



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 01:36 AM GMT

PDB ID : 3A4Z  
Title : Structure of cytochrome P450 Vdh mutant (Vdh-K1) obtained by directed evolution  
Authors : Yasutake, Y.; Fujii, Y.; Cheon, W.K.; Arisawa, A.; Tamura, T.  
Deposited on : 2009-07-24  
Resolution : 2.20 Å(reported)

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

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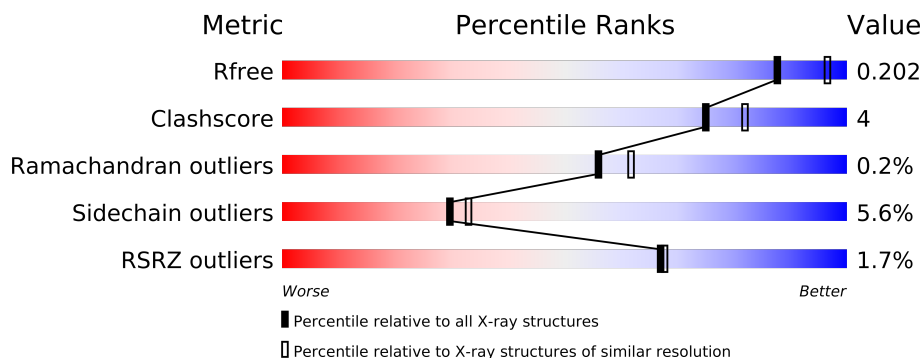
The following versions of software and data (see [references](#)) were used in the production of this report:

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

# 1 Overall quality at a glance

The reported resolution of this entry is 2.20 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	2938 (2.20-2.20)
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (2.20-2.20)

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	411	
1	B	411	
1	C	411	
1	D	411	
1	E	411	

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

Mol	Type	Chain	Res	Geometry	Electron density
3	CA	E	2504	-	X
5	GOL	A	3002	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16621 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 Vitamin D hydroxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	402	Total	C	N	O	S	0	0	0
			3113	1958	549	589	17			
1	B	402	Total	C	N	O	S	0	0	0
			3113	1958	549	589	17			
1	C	401	Total	C	N	O	S	0	0	0
			3108	1955	548	588	17			
1	D	401	Total	C	N	O	S	0	0	0
			3108	1955	548	588	17			
1	E	401	Total	C	N	O	S	0	0	0
			3108	1955	548	588	17			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	70	ARG	THR	ENGINEERED MUTATION	UNP C4B644
A	156	LEU	VAL	ENGINEERED MUTATION	UNP C4B644
A	216	MET	GLU	ENGINEERED MUTATION	UNP C4B644
A	384	ARG	GLU	ENGINEERED MUTATION	UNP C4B644
A	404	LEU	-	EXPRESSION TAG	UNP C4B644
A	405	GLU	-	EXPRESSION TAG	UNP C4B644
A	406	HIS	-	EXPRESSION TAG	UNP C4B644
A	407	HIS	-	EXPRESSION TAG	UNP C4B644
A	408	HIS	-	EXPRESSION TAG	UNP C4B644
A	409	HIS	-	EXPRESSION TAG	UNP C4B644
A	410	HIS	-	EXPRESSION TAG	UNP C4B644
A	411	HIS	-	EXPRESSION TAG	UNP C4B644
B	70	ARG	THR	ENGINEERED MUTATION	UNP C4B644
B	156	LEU	VAL	ENGINEERED MUTATION	UNP C4B644
B	216	MET	GLU	ENGINEERED MUTATION	UNP C4B644
B	384	ARG	GLU	ENGINEERED MUTATION	UNP C4B644
B	404	LEU	-	EXPRESSION TAG	UNP C4B644
B	405	GLU	-	EXPRESSION TAG	UNP C4B644
B	406	HIS	-	EXPRESSION TAG	UNP C4B644

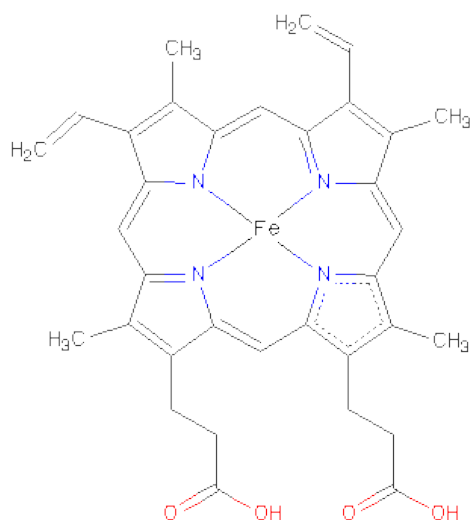
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Chain	Residue	Modelled	Actual	Comment	Reference
B	407	HIS	-	EXPRESSION TAG	UNP C4B644
B	408	HIS	-	EXPRESSION TAG	UNP C4B644
B	409	HIS	-	EXPRESSION TAG	UNP C4B644
B	410	HIS	-	EXPRESSION TAG	UNP C4B644
B	411	HIS	-	EXPRESSION TAG	UNP C4B644
C	70	ARG	THR	ENGINEERED MUTATION	UNP C4B644
C	156	LEU	VAL	ENGINEERED MUTATION	UNP C4B644
C	216	MET	GLU	ENGINEERED MUTATION	UNP C4B644
C	384	ARG	GLU	ENGINEERED MUTATION	UNP C4B644
C	404	LEU	-	EXPRESSION TAG	UNP C4B644
C	405	GLU	-	EXPRESSION TAG	UNP C4B644
C	406	HIS	-	EXPRESSION TAG	UNP C4B644
C	407	HIS	-	EXPRESSION TAG	UNP C4B644
C	408	HIS	-	EXPRESSION TAG	UNP C4B644
C	409	HIS	-	EXPRESSION TAG	UNP C4B644
C	410	HIS	-	EXPRESSION TAG	UNP C4B644
C	411	HIS	-	EXPRESSION TAG	UNP C4B644
D	70	ARG	THR	ENGINEERED MUTATION	UNP C4B644
D	156	LEU	VAL	ENGINEERED MUTATION	UNP C4B644
D	216	MET	GLU	ENGINEERED MUTATION	UNP C4B644
D	384	ARG	GLU	ENGINEERED MUTATION	UNP C4B644
D	404	LEU	-	EXPRESSION TAG	UNP C4B644
D	405	GLU	-	EXPRESSION TAG	UNP C4B644
D	406	HIS	-	EXPRESSION TAG	UNP C4B644
D	407	HIS	-	EXPRESSION TAG	UNP C4B644
D	408	HIS	-	EXPRESSION TAG	UNP C4B644
D	409	HIS	-	EXPRESSION TAG	UNP C4B644
D	410	HIS	-	EXPRESSION TAG	UNP C4B644
D	411	HIS	-	EXPRESSION TAG	UNP C4B644
E	70	ARG	THR	ENGINEERED MUTATION	UNP C4B644
E	156	LEU	VAL	ENGINEERED MUTATION	UNP C4B644
E	216	MET	GLU	ENGINEERED MUTATION	UNP C4B644
E	384	ARG	GLU	ENGINEERED MUTATION	UNP C4B644
E	404	LEU	-	EXPRESSION TAG	UNP C4B644
E	405	GLU	-	EXPRESSION TAG	UNP C4B644
E	406	HIS	-	EXPRESSION TAG	UNP C4B644
E	407	HIS	-	EXPRESSION TAG	UNP C4B644
E	408	HIS	-	EXPRESSION TAG	UNP C4B644
E	409	HIS	-	EXPRESSION TAG	UNP C4B644
E	410	HIS	-	EXPRESSION TAG	UNP C4B644
E	411	HIS	-	EXPRESSION TAG	UNP C4B644

