



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 01:16 AM GMT

PDB ID : 3GW9  
Title : Crystal structure of sterol 14-alpha demethylase (CYP51) from Trypanosoma brucei bound to an inhibitor N-(1-(2,4-dichlorophenyl)-2-(1H-imidazol-1-yl)ethyl)-4-(5-phenyl-1,3,4-oxadiazol-2-yl)benzamide  
Authors : Lepesheva, G.I.; Hargrove, T.Y.; Harp, J.; Wawrzak, Z.; Waterman, M.R.  
Deposited on : 2009-03-31  
Resolution : 1.87 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>

---

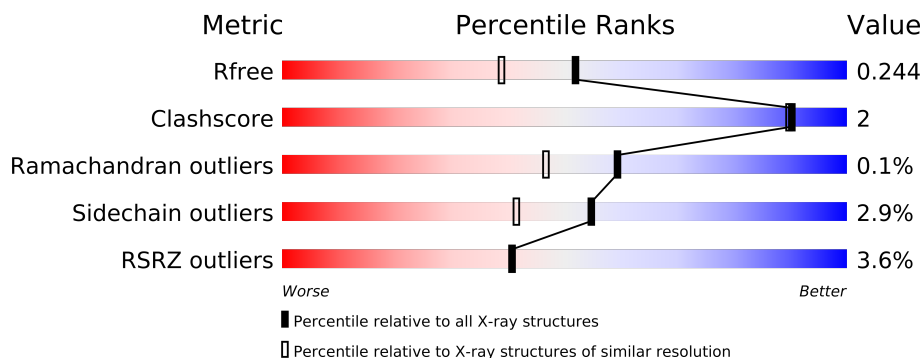
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.87 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	5260 (1.90-1.86)
Clashscore	79885	6268 (1.90-1.86)
Ramachandran outliers	78287	6195 (1.90-1.86)
Sidechain outliers	78261	6196 (1.90-1.86)
RSRZ outliers	66119	5262 (1.90-1.86)

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	450	
1	B	450	
1	C	450	
1	D	450	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15276 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.

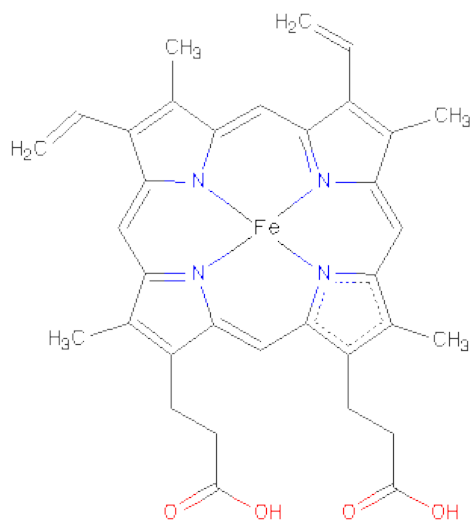
- Molecule 1 is a protein called STEROL 14ALPHA-DEMETHYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	450	Total	C	N	O	S	0	0	0
			3575	2283	625	640	27			
1	B	449	Total	C	N	O	S	0	0	0
			3566	2277	623	639	27			
1	C	449	Total	C	N	O	S	0	0	0
			3566	2277	623	639	27			
1	D	449	Total	C	N	O	S	0	0	0
			3566	2277	623	639	27			

There are 16 discrepancies between the modelled and reference sequences:

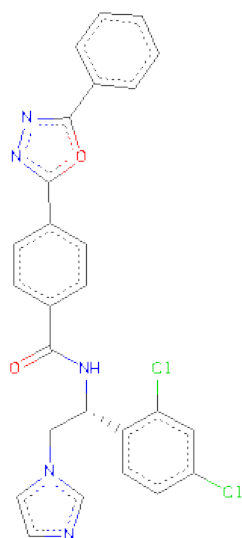
Chain	Residue	Modelled	Actual	Comment	Reference
A	28	LYS	ARG	ENGINEERED	UNP Q385E8
A	29	GLY	PRO	ENGINEERED	UNP Q385E8
A	30	LYS	THR	ENGINEERED	UNP Q385E8
A	31	LEU	ASP	ENGINEERED	UNP Q385E8
B	28	LYS	ARG	ENGINEERED	UNP Q385E8
B	29	GLY	PRO	ENGINEERED	UNP Q385E8
B	30	LYS	THR	ENGINEERED	UNP Q385E8
B	31	LEU	ASP	ENGINEERED	UNP Q385E8
C	28	LYS	ARG	ENGINEERED	UNP Q385E8
C	29	GLY	PRO	ENGINEERED	UNP Q385E8
C	30	LYS	THR	ENGINEERED	UNP Q385E8
C	31	LEU	ASP	ENGINEERED	UNP Q385E8
D	28	LYS	ARG	ENGINEERED	UNP Q385E8
D	29	GLY	PRO	ENGINEERED	UNP Q385E8
D	30	LYS	THR	ENGINEERED	UNP Q385E8
D	31	LEU	ASP	ENGINEERED	UNP Q385E8

