



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:03 am GMT

PDB ID : 4G7G  
Title : Sterol 14-alpha demethylase (CYP51) from Trypanosoma brucei in complex with the VNI derivative (R)-N-(1-(3,4'-difluorobiphenyl-4-yl)-2-(1H-imidazol-1-yl)ethyl)-4-(5-phenyl-1,3,4-oxadiazol-2-yl)benzamide [VNI/VNF (VFV)]  
Authors : Hargrove, T.Y.; Wawrzak, Z.; Waterman, M.R.; Lepesheva, G.I.  
Deposited on : 2012-07-20  
Resolution : 2.05 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

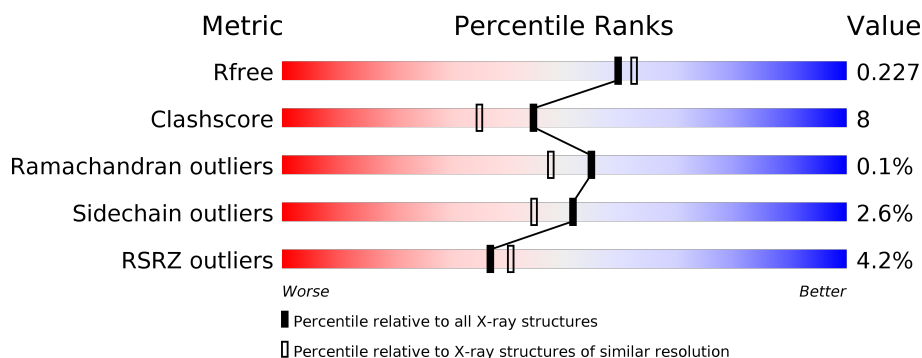
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.05 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	1316 (2.04-2.04)
Clashscore	112137	1394 (2.04-2.04)
Ramachandran outliers	110173	1383 (2.04-2.04)
Sidechain outliers	110143	1383 (2.04-2.04)
RSRZ outliers	101464	1319 (2.04-2.04)

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	448	<div> <div>4%</div> <div>88%</div> <div>12%</div> <div>.</div> </div>
1	B	448	<div> <div>4%</div> <div>81%</div> <div>17%</div> <div>.</div> </div>
1	C	448	<div> <div>5%</div> <div>84%</div> <div>15%</div> <div>.</div> </div>
1	D	448	<div> <div>4%</div> <div>83%</div> <div>16%</div> <div>.</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15068 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 sterol 14-alpha-demethylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	448	Total	C	N	O	S	0	0	0
			3557	2271	621	638	27			
1	B	448	Total	C	N	O	S	0	0	0
			3557	2271	621	638	27			
1	C	448	Total	C	N	O	S	0	0	0
			3557	2271	621	638	27			
1	D	448	Total	C	N	O	S	0	0	0
			3557	2271	621	638	27			

There are 12 discrepancies between the modelled and reference sequences:

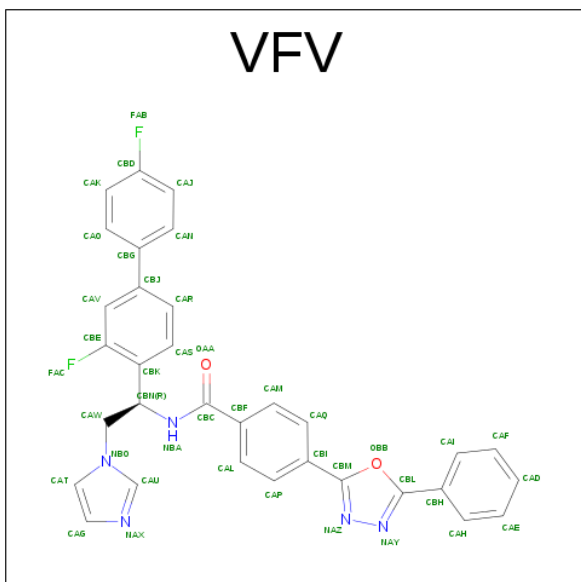
Chain	Residue	Modelled	Actual	Comment	Reference
A	29	GLY	PRO	ENGINEERED MUTATION	UNP Q385E8
A	30	LYS	THR	ENGINEERED MUTATION	UNP Q385E8
A	31	LEU	ASP	ENGINEERED MUTATION	UNP Q385E8
B	29	GLY	PRO	ENGINEERED MUTATION	UNP Q385E8
B	30	LYS	THR	ENGINEERED MUTATION	UNP Q385E8
B	31	LEU	ASP	ENGINEERED MUTATION	UNP Q385E8
C	29	GLY	PRO	ENGINEERED MUTATION	UNP Q385E8
C	30	LYS	THR	ENGINEERED MUTATION	UNP Q385E8
C	31	LEU	ASP	ENGINEERED MUTATION	UNP Q385E8
D	29	GLY	PRO	ENGINEERED MUTATION	UNP Q385E8
D	30	LYS	THR	ENGINEERED MUTATION	UNP Q385E8
D	31	LEU	ASP	ENGINEERED MUTATION	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 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is N-[(1R)-1-(3,4'-DIFLUOROBIPHENYL-4-YL)-2-(1H-IMIDAZOL-1-YL)ETHYL]-4-(5-PHENYL-1,3,4-OXADIAZOL-2-YL)BENZAMIDE (three-letter code: VFV) (formula: C<sub>32</sub>H<sub>23</sub>F<sub>2</sub>N<sub>5</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			41	32	2	5	2		
3	B	1	Total	C	F	N	O	0	0
			41	32	2	5	2		
3	C	1	Total	C	F	N	O	0	0
			41	32	2	5	2		
3	D	1	Total	C	F	N	O	0	0
			41	32	2	5	2		

