



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2018 – 03:41 pm 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 X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

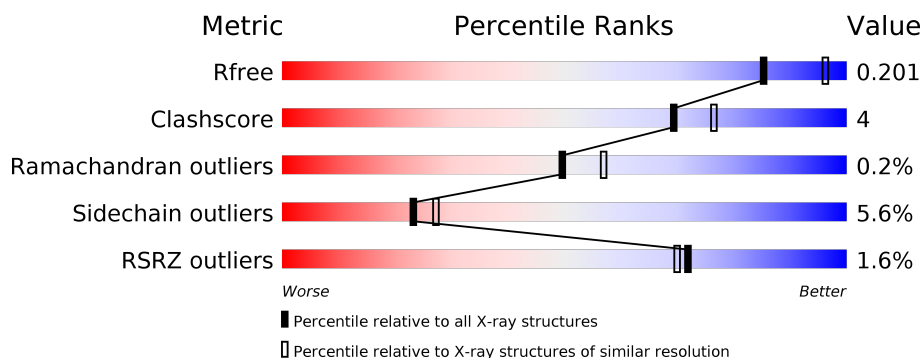
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	111664	4343 (2.20-2.20)
Clashscore	122126	5027 (2.20-2.20)
Ramachandran outliers	120053	4952 (2.20-2.20)
Sidechain outliers	120020	4953 (2.20-2.20)
RSRZ outliers	108989	4245 (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 ≥ 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>91%</div> <div>6% ..</div> </div>
1	B	411	<div> <div>2%</div> <div>86%</div> <div>9% ..</div> </div>
1	C	411	<div> <div>4%</div> <div>83%</div> <div>13% ..</div> </div>
1	D	411	<div> <div>%</div> <div>83%</div> <div>12% ..</div> </div>
1	E	411	<div> <div>%</div> <div>87%</div> <div>9% ..</div> </div>

2 Entry composition

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

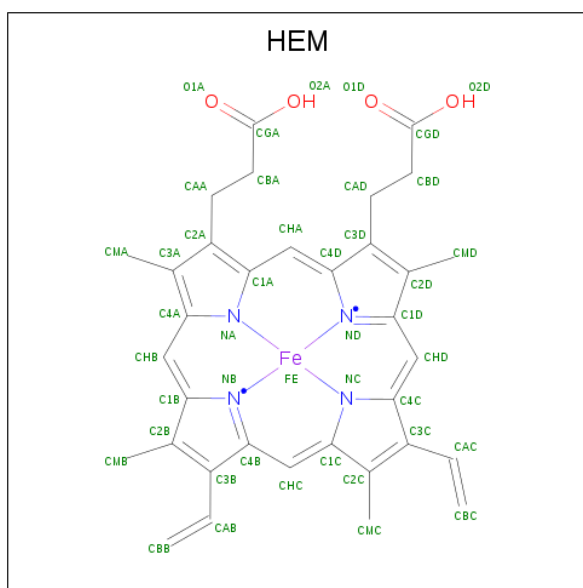
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Chain	Residue	Modelled	Actual	Comment	Reference
B	407	HIS	-	EXPRESSION TAG	UNP C4B644
B	408	HIS	-	EXPRESSION TAG	UNP C4B644
B	409	HIS	-	EXPRESSION TAG	UNP C4B644
B	410	HIS	-	EXPRESSION TAG	UNP C4B644
B	411	HIS	-	EXPRESSION TAG	UNP C4B644
C	70	ARG	THR	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: C₃H₈O₃).



