



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 06:59 AM GMT

PDB ID : 2D0T  
Title : Crystal structure of 4-phenylimidazole bound form of human indoleamine 2,3-dioxygenase  
Authors : Sugimoto, H.; Oda, S.; Otsuki, T.; Hino, T.; Yoshida, T.; Shiro, Y.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)  
Deposited on : 2005-08-08  
Resolution : 2.30 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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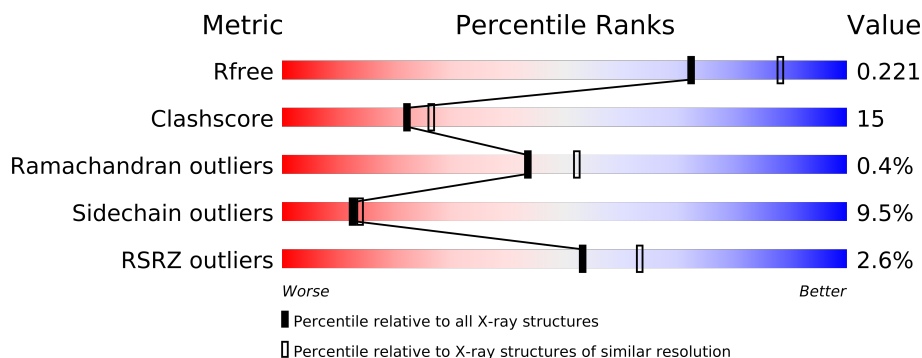
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	406	
1	B	406	

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

Mol	Type	Chain	Res	Geometry	Electron density
4	NHE	A	502	-	X
4	NHE	A	503	-	X
4	NHE	B	1502	-	X

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 6218 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

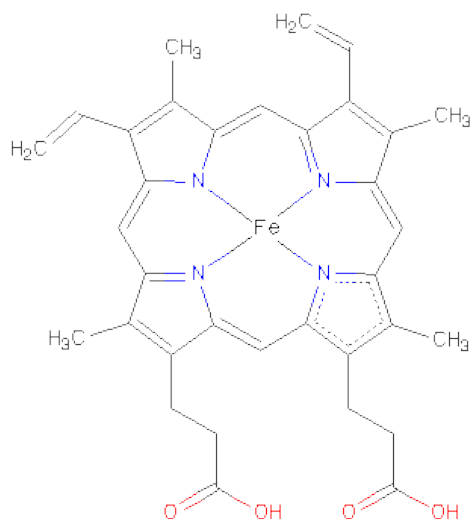
- Molecule 1 is a protein called Indoleamine 2,3-dioxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	373	Total	C	N	O	S	0	0	0
			2956	1899	504	536	17			
1	B	374	Total	C	N	O	S	0	0	0
			2964	1905	505	537	17			

There are 6 discrepancies between the modelled and reference sequences:

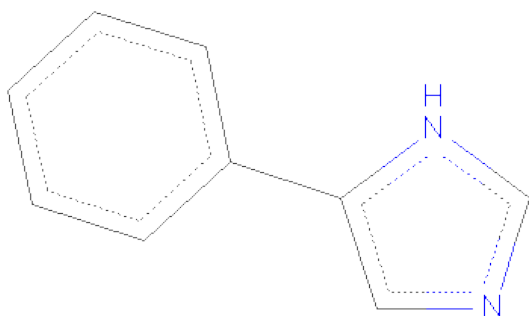
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	CLONING ARTIFACT	UNP P14902
A	-1	SER	-	CLONING ARTIFACT	UNP P14902
A	0	HIS	-	CLONING ARTIFACT	UNP P14902
B	-2	GLY	-	CLONING ARTIFACT	UNP P14902
B	-1	SER	-	CLONING ARTIFACT	UNP P14902
B	0	HIS	-	CLONING ARTIFACT	UNP P14902

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



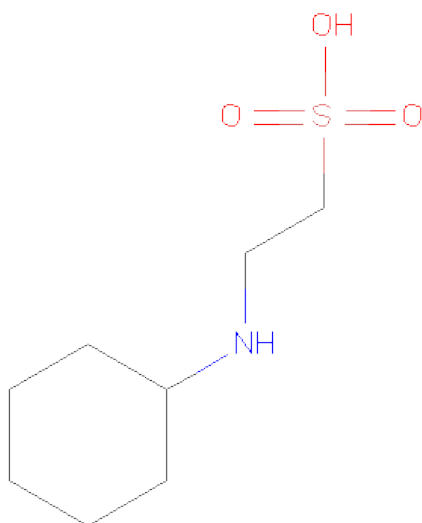
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is 4-PHENYL-1H-IMIDAZOLE (three-letter code: PIM) (formula: C<sub>9</sub>H<sub>8</sub>N<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			11	9	2		
3	B	1	Total	C	N	0	0
			11	9	2		

- Molecule 4 is 2-[N-CYCLOHEXYLAMINO]ETHANESULFONIC ACID (three-letter code: NHE) (formula: C<sub>8</sub>H<sub>17</sub>NO<sub>3</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			13	8	1	3	1		
4	A	1	Total	C	N	O	S	0	0
			13	8	1	3	1		
4	B	1	Total	C	N	O	S	0	0
			13	8	1	3	1		
4	B	1	Total	C	N	O	S	0	0
			13	8	1	3	1		

- Molecule 5 is water.

