



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 03:24 PM GMT

PDB ID : 1QW5  
Title : Murine inducible nitric oxide synthase oxygenase domain in complex with W1400 inhibitor.  
Authors : Fedorov, R.; Hartmann, E.; Ghosh, D.K.; Schlichting, I.  
Deposited on : 2003-08-31  
Resolution : 2.70 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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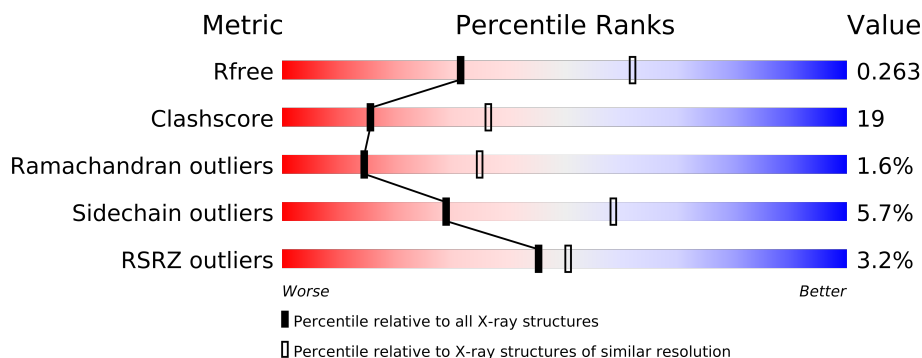
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	419	
1	B	419	

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

Mol	Type	Chain	Res	Geometry	Electron density
5	14W	B	904	-	X

## 2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 7241 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.

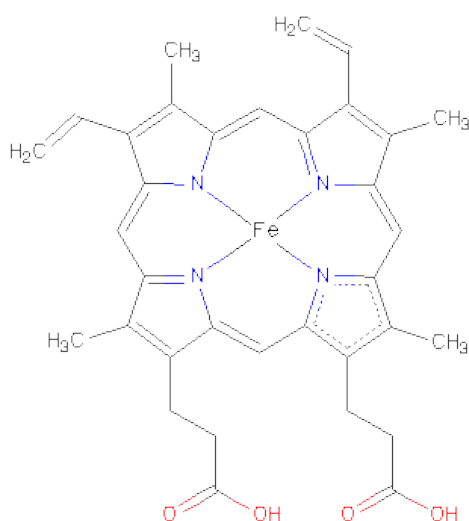
- Molecule 1 is a protein called Nitric oxide synthase, inducible.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	419	Total	C	N	O	S	0	0	0
			3415	2189	588	617	21			
1	B	419	Total	C	N	O	S	0	0	0
			3415	2189	588	617	21			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

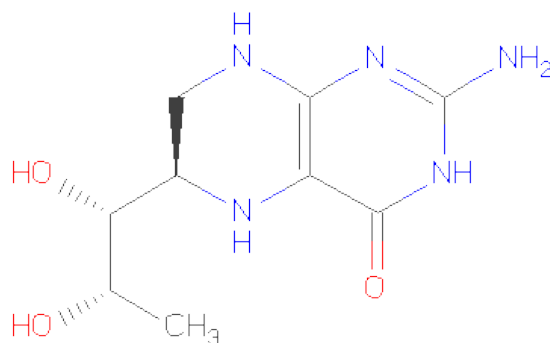
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



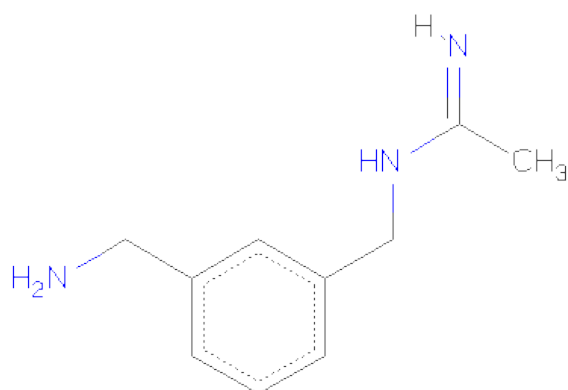
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 4 is 5,6,7,8-TETRAHYDROBIOPTERIN (three-letter code: H4B) (formula:  $C_9H_{15}N_5O_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			17	9	5	3		
4	B	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 5 is N-(3-(AMINOMETHYL)BENZYL)ACETAMIDINE (three-letter code: 14W) (formula:  $C_{10}H_{15}N_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	N	0	0
			13	10	3		
5	B	1	Total	C	N	0	0
			13	10	3		

- Molecule 6 is water.

