



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:25 PM GMT

PDB ID : 3ZBY  
Title : Ligand-free structure of CYP142 from Mycobacterium smegmatis  
Authors : Garcia-Fernandez, E.; Frank, D.J.; Galan, B.; Kells, P.M.; Podust, L.M.; Garcia, J.L.; Ortiz de Montellano, P.R.  
Deposited on : 2012-11-13  
Resolution : 1.93 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

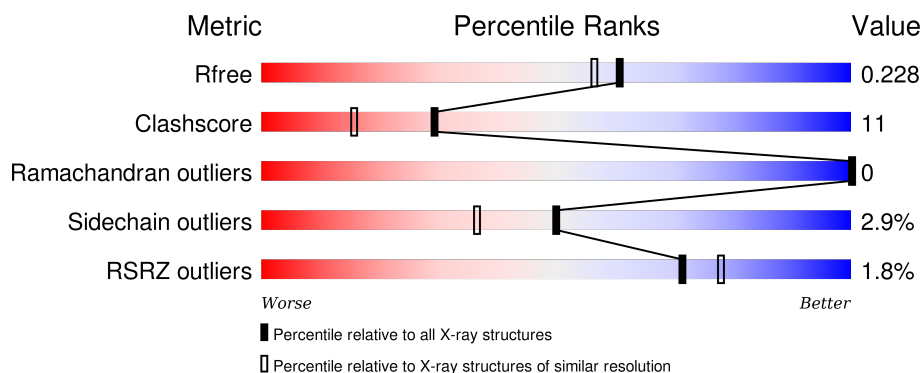
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.93 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	2910 (1.96-1.92)
Clashscore	102246	3095 (1.96-1.92)
Ramachandran outliers	100387	3062 (1.96-1.92)
Sidechain outliers	100360	3062 (1.96-1.92)
RSRZ outliers	91569	2915 (1.96-1.92)

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	407	<div> <div>2%</div> <div>84%</div> <div>13%</div> <div>..</div> </div>
1	B	407	<div> <div>%</div> <div>82%</div> <div>14%</div> <div>..</div> </div>
1	C	407	<div> <div>2%</div> <div>83%</div> <div>14%</div> <div>..</div> </div>
1	D	407	<div> <div>%</div> <div>82%</div> <div>14%</div> <div>..</div> </div>
1	E	407	<div> <div>2%</div> <div>83%</div> <div>13%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	407	

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	BCD	A	1403	X	-	-	X
3	BCD	B	1403	X	-	X	-
3	BCD	C	1403	X	-	X	-
3	BCD	D	1403	X	-	-	-
3	BCD	E	1403	X	-	X	-
3	BCD	F	1403	X	-	-	-
4	SO4	A	1404	-	-	X	X
4	SO4	B	1408	-	-	X	X
4	SO4	C	1406	-	-	X	X
4	SO4	D	1406	-	-	X	X
4	SO4	E	1406	-	-	X	X
4	SO4	F	1406	-	-	X	X
5	EDO	A	1406	-	-	-	X
5	EDO	B	1409	-	-	-	X
5	EDO	D	1407	-	-	-	X
5	EDO	E	1407	-	-	-	X
5	EDO	F	1407	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 22588 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 P 450 HEME-THIOLATE PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	402	Total	C	N	O	S	0	5	0
			3171	1990	561	595	25			
1	B	404	Total	C	N	O	S	0	5	0
			3181	1994	559	604	24			
1	C	402	Total	C	N	O	S	0	7	0
			3180	1995	561	600	24			
1	D	402	Total	C	N	O	S	0	7	0
			3205	2005	569	606	25			
1	E	402	Total	C	N	O	S	0	6	0
			3199	1999	574	602	24			
1	F	402	Total	C	N	O	S	0	6	0
			3186	1996	563	603	24			

There are 36 discrepancies between the modelled and reference sequences:

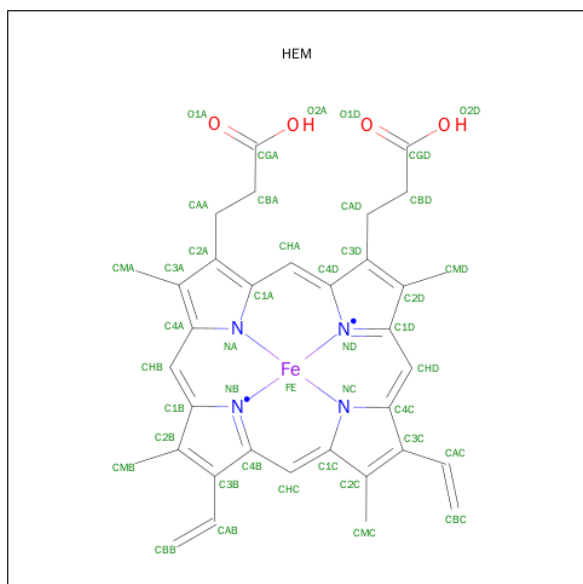
Chain	Residue	Modelled	Actual	Comment	Reference
A	402	HIS	-	EXPRESSION TAG	UNP A0R4Q6
A	403	HIS	-	EXPRESSION TAG	UNP A0R4Q6
A	404	HIS	-	EXPRESSION TAG	UNP A0R4Q6
A	405	HIS	-	EXPRESSION TAG	UNP A0R4Q6
A	406	HIS	-	EXPRESSION TAG	UNP A0R4Q6
A	407	HIS	-	EXPRESSION TAG	UNP A0R4Q6
B	402	HIS	-	EXPRESSION TAG	UNP A0R4Q6
B	403	HIS	-	EXPRESSION TAG	UNP A0R4Q6
B	404	HIS	-	EXPRESSION TAG	UNP A0R4Q6
B	405	HIS	-	EXPRESSION TAG	UNP A0R4Q6
B	406	HIS	-	EXPRESSION TAG	UNP A0R4Q6
B	407	HIS	-	EXPRESSION TAG	UNP A0R4Q6
C	402	HIS	-	EXPRESSION TAG	UNP A0R4Q6
C	403	HIS	-	EXPRESSION TAG	UNP A0R4Q6
C	404	HIS	-	EXPRESSION TAG	UNP A0R4Q6
C	405	HIS	-	EXPRESSION TAG	UNP A0R4Q6
C	406	HIS	-	EXPRESSION TAG	UNP A0R4Q6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	407	HIS	-	EXPRESSION TAG	UNP A0R4Q6
D	402	HIS	-	EXPRESSION TAG	UNP A0R4Q6
D	403	HIS	-	EXPRESSION TAG	UNP A0R4Q6
D	404	HIS	-	EXPRESSION TAG	UNP A0R4Q6
D	405	HIS	-	EXPRESSION TAG	UNP A0R4Q6
D	406	HIS	-	EXPRESSION TAG	UNP A0R4Q6
D	407	HIS	-	EXPRESSION TAG	UNP A0R4Q6
E	402	HIS	-	EXPRESSION TAG	UNP A0R4Q6
E	403	HIS	-	EXPRESSION TAG	UNP A0R4Q6
E	404	HIS	-	EXPRESSION TAG	UNP A0R4Q6
E	405	HIS	-	EXPRESSION TAG	UNP A0R4Q6
E	406	HIS	-	EXPRESSION TAG	UNP A0R4Q6
E	407	HIS	-	EXPRESSION TAG	UNP A0R4Q6
F	402	HIS	-	EXPRESSION TAG	UNP A0R4Q6
F	403	HIS	-	EXPRESSION TAG	UNP A0R4Q6
F	404	HIS	-	EXPRESSION TAG	UNP A0R4Q6
F	405	HIS	-	EXPRESSION TAG	UNP A0R4Q6
F	406	HIS	-	EXPRESSION TAG	UNP A0R4Q6
F	407	HIS	-	EXPRESSION TAG	UNP A0R4Q6

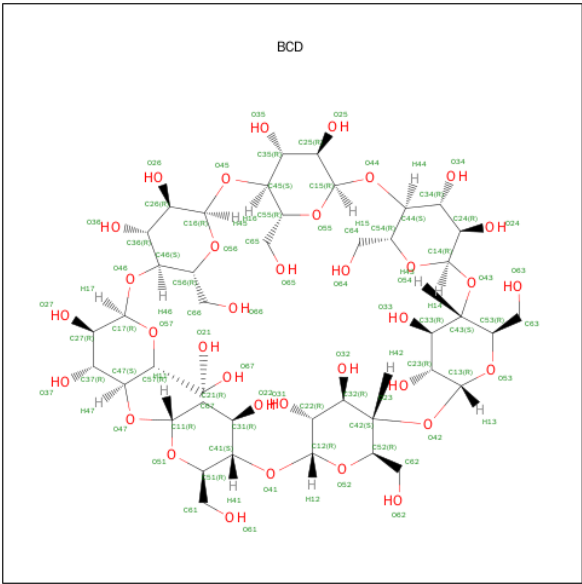
- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



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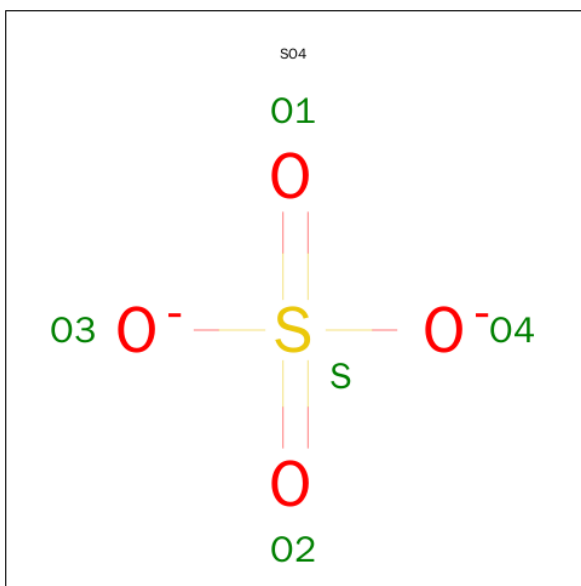
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is SUGAR (BETA-CYCLODEXTRIN) (three-letter code: BCD) (formula: C<sub>42</sub>H<sub>70</sub>O<sub>35</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			77	42	35		
3	B	1	Total	C	O	0	0
			77	42	35		
3	C	1	Total	C	O	0	0
			77	42	35		
3	D	1	Total	C	O	0	0
			77	42	35		
3	E	1	Total	C	O	0	0
			77	42	35		
3	F	1	Total	C	O	0	0
			77	42	35		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



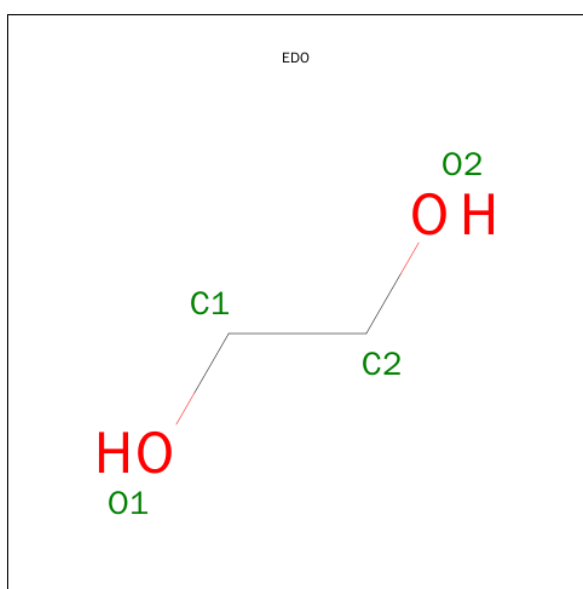
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

- Molecule 6 is water.

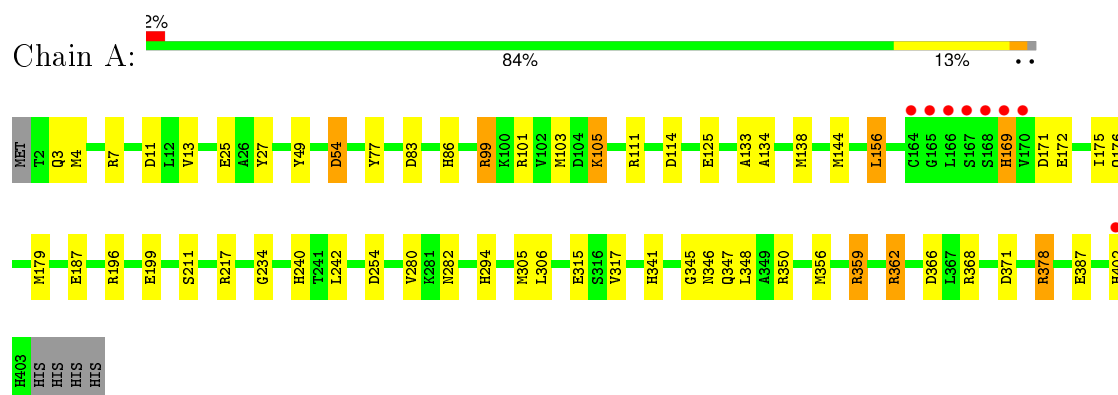


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	448	Total 448	O 448	0	0
6	B	439	Total 439	O 439	0	0
6	C	457	Total 457	O 457	0	0
6	D	431	Total 431	O 431	0	0
6	E	445	Total 445	O 445	0	0
6	F	417	Total 417	O 417	0	0

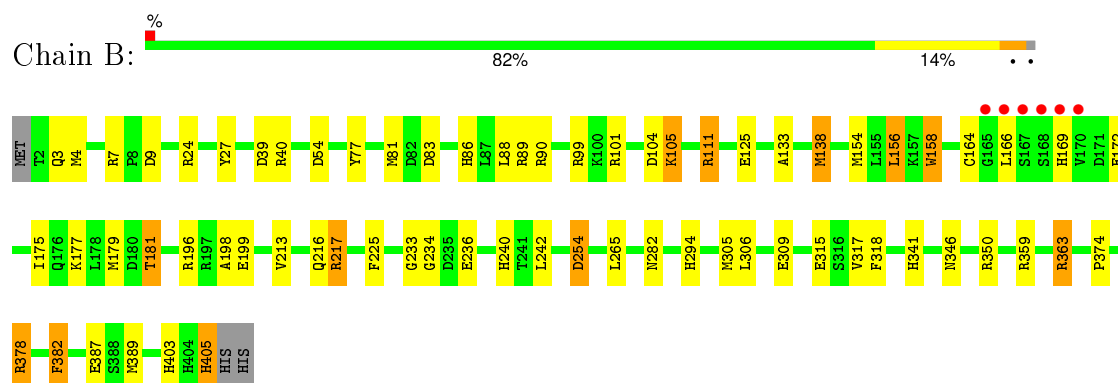
### 3 Residue-property plots [i](#)

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.