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		

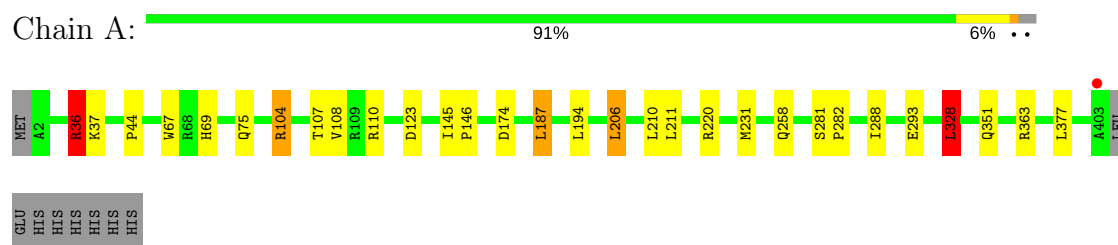
- Molecule 6 is water.

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		

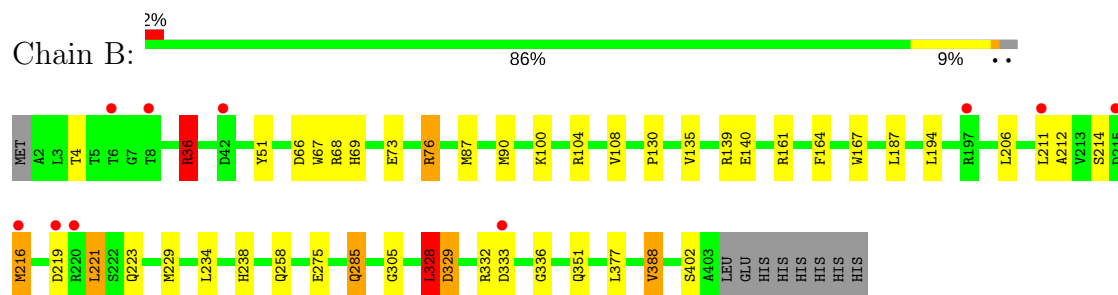
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

