



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:25 PM GMT

PDB ID : 4I8V  
Title : Human Cytochrome P450 1A1 in complex with alpha-naphthoflavone  
Authors : Walsh, A.A.; Scott, E.E.  
Deposited on : 2012-12-04  
Resolution : 2.60 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

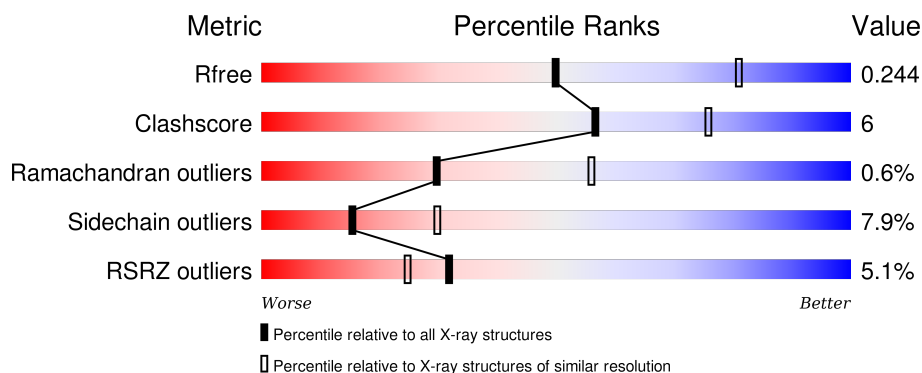
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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))
$R_{free}$	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	491	<div> <div> <div></div> <div>85%</div> <div>11%</div> <div>• •</div> </div> </div>
1	B	491	<div> <div> <div>2%</div> <div>78%</div> <div>16%</div> <div>• •</div> </div> </div>
1	C	491	<div> <div> <div>9%</div> <div>69%</div> <div>23%</div> <div>• 5%</div> </div> </div>
1	D	491	<div> <div> <div>8%</div> <div>77%</div> <div>16%</div> <div>• 5%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	BHF	D	601	-	-	-	X
4	NO3	A	604	-	-	-	X
4	NO3	B	603	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15532 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Cytochrome P450 1A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	477	Total	C	N	O	S	0	0	0
			3816	2442	664	689	21			
1	B	472	Total	C	N	O	S	0	0	0
			3776	2420	657	678	21			
1	C	468	Total	C	N	O	S	0	0	0
			3750	2404	652	673	21			
1	D	467	Total	C	N	O	S	0	0	0
			3741	2398	650	672	21			

There are 52 discrepancies between the modelled and reference sequences:

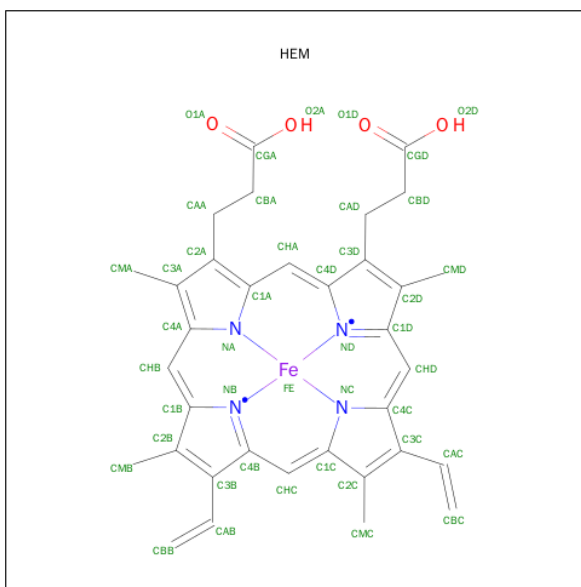
Chain	Residue	Modelled	Actual	Comment	Reference
A	28	MET	-	EXPRESSION TAG	UNP P04798
A	29	ALA	-	EXPRESSION TAG	UNP P04798
A	30	LYS	-	EXPRESSION TAG	UNP P04798
A	31	LYS	-	EXPRESSION TAG	UNP P04798
A	32	THR	-	EXPRESSION TAG	UNP P04798
A	33	SER	-	EXPRESSION TAG	UNP P04798
A	34	SER	-	EXPRESSION TAG	UNP P04798
A	513	HIS	-	EXPRESSION TAG	UNP P04798
A	514	HIS	-	EXPRESSION TAG	UNP P04798
A	515	HIS	-	EXPRESSION TAG	UNP P04798
A	516	HIS	-	EXPRESSION TAG	UNP P04798
A	517	HIS	-	EXPRESSION TAG	UNP P04798
A	518	HIS	-	EXPRESSION TAG	UNP P04798
B	28	MET	-	EXPRESSION TAG	UNP P04798
B	29	ALA	-	EXPRESSION TAG	UNP P04798
B	30	LYS	-	EXPRESSION TAG	UNP P04798
B	31	LYS	-	EXPRESSION TAG	UNP P04798
B	32	THR	-	EXPRESSION TAG	UNP P04798
B	33	SER	-	EXPRESSION TAG	UNP P04798
B	34	SER	-	EXPRESSION TAG	UNP P04798
B	513	HIS	-	EXPRESSION TAG	UNP P04798

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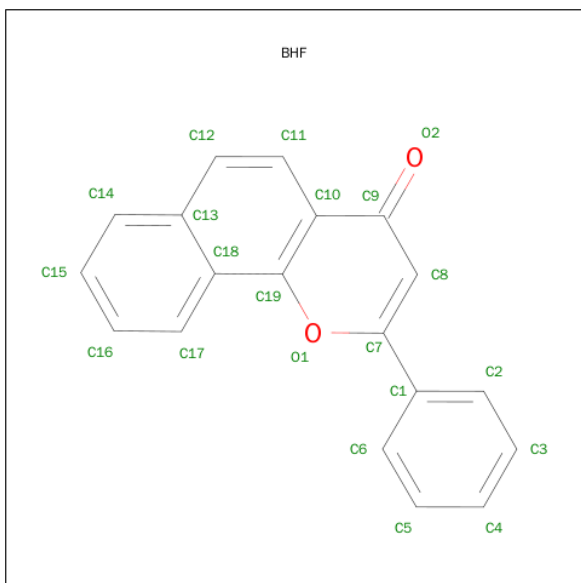
Chain	Residue	Modelled	Actual	Comment	Reference
B	514	HIS	-	EXPRESSION TAG	UNP P04798
B	515	HIS	-	EXPRESSION TAG	UNP P04798
B	516	HIS	-	EXPRESSION TAG	UNP P04798
B	517	HIS	-	EXPRESSION TAG	UNP P04798
B	518	HIS	-	EXPRESSION TAG	UNP P04798
C	28	MET	-	EXPRESSION TAG	UNP P04798
C	29	ALA	-	EXPRESSION TAG	UNP P04798
C	30	LYS	-	EXPRESSION TAG	UNP P04798
C	31	LYS	-	EXPRESSION TAG	UNP P04798
C	32	THR	-	EXPRESSION TAG	UNP P04798
C	33	SER	-	EXPRESSION TAG	UNP P04798
C	34	SER	-	EXPRESSION TAG	UNP P04798
C	513	HIS	-	EXPRESSION TAG	UNP P04798
C	514	HIS	-	EXPRESSION TAG	UNP P04798
C	515	HIS	-	EXPRESSION TAG	UNP P04798
C	516	HIS	-	EXPRESSION TAG	UNP P04798
C	517	HIS	-	EXPRESSION TAG	UNP P04798
C	518	HIS	-	EXPRESSION TAG	UNP P04798
D	28	MET	-	EXPRESSION TAG	UNP P04798
D	29	ALA	-	EXPRESSION TAG	UNP P04798
D	30	LYS	-	EXPRESSION TAG	UNP P04798
D	31	LYS	-	EXPRESSION TAG	UNP P04798
D	32	THR	-	EXPRESSION TAG	UNP P04798
D	33	SER	-	EXPRESSION TAG	UNP P04798
D	34	SER	-	EXPRESSION TAG	UNP P04798
D	513	HIS	-	EXPRESSION TAG	UNP P04798
D	514	HIS	-	EXPRESSION TAG	UNP P04798
D	515	HIS	-	EXPRESSION TAG	UNP P04798
D	516	HIS	-	EXPRESSION TAG	UNP P04798
D	517	HIS	-	EXPRESSION TAG	UNP P04798
D	518	HIS	-	EXPRESSION TAG	UNP P04798

