



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:16 AM GMT

PDB ID : 3A51  
Title : Structure of cytochrome P450 Vdh mutant (Vdh-K1) obtained by directed evolution with bound 25-hydroxyvitamin D3  
Authors : Yasutake, Y.; Fujii, Y.; Cheon, W.K.; Arisawa, A.; Tamura, T.  
Deposited on : 2009-07-24  
Resolution : 2.00 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

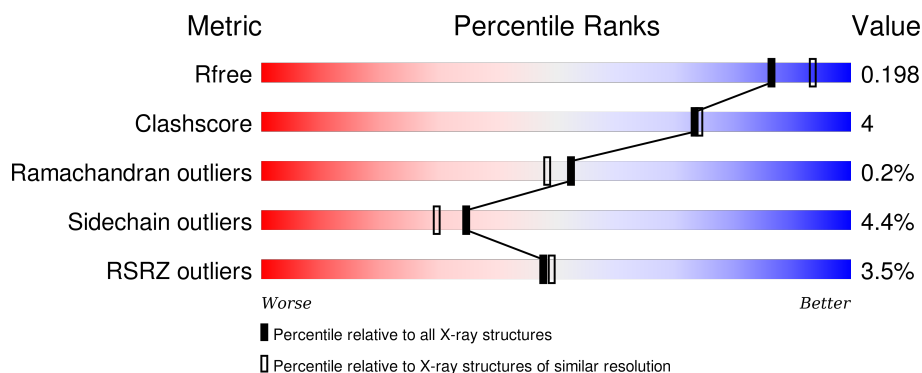
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	411	<div> <div>%</div> <div> <div></div> <div>92%</div> <div>6%</div> <div>.</div> </div> </div>
1	B	411	<div> <div>4%</div> <div> <div></div> <div>87%</div> <div>10%</div> <div>..</div> </div> </div>
1	C	411	<div> <div>8%</div> <div> <div></div> <div>85%</div> <div>11%</div> <div>..</div> </div> </div>
1	D	411	<div> <div>3%</div> <div> <div></div> <div>85%</div> <div>12%</div> <div>..</div> </div> </div>
1	E	411	<div> <div>%</div> <div> <div></div> <div>89%</div> <div>8%</div> <div>.</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	VDY	B	6178	-	-	-	X
3	VDY	D	6178	-	-	-	X
3	VDY	E	6178	-	-	-	X
5	GOL	A	3002	-	-	-	X
6	ACT	B	4009	-	-	-	X
6	ACT	C	4004	-	-	-	X
6	ACT	E	4005	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 17293 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 Vitamin D hydroxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	402	Total	C	N	O	S	0	2	0
			3126	1967	552	589	18			
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	402	Total	C	N	O	S	0	0	0
			3113	1958	549	589	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

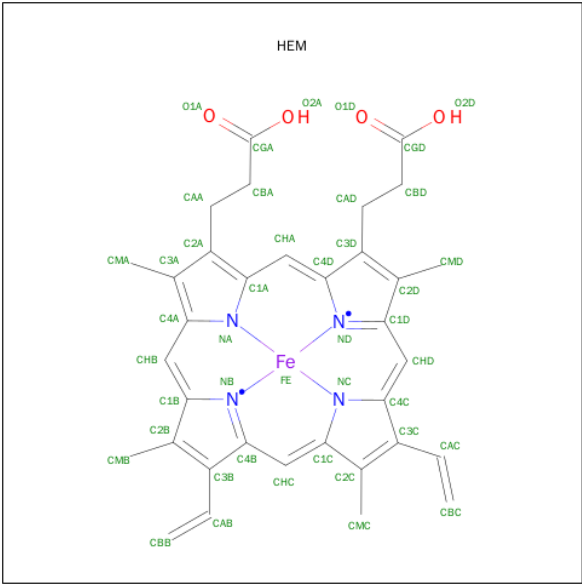
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Chain	Residue	Modelled	Actual	Comment	Reference
B	407	HIS	-	EXPRESSION TAG	UNP C4B644
B	408	HIS	-	EXPRESSION TAG	UNP C4B644
B	409	HIS	-	EXPRESSION TAG	UNP C4B644
B	410	HIS	-	EXPRESSION TAG	UNP C4B644
B	411	HIS	-	EXPRESSION TAG	UNP C4B644
C	70	ARG	THR	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

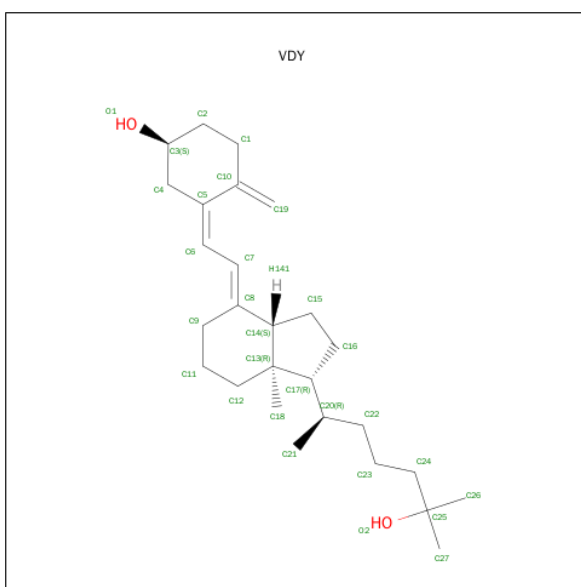
- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (for-

mula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).