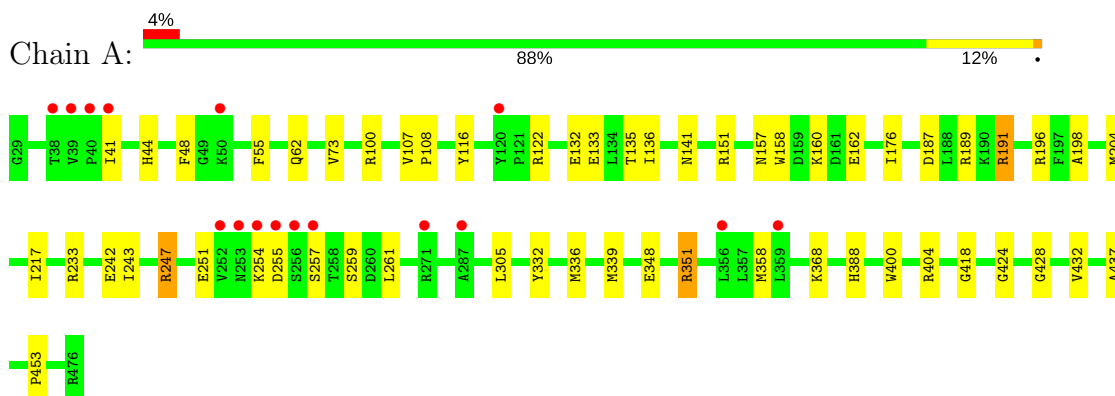
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	176	Total	O	0	0
			176	176		
4	B	123	Total	O	0	0
			123	123		
4	C	107	Total	O	0	0
			107	107		
4	D	98	Total	O	0	0
			98	98		

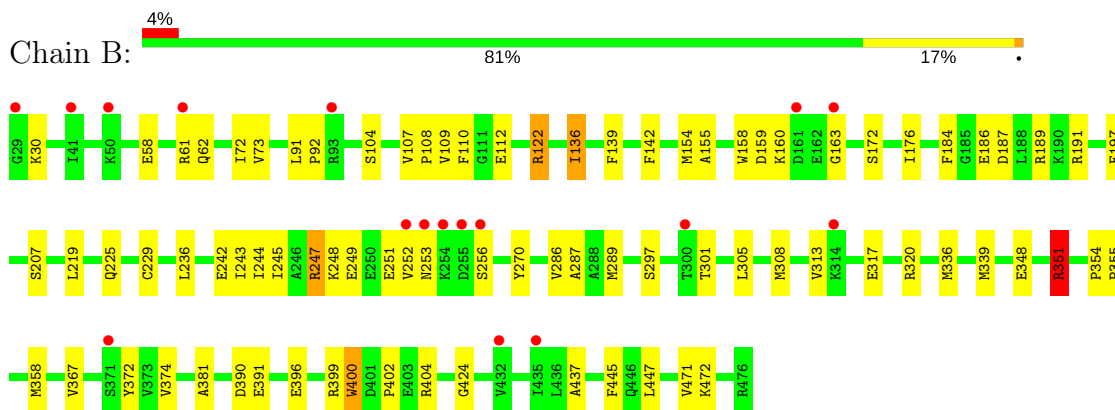
### 3 Residue-property plots

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.

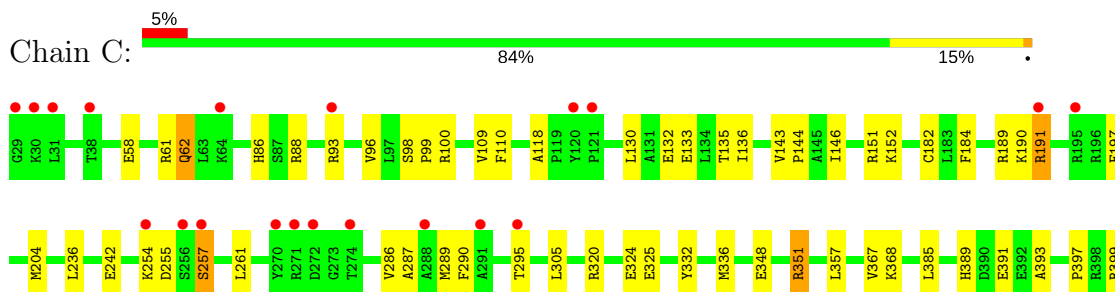
#### • Molecule 1: sterol 14-alpha-demethylase