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



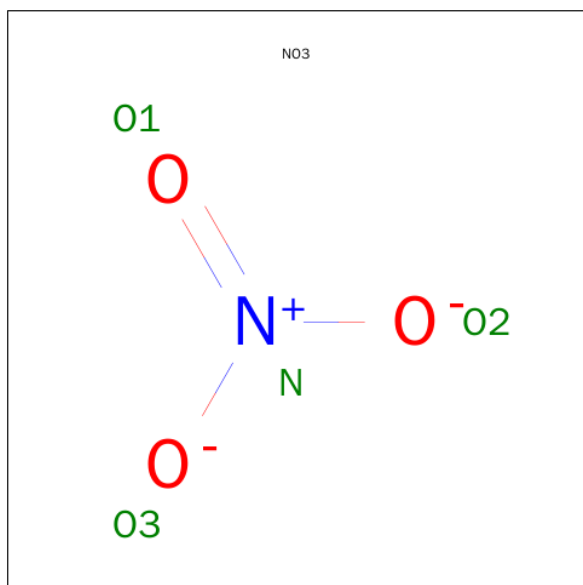
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is 2-PHENYL-4H-BENZO[H]CHROMEN-4-ONE (three-letter code: BHF) (formula:  $C_{19}H_{12}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			21	19	2		
3	B	1	Total	C	O	0	0
			21	19	2		
3	C	1	Total	C	O	0	0
			21	19	2		
3	D	1	Total	C	O	0	0
			21	19	2		

- Molecule 4 is NITRATE ION (three-letter code: NO3) (formula: NO<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	N	O	0	0
			4	1	3		
4	A	1	Total	N	O	0	0
			4	1	3		
4	B	1	Total	N	O	0	0
			4	1	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	87	Total	O	0	0
			87	87		
5	B	76	Total	O	0	0
			76	76		
5	C	10	Total	O	0	0
			10	10		

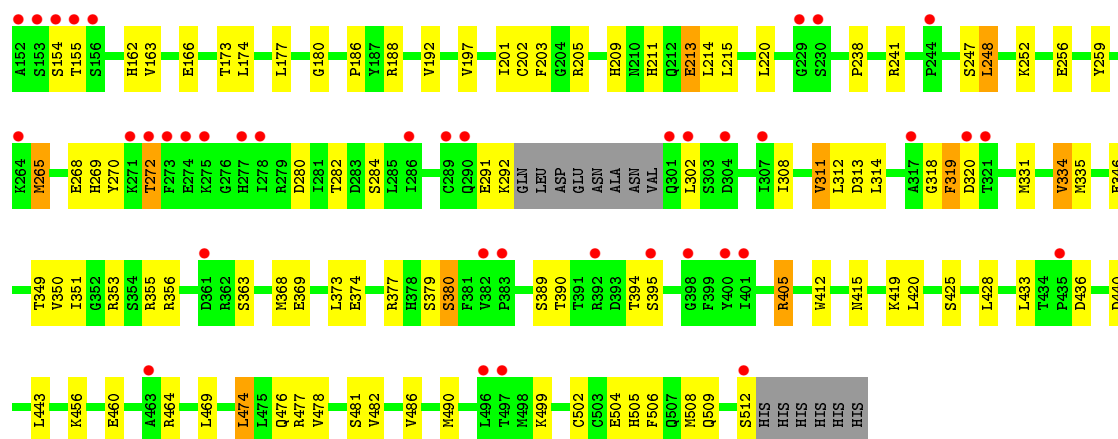
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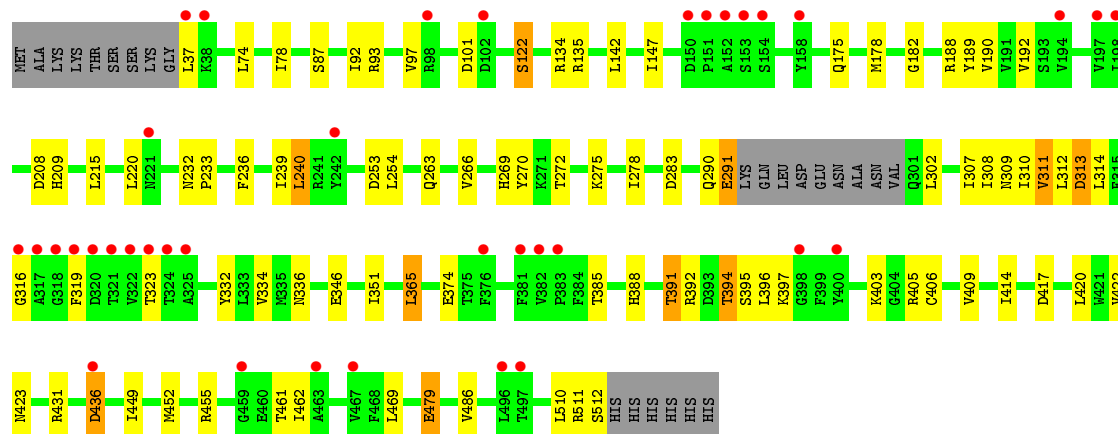
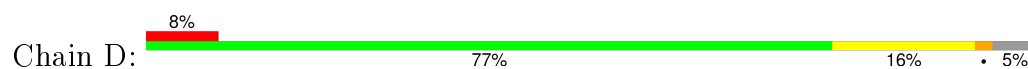
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	8	Total	O	0	0
			8	8		