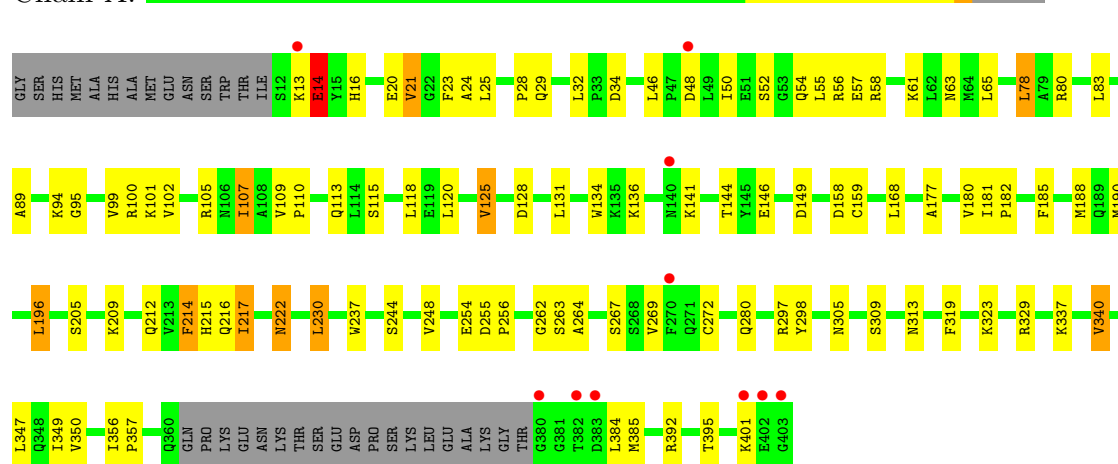
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	72	Total	O	0	0
			72	72		
5	B	66	Total	O	0	0
			66	66		

### 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.

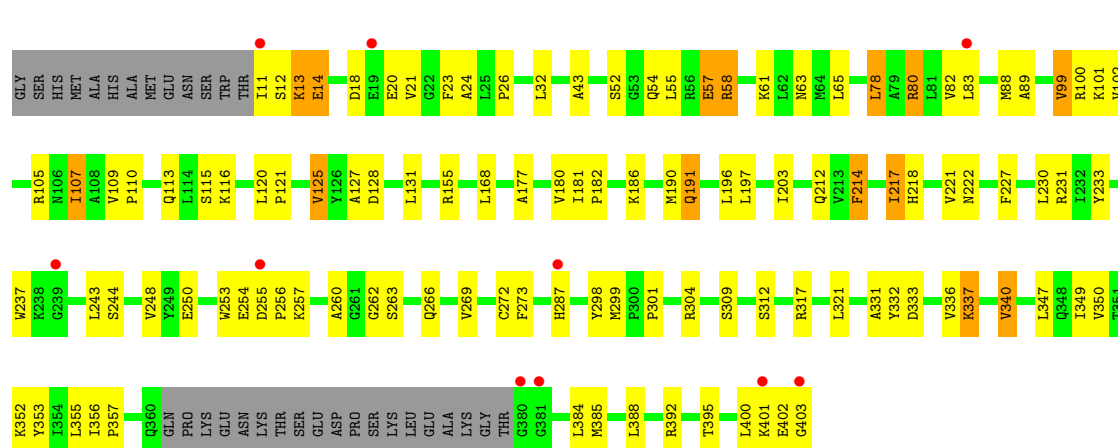
#### • Molecule 1: Indoleamine 2,3-dioxygenase

Chain A:



#### • Molecule 1: Indoleamine 2,3-dioxygenase

Chain B:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.07Å 98.03Å 130.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.94 – 2.30 20.01 – 2.30	Depositor EDS
% Data completeness (in resolution range)	90.7 (19.94-2.30) 90.8 (20.01-2.30)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.29 (at 2.30Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.191 , 0.221 0.192 , 0.221	Depositor DCC
$R_{free}$ test set	2179 reflections (5.06%)	DCC
Wilson B-factor (Å <sup>2</sup> )	46.3	Xtriage
Anisotropy	0.398	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 37.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 45262 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6218	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NHE, HEM, PIM

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	0.46	0/3024	0.65	0/4087
1	B	0.44	0/3032	0.63	0/4098
All	All	0.45	0/6056	0.64	0/8185

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2956	0	2967	84	1
1	B	2964	0	2978	91	1
2	A	43	0	30	6	0
2	B	43	0	30	5	0
3	A	11	0	8	2	0
3	B	11	0	8	2	0
4	A	26	0	32	8	0
4	B	26	0	33	5	0
5	A	72	0	0	5	0
5	B	66	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6218	0	6086	183	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 15.