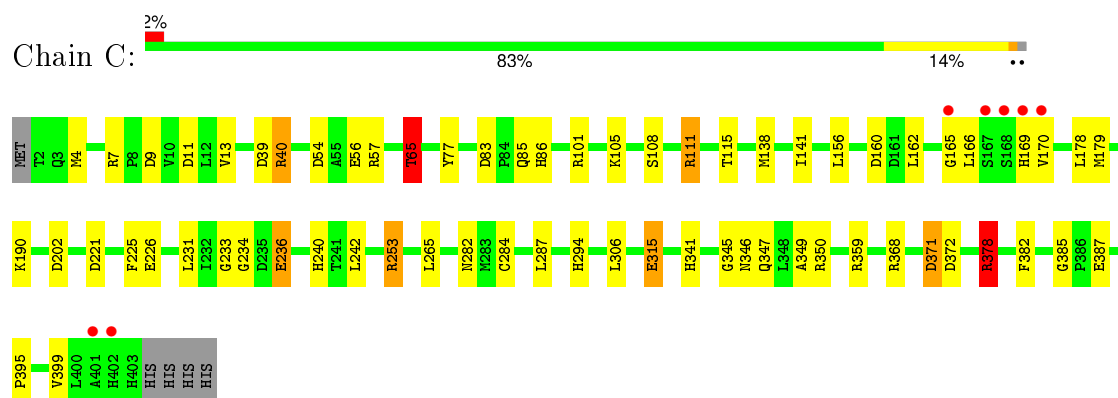
#### • Molecule 1: P450 HEME-THIOLATE PROTEIN



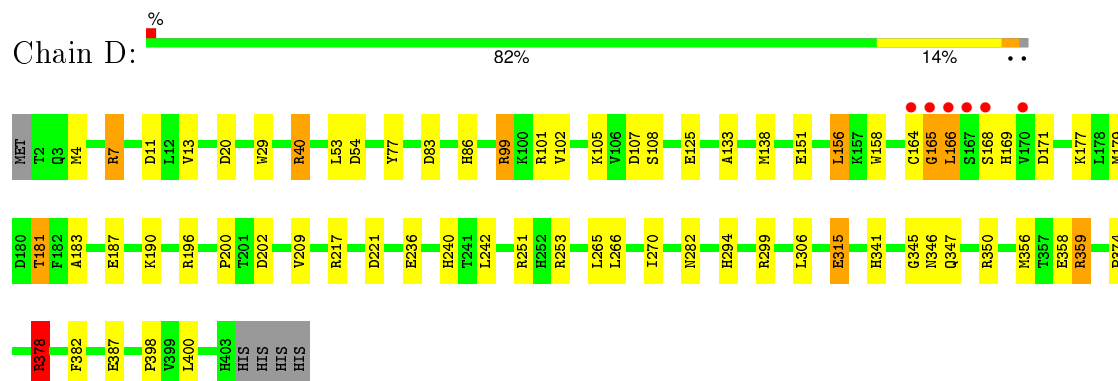
#### • Molecule 1: P450 HEME-THIOLATE PROTEIN



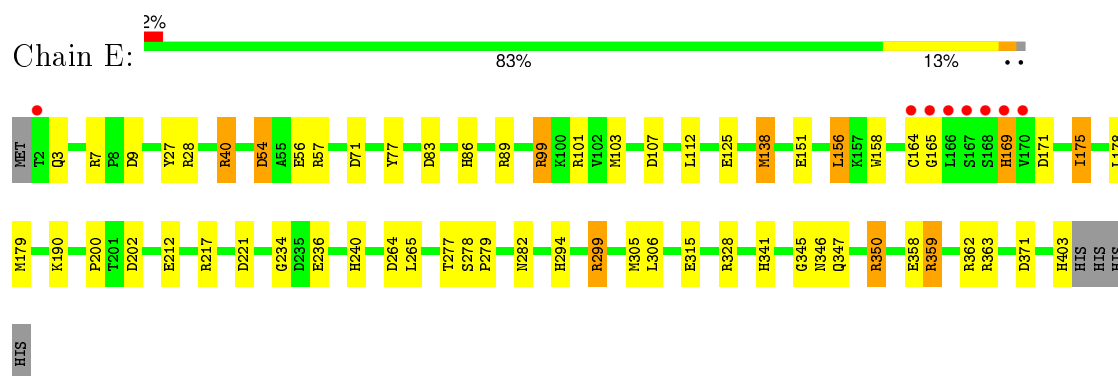
#### • Molecule 1: P450 HEME-THIOLATE PROTEIN



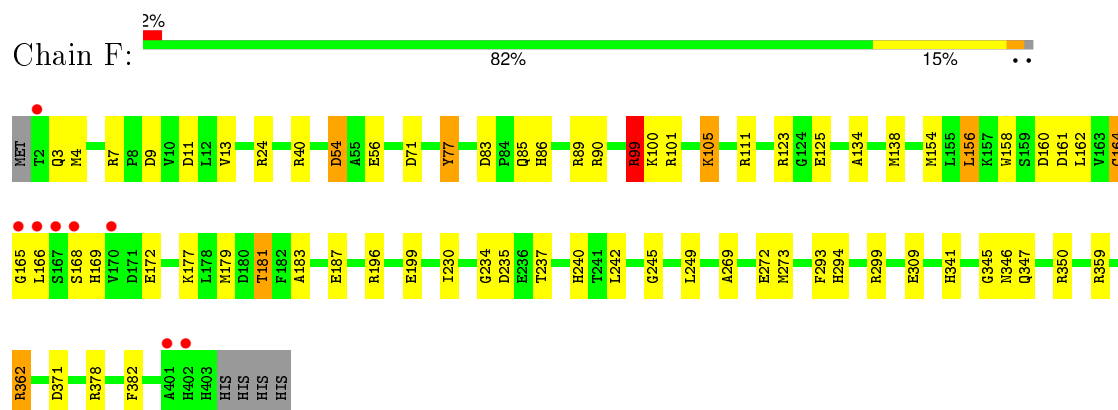
- Molecule 1: P450 HEME-THIOLATE PROTEIN



- Molecule 1: P450 HEME-THIOLATE PROTEIN



- Molecule 1: P450 HEME-THIOLATE PROTEIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.05Å 162.85Å 266.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	266.44 – 1.93 69.49 – 1.93	Depositor EDS
% Data completeness (in resolution range)	94.3 (266.44-1.93) 94.3 (69.49-1.93)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.16 (at 1.92Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.190 , 0.230 0.189 , 0.228	Depositor DCC
$R_{free}$ test set	14351 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	22.0	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 33.4	EDS
Estimated twinning fraction	0.460 for -1/2*h+1/2*k,3/2*h+1/2*k,-l 0.467 for -1/2*h-1/2*k,-3/2*h+1/2*k,-l 0.467 for 1/2*h+1/2*k,3/2*h-1/2*k,-l 0.467 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.467 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	3 of 283950 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	22588	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% 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: BCD, HEM, SO4, EDO

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	1.17	4/3237 (0.1%)	1.01	9/4391 (0.2%)
1	B	1.18	7/3251 (0.2%)	1.06	16/4414 (0.4%)
1	C	1.20	7/3255 (0.2%)	1.06	14/4416 (0.3%)
1	D	1.17	5/3274 (0.2%)	1.02	12/4439 (0.3%)
1	E	1.20	6/3265 (0.2%)	1.05	14/4427 (0.3%)
1	F	1.17	6/3258 (0.2%)	1.07	21/4420 (0.5%)
All	All	1.18	35/19540 (0.2%)	1.04	86/26507 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	236	GLU	CD-OE1	9.28	1.35	1.25
1	D	315	GLU	CD-OE1	8.82	1.35	1.25
1	F	272	GLU	CD-OE1	6.71	1.33	1.25
1	E	151	GLU	CD-OE2	-6.52	1.18	1.25
1	B	309	GLU	CB-CG	6.49	1.64	1.52
1	B	315	GLU	CD-OE1	6.41	1.32	1.25
1	E	158	TRP	CB-CG	-6.10	1.39	1.50
1	A	280	VAL	CB-CG2	6.08	1.65	1.52
1	F	309	GLU	CB-CG	6.02	1.63	1.52
1	C	236	GLU	CB-CG	-6.00	1.40	1.52
1	C	315	GLU	CD-OE1	5.93	1.32	1.25
1	F	293	PHE	CD2-CE2	5.88	1.51	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	317	VAL	CB-CG2	5.86	1.65	1.52
1	A	315	GLU	CD-OE1	5.85	1.32	1.25
1	B	27	TYR	CD1-CE1	5.79	1.48	1.39
1	C	226	GLU	CG-CD	5.75	1.60	1.51
1	C	284	CYS	CB-SG	-5.65	1.72	1.81
1	B	318	PHE	CE1-CZ	5.64	1.48	1.37
1	F	164	CYS	CB-SG	5.64	1.91	1.82
1	C	349	ALA	CA-CB	5.63	1.64	1.52
1	D	378	ARG	CG-CD	-5.62	1.37	1.51
1	E	27	TYR	CD1-CE1	5.56	1.47	1.39
1	B	158	TRP	CB-CG	-5.49	1.40	1.50
1	B	382	PHE	CE2-CZ	5.49	1.47	1.37
1	E	359	ARG	CZ-NH1	5.33	1.40	1.33
1	F	77	TYR	CD2-CE2	5.32	1.47	1.39
1	E	40	ARG	CG-CD	5.32	1.65	1.51
1	A	25	GLU	CD-OE2	-5.28	1.19	1.25
1	D	151	GLU	CD-OE2	-5.26	1.19	1.25
1	E	315	GLU	CD-OE1	5.22	1.31	1.25
1	C	382	PHE	CE2-CZ	5.22	1.47	1.37
1	F	382	PHE	CD1-CE1	5.17	1.49	1.39
1	D	158	TRP	CB-CG	-5.11	1.41	1.50
1	D	382	PHE	CE2-CZ	5.09	1.47	1.37
1	A	27	TYR	CD1-CE1	5.05	1.47	1.39

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	378	ARG	NE-CZ-NH1	10.78	125.69	120.30
1	B	363	ARG	NE-CZ-NH2	-10.43	115.09	120.30
1	F	242	LEU	CB-CG-CD2	-9.77	94.39	111.00
1	B	111	ARG	NE-CZ-NH1	9.31	124.96	120.30
1	B	363	ARG	NE-CZ-NH1	9.21	124.90	120.30
1	F	161	ASP	CB-CG-OD1	-8.82	110.36	118.30
1	C	287	LEU	CA-CB-CG	-8.38	96.04	115.30
1	C	111	ARG	NE-CZ-NH2	-8.19	116.21	120.30
1	B	359	ARG	NE-CZ-NH2	-8.05	116.27	120.30
1	F	101	ARG	NE-CZ-NH2	-7.93	116.34	120.30
1	A	111	ARG	NE-CZ-NH1	7.92	124.26	120.30
1	E	359	ARG	NE-CZ-NH2	-7.87	116.36	120.30
1	C	359	ARG	NE-CZ-NH2	-7.72	116.44	120.30
1	F	359	ARG	NE-CZ-NH2	-7.68	116.46	120.30
1	B	156	LEU	CB-CA-C	7.38	124.22	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	378	ARG	NE-CZ-NH2	-7.31	116.65	120.30
1	D	359	ARG	NE-CZ-NH2	-7.25	116.68	120.30
1	A	359	ARG	NE-CZ-NH2	-7.20	116.70	120.30
1	D	101	ARG	NE-CZ-NH2	-6.94	116.83	120.30
1	F	156	LEU	CB-CA-C	6.88	123.27	110.20
1	C	179	MET	CG-SD-CE	6.88	111.20	100.20
1	F	24	ARG	NE-CZ-NH1	-6.87	116.87	120.30
1	F	90	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	E	28	ARG	NE-CZ-NH1	6.69	123.65	120.30
1	E	179	MET	CG-SD-CE	6.64	110.82	100.20
1	F	111	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	B	101	ARG	NE-CZ-NH2	-6.45	117.08	120.30
1	F	179	MET	CG-SD-CE	6.44	110.50	100.20
1	E	112	LEU	CB-CG-CD1	-6.39	100.14	111.00
1	B	389	MET	CG-SD-CE	6.37	110.39	100.20
1	C	40	ARG	NE-CZ-NH1	6.25	123.43	120.30
1	F	111	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	C	287	LEU	CB-CG-CD1	6.17	121.49	111.00
1	A	362	ARG	NE-CZ-NH1	6.15	123.37	120.30
1	F	161	ASP	CB-CG-OD2	6.09	123.78	118.30
1	A	54	ASP	CB-CG-OD1	6.03	123.72	118.30
1	E	156	LEU	CB-CA-C	5.96	121.52	110.20
1	F	362	ARG	NE-CZ-NH1	5.95	123.27	120.30
1	E	107	ASP	CB-CG-OD1	5.87	123.58	118.30
1	A	156	LEU	CB-CA-C	5.86	121.33	110.20
1	A	179	MET	CG-SD-CE	5.85	109.56	100.20
1	E	54	ASP	CB-CG-OD1	5.85	123.56	118.30
1	A	362	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	C	39	ASP	CB-CG-OD1	5.74	123.47	118.30
1	E	101	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	D	156	LEU	CB-CA-C	5.71	121.06	110.20
1	F	99[A]	ARG	NE-CZ-NH2	-5.65	117.47	120.30
1	F	99[B]	ARG	NE-CZ-NH2	-5.65	117.47	120.30
1	B	254[A]	ASP	CB-CG-OD1	5.65	123.38	118.30
1	B	254[B]	ASP	CB-CG-OD1	5.65	123.38	118.30
1	B	105	LYS	CD-CE-NZ	-5.63	98.76	111.70
1	B	111	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	A	305	MET	CG-SD-CE	-5.60	91.25	100.20
1	D	251	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	E	89	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	F	89	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	D	20	ASP	CB-CG-OD1	5.50	123.25	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	179	MET	CG-SD-CE	5.49	108.98	100.20
1	A	101	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	B	24	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	F	378	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	F	156	LEU	CA-CB-CG	5.40	127.73	115.30
1	C	101	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	E	89	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	D	53	LEU	CB-CG-CD1	-5.34	101.92	111.00
1	C	57	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	F	89	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	B	90	ARG	NE-CZ-NH2	-5.33	117.63	120.30
1	F	362	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	D	7	ARG	NE-CZ-NH1	-5.26	117.67	120.30
1	E	350	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	E	264	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	F	54	ASP	CB-CG-OD1	5.21	122.99	118.30
1	E	28	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	B	39	ASP	CB-CG-OD1	5.20	122.98	118.30
1	E	328	ARG	NE-CZ-NH1	-5.19	117.70	120.30
1	F	235	ASP	CB-CG-OD1	5.17	122.96	118.30
1	C	236	GLU	CG-CD-OE2	-5.16	107.97	118.30
1	B	217	ARG	NE-CZ-NH1	-5.14	117.73	120.30
1	D	164[A]	CYS	C-N-CA	-5.11	111.57	122.30
1	D	164[B]	CYS	C-N-CA	-5.11	111.57	122.30
1	C	65	THR	OG1-CB-CG2	5.09	121.72	110.00
1	B	305	MET	CG-SD-CE	-5.06	92.10	100.20
1	D	107	ASP	CB-CG-OD2	-5.06	113.74	118.30
1	C	242	LEU	CA-CB-CG	-5.03	103.72	115.30
1	D	166	LEU	CB-CG-CD2	5.02	119.53	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	165	GLY	Peptide

## 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	3171	0	3105	53	0
1	B	3181	0	3091	65	0
1	C	3180	0	3116	49	0
1	D	3205	0	3134	59	0
1	E	3199	0	3132	52	0
1	F	3186	0	3126	64	0
2	A	43	0	30	6	0
2	B	43	0	30	6	0
2	C	43	0	30	5	0
2	D	43	0	30	6	0
2	E	43	0	30	6	0
2	F	43	0	30	10	0
3	A	77	0	70	16	0
3	B	77	0	70	23	0
3	C	77	0	70	22	0
3	D	77	0	70	10	0
3	E	77	0	67	23	0
3	F	77	0	68	6	0
4	A	10	0	0	8	0
4	B	15	0	0	5	0
4	C	15	0	0	3	0
4	D	15	0	0	5	0
4	E	15	0	0	5	0
4	F	15	0	0	5	0
5	A	4	0	5	0	0
5	B	4	0	5	1	0
5	C	4	0	5	1	0
5	D	4	0	5	0	0
5	E	4	0	5	0	0
5	F	4	0	5	0	0
6	A	448	0	0	17	0
6	B	439	0	0	15	0
6	C	457	0	0	13	0
6	D	431	0	0	12	0
6	E	445	0	0	14	1
6	F	417	0	0	20	1
All	All	22588	0	19329	442	1

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 11.