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
2	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is 3-{2-[1-(5-HYDROXY-1,5-DIMETHYL-HEXYL)-7A-METHYL-OCTA HYDRO-INDEN-4-YLIDENE]-ETHYLIDENE}-4-METHYLENE-CYCLOHEXANOL (three-letter code: VDY) (formula: C<sub>27</sub>H<sub>44</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 29 27 2	0	0
3	B	1	Total C O 29 27 2	0	0
3	C	1	Total C O 29 27 2	0	0
3	D	1	Total C O 29 27 2	0	0
3	E	1	Total C O 29 27 2	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

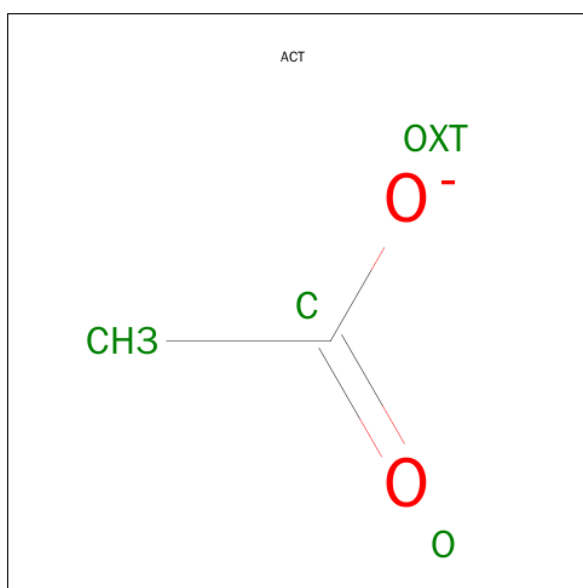
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	3	Total Ca 3 3	0	0
4	D	1	Total Ca 1 1	0	0
4	C	1	Total Ca 1 1	0	0
4	E	1	Total Ca 1 1	0	0

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		

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

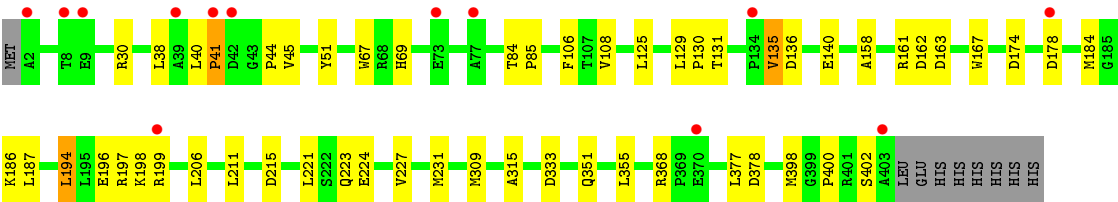
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	344	Total O 344 344	0	0
7	B	248	Total O 248 248	0	0
7	C	207	Total O 207 207	0	0
7	D	262	Total O 262 262	0	0
7	E	258	Total O 258 258	0	0

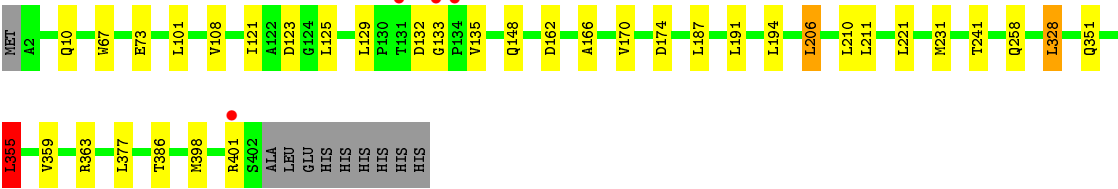
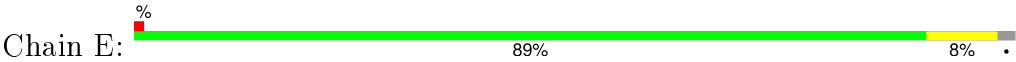


- Molecule 1: Vitamin D hydroxylase





• Molecule 1: Vitamin D hydroxylase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.17Å 171.80Å 189.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.60 – 2.00 45.59 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (45.60-2.00) 100.0 (45.59-2.00)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.37 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.197 , 0.234 0.199 , 0.198	Depositor DCC
$R_{free}$ test set	8490 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	27.3	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 46.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	2 of 169968 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	17293	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.81% 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: VDY, GOL, CA, HEM, ACT

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	0.72	0/3198	0.77	1/4349 (0.0%)
1	B	0.63	1/3179 (0.0%)	0.70	0/4325
1	C	0.62	0/3174	0.70	0/4318
1	D	0.65	0/3179	0.72	0/4325
1	E	0.64	0/3174	0.73	2/4318 (0.0%)
All	All	0.65	1/15904 (0.0%)	0.73	3/21635 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	378	ASP	CB-CG	5.04	1.62	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	132	ASP	CB-CG-OD1	5.31	123.08	118.30
1	A	30	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	E	355	LEU	CA-CB-CG	5.00	126.80	115.30

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	3126	0	3117	14	0
1	B	3113	0	3095	25	0
1	C	3108	0	3090	29	0
1	D	3113	0	3095	28	0
1	E	3108	0	3090	15	0
2	A	43	0	30	5	0
2	B	43	0	30	4	0
2	C	43	0	30	7	0
2	D	43	0	30	1	0
2	E	43	0	30	3	0
3	A	29	0	44	5	0
3	B	29	0	44	3	0
3	C	29	0	44	1	0
3	D	29	0	44	7	0
3	E	29	0	44	3	0
4	A	3	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
5	A	12	0	14	0	0
6	A	4	0	3	0	0
6	B	4	0	3	0	0
6	C	8	0	6	0	0
6	D	4	0	3	0	0
6	E	8	0	6	0	0
7	A	344	0	0	2	0
7	B	248	0	0	2	0
7	C	207	0	0	1	0
7	D	262	0	0	2	0
7	E	258	0	0	0	0
All	All	17293	0	15892	131	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 4.