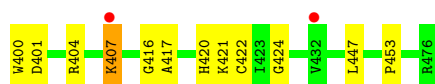


#### • Molecule 1: sterol 14-alpha-demethylase

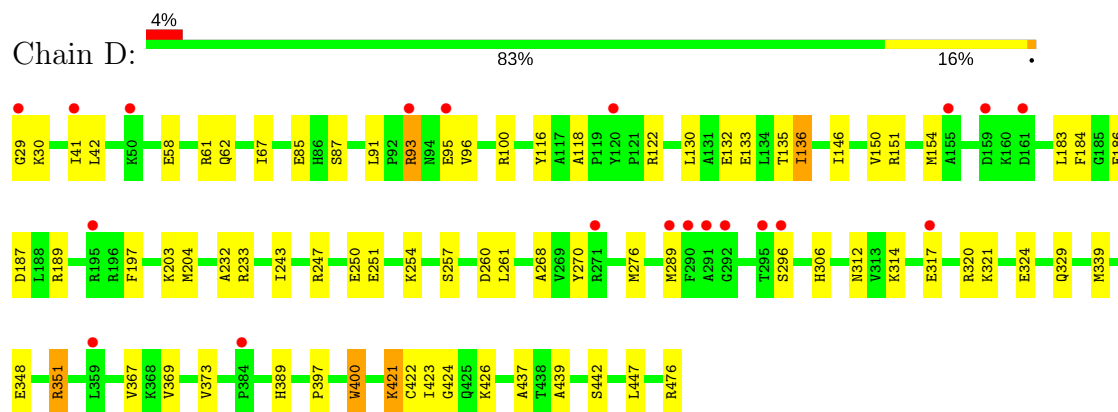


#### • Molecule 1: sterol 14-alpha-demethylase





- Molecule 1: sterol 14-alpha-demethylase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.95Å 79.71Å 117.87Å 74.64° 81.20° 68.96°	Depositor
Resolution (Å)	29.82 – 2.05 29.82 – 2.05	Depositor EDS
% Data completeness (in resolution range)	98.0 (29.82-2.05) 90.4 (29.82-2.05)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.79 (at 2.04Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.163 , 0.226 0.164 , 0.227	Depositor DCC
$R_{free}$ test set	6064 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	37.9	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 45.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	15068	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.36% 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.48	1/3639 (0.0%)	0.59	0/4922
1	B	0.47	1/3639 (0.0%)	0.61	2/4922 (0.0%)
1	C	0.45	1/3639 (0.0%)	0.56	0/4922
1	D	0.45	1/3639 (0.0%)	0.58	0/4922
All	All	0.46	4/14556 (0.0%)	0.59	2/19688 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	400	TRP	CD2-CE2	5.31	1.47	1.41
1	B	400	TRP	CD2-CE2	5.20	1.47	1.41
1	C	400	TRP	CD2-CE2	5.17	1.47	1.41
1	D	400	TRP	CD2-CE2	5.01	1.47	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	351	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	B	351	ARG	NE-CZ-NH1	5.22	122.91	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	3557	0	3594	40	0
1	B	3557	0	3594	62	0
1	C	3557	0	3594	43	0
1	D	3557	0	3594	66	0
2	A	43	0	30	5	0
2	B	43	0	30	8	0
2	C	43	0	30	8	0
2	D	43	0	30	8	0
3	A	41	0	23	2	0
3	B	41	0	22	1	0
3	C	41	0	23	0	0
3	D	41	0	23	1	0
4	A	176	0	0	3	0
4	B	123	0	0	10	0
4	C	107	0	0	5	0
4	D	98	0	0	3	0
All	All	15068	0	14587	219	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 (219) 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)
2:A:501:HEM:HHC	2:A:501:HEM:HBB2	1.28	1.10
1:D:187:ASP:OD2	1:D:247:ARG:HD3	1.49	1.09
1:C:133:GLU:HG3	1:C:261:LEU:HD12	1.39	1.04
2:B:501:HEM:HHC	2:B:501:HEM:HBB2	1.39	1.01
1:B:308:MET:SD	4:B:646:HOH:O	2.24	0.94
1:C:133:GLU:HG3	1:C:261:LEU:CD1	2.00	0.90
1:A:187:ASP:OD2	1:A:247:ARG:HD3	1.72	0.88
2:A:501:HEM:CHC	2:A:501:HEM:HBB2	2.07	0.80
1:B:136:ILE:HD11	1:B:336:MET:HE1	1.65	0.78
1:D:93:ARG:HH11	1:D:93:ARG:HB2	1.49	0.78
1:D:29:GLY:HA3	1:D:373:VAL:HG23	1.66	0.78
2:D:501:HEM:HHC	2:D:501:HEM:HBB2	1.65	0.77
1:D:67:ILE:HD13	1:D:369:VAL:HG12	1.67	0.77
1:B:245:ILE:O	1:B:249:GLU:HG3	1.87	0.74
1:C:58:GLU:OE1	1:C:61:ARG:NH1	2.22	0.73
1:D:187:ASP:OD2	1:D:247:ARG:CD	2.31	0.73
1:A:217:ILE:HD11	1:D:42:LEU:HD23	1.71	0.71
1:D:58:GLU:OE2	1:D:62:GLN:HG3	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:251:GLU:O	1:D:254:LYS:HE3	1.91	0.71
1:B:471:VAL:HB	4:B:646:HOH:O	1.89	0.70
1:C:184:PHE:O	1:C:189:ARG:NH1	2.25	0.70
2:B:501:HEM:CHC	2:B:501:HEM:HBB2	2.19	0.69
1:D:58:GLU:OE1	1:D:61:ARG:NH1	2.25	0.69
1:C:422:CYS:HB2	2:C:501:HEM:NA	2.08	0.68
1:A:100:ARG:HG3	1:A:116:TYR:O	1.94	0.67
1:A:191:ARG:HH21	1:A:196:ARG:HH12	1.41	0.67
1:A:217:ILE:HD11	1:D:42:LEU:CD2	2.24	0.67
1:C:320:ARG:O	1:C:324:GLU:HB2	1.95	0.67
1:B:236:LEU:CD2	1:B:286:VAL:HG23	2.25	0.66
1:A:348:GLU:OE1	1:A:351:ARG:HD3	1.95	0.66
1:B:256:SER:HB2	4:B:710:HOH:O	1.96	0.65
1:D:93:ARG:NH1	1:D:93:ARG:CB	2.59	0.65
1:C:348:GLU:OE1	1:C:351:ARG:HD3	1.96	0.65
1:C:86:HIS:HB2	4:C:650:HOH:O	1.96	0.64
1:D:348:GLU:OE1	1:D:351:ARG:HD3	1.98	0.63
1:B:252:VAL:HG13	1:B:253:ASN:N	2.13	0.63
1:B:399:ARG:O	1:B:404:ARG:NH2	2.31	0.63
2:D:501:HEM:HBC2	2:D:501:HEM:HMC2	1.81	0.62
1:A:157:ASN:O	1:A:158:TRP:HD1	1.83	0.61
1:C:88:ARG:HH21	1:C:368:LYS:HB3	1.65	0.61
1:D:100:ARG:NH2	1:D:118:ALA:O	2.33	0.61
1:C:152:LYS:NZ	4:C:659:HOH:O	2.31	0.61
2:B:501:HEM:HMC2	2:B:501:HEM:HBC2	1.83	0.61
1:A:332:TYR:CE2	1:A:336:MET:HG3	2.35	0.60
1:D:93:ARG:HH11	1:D:93:ARG:CB	2.13	0.60