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (for-

mula:  $C_{34}H_{32}FeN_4O_4$ ).

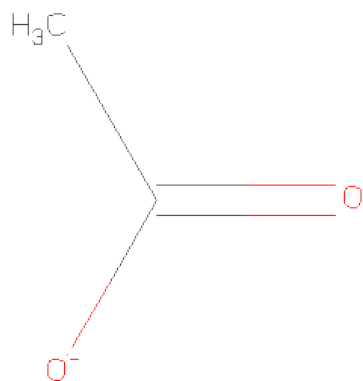


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	
			43	34	1	4	4	0
2	B	1	Total	C	Fe	N	O	
			43	34	1	4	4	0
2	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	0
2	D	1	Total	C	Fe	N	O	
			43	34	1	4	4	0
2	E	1	Total	C	Fe	N	O	
			43	34	1	4	4	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	Ca		
			3	3	0	0
3	D	1	Total	Ca		
			1	1	0	0
3	C	1	Total	Ca		
			1	1	0	0
3	E	1	Total	Ca		
			1	1	0	0

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is water.

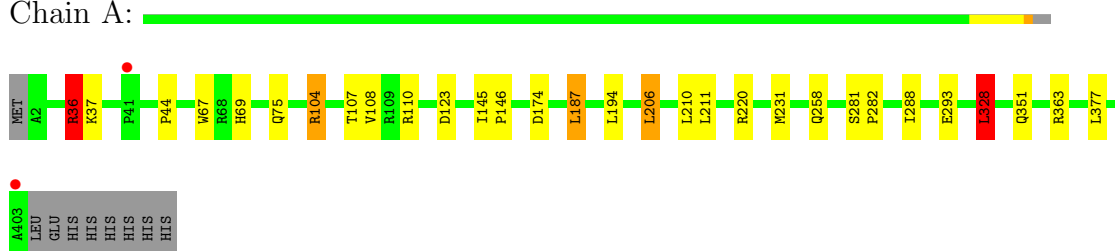
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	257	Total	O	0	0
			257	257		
6	B	127	Total	O	0	0
			127	127		
6	C	128	Total	O	0	0
			128	128		
6	D	148	Total	O	0	0
			148	148		
6	E	154	Total	O	0	0
			154	154		

### 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.

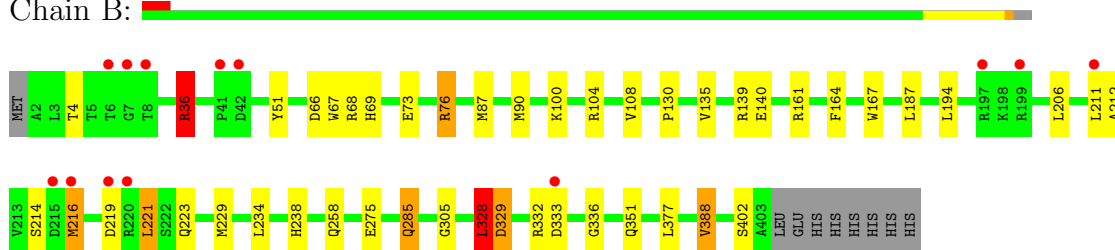
- Molecule 1: Vitamin D hydroxylase

Chain A:



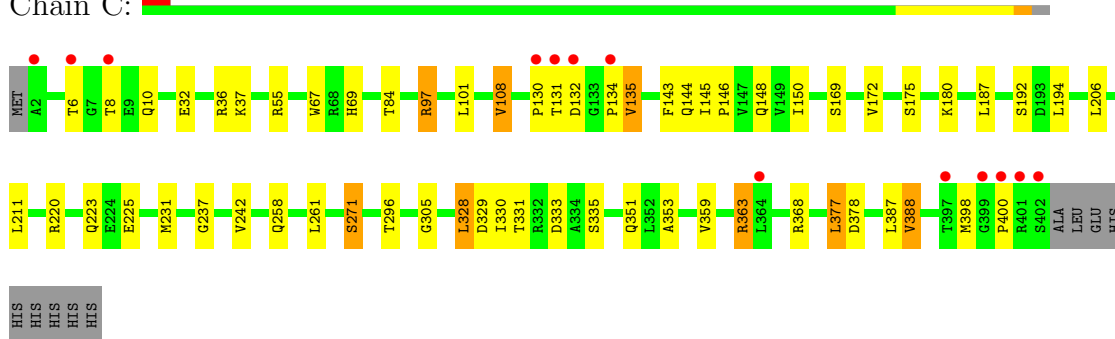
- Molecule 1: Vitamin D hydroxylase

Chain B:



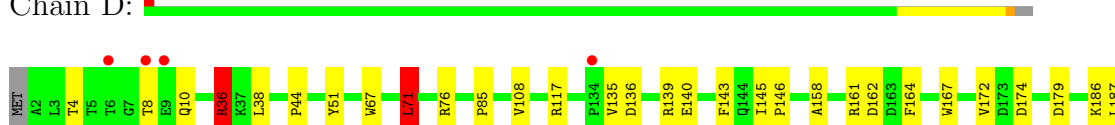
- Molecule 1: Vitamin D hydroxylase

Chain C:



- Molecule 1: Vitamin D hydroxylase

Chain D:

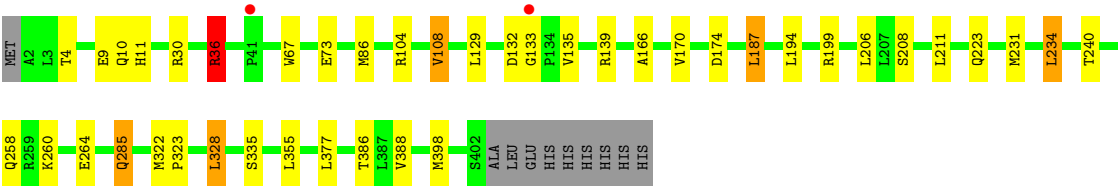






● Molecule 1: Vitamin D hydroxylase

Chain E:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.38Å 172.47Å 189.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.27 – 2.20 49.24 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.27-2.20) 99.9 (49.24-2.20)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.84 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.201 , 0.244 0.204 , 0.202	Depositor DCC
$R_{free}$ test set	6458 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	32.4	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 31.0	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 128913 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	16621	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% 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: GOL, CA, ACT, 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	0.76	0/3179	0.82	3/4325 (0.1%)
1	B	0.66	0/3179	0.74	5/4325 (0.1%)
1	C	0.69	0/3174	0.79	2/4318 (0.0%)
1	D	0.68	0/3174	0.77	3/4318 (0.1%)
1	E	0.71	0/3174	0.80	6/4318 (0.1%)
All	All	0.70	0/15880	0.78	19/21604 (0.1%)

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	36	ARG	NE-CZ-NH2	-12.37	114.12	120.30
1	C	97	ARG	NE-CZ-NH2	-12.35	114.12	120.30
1	A	36	ARG	NE-CZ-NH1	10.81	125.70	120.30
1	C	97	ARG	NE-CZ-NH1	10.09	125.35	120.30
1	E	234	LEU	CA-CB-CG	7.96	133.61	115.30
1	E	36	ARG	NE-CZ-NH2	-7.43	116.58	120.30
1	D	71	LEU	CA-CB-CG	7.21	131.89	115.30
1	E	36	ARG	NE-CZ-NH1	6.17	123.38	120.30
1	D	36	ARG	NE-CZ-NH1	5.97	123.28	120.30
1	D	36	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	B	328	LEU	CA-CB-CG	5.47	127.89	115.30
1	E	132	ASP	CB-CG-OD1	5.36	123.13	118.30
1	B	66	ASP	CB-CG-OD2	5.36	123.12	118.30
1	A	328	LEU	CA-CB-CG	5.36	127.62	115.30
1	B	285	GLN	CA-CB-CG	5.30	125.06	113.40
1	E	139	ARG	NE-CZ-NH1	-5.11	117.75	120.30
1	B	36	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	E	234	LEU	CB-CG-CD1	5.01	119.53	111.00
1	B	329	ASP	CB-CG-OD1	5.01	122.81	118.30

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	3113	0	3095	16	0
1	B	3113	0	3095	24	0
1	C	3108	0	3090	33	0
1	D	3108	0	3090	32	0
1	E	3108	0	3090	20	0
2	A	43	0	30	0	0
2	B	43	0	30	0	0
2	C	43	0	30	8	0
2	D	43	0	30	1	0
2	E	43	0	30	1	0
3	A	3	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
4	A	4	0	3	0	0
4	C	8	0	6	0	0
4	D	4	0	3	0	0
4	E	8	0	6	0	0
5	A	12	0	15	0	0
6	A	257	0	0	2	0
6	B	127	0	0	2	0
6	C	128	0	0	2	0
6	D	148	0	0	1	0
6	E	154	0	0	3	0
All	All	16621	0	15643	126	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 4.