• Molecule 1: Cytochrome P450 1A1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.00Å 195.49Å 235.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.24 – 2.60 38.21 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (38.24-2.60) 99.9 (38.21-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.42 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.7	Depositor
R, $R_{free}$	0.188 , 0.244 0.193 , 0.244	Depositor DCC
$R_{free}$ test set	4687 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	62.3	Xtriage
Anisotropy	0.273	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 58.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 93413 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	15532	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: HEM, NO3, BHF

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	0.83	0/3911	0.91	5/5300 (0.1%)
1	B	0.77	1/3870 (0.0%)	0.86	5/5241 (0.1%)
1	C	0.57	1/3844 (0.0%)	0.72	0/5207
1	D	0.58	0/3835	0.76	1/5196 (0.0%)
All	All	0.70	2/15460 (0.0%)	0.81	11/20944 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	44	TRP	CB-CG	5.97	1.60	1.50
1	B	42	GLY	C-O	-5.28	1.15	1.23

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	393	ASP	CB-CG-OD2	5.97	123.67	118.30
1	A	313	ASP	CB-CG-OD2	5.85	123.57	118.30
1	B	431	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	A	93	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	A	77	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	B	65	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	A	106	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	D	436	ASP	CB-CG-OD2	5.12	122.91	118.30
1	B	142	LEU	CB-CG-CD1	-5.05	102.42	111.00
1	A	77	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	B	65	ARG	NE-CZ-NH1	5.00	122.80	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3816	0	3809	28	0
1	B	3776	0	3780	43	0
1	C	3750	0	3750	64	0
1	D	3741	0	3737	43	0
2	A	43	0	30	6	0
2	B	43	0	30	4	0
2	C	43	0	30	3	0
2	D	43	0	30	5	0
3	A	21	0	12	0	0
3	B	21	0	12	0	0
3	C	21	0	12	0	0
3	D	21	0	12	1	0
4	A	8	0	0	0	0
4	B	4	0	0	0	0
5	A	87	0	0	3	0
5	B	76	0	0	5	0
5	C	10	0	0	1	0
5	D	8	0	0	0	0
All	All	15532	0	15244	188	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 6.