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

- Molecule 3 is N-[(1R)-1-(2,4-DICHLOROPHENYL)-2-(1H-IMIDAZOL-1-YL)ETHYL]-4-(5-PHENYL-1,3,4-OXADIAZOL-2-YL)BENZAMIDE (three-letter code: VNI) (formula:  $C_{26}H_{19}Cl_2N_5O_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 35	C 26	Cl 2	N 5	O 2	0	0
3	B	1	Total 35	C 26	Cl 2	N 5	O 2	0	0
3	C	1	Total 35	C 26	Cl 2	N 5	O 2	0	0
3	D	1	Total 35	C 26	Cl 2	N 5	O 2	0	0

- Molecule 4 is water.

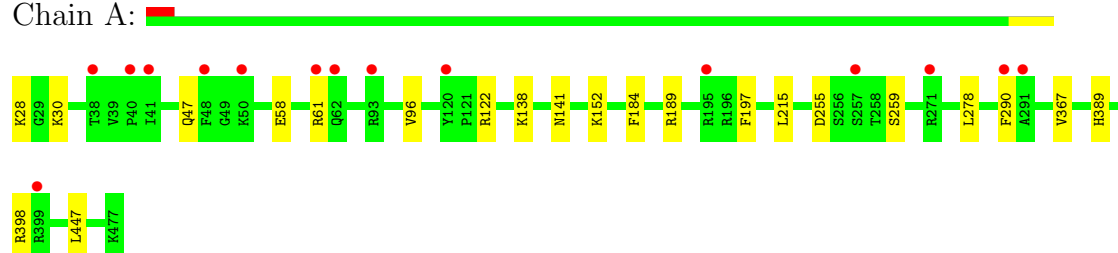
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	149	Total 149	O 149	0	0
4	B	195	Total 195	O 195	0	0
4	C	219	Total 219	O 219	0	0
4	D	128	Total 128	O 128	0	0

### 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 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.

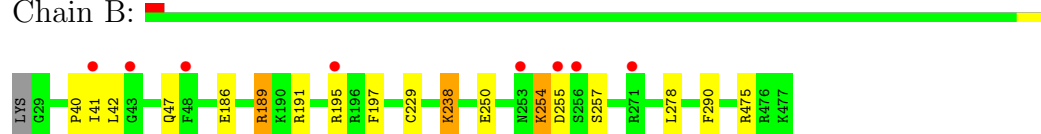
#### • Molecule 1: STEROL 14ALPHA-DEMETHYLASE

Chain A:



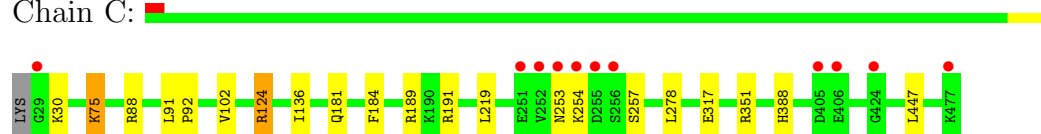
#### • Molecule 1: STEROL 14ALPHA-DEMETHYLASE

Chain B:



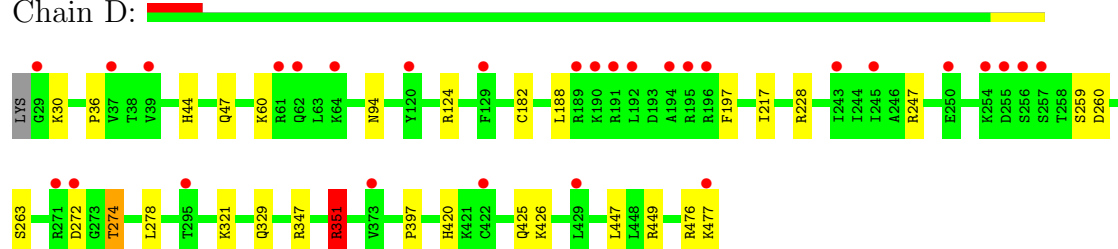
#### • Molecule 1: STEROL 14ALPHA-DEMETHYLASE

