



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 28, 2018 – 12:24 PM EST

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 : **FAILED**  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030736  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : rb-20030736

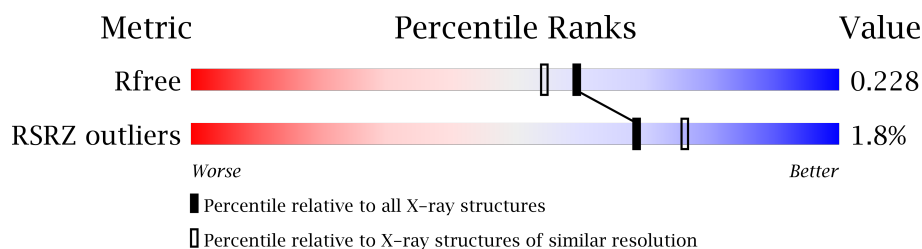
# 1 Overall quality at a glance

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))
$R_{free}$	100719	3233 (1.96-1.92)
RSRZ outliers	101464	3250 (1.96-1.92)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

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
4	SO4	A	1404	-	-	-	X
4	SO4	B	1408	-	-	-	X
4	SO4	C	1406	-	-	-	X
4	SO4	D	1406	-	-	-	X
4	SO4	E	1406	-	-	-	X
4	SO4	F	1406	-	-	-	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:

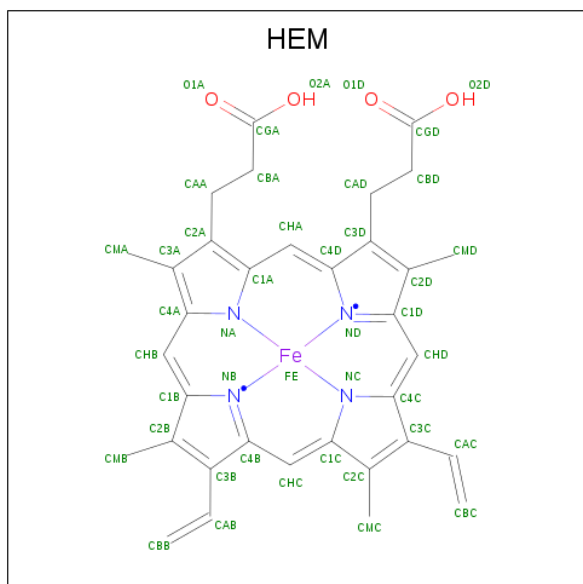
Chain	Residue	Modelled	Actual	Comment	Reference
A	402	HIS	-	expression tag	UNP A0R4Q6
A	403	HIS	-	expression tag	UNP A0R4Q6
A	404	HIS	-	expression tag	UNP A0R4Q6
A	405	HIS	-	expression tag	UNP A0R4Q6
A	406	HIS	-	expression tag	UNP A0R4Q6
A	407	HIS	-	expression tag	UNP A0R4Q6
B	402	HIS	-	expression tag	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:  $C_{34}H_{32}FeN_4O_4$ ).



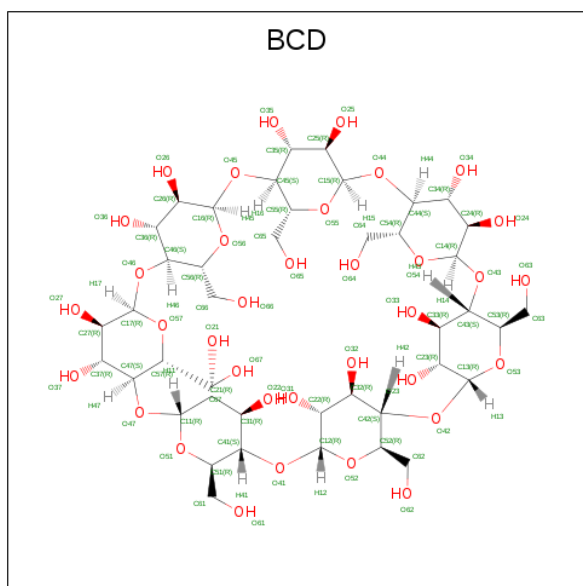
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	
			43	34	1	4	4	
							0	0

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

- Molecule 3 is BETA-CYCLODEXTRIN (three-letter code: BCD) (formula:  $C_{42}H_{70}O_{35}$ ).