All (131) 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:B:412:HEM:HBB2	2:B:412:HEM:HHC	1.42	0.98
1:C:353:ALA:CB	2:C:412:HEM:HBB2	1.94	0.97
1:C:353:ALA:HB1	2:C:412:HEM:CBB	1.95	0.96
1:D:40:LEU:HB3	1:D:41:PRO:HD2	1.50	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:LEU:HD13	1:A:231[A]:MET:HG3	1.57	0.86
1:A:107:THR:OG1	1:A:110:ARG:HG2	1.76	0.85
1:A:241:THR:HA	2:A:412:HEM:HBB1	1.58	0.84
1:C:187:LEU:HD13	1:C:231:MET:HG3	1.63	0.80
1:C:353:ALA:HB2	2:C:412:HEM:HBB2	1.60	0.80
1:C:353:ALA:HB1	2:C:412:HEM:HBB2	1.60	0.77
1:E:241:THR:HA	2:E:412:HEM:HBB1	1.66	0.76
1:D:135:VAL:HG21	1:D:398:MET:HG2	1.69	0.75
1:C:40:LEU:HB3	1:C:41:PRO:HD2	1.69	0.75
1:C:359:VAL:O	1:C:363:ARG:HG2	1.88	0.72
3:B:6178:VDY:H91	3:B:6178:VDY:H182	1.69	0.72
2:E:412:HEM:HBB2	2:E:412:HEM:HHC	1.76	0.67
1:D:184:MET:HE3	3:D:6178:VDY:H241	1.78	0.65
3:D:6178:VDY:H182	3:D:6178:VDY:H91	1.77	0.65
1:D:108:VAL:HA	1:D:351:GLN:HG2	1.80	0.63
1:D:85:PRO:HG3	1:D:224:GLU:HG3	1.79	0.63
3:B:6178:VDY:C9	3:B:6178:VDY:H182	2.29	0.62
1:E:191:LEU:HD12	1:E:231:MET:HG2	1.81	0.62
1:B:363:ARG:HD3	7:B:946:HOH:O	1.99	0.62
1:C:329:ASP:OD1	1:C:331:THR:HG22	1.99	0.61
1:D:69:HIS:HD2	7:D:486:HOH:O	1.84	0.59
1:E:359:VAL:O	1:E:363:ARG:HG2	2.01	0.59
1:D:40:LEU:HB3	1:D:41:PRO:CD	2.30	0.58
1:B:40:LEU:HD12	1:B:45:VAL:CG1	2.34	0.58
1:B:40:LEU:HD12	1:B:45:VAL:HG12	1.85	0.58
3:A:6178:VDY:H182	3:A:6178:VDY:H91	1.87	0.57
1:B:353:ALA:HB1	2:B:412:HEM:CBB	2.35	0.57
1:E:121:ILE:HD13	1:E:148:GLN:HG2	1.87	0.56
3:D:6178:VDY:C9	3:D:6178:VDY:H182	2.34	0.56
1:B:87:MET:CE	1:B:229:MET:CE	2.83	0.56
1:C:353:ALA:CB	2:C:412:HEM:CBB	2.62	0.55
1:A:187:LEU:HD13	1:A:231[A]:MET:CG	2.31	0.55
1:C:131:THR:HG23	1:C:400:PRO:HA	1.89	0.55
1:C:258:GLN:HG3	1:C:328:LEU:HD13	1.88	0.55
1:A:69:HIS:HD2	7:A:565:HOH:O	1.90	0.54
1:B:329:ASP:HB3	1:B:332:ARG:HG3	1.90	0.54
1:D:38:LEU:O	1:D:44:PRO:HA	2.07	0.54
1:D:30:ARG:NH2	7:D:475:HOH:O	2.39	0.54
1:A:241:THR:HA	2:A:412:HEM:CBB	2.32	0.53
1:C:296:THR:HG21	1:E:133:GLY:HA2	1.91	0.53
3:E:6178:VDY:H121	3:E:6178:VDY:H212	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:174:ASP:OD1	1:E:386:THR:HG23	2.10	0.52
1:E:101:LEU:HD21	1:E:221:LEU:HD22	1.91	0.52
1:A:191:LEU:HD12	1:A:231[B]:MET:HG3	1.92	0.51
1:D:196:GLU:O	1:D:199:ARG:HG3	2.12	0.49
1:D:106:PHE:CE2	2:D:412:HEM:HBC1	2.47	0.49
1:C:130:PRO:HG2	1:C:135:VAL:CG1	2.43	0.49
3:D:6178:VDY:H92	3:D:6178:VDY:C5	2.40	0.49
3:E:6178:VDY:H182	3:E:6178:VDY:H91	1.93	0.49
1:E:241:THR:CA	2:E:412:HEM:HBB1	2.38	0.49
3:E:6178:VDY:H182	3:E:6178:VDY:C9	2.43	0.49
1:B:217:ASP:HB2	1:B:220:ARG:HH21	1.77	0.49
3:A:6178:VDY:C5	3:A:6178:VDY:H92	2.41	0.48
1:B:87:MET:HE3	1:B:229:MET:CE	2.44	0.48
1:B:68:ARG:O	1:B:76:ARG:HD2	2.14	0.48
1:C:106:PHE:CE2	2:C:412:HEM:HBC1	2.48	0.48
1:D:40:LEU:CB	1:D:41:PRO:HD2	2.30	0.48
1:A:241:THR:CA	2:A:412:HEM:HBB1	2.38	0.48
1:B:353:ALA:CB	2:B:412:HEM:CBB	2.92	0.48
3:C:6178:VDY:C5	3:C:6178:VDY:H92	2.43	0.47
2:A:412:HEM:HHC	2:A:412:HEM:HBB2	1.96	0.47
1:D:199:ARG:HH22	1:D:215:ASP:CG	2.18	0.47
1:E:206:LEU:HD22	1:E:210:LEU:HG	1.96	0.46
1:B:217:ASP:HB2	1:B:220:ARG:NH2	2.30	0.46