Chain C:



#### • Molecule 1: STEROL 14ALPHA-DEMETHYLASE

Chain D:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.08Å 79.11Å 116.00Å 74.74° 79.13° 68.57°	Depositor
Resolution (Å)	37.48 – 1.87 37.46 – 1.87	Depositor EDS
% Data completeness (in resolution range)	97.0 (37.48-1.87) 97.0 (37.46-1.87)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.72 (at 1.87Å)	Xtriage
Refinement program	REFMAC 5.5.0070	Depositor
R, $R_{free}$	0.189 , 0.238 0.196 , 0.244	Depositor DCC
$R_{free}$ test set	7635 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	30.7	Xtriage
Anisotropy	0.288	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 41.6	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 152162 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	15276	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.65% 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, VNI

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	0.79	0/3657	0.76	0/4944
1	B	0.78	1/3648 (0.0%)	0.77	2/4933 (0.0%)
1	C	0.87	0/3648	0.82	2/4933 (0.0%)
1	D	0.71	1/3648 (0.0%)	0.72	1/4933 (0.0%)
All	All	0.79	2/14601 (0.0%)	0.77	5/19743 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	182	CYS	CB-SG	-5.63	1.72	1.81
1	B	229	CYS	CB-SG	-5.29	1.73	1.81

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	189	ARG	NE-CZ-NH2	-6.73	116.94	120.30
1	C	124	ARG	NE-CZ-NH2	-6.29	117.16	120.30
1	C	124	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	D	351	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	B	189	ARG	NE-CZ-NH1	5.01	122.81	120.30

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	3575	0	0	7	0
1	B	3566	0	0	5	0
1	C	3566	0	0	8	0
1	D	3566	0	0	9	0
2	A	43	0	0	0	0
2	B	43	0	0	0	0
2	C	43	0	0	0	0
2	D	43	0	0	3	0
3	A	35	0	0	0	0
3	B	35	0	0	0	0
3	C	35	0	0	0	0
3	D	35	0	0	0	0
4	A	149	0	0	2	0
4	B	195	0	0	0	0
4	C	219	0	0	3	0
4	D	128	0	0	0	0
All	All	15276	0	0	30	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 2.

All (30) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:186:GLU:OE2	1:B:189:ARG:NH2	2.33	0.62
1:A:58:GLU:OE1	1:A:61:ARG:NH1	2.35	0.59
1:A:122:ARG:NH2	4:A:602:HOH:O	2.41	0.53
1:A:184:PHE:O	1:A:189:ARG:NH1	2.43	0.52
1:C:91:LEU:N	1:C:92:PRO:CD	2.73	0.52
2:D:480:HEM:CMC	2:D:480:HEM:CBC	2.91	0.49
1:C:254:LYS:O	1:C:257:SER:OG	2.30	0.49
1:C:351:ARG:O	1:C:388:HIS:CD2	2.67	0.48
1:D:347:ARG:NH2	1:D:425:GLN:NE2	2.61	0.48
1:D:272:ASP:CB	1:D:274:THR:OG1	2.61	0.48
1:A:30:LYS:NZ	1:C:184:PHE:O	2.48	0.47
1:C:191:ARG:NH2	4:C:537:HOH:O	2.47	0.47
1:B:250:GLU:O	1:B:254:LYS:N	2.49	0.46
1:A:389:HIS:CE1	1:A:398:ARG:NH1	2.84	0.46
1:A:138:LYS:NZ	4:A:492:HOH:O	2.49	0.45
1:B:40:PRO:O	1:B:42:LEU:N	2.49	0.45