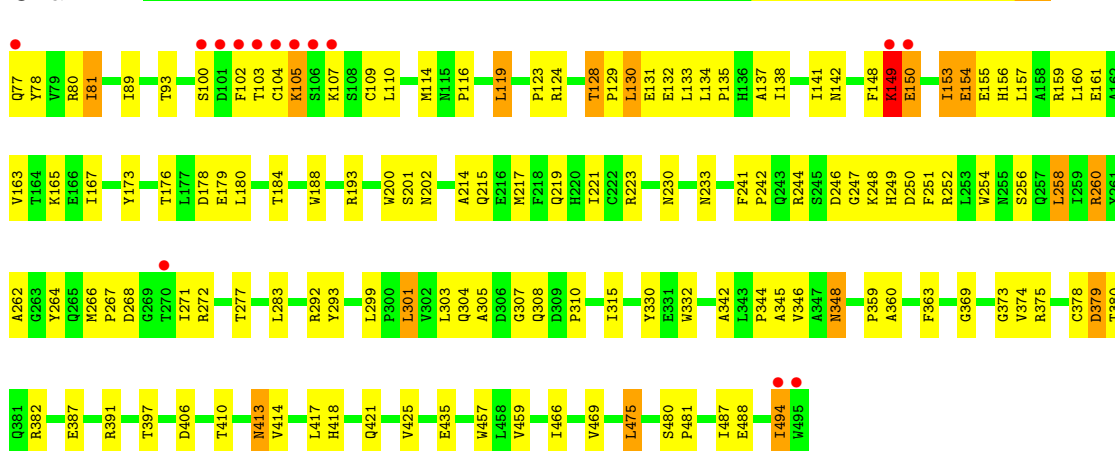
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	135	Total	O	0	0
			135	135		
6	B	128	Total	O	0	0
			128	128		

### 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.

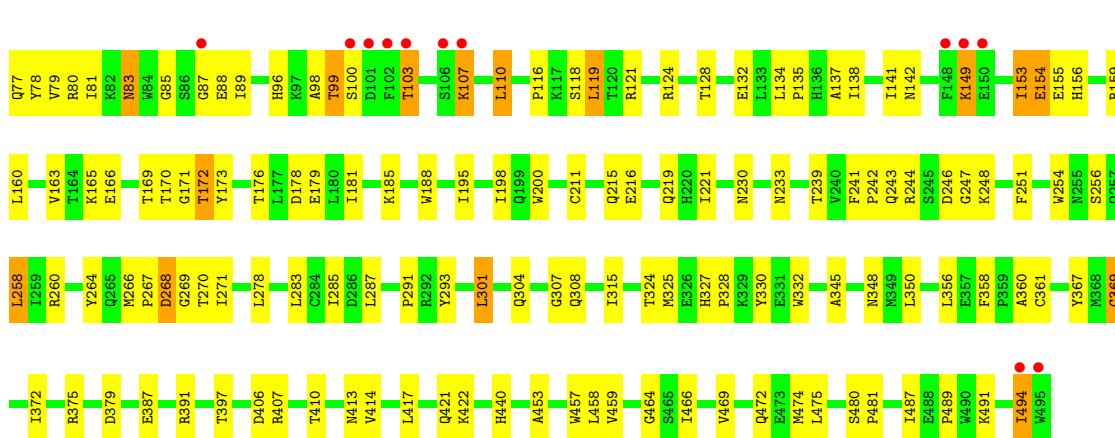
- Molecule 1: Nitric oxide synthase, inducible

Chain A:



- Molecule 1: Nitric oxide synthase, inducible

Chain B:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	214.56Å 214.56Å 117.39Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 2.70 19.69 – 2.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.70) 99.7 (19.69-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.11 (at 2.71Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.211 , 0.264 0.212 , 0.263	Depositor DCC
$R_{free}$ test set	2107 reflections (5.05%)	DCC
Wilson B-factor (Å <sup>2</sup> )	51.6	Xtriage
Anisotropy	0.579	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 48.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 43825 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7241	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% 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: HEM, ZN, H4B, 14W

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	0.39	0/3515	0.63	1/4778 (0.0%)
1	B	0.39	0/3515	0.63	0/4778
All	All	0.39	0/7030	0.63	1/9556 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	149	LYS	N-CA-C	-5.32	96.65	111.00

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	3415	0	3313	135	0
1	B	3415	0	3313	115	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	17	0	15	0	0
4	B	17	0	15	2	0
5	A	13	0	14	1	0
5	B	13	0	14	0	0
6	A	135	0	0	3	0
6	B	128	0	0	6	0
All	All	7241	0	6744	255	0

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 19.