1:E:351:GLN:HG3	1:E:355:LEU:HD22	1.96	0.46
1:C:119:THR:HG23	1:C:363:ARG:HE	1.79	0.46
1:B:259:ARG:HD2	7:B:704:HOH:O	2.15	0.46
1:D:51:TYR:HA	1:D:315:ALA:HB1	1.98	0.46
1:D:85:PRO:CG	1:D:224:GLU:HG3	2.45	0.46
1:D:45:VAL:HG11	1:D:309:MET:HG3	1.97	0.46
1:D:368:ARG:NH2	1:D:398:MET:HB3	2.31	0.46
1:D:194:LEU:HD22	1:D:198:LYS:HE2	1.98	0.46
1:C:30:ARG:NH2	7:C:497:HOH:O	2.48	0.45
1:B:327:ARG:O	1:B:332:ARG:NH1	2.49	0.45
1:C:206:LEU:HD22	1:C:210:LEU:HG	1.97	0.45
1:A:241:THR:CA	2:A:412:HEM:CBB	2.94	0.45
1:D:125:LEU:O	1:D:129:LEU:HG	2.16	0.45
1:C:261:LEU:HD22	1:C:268:LEU:CD1	2.47	0.45
1:C:322:MET:SD	1:C:332:ARG:HD3	2.57	0.45
1:E:123:ASP:OD1	1:E:363:ARG:NH2	2.47	0.45
3:A:6178:VDY:H182	3:A:6178:VDY:C9	2.46	0.45
1:B:164:PHE:HA	1:B:167:TRP:CE3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:115:GLU:N	1:C:116:PRO:CD	2.79	0.45
1:C:261:LEU:HD22	1:C:268:LEU:HD11	1.98	0.44
1:D:196:GLU:HA	1:D:199:ARG:HG3	1.99	0.44
1:D:136:ASP:O	1:D:140:GLU:CG	2.65	0.44
1:B:194:LEU:O	1:B:198:LYS:HG3	2.17	0.44
1:B:241:THR:HA	2:B:412:HEM:HBB1	2.00	0.44
3:A:6178:VDY:H61	3:A:6178:VDY:H192	1.55	0.44
1:D:227:VAL:HG12	1:D:231:MET:HE2	1.99	0.44
1:D:131:THR:HG23	1:D:400:PRO:HA	2.00	0.43
1:C:329:ASP:O	1:C:332:ARG:HB2	2.18	0.43
1:B:87:MET:CE	1:B:229:MET:HE1	2.48	0.43
1:C:130:PRO:HG2	1:C:135:VAL:HG12	2.00	0.43
3:B:6178:VDY:H92	3:B:6178:VDY:C5	2.41	0.43
1:C:143:PHE:CZ	1:C:147:VAL:HG21	2.54	0.43
1:C:139:ARG:NH2	1:C:140:GLU:OE1	2.51	0.43
1:D:167:TRP:NE1	1:D:186:LYS:HD2	2.34	0.43
1:C:129:LEU:HA	1:C:130:PRO:HD2	1.79	0.43
1:B:221:LEU:HD13	1:B:226:LEU:HB2	2.01	0.43
1:A:110:ARG:O	1:A:113:GLU:HG2	2.19	0.43
1:B:40:LEU:CD1	1:B:45:VAL:CG1	2.97	0.42
1:B:160:ASP:O	1:B:163:ASP:HB2	2.19	0.42
1:E:231:MET:HE3	1:E:231:MET:HB3	1.69	0.42
1:B:149:VAL:HG11	1:B:352:LEU:HD11	2.01	0.42
1:A:354:ARG:NH1	7:A:572:HOH:O	2.42	0.42
1:D:129:LEU:HA	1:D:130:PRO:HD3	1.92	0.42
1:B:51:TYR:HA	1:B:315:ALA:HB1	2.02	0.42
1:B:293:GLU:HA	1:B:304:ALA:HB2	2.01	0.41
1:C:248:GLY:O	1:C:251:ALA:HB3	2.20	0.41
1:C:108:VAL:HA	1:C:351:GLN:HG2	2.02	0.41
1:B:69:HIS:O	1:B:305:GLY:HA2	2.19	0.41
1:D:158:ALA:HA	1:D:161:ARG:HG3	2.02	0.41
3:D:6178:VDY:H61	3:D:6178:VDY:H192	1.74	0.41
1:A:206:LEU:HD22	1:A:210:LEU:HG	2.02	0.41
3:D:6178:VDY:H121	3:D:6178:VDY:H212	2.02	0.41
1:D:135:VAL:HG21	1:D:398:MET:CG	2.45	0.41
1:D:161:ARG:HE	1:D:161:ARG:HB3	1.70	0.41
2:C:412:HEM:HHC	2:C:412:HEM:HBB2	2.02	0.41
1:E:125:LEU:O	1:E:129:LEU:HG	2.21	0.41
3:D:6178:VDY:H231	3:D:6178:VDY:H211	1.91	0.40
1:C:281:SER:HA	1:C:282:PRO:HD3	1.95	0.40
1:A:180:LYS:HB3	3:A:6178:VDY:H261	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:GLU:HG3	1:B:328:LEU:HD12	2.04	0.40
1:E:258:GLN:HG3	1:E:328:LEU:HD13	2.02	0.40
1:E:166:ALA:O	1:E:170:VAL:HG23	2.22	0.40
1:A:51:TYR:HA	1:A:315:ALA:HB1	2.04	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	402/411 (98%)	389 (97%)	12 (3%)	1 (0%)	52	48
1	B	400/411 (97%)	384 (96%)	16 (4%)	0	100	100
1	C	399/411 (97%)	385 (96%)	14 (4%)	0	100	100
1	D	400/411 (97%)	382 (96%)	16 (4%)	2 (0%)	34	26
1	E	399/411 (97%)	387 (97%)	12 (3%)	0	100	100
All	All	2000/2055 (97%)	1927 (96%)	70 (4%)	3 (0%)	52	48