All (442) 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:E:169:HIS:O	1:E:175:ILE:HD11	1.28	1.29
3:E:1403:BCD:C37	3:E:1403:BCD:O21	1.84	1.25
3:E:1403:BCD:O37	3:E:1403:BCD:H21	1.40	1.21
3:E:1403:BCD:H37	3:E:1403:BCD:O21	1.37	1.19
3:C:1403:BCD:O36	3:C:1403:BCD:H27	1.43	1.15
1:D:40:ARG:HH11	1:D:40:ARG:CG	1.58	1.14
1:F:164:CYS:HB3	6:F:2237:HOH:O	1.49	1.12
3:E:1403:BCD:O37	3:E:1403:BCD:C21	1.97	1.12
1:F:230:ILE:HG23	2:F:1402:HEM:HBC1	1.27	1.12
3:C:1403:BCD:H13	3:C:1403:BCD:O32	1.36	1.11
3:C:1403:BCD:O51	3:C:1403:BCD:H672	1.48	1.10
3:E:1403:BCD:H53	3:E:1403:BCD:O23	1.46	1.08
1:F:138:MET:HE1	6:F:2215:HOH:O	1.52	1.08
3:B:1403:BCD:O37	3:B:1403:BCD:H21	1.53	1.08
1:F:99[A]:ARG:HA	1:F:99[A]:ARG:NE	1.64	1.08
1:C:7:ARG:HD2	4:C:1406:SO4:O3	1.55	1.07
1:F:99[A]:ARG:HA	1:F:99[A]:ARG:HE	1.12	1.06
3:B:1403:BCD:O32	3:B:1403:BCD:C23	2.02	1.06
1:E:299:ARG:HG3	1:E:299:ARG:HH11	1.18	1.04
1:E:7:ARG:HD2	4:E:1406:SO4:O2	1.55	1.04
3:A:1403:BCD:O32	3:A:1403:BCD:H13	1.55	1.04
3:C:1403:BCD:C67	3:C:1403:BCD:O51	2.06	1.03
3:B:1403:BCD:O32	3:B:1403:BCD:H23	1.58	1.03
1:D:7:ARG:HD2	4:D:1406:SO4:O3	1.59	1.00
3:D:1403:BCD:H632	3:D:1403:BCD:O64	1.61	1.00
3:B:1403:BCD:O37	3:B:1403:BCD:C21	2.09	1.00
1:D:99[B]:ARG:NH2	6:D:2170:HOH:O	1.92	1.00
1:D:40:ARG:NH1	1:D:40:ARG:HG3	1.59	0.99
1:F:4:MET:N	4:F:1406:SO4:O3	1.96	0.99
3:F:1403:BCD:HO32	3:F:1403:BCD:HO23	1.09	0.98
1:E:169:HIS:O	1:E:175:ILE:CD1	2.10	0.98
3:E:1403:BCD:O61	3:E:1403:BCD:H621	1.64	0.97
1:E:138:MET:HB3	1:E:156:LEU:HD13	1.47	0.97
1:F:7:ARG:HD2	4:F:1406:SO4:O2	1.65	0.96
3:C:1403:BCD:HO32	3:C:1403:BCD:H13	1.22	0.94
1:B:169:HIS:O	1:B:175:ILE:HD11	1.67	0.94
1:B:138:MET:HB3	1:B:156:LEU:HD13	1.50	0.93
3:C:1403:BCD:C27	3:C:1403:BCD:O36	2.17	0.92
3:E:1403:BCD:C53	3:E:1403:BCD:O23	2.16	0.92
3:C:1403:BCD:C13	3:C:1403:BCD:O32	2.17	0.92
3:E:1403:BCD:O37	3:E:1403:BCD:O21	1.84	0.92
1:C:138:MET:HB3	1:C:156:LEU:CD1	2.00	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1403:BCD:O26	3:C:1403:BCD:O35	1.88	0.91
3:E:1403:BCD:C21	3:E:1403:BCD:C37	2.43	0.91
1:D:40:ARG:HH11	1:D:40:ARG:HG3	0.76	0.90
3:B:1403:BCD:O32	3:B:1403:BCD:O23	1.90	0.89
3:D:1403:BCD:O64	3:D:1403:BCD:C63	2.21	0.88
1:B:7:ARG:NH1	4:B:1408:SO4:O1	2.07	0.88
3:B:1403:BCD:O26	3:B:1403:BCD:O35	1.91	0.88
3:E:1403:BCD:H56	3:E:1403:BCD:O57	1.75	0.86
1:F:99[A]:ARG:CA	1:F:99[A]:ARG:HE	1.67	0.86
1:B:81:MET:HE2	1:B:86:HIS:HA	1.55	0.86
1:E:138:MET:HB3	1:E:156:LEU:CD1	2.05	0.85
1:D:183:ALA:O	1:D:187[B]:GLU:HG3	1.76	0.85
1:E:299:ARG:HG3	1:E:299:ARG:NH1	1.92	0.84
1:D:138:MET:HB3	1:D:156:LEU:CD1	2.07	0.84
1:E:403:HIS:HD2	6:E:2441:HOH:O	1.60	0.84
1:C:4:MET:N	4:C:1406:SO4:O2	2.11	0.84
1:F:138:MET:HB3	1:F:156:LEU:HD13	1.57	0.84
1:F:230:ILE:HG23	2:F:1402:HEM:CBC	2.07	0.83
1:D:138:MET:HB3	1:D:156:LEU:HD13	1.61	0.82
1:F:138:MET:HB3	1:F:156:LEU:CD1	2.10	0.81
1:C:138:MET:HB3	1:C:156:LEU:HD13	1.62	0.81
1:A:99:ARG:HD3	1:A:347[A]:GLN:HE22	1.42	0.81
1:E:99:ARG:HE	1:E:347:GLN:HE22	1.28	0.80
1:B:378:ARG:NH1	1:B:387[A]:GLU:OE1	2.15	0.78
1:B:86:HIS:HE1	2:B:1402:HEM:O2D	1.64	0.78
1:E:359:ARG:HG2	1:E:362[B]:ARG:HH21	1.48	0.78
1:A:7:ARG:HD2	4:A:1404:SO4:O4	1.85	0.76
1:D:299:ARG:HD3	6:D:2347:HOH:O	1.85	0.76
3:E:1403:BCD:HO21	3:E:1403:BCD:H37	1.51	0.76
1:B:133:ALA:HA	1:B:242:LEU:HD23	1.66	0.75
1:A:3:GLN:HA	4:A:1404:SO4:O1	1.86	0.75
1:C:315:GLU:OE1	6:C:2080:HOH:O	2.04	0.75
3:C:1403:BCD:O26	3:C:1403:BCD:C45	2.35	0.74
1:A:144:MET:HE2	6:A:2096:HOH:O	1.87	0.74
1:B:111:ARG:HH22	1:B:405:HIS:CD2	2.05	0.74
3:B:1403:BCD:O34	3:B:1403:BCD:O25	2.03	0.74
1:D:99[A]:ARG:H	1:D:99[A]:ARG:CD	1.99	0.74
1:E:358:GLU:OE1	6:E:2413:HOH:O	2.06	0.74
1:F:160:ASP:OD2	6:F:2235:HOH:O	2.06	0.73
1:F:86:HIS:HE1	2:F:1402:HEM:O2D	1.70	0.73
1:B:81:MET:CE	1:B:86:HIS:HA	2.17	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:ARG:CD	6:B:2407:HOH:O	2.35	0.73
1:B:169:HIS:O	1:B:175:ILE:CD1	2.36	0.73
1:B:196:ARG:NH1	6:B:2272:HOH:O	2.19	0.73
1:E:221:ASP:OD2	3:E:1403:BCD:H14	1.90	0.72
3:A:1403:BCD:H672	3:A:1403:BCD:O51	1.88	0.72
1:B:138:MET:HB3	1:B:156:LEU:CD1	2.19	0.72
1:A:362:ARG:NH2	6:A:2415:HOH:O	2.21	0.72
1:D:165:GLY:O	1:D:169:HIS:HB3	1.90	0.71
1:F:249[B]:LEU:HD12	1:F:249[B]:LEU:N	2.04	0.71
1:E:86:HIS:HE1	2:E:1402:HEM:O2D	1.73	0.71
1:C:65:THR:HG21	6:C:2139:HOH:O	1.90	0.71
1:A:169:HIS:HD2	6:A:2136:HOH:O	1.73	0.71
1:D:221:ASP:HB3	3:D:1403:BCD:H612	1.72	0.71
1:D:86:HIS:HE1	2:D:1402:HEM:O2D	1.73	0.70
2:F:1402:HEM:HBB2	2:F:1402:HEM:HMB2	1.74	0.70
1:C:86:HIS:HE1	2:C:1402:HEM:O2D	1.74	0.70
3:F:1403:BCD:O61	3:F:1403:BCD:C11	2.32	0.69
1:A:86:HIS:HE1	2:A:1402:HEM:O2D	1.76	0.69
1:D:240:HIS:HE1	6:D:2292:HOH:O	1.74	0.69
3:E:1403:BCD:HO23	3:E:1403:BCD:H53	1.55	0.68
3:C:1403:BCD:O26	3:C:1403:BCD:C35	2.41	0.68
1:B:88:LEU:HD12	1:B:213:VAL:HG21	1.75	0.68
1:D:99[A]:ARG:H	1:D:99[A]:ARG:HD2	1.59	0.68
1:C:341:HIS:HD2	2:C:1402:HEM:O1D	1.77	0.68
3:B:1403:BCD:O37	3:B:1403:BCD:O21	2.11	0.68
3:A:1403:BCD:O41	3:A:1403:BCD:O61	2.10	0.68
1:D:29:TRP:HH2	4:D:1406:SO4:O1	1.77	0.67
1:B:341:HIS:HE1	6:B:2146:HOH:O	1.77	0.67
1:F:105:LYS:HG3	6:F:2080:HOH:O	1.94	0.67
3:A:1403:BCD:O32	3:A:1403:BCD:C13	2.35	0.66
1:E:341:HIS:HD2	2:E:1402:HEM:O1D	1.78	0.66
3:E:1403:BCD:HO37	3:E:1403:BCD:C21	2.05	0.66
1:A:387[A]:GLU:OE1	6:A:2436:HOH:O	2.13	0.66
1:B:179:MET:HE1	3:B:1403:BCD:H652	1.76	0.66
1:A:83:ASP:OD1	1:A:86:HIS:HD2	1.78	0.66
1:A:176:GLN:OE1	1:A:176:GLN:HA	1.95	0.66
3:D:1403:BCD:H632	3:D:1403:BCD:HO64	1.62	0.65
2:F:1402:HEM:HBB2	2:F:1402:HEM:CMB	2.26	0.65
3:B:1403:BCD:O47	3:B:1403:BCD:O67	2.11	0.65
1:B:172:GLU:CB	6:B:2259:HOH:O	2.45	0.65
1:F:181:THR:HG22	6:F:2243:HOH:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:29:TRP:CH2	4:D:1406:SO4:O1	2.50	0.64
3:C:1403:BCD:C23	3:C:1403:BCD:O32	2.46	0.64
1:F:85:GLN:HB3	6:F:2054:HOH:O	1.97	0.64
1:A:4:MET:N	4:A:1404:SO4:O1	2.30	0.64
1:D:315:GLU:OE1	6:D:2069:HOH:O	2.15	0.64
1:A:341:HIS:HD2	2:A:1402:HEM:O1D	1.81	0.63
1:A:346:ASN:HD22	1:A:350:ARG:HH11	1.46	0.63
1:F:341:HIS:HD2	2:F:1402:HEM:O1D	1.82	0.63
1:B:374:PRO:HD3	6:B:2220:HOH:O	1.97	0.63
3:C:1403:BCD:O34	3:C:1403:BCD:O25	2.17	0.63
3:E:1403:BCD:O35	3:E:1403:BCD:C16	2.33	0.63
1:A:11:ASP:OD1	1:A:13[B]:VAL:HG22	1.99	0.63
1:F:3:GLN:HA	4:F:1406:SO4:O3	1.99	0.62
1:F:187[B]:GLU:HG3	6:F:2246:HOH:O	1.98	0.62
1:F:245:GLY:O	1:F:249[B]:LEU:HD13	2.00	0.62
1:B:363:ARG:HD2	6:B:2416:HOH:O	1.98	0.62
1:E:7:ARG:CD	4:E:1406:SO4:O2	2.40	0.62
1:F:99[A]:ARG:CA	1:F:99[A]:ARG:NE	2.33	0.62
3:C:1403:BCD:HO61	3:C:1403:BCD:C12	2.13	0.62
3:D:1403:BCD:O21	3:D:1403:BCD:H51	1.99	0.62
1:B:88:LEU:CD1	1:B:213:VAL:CG2	2.78	0.61
1:A:105:LYS:HG3	6:A:2096:HOH:O	2.00	0.61
1:B:154:MET:HE2	1:B:158:TRP:CH2	2.36	0.61
1:B:240:HIS:HE1	6:B:2303:HOH:O	1.84	0.60
1:C:346:ASN:HD22	1:C:350:ARG:HH11	1.49	0.60
1:D:196:ARG:HD3	6:D:2256:HOH:O	2.01	0.60
1:D:358:GLU:OE1	6:D:2396:HOH:O	2.16	0.60
1:A:133:ALA:HA	1:A:242:LEU:HD23	1.83	0.60
3:C:1403:BCD:O51	3:C:1403:BCD:H671	2.01	0.60
1:E:99:ARG:HD3	1:E:103:MET:HG2	1.84	0.60
1:B:154:MET:CE	1:B:158:TRP:CH2	2.84	0.60
3:B:1403:BCD:O34	3:B:1403:BCD:C25	2.50	0.60
1:D:341:HIS:HD2	2:D:1402:HEM:O1D	1.84	0.59
1:E:341:HIS:HE1	6:E:2154:HOH:O	1.84	0.59
1:F:240:HIS:HE1	6:F:2282:HOH:O	1.85	0.59
1:F:341:HIS:HE1	6:F:2128:HOH:O	1.85	0.59
1:D:166:LEU:O	1:D:169:HIS:CE1	2.56	0.58
1:D:177:LYS:O	1:D:181:THR:HG23	2.03	0.58
3:C:1403:BCD:C12	3:C:1403:BCD:O61	2.51	0.58
1:F:99[A]:ARG:HH22	1:F:347:GLN:CB	2.16	0.58
1:E:346:ASN:HD22	1:E:350:ARG:HH11	1.49	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:177:LYS:O	1:F:181:THR:HG23	2.04	0.58
1:B:105:LYS:HG3	6:B:2190:HOH:O	2.04	0.58
1:B:225:PHE:CE2	3:B:1403:BCD:H622	2.39	0.58
1:F:7:ARG:CD	4:F:1406:SO4:O2	2.48	0.58
1:B:88:LEU:HD12	1:B:213:VAL:CG2	2.33	0.58
1:D:4:MET:N	4:D:1406:SO4:O2	2.36	0.58
1:F:346:ASN:HD22	1:F:350:ARG:HH11	1.51	0.57
1:B:88:LEU:CD1	1:B:213:VAL:HG23	2.34	0.57
1:E:9:ASP:OD1	1:E:40:ARG:HD3	2.05	0.57
1:F:83:ASP:OD1	1:F:86:HIS:HD2	1.87	0.57
2:E:1402:HEM:HBC2	2:E:1402:HEM:HMC1	1.87	0.57
1:D:374:PRO:O	6:D:2417:HOH:O	2.17	0.57
1:A:341:HIS:HE1	6:A:2146:HOH:O	1.86	0.57
1:C:11:ASP:OD1	1:C:13[A]:VAL:HG22	2.05	0.57
1:E:240:HIS:HE1	6:E:2302:HOH:O	1.87	0.57
1:D:99[B]:ARG:HG3	1:D:99[B]:ARG:HH11	1.70	0.56
3:D:1403:BCD:H662	3:D:1403:BCD:O57	2.05	0.56
1:D:341:HIS:HE1	6:D:2136:HOH:O	1.87	0.56
1:F:99[A]:ARG:HH22	1:F:347:GLN:HB2	1.70	0.56
1:D:99[B]:ARG:HG3	1:D:99[B]:ARG:NH1	2.19	0.56
1:F:249[B]:LEU:H	1:F:249[B]:LEU:CD1	2.18	0.56
1:C:9:ASP:OD1	1:C:40:ARG:HD3	2.06	0.56
1:F:249[B]:LEU:H	1:F:249[B]:LEU:HD12	1.70	0.56
3:B:1403:BCD:O41	3:B:1403:BCD:O61	2.24	0.55
3:F:1403:BCD:O62	6:F:2415:HOH:O	2.07	0.55
1:F:99[A]:ARG:HH12	1:F:347:GLN:HB3	1.71	0.55
1:C:378:ARG:NH1	1:C:387:GLU:HG2	2.20	0.55
1:C:341:HIS:HE1	6:C:2161:HOH:O	1.89	0.55
1:B:346:ASN:HD22	1:B:350:ARG:HH11	1.51	0.55
1:A:83:ASP:OD1	1:A:86:HIS:CD2	2.59	0.55
3:A:1403:BCD:H25	3:A:1403:BCD:O34	2.07	0.55
1:B:341:HIS:HD2	2:B:1402:HEM:O1D	1.90	0.55
1:F:249[B]:LEU:N	1:F:249[B]:LEU:CD1	2.69	0.55
1:B:179:MET:CE	3:B:1403:BCD:H652	2.36	0.55
1:F:362:ARG:NH2	6:F:2388:HOH:O	2.39	0.55
3:D:1403:BCD:H631	3:D:1403:BCD:O64	2.07	0.55
1:D:133:ALA:HA	1:D:242:LEU:HD23	1.87	0.55
1:B:86:HIS:CE1	2:B:1402:HEM:O2D	2.55	0.54
1:B:213:VAL:HG23	1:B:213:VAL:O	2.07	0.54
1:A:3:GLN:HG2	1:A:7:ARG:HD2	1.88	0.54
3:C:1403:BCD:C17	3:C:1403:BCD:O36	2.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:177:LYS:O	1:D:181:THR:CG2	2.56	0.54
1:E:71:ASP:CB	6:E:2142:HOH:O	2.56	0.54
1:C:54:ASP:OD2	1:C:294:HIS:HE1	1.91	0.54
3:C:1403:BCD:HO36	3:C:1403:BCD:H27	1.69	0.53
3:B:1403:BCD:O35	3:B:1403:BCD:C26	2.55	0.53
1:B:3:GLN:HA	4:B:1408:SO4:O2	2.08	0.53
1:C:236:GLU:OE1	1:C:240:HIS:HE1	1.91	0.53
1:F:371:ASP:O	6:F:2397:HOH:O	2.18	0.53
1:B:198:ALA:O	1:B:199[B]:GLU:OE1	2.25	0.53
1:D:102:VAL:HG11	1:D:347[A]:GLN:HG2	1.90	0.53
1:E:171:ASP:HB2	6:E:2262:HOH:O	2.07	0.53
3:B:1403:BCD:HO34	3:B:1403:BCD:HO25	1.41	0.53
3:A:1403:BCD:H32	3:A:1403:BCD:C23	2.39	0.53