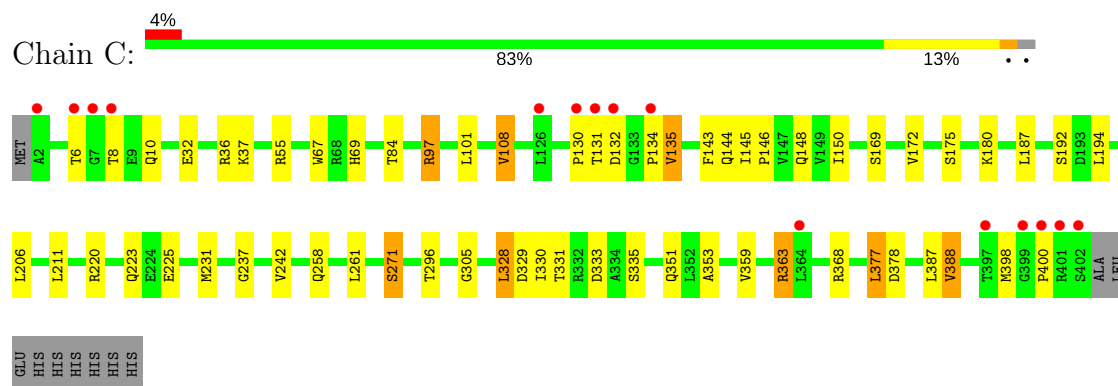
• Molecule 1: Vitamin D hydroxylase



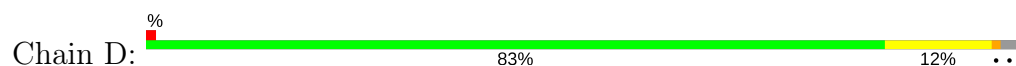
• Molecule 1: Vitamin D hydroxylase

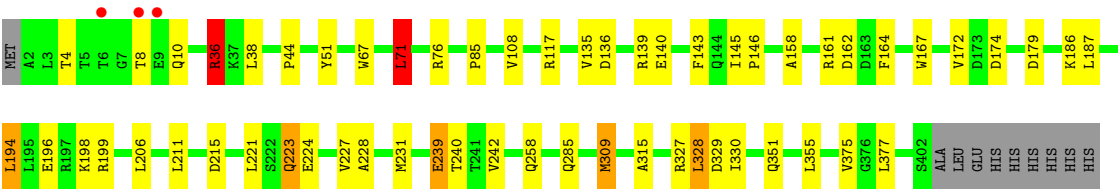


• Molecule 1: Vitamin D hydroxylase

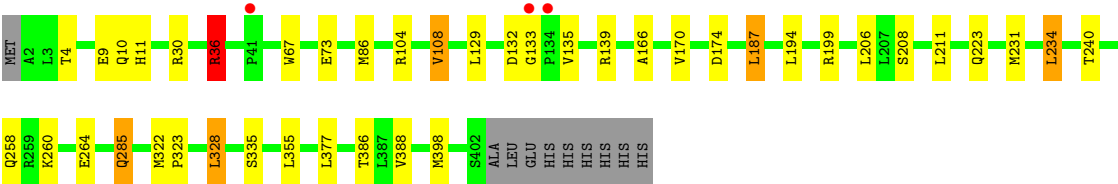
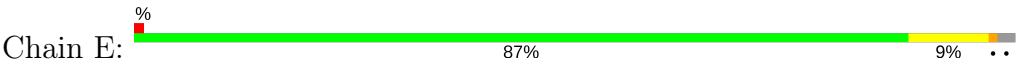


• Molecule 1: Vitamin D hydroxylase





● 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.84 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.201 , 0.244 0.202 , 0.201	Depositor DCC
R_{free} test set	6458 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	32.4	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 39.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16621	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

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 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	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

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 (126) 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: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:150:ILE:HG12	1:C:237:GLY:HA3	1.60	0.84
1:C:329:ASP:OD1	1:C:331:THR:HG22	1.77	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:108:VAL:HB	1:C:351:GLN:HG3	1.66	0.77
1:C:363:ARG:HH21	1:C:363:ARG:CG	1.96	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:196:GLU:O	1:D:199:ARG:HG3	1.99	0.63
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:135:VAL:HG21	1:E:398:MET:CE	2.34	0.57
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:C:388:VAL:HG22	6:C:644:HOH:O	2.09	0.51
1:D:161:ARG:HA	1:D:164:PHE:CZ	2.45	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:B:139:ARG:NH1	6:B:473:HOH:O	2.46	0.47
1:D:258:GLN:OE1	1:D:330:ILE:HG12	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:260:LYS:HE2	1:E:264:GLU:OE2	2.18	0.44
1:E:388:VAL:HG22	6:E:468:HOH:O	2.17	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:A:211:LEU:HD23	1:A:211:LEU:O	2.18	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:C:172:VAL:HG22	1:C:387:LEU:HD23	2.00	0.43
1:A:104:ARG:HA	1:A:104:ARG:HE	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: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:285:GLN:NE2	6:E:428:HOH:O	2.51	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:B:69:HIS:O	1:B:305:GLY:HA2	2.20	0.42
1:D:199:ARG:NH2	1:D:215:ASP:OD2	2.50	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: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:B:87:MET:HE3	1:B:229:MET:SD	2.60	0.42
1:D:136:ASP:O	1:D:140:GLU:CG	2.62	0.42
1:B:130:PRO:HD2	1:B:135:VAL:HG11	2.02	0.41
1:C:108:VAL:HA	1:C:351:GLN:HG3	2.02	0.41
1:D:117:ARG:HA	1:D:117:ARG:HD2	1.92	0.41
1:E:9:GLU:HB3	1:E:11:HIS:NE2	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 [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	400/411 (97%)	385 (96%)	14 (4%)	1 (0%)	43	48
1	B	400/411 (97%)	385 (96%)	15 (4%)	0	100	100
1	C	399/411 (97%)	383 (96%)	15 (4%)	1 (0%)	43	48
1	D	399/411 (97%)	381 (96%)	17 (4%)	1 (0%)	43	48
1	E	399/411 (97%)	383 (96%)	16 (4%)	0	100	100
All	All	1997/2055 (97%)	1917 (96%)	77 (4%)	3 (0%)	49	57