All (188) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:LEU:O	1:B:181:PRO:HD2	1.71	0.89
1:A:308:ILE:O	1:A:311:VAL:HG22	1.79	0.83
1:C:105:GLY:HA2	1:C:127:SER:OG	1.87	0.75
1:D:346:GLU:HG2	1:D:365:LEU:HD12	1.70	0.74
1:D:92:ILE:HD12	1:D:414:ILE:HD11	1.70	0.72
1:B:480:PHE:CE2	1:B:508:MET:HE3	2.25	0.72
1:D:302:LEU:HD12	1:D:302:LEU:O	1.90	0.72
1:C:460:GLU:O	1:C:464:ARG:HG3	1.91	0.71
2:D:600:HEM:HBB2	2:D:600:HEM:HMB2	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:205:ARG:NH2	1:C:268:GLU:OE1	2.25	0.69
1:B:361:ASP:O	1:B:365:LEU:HD22	1.92	0.69
2:A:601:HEM:HBB2	2:A:601:HEM:HMB2	1.75	0.69
1:B:474:LEU:O	1:B:478:VAL:HG22	1.94	0.68
1:A:308:ILE:O	1:A:311:VAL:CG2	2.43	0.67
2:A:601:HEM:HMC2	2:A:601:HEM:HBC2	1.76	0.66
1:C:203:PHE:CD1	1:C:265:MET:HG2	2.33	0.64
1:C:320:ASP:OD2	1:C:499:LYS:NZ	2.31	0.64
1:D:93:ARG:O	1:D:97:VAL:HG22	1.99	0.61
1:D:302:LEU:HD13	1:D:307:ILE:HG13	1.82	0.61
1:C:173:THR:O	1:C:177:LEU:HD12	2.01	0.60
1:C:331:MET:HB3	1:C:490:MET:CE	2.32	0.59
1:B:338:ARG:NH2	1:B:430:GLU:OE2	2.35	0.59
1:D:351:ILE:HD11	1:D:365:LEU:HD21	1.84	0.58
1:C:331:MET:HB3	1:C:490:MET:HE1	1.85	0.58
1:C:477:ARG:HB3	1:C:478:VAL:HG13	1.85	0.58
2:B:601:HEM:HMB2	2:B:601:HEM:HBB2	1.85	0.58
1:B:142:LEU:O	1:B:146:SER:CB	2.52	0.58
1:C:374:GLU:HA	1:C:374:GLU:OE1	2.02	0.58
1:B:174:LEU:HD22	1:B:184:PHE:CE1	2.38	0.58
1:B:92:ILE:HD12	1:B:414:ILE:HD11	1.86	0.57
1:B:478:VAL:HG21	1:B:508:MET:HE1	1.86	0.57
1:A:474:LEU:O	1:A:478:VAL:HG22	2.04	0.57
2:C:600:HEM:HBB2	2:C:600:HEM:HMB2	1.86	0.57
1:C:374:GLU:OE2	1:C:377:ARG:NH2	2.37	0.57
2:D:600:HEM:HBB2	2:D:600:HEM:CMB	2.34	0.56
1:A:461:THR:HG23	5:A:771:HOH:O	2.06	0.56
1:B:430:GLU:N	1:B:430:GLU:OE1	2.38	0.56
1:A:455:ARG:NH2	5:A:703:HOH:O	2.21	0.55
1:B:349:THR:HG22	1:B:349:THR:O	2.03	0.55
1:D:332:TYR:O	1:D:336:ASN:HB2	2.05	0.55
1:D:422:VAL:O	1:D:431:ARG:NH2	2.40	0.55
1:A:90:ASP:OD1	1:A:98:ARG:NH2	2.40	0.55
1:D:479:GLU:HG2	1:D:511:ARG:HG2	1.89	0.55
1:D:374:GLU:OE1	1:D:374:GLU:HA	2.07	0.55
1:B:285:LEU:CD1	1:B:311:VAL:CG1	2.86	0.54
1:C:84:VAL:HG23	1:C:405:ARG:HG2	1.89	0.53
1:A:455:ARG:O	2:A:601:HEM:HBA2	2.08	0.53
2:A:601:HEM:HBC2	2:A:601:HEM:CMC	2.38	0.53
1:C:350:VAL:HG12	1:C:351:ILE:HD12	1.90	0.53
1:B:285:LEU:HD12	1:B:311:VAL:CG1	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:600:HEM:HBC2	2:D:600:HEM:CMC	2.39	0.53
1:C:84:VAL:HG23	1:C:405:ARG:CG	2.39	0.53
1:B:394:THR:OG1	1:B:395:SER:N	2.41	0.53
1:C:103:PHE:CD1	1:C:390:THR:HG22	2.44	0.53
1:A:335:MET:HE3	1:A:488:VAL:HG11	1.92	0.52
2:D:600:HEM:HBC2	2:D:600:HEM:HMC2	1.90	0.52
1:D:239:ILE:CG2	1:D:240:LEU:N	2.73	0.52
1:C:509:GLN:OE1	1:C:509:GLN:HA	2.09	0.52
1:C:269:HIS:NE2	1:C:280:ASP:OD2	2.42	0.51
1:A:111:THR:HG23	1:A:235:ASP:OD1	2.11	0.51
1:B:142:LEU:O	1:B:146:SER:HB2	2.11	0.51
1:B:392:ARG:O	1:B:393:ASP:C	2.48	0.51
1:B:382:VAL:HG11	2:B:601:HEM:HMA2	1.93	0.51
1:D:278:ILE:HG23	1:D:283:ASP:HB3	1.92	0.51
1:B:509:GLN:OE1	1:B:509:GLN:HA	2.12	0.50
1:B:134:ARG:NH1	5:B:729:HOH:O	2.36	0.50
1:D:308:ILE:O	1:D:311:VAL:HG22	2.11	0.50
1:D:175:GLN:HE21	1:D:510:LEU:HD11	1.75	0.50
1:C:486:VAL:HG11	1:C:505:HIS:CG	2.46	0.50
1:C:490:MET:HA	1:C:490:MET:HE3	1.92	0.50
1:D:142:LEU:HD22	1:D:462:ILE:CD1	2.41	0.50
2:A:601:HEM:HBB2	2:A:601:HEM:CMB	2.40	0.49
1:A:74:LEU:C	1:A:74:LEU:HD12	2.32	0.49
1:B:142:LEU:O	1:B:146:SER:HB3	2.12	0.49
1:A:93:ARG:HD3	5:A:781:HOH:O	2.12	0.49
1:B:346:GLU:OE2	1:B:366:PRO:HD2	2.13	0.49
1:A:131:TRP:CZ2	1:A:455:ARG:HD3	2.47	0.49
1:C:202:CYS:O	1:C:282:THR:OG1	2.29	0.49
1:D:266:VAL:HG21	1:D:308:ILE:HG21	1.94	0.49
1:D:101:ASP:O	1:D:391:THR:OG1	2.29	0.49
1:C:308:ILE:O	1:C:311:VAL:HG22	2.13	0.49
1:C:197:VAL:O	1:C:201:ILE:HD12	2.13	0.48
1:A:203:PHE:CD1	1:A:265:MET:HG2	2.48	0.48
1:C:163:VAL:HG11	1:C:469:LEU:HB3	1.96	0.48
2:C:600:HEM:HMC2	2:C:600:HEM:HBC2	1.96	0.48
1:C:49:ILE:CD1	1:C:53:LEU:HD13	2.43	0.48
1:B:187:TYR:O	1:B:191:VAL:HG12	2.14	0.48
1:D:392:ARG:HA	1:D:403:LYS:HD2	1.95	0.47
1:C:379:SER:O	1:C:380:SER:C	2.51	0.47
1:C:346:GLU:O	1:C:349:THR:HG22	2.14	0.47
1:B:221:ASN:N	5:B:750:HOH:O	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:388:HIS:HE1	1:D:455:ARG:HB2	1.80	0.47
1:D:93:ARG:O	1:D:97:VAL:CG2	2.63	0.47
1:C:440:ASP:C	1:C:440:ASP:OD1	2.53	0.47
1:C:93:ARG:O	1:C:97:VAL:HG22	2.15	0.47
1:D:122:SER:OG	1:D:313:ASP:OD1	2.23	0.47
1:A:359:LEU:HD11	1:A:465:TRP:HB3	1.96	0.47
1:C:188:ARG:CZ	1:C:215:LEU:HD21	2.44	0.47
1:C:103:PHE:CE1	1:C:390:THR:HG22	2.50	0.47
1:D:190:VAL:HG12	1:D:323:THR:HG23	1.97	0.47
1:B:302:LEU:HD22	1:B:307:ILE:HG13	1.96	0.46
1:D:417:ASP:CB	1:D:420:LEU:HD12	2.46	0.46
1:C:419:LYS:HE2	1:C:420:LEU:HD12	1.98	0.46
1:B:285:LEU:CD1	1:B:311:VAL:HG13	2.46	0.45
1:B:111:THR:HG23	1:B:235:ASP:OD1	2.16	0.45
1:A:87:SER:HA	1:A:92:ILE:HD11	1.98	0.45
1:C:394:THR:OG1	1:C:395:SER:N	2.49	0.45
1:C:335:MET:HG3	1:C:490:MET:SD	2.57	0.45
1:B:216:SER:O	1:B:220:LEU:HB3	2.15	0.45
1:D:290:GLN:O	1:D:291:GLU:OE2	2.34	0.45
1:A:248:LEU:O	1:A:252:LYS:HG3	2.17	0.45
1:A:346:GLU:OE2	1:A:366:PRO:HD2	2.17	0.45
1:A:479:GLU:O	1:A:508:MET:HA	2.17	0.45
1:A:456:LYS:HB3	1:A:456:LYS:HE2	1.49	0.45
1:C:248:LEU:O	1:C:252:LYS:HG3	2.17	0.44
1:B:460:GLU:OE1	1:B:464:ARG:NH1	2.50	0.44
1:C:96:LEU:O	1:C:100:GLY:HA2	2.17	0.44
1:C:88:GLY:O	1:C:92:ILE:HB	2.16	0.44
1:B:349:THR:CG2	1:B:349:THR:O	2.66	0.44
1:D:396:LEU:O	1:D:397:LYS:C	2.56	0.44
1:A:292:LYS:HE2	1:A:304:ASP:OD1	2.17	0.44
1:B:75:GLN:HG2	5:B:712:HOH:O	2.18	0.44
1:A:262:MET:CE	1:A:263:GLN:HG3	2.48	0.44
1:B:353:ARG:O	1:B:355:ARG:N	2.50	0.44
1:B:478:VAL:HG21	1:B:508:MET:CE	2.47	0.43
1:D:511:ARG:O	1:D:512:SER:C	2.57	0.43
1:C:120:SER:O	1:C:121:MET:C	2.56	0.43
1:D:178:MET:O	1:D:182:GLY:HA2	2.18	0.43
1:B:175:GLN:OE1	1:B:510:LEU:HD23	2.19	0.43
1:C:104:LYS:O	1:C:127:SER:OG	2.35	0.43
1:C:380:SER:HB2	1:C:412:TRP:CD1	2.54	0.43
1:C:102:ASP:O	1:C:390:THR:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:394:THR:OG1	1:D:395:SER:N	2.52	0.43
1:B:186:PRO:O	1:B:190:VAL:HG23	2.18	0.43
1:B:318:GLY:HA2	2:B:601:HEM:HMC2	2.01	0.43
1:A:470:PHE:O	1:A:474:LEU:HB2	2.19	0.43
1:D:240:LEU:HD13	1:D:240:LEU:HA	1.89	0.43
1:C:213:GLU:CG	1:C:214:LEU:N	2.81	0.43
1:A:382:VAL:HG11	2:A:601:HEM:HMA2	2.00	0.43
1:B:338:ARG:HB3	5:B:745:HOH:O	2.18	0.43
1:C:186:PRO:HG2	1:C:506:PHE:CD2	2.54	0.43
1:B:77:ARG:NE	5:B:701:HOH:O	2.25	0.43
1:D:422:VAL:O	1:D:423:ASN:HB2	2.19	0.42
1:C:192:VAL:HG11	1:C:209:HIS:HA	2.02	0.42
1:B:488:VAL:HG23	1:B:488:VAL:O	2.18	0.42
1:B:176:GLU:CD	1:C:211:HIS:HE2	2.22	0.42
1:B:243:LEU:HB3	1:B:244:PRO:HD2	2.01	0.42
1:C:353:ARG:NH1	1:C:512:SER:O	2.52	0.42
1:A:166:GLU:OE2	1:A:206:ARG:NE	2.42	0.42
1:C:508:MET:HA	5:C:708:HOH:O	2.20	0.42
1:C:460:GLU:OE1	1:C:464:ARG:NH1	2.52	0.42
1:C:84:VAL:CG2	1:C:405:ARG:HG2	2.50	0.42
1:A:482:VAL:HG23	1:A:505:HIS:O	2.18	0.42
1:D:78:ILE:HG22	1:D:236:PHE:HB2	2.02	0.42
1:C:97:VAL:HG23	1:C:98:ARG:N	2.34	0.42
2:B:601:HEM:CMB	2:B:601:HEM:HBB2	2.48	0.42
1:C:270:TYR:C	1:C:272:THR:H	2.23	0.42
1:D:308:ILE:C	1:D:310:ILE:H	2.23	0.42
1:C:186:PRO:CG	1:C:506:PHE:CD2	3.03	0.42
1:C:312:LEU:HD12	1:C:312:LEU:HA	1.93	0.42
1:D:74:LEU:C	1:D:74:LEU:HD12	2.40	0.42
1:D:309:ASN:C	1:D:309:ASN:OD1	2.59	0.42
1:C:130:VAL:HG12	1:C:302:LEU:CD1	2.50	0.42
1:C:162:HIS:O	1:C:166:GLU:HG2	2.20	0.42
1:A:456:LYS:O	1:A:457:CYS:C	2.58	0.42
1:B:355:ARG:NH1	1:D:436:ASP:CG	2.74	0.41
1:C:334:VAL:HG21	1:C:506:PHE:CE1	2.55	0.41
1:B:163:VAL:HG11	1:B:469:LEU:HB3	2.01	0.41
1:D:188:ARG:HG2	1:D:189:TYR:CZ	2.55	0.41
1:A:146:SER:OG	1:A:147:ILE:N	2.54	0.41
1:D:455:ARG:NH1	2:D:600:HEM:O2D	2.54	0.41
1:C:110:TYR:O	1:C:113:THR:OG1	2.21	0.41
1:C:350:VAL:HG12	1:C:351:ILE:CD1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:MET:HE2	1:A:265:MET:HA	2.03	0.41
1:C:319:PHE:C	1:C:319:PHE:CD1	2.93	0.41
1:C:238:PRO:HA	1:C:241:ARG:NH1	2.36	0.41
1:D:134:ARG:O	1:D:135:ARG:C	2.59	0.41
1:C:318:GLY:HA2	2:C:600:HEM:HMC2	2.03	0.41
1:C:355:ARG:HG2	1:C:356:ARG:O	2.21	0.41
1:D:192:VAL:HB	1:D:209:HIS:CD2	2.56	0.41
1:C:369:GLU:O	1:C:373:LEU:HG	2.21	0.40
1:D:232:ASN:HA	1:D:233:PRO:HD3	1.92	0.40
1:C:474:LEU:O	1:C:478:VAL:HG22	2.21	0.40
1:D:178:MET:HA	1:D:182:GLY:HA2	2.03	0.40
1:B:434:THR:HG23	1:B:435:PRO:HD2	2.02	0.40
1:C:377:ARG:HD3	1:C:415:ASN:O	2.21	0.40
1:D:385:THR:OG1	1:D:409:VAL:HB	2.22	0.40
1:D:312:LEU:HD23	3:D:601:BHF:H15	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	475/491 (97%)	453 (95%)	22 (5%)	0	100	100
1	B	468/491 (95%)	447 (96%)	16 (3%)	5 (1%)	17	36
1	C	464/491 (94%)	426 (92%)	34 (7%)	4 (1%)	21	42
1	D	463/491 (94%)	426 (92%)	35 (8%)	2 (0%)	39	65
All	All	1870/1964 (95%)	1752 (94%)	107 (6%)	11 (1%)	30	56