2:A:501:HEM:CBB	2:A:501:HEM:HHC	2.18	0.59
1:B:256:SER:CB	4:B:710:HOH:O	2.49	0.59
1:C:93:ARG:HG2	1:C:96:VAL:HG23	1.85	0.58
2:D:501:HEM:HHC	2:D:501:HEM:CBB	2.32	0.58
2:D:501:HEM:CHC	2:D:501:HEM:HBB2	2.31	0.58
1:B:187:ASP:OD2	1:B:247:ARG:HD3	2.05	0.57
1:D:132:GLU:HA	1:D:135:THR:HG23	1.86	0.57
1:B:136:ILE:HD11	1:B:336:MET:CE	2.35	0.57
1:A:251:GLU:O	1:A:254:LYS:O	2.22	0.57
1:A:424:GLY:HA3	2:A:501:HEM:C3C	2.40	0.56
1:D:133:GLU:HG3	1:D:261:LEU:HD12	1.88	0.56
1:B:191:ARG:NH1	1:B:242:GLU:OE1	2.26	0.56
1:C:100:ARG:NH2	1:C:118:ALA:O	2.38	0.56
1:D:100:ARG:NH2	1:D:118:ALA:C	2.58	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:93:ARG:NH1	1:D:93:ARG:HB2	2.17	0.56
1:D:146:ILE:O	1:D:150:VAL:HG23	2.06	0.56
1:D:247:ARG:O	1:D:250:GLU:HG2	2.06	0.56
1:B:358:MET:CE	1:B:381:ALA:HB1	2.37	0.55
1:B:424:GLY:HA3	2:B:501:HEM:C3C	2.41	0.55
2:B:501:HEM:HBC2	2:B:501:HEM:CMC	2.37	0.55
1:C:191:ARG:NH1	1:C:242:GLU:OE1	2.39	0.55
1:D:442:SER:O	1:D:476:ARG:HB2	2.07	0.55
1:B:139:PHE:HA	1:B:142:PHE:HB2	1.89	0.55
1:D:197:PHE:CZ	1:D:289:MET:HG3	2.42	0.54
1:D:29:GLY:HA3	1:D:373:VAL:CG2	2.36	0.54
1:B:104:SER:HB3	1:B:219:LEU:CD1	2.38	0.54
1:D:93:ARG:NH1	1:D:93:ARG:HB3	2.23	0.54
1:B:112:GLU:HG2	4:B:654:HOH:O	2.08	0.54
1:D:151:ARG:HD2	4:D:616:HOH:O	2.08	0.54
1:D:243:ILE:O	1:D:247:ARG:HG3	2.09	0.53
1:C:295:THR:OG1	2:C:501:HEM:HBB2	2.09	0.53
1:B:58:GLU:OE1	1:B:61:ARG:NH1	2.42	0.53
1:D:306:HIS:O	1:D:312:ASN:ND2	2.34	0.53
1:D:122:ARG:O	1:D:122:ARG:HD3	2.08	0.53
1:D:422:CYS:HB2	2:D:501:HEM:NA	2.23	0.53
1:C:424:GLY:HA3	2:C:501:HEM:C3C	2.44	0.53
1:D:421:LYS:HB2	4:D:697:HOH:O	2.09	0.53
1:A:133:GLU:HG3	1:A:261:LEU:HD12	1.90	0.52
1:A:191:ARG:NH2	1:A:196:ARG:HH12	2.08	0.52
1:B:154:MET:HG2	1:B:158:TRP:CE3	2.44	0.52
1:C:146:ILE:HG13	1:C:182:CYS:SG	2.49	0.52
1:D:116:TYR:CE2	3:D:502:VFV:H1	2.44	0.52
1:B:186:GLU:HG3	1:B:189:ARG:HH21	1.75	0.52
1:B:110:PHE:CD1	1:B:287:ALA:HB2	2.44	0.52
1:D:204:MET:HE1	1:D:233:ARG:HG3	1.92	0.51
1:D:268:ALA:HB3	1:D:276:MET:HE3	1.93	0.51
1:A:254:LYS:HG3	1:A:255:ASP:N	2.26	0.51
1:B:308:MET:CE	4:B:646:HOH:O	2.56	0.51
1:B:308:MET:HE1	4:B:646:HOH:O	2.09	0.51
1:B:189:ARG:NH1	4:B:603:HOH:O	2.44	0.50
1:D:67:ILE:HD11	1:D:85:GLU:HG3	1.93	0.50
1:D:96:VAL:CG1	1:D:367:VAL:CG1	2.89	0.50
1:B:207:SER:O	1:B:225:GLN:HB3	2.12	0.50
1:C:422:CYS:HA	2:C:501:HEM:CHA	2.41	0.50
1:D:150:VAL:O	1:D:154:MET:HG3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:348:GLU:OE1	1:B:351:ARG:HD3	2.12	0.49
1:D:321:LYS:O	1:D:324:GLU:HB2	2.12	0.49
1:B:186:GLU:HG3	1:B:189:ARG:NH2	2.27	0.49
1:C:393:ALA:HA	1:C:407:LYS:HB2	1.93	0.49
1:B:244:ILE:O	1:B:248:LYS:HG3	2.11	0.49
1:B:348:GLU:HG3	1:B:400:TRP:CD1	2.48	0.49
1:C:332:TYR:CE1	1:C:336:MET:HG3	2.47	0.49
1:A:141:ASN:ND2	4:A:748:HOH:O	2.45	0.49
1:B:400:TRP:CH2	1:B:402:PRO:HG3	2.47	0.49
1:C:189:ARG:HG2	4:C:695:HOH:O	2.13	0.49
1:B:236:LEU:HD23	1:B:286:VAL:HG23	1.92	0.49
1:D:424:GLY:HA3	2:D:501:HEM:C3C	2.48	0.49
1:A:116:TYR:CE2	3:A:502:VFV:H1	2.49	0.48
2:B:501:HEM:NA	3:B:502:VFV:CAU	2.75	0.48
1:D:204:MET:HE3	1:D:233:ARG:HB2	1.96	0.48
1:A:191:ARG:NH1	1:A:242:GLU:OE1	2.45	0.48
1:D:29:GLY:CA	1:D:373:VAL:HG23	2.40	0.48
1:A:132:GLU:O	1:A:135:THR:HG23	2.14	0.48
1:B:243:ILE:O	1:B:247:ARG:CG	2.62	0.48
1:B:184:PHE:CE1	1:B:289:MET:HE2	2.48	0.48
1:C:130:LEU:O	1:C:133:GLU:HB2	2.14	0.47
1:A:358:MET:HB3	1:A:358:MET:HE3	1.86	0.47
1:D:197:PHE:CE2	1:D:289:MET:HG3	2.49	0.47
1:B:445:PHE:HB3	4:B:646:HOH:O	2.15	0.47
1:A:418:GLY:CA	1:B:253:ASN:HD21	2.28	0.47
1:A:44:HIS:HB3	1:A:55:PHE:CZ	2.49	0.47
1:B:252:VAL:CG1	1:B:253:ASN:N	2.77	0.47
1:A:351:ARG:O	1:A:388:HIS:HB3	2.15	0.47
1:D:96:VAL:CG1	1:D:367:VAL:HG11	2.45	0.47
1:B:243:ILE:O	1:B:247:ARG:HG3	2.15	0.46
1:D:100:ARG:HH22	1:D:118:ALA:C	2.18	0.46
1:A:254:LYS:HG3	1:A:255:ASP:H	1.80	0.46
1:B:155:ALA:O	1:B:159:ASP:HB3	2.14	0.46
1:A:424:GLY:HA3	2:A:501:HEM:C2C	2.51	0.46
1:C:110:PHE:CD1	1:C:287:ALA:HB2	2.51	0.46