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	74	ASP
1	D	174	ASP
1	D	41	PRO

### 5.3.2 Protein sidechains [i](#)

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	336/343 (98%)	326 (97%)	10 (3%)	48	47
1	B	334/343 (97%)	320 (96%)	14 (4%)	36	31
1	C	334/343 (97%)	317 (95%)	17 (5%)	29	23
1	D	334/343 (97%)	316 (95%)	18 (5%)	27	21
1	E	334/343 (97%)	319 (96%)	15 (4%)	34	29
All	All	1672/1715 (98%)	1598 (96%)	74 (4%)	35	30

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	TRP
1	A	84	THR
1	A	109	ARG
1	A	132	ASP
1	A	172	VAL
1	A	192	SER
1	A	194	LEU
1	A	206	LEU
1	A	377	LEU
1	A	389	ARG
1	B	9	GLU
1	B	10	GLN
1	B	67	TRP
1	B	76	ARG
1	B	84	THR
1	B	101	LEU
1	B	104	ARG
1	B	146	PRO
1	B	194	LEU
1	B	208	SER
1	B	221	LEU
1	B	333	ASP
1	B	335	SER
1	B	378	ASP
1	C	6	THR
1	C	55	ARG
1	C	67	TRP
1	C	84	THR

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Mol	Chain	Res	Type
1	C	135	VAL
1	C	172	VAL
1	C	194	LEU
1	C	206	LEU
1	C	211	LEU
1	C	261	LEU
1	C	267	SER
1	C	271	SER
1	C	328	LEU
1	C	332	ARG
1	C	335	SER
1	C	377	LEU
1	C	378	ASP
1	D	67	TRP
1	D	84	THR
1	D	135	VAL
1	D	162	ASP
1	D	163	ASP
1	D	178	ASP
1	D	187	LEU
1	D	194	LEU
1	D	197	ARG
1	D	206	LEU
1	D	211	LEU
1	D	221	LEU
1	D	223	GLN
1	D	333	ASP
1	D	355	LEU
1	D	377	LEU
1	D	378	ASP
1	D	402	SER
1	E	10	GLN
1	E	67	TRP
1	E	73	GLU
1	E	108	VAL
1	E	135	VAL
1	E	162	ASP
1	E	187	LEU
1	E	194	LEU
1	E	206	LEU
1	E	211	LEU
1	E	328	LEU

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Mol	Chain	Res	Type
1	E	355	LEU
1	E	377	LEU
1	E	398	MET
1	E	401	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	HIS
1	C	69	HIS
1	C	285	GLN
1	D	69	HIS
1	D	223	GLN
1	E	10	GLN
1	E	181	ASN
1	E	223	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](#)

Of 25 ligands modelled in this entry, 6 are monoatomic - leaving 19 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	0.32	0	5,5,5	0.46	0
5	GOL	A	3002	4	5,5,5	0.42	0	5,5,5	0.56	0
6	ACT	A	4006	-	1,3,3	2.00	0	0,3,3	0.00	-
2	HEM	A	412	1,3	30,50,50	2.29	10 (33%)	24,82,82	2.64	14 (58%)
3	VDY	A	6178	2	29,31,31	0.63	0	38,46,46	2.76	7 (18%)
6	ACT	B	4009	-	1,3,3	1.45	0	0,3,3	0.00	-
2	HEM	B	412	1,3	30,50,50	2.02	8 (26%)	24,82,82	2.79	16 (66%)
3	VDY	B	6178	2	29,31,31	0.55	0	38,46,46	2.77	6 (15%)
6	ACT	C	4004	4	1,3,3	1.71	0	0,3,3	0.00	-
6	ACT	C	4007	-	1,3,3	2.07	1 (100%)	0,3,3	0.00	-
2	HEM	C	412	1,3	30,50,50	2.03	9 (30%)	24,82,82	2.37	9 (37%)
3	VDY	C	6178	2	29,31,31	0.65	0	38,46,46	2.73	6 (15%)
6	ACT	D	4001	-	1,3,3	1.62	0	0,3,3	0.00	-
2	HEM	D	412	1,3	30,50,50	2.43	9 (30%)	24,82,82	2.45	10 (41%)
3	VDY	D	6178	2	29,31,31	0.49	0	38,46,46	2.34	5 (13%)
6	ACT	E	4005	4	1,3,3	2.03	1 (100%)	0,3,3	0.00	-
6	ACT	E	4008	-	1,3,3	1.23	0	0,3,3	0.00	-
2	HEM	E	412	1,3	30,50,50	2.30	12 (40%)	24,82,82	2.52	13 (54%)
3	VDY	E	6178	2	29,31,31	0.57	0	38,46,46	2.66	6 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	A	3001	-	-	0/4/4/4	0/0/0/0
5	GOL	A	3002	4	-	0/4/4/4	0/0/0/0
6	ACT	A	4006	-	-	0/0/0/0	0/0/0/0
2	HEM	A	412	1,3	-	0/10/54/54	0/0/8/8
3	VDY	A	6178	2	-	0/16/57/57	0/3/3/3
6	ACT	B	4009	-	-	0/0/0/0	0/0/0/0
2	HEM	B	412	1,3	-	0/10/54/54	0/0/8/8
3	VDY	B	6178	2	-	0/16/57/57	0/3/3/3
6	ACT	C	4004	4	-	0/0/0/0	0/0/0/0
6	ACT	C	4007	-	-	0/0/0/0	0/0/0/0
2	HEM	C	412	1,3	-	0/10/54/54	0/0/8/8
3	VDY	C	6178	2	-	1/16/57/57	0/3/3/3
6	ACT	D	4001	-	-	0/0/0/0	0/0/0/0
2	HEM	D	412	1,3	-	0/10/54/54	0/0/8/8