All (126) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:187:LEU:HD13	1:A:231:MET:HG3	1.44	0.98
1:C:363:ARG:HH21	1:C:363:ARG:HG3	1.34	0.92
1:C:258:GLN:HG3	1:C:328:LEU:HD13	1.53	0.90
1:C:329:ASP:OD1	1:C:331:THR:HG22	1.77	0.84
1:C:150:ILE:HG12	1:C:237:GLY:HA3	1.60	0.84
1:D:228:ALA:HA	1:D:231:MET:HE3	1.63	0.80
2:C:412:HEM:HHC	2:C:412:HEM:HBB2	1.65	0.78
1:E:129:LEU:HB3	1:E:398:MET:HE3	1.65	0.78
1:C:363:ARG:HH21	1:C:363:ARG:CG	1.96	0.77
1:C:108:VAL:HB	1:C:351:GLN:HG3	1.66	0.77
1:A:107:THR:OG1	1:A:110:ARG:HG2	1.84	0.77
1:D:136:ASP:O	1:D:140:GLU:HG2	1.84	0.76
1:E:187:LEU:HD13	1:E:231:MET:HG3	1.69	0.75
1:E:285:GLN:HG2	1:E:386:THR:O	1.87	0.74
1:C:353:ALA:HB1	2:C:412:HEM:CBB	2.17	0.74
1:E:4:THR:O	1:E:36:ARG:NH2	2.22	0.72
1:E:135:VAL:HG21	1:E:398:MET:HE1	1.71	0.71
1:D:4:THR:O	1:D:36:ARG:NH2	2.25	0.70
1:C:359:VAL:O	1:C:363:ARG:HG2	1.91	0.70
1:C:97:ARG:NH2	1:C:225:GLU:OE2	2.25	0.69
1:E:199:ARG:HH22	1:E:223:GLN:HE22	1.41	0.69
1:B:108:VAL:HG22	1:B:351:GLN:HG3	1.75	0.69
1:D:172:VAL:HG21	1:D:239:GLU:HG2	1.75	0.68
1:D:242:VAL:HG23	6:D:432:HOH:O	1.92	0.68
1:C:97:ARG:HH22	1:C:225:GLU:CD	1.98	0.66
1:C:143:PHE:HA	1:C:242:VAL:HG22	1.78	0.65
1:B:388:VAL:HG22	6:B:818:HOH:O	1.97	0.64
1:D:227:VAL:HG12	1:D:231:MET:HE2	1.80	0.63
1:D:285:GLN:HB3	1:D:309:MET:HG2	1.79	0.63
1:D:196:GLU:O	1:D:199:ARG:HG3	1.99	0.63
1:B:87:MET:CE	1:B:229:MET:CE	2.78	0.62
1:B:87:MET:HE3	1:B:229:MET:CE	2.30	0.62
2:C:412:HEM:HBC2	2:C:412:HEM:HHD	1.82	0.62
1:D:143:PHE:HA	1:D:242:VAL:HG22	1.83	0.60
1:A:36:ARG:HD2	1:A:37:LYS:O	2.02	0.60
1:B:258:GLN:HG3	1:B:328:LEU:HD13	1.84	0.59
1:D:258:GLN:HG3	1:D:328:LEU:HD13	1.84	0.59
1:C:108:VAL:CB	1:C:351:GLN:HG3	2.32	0.59
1:D:158:ALA:HA	1:D:161:ARG:HG3	1.83	0.59
1:C:363:ARG:HG3	1:C:363:ARG:NH2	2.08	0.58
1:A:187:LEU:HD13	1:A:231:MET:CG	2.27	0.58
1:C:187:LEU:HD13	1:C:231:MET:HG3	1.87	0.57
1:E:135:VAL:HG21	1:E:398:MET:CE	2.34	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:145:ILE:HB	1:C:146:PRO:HD3	1.87	0.57
1:D:71:LEU:CD2	1:D:76:ARG:HG2	2.36	0.55
1:C:242:VAL:HG23	6:C:455:HOH:O	2.06	0.55
1:B:219:ASP:HB3	1:C:108:VAL:HG11	1.88	0.55
1:C:353:ALA:CB	2:C:412:HEM:CBB	2.86	0.54
1:C:131:THR:HG23	1:C:400:PRO:HA	1.90	0.53
1:D:85:PRO:HG3	1:D:224:GLU:HG3	1.90	0.53
1:A:258:GLN:HG3	1:A:328:LEU:HD13	1.90	0.53
1:E:258:GLN:HG3	1:E:328:LEU:HD13	1.91	0.52
1:D:161:ARG:HA	1:D:164:PHE:CZ	2.45	0.51
1:C:388:VAL:HG22	6:C:644:HOH:O	2.09	0.51
1:B:4:THR:O	1:B:36:ARG:NH2	2.43	0.51
1:D:194:LEU:HD22	1:D:198:LYS:HE2	1.91	0.50
1:D:145:ILE:HB	1:D:146:PRO:HD3	1.93	0.50
1:A:37:LYS:HE3	1:A:44:PRO:HB2	1.94	0.50
1:D:139:ARG:NH2	1:D:140:GLU:OE2	2.45	0.50
1:B:164:PHE:HA	1:B:167:TRP:CE3	2.47	0.50
1:D:71:LEU:HD22	1:D:76:ARG:HG2	1.94	0.49
1:A:69:HIS:HD2	6:A:513:HOH:O	1.95	0.49
1:C:353:ALA:CB	2:C:412:HEM:HBB2	2.42	0.49
1:E:174:ASP:OD1	1:E:386:THR:HG23	2.13	0.49
1:B:87:MET:CE	1:B:229:MET:HE3	2.43	0.49
1:B:212:ALA:O	1:B:216:MET:HG3	2.13	0.48
1:C:296:THR:HG21	1:E:133:GLY:HA2	1.95	0.48
1:B:51:TYR:OH	1:B:336:GLY:O	2.30	0.48
1:C:368:ARG:HG3	1:C:398:MET:HE3	1.96	0.47
1:D:258:GLN:OE1	1:D:330:ILE:HG12	2.15	0.47
1:B:139:ARG:NH1	6:B:473:HOH:O	2.46	0.47
1:D:164:PHE:HA	1:D:167:TRP:CE3	2.50	0.47
1:D:375:VAL:HG12	1:E:108:VAL:HG11	1.97	0.46
1:A:281:SER:HA	1:A:282:PRO:HD3	1.76	0.46
1:C:220:ARG:HG2	1:C:220:ARG:HH11	1.81	0.45
1:C:144:GLN:O	1:C:148:GLN:HG3	2.17	0.45
1:D:108:VAL:HA	1:D:351:GLN:HG2	1.98	0.45
1:A:145:ILE:HB	1:A:146:PRO:HD3	1.98	0.45
1:E:322:MET:HA	1:E:323:PRO:HD2	1.89	0.45
1:C:353:ALA:HB2	2:C:412:HEM:HBB2	1.99	0.45
1:C:175:SER:HB2	1:C:180:LYS:HE2	1.99	0.44
1:C:36:ARG:NH1	1:C:37:LYS:O	2.50	0.44
1:A:123:ASP:OD2	1:A:363:ARG:HD2	2.16	0.44
1:B:139:ARG:HH22	1:B:140:GLU:CD	2.21	0.44
1:B:68:ARG:O	1:B:76:ARG:HD2	2.18	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:87:MET:CE	1:B:229:MET:HE1	2.47	0.44
1:C:69:HIS:O	1:C:305:GLY:HA2	2.17	0.44
1:E:388:VAL:HG22	6:E:468:HOH:O	2.17	0.44
1:E:260:LYS:HE2	1:E:264:GLU:OE2	2.18	0.44
2:C:412:HEM:HHD	2:C:412:HEM:CBC	2.48	0.44
1:D:327:ARG:NH1	1:D:329:ASP:HB2	2.33	0.43
1:D:51:TYR:HA	1:D:315:ALA:HB1	2.00	0.43
1:D:38:LEU:O	1:D:44:PRO:HA	2.18	0.43
1:A:211:LEU:HD23	1:A:211:LEU:O	2.18	0.43
1:C:172:VAL:HG22	1:C:387:LEU:HD23	2.00	0.43
1:A:104:ARG:HE	1:A:104:ARG:HA	1.83	0.43
1:A:37:LYS:HE3	1:A:44:PRO:CB	2.49	0.43
1:B:214:SER:HB2	1:B:221:LEU:HD12	2.01	0.43
1:E:285:GLN:NE2	6:E:428:HOH:O	2.51	0.43
1:B:73:GLU:HA	1:B:76:ARG:HB2	2.01	0.43
1:D:240:THR:HB	2:D:412:HEM:C3B	2.54	0.43
1:E:86:MET:HE2	1:E:86:MET:HB2	1.73	0.43
1:A:37:LYS:NZ	6:A:581:HOH:O	2.52	0.42
1:D:199:ARG:NH2	1:D:215:ASP:OD2	2.50	0.42
1:B:69:HIS:O	1:B:305:GLY:HA2	2.20	0.42
1:C:130:PRO:HG2	1:C:135:VAL:CG1	2.49	0.42
1:E:166:ALA:O	1:E:170:VAL:HG23	2.19	0.42
1:E:30:ARG:NH2	6:E:437:HOH:O	2.50	0.42
1:D:136:ASP:O	1:D:140:GLU:CG	2.62	0.42
1:B:87:MET:HE3	1:B:229:MET:SD	2.60	0.42
1:A:206:LEU:HD22	1:A:210:LEU:HG	2.01	0.42
1:A:108:VAL:HA	1:A:351:GLN:OE1	2.20	0.42
1:C:108:VAL:HA	1:C:351:GLN:HG3	2.02	0.41
1:B:130:PRO:HD2	1:B:135:VAL:HG11	2.02	0.41
1:E:9:GLU:HB3	1:E:11:HIS:NE2	2.34	0.41
1:D:117:ARG:HA	1:D:117:ARG:HD2	1.92	0.41
1:C:271:SER:HB3	1:C:330:ILE:O	2.21	0.41
1:B:161:ARG:HA	1:B:164:PHE:CZ	2.55	0.41
1:B:329:ASP:HB3	1:B:332:ARG:HG3	2.03	0.41
1:B:275:GLU:HG3	1:B:328:LEU:CD2	2.52	0.40
1:D:161:ARG:HE	1:D:161:ARG:HB3	1.73	0.40
1:D:223:GLN:HE21	1:D:223:GLN:HB3	1.68	0.40
2:C:412:HEM:HBC2	2:C:412:HEM:CHD	2.49	0.40
1:E:240:THR:HB	2:E:412:HEM:C3B	2.57	0.40
1:D:167:TRP:NE1	1:D:186:LYS:HD2	2.36	0.40
1:B:234:LEU:O	1:B:238:HIS:HD2	2.05	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	400/411 (97%)	385 (96%)	14 (4%)	1 (0%)	50	53
1	B	400/411 (97%)	385 (96%)	15 (4%)	0	100	100
1	C	399/411 (97%)	383 (96%)	15 (4%)	1 (0%)	50	53
1	D	399/411 (97%)	381 (96%)	17 (4%)	1 (0%)	50	53
1	E	399/411 (97%)	383 (96%)	16 (4%)	0	100	100
All	All	1997/2055 (97%)	1917 (96%)	77 (4%)	3 (0%)	56	62