1:C:83:ASP:OD1	1:C:86:HIS:HD2	1.92	0.53
1:F:71:ASP:CB	6:F:2120:HOH:O	2.55	0.53
1:D:54:ASP:OD2	1:D:294:HIS:HE1	1.91	0.53
3:A:1403:BCD:O32	3:A:1403:BCD:H23	2.08	0.53
1:B:54:ASP:OD2	1:B:294:HIS:HE1	1.92	0.53
1:C:7:ARG:CD	4:C:1406:SO4:O3	2.45	0.53
1:D:221:ASP:CB	3:D:1403:BCD:H612	2.38	0.53
3:D:1403:BCD:C51	3:D:1403:BCD:O21	2.54	0.53
1:A:359:ARG:HG2	6:A:2205:HOH:O	2.09	0.52
1:B:225:PHE:HE2	3:B:1403:BCD:H622	1.73	0.52
3:A:1403:BCD:H23	3:A:1403:BCD:H32	1.90	0.52
1:B:88:LEU:HD11	1:B:213:VAL:HG23	1.91	0.52
1:F:154:MET:HE2	1:F:158:TRP:CH2	2.44	0.52
2:B:1402:HEM:HBC2	2:B:1402:HEM:HMC1	1.92	0.52
3:B:1403:BCD:HO35	3:B:1403:BCD:HO26	1.47	0.52
3:B:1403:BCD:C37	3:B:1403:BCD:C21	2.87	0.52
1:F:11:ASP:OD1	1:F:13[A]:VAL:HG22	2.09	0.52
1:E:54:ASP:OD2	1:E:294:HIS:HE1	1.92	0.52
1:A:172:GLU:HA	1:A:175:ILE:HD12	1.91	0.52
1:D:166:LEU:O	1:D:169:HIS:ND1	2.43	0.52
1:A:346:ASN:HD22	1:A:350:ARG:NH1	2.08	0.52
1:F:154:MET:CE	1:F:158:TRP:CH2	2.93	0.52
1:E:200:PRO:HG3	6:E:2286:HOH:O	2.09	0.52
1:E:403:HIS:CD2	6:E:2441:HOH:O	2.46	0.52
1:D:346:ASN:HD22	1:D:350:ARG:HH11	1.56	0.51
1:A:240:HIS:HE1	6:A:2305:HOH:O	1.92	0.51
1:D:4:MET:HG3	4:D:1406:SO4:O2	2.10	0.51
1:C:395:PRO:O	6:C:2453:HOH:O	2.18	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:162:LEU:O	1:F:166:LEU:HG	2.10	0.51
1:A:3:GLN:CA	4:A:1404:SO4:O1	2.59	0.51
1:C:165:GLY:HA3	1:C:178:LEU:HD13	1.93	0.51
1:F:83:ASP:OD1	1:F:86:HIS:CD2	2.63	0.51
1:D:190:LYS:NZ	1:D:221:ASP:OD1	2.44	0.51
1:C:347[B]:GLN:HG3	6:C:2422:HOH:O	2.10	0.51
1:E:3:GLN:HA	4:E:1406:SO4:O4	2.11	0.51
1:B:4:MET:HB2	4:B:1408:SO4:O4	2.11	0.51
3:C:1403:BCD:H23	3:C:1403:BCD:O32	2.11	0.50
3:A:1403:BCD:HO32	3:A:1403:BCD:H13	1.71	0.50
1:A:171:ASP:CG	6:A:2263:HOH:O	2.49	0.50
3:E:1403:BCD:O35	3:E:1403:BCD:H16	2.11	0.50
1:F:245:GLY:O	1:F:249[B]:LEU:CD1	2.60	0.50
1:E:56:GLU:OE2	2:E:1402:HEM:O2A	2.29	0.50
3:A:1403:BCD:O32	3:A:1403:BCD:C23	2.60	0.50
1:D:341:HIS:O	2:D:1402:HEM:HBA2	2.11	0.50
1:A:134:ALA:O	1:A:138:MET:HG3	2.12	0.50
1:E:99:ARG:HD3	1:E:103:MET:CG	2.41	0.50
1:E:236:GLU:HG3	6:E:2299:HOH:O	2.11	0.50
3:B:1403:BCD:HO34	3:B:1403:BCD:C25	2.24	0.49
1:A:254:ASP:HB2	6:A:2326:HOH:O	2.12	0.49
1:B:83:ASP:OD1	1:B:86:HIS:HD2	1.96	0.49
1:F:56:GLU:OE2	2:F:1402:HEM:O2A	2.29	0.49
1:E:83:ASP:OD1	1:E:86:HIS:HD2	1.95	0.49
1:C:170:VAL:N	6:C:2274:HOH:O	2.42	0.49
1:B:88:LEU:HD11	1:B:213:VAL:CG2	2.43	0.49
1:F:345:GLY:HA3	2:F:1402:HEM:C3C	2.48	0.49
2:A:1402:HEM:CMB	2:A:1402:HEM:HBB2	2.43	0.49
2:A:1402:HEM:HMB2	2:A:1402:HEM:HBB2	1.95	0.49
1:F:346:ASN:HD22	1:F:350:ARG:NH1	2.10	0.49
1:A:402:HIS:O	6:A:2445:HOH:O	2.20	0.49
1:B:166:LEU:O	1:B:169:HIS:ND1	2.45	0.48
1:D:11:ASP:OD1	1:D:13:VAL:HG22	2.13	0.48
1:D:190:LYS:CE	1:D:221:ASP:OD1	2.61	0.48
1:D:83:ASP:OD1	1:D:86:HIS:HD2	1.96	0.48
1:A:378:ARG:HD3	1:A:387[B]:GLU:CD	2.34	0.48
1:A:4:MET:HB2	4:A:1404:SO4:O2	2.13	0.48
1:A:378:ARG:HD3	1:A:387[B]:GLU:OE1	2.12	0.48
1:D:266:LEU:O	1:D:270:ILE:HG12	2.13	0.48
3:E:1403:BCD:C66	3:E:1403:BCD:C26	2.85	0.48
3:A:1403:BCD:H23	3:A:1403:BCD:C32	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:GLN:CA	4:B:1408:SO4:O2	2.61	0.48
1:A:7:ARG:CD	4:A:1404:SO4:O4	2.58	0.48
1:A:138:MET:HB3	1:A:156:LEU:HD13	1.96	0.48
1:C:105[A]:LYS:HE2	6:C:2206:HOH:O	2.12	0.48
1:B:254[A]:ASP:OD1	6:B:2323:HOH:O	2.19	0.48
1:E:57:ARG:NH1	6:E:2116:HOH:O	2.18	0.48
1:A:345:GLY:HA3	2:A:1402:HEM:C3C	2.49	0.48
1:C:346:ASN:HD22	1:C:350:ARG:NH1	2.11	0.48
1:A:242:LEU:HD21	1:A:356:MET:HG2	1.94	0.48
1:D:346:ASN:HD22	1:D:350:ARG:NH1	2.12	0.48
1:F:9:ASP:OD1	1:F:40:ARG:HD3	2.14	0.48
3:A:1403:BCD:C32	3:A:1403:BCD:C23	2.88	0.48
1:B:54:ASP:OD2	1:B:294:HIS:CE1	2.66	0.48
1:E:99:ARG:HE	1:E:347:GLN:NE2	2.03	0.48
1:B:240:HIS:HD2	6:B:2306:HOH:O	1.97	0.48
1:F:165:GLY:O	1:F:169:HIS:HB3	2.14	0.48
1:C:371:ASP:C	1:C:371:ASP:OD1	2.53	0.47
1:B:166:LEU:O	1:B:169:HIS:CE1	2.67	0.47
1:C:13[B]:VAL:O	1:C:13[B]:VAL:HG12	2.13	0.47
3:C:1403:BCD:O41	3:C:1403:BCD:O61	2.32	0.47
1:C:56:GLU:OE2	2:C:1402:HEM:O2A	2.32	0.47
2:B:1402:HEM:HBB2	2:B:1402:HEM:CMB	2.45	0.47
2:D:1402:HEM:HBB2	2:D:1402:HEM:CMB	2.45	0.47
1:A:234:GLY:HA2	2:A:1402:HEM:C2C	2.49	0.47
1:B:217:ARG:NE	6:B:2284:HOH:O	2.46	0.47
1:D:378:ARG:HB2	1:D:387[A]:GLU:HG2	1.95	0.47
1:D:105:LYS:HE3	1:D:108:SER:OG	2.15	0.47
1:D:40:ARG:CG	1:D:40:ARG:NH1	2.34	0.47
1:C:54:ASP:OD2	1:C:294:HIS:CE1	2.67	0.47
3:B:1403:BCD:H27	3:B:1403:BCD:H46	1.78	0.47
3:B:1403:BCD:C12	3:B:1403:BCD:C61	2.93	0.47
1:B:234:GLY:HA2	2:B:1402:HEM:C2C	2.50	0.46
1:A:144:MET:HE1	1:A:348:LEU:HD22	1.97	0.46
1:B:387[B]:GLU:OE2	6:B:2435:HOH:O	2.19	0.46
1:F:172:GLU:CG	6:F:2241:HOH:O	2.63	0.46
3:E:1403:BCD:C62	3:E:1403:BCD:O61	2.26	0.46
1:F:234:GLY:HA2	2:F:1402:HEM:C2C	2.50	0.46
1:E:165:GLY:HA3	1:E:178:LEU:HD13	1.98	0.46
3:E:1403:BCD:C56	3:E:1403:BCD:O57	2.55	0.46
1:B:3:GLN:CB	4:B:1408:SO4:O2	2.63	0.46
1:C:378:ARG:NH1	1:C:387:GLU:OE2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:190:LYS:NZ	1:E:221:ASP:OD1	2.48	0.46
1:F:138:MET:HE2	6:F:2214:HOH:O	2.16	0.46
1:C:240:HIS:CG	1:C:385:GLY:HA3	2.51	0.46
1:A:282:ASN:HA	1:A:306:LEU:O	2.16	0.46
1:A:169:HIS:CD2	6:A:2136:HOH:O	2.56	0.46
1:F:54:ASP:OD2	1:F:294:HIS:HE1	1.98	0.46
1:C:85[A]:GLN:HG3	6:C:2175:HOH:O	2.15	0.46
1:D:345:GLY:HA3	2:D:1402:HEM:C3C	2.51	0.46
1:F:240:HIS:HD2	6:F:2285:HOH:O	1.98	0.46
1:B:9:ASP:OD1	1:B:40:ARG:HD3	2.16	0.45
1:E:190:LYS:CE	1:E:221:ASP:OD1	2.63	0.45
3:A:1403:BCD:O35	3:A:1403:BCD:C16	2.64	0.45
1:A:196:ARG:HD3	6:A:2277:HOH:O	2.16	0.45
1:D:165:GLY:CA	1:D:168:SER:H	2.29	0.45
1:C:111:ARG:NH2	6:C:2226:HOH:O	2.43	0.45
1:A:4:MET:SD	4:A:1404:SO4:O2	2.75	0.45
1:D:242:LEU:HD21	1:D:356:MET:HG2	1.99	0.45
3:E:1403:BCD:H26	3:E:1403:BCD:C66	2.47	0.45
3:A:1403:BCD:C25	3:A:1403:BCD:O34	2.64	0.45
1:E:240:HIS:HD2	6:E:2305:HOH:O	1.98	0.45
1:C:160:ASP:OD2	6:C:2270:HOH:O	2.21	0.45
1:E:3:GLN:CA	4:E:1406:SO4:O4	2.65	0.45
1:A:240:HIS:HD2	6:A:2308:HOH:O	2.00	0.45
1:B:382:PHE:HB3	6:B:2433:HOH:O	2.17	0.45
1:E:403:HIS:HB2	6:E:2439:HOH:O	2.17	0.44
1:E:347:GLN:HG3	6:E:2403:HOH:O	2.17	0.44
1:D:378:ARG:NH1	1:D:387[A]:GLU:OE1	2.49	0.44
1:F:237:THR:HG23	6:F:2280:HOH:O	2.16	0.44
1:B:346:ASN:HD22	1:B:350:ARG:NH1	2.13	0.44
1:C:166:LEU:O	1:C:169:HIS:ND1	2.50	0.44
1:A:54:ASP:OD2	1:A:294:HIS:HE1	2.01	0.44
2:D:1402:HEM:HBB2	2:D:1402:HEM:HMB2	2.00	0.44
1:C:282:ASN:HA	1:C:306:LEU:O	2.18	0.44
1:F:138:MET:CE	6:F:2214:HOH:O	2.65	0.44
1:D:359:ARG:HG2	6:D:2195:HOH:O	2.18	0.44
1:E:345:GLY:HA3	2:E:1402:HEM:C3C	2.53	0.43
3:E:1403:BCD:H16	3:E:1403:BCD:H661	1.68	0.43
3:B:1403:BCD:O61	3:B:1403:BCD:C12	2.66	0.43
1:C:345:GLY:HA3	2:C:1402:HEM:C3C	2.52	0.43
1:A:156:LEU:HB3	6:A:2254:HOH:O	2.18	0.43
1:D:236:GLU:HG3	6:D:2290:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:ARG:NH2	1:B:405:HIS:NE2	2.67	0.43
3:D:1403:BCD:C66	3:D:1403:BCD:O57	2.67	0.43
1:E:282:ASN:HA	1:E:306:LEU:O	2.19	0.43
1:C:234:GLY:HA2	2:C:1402:HEM:C2C	2.54	0.43
1:E:346:ASN:HD22	1:E:350:ARG:NH1	2.15	0.43
1:C:221:ASP:OD2	3:C:1403:BCD:O23	2.17	0.43
1:E:359:ARG:HG2	1:E:362[B]:ARG:NH2	2.25	0.43
1:D:398:PRO:HB2	1:D:400:LEU:HG	1.99	0.43
3:E:1403:BCD:H662	3:E:1403:BCD:H26	1.99	0.43
3:E:1403:BCD:H622	3:E:1403:BCD:H611	1.24	0.43
3:A:1403:BCD:O35	3:A:1403:BCD:H16	2.19	0.43
1:F:85:GLN:CB	6:F:2054:HOH:O	2.61	0.43
1:F:123:ARG:HG2	1:F:125:GLU:OE2	2.19	0.43
3:A:1403:BCD:H46	3:A:1403:BCD:H27	1.66	0.43
1:B:233:GLY:HA2	5:B:1409:EDO:H22	2.00	0.43
3:F:1403:BCD:H46	3:F:1403:BCD:H16	1.12	0.43
1:E:234:GLY:HA2	2:E:1402:HEM:C2C	2.54	0.43
1:C:233:GLY:HA2	5:C:1407:EDO:H22	2.01	0.43
1:C:141:ILE:HG21	1:C:231:LEU:HD23	2.00	0.43
1:B:177:LYS:O	1:B:181:THR:HG23	2.19	0.42
1:E:99:ARG:NE	1:E:347:GLN:HE22	2.05	0.42
1:B:378:ARG:HD3	1:B:387[A]:GLU:CD	2.39	0.42
1:F:183:ALA:O	1:F:187[B]:GLU:HG2	2.19	0.42
1:C:294:HIS:HD2	6:C:2367:HOH:O	2.02	0.42
1:D:200:PRO:HG3	6:D:2275:HOH:O	2.19	0.42
1:D:181:THR:HB	6:D:2243:HOH:O	2.19	0.42
1:A:4:MET:CG	4:A:1404:SO4:O2	2.68	0.42
1:A:211:SER:O	1:A:217:ARG:HG2	2.19	0.42
1:C:240:HIS:HD2	6:C:2320:HOH:O	2.01	0.42
1:A:366:ASP:O	1:A:368[A]:ARG:HG3	2.19	0.42
1:E:299:ARG:CG	1:E:299:ARG:HH11	2.05	0.42
1:A:144:MET:HE1	1:A:348:LEU:CD2	2.49	0.42
1:E:212:GLU:OE1	1:E:217[A]:ARG:CZ	2.68	0.42
1:A:49:TYR:CD1	1:A:317:VAL:HG21	2.55	0.42
1:D:209:VAL:O	1:D:217:ARG:NH2	2.52	0.42
3:C:1403:BCD:C45	3:C:1403:BCD:HO26	2.31	0.42
1:B:105:LYS:HD3	1:B:105:LYS:HA	1.75	0.42
1:C:190:LYS:NZ	1:C:221:ASP:OD1	2.45	0.41
1:B:198:ALA:C	1:B:199[B]:GLU:OE1	2.58	0.41
1:C:162:LEU:O	1:C:166:LEU:HG	2.19	0.41
1:B:282:ASN:HA	1:B:306:LEU:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:277:THR:O	1:E:278:SER:C	2.57	0.41
1:E:362[B]:ARG:HG2	1:E:363:ARG:HG3	2.01	0.41
1:D:282:ASN:HA	1:D:306:LEU:O	2.20	0.41
1:F:86:HIS:CE1	2:F:1402:HEM:O2D	2.60	0.41
1:F:3:GLN:CA	4:F:1406:SO4:O3	2.67	0.41
1:B:213:VAL:O	1:B:213:VAL:CG2	2.69	0.41
1:B:199[B]:GLU:OE1	1:B:199[B]:GLU:CA	2.66	0.41
1:E:278:SER:N	1:E:279:PRO:HD3	2.35	0.41
1:C:225:PHE:CE2	3:C:1403:BCD:H622	2.54	0.41
1:E:294:HIS:HD2	6:E:2357:HOH:O	2.03	0.41
1:A:144:MET:HB2	1:A:144:MET:HE2	1.60	0.41
1:A:187:GLU:OE1	6:A:2267:HOH:O	2.22	0.41
1:F:134:ALA:O	1:F:138:MET:HG3	2.21	0.41
1:A:99:ARG:HD2	1:A:103:MET:HG3	2.03	0.41
1:B:236:GLU:HG3	6:B:2302:HOH:O	2.21	0.41
1:B:81:MET:CE	1:B:89:ARG:HB3	2.50	0.41
1:C:83:ASP:OD1	1:C:86:HIS:CD2	2.71	0.41
1:A:114:ASP:OD1	6:A:2205:HOH:O	2.22	0.41
1:C:166:LEU:O	1:C:169:HIS:CE1	2.74	0.41
1:D:253:ARG:HA	1:D:253:ARG:HD2	1.78	0.41
1:F:138:MET:HE3	6:F:2211:HOH:O	2.21	0.40
1:F:196:ARG:HD3	1:F:196:ARG:HA	1.95	0.40
1:F:269:ALA:O	1:F:273:MET:HG3	2.21	0.40
1:B:199[A]:GLU:OE1	6:B:2278:HOH:O	2.22	0.40
1:E:7:ARG:NH1	4:E:1406:SO4:O2	2.45	0.40
1:C:253:ARG:HD2	1:C:253:ARG:HA	1.81	0.40
3:F:1403:BCD:H611	3:F:1403:BCD:H11	1.49	0.40
3:F:1403:BCD:H11	3:F:1403:BCD:O61	2.06	0.40
1:C:111:ARG:NE	6:C:2226:HOH:O	2.46	0.40
1:C:111:ARG:O	1:C:115:THR:HG23	2.20	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:2187:HOH:O	6:F:2414:HOH:O[3_545]	1.89	0.31