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	VDY	D	6178	2	-	0/16/57/57	0/3/3/3
6	ACT	E	4005	4	-	0/0/0/0	0/0/0/0
6	ACT	E	4008	-	-	0/0/0/0	0/0/0/0
2	HEM	E	412	1,3	-	0/10/54/54	0/0/8/8
3	VDY	E	6178	2	-	0/16/57/57	0/3/3/3

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	412	HEM	C3B-C4B	-9.30	1.43	1.51
2	E	412	HEM	C3B-C4B	-7.43	1.45	1.51
2	A	412	HEM	C3B-C4B	-7.14	1.45	1.51
2	B	412	HEM	C3B-C4B	-5.90	1.46	1.51
2	C	412	HEM	C3B-C4B	-5.84	1.46	1.51
2	A	412	HEM	C3D-C4D	-5.18	1.44	1.51
2	E	412	HEM	C3D-C4D	-5.02	1.45	1.51
2	D	412	HEM	C3D-C4D	-4.49	1.45	1.51
2	B	412	HEM	C3D-C4D	-4.39	1.45	1.51
2	E	412	HEM	C2C-C1C	-4.22	1.44	1.52
2	C	412	HEM	C3D-C4D	-4.17	1.46	1.51
2	D	412	HEM	C2C-C1C	-4.10	1.44	1.52
2	C	412	HEM	C2C-C1C	-3.67	1.45	1.52
2	A	412	HEM	C2C-C1C	-3.50	1.45	1.52
2	B	412	HEM	C2C-C1C	-3.19	1.46	1.52
2	D	412	HEM	C2B-C1B	-2.40	1.44	1.51
2	C	412	HEM	C2D-C1D	-2.33	1.44	1.51
2	D	412	HEM	C2D-C1D	-2.32	1.44	1.51
2	E	412	HEM	C2B-C1B	-2.31	1.44	1.51
2	A	412	HEM	C2B-C1B	-2.29	1.44	1.51
2	A	412	HEM	C2D-C1D	-2.28	1.44	1.51
2	E	412	HEM	C2D-C1D	-2.15	1.44	1.51
6	E	4005	ACT	CH3-C	2.03	1.51	1.48
6	C	4007	ACT	CH3-C	2.07	1.51	1.48
2	C	412	HEM	FE-NB	2.09	2.08	1.97
2	E	412	HEM	C3C-CAC	2.11	1.55	1.51
2	C	412	HEM	C3B-CAB	2.13	1.55	1.51
2	E	412	HEM	CAA-C2A	2.15	1.55	1.52
2	D	412	HEM	FE-NB	2.15	2.08	1.97
2	A	412	HEM	C3C-CAC	2.19	1.55	1.51
2	B	412	HEM	CAA-C2A	2.20	1.55	1.52
2	E	412	HEM	C3B-CAB	2.21	1.55	1.51
2	C	412	HEM	C1C-NC	2.22	1.38	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	412	HEM	C1C-NC	2.23	1.38	1.36
2	E	412	HEM	C4C-NC	2.23	1.38	1.36
2	D	412	HEM	C3B-CAB	2.24	1.55	1.51
2	A	412	HEM	FE-NB	2.31	2.09	1.97
2	A	412	HEM	C3B-CAB	2.31	1.55	1.51
2	C	412	HEM	FE-ND	2.31	2.09	1.97
2	B	412	HEM	C3C-CAC	2.32	1.55	1.51
2	B	412	HEM	FE-NB	2.33	2.09	1.97
2	E	412	HEM	FE-NB	2.44	2.10	1.97
2	B	412	HEM	FE-ND	2.55	2.11	1.97
2	E	412	HEM	C1C-NC	2.61	1.39	1.36
2	A	412	HEM	FE-ND	2.77	2.12	1.97
2	E	412	HEM	FE-ND	2.81	2.12	1.97
2	A	412	HEM	FE-NC	3.34	2.09	1.95
2	B	412	HEM	FE-NC	3.43	2.09	1.95
2	D	412	HEM	FE-NC	3.52	2.09	1.95
2	C	412	HEM	C4C-NC	3.66	1.40	1.36