2:C:501:HEM:HBC2	2:C:501:HEM:CMC	2.45	0.46
1:B:176:ILE:HD11	1:B:197:PHE:CD2	2.51	0.46
1:D:348:GLU:HG3	1:D:400:TRP:CD1	2.50	0.46
1:B:110:PHE:HD1	1:B:287:ALA:HB2	1.81	0.46
1:A:339:MET:HE3	1:A:437:ALA:HB2	1.99	0.45
1:C:357:LEU:HD22	1:C:385:LEU:HD22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:270:TYR:OH	1:D:276:MET:HG3	2.15	0.45
1:A:107:VAL:N	1:A:108:PRO:CD	2.80	0.45
1:A:351:ARG:HD2	1:A:404:ARG:HD2	1.98	0.45
2:B:501:HEM:HHC	2:B:501:HEM:CBB	2.27	0.45
1:D:93:ARG:HB3	1:D:93:ARG:CZ	2.46	0.45
1:A:189:ARG:NH1	4:A:653:HOH:O	2.49	0.45
1:B:122:ARG:HD2	1:B:270:TYR:CE1	2.52	0.44
1:D:187:ASP:OD1	1:D:187:ASP:N	2.47	0.44
1:D:389:HIS:CD2	1:D:397:PRO:HB2	2.51	0.44
1:A:73:VAL:O	1:A:73:VAL:HG12	2.17	0.44
1:D:136:ILE:HD13	1:D:426:LYS:HD2	1.98	0.44
1:C:401:ASP:O	1:C:404:ARG:HG2	2.18	0.44
1:A:48:PHE:CE1	3:A:502:VFV:H21	2.52	0.44
1:C:422:CYS:HB2	2:C:501:HEM:C1A	2.52	0.44
1:B:424:GLY:HA3	2:B:501:HEM:C2C	2.53	0.44
1:A:428:GLY:O	1:A:432:VAL:HG23	2.18	0.44
1:B:109:VAL:HG13	1:B:286:VAL:CG1	2.48	0.44
1:D:184:PHE:O	1:D:189:ARG:NH1	2.51	0.44
1:A:160:LYS:HB2	1:A:162:GLU:O	2.17	0.44
1:B:30:LYS:HE3	1:B:372:TYR:CE1	2.53	0.44
1:A:243:ILE:O	1:A:247:ARG:CG	2.66	0.43
1:B:107:VAL:N	1:B:108:PRO:CD	2.82	0.43
1:C:254:LYS:O	1:C:255:ASP:HB2	2.18	0.43
1:C:422:CYS:HA	2:C:501:HEM:C4D	2.52	0.43
1:B:58:GLU:OE2	1:B:62:GLN:HG3	2.18	0.43
1:B:320:ARG:O	4:B:662:HOH:O	2.21	0.43
1:D:317:GLU:CD	4:D:657:HOH:O	2.57	0.43
1:C:99:PRO:HG3	1:C:420:HIS:CE1	2.54	0.43
1:D:183:LEU:O	1:D:260:ASP:HB2	2.19	0.43
1:C:58:GLU:O	1:C:62:GLN:HB2	2.19	0.43
1:A:191:ARG:HG3	1:A:243:ILE:HD11	1.99	0.43
1:C:325:GLU:HB2	4:C:626:HOH:O	2.19	0.43
1:C:389:HIS:CD2	1:C:397:PRO:HB2	2.54	0.43
1:B:313:VAL:O	1:B:317:GLU:HB2	2.18	0.43
1:C:416:GLY:O	1:C:417:ALA:HB2	2.18	0.43
1:A:204:MET:HE3	1:A:233:ARG:HB2	2.00	0.42
1:B:160:LYS:HA	1:B:160:LYS:HD3	1.85	0.42
1:C:109:VAL:HA	1:C:204:MET:HE2	2.01	0.42
1:D:296:SER:OG	2:D:501:HEM:CBB	2.68	0.42
1:A:217:ILE:HD11	1:D:42:LEU:HD21	2.01	0.42
1:A:418:GLY:C	1:B:253:ASN:HD21	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:29:GLY:N	1:D:373:VAL:HG21	2.34	0.42
1:A:176:ILE:HD13	1:A:198:ALA:HB2	2.01	0.42
1:D:186:GLU:HG3	1:D:189:ARG:NH2	2.35	0.42
1:D:154:MET:CE	1:D:439:ALA:HA	2.50	0.42
1:B:91:LEU:N	1:B:92:PRO:CD	2.83	0.42
1:A:305:LEU:HD13	1:A:453:PRO:HD2	2.01	0.42
1:C:257:SER:HA	4:C:618:HOH:O	2.19	0.42
1:D:29:GLY:CA	1:D:373:VAL:CG2	2.97	0.42
1:C:143:VAL:N	1:C:144:PRO:HD2	2.35	0.42
1:B:172:SER:HA	1:B:297:SER:OG	2.19	0.42
1:D:339:MET:HE3	1:D:437:ALA:HB2	2.01	0.42
1:C:236:LEU:CD2	1:C:286:VAL:CG2	2.98	0.42
1:D:203:LYS:HD3	1:D:232:ALA:HB2	2.02	0.41
1:B:367:VAL:HG23	1:B:374:VAL:HB	2.02	0.41
1:D:422:CYS:HA	2:D:501:HEM:CHA	2.49	0.41
1:C:132:GLU:O	1:C:135:THR:HG23	2.21	0.41
1:B:163:GLY:O	1:B:472:LYS:HA	2.20	0.41
1:B:358:MET:HE1	1:B:381:ALA:HB1	2.02	0.41
1:B:396:GLU:HG2	1:B:396:GLU:O	2.20	0.41
1:D:130:LEU:HD23	1:D:423:ILE:HD11	2.03	0.41
1:C:424:GLY:HA3	2:C:501:HEM:C2C	2.56	0.41
1:D:87:SER:HB2	1:D:91:LEU:HD12	2.01	0.41
1:D:93:ARG:CD	1:D:95:GLU:HB2	2.51	0.41
1:D:136:ILE:CD1	1:D:426:LYS:HD2	2.51	0.41
1:A:257:SER:HA	4:A:697:HOH:O	2.20	0.41
1:B:354:PRO:HA	1:B:355:PRO:HD3	1.87	0.41
1:B:400:TRP:CZ2	1:B:402:PRO:HG3	2.56	0.41
1:B:339:MET:HE1	1:B:437:ALA:HB2	2.02	0.41
1:C:417:ALA:HA	1:C:421:LYS:HB3	2.02	0.41
1:B:72:ILE:HG22	1:B:73:VAL:HG23	2.02	0.41
1:D:320:ARG:HG3	1:D:320:ARG:HH11	1.86	0.41
1:C:98:SER:HA	1:C:99:PRO:HD3	1.99	0.40
1:C:351:ARG:HD2	1:C:404:ARG:HD2	2.03	0.40
1:B:301:THR:O	1:B:305:LEU:HG	2.21	0.40
1:C:305:LEU:HD13	1:C:453:PRO:HD2	2.02	0.40
1:A:418:GLY:HA2	1:B:253:ASN:HD21	1.87	0.40
1:C:197:PHE:CE2	1:C:289:MET:HG3	2.56	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	446/448 (100%)	435 (98%)	10 (2%)	1 (0%)	51	42
1	B	446/448 (100%)	434 (97%)	12 (3%)	0	100	100
1	C	446/448 (100%)	429 (96%)	17 (4%)	0	100	100
1	D	446/448 (100%)	435 (98%)	11 (2%)	0	100	100
All	All	1784/1792 (100%)	1733 (97%)	50 (3%)	1 (0%)	55	47