## 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	405/407 (100%)	393 (97%)	12 (3%)	0	100	100
1	B	407/407 (100%)	394 (97%)	13 (3%)	0	100	100
1	C	407/407 (100%)	391 (96%)	16 (4%)	0	100	100
1	D	407/407 (100%)	395 (97%)	12 (3%)	0	100	100
1	E	406/407 (100%)	395 (97%)	11 (3%)	0	100	100
1	F	406/407 (100%)	397 (98%)	9 (2%)	0	100	100
All	All	2438/2442 (100%)	2365 (97%)	73 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	340/349 (97%)	332 (98%)	8 (2%)	57	46
1	B	341/349 (98%)	330 (97%)	11 (3%)	46	32
1	C	343/349 (98%)	330 (96%)	13 (4%)	40	24
1	D	346/349 (99%)	336 (97%)	10 (3%)	50	36
1	E	345/349 (99%)	333 (96%)	12 (4%)	43	28
1	F	346/349 (99%)	337 (97%)	9 (3%)	54	42
All	All	2061/2094 (98%)	1998 (97%)	63 (3%)	50	33

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	TYR
1	A	99	ARG
1	A	105	LYS
1	A	125	GLU
1	A	169	HIS
1	A	199	GLU
1	A	371	ASP
1	A	378	ARG
1	B	77	TYR
1	B	104	ASP
1	B	125	GLU
1	B	138	MET
1	B	164	CYS
1	B	181	THR
1	B	216	GLN
1	B	265	LEU
1	B	378	ARG
1	B	403	HIS
1	B	405	HIS
1	C	65	THR
1	C	77	TYR
1	C	108	SER
1	C	202	ASP
1	C	253	ARG
1	C	265	LEU
1	C	368[A]	ARG
1	C	368[B]	ARG
1	C	371	ASP
1	C	372[A]	ASP
1	C	372[B]	ASP
1	C	378	ARG
1	C	399	VAL
1	D	40	ARG
1	D	77	TYR
1	D	99[A]	ARG
1	D	99[B]	ARG
1	D	125	GLU
1	D	171	ASP
1	D	181	THR
1	D	202	ASP
1	D	265	LEU
1	D	378	ARG

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Mol	Chain	Res	Type
1	E	77	TYR
1	E	99	ARG
1	E	125	GLU
1	E	138	MET
1	E	164	CYS
1	E	169	HIS
1	E	175	ILE
1	E	202	ASP
1	E	265	LEU
1	E	299	ARG
1	E	305	MET
1	E	371	ASP
1	F	77	TYR
1	F	99[A]	ARG
1	F	99[B]	ARG
1	F	100	LYS
1	F	105	LYS
1	F	168	SER
1	F	181	THR
1	F	199	GLU
1	F	299	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	HIS
1	A	94	ASN
1	A	216	GLN
1	A	240	HIS
1	A	294	HIS
1	A	323	ASN
1	A	341	HIS
1	A	346	ASN
1	B	3	GLN
1	B	72	GLN
1	B	86	HIS
1	B	240	HIS
1	B	294	HIS
1	B	323	ASN
1	B	341	HIS
1	B	346	ASN
1	C	72	GLN

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Mol	Chain	Res	Type
1	C	86	HIS
1	C	240	HIS
1	C	294	HIS
1	C	323	ASN
1	C	341	HIS
1	C	346	ASN
1	D	86	HIS
1	D	240	HIS
1	D	294	HIS
1	D	323	ASN
1	D	341	HIS
1	D	346	ASN
1	E	86	HIS
1	E	216	GLN
1	E	240	HIS
1	E	294	HIS
1	E	323	ASN
1	E	341	HIS
1	E	346	ASN
1	E	347	GLN
1	F	86	HIS
1	F	216	GLN
1	F	240	HIS
1	F	294	HIS
1	F	323	ASN
1	F	341	HIS
1	F	346	ASN
1	F	347	GLN
1	F	403	HIS