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	6178	VDY	C6-C7-C8	-12.23	107.21	125.87
3	A	6178	VDY	C6-C7-C8	-11.66	108.09	125.87
3	C	6178	VDY	C6-C7-C8	-11.04	109.02	125.87
3	E	6178	VDY	C6-C7-C8	-10.83	109.35	125.87
3	D	6178	VDY	C6-C7-C8	-10.11	110.45	125.87
3	D	6178	VDY	C9-C8-C7	-5.34	118.09	125.36
2	B	412	HEM	C3B-CAB-CBB	-4.77	117.15	124.46
3	B	6178	VDY	C9-C8-C7	-4.61	119.08	125.36
3	A	6178	VDY	C15-C14-C8	-4.52	114.21	120.68
3	E	6178	VDY	C9-C8-C7	-4.48	119.26	125.36
2	A	412	HEM	C3B-CAB-CBB	-4.23	117.96	124.46
3	C	6178	VDY	C15-C14-C8	-4.06	114.86	120.68
2	B	412	HEM	CMA-C3A-C4A	-4.04	121.67	128.36
2	E	412	HEM	C3C-CAC-CBC	-4.02	118.30	124.46
2	D	412	HEM	C3C-CAC-CBC	-3.90	118.48	124.46
3	A	6178	VDY	C9-C8-C7	-3.89	120.06	125.36
2	E	412	HEM	C3B-CAB-CBB	-3.86	118.54	124.46
3	B	6178	VDY	C15-C14-C8	-3.45	115.73	120.68
3	C	6178	VDY	C9-C8-C7	-3.45	120.67	125.36
2	C	412	HEM	CBD-CAD-C3D	-3.37	103.76	113.55
2	A	412	HEM	CAA-C2A-C1A	-3.29	123.44	127.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	412	HEM	C3B-C4B-NB	-2.99	105.92	111.63
2	A	412	HEM	CBA-CAA-C2A	-2.95	107.25	112.53
2	B	412	HEM	CAA-C2A-C1A	-2.90	123.86	127.01
3	E	6178	VDY	C15-C14-C8	-2.88	116.56	120.68
2	D	412	HEM	CMA-C3A-C4A	-2.87	123.62	128.36
2	A	412	HEM	CBD-CAD-C3D	-2.83	105.31	113.55
2	E	412	HEM	C3B-C4B-NB	-2.70	106.46	111.63
2	B	412	HEM	C3B-C4B-NB	-2.66	106.54	111.63
3	D	6178	VDY	C13-C14-C8	-2.64	108.10	112.85
2	E	412	HEM	CMA-C3A-C4A	-2.43	124.35	128.36
2	E	412	HEM	CBD-CAD-C3D	-2.36	106.68	113.55
2	B	412	HEM	C3C-CAC-CBC	-2.35	120.85	124.46
2	C	412	HEM	C3B-C4B-NB	-2.35	107.14	111.63
2	D	412	HEM	CBD-CAD-C3D	-2.29	106.88	113.55
2	B	412	HEM	CBD-CAD-C3D	-2.26	106.98	113.55
2	A	412	HEM	CMA-C3A-C4A	-2.15	124.80	128.36
2	E	412	HEM	CAA-C2A-C1A	-2.05	124.79	127.01
2	A	412	HEM	C2C-C1C-CHC	2.11	126.89	123.68
2	B	412	HEM	C4B-CHC-C1C	2.12	129.37	125.82
3	C	6178	VDY	C9-C8-C14	2.14	118.46	113.39
3	E	6178	VDY	C2-C3-C4	2.20	114.23	110.32
2	C	412	HEM	C2D-C3D-C4D	2.21	105.25	101.50
2	B	412	HEM	C2D-C3D-C4D	2.24	105.30	101.50
3	B	6178	VDY	C18-C13-C14	2.28	114.00	110.07
2	D	412	HEM	C2C-C1C-CHC	2.40	127.33	123.68
2	B	412	HEM	C2C-C1C-CHC	2.41	127.35	123.68
2	B	412	HEM	CMA-C3A-C2A	2.50	130.46	125.24
2	A	412	HEM	CMB-C2B-C3B	2.54	122.88	116.53
2	A	412	HEM	C2D-C3D-C4D	2.63	105.97	101.50
2	D	412	HEM	CMD-C2D-C3D	2.66	126.12	114.35
2	E	412	HEM	CMB-C2B-C3B	2.74	123.36	116.53
3	A	6178	VDY	C2-C3-C4	2.78	115.26	110.32
2	D	412	HEM	C2D-C3D-C4D	2.82	106.27	101.50
2	E	412	HEM	C2D-C3D-C4D	2.88	106.38	101.50
2	A	412	HEM	CMD-C2D-C3D	2.96	127.43	114.35
2	C	412	HEM	CMD-C2D-C3D	2.96	127.44	114.35
2	B	412	HEM	C3B-C4B-CHC	3.01	127.40	123.16
2	E	412	HEM	CMC-C2C-C3C	3.02	124.06	116.53
2	B	412	HEM	CMD-C2D-C3D	3.03	127.74	114.35
2	C	412	HEM	C3B-C4B-CHC	3.04	127.45	123.16
3	A	6178	VDY	C18-C13-C14	3.10	115.40	110.07
2	E	412	HEM	CMD-C2D-C3D	3.34	129.13	114.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	412	HEM	C3B-C4B-CHC	3.41	127.97	123.16
2	E	412	HEM	C3B-C4B-CHC	3.50	128.09	123.16
2	B	412	HEM	CMB-C2B-C3B	3.65	125.65	116.53
2	D	412	HEM	CMC-C2C-C3C	3.74	125.86	116.53
3	D	6178	VDY	C4-C5-C6	3.85	126.00	120.64
2	B	412	HEM	CMC-C2C-C3C	4.12	126.82	116.53
2	A	412	HEM	CAD-C3D-C2D	4.17	125.22	113.22
2	E	412	HEM	CAD-C3D-C4D	4.19	127.24	112.47
2	C	412	HEM	CMB-C2B-C3B	4.21	127.04	116.53
2	D	412	HEM	CAD-C3D-C2D	4.21	125.33	113.22
2	B	412	HEM	CAD-C3D-C4D	4.24	127.42	112.47
2	C	412	HEM	CMC-C2C-C3C	4.41	127.53	116.53
3	A	6178	VDY	C4-C5-C6	4.43	126.81	120.64
2	A	412	HEM	CMC-C2C-C3C	4.50	127.77	116.53
2	D	412	HEM	CAD-C3D-C4D	4.51	128.36	112.47
2	C	412	HEM	CAD-C3D-C2D	4.53	126.24	113.22
2	C	412	HEM	CAD-C3D-C4D	4.55	128.50	112.47
2	E	412	HEM	CAD-C3D-C2D	4.58	126.38	113.22
2	A	412	HEM	CAD-C3D-C4D	4.63	128.80	112.47
2	D	412	HEM	CMB-C2B-C3B	4.67	128.18	116.53
3	B	6178	VDY	C4-C5-C6	4.78	127.29	120.64
2	B	412	HEM	CAD-C3D-C2D	4.89	127.26	113.22
3	C	6178	VDY	C4-C5-C6	4.95	127.52	120.64
3	E	6178	VDY	C4-C5-C6	5.48	128.25	120.64
3	D	6178	VDY	C7-C6-C5	5.82	137.46	126.81
3	B	6178	VDY	C7-C6-C5	7.72	140.94	126.81
3	E	6178	VDY	C7-C6-C5	7.89	141.27	126.81
3	A	6178	VDY	C7-C6-C5	7.91	141.29	126.81
3	C	6178	VDY	C7-C6-C5	8.52	142.41	126.81

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	6178	VDY	C8-C7-C6-C5

There are no ring outliers.