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	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	390/390 (100%)	381 (98%)	9 (2%)	56	49
1	B	390/390 (100%)	381 (98%)	9 (2%)	56	49
1	C	390/390 (100%)	377 (97%)	13 (3%)	43	36
1	D	390/390 (100%)	380 (97%)	10 (3%)	51	44
All	All	1560/1560 (100%)	1519 (97%)	41 (3%)	51	44

All (41) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	A	62	GLN
1	A	122	ARG
1	A	136	ILE
1	A	151	ARG
1	A	191	ARG
1	A	247	ARG
1	A	259	SER
1	A	351	ARG
1	A	368	LYS
1	B	122	ARG
1	B	136	ILE
1	B	229	CYS
1	B	247	ARG
1	B	251	GLU
1	B	351	ARG
1	B	390	ASP
1	B	391	GLU
1	B	447	LEU
1	C	62	GLN
1	C	136	ILE
1	C	151	ARG
1	C	190	LYS
1	C	191	ARG
1	C	257	SER
1	C	290	PHE
1	C	351	ARG
1	C	367	VAL
1	C	391	GLU
1	C	399	ARG
1	C	407	LYS
1	C	447	LEU
1	D	30	LYS
1	D	41	ILE
1	D	93	ARG
1	D	136	ILE
1	D	257	SER
1	D	314	LYS
1	D	329	GLN
1	D	351	ARG
1	D	421	LYS
1	D	447	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	253	ASN
1	B	312	ASN
1	C	157	ASN
1	D	148	HIS
1	D	199	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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	501	1,3	28,50,50	2.84	11 (39%)	17,82,82	2.72	6 (35%)
3	VFV	A	502	2	39,46,46	1.63	5 (12%)	53,64,64	1.22	7 (13%)
2	HEM	B	501	1,3	28,50,50	2.91	11 (39%)	17,82,82	3.16	7 (41%)
3	VFV	B	502	2	39,46,46	2.88	6 (15%)	53,64,64	1.50	10 (18%)
2	HEM	C	501	1,3	28,50,50	3.16	12 (42%)	17,82,82	3.04	8 (47%)
3	VFV	C	502	2	39,46,46	2.05	7 (17%)	53,64,64	1.21	5 (9%)
2	HEM	D	501	1,3	28,50,50	2.83	11 (39%)	17,82,82	2.78	7 (41%)
3	VFV	D	502	2	39,46,46	3.89	10 (25%)	53,64,64	1.69	11 (20%)

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	501	1,3	-	0/6/54/54	0/0/8/8
3	VFV	A	502	2	-	0/24/28/28	0/5/6/6
2	HEM	B	501	1,3	-	0/6/54/54	0/0/8/8
3	VFV	B	502	2	-	0/24/28/28	0/5/6/6
2	HEM	C	501	1,3	-	0/6/54/54	0/0/8/8
3	VFV	C	502	2	-	0/24/28/28	0/5/6/6
2	HEM	D	501	1,3	-	0/6/54/54	0/0/8/8
3	VFV	D	502	2	-	0/24/28/28	0/5/6/6