### 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 ⓘ

35 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	HEM	A	1402	1,5	30,50,50	2.50	13 (43%)	24,82,82	2.81	12 (50%)
3	BCD	A	1403	-	84,84,84	0.77	1 (1%)	126,126,126	2.31	49 (38%)
4	SO4	A	1404	-	4,4,4	0.84	0	6,6,6	1.46	1 (16%)
4	SO4	A	1405	-	4,4,4	0.72	0	6,6,6	0.72	0
5	EDO	A	1406	2	3,3,3	1.32	0	2,2,2	0.93	0
2	HEM	B	1402	1,5	30,50,50	2.54	12 (40%)	24,82,82	2.72	13 (54%)
3	BCD	B	1403	-	84,84,84	0.92	3 (3%)	126,126,126	2.69	59 (46%)
4	SO4	B	1406	-	4,4,4	1.16	0	6,6,6	0.66	0
4	SO4	B	1407	-	4,4,4	0.86	0	6,6,6	0.54	0
4	SO4	B	1408	-	4,4,4	1.16	0	6,6,6	0.95	0
5	EDO	B	1409	2	3,3,3	1.37	0	2,2,2	0.98	0
2	HEM	C	1402	1,5	30,50,50	2.58	9 (30%)	24,82,82	2.55	9 (37%)
3	BCD	C	1403	-	84,84,84	0.99	2 (2%)	126,126,126	2.47	53 (42%)
4	SO4	C	1404	-	4,4,4	1.19	0	6,6,6	0.97	0
4	SO4	C	1405	-	4,4,4	1.08	0	6,6,6	0.35	0
4	SO4	C	1406	-	4,4,4	0.77	0	6,6,6	0.61	0
5	EDO	C	1407	2	3,3,3	0.84	0	2,2,2	0.04	0
2	HEM	D	1402	1,5	30,50,50	2.40	12 (40%)	24,82,82	2.81	12 (50%)
3	BCD	D	1403	-	84,84,84	0.70	1 (1%)	126,126,126	2.03	42 (33%)
4	SO4	D	1404	-	4,4,4	1.12	0	6,6,6	0.59	0
4	SO4	D	1405	-	4,4,4	1.41	0	6,6,6	0.49	0
4	SO4	D	1406	-	4,4,4	0.99	0	6,6,6	1.25	1 (16%)
5	EDO	D	1407	2	3,3,3	1.15	0	2,2,2	0.84	0
2	HEM	E	1402	1,5	30,50,50	2.44	12 (40%)	24,82,82	2.68	11 (45%)
3	BCD	E	1403	-	84,84,84	0.92	0	126,126,126	2.96	55 (43%)
4	SO4	E	1404	-	4,4,4	1.11	0	6,6,6	0.78	0
4	SO4	E	1405	-	4,4,4	1.17	0	6,6,6	0.63	0
4	SO4	E	1406	1	4,4,4	0.85	0	6,6,6	0.83	0
5	EDO	E	1407	2	3,3,3	1.38	0	2,2,2	0.91	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	HEM	F	1402	1,5	30,50,50	2.37	7 (23%)	24,82,82	3.05	12 (50%)
3	BCD	F	1403	-	84,84,84	0.69	1 (1%)	126,126,126	2.34	53 (42%)
4	SO4	F	1404	-	4,4,4	0.91	0	6,6,6	0.53	0
4	SO4	F	1405	-	4,4,4	1.57	1 (25%)	6,6,6	1.01	1 (16%)
4	SO4	F	1406	-	4,4,4	0.77	0	6,6,6	0.59	0
5	EDO	F	1407	2	3,3,3	1.30	0	2,2,2	0.73	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	1402	1,5	-	0/10/54/54	0/0/8/8
3	BCD	A	1403	-	2/2/35/35	0/42/182/182	0/0/8/8
4	SO4	A	1404	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1405	-	-	0/0/0/0	0/0/0/0
5	EDO	A	1406	2	-	0/1/1/1	0/0/0/0
2	HEM	B	1402	1,5	-	0/10/54/54	0/0/8/8
3	BCD	B	1403	-	2/2/35/35	0/42/182/182	0/0/8/8
4	SO4	B	1406	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1407	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1408	-	-	0/0/0/0	0/0/0/0
5	EDO	B	1409	2	-	0/1/1/1	0/0/0/0
2	HEM	C	1402	1,5	-	0/10/54/54	0/0/8/8
3	BCD	C	1403	-	2/2/35/35	0/42/182/182	0/0/8/8
4	SO4	C	1404	-	-	0/0/0/0	0/0/0/0
4	SO4	C	1405	-	-	0/0/0/0	0/0/0/0
4	SO4	C	1406	-	-	0/0/0/0	0/0/0/0
5	EDO	C	1407	2	-	0/1/1/1	0/0/0/0
2	HEM	D	1402	1,5	-	0/10/54/54	0/0/8/8
3	BCD	D	1403	-	1/1/35/35	0/42/182/182	0/0/8/8
4	SO4	D	1404	-	-	0/0/0/0	0/0/0/0
4	SO4	D	1405	-	-	0/0/0/0	0/0/0/0
4	SO4	D	1406	-	-	0/0/0/0	0/0/0/0
5	EDO	D	1407	2	-	0/1/1/1	0/0/0/0
2	HEM	E	1402	1,5	-	0/10/54/54	0/0/8/8
3	BCD	E	1403	-	3/3/35/35	0/42/182/182	0/0/8/8
4	SO4	E	1404	-	-	0/0/0/0	0/0/0/0
4	SO4	E	1405	-	-	0/0/0/0	0/0/0/0
4	SO4	E	1406	1	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	E	1407	2	-	0/1/1/1	0/0/0/0
2	HEM	F	1402	1,5	-	0/10/54/54	0/0/8/8
3	BCD	F	1403	-	2/2/35/35	1/42/182/182	0/0/8/8
4	SO4	F	1404	-	-	0/0/0/0	0/0/0/0
4	SO4	F	1405	-	-	0/0/0/0	0/0/0/0
4	SO4	F	1406	-	-	0/0/0/0	0/0/0/0
5	EDO	F	1407	2	-	0/1/1/1	0/0/0/0

All (74) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1402	HEM	C3B-C4B	-9.42	1.43	1.51
2	B	1402	HEM	C3B-C4B	-9.07	1.43	1.51
2	F	1402	HEM	C3B-C4B	-8.91	1.43	1.51
2	D	1402	HEM	C3B-C4B	-8.71	1.44	1.51
2	E	1402	HEM	C3B-C4B	-8.49	1.44	1.51
2	A	1402	HEM	C3B-C4B	-7.43	1.45	1.51
2	C	1402	HEM	C3D-C4D	-5.72	1.44	1.51
2	A	1402	HEM	C3D-C4D	-5.51	1.44	1.51
2	F	1402	HEM	C3D-C4D	-5.47	1.44	1.51
2	B	1402	HEM	C3D-C4D	-4.44	1.45	1.51
2	D	1402	HEM	C3D-C4D	-4.26	1.46	1.51
2	D	1402	HEM	C2C-C1C	-3.68	1.45	1.52
2	E	1402	HEM	C3D-C4D	-3.45	1.47	1.51
2	C	1402	HEM	C2C-C1C	-3.44	1.46	1.52
2	A	1402	HEM	C2C-C1C	-3.40	1.46	1.52
2	E	1402	HEM	C2C-C1C	-3.27	1.46	1.52
2	B	1402	HEM	C2C-C1C	-2.72	1.47	1.52
2	F	1402	HEM	C2C-C1C	-2.72	1.47	1.52
2	E	1402	HEM	C2B-C1B	-2.61	1.43	1.51
2	A	1402	HEM	C2B-C1B	-2.30	1.44	1.51
2	A	1402	HEM	C2D-C1D	-2.29	1.44	1.51
2	F	1402	HEM	C2B-C1B	-2.23	1.44	1.51
2	B	1402	HEM	C2B-C1B	-2.20	1.44	1.51
2	C	1402	HEM	C2D-C1D	-2.19	1.44	1.51
2	A	1402	HEM	CAD-C3D	-2.19	1.49	1.54
2	C	1402	HEM	CAD-C3D	-2.12	1.49	1.54
2	F	1402	HEM	C4C-NC	2.01	1.38	1.36
2	E	1402	HEM	CMD-C2D	2.02	1.57	1.53
2	D	1402	HEM	C4C-NC	2.02	1.38	1.36
2	F	1402	HEM	CMB-C2B	2.04	1.57	1.53
2	D	1402	HEM	FE-NC	2.06	2.03	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1403	BCD	O42-C13	2.07	1.47	1.41
2	E	1402	HEM	CMA-C3A	2.10	1.56	1.51
2	B	1402	HEM	CMD-C2D	2.11	1.58	1.53
2	D	1402	HEM	C3C-CAC	2.14	1.55	1.51
2	B	1402	HEM	CMC-C2C	2.14	1.58	1.53
3	F	1403	BCD	O51-C11	2.15	1.47	1.41
2	D	1402	HEM	C1C-NC	2.20	1.38	1.36
2	C	1402	HEM	FE-NB	2.21	2.09	1.97
2	D	1402	HEM	C3B-CAB	2.22	1.55	1.51
2	D	1402	HEM	CMC-C2C	2.25	1.58	1.53
3	A	1403	BCD	O52-C12	2.26	1.47	1.41
3	B	1403	BCD	O25-C25	2.27	1.48	1.43
4	F	1405	SO4	O3-S	2.29	1.55	1.47
2	E	1402	HEM	CMB-C2B	2.29	1.58	1.53
3	B	1403	BCD	O56-C16	2.30	1.47	1.41
3	C	1403	BCD	C33-C23	2.32	1.58	1.52
2	B	1402	HEM	CMA-C3A	2.33	1.56	1.51
2	E	1402	HEM	FE-NC	2.35	2.05	1.95
2	D	1402	HEM	CMD-C2D	2.39	1.58	1.53
2	A	1402	HEM	CMC-C2C	2.43	1.58	1.53
2	B	1402	HEM	CMB-C2B	2.49	1.58	1.53
2	B	1402	HEM	FE-NC	2.51	2.05	1.95
2	A	1402	HEM	FE-NC	2.56	2.05	1.95
2	D	1402	HEM	CMB-C2B	2.57	1.59	1.53
2	E	1402	HEM	CAA-C2A	2.58	1.56	1.52
2	E	1402	HEM	C1C-NC	2.71	1.39	1.36
2	F	1402	HEM	C3C-CAC	2.74	1.56	1.51
2	C	1402	HEM	FE-NC	2.78	2.06	1.95
2	A	1402	HEM	C4C-NC	2.82	1.39	1.36
2	A	1402	HEM	CMB-C2B	2.83	1.59	1.53
2	C	1402	HEM	C3C-CAC	2.85	1.56	1.51
2	D	1402	HEM	CAA-C2A	2.90	1.57	1.52
2	B	1402	HEM	C1C-NC	2.90	1.39	1.36
2	A	1402	HEM	C1C-NC	2.95	1.39	1.36
2	E	1402	HEM	FE-ND	2.97	2.13	1.97
2	B	1402	HEM	CAA-C2A	3.02	1.57	1.52
2	A	1402	HEM	C3C-CAC	3.14	1.57	1.51
2	A	1402	HEM	FE-ND	3.14	2.14	1.97
2	B	1402	HEM	C3C-CAC	3.35	1.57	1.51
2	C	1402	HEM	FE-ND	3.59	2.16	1.97
2	E	1402	HEM	C3C-CAC	3.72	1.58	1.51
3	B	1403	BCD	O52-C12	3.75	1.51	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1403	BCD	O52-C12	3.93	1.51	1.41