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	354	SER
1	B	209	HIS
1	C	180	GLY
1	C	291	GLU
1	D	275	LYS
1	C	363	SER
1	C	380	SER
1	B	380	SER
1	D	316	GLY
1	B	449	ILE
1	B	422	VAL

### 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	426/439 (97%)	401 (94%)	25 (6%)	24	47
1	B	422/439 (96%)	388 (92%)	34 (8%)	15	28
1	C	419/439 (95%)	376 (90%)	43 (10%)	9	16
1	D	418/439 (95%)	387 (93%)	31 (7%)	17	34
All	All	1685/1756 (96%)	1552 (92%)	133 (8%)	15	30

All (133) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	87	SER
1	A	89	LEU
1	A	147	ILE
1	A	215	LEU
1	A	221	ASN
1	A	228	VAL
1	A	247	SER
1	A	254	LEU
1	A	265	MET
1	A	290	GLN
1	A	294	LEU

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Mol	Chain	Res	Type
1	A	311	VAL
1	A	314	LEU
1	A	319	PHE
1	A	354	SER
1	A	359	LEU
1	A	365	LEU
1	A	418	GLN
1	A	428	LEU
1	A	433	LEU
1	A	436	ASP
1	A	456	LYS
1	A	461	THR
1	A	470	PHE
1	A	490	MET
1	B	87	SER
1	B	101	ASP
1	B	130	VAL
1	B	155	THR
1	B	161	GLU
1	B	164	SER
1	B	172	SER
1	B	177	LEU
1	B	183	HIS
1	B	185	ASN
1	B	241	ARG
1	B	254	LEU
1	B	256	GLU
1	B	259	TYR
1	B	263	GLN
1	B	265	MET
1	B	281	ILE
1	B	302	LEU
1	B	313	ASP
1	B	314	LEU
1	B	319	PHE
1	B	338	ARG
1	B	353	ARG
1	B	365	LEU
1	B	368	MET
1	B	405	ARG
1	B	418	GLN
1	B	428	LEU