All (255) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:153:ILE:H	1:B:153:ILE:HD12	1.13	1.14
1:A:153:ILE:HD12	1:A:153:ILE:H	1.28	0.96
1:B:494:ILE:H	1:B:494:ILE:HD12	1.36	0.91
1:B:285:ILE:HD11	1:B:291:PRO:HB3	1.53	0.91
1:A:494:ILE:H	1:A:494:ILE:HD12	1.34	0.91
1:A:80:ARG:HE	1:A:89:ILE:HG21	1.38	0.89
1:A:77:GLN:HG2	1:A:78:TYR:H	1.37	0.88
1:A:81:ILE:HD11	1:A:475:LEU:HD13	1.61	0.83
1:A:134:LEU:O	1:A:138:ILE:HG12	1.80	0.81
1:B:153:ILE:H	1:B:153:ILE:CD1	1.90	0.80
1:A:103:THR:HG22	1:A:110:LEU:HB2	1.63	0.79
1:B:83:ASN:ND2	1:B:85:GLY:H	1.81	0.79
1:B:301:LEU:HD13	1:B:315:ILE:HD11	1.66	0.78
1:B:83:ASN:HD22	1:B:83:ASN:C	1.87	0.78
1:B:83:ASN:HD22	1:B:85:GLY:H	1.34	0.76
1:B:103:THR:HG21	1:B:116:PRO:HB2	1.66	0.76
1:B:387:GLU:OE1	1:B:397:THR:HG21	1.86	0.75
1:B:387:GLU:OE2	1:B:391:ARG:HD2	1.85	0.75
1:A:149:LYS:O	1:A:150:GLU:HG2	1.86	0.75
1:A:77:GLN:HG2	1:A:78:TYR:N	2.01	0.75
1:B:107:LYS:HB3	1:B:107:LYS:NZ	2.03	0.74
1:A:130:LEU:HD13	1:A:167:ILE:HG22	1.69	0.74
1:B:494:ILE:N	1:B:494:ILE:HD12	2.03	0.73
1:A:221:ILE:HG21	1:A:301:LEU:HD21	1.68	0.73
1:A:129:PRO:HB2	1:A:132:GLU:HG3	1.72	0.71
1:B:110:LEU:HD23	1:B:110:LEU:N	2.05	0.70
1:A:104:CYS:HA	1:A:110:LEU:HD12	1.74	0.70
1:A:134:LEU:HB3	1:A:135:PRO:HD3	1.74	0.70
1:B:103:THR:O	1:B:110:LEU:HG	1.92	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:165:LYS:O	1:B:169:THR:HG23	1.93	0.69
1:A:159:ARG:O	1:A:163:VAL:HG23	1.93	0.69
1:A:154:GLU:H	1:A:154:GLU:CD	1.96	0.68
1:A:104:CYS:HA	1:A:110:LEU:CD1	2.24	0.67
1:A:188:TRP:CE3	1:A:200:TRP:HA	2.31	0.65
1:A:176:THR:OG1	1:A:179:GLU:HG3	1.96	0.65
1:B:375:ARG:O	1:B:379:ASP:HB2	1.96	0.65
1:A:138:ILE:HG22	1:A:142:ASN:HD21	1.62	0.65
1:A:262:ALA:HB2	1:A:299:LEU:CD2	2.27	0.64
1:B:153:ILE:N	1:B:153:ILE:HD12	1.98	0.64
1:A:387:GLU:O	1:A:391:ARG:HG3	1.98	0.63
1:A:138:ILE:HG23	1:A:160:LEU:HD22	1.81	0.63
1:B:110:LEU:HD23	1:B:110:LEU:H	1.62	0.62
1:A:215:GLN:HG3	1:A:219:GLN:NE2	2.14	0.62
1:A:252:ARG:HD3	1:A:359:PRO:HB2	1.80	0.62
1:A:330:TYR:HB3	1:A:332:TRP:CE2	2.34	0.62
1:B:260:ARG:HG3	6:B:986:HOH:O	1.99	0.62
1:B:88:GLU:C	1:B:89:ILE:HD12	2.21	0.61
1:A:271:ILE:HD12	1:A:271:ILE:N	2.16	0.61
1:B:285:ILE:HD11	1:B:291:PRO:CB	2.28	0.61
1:B:171:GLY:O	1:B:172:THR:HB	2.01	0.61
1:A:375:ARG:O	1:A:379:ASP:HB2	2.00	0.61
3:B:900:HEM:HMC1	3:B:900:HEM:HBC2	1.83	0.60
1:A:258:LEU:HB2	1:A:345:ALA:HB3	1.83	0.60
1:B:149:LYS:HD2	1:B:149:LYS:O	2.01	0.60
1:B:81:ILE:HD11	1:B:475:LEU:CD1	2.32	0.59
1:A:132:GLU:O	1:A:135:PRO:HD2	2.02	0.59
1:A:116:PRO:HG2	1:A:119:LEU:HB2	1.85	0.59
1:B:264:TYR:CE2	1:B:293:TYR:HA	2.38	0.59
1:B:116:PRO:CG	1:B:119:LEU:HD22	2.33	0.59
1:A:217:MET:HB3	1:A:303:LEU:HD13	1.83	0.58
3:A:900:HEM:HBA2	6:A:963:HOH:O	2.02	0.58
1:A:266:MET:CE	1:A:272:ARG:HH11	2.15	0.58
1:A:251:PHE:O	1:A:360:ALA:HB2	2.02	0.58
1:A:103:THR:HG23	1:A:116:PRO:HB3	1.84	0.58