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:260:ASP:OD1	1:D:263:SER:N	2.49	0.45
2:D:480:HEM:CMB	2:D:480:HEM:CBB	2.95	0.45
1:B:238:LYS:N	1:B:238:LYS:CD	2.81	0.44
1:A:96:VAL:CG1	1:A:367:VAL:CG1	2.97	0.43
1:D:36:PRO:O	1:D:44:HIS:CE1	2.72	0.42
1:D:247:ARG:NH2	1:D:260:ASP:OD2	2.52	0.42
1:C:75:LYS:NZ	4:C:675:HOH:O	2.53	0.42
1:C:124:ARG:NH2	4:C:640:HOH:O	2.53	0.41
1:B:255:ASP:O	1:B:257:SER:N	2.53	0.41
1:D:476:ARG:O	1:D:477:LYS:C	2.58	0.41
1:D:94:ASN:OD1	1:D:420:HIS:NE2	2.54	0.41
1:C:181:GLN:OE1	1:C:189:ARG:NH1	2.55	0.40
1:D:351:ARG:NH2	1:D:397:PRO:O	2.55	0.40
1:D:124:ARG:NH2	2:D:480:HEM:O1D	2.54	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	448/450 (100%)	436 (97%)	12 (3%)	0	100	100
1	B	447/450 (99%)	432 (97%)	14 (3%)	1 (0%)	56	43
1	C	447/450 (99%)	435 (97%)	11 (2%)	1 (0%)	56	43
1	D	447/450 (99%)	438 (98%)	9 (2%)	0	100	100
All	All	1789/1800 (99%)	1741 (97%)	46 (3%)	2 (0%)	59	47

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	253	ASN
1	B	41	ILE

### 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	392/392 (100%)	381 (97%)	11 (3%)	56	43
1	B	391/392 (100%)	382 (98%)	9 (2%)	63	52
1	C	391/392 (100%)	382 (98%)	9 (2%)	63	52
1	D	391/392 (100%)	375 (96%)	16 (4%)	41	26
All	All	1565/1568 (100%)	1520 (97%)	45 (3%)	55	41

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	LYS
1	A	47	GLN
1	A	141	ASN
1	A	152	LYS
1	A	197	PHE
1	A	215	LEU
1	A	255	ASP
1	A	259	SER
1	A	278	LEU
1	A	290	PHE
1	A	447	LEU
1	B	47	GLN
1	B	191	ARG
1	B	195	ARG
1	B	197	PHE
1	B	238	LYS
1	B	254	LYS
1	B	278	LEU
1	B	290	PHE
1	B	475	ARG
1	C	30	LYS
1	C	75	LYS
1	C	88	ARG
1	C	102	VAL
1	C	136	ILE
1	C	219	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	278	LEU
1	C	317	GLU
1	C	447	LEU
1	D	30	LYS
1	D	47	GLN
1	D	60	LYS
1	D	188	LEU
1	D	197	PHE
1	D	217	ILE
1	D	228	ARG
1	D	259	SER
1	D	274	THR
1	D	278	LEU
1	D	321	LYS
1	D	329	GLN
1	D	351	ARG
1	D	426	LYS
1	D	447	LEU
1	D	449	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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	480	1,3	49,50,50	2.45	17 (34%)	46,82,82	2.20	16 (34%)
3	VNI	A	490	2	39,39,39	2.03	4 (10%)	51,54,54	1.85	9 (17%)
2	HEM	B	480	1,3	49,50,50	2.33	14 (28%)	46,82,82	2.17	11 (23%)
3	VNI	B	490	2	39,39,39	2.10	6 (15%)	51,54,54	1.83	12 (23%)
2	HEM	C	480	1,3	49,50,50	2.58	15 (30%)	46,82,82	2.21	13 (28%)
3	VNI	C	490	2	39,39,39	2.42	5 (12%)	51,54,54	2.31	15 (29%)
2	HEM	D	480	1,3	49,50,50	2.79	20 (40%)	46,82,82	1.55	8 (17%)
3	VNI	D	490	2	39,39,39	2.05	4 (10%)	51,54,54	1.64	8 (15%)

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	480	1,3	-	0/14/114/114	0/0/8/8
3	VNI	A	490	2	-	0/24/24/24	0/4/5/5
2	HEM	B	480	1,3	-	0/14/114/114	0/0/8/8
3	VNI	B	490	2	-	0/24/24/24	0/4/5/5
2	HEM	C	480	1,3	-	0/14/114/114	0/0/8/8
3	VNI	C	490	2	-	0/24/24/24	0/4/5/5
2	HEM	D	480	1,3	-	0/14/114/114	0/0/8/8
3	VNI	D	490	2	-	0/24/24/24	0/4/5/5