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Mol	Chain	Res	Type
1	B	433	LEU
1	B	434	THR
1	B	436	ASP
1	B	490	MET
1	B	508	MET
1	B	510	LEU
1	C	44	TRP
1	C	77	ARG
1	C	80	SER
1	C	90	ASP
1	C	91	THR
1	C	92	ILE
1	C	127	SER
1	C	130	VAL
1	C	143	LYS
1	C	149	SER
1	C	154	SER
1	C	155	THR
1	C	174	LEU
1	C	213	GLU
1	C	220	LEU
1	C	247	SER
1	C	248	LEU
1	C	256	GLU
1	C	259	TYR
1	C	265	MET
1	C	272	THR
1	C	284	SER
1	C	292	LYS
1	C	311	VAL
1	C	313	ASP
1	C	314	LEU
1	C	319	PHE
1	C	334	VAL
1	C	368	MET
1	C	389	SER
1	C	405	ARG
1	C	425	SER
1	C	428	LEU
1	C	433	LEU
1	C	436	ASP
1	C	443	LEU

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Mol	Chain	Res	Type
1	C	456	LYS
1	C	474	LEU
1	C	476	GLN
1	C	481	SER
1	C	482	VAL
1	C	502	CYS
1	C	504	GLU
1	D	37	LEU
1	D	87	SER
1	D	122	SER
1	D	147	ILE
1	D	208	ASP
1	D	215	LEU
1	D	220	LEU
1	D	240	LEU
1	D	253	ASP
1	D	254	LEU
1	D	263	GLN
1	D	269	HIS
1	D	270	TYR
1	D	272	THR
1	D	291	GLU
1	D	311	VAL
1	D	313	ASP
1	D	314	LEU
1	D	319	PHE
1	D	334	VAL
1	D	365	LEU
1	D	391	THR
1	D	394	THR
1	D	405	ARG
1	D	406	CYS
1	D	449	ILE
1	D	452	MET
1	D	461	THR
1	D	469	LEU
1	D	479	GLU
1	D	486	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	209	HIS
1	C	344	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

11 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	601	1	30,50,50	2.46	8 (26%)	24,82,82	2.36	10 (41%)
3	BHF	A	602	-	23,24,24	2.08	8 (34%)	29,34,34	2.29	12 (41%)
4	NO3	A	603	-	3,3,3	2.58	2 (66%)	3,3,3	0.18	0
4	NO3	A	604	-	3,3,3	3.36	2 (66%)	3,3,3	0.67	0
2	HEM	B	601	1	30,50,50	2.50	8 (26%)	24,82,82	2.37	9 (37%)
3	BHF	B	602	-	23,24,24	2.35	7 (30%)	29,34,34	2.38	12 (41%)
4	NO3	B	603	-	3,3,3	3.40	2 (66%)	3,3,3	1.31	0
2	HEM	C	600	1	30,50,50	2.20	9 (30%)	24,82,82	2.49	11 (45%)
3	BHF	C	601	-	23,24,24	2.31	6 (26%)	29,34,34	1.43	5 (17%)
2	HEM	D	600	1	30,50,50	2.57	9 (30%)	24,82,82	2.28	8 (33%)
3	BHF	D	601	-	23,24,24	2.30	6 (26%)	29,34,34	1.51	7 (24%)

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	601	1	-	0/10/54/54	0/0/8/8
3	BHF	A	602	-	-	0/4/4/4	0/4/4/4
4	NO3	A	603	-	-	0/0/0/0	0/0/0/0
4	NO3	A	604	-	-	0/0/0/0	0/0/0/0
2	HEM	B	601	1	-	0/10/54/54	0/0/8/8
3	BHF	B	602	-	-	0/4/4/4	0/4/4/4
4	NO3	B	603	-	-	0/0/0/0	0/0/0/0
2	HEM	C	600	1	-	0/10/54/54	0/0/8/8
3	BHF	C	601	-	-	0/4/4/4	0/4/4/4
2	HEM	D	600	1	-	0/10/54/54	0/0/8/8
3	BHF	D	601	-	-	0/4/4/4	0/4/4/4