1:A:494:ILE:N	1:A:494:ILE:HD12	2.13	0.58
1:A:103:THR:HG22	1:A:110:LEU:CB	2.34	0.57
1:B:407:ARG:HD3	6:B:983:HOH:O	2.05	0.57
1:B:188:TRP:CE3	1:B:200:TRP:HA	2.39	0.57
1:B:166:GLU:OE2	1:B:173:TYR:HA	2.05	0.57
1:A:417:LEU:O	1:A:421:GLN:HG3	2.05	0.56
1:A:154:GLU:HG2	1:A:155:GLU:H	1.71	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:271:ILE:HD12	1:A:271:ILE:H	1.71	0.56
1:A:223:ARG:HG2	1:A:223:ARG:HH11	1.70	0.56
1:A:254:TRP:HE3	1:A:283:LEU:HD21	1.70	0.56
1:A:163:VAL:HG13	1:A:173:TYR:CD2	2.41	0.56
1:B:304:GLN:HG3	1:B:308:GLN:O	2.06	0.56
1:A:230:ASN:HB3	1:A:233:ASN:O	2.06	0.56
1:B:103:THR:CG2	1:B:116:PRO:HB2	2.35	0.55
1:A:138:ILE:HG23	1:A:160:LEU:CD2	2.36	0.55
1:A:303:LEU:O	1:A:310:PRO:HA	2.07	0.55
1:B:107:LYS:HZ3	1:B:107:LYS:HB3	1.70	0.55
1:B:254:TRP:HE3	1:B:283:LEU:HD21	1.72	0.55
1:B:137:ALA:O	1:B:141:ILE:HG12	2.07	0.55
1:A:124:ARG:HH22	1:A:128:THR:HG22	1.72	0.55
1:B:153:ILE:O	1:B:156:HIS:HB3	2.06	0.55
1:A:153:ILE:O	1:A:157:LEU:HG	2.07	0.55
1:B:176:THR:OG1	1:B:179:GLU:HG3	2.06	0.55
1:A:133:LEU:HD22	1:A:167:ILE:HD13	1.88	0.55
1:A:131:GLU:O	1:A:135:PRO:HG2	2.07	0.54
1:A:105:LYS:HG3	1:A:110:LEU:HD11	1.88	0.54
1:B:301:LEU:CD1	1:B:315:ILE:HD11	2.36	0.54
1:B:103:THR:HG23	1:B:118:SER:HB3	1.90	0.54
1:B:283:LEU:O	1:B:287:LEU:HG	2.08	0.54
1:A:344:PRO:HB2	5:A:902:14W:H6	1.90	0.54
1:B:221:ILE:HG21	1:B:301:LEU:HD21	1.89	0.53
1:B:116:PRO:HG2	1:B:119:LEU:HD22	1.90	0.53
1:A:459:VAL:HG22	1:A:469:VAL:HG23	1.90	0.53
1:B:241:PHE:HB3	1:B:242:PRO:CD	2.38	0.53
1:A:107:LYS:HB2	1:A:107:LYS:NZ	2.22	0.53
1:B:134:LEU:O	1:B:138:ILE:HG13	2.08	0.53
1:B:83:ASN:C	1:B:83:ASN:ND2	2.60	0.52
1:A:246:ASP:OD2	1:A:248:LYS:HB2	2.09	0.52
1:B:78:TYR:CD1	1:B:78:TYR:C	2.83	0.52
1:A:342:ALA:HB1	1:A:425:VAL:HG11	1.92	0.52
1:B:330:TYR:HD2	1:B:332:TRP:NE1	2.08	0.51
1:B:244:ARG:HA	6:B:1002:HOH:O	2.10	0.51
1:B:124:ARG:HB2	1:B:247:GLY:HA3	1.92	0.51
1:B:251:PHE:O	1:B:360:ALA:HB2	2.10	0.51
1:A:138:ILE:O	1:A:142:ASN:ND2	2.43	0.51
1:A:104:CYS:CB	1:A:109:CYS:HA	2.40	0.51
1:B:198:ILE:HB	1:B:440:HIS:HB2	1.91	0.51
1:A:124:ARG:NH2	1:A:128:THR:HG22	2.25	0.51
1:B:417:LEU:O	1:B:421:GLN:HG3	2.11	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:81:ILE:HD11	1:B:475:LEU:HD12	1.93	0.51
1:A:148:PHE:N	1:A:148:PHE:CD2	2.79	0.51
1:A:153:ILE:HG22	1:A:157:LEU:HD11	1.92	0.50
1:A:330:TYR:CD2	1:A:330:TYR:N	2.76	0.50
1:B:132:GLU:O	1:B:135:PRO:HD2	2.11	0.50
1:B:266:MET:HB3	1:B:267:PRO:HD2	1.93	0.50
1:B:268:ASP:O	1:B:270:THR:N	2.37	0.50
1:A:410:THR:O	1:A:414:VAL:HG23	2.12	0.50
1:B:138:ILE:HG22	1:B:142:ASN:HD21	1.77	0.50
1:B:327:HIS:ND1	1:B:328:PRO:HD2	2.27	0.50
1:B:330:TYR:HD2	1:B:332:TRP:HE1	1.58	0.50
1:A:241:PHE:HB3	1:A:242:PRO:HD2	1.93	0.50
1:B:215:GLN:HG3	1:B:219:GLN:NE2	2.27	0.50
1:B:410:THR:O	1:B:414:VAL:HG23	2.11	0.49
1:A:104:CYS:HA	1:A:110:LEU:H	1.76	0.49
1:A:262:ALA:HB2	1:A:299:LEU:HD21	1.91	0.49