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	174	ASP
1	C	377	LEU
1	D	174	ASP

### 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	334/343 (97%)	322 (96%)	12 (4%)	47	56
1	B	334/343 (97%)	315 (94%)	19 (6%)	29	32
1	C	334/343 (97%)	307 (92%)	27 (8%)	17	16
1	D	334/343 (97%)	315 (94%)	19 (6%)	29	32
1	E	334/343 (97%)	317 (95%)	17 (5%)	33	38
All	All	1670/1715 (97%)	1576 (94%)	94 (6%)	30	33

All (94) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	A	36	ARG
1	A	67	TRP
1	A	75	GLN
1	A	104	ARG
1	A	187	LEU
1	A	194	LEU
1	A	206	LEU
1	A	220	ARG
1	A	288	ILE
1	A	293	GLU
1	A	328	LEU
1	A	377	LEU
1	B	36	ARG
1	B	67	TRP
1	B	76	ARG
1	B	90	MET
1	B	100	LYS
1	B	104	ARG
1	B	187	LEU
1	B	194	LEU
1	B	206	LEU
1	B	211	LEU
1	B	216	MET
1	B	221	LEU
1	B	223	GLN
1	B	285	GLN
1	B	328	LEU
1	B	333	ASP
1	B	377	LEU
1	B	388	VAL
1	B	402	SER
1	C	6	THR
1	C	8	THR
1	C	10	GLN
1	C	32	GLU
1	C	55	ARG
1	C	67	TRP
1	C	84	THR
1	C	101	LEU
1	C	108	VAL
1	C	132	ASP
1	C	134	PRO
1	C	135	VAL