All (85) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	490	VNI	C21-C20	-9.65	1.38	1.47
3	C	490	VNI	C16-C19	-9.55	1.38	1.47
3	D	490	VNI	C16-C19	-8.51	1.39	1.47
3	B	490	VNI	C16-C19	-8.07	1.39	1.47
2	D	480	HEM	C2D-C1D	-7.88	1.42	1.44
3	B	490	VNI	C21-C20	-7.84	1.40	1.47
2	D	480	HEM	C3B-C2B	-7.70	1.30	1.43
2	B	480	HEM	C2D-C1D	7.66	1.46	1.44

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	490	VNI	C21-C20	-7.52	1.40	1.47
3	A	490	VNI	C16-C19	-7.50	1.40	1.47
2	D	480	HEM	C3C-C2C	-7.48	1.30	1.43
2	C	480	HEM	C3D-C4D	-7.44	1.42	1.44
3	D	490	VNI	C21-C20	-7.36	1.40	1.47
2	A	480	HEM	C3C-C2C	-6.67	1.32	1.43
2	C	480	HEM	C3C-C2C	-6.55	1.32	1.43
2	C	480	HEM	C3B-C2B	-6.28	1.32	1.43
2	B	480	HEM	C3B-C2B	-5.99	1.33	1.43
2	A	480	HEM	C3B-C2B	-5.79	1.33	1.43
2	C	480	HEM	C2D-C1D	-5.38	1.43	1.44
2	A	480	HEM	C4A-C3A	5.14	1.46	1.40
2	A	480	HEM	C3C-CAC	4.97	1.56	1.40
2	D	480	HEM	C4A-C3A	4.89	1.46	1.40
2	D	480	HEM	FE-NB	-4.64	1.81	1.97
2	B	480	HEM	C3C-C2C	-4.54	1.35	1.43
2	D	480	HEM	C2B-C1B	-4.53	1.43	1.44
2	C	480	HEM	C4A-C3A	4.41	1.45	1.40
2	B	480	HEM	C4A-C3A	4.40	1.45	1.40
2	D	480	HEM	C4C-NC	-4.29	1.32	1.38
2	C	480	HEM	C3B-CAB	4.27	1.53	1.40
2	B	480	HEM	C3C-CAC	4.22	1.53	1.40
2	C	480	HEM	C2B-C1B	4.14	1.45	1.44
2	B	480	HEM	C3B-CAB	4.14	1.53	1.40
2	A	480	HEM	C3B-CAB	3.98	1.52	1.40
2	B	480	HEM	C3D-C2D	3.90	1.50	1.43
2	C	480	HEM	C3C-CAC	3.85	1.52	1.40
2	A	480	HEM	C3D-C2D	3.85	1.50	1.43
2	D	480	HEM	C1C-NC	-3.83	1.32	1.38
3	A	490	VNI	C6-N2	-3.77	1.31	1.36
2	A	480	HEM	C2B-C1B	-3.75	1.43	1.44
2	A	480	HEM	CMC-C2C	3.70	1.58	1.47
2	D	480	HEM	C3B-CAB	3.62	1.51	1.40
2	A	480	HEM	C2D-C1D	-3.59	1.43	1.44
3	B	490	VNI	C6-N2	-3.59	1.31	1.36
2	B	480	HEM	CMC-C2C	3.46	1.58	1.47
2	A	480	HEM	CMD-C2D	3.39	1.58	1.47
2	C	480	HEM	CAA-C2A	3.34	1.57	1.52
2	C	480	HEM	C4C-NC	-3.27	1.33	1.38
2	D	480	HEM	C3C-CAC	3.25	1.50	1.40
3	A	490	VNI	C7-C2	-3.22	1.46	1.51
2	A	480	HEM	C3B-C4B	-3.08	1.40	1.44