10 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	412	HEM	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	6178	VDY	5	0
2	B	412	HEM	4	0
3	B	6178	VDY	3	0
2	C	412	HEM	7	0
3	C	6178	VDY	1	0
2	D	412	HEM	1	0
3	D	6178	VDY	7	0
2	E	412	HEM	3	0
3	E	6178	VDY	3	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	402/411 (97%)	-0.10	4 (0%) 84 84	12, 21, 36, 50	0
1	B	402/411 (97%)	0.15	16 (3%) 42 44	17, 30, 51, 62	0
1	C	401/411 (97%)	0.37	33 (8%) 14 15	15, 31, 56, 72	0
1	D	402/411 (97%)	-0.00	13 (3%) 51 52	15, 30, 51, 61	0
1	E	401/411 (97%)	-0.09	4 (0%) 84 84	19, 28, 44, 56	0
All	All	2008/2055 (97%)	0.07	70 (3%) 48 49	12, 28, 50, 72	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	403	ALA	6.0
1	D	8	THR	4.5
1	C	6	THR	4.1
1	B	6	THR	4.1
1	D	42	ASP	4.0
1	D	403	ALA	4.0
1	C	402	SER	3.9
1	C	7	GLY	3.9
1	C	2	ALA	3.8
1	C	397	THR	3.8
1	B	216	MET	3.8
1	C	400	PRO	3.8
1	D	2	ALA	3.8
1	C	132	ASP	3.7
1	E	133	GLY	3.6
1	C	399	GLY	3.4
1	C	370	GLU	3.3
1	C	8	THR	3.2
1	E	134	PRO	3.2
1	C	364	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	199	ARG	3.1
1	B	8	THR	3.1
1	B	159	GLU	3.1
1	C	262	LEU	3.0
1	D	77	ALA	3.0
1	C	134	PRO	3.0
1	B	7	GLY	3.0
1	A	41	PRO	2.9
1	C	266	PRO	2.8
1	D	134	PRO	2.8
1	D	73	GLU	2.7
1	C	253	LEU	2.7
1	C	254	THR	2.7
1	C	256	PRO	2.7
1	D	178	ASP	2.7
1	D	370	GLU	2.6
1	B	204	ASP	2.6
1	C	32	GLU	2.6
1	D	41	PRO	2.5
1	B	9	GLU	2.5
1	C	268	LEU	2.5
1	B	200	THR	2.5
1	C	9	GLU	2.5
1	C	129	LEU	2.5
1	B	403	ALA	2.5
1	B	333	ASP	2.5
1	D	39	ALA	2.5
1	D	199	ARG	2.5
1	C	401	ARG	2.4
1	C	263	ALA	2.4
1	B	197	ARG	2.3
1	C	126	LEU	2.3
1	C	369	PRO	2.3
1	B	2	ALA	2.3
1	C	139	ARG	2.3
1	C	159	GLU	2.3
1	E	131	THR	2.3
1	C	261	LEU	2.3
1	C	396	VAL	2.2
1	C	131	THR	2.2
1	C	365	PHE	2.2
1	A	2	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	109	ARG	2.1
1	E	401	ARG	2.1
1	C	264	GLU	2.1
1	C	130	PRO	2.1
1	B	101	LEU	2.1
1	B	211	LEU	2.1
1	D	9	GLU	2.0
1	B	41	PRO	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(Å <sup>2</sup> )	Q<0.9
5	GOL	A	3002	6/6	0.93	0.16	5.89	30,31,34,37	0
3	VDY	D	6178	29/29	0.85	0.23	5.64	43,46,57,57	0
3	VDY	E	6178	29/29	0.87	0.20	4.59	37,39,53,54	0
3	VDY	B	6178	29/29	0.86	0.21	3.07	39,46,58,59	0
6	ACT	E	4005	4/4	0.78	0.18	3.03	41,41,41,42	0
6	ACT	B	4009	4/4	0.68	0.19	3.02	42,42,42,42	0
6	ACT	C	4004	4/4	0.85	0.14	2.21	40,40,41,41	0
3	VDY	C	6178	29/29	0.89	0.17	1.41	28,33,43,45	0
2	HEM	C	412	43/43	0.98	0.17	1.21	14,18,21,29	0
2	HEM	D	412	43/43	0.99	0.11	1.03	12,16,19,26	0
2	HEM	E	412	43/43	0.98	0.14	0.99	16,19,21,31	0
3	VDY	A	6178	29/29	0.90	0.14	0.86	27,31,42,44	0
6	ACT	A	4006	4/4	0.94	0.15	0.52	24,27,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	HEM	A	412	43/43	0.99	0.16	0.26	9,13,18,27	0
2	HEM	B	412	43/43	0.97	0.12	0.11	18,25,27,32	0
6	ACT	C	4007	4/4	0.89	0.15	-0.08	36,37,37,37	0
5	GOL	A	3001	6/6	0.97	0.11	-0.25	23,23,25,25	0
4	CA	E	2504	1/1	0.96	0.09	-0.34	35,35,35,35	0
4	CA	C	2503	1/1	0.97	0.05	-1.95	32,32,32,32	0
4	CA	D	2502	1/1	0.98	0.05	-2.56	35,35,35,35	0
4	CA	A	2501	1/1	0.98	0.04	-3.28	29,29,29,29	0
4	CA	A	2506	1/1	0.93	0.06	-	45,45,45,45	0
4	CA	A	2505	1/1	0.98	0.05	-	30,30,30,30	0
6	ACT	D	4001	4/4	0.96	0.13	-	21,22,22,22	0
6	ACT	E	4008	4/4	0.91	0.14	-	40,40,40,40	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.