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Mol	Chain	Res	Type
1	C	169	SER
1	C	192	SER
1	C	194	LEU
1	C	206	LEU
1	C	211	LEU
1	C	223	GLN
1	C	261	LEU
1	C	271	SER
1	C	328	LEU
1	C	333	ASP
1	C	335	SER
1	C	363	ARG
1	C	377	LEU
1	C	378	ASP
1	C	388	VAL
1	D	8	THR
1	D	10	GLN
1	D	36	ARG
1	D	67	TRP
1	D	71	LEU
1	D	135	VAL
1	D	162	ASP
1	D	179	ASP
1	D	187	LEU
1	D	194	LEU
1	D	206	LEU
1	D	211	LEU
1	D	221	LEU
1	D	223	GLN
1	D	239	GLU
1	D	309	MET
1	D	328	LEU
1	D	355	LEU
1	D	377	LEU
1	E	10	GLN
1	E	36	ARG
1	E	67	TRP
1	E	73	GLU
1	E	104	ARG
1	E	108	VAL
1	E	187	LEU
1	E	194	LEU

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Mol	Chain	Res	Type
1	E	206	LEU
1	E	208	SER
1	E	211	LEU
1	E	234	LEU
1	E	285	GLN
1	E	328	LEU
1	E	335	SER
1	E	355	LEU
1	E	377	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	HIS
1	B	69	HIS
1	B	238	HIS
1	C	10	GLN
1	C	20	GLN
1	C	69	HIS
1	C	223	GLN
1	C	238	HIS
1	C	285	GLN
1	D	10	GLN
1	D	69	HIS
1	D	223	GLN
1	D	285	GLN
1	E	10	GLN
1	E	223	GLN
1	E	285	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 19 ligands modelled in this entry, 6 are monoatomic - leaving 13 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
5	GOL	A	3001	-	5,5,5	0.50	0	5,5,5	0.21	0
5	GOL	A	3002	3	5,5,5	0.31	0	5,5,5	1.73	1 (20%)
4	ACT	A	4006	-	1,3,3	2.30	1 (100%)	0,3,3	0.00	-
2	HEM	A	412	1	49,50,50	2.58	21 (42%)	46,82,82	2.52	10 (21%)
2	HEM	B	412	1	49,50,50	2.82	16 (32%)	46,82,82	2.15	7 (15%)
4	ACT	C	4004	3	1,3,3	1.49	0	0,3,3	0.00	-
4	ACT	C	4007	-	1,3,3	2.25	1 (100%)	0,3,3	0.00	-
2	HEM	C	412	1	49,50,50	2.41	19 (38%)	46,82,82	2.49	11 (23%)
4	ACT	D	4001	-	1,3,3	2.53	1 (100%)	0,3,3	0.00	-
2	HEM	D	412	1	49,50,50	2.45	18 (36%)	46,82,82	2.26	8 (17%)
4	ACT	E	4005	3	1,3,3	1.78	0	0,3,3	0.00	-
4	ACT	E	4008	-	1,3,3	1.20	0	0,3,3	0.00	-
2	HEM	E	412	1	49,50,50	2.49	16 (32%)	46,82,82	2.37	10 (21%)

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
5	GOL	A	3001	-	-	0/4/4/4	0/0/0/0
5	GOL	A	3002	3	-	0/4/4/4	0/0/0/0
4	ACT	A	4006	-	-	0/0/0/0	0/0/0/0
2	HEM	A	412	1	-	0/14/114/114	0/0/8/8
2	HEM	B	412	1	-	0/14/114/114	0/0/8/8

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ACT	C	4004	3	-	0/0/0/0	0/0/0/0
4	ACT	C	4007	-	-	0/0/0/0	0/0/0/0
2	HEM	C	412	1	-	0/14/114/114	0/0/8/8
4	ACT	D	4001	-	-	0/0/0/0	0/0/0/0
2	HEM	D	412	1	-	0/14/114/114	0/0/8/8
4	ACT	E	4005	3	-	0/0/0/0	0/0/0/0
4	ACT	E	4008	-	-	0/0/0/0	0/0/0/0
2	HEM	E	412	1	-	0/14/114/114	0/0/8/8