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 [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	334/343 (97%)	322 (96%)	12 (4%)	38	48
1	B	334/343 (97%)	315 (94%)	19 (6%)	23	26
1	C	334/343 (97%)	307 (92%)	27 (8%)	13	13
1	D	334/343 (97%)	315 (94%)	19 (6%)	23	26
1	E	334/343 (97%)	317 (95%)	17 (5%)	26	31
All	All	1670/1715 (97%)	1576 (94%)	94 (6%)	23	27

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 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 ⓘ

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	0.56	0	5,5,5	0.26	0
5	GOL	A	3002	3	5,5,5	0.33	0	5,5,5	1.69	1 (20%)
4	ACT	A	4006	-	1,3,3	2.63	1 (100%)	0,3,3	0.00	-
2	HEM	A	412	1	27,50,50	2.21	11 (40%)	17,82,82	1.68	4 (23%)
2	HEM	B	412	1	27,50,50	2.07	7 (25%)	17,82,82	1.87	6 (35%)
4	ACT	C	4004	3	1,3,3	1.74	0	0,3,3	0.00	-
4	ACT	C	4007	-	1,3,3	2.58	1 (100%)	0,3,3	0.00	-
2	HEM	C	412	1	27,50,50	2.14	8 (29%)	17,82,82	1.82	4 (23%)
4	ACT	D	4001	-	1,3,3	2.89	1 (100%)	0,3,3	0.00	-
2	HEM	D	412	1	27,50,50	2.18	9 (33%)	17,82,82	1.61	4 (23%)
4	ACT	E	4005	3	1,3,3	2.06	1 (100%)	0,3,3	0.00	-
4	ACT	E	4008	-	1,3,3	1.42	0	0,3,3	0.00	-
2	HEM	E	412	1	27,50,50	2.24	9 (33%)	17,82,82	1.93	5 (29%)

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	-	0/6/54/54	0/0/8/8
2	HEM	B	412	1	-	0/6/54/54	0/0/8/8
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	-	0/6/54/54	0/0/8/8
4	ACT	D	4001	-	-	0/0/0/0	0/0/0/0
2	HEM	D	412	1	-	0/6/54/54	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	-	0/6/54/54	0/0/8/8