All (183) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:401:LYS:HA	1:A:401:LYS:HE2	1.17	1.15
1:B:21:VAL:HG13	1:B:24:ALA:HB3	1.39	0.99
1:B:13:LYS:HD2	1:B:14:GLU:H	1.25	0.99
1:A:21:VAL:HG13	1:A:24:ALA:HB3	1.43	0.97
4:A:502:NHE:HC21	4:A:503:NHE:HN	1.31	0.95
1:B:105:ARG:HB3	1:B:250:GLU:HG2	1.57	0.86
1:A:401:LYS:CE	1:A:401:LYS:HA	2.06	0.83
1:A:329:ARG:HE	1:A:401:LYS:HD2	1.44	0.82
1:A:401:LYS:HE2	1:A:401:LYS:CA	2.02	0.81
1:A:136:LYS:HE2	1:A:141:LYS:O	1.80	0.81
1:A:188:MET:HG2	1:A:319:PHE:CD2	2.16	0.81
1:B:21:VAL:CG1	1:B:24:ALA:HB3	2.14	0.77
1:A:385:MET:HE2	1:A:385:MET:HA	1.66	0.76
1:B:80:ARG:NH2	1:B:121:PRO:O	2.20	0.75
1:B:13:LYS:HD2	1:B:14:GLU:N	2.02	0.75
1:A:329:ARG:NE	1:A:401:LYS:HD2	2.01	0.74
1:A:102:VAL:HG22	1:A:248:VAL:HG11	1.70	0.71
1:B:109:VAL:O	1:B:113:GLN:HG3	1.90	0.71
1:B:88:MET:SD	5:B:1511:HOH:O	2.49	0.69
1:B:102:VAL:HG22	1:B:248:VAL:HG11	1.72	0.69
1:A:23:PHE:HD2	1:A:269:VAL:HG23	1.58	0.69
1:B:13:LYS:CD	1:B:14:GLU:H	2.04	0.67
4:A:503:NHE:H6'1	4:A:503:NHE:C2	2.25	0.67
1:A:255:ASP:HB3	1:A:256:PRO:HD2	1.78	0.66
1:B:255:ASP:HB3	1:B:256:PRO:HD2	1.76	0.66
1:A:125:VAL:HG13	5:A:504:HOH:O	1.94	0.66
1:A:32:LEU:HG	1:A:78:LEU:HD13	1.79	0.65
1:A:102:VAL:HG22	1:A:248:VAL:CG1	2.26	0.65
1:B:23:PHE:HD2	1:B:269:VAL:HG23	1.61	0.64
1:A:262:GLY:O	4:A:502:NHE:HC'1	1.97	0.64
1:B:102:VAL:HG22	1:B:248:VAL:CG1	2.27	0.64
1:A:347:LEU:HD12	1:A:392:ARG:HH11	1.63	0.64
1:B:262:GLY:O	4:B:1502:NHE:HC'1	1.98	0.63
1:A:181:ILE:HB	1:A:182:PRO:HD3	1.81	0.63
1:A:263:SER:HA	3:A:501:PIM:HN1	1.64	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:218:HIS:HD2	1:B:352:LYS:NZ	1.99	0.61
1:A:14:GLU:C	1:A:16:HIS:H	2.05	0.61
1:A:217:ILE:HG21	1:A:349:ILE:HD13	1.82	0.60
1:B:401:LYS:O	1:B:402:GLU:HG2	2.02	0.59
1:B:83:LEU:HD22	1:B:107:ILE:HD11	1.83	0.59
1:A:217:ILE:O	1:A:217:ILE:HD13	2.03	0.59
1:B:260:ALA:HB1	4:B:1502:NHE:O3	2.03	0.59
1:B:340:VAL:HG12	1:B:395:THR:HG22	1.85	0.58
1:B:102:VAL:HA	1:B:248:VAL:HG13	1.85	0.58
1:B:11:ILE:HG22	1:B:12:SER:N	2.19	0.58
2:B:404:HEM:HBA1	4:B:1503:NHE:H6'2	1.85	0.57
1:B:321:LEU:HD21	1:B:400:LEU:HD22	1.87	0.57
1:B:356:ILE:HB	1:B:357:PRO:HD3	1.86	0.57
1:B:180:VAL:HG21	1:B:203:ILE:HG13	1.86	0.57
1:B:401:LYS:HG2	1:B:402:GLU:N	2.20	0.56
1:A:347:LEU:HD12	1:A:392:ARG:NH1	2.19	0.56
1:B:402:GLU:O	1:B:402:GLU:HG3	2.04	0.56
4:A:503:NHE:H6'1	4:A:503:NHE:HC21	1.86	0.56
1:B:24:ALA:HA	1:B:131:LEU:HD22	1.87	0.55
1:B:57:GLU:HG3	1:B:58:ARG:N	2.20	0.55
1:B:57:GLU:O	1:B:61:LYS:HG2	2.07	0.55
1:B:23:PHE:CD2	1:B:269:VAL:HG23	2.42	0.55
1:A:217:ILE:HG21	1:A:349:ILE:CD1	2.37	0.54
1:B:191:GLN:CA	1:B:191:GLN:HE21	2.19	0.54
1:B:115:SER:HB3	1:B:120:LEU:O	2.07	0.54
1:A:83:LEU:HD22	1:A:107:ILE:HD11	1.90	0.54