1:A:241:PHE:HB3	1:A:242:PRO:CD	2.42	0.49
1:B:154:GLU:CD	1:B:154:GLU:N	2.66	0.49
1:B:246:ASP:OD2	1:B:248:LYS:HB2	2.12	0.49
1:A:180:LEU:O	1:A:184:THR:HG23	2.12	0.49
1:A:130:LEU:CD1	1:A:167:ILE:HG22	2.42	0.49
1:B:489:PRO:C	1:B:491:LYS:H	2.16	0.48
1:B:453:ALA:HB1	1:B:458:LEU:CD1	2.43	0.48
1:A:305:ALA:O	1:A:308:GLN:HB2	2.14	0.48
1:A:264:TYR:CD2	1:A:293:TYR:HA	2.47	0.48
1:B:110:LEU:CD2	1:B:110:LEU:N	2.75	0.48
1:B:215:GLN:HG3	1:B:219:GLN:HE22	1.79	0.48
1:A:153:ILE:HD12	1:A:153:ILE:N	2.11	0.48
1:A:379:ASP:HB3	1:A:382:ARG:HG2	1.94	0.48
1:B:173:TYR:CE1	1:B:356:LEU:HD21	2.48	0.48
1:A:304:GLN:HG3	1:A:308:GLN:O	2.13	0.48
1:A:494:ILE:CD1	1:A:494:ILE:H	2.11	0.48
1:A:301:LEU:HD13	1:A:315:ILE:HD11	1.96	0.48
1:B:271:ILE:HD13	1:B:278:LEU:HD11	1.96	0.48
1:B:195:ILE:N	6:B:1021:HOH:O	2.44	0.48
1:A:132:GLU:C	1:A:135:PRO:HD2	2.33	0.47
1:B:124:ARG:HG3	1:B:244:ARG:HD3	1.96	0.47
1:B:267:PRO:HG2	1:B:268:ASP:OD1	2.14	0.47
1:A:138:ILE:HG22	1:A:142:ASN:ND2	2.26	0.47
1:A:252:ARG:CD	1:A:359:PRO:HB2	2.44	0.47
1:A:104:CYS:HB2	1:A:109:CYS:HA	1.96	0.47
1:A:379:ASP:CB	1:A:382:ARG:HG2	2.44	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:239:THR:O	1:B:361:CYS:HA	2.15	0.47
1:A:81:ILE:HD12	1:A:475:LEU:HD22	1.97	0.47
1:A:102:PHE:CG	1:A:103:THR:N	2.82	0.47
1:A:457:TRP:HZ3	6:A:963:HOH:O	1.97	0.47
1:B:241:PHE:HB3	1:B:242:PRO:HD2	1.96	0.47
1:B:98:ALA:O	1:B:99:THR:O	2.32	0.47
1:B:487:ILE:HD12	1:B:487:ILE:N	2.30	0.46
3:A:900:HEM:HBD1	6:A:963:HOH:O	2.15	0.46
1:A:254:TRP:CE3	1:A:283:LEU:HD21	2.50	0.46
1:B:230:ASN:HB3	1:B:233:ASN:O	2.16	0.46
1:A:161:GLU:OE2	1:A:165:LYS:NZ	2.47	0.46
1:A:348:ASN:ND2	1:A:348:ASN:H	2.14	0.46
1:B:154:GLU:CD	1:B:155:GLU:H	2.18	0.46
1:B:83:ASN:HB2	1:B:472:GLN:OE1	2.15	0.46
1:B:89:ILE:HD12	1:B:89:ILE:N	2.31	0.46
1:B:80:ARG:NH2	6:B:1042:HOH:O	2.44	0.46
3:A:900:HEM:HHC	3:A:900:HEM:HBB2	1.97	0.45
1:A:264:TYR:CE2	1:A:293:TYR:HA	2.52	0.45
1:A:103:THR:HG23	1:A:116:PRO:CB	2.47	0.45
1:A:114:MET:HE2	1:A:457:TRP:HZ2	1.82	0.45
1:B:466:ILE:O	1:B:466:ILE:HG22	2.16	0.45
1:A:249:HIS:HA	1:A:307:GLY:HA3	1.99	0.45
1:B:387:GLU:CD	1:B:391:ARG:HD2	2.36	0.45
1:B:79:VAL:HG11	1:B:475:LEU:HD11	1.98	0.45
1:A:330:TYR:HB3	1:A:332:TRP:NE1	2.32	0.45
1:B:83:ASN:ND2	1:B:85:GLY:N	2.59	0.44
1:B:258:LEU:HD22	1:B:345:ALA:HB1	1.98	0.44
3:B:900:HEM:CMC	3:B:900:HEM:HBC2	2.46	0.44
1:B:264:TYR:CD2	1:B:293:TYR:HA	2.52	0.44
1:A:78:TYR:CD1	1:A:78:TYR:C	2.91	0.44
1:A:104:CYS:HA	1:A:110:LEU:HD13	1.99	0.44
1:A:137:ALA:O	1:A:141:ILE:HG12	2.17	0.44
1:A:134:LEU:HD11	1:A:138:ILE:HD11	1.99	0.44
1:A:116:PRO:CG	1:A:119:LEU:HD22	2.48	0.44
1:B:181:ILE:O	1:B:185:LYS:HG3	2.17	0.44
1:A:131:GLU:O	1:A:135:PRO:CD	2.65	0.44
1:A:130:LEU:HD13	1:A:167:ILE:CG2	2.44	0.44
1:A:103:THR:CG2	1:A:116:PRO:HB3	2.48	0.43
1:B:350:LEU:HD23	1:B:350:LEU:C	2.38	0.43
1:A:346:VAL:HB	1:A:363:PHE:CZ	2.53	0.43