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	480	HEM	C3D-C2D	3.07	1.49	1.43
2	C	480	HEM	C3D-C2D	2.98	1.49	1.43
2	C	480	HEM	CMC-C2C	2.96	1.56	1.47
3	D	490	VNI	C6-N2	-2.96	1.32	1.36
2	B	480	HEM	C3B-C4B	-2.89	1.41	1.44
2	C	480	HEM	CMB-C2B	2.81	1.56	1.47
2	B	480	HEM	CAA-C2A	2.81	1.57	1.52
3	D	490	VNI	C7-C2	-2.74	1.47	1.51
2	A	480	HEM	FE-NA	2.73	2.04	1.92
2	C	480	HEM	FE-NB	-2.67	1.88	1.97
2	A	480	HEM	CMB-C2B	2.62	1.55	1.47
3	C	490	VNI	C6-N2	-2.62	1.32	1.36
3	B	490	VNI	C7-C2	-2.61	1.47	1.51
2	D	480	HEM	O2D-CGD	-2.58	1.21	1.30
2	B	480	HEM	C4C-NC	-2.55	1.34	1.38
3	B	490	VNI	C3-N2	-2.50	1.45	1.48
2	B	480	HEM	CMD-C2D	2.47	1.55	1.47
2	D	480	HEM	C4A-NA	-2.45	1.31	1.36
2	A	480	HEM	CHA-C4D	2.43	1.39	1.35
2	A	480	HEM	CAA-C2A	2.38	1.56	1.52
2	D	480	HEM	C2A-C3A	-2.35	1.30	1.37
2	A	480	HEM	CMA-C3A	2.34	1.56	1.51
2	B	480	HEM	C1A-NA	2.34	1.41	1.36
2	D	480	HEM	C1A-CHA	-2.30	1.33	1.39
2	C	480	HEM	FE-NA	2.25	2.02	1.92
3	C	490	VNI	C6-N3	2.18	1.38	1.34
2	D	480	HEM	CHD-C1D	-2.18	1.34	1.39
3	B	490	VNI	N4-N5	2.18	1.42	1.37
2	D	480	HEM	O2A-CGA	-2.17	1.22	1.30
2	D	480	HEM	CMC-C2C	2.13	1.54	1.47
2	A	480	HEM	O2A-CGA	-2.11	1.22	1.30
3	C	490	VNI	C12-CL2	2.05	1.78	1.73
2	B	480	HEM	CMB-C2B	2.04	1.53	1.47
2	D	480	HEM	C4A-CHB	-2.04	1.34	1.39
2	D	480	HEM	FE-NA	2.03	2.01	1.92

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	490	VNI	O2-C20-C21	6.97	126.43	119.23
2	C	480	HEM	CHC-C4B-NB	6.96	130.37	124.58
2	B	480	HEM	C3B-C4B-NB	-6.94	109.03	114.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	480	HEM	C3B-C4B-NB	-6.77	109.16	114.00
3	B	490	VNI	C3-C2-N1	-6.52	96.18	109.84
3	C	490	VNI	C12-C7-C2	-6.34	117.18	121.89
2	A	480	HEM	C3B-C4B-NB	-6.08	109.65	114.00
3	C	490	VNI	O2-C19-C16	5.77	125.19	119.23
2	B	480	HEM	CHC-C4B-NB	5.52	129.17	124.58
3	D	490	VNI	O2-C20-C21	5.36	124.76	119.23
3	C	490	VNI	C3-C2-N1	-5.33	98.67	109.84
2	A	480	HEM	CAD-C3D-C4D	5.05	133.62	124.53
3	A	490	VNI	C3-C2-N1	-5.02	99.32	109.84
2	A	480	HEM	CHD-C1D-ND	4.86	128.62	124.58
3	A	490	VNI	C12-C7-C2	-4.85	118.28	121.89
2	B	480	HEM	C4D-ND-C1D	4.82	110.09	105.16
3	C	490	VNI	C2-C3-N2	4.67	117.80	112.16
3	A	490	VNI	O2-C19-C16	4.65	124.03	119.23
3	A	490	VNI	O2-C20-C21	4.64	124.02	119.23
2	C	480	HEM	C4A-CHB-C1B	-4.32	121.78	127.47
2	B	480	HEM	CMA-C3A-C4A	-4.28	122.03	128.62
2	C	480	HEM	C4D-ND-C1D	4.20	109.46	105.16
3	D	490	VNI	C3-C2-N1	-4.19	101.05	109.84
2	B	480	HEM	C4A-CHB-C1B	-4.19	121.96	127.47
2	C	480	HEM	CMA-C3A-C4A	-4.17	122.20	128.62
3	B	490	VNI	C4-N2-C6	4.09	110.24	106.37
2	D	480	HEM	CAD-C3D-C4D	4.05	131.81	124.53
3	D	490	VNI	C12-C7-C2	-4.02	118.90	121.89
2	A	480	HEM	CMA-C3A-C4A	-4.01	122.46	128.62
3	D	490	VNI	O2-C19-C16	3.95	123.31	119.23
3	B	490	VNI	C12-C7-C2	-3.91	118.99	121.89
2	A	480	HEM	C1A-CHA-C4D	-3.81	122.45	127.47
3	C	490	VNI	C11-C10-CL1	-3.71	114.57	119.14
2	A	480	HEM	CHC-C4B-NB	3.58	127.56	124.58
2	D	480	HEM	C3B-C4B-NB	-3.50	111.50	114.00
2	D	480	HEM	C1B-NB-C4B	-3.44	101.64	105.16
3	C	490	VNI	C13-C1-N1	-3.35	111.31	116.89
3	B	490	VNI	C21-C20-N5	3.35	130.42	122.26
2	B	480	HEM	CAD-C3D-C4D	3.06	130.03	124.53
3	A	490	VNI	C4-N2-C6	3.02	109.23	106.37
2	A	480	HEM	CAD-C3D-C2D	-2.98	120.61	127.25
3	B	490	VNI	C16-C19-N4	2.97	129.49	122.26
2	A	480	HEM	C4A-CHB-C1B	-2.96	123.58	127.47
3	A	490	VNI	C13-C1-N1	-2.95	111.97	116.89
3	C	490	VNI	C8-C7-C12	2.90	119.98	116.81