1:A:23:PHE:CD2	1:A:269:VAL:HG23	2.42	0.54
1:B:287:HIS:HE1	4:B:1503:NHE:H4'2	1.72	0.54
1:B:287:HIS:CE1	4:B:1503:NHE:H4'2	2.42	0.54
1:A:109:VAL:HB	1:A:110:PRO:HD3	1.89	0.53
1:A:401:LYS:CE	1:A:401:LYS:CA	2.78	0.53
1:B:384:LEU:HD11	2:B:404:HEM:HMA3	1.90	0.53
1:A:350:VAL:HG11	1:A:385:MET:CE	2.39	0.53
1:A:136:LYS:CE	1:A:141:LYS:O	2.53	0.53
1:A:384:LEU:HD22	4:A:503:NHE:O3	2.09	0.53
1:A:384:LEU:HD11	2:A:404:HEM:HMA3	1.91	0.52
1:B:52:SER:OG	1:B:54:GLN:HG3	2.09	0.52
1:B:13:LYS:CD	1:B:14:GLU:N	2.68	0.52
1:B:80:ARG:NH1	1:B:128:ASP:OD2	2.42	0.52
1:A:216:GLN:NE2	5:A:545:HOH:O	2.42	0.52
1:B:401:LYS:HG2	1:B:402:GLU:H	1.73	0.52
1:A:102:VAL:HA	1:A:248:VAL:HG13	1.90	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:266:GLN:O	1:B:299:MET:HG2	2.10	0.52
1:A:14:GLU:C	1:A:14:GLU:CD	2.69	0.51
1:A:222:ASN:ND2	5:A:528:HOH:O	2.43	0.51
1:B:83:LEU:HD22	1:B:107:ILE:CD1	2.41	0.51
1:B:214:PHE:HD1	1:B:214:PHE:O	1.94	0.51
1:B:191:GLN:NE2	1:B:191:GLN:HA	2.26	0.51
1:B:253:TRP:CE3	1:B:257:LYS:HG3	2.46	0.51
1:A:55:LEU:CD2	1:A:89:ALA:HB1	2.41	0.50
1:A:146:GLU:H	1:A:146:GLU:CD	2.14	0.50
1:B:218:HIS:HD2	1:B:352:LYS:HZ3	1.58	0.50
1:B:336:VAL:O	1:B:340:VAL:HG13	2.12	0.50
1:A:115:SER:HB3	1:A:120:LEU:O	2.10	0.50
1:A:109:VAL:O	1:A:113:GLN:HG3	2.12	0.50
1:A:205:SER:O	1:A:209:LYS:HG3	2.12	0.49
1:A:50:ILE:HG12	1:A:55:LEU:HD22	1.95	0.49
1:A:340:VAL:HG12	1:A:395:THR:HG22	1.93	0.49
1:B:385:MET:HA	1:B:385:MET:HE2	1.94	0.49
1:A:101:LYS:O	1:A:248:VAL:HG12	2.13	0.49
1:B:317:ARG:HD2	1:B:332:TYR:OH	2.11	0.49
1:A:188:MET:HG2	1:A:319:PHE:CE2	2.46	0.49
1:B:88:MET:HG2	5:B:1511:HOH:O	2.13	0.48
1:B:217:ILE:HG21	1:B:349:ILE:HD12	1.94	0.48
1:A:305:ASN:CG	1:B:312:SER:HB2	2.33	0.48
1:A:29:GLN:O	1:A:78:LEU:HG	2.14	0.48
1:A:25:LEU:HD23	1:A:28:PRO:HB3	1.95	0.48
1:B:155:ARG:HD2	1:B:233:TYR:OH	2.13	0.48
1:A:28:PRO:HG2	1:A:134:TRP:O	2.14	0.48
1:A:347:LEU:CD1	1:A:392:ARG:HH11	2.25	0.48
1:B:191:GLN:HA	1:B:191:GLN:HE21	1.79	0.48
1:B:301:PRO:HA	1:B:304:ARG:NH1	2.28	0.48
1:B:43:ALA:HB2	1:B:82:VAL:HG13	1.95	0.48
1:A:347:LEU:CD1	1:A:392:ARG:NH1	2.76	0.47
1:B:125:VAL:HG13	5:B:1506:HOH:O	2.14	0.47
1:A:24:ALA:HA	1:A:131:LEU:HD22	1.97	0.47
1:B:121:PRO:HG3	1:B:298:TYR:CD2	2.50	0.47
1:A:356:ILE:HB	1:A:357:PRO:HD3	1.96	0.47
1:B:14:GLU:CD	1:B:14:GLU:N	2.68	0.47
1:A:83:LEU:HD22	1:A:107:ILE:CD1	2.45	0.47
1:A:21:VAL:CG1	1:A:24:ALA:HB3	2.29	0.47
1:B:350:VAL:HG11	1:B:385:MET:CE	2.45	0.46
1:A:264:ALA:O	1:A:267:SER:HB3	2.15	0.46
1:A:350:VAL:HG11	1:A:385:MET:HE1	1.96	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:263:SER:HA	3:B:1501:PIM:HN1	1.80	0.46
1:B:125:VAL:HG13	1:B:127:ALA:H	1.80	0.46
1:B:13:LYS:NZ	1:B:14:GLU:HB2	2.30	0.46