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	412	HEM	C3C-C2C	-5.47	1.32	1.40
2	A	412	HEM	C3C-C2C	-4.88	1.33	1.40
2	D	412	HEM	C3C-C2C	-4.86	1.33	1.40
2	C	412	HEM	C3B-C2B	-4.12	1.34	1.40
2	C	412	HEM	C3C-C2C	-3.90	1.35	1.40
2	D	412	HEM	C3B-C2B	-3.73	1.35	1.40
2	E	412	HEM	C3B-C2B	-3.53	1.35	1.40
2	B	412	HEM	C3B-C2B	-3.47	1.35	1.40
2	B	412	HEM	C3C-C2C	-3.34	1.35	1.40
2	A	412	HEM	C3B-C2B	-2.71	1.36	1.40
2	E	412	HEM	CAA-C2A	2.01	1.55	1.52
2	B	412	HEM	CAA-C2A	2.03	1.55	1.52
4	E	4005	ACT	CH3-C	2.06	1.51	1.48
2	D	412	HEM	CMA-C3A	2.06	1.55	1.51
2	C	412	HEM	CMA-C3A	2.09	1.55	1.51
2	A	412	HEM	C1D-ND	2.12	1.40	1.36
2	C	412	HEM	C4B-NB	2.17	1.40	1.36
2	D	412	HEM	C1D-ND	2.19	1.40	1.36
2	B	412	HEM	CMC-C2C	2.22	1.56	1.51
2	A	412	HEM	CAA-C2A	2.23	1.55	1.52
2	E	412	HEM	CMA-C3A	2.23	1.56	1.51
2	A	412	HEM	CMD-C2D	2.24	1.56	1.51
2	D	412	HEM	CAA-C2A	2.33	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	412	HEM	CMA-C3A	2.34	1.56	1.51
2	A	412	HEM	C4A-NA	2.35	1.41	1.36
2	E	412	HEM	CMC-C2C	2.35	1.57	1.51
2	A	412	HEM	CMC-C2C	2.42	1.57	1.51
4	C	4007	ACT	CH3-C	2.58	1.52	1.48
4	A	4006	ACT	CH3-C	2.63	1.52	1.48
2	E	412	HEM	CMD-C2D	2.69	1.57	1.51
2	C	412	HEM	CAA-C2A	2.71	1.56	1.52
2	D	412	HEM	CMD-C2D	2.72	1.57	1.51
4	D	4001	ACT	CH3-C	2.89	1.52	1.48
2	D	412	HEM	C3B-CAB	3.31	1.54	1.47
2	D	412	HEM	C3C-CAC	3.36	1.54	1.47
2	C	412	HEM	C3B-CAB	3.52	1.54	1.47
2	A	412	HEM	C3B-CAB	3.60	1.55	1.47
2	E	412	HEM	C3C-CAC	3.70	1.55	1.47
2	A	412	HEM	C3C-CAC	3.77	1.55	1.47
2	C	412	HEM	C3C-CAC	3.81	1.55	1.47
2	B	412	HEM	C3C-CAC	3.82	1.55	1.47
2	B	412	HEM	C3B-CAB	4.03	1.55	1.47
2	E	412	HEM	C3B-CAB	4.08	1.56	1.47
2	C	412	HEM	C3D-C2D	4.93	1.52	1.37
2	E	412	HEM	C3D-C2D	5.08	1.52	1.37
2	A	412	HEM	C3D-C2D	5.34	1.53	1.37
2	D	412	HEM	C3D-C2D	5.43	1.53	1.37
2	B	412	HEM	C3D-C2D	5.45	1.53	1.37