All (383) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1403	BCD	O54-C54-C44	-10.39	87.79	109.75
3	E	1403	BCD	O55-C55-C45	-9.36	89.97	109.75
3	E	1403	BCD	C15-O44-C44	-8.50	95.79	118.01
3	C	1403	BCD	O53-C53-C43	-8.45	91.90	109.75
3	F	1403	BCD	C37-C47-C57	-8.14	92.44	110.84
2	F	1402	HEM	C3C-CAC-CBC	-7.89	112.36	124.46
3	A	1403	BCD	C36-C46-C56	-7.75	93.32	110.84
3	A	1403	BCD	C14-O43-C43	-7.47	98.50	118.01
3	B	1403	BCD	C36-C46-C56	-7.00	95.01	110.84
3	E	1403	BCD	C12-O41-C41	-6.91	99.95	118.01
3	E	1403	BCD	C16-O45-C45	-6.84	100.15	118.01
3	B	1403	BCD	C33-C43-C53	-6.24	96.72	110.84
2	D	1402	HEM	C3B-CAB-CBB	-5.96	115.31	124.46
3	B	1403	BCD	C13-C23-C33	-5.93	98.28	109.97
3	C	1403	BCD	C13-O42-C42	-5.87	102.68	118.01
3	B	1403	BCD	O53-C53-C43	-5.66	97.79	109.75
3	C	1403	BCD	C15-O44-C44	-5.61	103.35	118.01
2	F	1402	HEM	C3B-CAB-CBB	-5.40	116.17	124.46
3	E	1403	BCD	C17-O57-C57	-5.40	103.26	113.75
3	C	1403	BCD	O54-C54-C44	-5.34	98.47	109.75
3	C	1403	BCD	C17-O57-C57	-5.31	103.43	113.75
3	B	1403	BCD	O27-C27-C37	-5.26	98.49	110.34
3	E	1403	BCD	O53-C13-C23	-5.24	99.52	110.28
3	F	1403	BCD	O51-C51-C61	-5.21	93.17	106.36
3	D	1403	BCD	C27-C37-C47	-5.16	98.27	109.60
3	A	1403	BCD	C13-O42-C42	-5.07	104.76	118.01
3	B	1403	BCD	C15-O44-C44	-5.02	104.89	118.01
3	B	1403	BCD	O41-C12-C22	-4.99	95.95	108.10
3	E	1403	BCD	C35-C45-C55	-4.95	99.65	110.84
3	B	1403	BCD	C12-O41-C41	-4.89	105.23	118.01
2	A	1402	HEM	C3B-CAB-CBB	-4.81	117.08	124.46
3	F	1403	BCD	C14-O54-C54	-4.78	104.47	113.75
3	F	1403	BCD	O56-C56-C46	-4.75	99.72	109.75
2	E	1402	HEM	C3B-CAB-CBB	-4.65	117.32	124.46
3	F	1403	BCD	C12-O41-C41	-4.64	105.89	118.01
3	B	1403	BCD	C32-C42-C52	-4.63	100.36	110.84
3	B	1403	BCD	O53-C13-C23	-4.63	100.78	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1403	BCD	C37-C47-C57	-4.62	100.39	110.84
3	A	1403	BCD	O44-C44-C34	-4.49	95.59	107.17
3	F	1403	BCD	C16-C26-C36	-4.46	101.19	109.97
3	E	1403	BCD	O23-C23-C13	-4.39	100.39	110.02
3	B	1403	BCD	O52-C52-C42	-4.34	100.57	109.75
3	F	1403	BCD	C26-C36-C46	-4.32	100.11	109.60
2	C	1402	HEM	C3B-CAB-CBB	-4.30	117.86	124.46
3	B	1403	BCD	C15-C25-C35	-4.29	101.53	109.97
2	B	1402	HEM	CBA-CAA-C2A	-4.28	104.85	112.53
3	D	1403	BCD	C17-C27-C37	-4.25	101.60	109.97
3	A	1403	BCD	O22-C22-C32	-4.22	100.83	110.34
3	E	1403	BCD	C32-C42-C52	-4.12	101.52	110.84
2	B	1402	HEM	C3B-CAB-CBB	-4.01	118.31	124.46
3	A	1403	BCD	O42-C13-O53	-3.98	100.62	110.68
3	B	1403	BCD	O66-C66-C56	-3.97	98.21	111.33
3	F	1403	BCD	C16-O56-C56	-3.93	106.12	113.75
3	C	1403	BCD	O57-C17-C27	-3.88	102.31	110.28
3	E	1403	BCD	O57-C57-C47	-3.87	101.57	109.75
3	A	1403	BCD	O35-C35-C45	-3.83	100.81	109.87
3	D	1403	BCD	C26-C36-C46	-3.80	101.25	109.60
3	F	1403	BCD	C16-O45-C45	-3.78	108.14	118.01
3	C	1403	BCD	C16-O45-C45	-3.77	108.17	118.01
3	D	1403	BCD	C14-O54-C54	-3.69	106.58	113.75
2	A	1402	HEM	CBA-CAA-C2A	-3.60	106.07	112.53
3	D	1403	BCD	O52-C52-C62	-3.54	97.40	106.36
3	C	1403	BCD	O34-C34-C44	-3.48	101.65	109.87
3	A	1403	BCD	O47-C47-C37	-3.46	98.22	107.17
3	F	1403	BCD	O67-C67-C57	-3.43	100.01	111.33
3	F	1403	BCD	C27-C37-C47	-3.42	102.08	109.60
3	B	1403	BCD	C13-O42-C42	-3.40	109.11	118.01
3	A	1403	BCD	C37-C47-C57	-3.40	103.15	110.84
3	B	1403	BCD	C67-C57-C47	-3.33	103.56	113.25
3	D	1403	BCD	C11-O47-C47	-3.33	109.31	118.01
3	F	1403	BCD	C17-O46-C46	-3.30	109.38	118.01
3	E	1403	BCD	C15-O55-C55	-3.30	107.35	113.75
3	C	1403	BCD	C36-C46-C56	-3.28	103.42	110.84
3	C	1403	BCD	C16-C26-C36	-3.24	103.58	109.97
3	E	1403	BCD	O44-C15-O55	-3.21	102.55	110.68
3	E	1403	BCD	C16-C26-C36	-3.18	103.70	109.97
3	C	1403	BCD	O56-C16-C26	-3.18	103.75	110.28
3	F	1403	BCD	O46-C17-O57	-3.17	102.65	110.68
3	A	1403	BCD	C34-C44-C54	-3.16	103.70	110.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1403	BCD	C32-C42-C52	-3.15	103.70	110.84
3	E	1403	BCD	C33-C43-C53	-3.14	103.75	110.84
3	B	1403	BCD	O34-C34-C44	-3.12	102.50	109.87
2	F	1402	HEM	CAA-CBA-CGA	-3.11	107.05	112.75
3	B	1403	BCD	O21-C21-C11	-3.10	103.23	110.02
3	A	1403	BCD	O53-C53-C43	-3.09	103.23	109.75
2	B	1402	HEM	CAA-C2A-C1A	-3.07	123.67	127.01
3	C	1403	BCD	C35-C45-C55	-3.05	103.94	110.84
3	D	1403	BCD	C17-O46-C46	-3.05	110.05	118.01
3	F	1403	BCD	O61-C61-C51	-3.01	101.38	111.33
3	A	1403	BCD	C31-C41-C51	-3.00	104.05	110.84
3	D	1403	BCD	O54-C54-C64	-3.00	98.78	106.36
3	E	1403	BCD	C36-C46-C56	-2.99	104.07	110.84
3	E	1403	BCD	O56-C16-C26	-2.98	104.16	110.28
3	B	1403	BCD	C22-C32-C42	-2.96	103.09	109.60
3	F	1403	BCD	C36-C46-C56	-2.96	104.15	110.84
3	F	1403	BCD	O55-C15-C25	-2.94	104.25	110.28
3	D	1403	BCD	O31-C31-C21	-2.92	103.76	110.34
3	C	1403	BCD	C32-C42-C52	-2.92	104.24	110.84
3	F	1403	BCD	O62-C62-C52	-2.92	101.70	111.33
3	B	1403	BCD	C16-O45-C45	-2.90	110.43	118.01
3	E	1403	BCD	C24-C34-C44	-2.86	103.32	109.60
3	E	1403	BCD	O43-C14-O54	-2.86	103.45	110.68
2	D	1402	HEM	CBD-CAD-C3D	-2.85	105.25	113.55
3	F	1403	BCD	O54-C14-C24	-2.83	104.47	110.28
3	B	1403	BCD	O55-C55-C45	-2.82	103.78	109.75
4	D	1406	SO4	O2-S-O1	-2.76	100.76	109.50
3	A	1403	BCD	C11-O51-C51	-2.74	108.42	113.75
2	A	1402	HEM	CBD-CAD-C3D	-2.73	105.60	113.55
2	C	1402	HEM	CAA-C2A-C1A	-2.71	124.07	127.01
3	E	1403	BCD	O61-C61-C51	-2.70	102.40	111.33
3	B	1403	BCD	C16-O56-C56	-2.65	108.59	113.75
3	E	1403	BCD	C11-O51-C51	-2.65	108.61	113.75
3	D	1403	BCD	C14-O43-C43	-2.64	111.10	118.01
2	D	1402	HEM	CAA-CBA-CGA	-2.62	107.95	112.75
3	A	1403	BCD	O45-C16-O56	-2.62	104.06	110.68
2	D	1402	HEM	CMA-C3A-C4A	-2.62	124.04	128.36
3	B	1403	BCD	O55-C15-C25	-2.58	104.98	110.28
3	C	1403	BCD	O56-C56-C46	-2.57	104.31	109.75
3	B	1403	BCD	O43-C14-O54	-2.57	104.19	110.68
3	A	1403	BCD	C17-O46-C46	-2.56	111.31	118.01
3	E	1403	BCD	C25-C35-C45	-2.56	103.97	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1403	BCD	C15-O44-C44	-2.54	111.38	118.01
3	C	1403	BCD	C33-C43-C53	-2.53	105.11	110.84
3	D	1403	BCD	C15-O44-C44	-2.52	111.43	118.01
3	E	1403	BCD	O65-C65-C55	-2.51	103.04	111.33
2	F	1402	HEM	CBD-CAD-C3D	-2.51	106.26	113.55
3	C	1403	BCD	O52-C52-C42	-2.50	104.47	109.75
3	B	1403	BCD	C24-C34-C44	-2.49	104.12	109.60
3	A	1403	BCD	C17-C27-C37	-2.47	105.10	109.97
3	B	1403	BCD	C11-O51-C51	-2.45	108.99	113.75
3	D	1403	BCD	O31-C31-C41	-2.42	104.14	109.87
3	F	1403	BCD	C25-C35-C45	-2.42	104.29	109.60
3	B	1403	BCD	O67-C67-C57	-2.41	103.36	111.33
2	E	1402	HEM	CBD-CAD-C3D	-2.39	106.59	113.55
3	D	1403	BCD	C11-C21-C31	-2.38	105.28	109.97
2	E	1402	HEM	CAA-CBA-CGA	-2.38	108.39	112.75
3	B	1403	BCD	O51-C51-C41	-2.34	104.81	109.75
3	D	1403	BCD	C33-C43-C53	-2.33	105.57	110.84
4	F	1405	SO4	O2-S-O1	-2.32	102.14	109.50
3	D	1403	BCD	C12-O41-C41	-2.32	111.94	118.01
2	A	1402	HEM	C3B-C4B-NB	-2.32	107.20	111.63
3	C	1403	BCD	C37-C47-C57	-2.31	105.62	110.84
3	F	1403	BCD	C11-O51-C51	-2.27	109.33	113.75
2	F	1402	HEM	CBA-CAA-C2A	-2.26	108.47	112.53
3	F	1403	BCD	C33-C43-C53	-2.26	105.73	110.84
3	F	1403	BCD	O33-C33-C23	-2.26	105.26	110.34
3	A	1403	BCD	C13-C23-C33	-2.25	105.53	109.97
3	D	1403	BCD	C35-C45-C55	-2.24	105.77	110.84
3	F	1403	BCD	O21-C21-C31	-2.23	105.31	110.34
3	C	1403	BCD	O26-C26-C16	-2.23	105.14	110.02
3	F	1403	BCD	O34-C34-C44	-2.22	104.61	109.87
3	D	1403	BCD	C14-C24-C34	-2.20	105.63	109.97
2	B	1402	HEM	CBD-CAD-C3D	-2.20	107.16	113.55
3	B	1403	BCD	C27-C37-C47	-2.19	104.80	109.60
3	C	1403	BCD	C14-O43-C43	-2.18	112.30	118.01
3	A	1403	BCD	O52-C52-C42	-2.18	105.14	109.75
3	B	1403	BCD	O54-C54-C44	-2.17	105.16	109.75
2	F	1402	HEM	CAA-C2A-C1A	-2.16	124.66	127.01
3	B	1403	BCD	O47-C47-C57	-2.15	103.66	109.32
2	C	1402	HEM	CAA-CBA-CGA	-2.15	108.80	112.75
2	A	1402	HEM	CMA-C3A-C4A	-2.15	124.80	128.36
3	F	1403	BCD	O27-C27-C37	-2.15	105.49	110.34
3	F	1403	BCD	C12-C22-C32	-2.14	105.75	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1402	HEM	CBA-CAA-C2A	-2.14	108.70	112.53
3	C	1403	BCD	O67-C67-C57	-2.13	104.28	111.33
2	B	1402	HEM	CAA-CBA-CGA	-2.13	108.84	112.75
3	E	1403	BCD	O51-C11-C21	-2.13	105.90	110.28
3	E	1403	BCD	C21-C31-C41	-2.12	104.95	109.60
3	C	1403	BCD	O23-C23-C13	-2.10	105.42	110.02
3	E	1403	BCD	O56-C56-C46	-2.08	105.34	109.75
3	C	1403	BCD	O31-C31-C21	-2.07	105.67	110.34
2	E	1402	HEM	C3B-C4B-NB	-2.07	107.67	111.63
3	A	1403	BCD	O45-C45-C35	-2.07	101.82	107.17
2	B	1402	HEM	C3C-CAC-CBC	-2.07	121.28	124.46
2	B	1402	HEM	C3B-C4B-NB	-2.06	107.69	111.63
3	F	1403	BCD	C35-C45-C55	-2.05	106.20	110.84
3	A	1403	BCD	O21-C21-C11	-2.04	105.55	110.02
2	D	1402	HEM	CBA-CAA-C2A	-2.04	108.87	112.53
3	F	1403	BCD	O57-C57-C67	-2.03	101.22	106.36
3	A	1403	BCD	O43-C43-C53	-2.03	103.98	109.32
3	D	1403	BCD	O45-C16-O56	-2.01	105.60	110.68
3	E	1403	BCD	O24-C24-C34	-2.01	105.82	110.34
3	A	1403	BCD	O56-C56-C46	-2.00	105.51	109.75
3	C	1403	BCD	C13-O53-C53	-2.00	109.86	113.75
3	A	1403	BCD	O44-C15-C25	2.01	112.99	108.10
3	E	1403	BCD	O21-C21-C31	2.01	114.86	110.34
3	F	1403	BCD	O56-C56-C66	2.01	111.44	106.36
3	B	1403	BCD	O46-C17-O57	2.01	115.78	110.68
3	E	1403	BCD	O43-C43-C53	2.02	114.62	109.32
3	A	1403	BCD	C16-O56-C56	2.02	117.67	113.75
3	F	1403	BCD	O52-C12-C22	2.03	114.44	110.28
3	D	1403	BCD	O44-C44-C34	2.04	112.43	107.17
3	D	1403	BCD	O56-C16-C26	2.04	114.47	110.28
3	A	1403	BCD	C15-O55-C55	2.04	117.71	113.75
3	D	1403	BCD	O63-C63-C53	2.06	118.15	111.33
3	F	1403	BCD	O45-C16-C26	2.08	113.16	108.10
3	E	1403	BCD	O46-C17-C27	2.09	113.19	108.10
3	A	1403	BCD	O55-C15-C25	2.10	114.58	110.28
3	F	1403	BCD	O41-C41-C51	2.11	114.87	109.32
3	B	1403	BCD	O51-C11-C21	2.11	114.61	110.28
3	B	1403	BCD	O51-C51-C61	2.12	111.70	106.36
3	C	1403	BCD	C62-C52-C42	2.12	119.41	113.25
3	A	1403	BCD	O56-C56-C66	2.13	111.74	106.36
3	C	1403	BCD	O45-C45-C35	2.13	112.67	107.17
3	B	1403	BCD	O31-C31-C41	2.14	114.94	109.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1403	BCD	O47-C47-C57	2.16	114.99	109.32
3	C	1403	BCD	O31-C31-C41	2.16	114.98	109.87
3	B	1403	BCD	C25-C35-C45	2.16	114.34	109.60
3	C	1403	BCD	O47-C11-O51	2.17	116.17	110.68
3	F	1403	BCD	O44-C44-C34	2.20	112.86	107.17
3	A	1403	BCD	O57-C57-C67	2.21	111.94	106.36
3	B	1403	BCD	O36-C36-C46	2.21	115.10	109.87
3	F	1403	BCD	O25-C25-C35	2.21	115.31	110.34
3	A	1403	BCD	C12-C22-C32	2.21	114.33	109.97
3	C	1403	BCD	O35-C35-C45	2.22	115.13	109.87
3	C	1403	BCD	C12-C22-C32	2.23	114.38	109.97
3	C	1403	BCD	O23-C23-C33	2.24	115.37	110.34
3	A	1403	BCD	O44-C44-C54	2.25	115.25	109.32
3	D	1403	BCD	O43-C43-C53	2.26	115.26	109.32
3	E	1403	BCD	O33-C33-C43	2.27	115.24	109.87
3	D	1403	BCD	O34-C34-C24	2.28	115.47	110.34
3	C	1403	BCD	O54-C54-C64	2.29	112.13	106.36
3	C	1403	BCD	O51-C51-C61	2.30	112.16	106.36
3	C	1403	BCD	O27-C27-C17	2.30	115.06	110.02
2	D	1402	HEM	C2C-C1C-CHC	2.32	127.22	123.68
3	A	1403	BCD	O33-C33-C43	2.34	115.41	109.87
3	B	1403	BCD	O32-C32-C42	2.35	115.43	109.87
3	B	1403	BCD	O54-C54-C64	2.36	112.32	106.36
2	D	1402	HEM	C2D-C3D-C4D	2.36	105.50	101.50
3	D	1403	BCD	O22-C22-C12	2.36	115.20	110.02
3	F	1403	BCD	O31-C31-C21	2.37	115.67	110.34
3	C	1403	BCD	C63-C53-C43	2.37	120.14	113.25
3	F	1403	BCD	O65-C65-C55	2.37	119.18	111.33
2	A	1402	HEM	C1D-CHD-C4C	2.37	129.79	125.82
3	A	1403	BCD	C62-C52-C42	2.41	120.25	113.25
3	E	1403	BCD	C14-C24-C34	2.42	114.75	109.97
3	A	1403	BCD	O23-C23-C13	2.43	115.34	110.02
3	D	1403	BCD	O41-C12-C22	2.45	114.06	108.10
3	C	1403	BCD	O46-C46-C36	2.47	113.53	107.17
3	A	1403	BCD	C11-O47-C47	2.48	124.48	118.01
3	C	1403	BCD	C13-C23-C33	2.49	114.88	109.97
3	F	1403	BCD	O35-C35-C25	2.50	115.97	110.34
3	E	1403	BCD	O46-C17-O57	2.51	117.03	110.68
3	D	1403	BCD	O25-C25-C15	2.51	115.53	110.02
3	C	1403	BCD	O53-C13-C23	2.53	115.47	110.28
3	F	1403	BCD	O36-C36-C26	2.56	116.09	110.34
3	D	1403	BCD	O32-C32-C42	2.56	115.93	109.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1403	BCD	O45-C45-C35	2.57	113.79	107.17
3	B	1403	BCD	C13-O53-C53	2.57	118.74	113.75
3	F	1403	BCD	O46-C46-C36	2.58	113.83	107.17
3	E	1403	BCD	O45-C16-O56	2.59	117.23	110.68
3	B	1403	BCD	O47-C47-C37	2.59	113.85	107.17
3	D	1403	BCD	O44-C44-C54	2.60	116.15	109.32
3	F	1403	BCD	O55-C55-C65	2.62	112.97	106.36
3	E	1403	BCD	O54-C14-C24	2.62	115.65	110.28
3	C	1403	BCD	C11-C21-C31	2.64	115.17	109.97
3	D	1403	BCD	O46-C17-C27	2.66	114.58	108.10
3	A	1403	BCD	O52-C12-C22	2.68	115.78	110.28
3	F	1403	BCD	O47-C47-C57	2.71	116.44	109.32
3	F	1403	BCD	O23-C23-C13	2.75	116.05	110.02
2	C	1402	HEM	CMD-C2D-C3D	2.75	126.53	114.35
3	C	1403	BCD	O26-C26-C36	2.76	116.54	110.34
3	D	1403	BCD	O26-C26-C16	2.79	116.13	110.02
3	C	1403	BCD	C67-C57-C47	2.81	121.42	113.25
3	B	1403	BCD	O55-C55-C65	2.81	113.46	106.36
3	D	1403	BCD	O45-C45-C55	2.87	116.86	109.32
3	B	1403	BCD	O43-C43-C53	2.87	116.86	109.32
3	A	1403	BCD	O32-C32-C42	2.88	116.68	109.87
3	D	1403	BCD	O53-C13-C23	2.88	116.18	110.28
3	D	1403	BCD	O43-C14-C24	2.91	115.18	108.10
3	B	1403	BCD	O34-C34-C24	2.92	116.92	110.34
3	F	1403	BCD	O33-C33-C43	2.94	116.83	109.87
3	E	1403	BCD	C64-C54-C44	2.94	121.80	113.25
4	A	1404	SO4	O2-S-O1	2.95	118.83	109.50
3	A	1403	BCD	C11-C21-C31	2.95	115.78	109.97
3	C	1403	BCD	O41-C12-O52	2.95	118.14	110.68
3	C	1403	BCD	C14-C24-C34	2.95	115.79	109.97
3	C	1403	BCD	O22-C22-C12	2.98	116.54	110.02
3	E	1403	BCD	C13-C23-C33	2.98	115.85	109.97
3	E	1403	BCD	O41-C12-C22	2.98	115.36	108.10
2	E	1402	HEM	C2D-C3D-C4D	3.00	106.58	101.50
3	A	1403	BCD	O47-C11-O51	3.06	118.42	110.68
3	E	1403	BCD	O45-C45-C35	3.07	115.09	107.17
3	A	1403	BCD	O36-C36-C26	3.09	117.30	110.34
3	A	1403	BCD	O62-C62-C52	3.11	121.61	111.33
3	B	1403	BCD	O25-C25-C15	3.13	116.88	110.02
3	B	1403	BCD	C66-C56-C46	3.13	122.36	113.25
3	F	1403	BCD	O47-C47-C37	3.16	115.31	107.17
3	E	1403	BCD	O45-C16-C26	3.21	115.91	108.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1402	HEM	C2D-C3D-C4D	3.23	106.98	101.50
3	E	1403	BCD	O46-C46-C56	3.25	117.85	109.32
3	A	1403	BCD	O56-C16-C26	3.31	117.07	110.28
2	A	1402	HEM	CMD-C2D-C3D	3.32	129.01	114.35
2	B	1402	HEM	C2D-C3D-C4D	3.32	107.12	101.50
3	F	1403	BCD	O26-C26-C36	3.34	117.86	110.34
3	C	1403	BCD	O55-C55-C65	3.35	114.81	106.36
3	A	1403	BCD	C66-C56-C46	3.38	123.07	113.25
2	F	1402	HEM	CMD-C2D-C3D	3.39	129.33	114.35
3	B	1403	BCD	O41-C12-O52	3.45	119.41	110.68
3	E	1403	BCD	O26-C26-C36	3.47	118.15	110.34
2	D	1402	HEM	CMD-C2D-C3D	3.49	129.78	114.35
2	A	1402	HEM	C2D-C3D-C4D	3.53	107.48	101.50
2	F	1402	HEM	CMC-C2C-C3C	3.54	125.38	116.53
3	A	1403	BCD	O25-C25-C15	3.56	117.82	110.02
2	B	1402	HEM	CAD-C3D-C4D	3.60	125.15	112.47
2	B	1402	HEM	CMD-C2D-C3D	3.60	130.28	114.35
3	D	1403	BCD	C62-C52-C42	3.66	123.90	113.25
2	E	1402	HEM	CMD-C2D-C3D	3.66	130.55	114.35
3	E	1403	BCD	C17-C27-C37	3.67	117.20	109.97
3	E	1403	BCD	O52-C52-C62	3.71	115.73	106.36
3	D	1403	BCD	O47-C47-C37	3.71	116.75	107.17
2	C	1402	HEM	C2D-C3D-C4D	3.71	107.79	101.50
2	A	1402	HEM	CAD-C3D-C4D	3.71	125.57	112.47
3	B	1403	BCD	O54-C14-C24	3.72	117.90	110.28
3	B	1403	BCD	C16-C26-C36	3.74	117.34	109.97
3	A	1403	BCD	C63-C53-C43	3.74	124.13	113.25
3	C	1403	BCD	O44-C44-C54	3.75	119.19	109.32
3	F	1403	BCD	O47-C11-C21	3.76	117.25	108.10
2	F	1402	HEM	CAD-C3D-C4D	3.77	125.75	112.47
3	B	1403	BCD	O56-C16-C26	3.77	118.00	110.28
3	C	1403	BCD	O54-C14-C24	3.81	118.09	110.28
3	D	1403	BCD	O23-C23-C13	3.84	118.44	110.02
3	E	1403	BCD	O46-C46-C36	3.85	117.10	107.17
3	B	1403	BCD	C63-C53-C43	3.86	124.48	113.25
2	C	1402	HEM	CAD-C3D-C4D	3.92	126.29	112.47
3	F	1403	BCD	C17-C27-C37	3.93	117.72	109.97
3	A	1403	BCD	O51-C51-C61	3.97	116.38	106.36
3	F	1403	BCD	O41-C12-C22	3.98	117.79	108.10
3	D	1403	BCD	O42-C42-C52	3.98	119.79	109.32
2	C	1402	HEM	CMC-C2C-C3C	4.03	126.59	116.53
3	D	1403	BCD	O44-C15-C25	4.03	117.92	108.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1403	BCD	O44-C15-C25	4.04	117.94	108.10
3	F	1403	BCD	O27-C27-C17	4.06	118.92	110.02
3	F	1403	BCD	O43-C14-C24	4.08	118.04	108.10
2	E	1402	HEM	CAD-C3D-C4D	4.14	127.08	112.47
3	E	1403	BCD	C65-C55-C45	4.17	125.39	113.25
3	C	1403	BCD	O53-C53-C63	4.20	116.98	106.36
3	B	1403	BCD	O46-C46-C36	4.23	118.08	107.17
3	B	1403	BCD	O33-C33-C23	4.26	119.92	110.34
3	C	1403	BCD	O52-C12-C22	4.27	119.04	110.28
2	D	1402	HEM	CAD-C3D-C4D	4.29	127.59	112.47
3	B	1403	BCD	O42-C13-C23	4.33	118.64	108.10
3	E	1403	BCD	O57-C57-C67	4.40	117.47	106.36
3	C	1403	BCD	O41-C41-C31	4.41	118.54	107.17
3	E	1403	BCD	O41-C41-C31	4.41	118.56	107.17
2	C	1402	HEM	CAD-C3D-C2D	4.42	125.92	113.22
3	D	1403	BCD	C16-O56-C56	4.42	122.33	113.75
3	A	1403	BCD	O42-C13-C23	4.47	118.97	108.10
3	D	1403	BCD	O42-C13-C23	4.48	118.99	108.10
2	E	1402	HEM	CAD-C3D-C2D	4.54	126.27	113.22
3	D	1403	BCD	C13-O53-C53	4.58	122.64	113.75
2	D	1402	HEM	CMC-C2C-C3C	4.61	128.03	116.53
3	E	1403	BCD	O42-C42-C32	4.61	119.06	107.17
3	B	1403	BCD	O42-C42-C32	4.62	119.11	107.17
2	D	1402	HEM	CAD-C3D-C2D	4.69	126.70	113.22
2	B	1402	HEM	CMC-C2C-C3C	4.72	128.31	116.53
2	E	1402	HEM	CMC-C2C-C3C	4.73	128.33	116.53
3	E	1403	BCD	O43-C14-C24	4.75	119.65	108.10
2	B	1402	HEM	CMB-C2B-C3B	4.75	128.39	116.53
2	F	1402	HEM	CMB-C2B-C3B	4.75	128.39	116.53
2	A	1402	HEM	CAD-C3D-C2D	4.77	126.93	113.22
2	F	1402	HEM	CAD-C3D-C2D	4.87	127.22	113.22
3	B	1403	BCD	O41-C41-C31	4.90	119.81	107.17
2	A	1402	HEM	CMC-C2C-C3C	4.91	128.78	116.53
3	F	1403	BCD	O22-C22-C12	4.92	120.80	110.02
2	B	1402	HEM	CAD-C3D-C2D	5.04	127.70	113.22
3	C	1403	BCD	O42-C42-C52	5.10	122.72	109.32
2	D	1402	HEM	CMB-C2B-C3B	5.10	129.26	116.53
3	E	1403	BCD	O55-C15-C25	5.10	120.75	110.28
3	A	1403	BCD	O46-C46-C56	5.17	122.91	109.32
3	F	1403	BCD	O46-C17-C27	5.23	120.83	108.10
3	E	1403	BCD	O53-C53-C43	5.28	120.90	109.75
2	A	1402	HEM	CMB-C2B-C3B	5.29	129.73	116.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1403	BCD	O52-C52-C62	5.30	119.76	106.36
3	B	1403	BCD	O52-C12-C22	5.57	121.70	110.28
3	C	1403	BCD	O43-C43-C33	5.58	121.58	107.17
2	C	1402	HEM	CMB-C2B-C3B	5.60	130.52	116.53
3	C	1403	BCD	O42-C13-C23	5.62	121.78	108.10
3	E	1403	BCD	O47-C47-C37	5.62	121.68	107.17
2	E	1402	HEM	CMB-C2B-C3B	5.79	130.99	116.53
3	A	1403	BCD	O54-C14-C24	5.84	122.27	110.28
3	C	1403	BCD	O46-C17-C27	5.95	122.58	108.10
3	E	1403	BCD	O45-C45-C55	6.25	125.74	109.32