All (73) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	502	VFV	FAB-CBD	-20.00	0.88	1.36
3	B	502	VFV	NAZ-NAY	-12.45	1.14	1.37
3	B	502	VFV	CBK-CBN	-8.76	1.38	1.52
3	C	502	VFV	CBK-CBN	-8.12	1.39	1.52
3	D	502	VFV	CBK-CBN	-6.41	1.41	1.52
3	A	502	VFV	CBK-CBN	-6.18	1.42	1.52
3	D	502	VFV	CBF-CBC	-5.44	1.38	1.50
3	D	502	VFV	FAC-CBE	-5.20	1.22	1.35
3	B	502	VFV	CAW-NBO	-5.16	1.43	1.48
3	D	502	VFV	CBJ-CBG	-4.85	1.36	1.49
3	B	502	VFV	CBF-CBC	-4.78	1.40	1.50
3	C	502	VFV	CBF-CBC	-4.73	1.40	1.50
3	C	502	VFV	NAZ-NAY	-4.72	1.28	1.37
3	D	502	VFV	CAT-NBO	-4.52	1.29	1.37
3	B	502	VFV	CBJ-CBG	-4.34	1.37	1.49
3	A	502	VFV	CBF-CBC	-4.17	1.41	1.50
3	C	502	VFV	CBJ-CBG	-4.04	1.38	1.49
2	D	501	HEM	C4D-ND	-3.51	1.32	1.36
3	A	502	VFV	CBJ-CBG	-3.40	1.40	1.49
3	D	502	VFV	CAS-CBK	-3.24	1.35	1.39
3	C	502	VFV	FAC-CBE	-3.12	1.27	1.35
2	B	501	HEM	C4D-ND	-3.03	1.33	1.36
3	C	502	VFV	FAB-CBD	-2.91	1.29	1.36
2	A	501	HEM	C4D-ND	-2.58	1.33	1.36
3	D	502	VFV	NAZ-NAY	-2.57	1.32	1.37
3	D	502	VFV	CBN-NBA	-2.53	1.43	1.46
2	C	501	HEM	C4D-ND	-2.38	1.34	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	502	VFV	CAT-NBO	-2.30	1.33	1.37
3	A	502	VFV	CAT-NBO	-2.15	1.33	1.37
3	A	502	VFV	FAC-CBE	-2.06	1.30	1.35
3	D	502	VFV	CAV-CBJ	-2.02	1.36	1.39
2	B	501	HEM	C1D-CHD	2.21	1.46	1.40
2	C	501	HEM	C4B-CHC	2.51	1.46	1.40
2	B	501	HEM	C1A-CHA	2.51	1.46	1.40
2	D	501	HEM	C1D-CHD	2.58	1.47	1.40
2	C	501	HEM	C1A-CHA	2.61	1.47	1.40
2	A	501	HEM	C1D-CHD	2.65	1.47	1.40
2	C	501	HEM	C1D-CHD	2.74	1.47	1.40
2	D	501	HEM	C1A-CHA	2.78	1.47	1.40
2	A	501	HEM	C3D-C2D	2.80	1.46	1.37
3	B	502	VFV	CAW-CBN	2.80	1.57	1.53
2	A	501	HEM	C2A-C3A	2.91	1.46	1.37
2	B	501	HEM	C3B-C2B	2.93	1.44	1.40
2	A	501	HEM	C4B-CHC	3.05	1.48	1.40
2	D	501	HEM	C3D-C2D	3.08	1.46	1.37
2	B	501	HEM	C3D-C2D	3.29	1.47	1.37
2	C	501	HEM	C3D-C2D	3.39	1.47	1.37
2	A	501	HEM	C3B-C2B	3.40	1.44	1.40
2	C	501	HEM	C2A-C3A	3.47	1.47	1.37
2	D	501	HEM	C2A-C3A	3.59	1.48	1.37
2	D	501	HEM	C4A-NA	3.65	1.44	1.36
2	D	501	HEM	C3B-C2B	3.84	1.45	1.40
2	B	501	HEM	C2A-C3A	3.88	1.49	1.37
2	C	501	HEM	C3B-C2B	3.88	1.45	1.40
2	A	501	HEM	C4A-NA	4.01	1.44	1.36
2	B	501	HEM	C4A-NA	4.18	1.45	1.36
2	C	501	HEM	C4A-NA	4.59	1.46	1.36
2	A	501	HEM	C1A-NA	4.61	1.46	1.36
2	C	501	HEM	C1A-NA	4.72	1.46	1.36
2	B	501	HEM	C1A-NA	4.90	1.46	1.36
2	D	501	HEM	C1A-NA	5.03	1.46	1.36
2	D	501	HEM	C1C-NC	5.12	1.42	1.36
2	D	501	HEM	C3C-C2C	5.90	1.48	1.40
2	B	501	HEM	C3C-C2C	5.93	1.48	1.40
2	C	501	HEM	C3C-C2C	6.07	1.48	1.40
2	A	501	HEM	C1C-NC	6.15	1.44	1.36
2	A	501	HEM	C4C-NC	6.39	1.44	1.36
2	B	501	HEM	C4C-NC	6.60	1.44	1.36
2	A	501	HEM	C3C-C2C	6.82	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	HEM	C1C-NC	7.10	1.45	1.36
2	D	501	HEM	C4C-NC	7.14	1.45	1.36
2	C	501	HEM	C1C-NC	7.77	1.45	1.36
2	C	501	HEM	C4C-NC	8.17	1.46	1.36

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	HEM	C1D-C2D-C3D	-7.73	101.61	107.00
2	A	501	HEM	C1D-C2D-C3D	-7.49	101.78	107.00
2	C	501	HEM	C1D-C2D-C3D	-7.09	102.06	107.00
2	B	501	HEM	C1D-C2D-C3D	-7.02	102.11	107.00
2	B	501	HEM	CAD-CBD-CGD	-5.02	104.08	112.66
2	C	501	HEM	CAD-CBD-CGD	-4.74	104.57	112.66
2	B	501	HEM	CBA-CAA-C2A	-4.57	103.74	112.48
2	A	501	HEM	CAD-CBD-CGD	-3.77	106.21	112.66
3	C	502	VFV	CBN-NBA-CBC	-3.64	117.16	122.15
2	D	501	HEM	CAD-CBD-CGD	-3.51	106.66	112.66
2	C	501	HEM	C4A-C3A-C2A	-3.50	104.56	107.00
2	A	501	HEM	C4A-C3A-C2A	-3.50	104.56	107.00
3	B	502	VFV	CAV-CBE-CBK	-3.32	119.32	123.66
2	C	501	HEM	CAA-CBA-CGA	-3.27	107.07	112.66
2	B	501	HEM	C4A-C3A-C2A	-3.09	104.85	107.00
3	B	502	VFV	CAM-CBF-CAL	-3.06	114.34	118.58
3	D	502	VFV	CAV-CBE-CBK	-2.86	119.91	123.66
3	A	502	VFV	CBN-NBA-CBC	-2.71	118.44	122.15
3	B	502	VFV	CAR-CBJ-CBG	-2.37	117.19	121.38
3	C	502	VFV	CAV-CBE-CBK	-2.27	120.69	123.66
2	A	501	HEM	CAA-CBA-CGA	-2.24	108.83	112.66
2	D	501	HEM	C4A-C3A-C2A	-2.16	105.49	107.00
3	C	502	VFV	CAN-CBG-CBJ	-2.16	117.56	121.38
3	A	502	VFV	CAJ-CBD-CAK	-2.09	119.95	122.86
3	D	502	VFV	CAR-CBJ-CBG	-2.01	117.84	121.38
3	D	502	VFV	CBF-CBC-NBA	2.06	120.77	116.97
3	C	502	VFV	CAR-CBJ-CAV	2.07	120.83	118.16
2	C	501	HEM	CMB-C2B-C3B	2.12	128.83	124.89
3	B	502	VFV	CAP-CBI-CBM	2.14	124.02	120.51
3	A	502	VFV	CBL-NAY-NAZ	2.14	109.81	105.22
2	C	501	HEM	C4C-C3C-C2C	2.20	108.44	106.90
3	D	502	VFV	CAR-CBJ-CAV	2.21	121.02	118.16
3	A	502	VFV	CAS-CBK-CBE	2.31	118.95	116.11
3	B	502	VFV	CAR-CBJ-CAV	2.36	121.21	118.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502	VFV	CBI-CBM-NAZ	2.53	127.52	124.20
3	B	502	VFV	CAE-CAH-CBH	2.56	123.81	120.57
3	D	502	VFV	CAF-CAI-CBH	2.61	123.87	120.57
3	D	502	VFV	CAS-CBK-CBN	2.62	126.12	120.28
2	D	501	HEM	CMB-C2B-C3B	2.62	129.75	124.89
3	A	502	VFV	CBH-CBL-NAY	2.68	127.73	124.20
3	A	502	VFV	CBK-CBN-NBA	2.71	117.34	111.93
3	D	502	VFV	CAH-CBH-CBL	2.72	124.97	120.51
2	D	501	HEM	CMC-C2C-C3C	2.78	130.05	124.89
2	D	501	HEM	CMD-C2D-C3D	2.94	130.48	124.94
3	B	502	VFV	CBK-CBN-NBA	2.95	117.82	111.93
2	A	501	HEM	C3B-C4B-NB	3.22	113.37	109.21
3	C	502	VFV	CBI-CBM-NAZ	3.27	128.50	124.20
3	D	502	VFV	CAS-CBK-CBE	3.37	120.25	116.11
2	B	501	HEM	CMC-C2C-C3C	3.37	131.14	124.89
3	A	502	VFV	CBI-CBM-NAZ	3.40	128.67	124.20
3	B	502	VFV	CAQ-CAM-CBF	3.48	124.68	120.79
3	B	502	VFV	CAS-CBK-CBE	3.72	120.68	116.11
2	A	501	HEM	CMC-C2C-C3C	3.80	131.95	124.89
2	B	501	HEM	CMD-C2D-C3D	3.85	132.20	124.94
3	D	502	VFV	FAC-CBE-CBK	4.01	124.42	118.28
2	C	501	HEM	CBD-CAD-C3D	4.35	120.76	112.47
2	C	501	HEM	C3B-C4B-NB	4.55	115.09	109.21
3	D	502	VFV	CBH-CBL-NAY	4.60	130.25	124.20
3	D	502	VFV	CBI-CBM-NAZ	4.63	130.29	124.20
2	D	501	HEM	C3B-C4B-NB	5.17	115.89	109.21
2	B	501	HEM	C3B-C4B-NB	5.42	116.21	109.21