1:A:50:ILE:HD11	1:A:89:ALA:HB1	1.96	0.46
1:A:13:LYS:HB3	1:A:13:LYS:NZ	2.30	0.46
1:B:384:LEU:HD11	2:B:404:HEM:CMA	2.45	0.46
2:A:404:HEM:HBA1	4:A:503:NHE:H6'2	1.99	0.45
1:A:177:ALA:O	1:A:180:VAL:HG13	2.16	0.45
1:B:384:LEU:HD21	2:B:404:HEM:HMA3	1.98	0.45
1:B:355:LEU:HD11	1:B:385:MET:SD	2.57	0.45
1:A:385:MET:HE2	1:A:385:MET:CA	2.41	0.45
1:A:384:LEU:HD11	2:A:404:HEM:CMA	2.47	0.45
1:A:102:VAL:HA	1:A:248:VAL:CG1	2.46	0.45
1:A:329:ARG:HE	1:A:401:LYS:CD	2.23	0.45
1:B:177:ALA:HB3	1:B:273:PHE:HZ	1.82	0.45
1:B:125:VAL:CG2	1:B:298:TYR:HB3	2.47	0.44
1:A:80:ARG:HG3	1:A:118:LEU:HD12	1.99	0.44
1:B:32:LEU:HG	1:B:78:LEU:HD13	2.00	0.44
1:A:52:SER:OG	1:A:54:GLN:HG2	2.17	0.44
1:A:100:ARG:HA	1:A:100:ARG:HD3	1.85	0.44
2:A:404:HEM:O2A	4:A:503:NHE:H6'2	2.18	0.44
1:B:333:ASP:O	1:B:337:LYS:HB2	2.18	0.44
1:B:218:HIS:CD2	1:B:352:LYS:NZ	2.84	0.44
1:A:63:ASN:O	1:A:65:LEU:HD13	2.18	0.44
1:B:101:LYS:O	1:B:248:VAL:HG12	2.19	0.43
1:A:297:ARG:NH2	5:A:575:HOH:O	2.50	0.43
1:B:197:LEU:HD12	1:B:331:ALA:HB2	2.00	0.43
1:B:11:ILE:CG2	1:B:12:SER:N	2.82	0.43
1:A:14:GLU:N	1:A:14:GLU:OE1	2.52	0.43
1:B:63:ASN:O	1:B:65:LEU:HD13	2.19	0.43
1:B:100:ARG:HA	1:B:100:ARG:HD3	1.80	0.43
1:B:109:VAL:HB	1:B:110:PRO:HD3	2.00	0.43
1:A:196:LEU:HD12	1:A:319:PHE:CE2	2.54	0.42
1:A:50:ILE:CG1	1:A:55:LEU:HD22	2.49	0.42
1:B:221:VAL:HG12	1:B:353:TYR:CE2	2.55	0.42
2:A:404:HEM:C1A	3:A:501:PIM:H2	2.55	0.42
1:A:14:GLU:C	1:A:16:HIS:N	2.70	0.42
1:A:214:PHE:CE1	1:A:349:ILE:HD12	2.55	0.42
1:B:221:VAL:HG12	1:B:353:TYR:HE2	1.84	0.42
1:B:101:LYS:HG2	1:B:243:LEU:HD23	2.01	0.42
1:A:264:ALA:HB3	2:A:404:HEM:C1D	2.55	0.42
1:B:181:ILE:HB	1:B:182:PRO:HD3	2.01	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:340:VAL:HG12	1:B:395:THR:CG2	2.50	0.42
2:B:404:HEM:C1A	3:B:1501:PIM:H2	2.55	0.42
1:B:99:VAL:CG2	1:B:100:ARG:N	2.82	0.42
1:B:88:MET:CG	5:B:1511:HOH:O	2.68	0.41
1:A:80:ARG:NH2	1:A:128:ASP:OD2	2.53	0.41
1:B:401:LYS:CG	1:B:402:GLU:H	2.32	0.41
1:B:227:PHE:O	1:B:231:ARG:NH1	2.53	0.41
4:A:503:NHE:H6'1	4:A:503:NHE:HC22	1.99	0.41
1:B:347:LEU:HD21	1:B:388:LEU:CB	2.50	0.41
1:B:401:LYS:CG	1:B:402:GLU:N	2.83	0.41
1:A:56:ARG:CZ	1:A:100:ARG:HG2	2.51	0.41
1:B:18:ASP:HB2	1:B:26:PRO:HG3	2.02	0.41
1:A:185:PHE:CE1	1:A:313:ASN:HB3	2.55	0.41
1:A:158:ASP:O	1:A:159:CYS:HB2	2.21	0.41
1:A:298:TYR:N	1:A:298:TYR:CD1	2.89	0.41
1:B:102:VAL:HA	1:B:248:VAL:CG1	2.50	0.41
1:B:347:LEU:HA	1:B:347:LEU:HD23	1.78	0.41
1:A:230:LEU:HA	1:A:230:LEU:HD23	1.82	0.41
1:A:196:LEU:HD12	1:A:319:PHE:HE2	1.86	0.40
1:B:55:LEU:HD22	1:B:89:ALA:HB1	2.03	0.40
1:A:55:LEU:HD22	1:A:89:ALA:HB1	2.03	0.40
1:A:95:GLY:HA2	5:A:525:HOH:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:94:LYS:N	1:B:403:GLY:OXT[3.655]	2.02	0.18