All (93) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	412	HEM	C2D-C1D	10.33	1.47	1.44
2	E	412	HEM	C3C-C2C	-6.28	1.32	1.43
2	A	412	HEM	C3C-C2C	-5.80	1.33	1.43
2	D	412	HEM	C3C-C2C	-5.79	1.33	1.43
2	B	412	HEM	C3D-C2D	5.75	1.53	1.43
2	D	412	HEM	C3D-C2D	5.72	1.53	1.43
2	A	412	HEM	C3D-C2D	5.56	1.53	1.43
2	E	412	HEM	FE-NA	5.55	2.16	1.92
2	C	412	HEM	C3B-C2B	-5.20	1.34	1.43
2	A	412	HEM	FE-NA	5.14	2.14	1.92
2	E	412	HEM	C3D-C2D	5.13	1.52	1.43
2	C	412	HEM	C3C-C2C	-5.03	1.35	1.43
2	E	412	HEM	C3B-CAB	4.95	1.56	1.40
2	B	412	HEM	C3B-CAB	4.92	1.55	1.40
2	D	412	HEM	C3B-C2B	-4.89	1.35	1.43
2	C	412	HEM	C3D-C2D	4.87	1.52	1.43
2	D	412	HEM	C4A-C3A	4.85	1.46	1.40
2	A	412	HEM	FE-ND	4.75	2.15	1.97
2	B	412	HEM	C3C-CAC	4.74	1.55	1.40
2	E	412	HEM	C3B-C2B	-4.74	1.35	1.43
2	C	412	HEM	C3C-CAC	4.73	1.55	1.40
2	A	412	HEM	C3C-CAC	4.71	1.55	1.40
2	A	412	HEM	C4A-C3A	4.69	1.46	1.40
2	B	412	HEM	C3B-C2B	-4.69	1.35	1.43
2	E	412	HEM	FE-ND	4.67	2.14	1.97
2	E	412	HEM	C3C-CAC	4.66	1.55	1.40
2	A	412	HEM	C3B-CAB	4.65	1.55	1.40
2	C	412	HEM	C3B-CAB	4.60	1.54	1.40
2	B	412	HEM	C3C-C2C	-4.58	1.35	1.43
2	B	412	HEM	FE-ND	4.50	2.14	1.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	412	HEM	C3B-CAB	4.47	1.54	1.40
2	A	412	HEM	FE-NB	4.46	2.14	1.97
2	D	412	HEM	C3C-CAC	4.45	1.54	1.40
2	E	412	HEM	FE-NB	4.42	2.13	1.97
2	B	412	HEM	C4A-C3A	4.40	1.45	1.40
2	D	412	HEM	FE-NC	4.30	2.14	1.97
2	B	412	HEM	FE-NB	4.18	2.13	1.97
2	C	412	HEM	FE-NA	4.13	2.10	1.92
2	A	412	HEM	C3B-C2B	-4.09	1.36	1.43
2	C	412	HEM	FE-ND	4.05	2.12	1.97
2	B	412	HEM	FE-NA	3.98	2.09	1.92
2	D	412	HEM	FE-NA	3.94	2.09	1.92
2	C	412	HEM	C3D-C4D	3.93	1.45	1.44
2	E	412	HEM	C4A-C3A	3.87	1.45	1.40
2	B	412	HEM	C3D-C4D	3.81	1.45	1.44
2	C	412	HEM	C2B-C1B	3.78	1.45	1.44
2	D	412	HEM	FE-NB	3.70	2.11	1.97
2	C	412	HEM	C2D-C1D	3.65	1.45	1.44
2	C	412	HEM	FE-NB	3.63	2.11	1.97
2	A	412	HEM	CHA-C4D	3.56	1.40	1.35
2	D	412	HEM	FE-ND	3.23	2.09	1.97
2	A	412	HEM	CMC-C2C	3.19	1.57	1.47
2	E	412	HEM	CMC-C2C	3.14	1.57	1.47
2	D	412	HEM	CMD-C2D	3.13	1.57	1.47
2	E	412	HEM	CMD-C2D	3.11	1.57	1.47
2	A	412	HEM	FE-NC	3.06	2.09	1.97
2	B	412	HEM	CMC-C2C	3.04	1.56	1.47
2	A	412	HEM	C2B-C1B	3.03	1.45	1.44
2	E	412	HEM	CHA-C4D	2.90	1.40	1.35
2	B	412	HEM	FE-NC	2.89	2.08	1.97
2	A	412	HEM	C2D-C1D	2.88	1.45	1.44
2	A	412	HEM	CMD-C2D	2.82	1.56	1.47
2	A	412	HEM	CMB-C2B	2.81	1.56	1.47
2	D	412	HEM	CHB-C1B	2.76	1.39	1.35
2	C	412	HEM	CMB-C2B	2.71	1.55	1.47
2	C	412	HEM	CHA-C4D	2.70	1.39	1.35
2	D	412	HEM	CMC-C2C	2.65	1.55	1.47
2	D	412	HEM	CMB-C2B	2.63	1.55	1.47
2	E	412	HEM	CHB-C1B	2.62	1.39	1.35
2	C	412	HEM	CAA-C2A	2.57	1.56	1.52
2	E	412	HEM	C3D-C4D	2.55	1.45	1.44
2	C	412	HEM	FE-NC	2.54	2.07	1.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	4001	ACT	CH3-C	2.53	1.52	1.48
2	A	412	HEM	CHB-C1B	2.44	1.39	1.35
2	C	412	HEM	CMD-C2D	2.43	1.55	1.47
2	B	412	HEM	CHB-C1B	2.41	1.39	1.35
2	D	412	HEM	C2B-C1B	-2.41	1.44	1.44
2	B	412	HEM	CMB-C2B	2.39	1.54	1.47
2	C	412	HEM	CMC-C2C	2.38	1.54	1.47
2	B	412	HEM	CMD-C2D	2.38	1.54	1.47
2	D	412	HEM	C3D-C4D	2.36	1.45	1.44
2	C	412	HEM	C4C-NC	2.35	1.41	1.38
2	A	412	HEM	CHD-C4C	2.33	1.40	1.36
4	A	4006	ACT	CH3-C	2.30	1.52	1.48
2	A	412	HEM	C4A-NA	2.26	1.41	1.36
2	A	412	HEM	CMA-C3A	2.26	1.56	1.51
4	C	4007	ACT	CH3-C	2.25	1.52	1.48
2	E	412	HEM	CMB-C2B	2.21	1.54	1.47
2	D	412	HEM	CAA-C2A	2.21	1.55	1.52
2	D	412	HEM	CHA-C4D	2.19	1.39	1.35
2	E	412	HEM	CMA-C3A	2.15	1.56	1.51
2	A	412	HEM	CAA-C2A	2.11	1.55	1.52
2	C	412	HEM	CMA-C3A	2.02	1.55	1.51