All (67) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	HEM	C2C-C1C	-7.50	1.38	1.52
2	D	600	HEM	C2C-C1C	-7.48	1.38	1.52
2	D	600	HEM	C2D-C3D	-7.44	1.32	1.54
2	B	601	HEM	C2D-C3D	-7.32	1.32	1.54
2	A	601	HEM	C2D-C3D	-6.96	1.33	1.54
2	A	601	HEM	C2C-C1C	-6.44	1.40	1.52
2	C	600	HEM	C2D-C3D	-6.24	1.35	1.54
2	C	600	HEM	C2C-C1C	-6.13	1.40	1.52
2	D	600	HEM	C3D-C4D	-4.84	1.45	1.51
2	A	601	HEM	C3B-C4B	-4.26	1.48	1.51
2	A	601	HEM	C3D-C4D	-4.06	1.46	1.51
2	B	601	HEM	C3B-C4B	-3.86	1.48	1.51
2	A	601	HEM	C3B-CAB	-3.41	1.44	1.51
2	B	601	HEM	C3D-C4D	-3.30	1.47	1.51
2	B	601	HEM	C3B-CAB	-3.13	1.45	1.51
2	A	601	HEM	C2B-C1B	-3.03	1.41	1.51
2	C	600	HEM	C3B-C4B	-2.87	1.49	1.51
2	B	601	HEM	C2B-C1B	-2.82	1.42	1.51
2	D	600	HEM	C3B-C4B	-2.75	1.49	1.51
2	D	600	HEM	C2B-C1B	-2.67	1.43	1.51
2	C	600	HEM	C2B-C1B	-2.44	1.43	1.51
2	A	601	HEM	C2D-C1D	-2.32	1.44	1.51
2	C	600	HEM	C2D-C1D	-2.30	1.44	1.51
2	C	600	HEM	FE-ND	-2.26	1.85	1.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	600	HEM	C4C-NC	-2.21	1.33	1.36
2	D	600	HEM	C3B-CAB	-2.20	1.47	1.51
2	C	600	HEM	C3B-CAB	-2.12	1.47	1.51
2	C	600	HEM	C3D-C4D	-2.12	1.48	1.51
2	D	600	HEM	CMC-C2C	-2.11	1.48	1.53
2	B	601	HEM	CAD-C3D	-2.09	1.49	1.54
3	A	602	BHF	C1-C7	2.12	1.48	1.46
3	A	602	BHF	O1-C7	2.15	1.38	1.35
3	B	602	BHF	C8-C9	2.18	1.42	1.37
3	B	602	BHF	C12-C11	2.20	1.41	1.34
3	A	602	BHF	C12-C11	2.25	1.41	1.34
3	B	602	BHF	C1-C7	2.26	1.49	1.46
3	C	601	BHF	C1-C7	2.30	1.49	1.46
3	B	602	BHF	C18-C19	2.32	1.44	1.41
2	D	600	HEM	FE-NC	2.39	2.05	1.95
3	A	602	BHF	C18-C13	2.42	1.47	1.42
3	D	601	BHF	C8-C7	2.68	1.42	1.36
3	C	601	BHF	C8-C7	2.76	1.42	1.36
3	A	602	BHF	C8-C9	2.82	1.43	1.37
2	B	601	HEM	FE-NC	3.02	2.07	1.95
4	B	603	NO3	O3-N	3.06	1.41	1.25
3	C	601	BHF	C18-C13	3.08	1.48	1.42
4	A	603	NO3	O2-N	3.10	1.41	1.25
2	A	601	HEM	FE-NC	3.19	2.08	1.95
4	A	603	NO3	O3-N	3.22	1.42	1.25
3	D	601	BHF	C1-C7	3.39	1.50	1.46
3	D	601	BHF	C18-C13	3.45	1.49	1.42
4	A	604	NO3	O2-N	3.54	1.43	1.25
3	B	602	BHF	C8-C7	3.55	1.44	1.36
3	D	601	BHF	C18-C19	3.74	1.46	1.41
2	C	600	HEM	FE-NC	3.93	2.11	1.95
3	A	602	BHF	C8-C7	4.03	1.45	1.36
3	C	601	BHF	C18-C19	4.10	1.46	1.41
3	A	602	BHF	C10-C19	4.28	1.47	1.41
4	A	604	NO3	O3-N	4.41	1.48	1.25
3	A	602	BHF	C9-C10	4.76	1.47	1.41
4	B	603	NO3	O2-N	4.90	1.50	1.25
3	C	601	BHF	C9-C10	5.07	1.48	1.41
3	D	601	BHF	C9-C10	5.12	1.48	1.41
3	D	601	BHF	C10-C19	5.46	1.48	1.41
3	C	601	BHF	C10-C19	6.10	1.49	1.41
3	B	602	BHF	C9-C10	6.21	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	BHF	C10-C19	6.28	1.49	1.41