## 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	369/406 (91%)	353 (96%)	14 (4%)	2 (0%)	38	45
1	B	370/406 (91%)	355 (96%)	14 (4%)	1 (0%)	50	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	739/812 (91%)	708 (96%)	28 (4%)	3 (0%)	43	52

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	GLU
1	A	244	SER
1	B	244	SER

### 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	322/350 (92%)	289 (90%)	33 (10%)	11	12
1	B	323/350 (92%)	295 (91%)	28 (9%)	15	17
All	All	645/700 (92%)	584 (90%)	61 (10%)	12	14

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	GLU
1	A	20	GLU
1	A	21	VAL
1	A	34	ASP
1	A	46	LEU
1	A	48	ASP
1	A	57	GLU
1	A	58	ARG
1	A	61	LYS
1	A	78	LEU
1	A	99	VAL
1	A	105	ARG
1	A	107	ILE
1	A	125	VAL
1	A	144	THR
1	A	149	ASP

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Mol	Chain	Res	Type
1	A	168	LEU
1	A	190	MET
1	A	196	LEU
1	A	212	GLN
1	A	214	PHE
1	A	215	HIS
1	A	217	ILE
1	A	222	ASN
1	A	230	LEU
1	A	237	TRP
1	A	254	GLU
1	A	272	CYS
1	A	280	GLN
1	A	309	SER
1	A	323	LYS
1	A	337	LYS
1	A	340	VAL
1	B	13	LYS
1	B	14	GLU
1	B	20	GLU
1	B	57	GLU
1	B	58	ARG
1	B	78	LEU
1	B	80	ARG
1	B	99	VAL
1	B	107	ILE
1	B	116	LYS
1	B	125	VAL
1	B	168	LEU
1	B	186	LYS
1	B	190	MET
1	B	191	GLN
1	B	196	LEU
1	B	212	GLN
1	B	214	PHE
1	B	217	ILE
1	B	222	ASN
1	B	230	LEU
1	B	237	TRP
1	B	254	GLU
1	B	272	CYS
1	B	309	SER

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Mol	Chain	Res	Type
1	B	337	LYS
1	B	340	VAL
1	B	392	ARG

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	37	ASN
1	A	69	HIS
1	A	191	GLN
1	A	242	GLN
1	A	293	GLN
1	B	37	ASN
1	B	63	ASN
1	B	73	HIS
1	B	191	GLN
1	B	212	GLN
1	B	218	HIS
1	B	287	HIS
1	B	293	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

8 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	404	1,3	49,50,50	1.88	14 (28%)	46,82,82	1.59	9 (19%)
3	PIM	A	501	2	12,12,12	1.84	4 (33%)	15,15,15	2.95	7 (46%)
4	NHE	A	502	-	13,13,13	2.97	1 (7%)	17,17,17	1.08	1 (5%)
4	NHE	A	503	-	13,13,13	3.20	4 (30%)	17,17,17	1.80	4 (23%)
3	PIM	B	1501	2	12,12,12	1.73	4 (33%)	15,15,15	2.95	7 (46%)
4	NHE	B	1502	-	13,13,13	2.23	2 (15%)	17,17,17	1.46	4 (23%)
4	NHE	B	1503	-	13,13,13	2.10	2 (15%)	17,17,17	1.46	1 (5%)
2	HEM	B	404	1,3	49,50,50	2.27	18 (36%)	46,82,82	1.64	9 (19%)