1:A:154:GLU:N	1:A:154:GLU:CD	2.69	0.43
1:A:262:ALA:CB	1:A:299:LEU:HD21	2.48	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:258:LEU:HB2	1:B:345:ALA:HB3	1.99	0.43
1:A:244:ARG:HG3	1:A:250:ASP:OD1	2.18	0.43
1:A:373:GLY:HA3	1:A:413:ASN:ND2	2.34	0.43
1:B:327:HIS:ND1	1:B:328:PRO:CD	2.80	0.43
1:B:494:ILE:CD1	1:B:494:ILE:H	2.17	0.43
1:B:480:SER:HA	1:B:481:PRO:C	2.39	0.43
1:A:131:GLU:O	1:A:135:PRO:CG	2.67	0.43
1:B:327:HIS:CG	1:B:328:PRO:HD2	2.53	0.43
1:A:80:ARG:HG3	1:A:89:ILE:CG2	2.49	0.43
1:B:138:ILE:HG23	1:B:160:LEU:HD22	2.01	0.43
1:A:148:PHE:N	1:A:148:PHE:HD2	2.17	0.42
1:A:202:ASN:N	1:A:202:ASN:HD22	2.16	0.42
1:A:154:GLU:HG2	1:A:155:GLU:N	2.34	0.42
1:B:159:ARG:O	1:B:163:VAL:HG23	2.19	0.42
1:A:114:MET:CE	1:A:457:TRP:HZ2	2.32	0.42
1:A:466:ILE:O	1:A:466:ILE:HG22	2.18	0.42
1:A:123:PRO:HD2	1:A:487:ILE:HD12	2.01	0.42
1:A:260:ARG:HD2	1:A:277:THR:HG21	2.02	0.42
1:B:367:TYR:CD2	1:B:372:ILE:HD11	2.54	0.42
1:A:266:MET:HB3	1:A:267:PRO:HD2	2.02	0.42
1:A:266:MET:HE2	1:A:272:ARG:HH11	1.82	0.42
1:A:344:PRO:O	1:A:344:PRO:HG2	2.19	0.42
1:B:327:HIS:CE1	1:B:330:TYR:HD1	2.37	0.42
1:A:103:THR:HG21	1:A:110:LEU:O	2.20	0.41
1:B:256:SER:HA	1:B:348:ASN:ND2	2.35	0.41
1:B:459:VAL:HG22	1:B:469:VAL:HG23	2.01	0.41
1:B:375:ARG:HH12	4:B:903:H4B:C4	2.33	0.41
1:B:121:ARG:HD3	1:B:121:ARG:HA	1.90	0.41
1:A:153:ILE:O	1:A:156:HIS:HB3	2.21	0.41
1:B:166:GLU:O	1:B:170:THR:OG1	2.31	0.41
1:A:330:TYR:HD1	1:A:332:TRP:CZ2	2.38	0.41
1:A:193:ARG:HD3	1:A:457:TRP:CD2	2.56	0.41
1:A:413:ASN:HA	1:A:413:ASN:HD22	1.56	0.41
1:A:248:LYS:HE3	1:A:248:LYS:HB3	1.81	0.41
1:B:422:LYS:HB3	1:B:422:LYS:NZ	2.36	0.41
1:B:83:ASN:O	1:B:87:GLY:N	2.53	0.41
1:A:266:MET:HE1	1:A:272:ARG:HD3	2.03	0.41
1:B:77:GLN:O	1:B:96:HIS:HE1	2.02	0.41
1:B:103:THR:HG23	1:B:118:SER:CB	2.50	0.41
1:A:214:ALA:O	1:A:217:MET:HB2	2.20	0.41
1:B:195:ILE:O	1:B:195:ILE:HG12	2.20	0.41
1:B:211:CYS:SG	1:B:216:GLU:HB3	2.60	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:110:LEU:HD12	1:A:110:LEU:N	2.35	0.41
1:B:457:TRP:HA	4:B:903:H4B:N1	2.36	0.41
1:A:330:TYR:HD2	1:A:330:TYR:N	2.17	0.41
1:A:330:TYR:CD1	1:A:332:TRP:CZ2	3.09	0.41
1:A:418:HIS:HA	1:A:421:GLN:OE1	2.21	0.41
1:A:494:ILE:CD1	1:A:494:ILE:N	2.79	0.40
1:B:116:PRO:HG2	1:B:119:LEU:HB2	2.02	0.40
1:A:78:TYR:HB3	1:A:93:THR:HG22	2.04	0.40
1:B:243:GLN:HB3	1:B:358:PHE:CE2	2.56	0.40
1:B:369:GLY:HA3	6:B:1004:HOH:O	2.21	0.40
1:A:134:LEU:CD1	1:A:138:ILE:HD11	2.50	0.40
1:A:244:ARG:HG3	1:A:247:GLY:HA2	2.04	0.40
1:A:480:SER:HA	1:A:481:PRO:C	2.41	0.40
1:B:103:THR:HG21	1:B:116:PRO:CB	2.46	0.40
1:B:138:ILE:O	1:B:142:ASN:ND2	2.55	0.40
1:A:374:VAL:O	1:A:378:CYS:HB2	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	417/419 (100%)	374 (90%)	37 (9%)	6 (1%)	16	41
1	B	417/419 (100%)	376 (90%)	34 (8%)	7 (2%)	14	33
All	All	834/838 (100%)	750 (90%)	71 (8%)	13 (2%)	14	35