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	480	HEM	C4A-CHB-C1B	-2.89	123.67	127.47
2	C	480	HEM	C2D-C1D-ND	-2.87	109.55	112.93
3	D	490	VNI	C16-C19-N4	2.84	129.17	122.26
2	A	480	HEM	CMC-C2C-C3C	2.81	132.78	126.16
2	C	480	HEM	CAD-C3D-C4D	2.78	129.53	124.53
2	A	480	HEM	C4D-ND-C1D	2.73	107.95	105.16
2	D	480	HEM	CMA-C3A-C4A	-2.73	124.43	128.62
2	B	480	HEM	CBD-CAD-C3D	-2.72	108.43	114.37
3	B	490	VNI	O2-C20-C21	2.69	122.01	119.23
2	B	480	HEM	C2D-C1D-ND	-2.68	109.77	112.93
3	C	490	VNI	C7-C2-N1	2.66	117.63	111.97
2	C	480	HEM	CBA-CAA-C2A	-2.59	108.12	112.69
3	B	490	VNI	O2-C19-C16	2.59	121.91	119.23
2	C	480	HEM	CHD-C1D-ND	2.58	126.73	124.58
2	B	480	HEM	C4A-C3A-C2A	2.58	108.79	107.00
2	C	480	HEM	CHC-C1C-NC	-2.57	122.50	124.73
2	B	480	HEM	CHD-C4C-NC	2.56	126.96	124.73
2	A	480	HEM	CMA-C3A-C2A	2.53	129.71	124.94
2	C	480	HEM	CMA-C3A-C2A	2.52	129.69	124.94
3	B	490	VNI	C2-N1-C1	-2.52	118.63	122.41
2	D	480	HEM	CHD-C1D-ND	2.52	126.67	124.58
3	A	490	VNI	C18-C13-C1	-2.47	112.90	120.56
3	C	490	VNI	C9-C10-CL1	2.47	123.41	119.34
3	A	490	VNI	C21-C20-N5	2.45	128.22	122.26
2	D	480	HEM	O2D-CGD-CBD	2.44	122.85	114.22
3	D	490	VNI	C21-C20-N5	2.38	128.04	122.26
2	A	480	HEM	O2D-CGD-CBD	2.35	122.51	114.22
3	C	490	VNI	C4-N2-C6	2.33	108.58	106.37
3	A	490	VNI	C16-C19-N4	2.27	127.80	122.26
3	C	490	VNI	O1-C1-N1	2.25	126.50	122.44
2	C	480	HEM	O2D-CGD-CBD	2.24	122.12	114.22
2	A	480	HEM	CBD-CAD-C3D	-2.21	109.56	114.37
2	B	480	HEM	CMA-C3A-C2A	2.20	129.09	124.94
3	B	490	VNI	C3-C2-C7	2.19	115.67	110.75
3	D	490	VNI	C7-C12-CL2	-2.18	117.83	120.44
3	C	490	VNI	C7-C12-CL2	2.16	123.02	120.44
2	A	480	HEM	O1D-CGD-CBD	-2.16	115.61	123.03
2	A	480	HEM	C4C-NC-C1C	2.15	107.77	105.53
3	C	490	VNI	C15-C14-C13	-2.15	118.19	120.76
2	C	480	HEM	CBD-CAD-C3D	-2.14	109.70	114.37
3	B	490	VNI	C11-C12-CL2	-2.10	115.25	118.55
2	A	480	HEM	C2D-C1D-ND	-2.08	110.48	112.93