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	404	1,3	-	0/14/114/114	0/0/8/8
3	PIM	A	501	2	-	0/4/4/4	0/2/2/2
4	NHE	A	502	-	-	0/7/15/15	0/1/1/1
4	NHE	A	503	-	-	0/7/15/15	0/1/1/1
3	PIM	B	1501	2	-	0/4/4/4	0/2/2/2
4	NHE	B	1502	-	-	0/7/15/15	0/1/1/1
4	NHE	B	1503	-	-	0/7/15/15	0/1/1/1
2	HEM	B	404	1,3	-	0/14/114/114	0/0/8/8

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	502	NHE	C2-S	-10.43	1.61	1.77
4	A	503	NHE	C1-N	9.30	1.67	1.47
4	B	1502	NHE	C2-S	-6.92	1.67	1.77
4	B	1503	NHE	C2-S	-6.42	1.67	1.77
2	B	404	HEM	C2D-C1D	6.07	1.46	1.44
4	A	503	NHE	C2'-C1'	4.73	1.64	1.51
2	B	404	HEM	C2B-C1B	4.60	1.45	1.44
2	B	404	HEM	C4A-C3A	4.44	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	404	HEM	FE-NC	4.33	2.14	1.97
2	B	404	HEM	CHD-C4C	4.27	1.44	1.36
2	B	404	HEM	FE-NC	4.14	2.13	1.97
2	B	404	HEM	C3C-C2C	-4.06	1.36	1.43
2	A	404	HEM	C3D-C2D	-4.03	1.36	1.43
2	B	404	HEM	CHB-C1B	3.76	1.41	1.35
2	B	404	HEM	CHA-C4D	3.53	1.40	1.35
2	A	404	HEM	CHA-C4D	3.42	1.40	1.35
2	A	404	HEM	C3C-C2C	-3.28	1.38	1.43
4	A	503	NHE	C2-S	-3.25	1.72	1.77
3	A	501	PIM	C6-C5	3.23	1.52	1.47
2	B	404	HEM	FE-NA	3.24	2.06	1.92
2	A	404	HEM	CHB-C1B	3.22	1.40	1.35
2	A	404	HEM	CHC-C1C	3.22	1.42	1.36
2	B	404	HEM	C3D-C2D	-3.00	1.38	1.43
2	A	404	HEM	C4A-C3A	2.93	1.43	1.40
2	A	404	HEM	CMB-C2B	2.90	1.56	1.47
2	A	404	HEM	CHD-C4C	2.90	1.41	1.36
4	A	503	NHE	O3-S	-2.87	1.39	1.46
3	A	501	PIM	C8-C7	2.82	1.45	1.39
3	B	1501	PIM	C8-C7	2.81	1.45	1.39
2	B	404	HEM	CMB-C2B	2.75	1.55	1.47
3	A	501	PIM	C2-N3	-2.68	1.29	1.34
2	A	404	HEM	C3B-C4B	2.65	1.47	1.44
2	B	404	HEM	CHC-C1C	2.65	1.41	1.36
3	B	1501	PIM	C2-N3	-2.63	1.30	1.34
3	A	501	PIM	C4-N3	-2.59	1.27	1.35
2	A	404	HEM	CMC-C2C	2.44	1.55	1.47
4	B	1503	NHE	C2'-C1'	2.40	1.58	1.51
2	B	404	HEM	CHD-C1D	2.31	1.44	1.39
2	A	404	HEM	FE-NA	2.29	2.02	1.92
2	B	404	HEM	CBB-CAB	2.28	1.42	1.28
2	A	404	HEM	CBB-CAB	2.28	1.42	1.28
3	B	1501	PIM	C4-N3	-2.20	1.28	1.35
4	B	1502	NHE	O1-S	-2.19	1.38	1.45
2	B	404	HEM	C1C-NC	-2.14	1.35	1.38
2	B	404	HEM	CMC-C2C	2.14	1.54	1.47
2	B	404	HEM	C3B-C4B	2.11	1.46	1.44
2	B	404	HEM	CBD-CGD	2.05	1.55	1.50
2	A	404	HEM	O1A-CGA	2.04	1.29	1.22
3	B	1501	PIM	C6-C5	2.03	1.50	1.47