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	100	SER
1	A	105	LYS
1	B	99	THR
1	B	172	THR

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Mol	Chain	Res	Type
1	B	269	GLY
1	A	150	GLU
1	A	369	GLY
1	A	397	THR
1	B	100	SER
1	A	268	ASP
1	B	464	GLY
1	B	307	GLY
1	B	369	GLY

### 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	367/367 (100%)	344 (94%)	23 (6%)	25	53
1	B	367/367 (100%)	348 (95%)	19 (5%)	32	63
All	All	734/734 (100%)	692 (94%)	42 (6%)	29	58

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	ILE
1	A	119	LEU
1	A	128	THR
1	A	130	LEU
1	A	149	LYS
1	A	153	ILE
1	A	154	GLU
1	A	178	ASP
1	A	201	SER
1	A	256	SER
1	A	258	LEU
1	A	260	ARG
1	A	292	ARG
1	A	301	LEU
1	A	348	ASN
1	A	379	ASP

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Mol	Chain	Res	Type
1	A	380	THR
1	A	406	ASP
1	A	413	ASN
1	A	435	GLU
1	A	475	LEU
1	A	488	GLU
1	A	494	ILE
1	B	83	ASN
1	B	103	THR
1	B	107	LYS
1	B	110	LEU
1	B	119	LEU
1	B	128	THR
1	B	149	LYS
1	B	153	ILE
1	B	154	GLU
1	B	178	ASP
1	B	258	LEU
1	B	268	ASP
1	B	301	LEU
1	B	324	THR
1	B	325	MET
1	B	406	ASP
1	B	413	ASN
1	B	474	MET
1	B	494	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	ASN
1	A	142	ASN
1	A	174	GLN
1	A	202	ASN
1	A	215	GLN
1	A	219	GLN
1	A	231	ASN
1	A	348	ASN
1	A	413	ASN
1	B	83	ASN
1	B	96	HIS
1	B	142	ASN

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Mol	Chain	Res	Type
1	B	143	GLN
1	B	174	GLN
1	B	202	ASN
1	B	215	GLN
1	B	219	GLN
1	B	231	ASN
1	B	249	HIS
1	B	486	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 ⓘ

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	HEM	A	900	1	49,50,50	2.84	12 (24%)	46,82,82	1.40	8 (17%)
4	H4B	A	901	-	18,18,18	1.60	5 (27%)	24,26,26	2.60	9 (37%)
5	14W	A	902	-	13,13,13	1.39	1 (7%)	16,16,16	0.71	0
3	HEM	B	900	1	49,50,50	2.09	13 (26%)	46,82,82	1.28	4 (8%)
4	H4B	B	903	-	18,18,18	1.69	5 (27%)	24,26,26	2.50	9 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	14W	B	904	-	13,13,13	1.51	2 (15%)	16,16,16	0.59	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEM	A	900	1	-	0/14/114/114	0/0/8/8
4	H4B	A	901	-	-	0/8/17/17	0/0/2/2
5	14W	A	902	-	-	0/7/7/7	0/1/1/1
3	HEM	B	900	1	-	0/14/114/114	0/0/8/8
4	H4B	B	903	-	-	0/8/17/17	0/0/2/2
5	14W	B	904	-	-	0/7/7/7	0/1/1/1

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	900	HEM	C2D-C1D	10.51	1.47	1.44
3	A	900	HEM	C3D-C4D	8.13	1.46	1.44
3	A	900	HEM	C3D-C2D	-6.61	1.32	1.43
3	B	900	HEM	C3D-C4D	6.43	1.46	1.44
3	A	900	HEM	C4A-C3A	6.20	1.47	1.40
3	B	900	HEM	C2D-C1D	-4.88	1.43	1.44
3	A	900	HEM	C3C-C2C	-4.67	1.35	1.43
3	B	900	HEM	C3D-C2D	-4.58	1.35	1.43
3	A	900	HEM	C2B-C1B	4.43	1.45	1.44
3	B	900	HEM	FE-NB	4.05	2.12	1.97
4	B	903	H4B	C4-N3	3.95	1.43	1.37
3	A	900	HEM	C3B-C4B	3.89	1.49	1.44
3	B	900	HEM	C4A-C3A	3.75	1.44	1.40
3	B	900	HEM	CHA-C4D	3.58	1.40	1.35
4	A	901	H4B	C2-N1	3.36	1.37	1.33
3	A	900	HEM	FE-NB	3.30	2.09	1.97
3	B	900	HEM	C3B-C4B	3.20	1.48	1.44
4	A	901	H4B	C4-N3	3.16	1.42	1.37
3	A	900	HEM	C3B-C2B	-3.10	1.38	1.43
3	B	900	HEM	C3B-C2B	-3.06	1.38	1.43
4	B	903	H4B	C2-N1	2.91	1.37	1.33
3	B	900	HEM	FE-ND	-2.88	1.87	1.97
4	B	903	H4B	C6-N5	2.87	1.52	1.46
5	B	904	14W	C10-C9	2.86	1.52	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	900	HEM	CHB-C1B	2.85	1.39	1.35
4	A	901	H4B	C6-N5	2.78	1.51	1.46
3	B	900	HEM	C3C-C2C	-2.60	1.39	1.43
4	A	901	H4B	C8A-N1	2.60	1.39	1.34
3	A	900	HEM	CHA-C4D	2.51	1.39	1.35
3	B	900	HEM	CMC-C2C	2.48	1.55	1.47
4	B	903	H4B	C4A-N5	2.41	1.46	1.38
4	B	903	H4B	C8A-N1	2.40	1.39	1.34
3	A	900	HEM	FE-ND	-2.31	1.89	1.97
5	A	902	14W	C2-C3	2.30	1.43	1.39
5	B	904	14W	C6-C1	2.16	1.43	1.38
3	B	900	HEM	CHC-C1C	2.14	1.40	1.36
3	B	900	HEM	FE-NA	2.12	2.01	1.92
4	A	901	H4B	C4A-N5	2.09	1.45	1.38