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	480	HEM	C4C-NC-C1C	2.05	107.67	105.53
3	B	490	VNI	C13-C1-N1	-2.03	113.52	116.89
3	B	490	VNI	C18-C13-C14	2.02	121.53	118.63
3	C	490	VNI	C11-C12-CL2	-2.02	115.37	118.55
3	D	490	VNI	C2-C3-N2	2.02	114.60	112.16

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	450/450 (100%)	0.23	15 (3%) 44 44	22, 35, 51, 61	0
1	B	449/450 (99%)	0.11	8 (1%) 65 66	21, 32, 45, 57	0
1	C	449/450 (99%)	0.13	11 (2%) 56 57	20, 30, 42, 61	0
1	D	449/450 (99%)	0.39	29 (6%) 18 18	23, 38, 61, 71	0
All	All	1797/1800 (99%)	0.21	63 (3%) 41 42	20, 33, 52, 71	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	29	GLY	8.2
1	B	256	SER	5.9
1	B	255	ASP	5.5
1	D	194	ALA	4.9
1	C	255	ASP	4.6
1	D	243	ILE	4.4
1	D	257	SER	3.9
1	C	253	ASN	3.8
1	C	256	SER	3.8
1	D	256	SER	3.7
1	C	29	GLY	3.6
1	C	254	LYS	3.4
1	D	191	ARG	3.3
1	C	477	LYS	3.3
1	C	252	VAL	3.1
1	A	257	SER	3.0
1	B	41	ILE	3.0
1	D	477	LYS	3.0
1	C	405	ASP	3.0
1	D	120	TYR	3.0
1	D	62	GLN	3.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	271	ARG	2.9
1	D	37	VAL	2.8
1	D	190	LYS	2.8
1	D	61	ARG	2.8
1	A	41	ILE	2.8
1	B	271	ARG	2.7
1	D	64	LYS	2.7
1	C	251	GLU	2.7
1	D	254	LYS	2.5
1	D	39	VAL	2.5
1	D	373	VAL	2.5
1	C	424	GLY	2.5
1	B	253	ASN	2.5
1	D	195	ARG	2.5
1	C	406	GLU	2.4
1	B	195	ARG	2.4
1	B	48	PHE	2.4
1	D	271	ARG	2.4
1	A	399	ARG	2.4
1	A	290	PHE	2.4
1	A	120	TYR	2.3
1	D	250	GLU	2.3
1	A	93	ARG	2.3
1	D	192	LEU	2.3
1	D	245	ILE	2.2
1	A	48	PHE	2.2
1	D	189	ARG	2.2
1	B	43	GLY	2.2
1	A	40	PRO	2.2
1	A	50	LYS	2.2
1	D	429	LEU	2.2
1	A	38	THR	2.2
1	D	295	THR	2.2
1	A	61	ARG	2.1
1	D	129	PHE	2.1
1	A	291	ALA	2.1
1	D	255	ASP	2.1
1	D	272	ASP	2.1
1	D	422	CYS	2.1
1	A	195	ARG	2.1
1	A	62	GLN	2.1
1	D	196	ARG	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
2	HEM	A	480	43/43	0.20	1.48	16,22,28,33	0
2	HEM	B	480	43/43	0.18	1.31	19,22,25,30	0
2	HEM	D	480	43/43	0.17	0.80	24,28,37,42	0
3	VNI	A	490	35/35	0.15	0.34	21,31,50,50	0
3	VNI	D	490	35/35	0.13	0.32	23,31,45,45	0
3	VNI	B	490	35/35	0.13	0.30	23,32,53,53	0
3	VNI	C	490	35/35	0.12	0.14	20,25,40,43	0
2	HEM	C	480	43/43	0.15	0.00	16,20,26,30	0

## 6.5 Other polymers

There are no such residues in this entry.