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	PIM	C2-N1-C5	-8.43	103.46	108.58
3	B	1501	PIM	C2-N1-C5	-8.40	103.48	108.58
2	B	404	HEM	CBA-CAA-C2A	5.70	122.74	112.69
2	A	404	HEM	CBA-CAA-C2A	5.53	122.43	112.69
4	B	1503	NHE	O1-S-C2	-5.08	102.46	106.81
4	B	1502	NHE	O1-S-C2	-4.49	102.96	106.81
4	A	503	NHE	O2-S-C2	-4.48	102.97	106.81
2	A	404	HEM	C3B-C4B-NB	-4.11	111.06	114.00
3	A	501	PIM	C6-C5-N1	3.89	126.70	121.45
3	B	1501	PIM	C6-C5-N1	3.77	126.54	121.45
2	B	404	HEM	C3B-C4B-NB	-3.74	111.32	114.00
2	B	404	HEM	CBD-CAD-C3D	3.61	122.26	114.37
2	A	404	HEM	CBD-CAD-C3D	3.46	121.92	114.37
4	A	503	NHE	C1-C2-S	-3.20	105.29	113.66
4	A	503	NHE	O3-S-O2	3.20	118.70	111.78
3	B	1501	PIM	C11-C6-C7	2.97	123.12	117.58
3	A	501	PIM	C11-C6-C7	2.96	123.09	117.58
2	A	404	HEM	CAD-CBD-CGD	2.92	122.58	113.48
2	B	404	HEM	C2D-C1D-ND	-2.80	109.62	112.93
3	B	1501	PIM	C10-C9-C8	2.76	125.73	119.97
4	A	503	NHE	C1-N-C1'	2.72	119.73	113.98
3	A	501	PIM	C10-C9-C8	2.67	125.53	119.97
2	B	404	HEM	CAD-CBD-CGD	2.66	121.79	113.48
3	A	501	PIM	C4-C5-C6	-2.47	125.31	129.77
3	B	1501	PIM	C4-C5-C6	-2.42	125.41	129.77
3	B	1501	PIM	C9-C10-C11	-2.35	116.26	120.17
2	A	404	HEM	CAA-CBA-CGA	2.34	120.97	113.47
2	B	404	HEM	CHC-C4B-NB	-2.32	122.65	124.58
4	A	502	NHE	C2-C1-N	-2.32	104.34	111.21
3	A	501	PIM	C9-C10-C11	-2.30	116.34	120.17
2	B	404	HEM	CAA-CBA-CGA	2.25	120.71	113.47
2	B	404	HEM	O2D-CGD-CBD	2.17	121.89	114.22
2	B	404	HEM	O1D-CGD-CBD	-2.13	115.71	123.03
4	B	1502	NHE	O3-S-C2	-2.12	103.24	105.93
4	B	1502	NHE	O2-S-C2	2.12	108.62	106.81
2	A	404	HEM	C2D-C1D-ND	-2.11	110.44	112.93
2	A	404	HEM	O2D-CGD-CBD	2.08	121.56	114.22
2	A	404	HEM	CMA-C3A-C4A	-2.06	125.45	128.62
2	A	404	HEM	O1D-CGD-CBD	-2.06	115.94	123.03
3	B	1501	PIM	C9-C8-C7	-2.05	116.75	120.17
3	A	501	PIM	C9-C8-C7	-2.02	116.81	120.17
4	B	1502	NHE	O3-S-O2	2.02	116.15	111.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	373/406 (91%)	-0.04	10 (2%)	52 62	36, 54, 82, 127	0
1	B	374/406 (92%)	-0.01	10 (2%)	52 62	35, 55, 85, 109	0
All	All	747/812 (91%)	-0.03	20 (2%)	53 62	35, 54, 84, 127	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	403	GLY	13.2
1	A	402	GLU	5.4
1	B	11	ILE	4.9
1	B	19	GLU	3.1
1	A	13	LYS	2.9
1	A	140	ASN	2.8
1	A	380	GLY	2.7
1	A	401	LYS	2.7
1	B	380	GLY	2.6
1	B	403	GLY	2.6
1	B	83	LEU	2.5
1	B	239	GLY	2.5
1	A	48	ASP	2.4
1	B	381	GLY	2.4
1	A	382	THR	2.3
1	B	255	ASP	2.3
1	B	287	HIS	2.2
1	B	401	LYS	2.0
1	A	270	PHE	2.0
1	A	383	ASP	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	NHE	A	503	13/13	0.24	4.26	70,88,127,128	0
4	NHE	A	502	13/13	0.21	3.33	66,83,109,111	0
4	NHE	B	1502	13/13	0.21	3.27	66,76,110,116	0
2	HEM	B	404	43/43	0.18	1.68	33,42,55,60	0
3	PIM	B	1501	11/11	0.17	1.35	35,40,45,47	0
2	HEM	A	404	43/43	0.17	1.07	28,41,48,55	0
3	PIM	A	501	11/11	0.12	0.35	28,34,39,40	0
4	NHE	B	1503	13/13	0.12	-0.29	66,72,110,111	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.