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	901	H4B	C4-C4A-C8A	8.65	122.57	114.56
4	B	903	H4B	C4-C4A-C8A	8.38	122.33	114.56
3	B	900	HEM	CHC-C4B-NB	-4.43	120.91	124.58
3	A	900	HEM	CHC-C4B-NB	-3.70	121.51	124.58
4	B	903	H4B	C4-N3-C2	3.46	125.57	119.51
4	A	901	H4B	C2-N1-C8A	3.43	122.49	117.61
4	B	903	H4B	C2-N1-C8A	3.41	122.46	117.61
4	B	903	H4B	C4A-N5-C6	-3.37	112.00	121.16
4	A	901	H4B	N3-C2-N1	-3.33	117.11	121.78
4	A	901	H4B	C4-N3-C2	3.30	125.29	119.51
3	A	900	HEM	CHD-C4C-NC	-3.08	122.06	124.73
4	A	901	H4B	C4A-N5-C6	-3.02	112.95	121.16
4	B	903	H4B	N3-C2-N1	-3.01	117.57	121.78
4	A	901	H4B	C9-C6-N5	-2.85	104.38	109.69
4	A	901	H4B	C7-C6-C9	2.74	117.88	113.66
3	A	900	HEM	C3B-C4B-NB	-2.72	112.05	114.00
3	A	900	HEM	CBD-CAD-C3D	-2.64	108.60	114.37
3	B	900	HEM	CHD-C4C-NC	-2.60	122.47	124.73
3	A	900	HEM	CAD-C3D-C4D	2.59	129.19	124.53
3	A	900	HEM	CAD-C3D-C2D	-2.44	121.81	127.25
4	A	901	H4B	N8-C8A-N1	2.39	119.32	115.82
4	B	903	H4B	C7-C6-C9	2.28	117.17	113.66
3	B	900	HEM	C4A-NA-C1A	-2.23	103.82	106.76
4	A	901	H4B	C4A-C8A-N8	2.22	122.28	119.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	900	HEM	C3B-C4B-NB	-2.22	112.41	114.00
4	B	903	H4B	N8-C8A-N1	2.17	119.00	115.82
4	B	903	H4B	C4A-C8A-N8	2.14	122.17	119.23
4	B	903	H4B	C9-C6-N5	-2.13	105.71	109.69
3	A	900	HEM	C4A-NA-C1A	-2.13	103.96	106.76
3	A	900	HEM	C4C-NC-C1C	-2.08	103.37	105.53

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	419/419 (100%)	-0.19	14 (3%)	44 49	32, 49, 72, 89	0
1	B	419/419 (100%)	-0.20	12 (2%)	49 55	32, 49, 69, 93	0
All	All	838/838 (100%)	-0.19	26 (3%)	45 52	32, 49, 71, 93	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	106	SER	6.2
1	A	103	THR	6.1
1	B	103	THR	5.3
1	A	102	PHE	5.1
1	B	102	PHE	5.1
1	A	104	CYS	4.8
1	B	101	ASP	4.8
1	A	106	SER	4.2
1	B	107	LYS	4.2
1	A	100	SER	3.4
1	A	150	GLU	3.3
1	B	150	GLU	3.2
1	A	149	LYS	3.1
1	B	100	SER	3.0
1	A	107	LYS	2.8
1	B	87	GLY	2.6
1	A	105	LYS	2.5
1	B	149	LYS	2.4
1	B	495	TRP	2.4
1	A	101	ASP	2.4
1	A	270	THR	2.2
1	A	494	ILE	2.2
1	A	495	TRP	2.1
1	B	148	PHE	2.1

*Continued on next page...*

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Mol	Chain	Res	Type	RSRZ
1	A	77	GLN	2.0
1	B	494	ILE	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
5	14W	B	904	13/13	0.25	4.54	38,40,43,43	0
2	ZN	B	950	1/1	0.28	1.80	45,45,45,45	1
5	14W	A	902	13/13	0.20	1.75	37,39,40,41	0
2	ZN	A	950	1/1	0.32	0.35	49,49,49,49	1
3	HEM	B	900	43/43	0.14	-0.12	30,42,48,53	0
4	H4B	B	903	17/17	0.12	-0.33	22,35,40,42	0
4	H4B	A	901	17/17	0.12	-0.47	18,35,47,48	0
3	HEM	A	900	43/43	0.13	-0.62	26,43,57,64	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.