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	412	HEM	C3B-C4B-NB	-9.98	106.86	114.00
2	C	412	HEM	C3B-C4B-NB	-9.84	106.96	114.00
2	A	412	HEM	C3B-C4B-NB	-9.61	107.12	114.00
2	E	412	HEM	C3B-C4B-NB	-9.29	107.36	114.00
2	B	412	HEM	C3B-C4B-NB	-8.71	107.77	114.00
2	E	412	HEM	C4D-ND-C1D	7.68	113.02	105.16
2	A	412	HEM	C4D-ND-C1D	7.67	113.01	105.16
2	C	412	HEM	C4D-ND-C1D	7.60	112.93	105.16
2	D	412	HEM	C4D-ND-C1D	6.87	112.19	105.16
2	B	412	HEM	C4D-ND-C1D	6.51	111.83	105.16
2	A	412	HEM	C2D-C1D-ND	-4.70	107.38	112.93
2	C	412	HEM	C2D-C1D-ND	-4.68	107.40	112.93
2	C	412	HEM	CBD-CAD-C3D	-4.68	104.15	114.37
2	A	412	HEM	C4C-NC-C1C	4.08	109.78	105.53
2	E	412	HEM	C1B-NB-C4B	3.94	109.19	105.16
2	D	412	HEM	C2D-C1D-ND	-3.91	108.31	112.93
2	B	412	HEM	CBD-CAD-C3D	-3.83	106.01	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	412	HEM	C2D-C1D-ND	-3.76	108.49	112.93
2	C	412	HEM	CMA-C3A-C4A	-3.65	123.00	128.62
2	D	412	HEM	C4C-NC-C1C	3.61	109.29	105.53
2	B	412	HEM	C2D-C1D-ND	-3.60	108.68	112.93
2	A	412	HEM	C1B-NB-C4B	3.60	108.84	105.16
2	B	412	HEM	C4C-NC-C1C	3.44	109.11	105.53
2	D	412	HEM	C1B-NB-C4B	3.43	108.67	105.16
2	E	412	HEM	CBD-CAD-C3D	-3.41	106.94	114.37
2	B	412	HEM	C1B-NB-C4B	3.38	108.62	105.16
2	A	412	HEM	C3A-C4A-NA	-3.36	106.87	109.41
2	A	412	HEM	CBD-CAD-C3D	-3.35	107.06	114.37
2	A	412	HEM	CBA-CAA-C2A	-3.18	107.09	112.69
2	A	412	HEM	CHD-C1D-ND	2.99	127.07	124.58
2	E	412	HEM	CMA-C3A-C4A	-2.95	124.08	128.62
2	C	412	HEM	CHD-C1D-ND	2.78	126.89	124.58
2	E	412	HEM	C3A-C4A-NA	-2.65	107.41	109.41
2	C	412	HEM	C4A-CHB-C1B	-2.65	123.99	127.47
5	A	3002	GOL	O2-C2-C3	2.62	120.17	108.22
2	A	412	HEM	CHC-C4B-NB	2.61	126.76	124.58
2	E	412	HEM	CHD-C1D-ND	2.61	126.75	124.58
2	D	412	HEM	CHC-C4B-NB	2.59	126.73	124.58
2	D	412	HEM	CBD-CAD-C3D	-2.59	108.72	114.37
2	C	412	HEM	C1B-NB-C4B	2.57	107.80	105.16
2	C	412	HEM	C4C-NC-C1C	2.57	108.21	105.53
2	D	412	HEM	CBA-CAA-C2A	-2.55	108.19	112.69
2	C	412	HEM	CHC-C4B-NB	2.42	126.59	124.58
2	B	412	HEM	C3A-C4A-NA	-2.16	107.78	109.41
2	E	412	HEM	CAD-C3D-C4D	2.13	128.36	124.53
2	C	412	HEM	C4A-C3A-C2A	2.07	108.44	107.00
2	E	412	HEM	C2A-C1A-NA	-2.06	106.87	109.73

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	402/411 (97%)	-0.30	2 (0%) 88 90	15, 26, 42, 53	0
1	B	402/411 (97%)	-0.01	13 (3%) 45 46	23, 36, 62, 75	0
1	C	401/411 (97%)	-0.13	13 (3%) 45 46	20, 35, 58, 69	0
1	D	401/411 (97%)	-0.24	4 (0%) 79 80	17, 35, 55, 64	0
1	E	401/411 (97%)	-0.32	2 (0%) 88 90	22, 32, 47, 59	0
All	All	2007/2055 (97%)	-0.20	34 (1%) 67 68	15, 33, 55, 75	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	134	PRO	4.3
1	A	403	ALA	4.2
1	E	133	GLY	3.7
1	C	399	GLY	3.5
1	C	402	SER	3.4
1	C	6	THR	3.2
1	B	197	ARG	3.1
1	C	397	THR	3.1
1	C	132	ASP	3.0
1	D	8	THR	2.9
1	B	333	ASP	2.9
1	E	41	PRO	2.9
1	C	364	LEU	2.8
1	C	400	PRO	2.7
1	B	216	MET	2.7
1	C	130	PRO	2.7
1	A	41	PRO	2.7
1	B	211	LEU	2.6
1	C	401	ARG	2.6
1	B	7	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	2	ALA	2.6
1	B	199	ARG	2.5
1	B	42	ASP	2.4
1	B	6	THR	2.4
1	B	220	ARG	2.4
1	D	9	GLU	2.4
1	B	219	ASP	2.3
1	B	8	THR	2.3
1	B	215	ASP	2.3
1	D	134	PRO	2.2
1	C	131	THR	2.2
1	C	8	THR	2.1
1	B	41	PRO	2.1
1	D	6	THR	2.1

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	GOL	A	3002	6/6	0.17	4.18	36,38,39,45	0
3	CA	E	2504	1/1	0.15	2.78	43,43,43,43	0
4	ACT	E	4005	4/4	0.13	1.41	47,48,48,48	0
4	ACT	C	4004	4/4	0.14	1.21	49,50,50,50	0
3	CA	D	2502	1/1	0.12	0.75	44,44,44,44	0
2	HEM	C	412	43/43	0.12	0.65	14,21,24,30	0
2	HEM	E	412	43/43	0.14	0.56	20,22,24,29	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	HEM	A	412	43/43	0.13	0.49	15,19,20,26	0
3	CA	A	2506	1/1	0.13	0.42	50,50,50,50	0
2	HEM	D	412	43/43	0.10	0.14	19,21,23,26	0
4	ACT	D	4001	4/4	0.09	0.10	23,23,23,24	0
4	ACT	C	4007	4/4	0.13	0.05	34,35,35,36	0
2	HEM	B	412	43/43	0.12	0.05	27,31,34,36	0
5	GOL	A	3001	6/6	0.09	-0.01	24,27,29,30	0
3	CA	C	2503	1/1	0.08	-0.60	43,43,43,43	0
4	ACT	A	4006	4/4	0.12	-0.92	22,23,23,23	0
3	CA	A	2501	1/1	0.09	-0.97	39,39,39,39	0
4	ACT	E	4008	4/4	0.12	-0.99	32,32,33,33	0
3	CA	A	2505	1/1	0.05	-2.47	37,37,37,37	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.