
2	HEM	A	417	43/43	0.98	0.10	0.60	2,6,12,21	0
2	HEM	C	417	43/43	0.98	0.09	-0.03	6,10,14,23	0

## 6.5 Other polymers

There are no such residues in this entry.