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	HEM	5	0
3	A	502	VFV	2	0
2	B	501	HEM	8	0
3	B	502	VFV	1	0
2	C	501	HEM	8	0
2	D	501	HEM	8	0
3	D	502	VFV	1	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

### 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	448/448 (100%)	-0.04	16 (3%) 43 48	22, 37, 58, 107	0
1	B	448/448 (100%)	0.12	17 (3%) 41 45	23, 41, 67, 132	0
1	C	448/448 (100%)	0.13	22 (4%) 30 33	29, 46, 68, 109	0
1	D	448/448 (100%)	0.21	20 (4%) 34 37	26, 46, 73, 99	0
All	All	1792/1792 (100%)	0.11	75 (4%) 37 40	22, 42, 69, 132	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	253	ASN	10.0
1	B	254	LYS	8.0
1	B	252	VAL	7.8
1	C	256	SER	7.0
1	B	256	SER	5.6
1	C	407	LYS	4.6
1	A	255	ASP	4.5
1	A	256	SER	4.5
1	C	29	GLY	4.2
1	D	120	TYR	4.2
1	C	271	ARG	4.1
1	C	120	TYR	3.9
1	A	41	ILE	3.9
1	C	257	SER	3.9
1	C	93	ARG	3.8
1	D	29	GLY	3.6
1	D	195	ARG	3.6
1	D	159	ASP	3.6
1	C	254	LYS	3.6
1	B	255	ASP	3.4
1	D	271	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	121	PRO	3.2
1	B	163	GLY	3.2
1	C	274	THR	3.1
1	B	435	ILE	2.9
1	C	291	ALA	2.9
1	D	292	GLY	2.9
1	D	95	GLU	2.8
1	A	40	PRO	2.8
1	A	257	SER	2.7
1	D	93	ARG	2.7
1	B	61	ARG	2.7
1	A	356	LEU	2.7
1	D	161	ASP	2.7
1	D	50	LYS	2.6
1	C	272	ASP	2.6
1	D	296	SER	2.6
1	A	253	ASN	2.6
1	C	64	LYS	2.5
1	C	38	THR	2.5
1	C	195	ARG	2.5
1	D	317	GLU	2.5
1	A	271	ARG	2.5
1	A	359	LEU	2.5
1	B	432	VAL	2.5
1	B	50	LYS	2.5
1	C	270	TYR	2.4
1	D	291	ALA	2.3
1	D	295	THR	2.3
1	A	120	TYR	2.3
1	C	288	ALA	2.3
1	C	432	VAL	2.3
1	B	29	GLY	2.3
1	D	289	MET	2.2
1	B	371	SER	2.2
1	D	41	ILE	2.2
1	A	254	LYS	2.2
1	C	30	LYS	2.2
1	D	359	LEU	2.2
1	D	290	PHE	2.2
1	B	161	ASP	2.2
1	A	50	LYS	2.2
1	D	384	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	314	LYS	2.1
1	A	252	VAL	2.1
1	A	38	THR	2.1
1	B	41	ILE	2.1
1	C	191	ARG	2.1
1	A	39	VAL	2.1
1	A	287	ALA	2.1
1	C	295	THR	2.1
1	C	31	LEU	2.0
1	D	155	ALA	2.0
1	B	300	THR	2.0
1	B	93	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( $\text{\AA}^2$ )	Q<0.9
2	HEM	A	501	43/43	0.98	0.19	0.78	19,24,33,46	0
3	VFV	C	502	41/41	0.95	0.18	0.67	25,40,58,68	0
2	HEM	B	501	43/43	0.98	0.17	0.62	22,26,34,44	0
2	HEM	D	501	43/43	0.98	0.19	0.53	22,27,39,55	0
2	HEM	C	501	43/43	0.96	0.18	0.50	29,35,44,75	0
3	VFV	A	502	41/41	0.97	0.18	0.45	21,34,43,49	0
3	VFV	B	502	41/41	0.96	0.16	0.42	23,33,65,71	0
3	VFV	D	502	41/41	0.90	0.16	0.07	24,37,53,60	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.