All (12) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	E	1403	BCD	C11
3	E	1403	BCD	C14
3	E	1403	BCD	C17
3	A	1403	BCD	C11
3	A	1403	BCD	C17
3	C	1403	BCD	C11
3	C	1403	BCD	C17
3	D	1403	BCD	C17
3	F	1403	BCD	C14
3	F	1403	BCD	C26
3	B	1403	BCD	C11
3	B	1403	BCD	C17

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	1403	BCD	C44-O44-C15-C25

There are no ring outliers.

20 monomers are involved in 172 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1402	HEM	6	0
3	A	1403	BCD	16	0
4	A	1404	SO4	8	0
2	B	1402	HEM	6	0
3	B	1403	BCD	23	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1408	SO4	5	0
5	B	1409	EDO	1	0
2	C	1402	HEM	5	0
3	C	1403	BCD	22	0
4	C	1406	SO4	3	0
5	C	1407	EDO	1	0
2	D	1402	HEM	6	0
3	D	1403	BCD	10	0
4	D	1406	SO4	5	0
2	E	1402	HEM	6	0
3	E	1403	BCD	23	0
4	E	1406	SO4	5	0
2	F	1402	HEM	10	0
3	F	1403	BCD	6	0
4	F	1406	SO4	5	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	402/407 (98%)	-0.30	8 (1%) 68 75	12, 22, 44, 60	0
1	B	404/407 (99%)	-0.29	6 (1%) 76 82	12, 22, 44, 64	0
1	C	402/407 (98%)	-0.27	7 (1%) 73 79	12, 22, 43, 57	0
1	D	402/407 (98%)	-0.25	6 (1%) 76 82	12, 22, 43, 61	0
1	E	402/407 (98%)	-0.27	8 (1%) 68 75	12, 22, 43, 56	0
1	F	402/407 (98%)	-0.27	8 (1%) 68 75	12, 22, 44, 55	0
All	All	2414/2442 (98%)	-0.28	43 (1%) 71 78	12, 22, 44, 64	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	165	GLY	5.5
1	F	170	VAL	4.8
1	C	170	VAL	4.4
1	D	167	SER	4.3
1	B	165	GLY	4.2
1	D	168	SER	4.1
1	A	165	GLY	4.0
1	B	167	SER	3.9
1	E	170	VAL	3.9
1	B	168	SER	3.8
1	C	165	GLY	3.6
1	B	170	VAL	3.6
1	D	166	LEU	3.5
1	A	170	VAL	3.5
1	C	168	SER	3.4
1	F	165	GLY	3.2
1	D	170	VAL	3.2
1	A	169	HIS	3.0
1	E	168	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	F	166	LEU	2.8
1	F	168	SER	2.8
1	A	168	SER	2.8
1	F	401	ALA	2.6
1	E	167	SER	2.6
1	A	166	LEU	2.6
1	B	166	LEU	2.6
1	A	167	SER	2.5
1	F	167	SER	2.5
1	E	169	HIS	2.5
1	F	402	HIS	2.5
1	C	401	ALA	2.4
1	A	402	HIS	2.4
1	B	169	HIS	2.4
1	C	169	HIS	2.4
1	D	165	GLY	2.3
1	E	164	CYS	2.3
1	A	164[A]	CYS	2.3
1	C	167	SER	2.3
1	E	2	THR	2.3
1	E	166	LEU	2.2
1	F	2	THR	2.2
1	D	164[A]	CYS	2.2
1	C	402	HIS	2.1

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	SO4	C	1406	5/5	0.95	0.57	16.08	32,42,45,47	0
4	SO4	D	1406	5/5	0.96	0.55	10.04	29,44,46,47	0
4	SO4	A	1404	5/5	0.98	0.50	10.00	27,42,43,44	0
5	EDO	B	1409	4/4	0.89	0.15	9.94	19,20,22,32	0
4	SO4	B	1408	5/5	0.95	0.50	8.57	30,43,45,49	0
4	SO4	F	1406	5/5	0.98	0.54	8.55	27,41,41,48	0
4	SO4	E	1406	5/5	0.96	0.50	8.21	29,41,44,49	0
5	EDO	E	1407	4/4	0.95	0.14	5.60	22,23,23,31	0
5	EDO	F	1407	4/4	0.97	0.12	3.55	18,21,22,27	0
5	EDO	D	1407	4/4	0.97	0.11	3.27	19,20,21,34	0
3	BCD	A	1403	77/77	0.89	0.17	2.10	21,40,45,49	77
5	EDO	A	1406	4/4	0.96	0.10	2.04	19,22,23,30	0
3	BCD	F	1403	77/77	0.91	0.15	1.83	26,39,45,48	77
3	BCD	D	1403	77/77	0.91	0.15	1.78	24,39,44,51	77
3	BCD	E	1403	77/77	0.91	0.15	1.68	25,38,42,49	77
3	BCD	B	1403	77/77	0.90	0.15	1.67	21,38,43,46	77
5	EDO	C	1407	4/4	0.98	0.11	1.50	21,23,26,30	0
2	HEM	A	1402	43/43	0.98	0.09	1.14	11,14,17,22	0
2	HEM	D	1402	43/43	0.99	0.09	0.80	8,14,16,22	0
2	HEM	B	1402	43/43	0.99	0.09	0.77	10,13,16,24	0
2	HEM	C	1402	43/43	0.99	0.09	0.77	9,14,17,24	0
2	HEM	E	1402	43/43	0.99	0.09	0.74	9,14,17,22	0
2	HEM	F	1402	43/43	0.98	0.09	0.72	10,14,19,28	0
3	BCD	C	1403	77/77	0.90	0.13	0.66	22,37,45,50	77
4	SO4	F	1404	5/5	0.98	0.16	-	25,25,31,32	0
4	SO4	C	1404	5/5	0.98	0.12	-	26,28,29,32	0
4	SO4	B	1406	5/5	0.97	0.14	-	30,30,35,36	0
4	SO4	B	1407	5/5	0.98	0.12	-	23,29,30,31	0
4	SO4	A	1405	5/5	0.98	0.14	-	27,30,31,33	0
4	SO4	E	1405	5/5	0.97	0.20	-	34,34,35,38	0
4	SO4	D	1405	5/5	0.95	0.18	-	30,31,35,35	0
4	SO4	D	1404	5/5	0.98	0.14	-	25,26,31,31	0
4	SO4	E	1404	5/5	0.97	0.15	-	27,28,31,32	0
4	SO4	F	1405	5/5	0.96	0.21	-	33,34,36,37	0
4	SO4	C	1405	5/5	0.97	0.17	-	33,33,35,36	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.