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	412	HEM	CBD-CAD-C3D	-4.36	104.15	112.47
2	C	412	HEM	CMA-C3A-C4A	-3.56	123.00	128.46
2	B	412	HEM	CBD-CAD-C3D	-3.39	106.01	112.47
2	E	412	HEM	C1D-C2D-C3D	-3.10	104.84	107.00
2	B	412	HEM	C1D-C2D-C3D	-2.91	104.97	107.00
2	E	412	HEM	CBD-CAD-C3D	-2.90	106.94	112.47
2	E	412	HEM	CMA-C3A-C4A	-2.85	124.08	128.46
2	A	412	HEM	CBD-CAD-C3D	-2.83	107.06	112.47
2	A	412	HEM	CBA-CAA-C2A	-2.82	107.09	112.48
2	A	412	HEM	C3C-C4C-NC	-2.55	106.13	110.94
2	E	412	HEM	CAA-CBA-CGA	-2.51	108.37	112.66
2	D	412	HEM	C3C-C4C-NC	-2.46	106.30	110.94
2	D	412	HEM	C1D-C2D-C3D	-2.25	105.43	107.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	412	HEM	CBA-CAA-C2A	-2.24	108.19	112.48
2	B	412	HEM	CAD-CBD-CGD	-2.15	108.98	112.66
2	C	412	HEM	C4A-C3A-C2A	2.07	108.44	107.00
2	C	412	HEM	C4C-C3C-C2C	2.12	108.38	106.90
2	B	412	HEM	CMC-C2C-C3C	2.19	128.87	124.88
2	B	412	HEM	CMB-C2B-C3B	2.27	129.01	124.88
5	A	3002	GOL	O2-C2-C3	2.45	120.17	109.00
2	A	412	HEM	C4C-C3C-C2C	2.83	108.87	106.90
2	B	412	HEM	C4C-C3C-C2C	3.16	109.10	106.90
2	E	412	HEM	C4C-C3C-C2C	3.28	109.19	106.90
2	D	412	HEM	C4C-C3C-C2C	3.45	109.31	106.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	412	HEM	8	0
2	D	412	HEM	1	0
2	E	412	HEM	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, 95th 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 ²)	Q<0.9
1	A	402/411 (97%)	-0.19	1 (0%) 94 94	15, 26, 42, 53	0
1	B	402/411 (97%)	-0.06	10 (2%) 57 55	23, 36, 62, 75	0
1	C	401/411 (97%)	-0.17	15 (3%) 41 39	20, 35, 58, 69	0
1	D	401/411 (97%)	-0.28	3 (0%) 87 86	17, 35, 55, 64	0
1	E	401/411 (97%)	-0.36	3 (0%) 87 86	22, 32, 47, 59	0
All	All	2007/2055 (97%)	-0.21	32 (1%) 72 70	15, 33, 55, 75	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	399	GLY	4.7
1	D	8	THR	4.5
1	C	134	PRO	4.2
1	C	6	THR	3.9
1	A	403	ALA	3.6
1	C	130	PRO	3.5
1	E	133	GLY	3.5
1	C	400	PRO	3.4
1	B	197	ARG	3.2
1	B	6	THR	3.2
1	C	8	THR	3.2
1	B	333	ASP	3.1
1	C	132	ASP	3.0
1	B	219	ASP	2.9
1	C	402	SER	2.9
1	D	9	GLU	2.9
1	C	7	GLY	2.9
1	C	401	ARG	2.9
1	D	6	THR	2.6
1	C	364	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	2	ALA	2.5
1	C	397	THR	2.5
1	B	216	MET	2.4
1	B	8	THR	2.2
1	B	215	ASP	2.2
1	B	211	LEU	2.2
1	B	220	ARG	2.2
1	E	134	PRO	2.2
1	C	126	LEU	2.1
1	B	42	ASP	2.1
1	E	41	PRO	2.0
1	C	131	THR	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. The B-factors column lists the minimum, median, 95th 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	B-factors(Å ²)	Q<0.9
4	ACT	E	4005	4/4	0.82	0.14	47,48,48,48	0
4	ACT	C	4004	4/4	0.85	0.14	49,50,50,50	0
3	CA	A	2506	1/1	0.87	0.12	50,50,50,50	0
4	ACT	C	4007	4/4	0.91	0.12	34,35,35,36	0
3	CA	D	2502	1/1	0.94	0.12	44,44,44,44	0
5	GOL	A	3002	6/6	0.94	0.16	36,38,39,45	0
5	GOL	A	3001	6/6	0.95	0.11	24,27,29,30	0
2	HEM	B	412	43/43	0.96	0.12	27,31,34,36	0
3	CA	C	2503	1/1	0.96	0.10	43,43,43,43	0
3	CA	A	2505	1/1	0.97	0.06	37,37,37,37	0
2	HEM	C	412	43/43	0.97	0.12	14,21,24,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	ACT	A	4006	4/4	0.98	0.11	22,23,23,23	0
3	CA	E	2504	1/1	0.98	0.12	43,43,43,43	0
2	HEM	D	412	43/43	0.98	0.11	19,21,23,26	0
4	ACT	D	4001	4/4	0.98	0.11	23,23,23,24	0
2	HEM	A	412	43/43	0.98	0.13	15,19,20,26	0
4	ACT	E	4008	4/4	0.98	0.12	32,32,33,33	0
2	HEM	E	412	43/43	0.99	0.13	20,22,24,29	0
3	CA	A	2501	1/1	0.99	0.12	39,39,39,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.