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	BHF	C13-C18-C19	-5.20	114.88	118.67
3	A	602	BHF	C2-C1-C7	-4.96	115.65	120.45
3	B	602	BHF	C2-C1-C7	-4.65	115.95	120.45
3	B	602	BHF	O1-C7-C1	-3.87	108.52	113.42
3	A	602	BHF	C7-O1-C19	-3.53	117.33	122.30
3	A	602	BHF	O1-C7-C1	-3.47	109.03	113.42
3	A	602	BHF	C17-C18-C19	-3.41	117.72	122.61
3	B	602	BHF	C14-C13-C18	-3.21	114.56	119.57
3	C	601	BHF	C2-C1-C7	-3.16	117.40	120.45
3	A	602	BHF	C14-C13-C18	-2.97	114.93	119.57
3	C	601	BHF	C13-C18-C19	-2.92	116.55	118.67
3	D	601	BHF	C2-C1-C7	-2.74	117.80	120.45
2	C	600	HEM	C1D-CHD-C4C	-2.71	121.29	125.82
3	D	601	BHF	C9-C10-C19	-2.68	115.57	118.79
2	A	601	HEM	C3B-C4B-NB	-2.67	106.53	111.63
3	A	602	BHF	C16-C17-C18	-2.62	116.28	120.79
2	C	600	HEM	C3B-C4B-NB	-2.57	106.72	111.63
3	C	601	BHF	C8-C7-C1	-2.57	124.56	127.32
3	B	602	BHF	C12-C11-C10	-2.46	118.21	121.42
3	D	601	BHF	C13-C18-C19	-2.42	116.91	118.67
3	B	602	BHF	C9-C10-C19	-2.38	115.94	118.79
3	D	601	BHF	C8-C7-C1	-2.37	124.78	127.32
2	A	601	HEM	C1D-CHD-C4C	-2.28	122.01	125.82
3	A	602	BHF	C13-C18-C19	-2.16	117.10	118.67
3	B	602	BHF	C7-O1-C19	-2.15	119.29	122.30
2	D	600	HEM	C3B-C4B-NB	-2.12	107.57	111.63
2	B	601	HEM	C3B-C4B-NB	-2.10	107.61	111.63
3	A	602	BHF	C9-C10-C19	-2.07	116.31	118.79
3	D	601	BHF	C16-C17-C18	-2.01	117.32	120.79
2	B	601	HEM	CAA-C2A-C1A	2.01	129.19	127.01
2	C	600	HEM	C2C-C1C-CHC	2.04	126.78	123.68
2	C	600	HEM	C2D-C3D-C4D	2.04	104.96	101.50
2	D	600	HEM	CHD-C1D-ND	2.11	129.60	124.52
2	B	601	HEM	CHC-C4B-NB	2.11	129.61	124.52
2	A	601	HEM	CHC-C4B-NB	2.15	129.69	124.52
2	B	601	HEM	CMD-C2D-C3D	2.16	123.91	114.35
2	B	601	HEM	C2D-C3D-C4D	2.16	105.16	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	600	HEM	CBA-CAA-C2A	2.25	116.56	112.53
3	B	602	BHF	C6-C1-C2	2.26	121.82	117.55
2	A	601	HEM	CMD-C2D-C3D	2.36	124.79	114.35
3	C	601	BHF	C17-C18-C13	2.42	121.83	117.65
3	C	601	BHF	O1-C7-C8	2.44	122.18	119.29
3	D	601	BHF	C6-C1-C7	2.45	122.82	120.45
3	A	602	BHF	C6-C1-C2	2.52	122.31	117.55
3	B	602	BHF	O1-C19-C10	2.57	123.93	121.21
2	C	600	HEM	CHC-C4B-NB	2.81	131.28	124.52
3	A	602	BHF	O1-C7-C8	2.86	122.67	119.29
2	D	600	HEM	CMD-C2D-C3D	2.96	127.42	114.35
3	D	601	BHF	C17-C18-C13	3.00	122.84	117.65
2	A	601	HEM	C2D-C3D-C4D	3.10	106.76	101.50
2	A	601	HEM	CBA-CAA-C2A	3.11	118.10	112.53
3	B	602	BHF	O1-C7-C8	3.17	123.04	119.29
2	C	600	HEM	CMD-C2D-C3D	3.21	128.54	114.35
3	B	602	BHF	C18-C19-C10	3.42	122.75	119.88
2	C	600	HEM	CHD-C1D-ND	3.57	133.11	124.52
2	B	601	HEM	CAD-C3D-C2D	3.73	123.94	113.22
2	C	600	HEM	CAD-C3D-C2D	3.83	124.22	113.22
3	A	602	BHF	O1-C19-C10	3.92	125.36	121.21
2	A	601	HEM	CAD-C3D-C2D	3.98	124.65	113.22
3	B	602	BHF	C17-C18-C13	4.01	124.59	117.65
2	B	601	HEM	CMB-C2B-C3B	4.04	126.62	116.53
2	D	600	HEM	CMB-C2B-C3B	4.07	126.68	116.53
2	C	600	HEM	CMB-C2B-C3B	4.22	127.06	116.53
3	A	602	BHF	C17-C18-C13	4.35	125.17	117.65
2	A	601	HEM	CMC-C2C-C3C	4.41	127.53	116.53
2	A	601	HEM	CMB-C2B-C3B	4.53	127.84	116.53
2	A	601	HEM	CAD-C3D-C4D	4.57	128.59	112.47
2	D	600	HEM	CAD-C3D-C4D	4.57	128.60	112.47
2	C	600	HEM	CMC-C2C-C3C	4.71	128.28	116.53
2	D	600	HEM	CMC-C2C-C3C	4.71	128.28	116.53
2	D	600	HEM	CAD-C3D-C2D	4.72	126.78	113.22
2	B	601	HEM	CAD-C3D-C4D	5.18	130.72	112.47
2	C	600	HEM	CAD-C3D-C4D	5.20	130.81	112.47
2	B	601	HEM	CMC-C2C-C3C	5.85	131.14	116.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	HEM	6	0
2	B	601	HEM	4	0
2	C	600	HEM	3	0
2	D	600	HEM	5	0
3	D	601	BHF	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	477/491 (97%)	-0.20	3 (0%) 90 88	31, 52, 91, 131	0
1	B	472/491 (96%)	-0.08	12 (2%) 61 54	35, 60, 100, 148	0
1	C	468/491 (95%)	0.36	45 (9%) 10 6	59, 90, 118, 146	0
1	D	467/491 (95%)	0.32	37 (7%) 15 11	51, 84, 117, 148	0
All	All	1884/1964 (95%)	0.10	97 (5%) 32 25	31, 73, 113, 148	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	36	GLY	6.5
1	B	301	GLN	6.3
1	C	273	PHE	5.2
1	C	302	LEU	4.7
1	D	317	ALA	4.5
1	C	398	GLY	4.4
1	D	321	THR	4.3
1	D	152	ALA	4.2
1	D	318	GLY	4.1
1	D	436	ASP	3.9
1	C	301	GLN	3.9
1	C	37	LEU	3.9
1	C	277	HIS	3.9
1	D	37	LEU	3.8
1	D	322	VAL	3.7
1	D	382	VAL	3.7
1	C	278	ILE	3.7
1	D	496	LEU	3.6
1	C	244	PRO	3.6
1	D	497	THR	3.6
1	D	153	SER	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	38	LYS	3.5
1	C	307	ILE	3.5
1	C	152	ALA	3.4
1	C	155	THR	3.3
1	D	150	ASP	3.3
1	D	198	ILE	3.3
1	D	381	PHE	3.3
1	C	230	SER	3.3
1	D	221	ASN	3.2
1	C	274	GLU	3.2
1	C	321	THR	3.1
1	D	467	VAL	3.1
1	C	271	LYS	3.1
1	B	155	THR	3.1
1	C	154	SER	3.0
1	D	194	VAL	3.0
1	D	324	THR	3.0
1	B	154	SER	3.0
1	C	272	THR	3.0
1	D	154	SER	3.0
1	B	321	THR	2.9
1	D	319	PHE	2.8
1	B	302	LEU	2.8
1	C	286	ILE	2.8
1	A	152	ALA	2.8
1	D	151	PRO	2.8
1	C	401	ILE	2.7
1	B	152	ALA	2.7
1	C	156	SER	2.7
1	C	275	LYS	2.7
1	D	323	THR	2.7
1	D	98	ARG	2.6
1	D	325	ALA	2.6
1	A	181	PRO	2.6
1	D	320	ASP	2.6
1	C	150	ASP	2.6
1	C	392	ARG	2.5
1	D	102	ASP	2.5
1	C	395	SER	2.5
1	D	383	PRO	2.5
1	B	271	LYS	2.4
1	D	197	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	383	PRO	2.4
1	C	320	ASP	2.4
1	C	304	ASP	2.4
1	C	496	LEU	2.4
1	B	322	VAL	2.4
1	C	512	SER	2.4
1	C	497	THR	2.4
1	C	129	PRO	2.3
1	C	229	GLY	2.3
1	B	149	SER	2.3
1	C	290	GLN	2.3
1	D	398	GLY	2.3
1	C	289	CYS	2.3
1	C	44	TRP	2.3
1	D	400	TYR	2.2
1	C	382	VAL	2.2
1	C	361	ASP	2.2
1	D	316	GLY	2.1
1	C	400	TYR	2.1
1	B	325	ALA	2.1
1	B	323	THR	2.1
1	C	435	PRO	2.1
1	D	376	PHE	2.1
1	C	264	LYS	2.1
1	B	382	VAL	2.1
1	D	38	LYS	2.1
1	D	158	TYR	2.1
1	D	459	GLY	2.1
1	D	463	ALA	2.1
1	C	153	SER	2.1
1	D	242	TYR	2.1
1	C	317	ALA	2.0
1	C	463	ALA	2.0
1	C	39	ASN	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 [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
4	NO3	B	603	4/4	0.72	0.28	5.85	51,68,73,86	0
4	NO3	A	604	4/4	0.63	0.21	4.23	64,66,70,101	0
3	BHF	D	601	21/21	0.89	0.48	1.72	94,106,115,121	0
3	BHF	A	602	21/21	0.91	0.29	1.30	43,55,72,81	0
3	BHF	C	601	21/21	0.88	0.30	1.03	88,104,120,122	0
2	HEM	B	601	43/43	0.98	0.23	0.23	36,46,54,60	0
3	BHF	B	602	21/21	0.92	0.22	0.22	58,62,67,79	0
2	HEM	A	601	43/43	0.99	0.23	0.11	32,38,44,52	0
2	HEM	D	600	43/43	0.97	0.28	-0.07	40,53,73,80	0
2	HEM	C	600	43/43	0.98	0.21	-0.42	43,56,80,103	0
4	NO3	A	603	4/4	0.61	0.38	-	103,103,111,118	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.