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

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



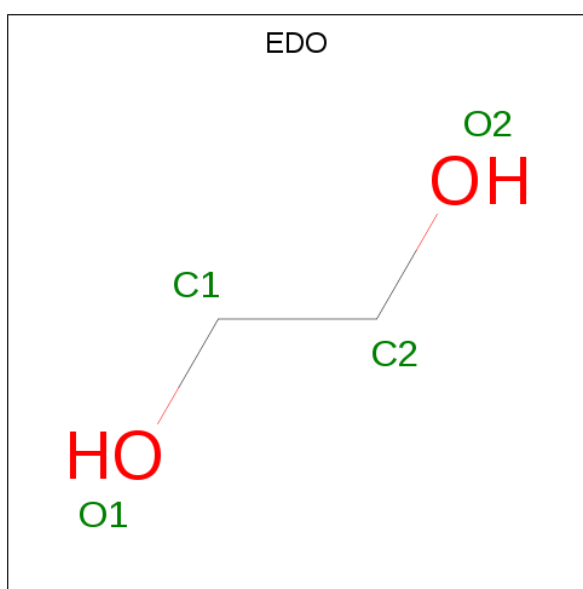
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total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

MolProbity failed to run properly - this section is therefore empty.



### 3 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
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
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
$F_o, F_c$ 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 4 Model quality [i](#)

### 4.1 Standard geometry [i](#)

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### 4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

### 4.3 Torsion angles [i](#)

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

MolProbity failed to run properly - this section is therefore empty.

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

MolProbity failed to run properly - this section is therefore empty.

#### 4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

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

### 4.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 4.6 Ligand geometry [i](#)

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	28,50,50	2.38	10 (35%)	17,82,82	2.53	11 (64%)
3	BCD	A	1403	-	84,84,84	0.80	1 (1%)	126,126,126	2.44	52 (41%)
4	SO4	A	1404	-	4,4,4	0.72	0	6,6,6	1.08	0
4	SO4	A	1405	-	4,4,4	0.64	0	6,6,6	0.76	0
5	EDO	A	1406	2	3,3,3	1.33	0	2,2,2	0.96	0
2	HEM	B	1402	1,5	28,50,50	2.49	14 (50%)	17,82,82	2.14	6 (35%)
3	BCD	B	1403	-	84,84,84	0.95	3 (3%)	126,126,126	2.84	63 (50%)
4	SO4	B	1406	-	4,4,4	0.76	0	6,6,6	0.70	0
4	SO4	B	1407	-	4,4,4	0.61	0	6,6,6	0.60	0
4	SO4	B	1408	-	4,4,4	0.77	0	6,6,6	0.86	0
5	EDO	B	1409	2	3,3,3	1.38	0	2,2,2	1.00	0
2	HEM	C	1402	1,5	28,50,50	2.06	8 (28%)	17,82,82	1.98	6 (35%)
3	BCD	C	1403	-	84,84,84	1.02	2 (2%)	126,126,126	2.61	56 (44%)
4	SO4	C	1404	-	4,4,4	0.75	0	6,6,6	0.88	0
4	SO4	C	1405	-	4,4,4	0.78	0	6,6,6	0.54	0
4	SO4	C	1406	-	4,4,4	0.61	0	6,6,6	0.81	0
5	EDO	C	1407	2	3,3,3	0.84	0	2,2,2	0.09	0
2	HEM	D	1402	1,5	28,50,50	2.43	12 (42%)	17,82,82	2.31	8 (47%)
3	BCD	D	1403	-	84,84,84	0.72	1 (1%)	126,126,126	2.15	46 (36%)
4	SO4	D	1404	-	4,4,4	0.80	0	6,6,6	0.58	0
4	SO4	D	1405	-	4,4,4	0.99	0	6,6,6	0.54	0
4	SO4	D	1406	-	4,4,4	0.81	0	6,6,6	1.06	0
5	EDO	D	1407	2	3,3,3	1.16	0	2,2,2	0.85	0
2	HEM	E	1402	1,5	28,50,50	2.48	14 (50%)	17,82,82	2.28	7 (41%)
3	BCD	E	1403	-	84,84,84	0.95	0	126,126,126	3.12	56 (44%)
4	SO4	E	1404	-	4,4,4	0.67	0	6,6,6	0.61	0
4	SO4	E	1405	-	4,4,4	0.84	0	6,6,6	0.50	0
4	SO4	E	1406	1	4,4,4	0.56	0	6,6,6	0.64	0
5	EDO	E	1407	2	3,3,3	1.38	0	2,2,2	0.93	0
2	HEM	F	1402	1,5	28,50,50	2.21	9 (32%)	17,82,82	2.17	7 (41%)
3	BCD	F	1403	-	84,84,84	0.71	2 (2%)	126,126,126	2.47	57 (45%)
4	SO4	F	1404	-	4,4,4	0.72	0	6,6,6	0.57	0
4	SO4	F	1405	-	4,4,4	0.91	0	6,6,6	0.72	0
4	SO4	F	1406	-	4,4,4	0.47	0	6,6,6	0.55	0
5	EDO	F	1407	2	3,3,3	1.31	0	2,2,2	0.76	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	-	0/6/54/54	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	-	0/6/54/54	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	-	0/6/54/54	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	-	0/6/54/54	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	-	0/6/54/54	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
5	EDO	E	1407	2	-	0/1/1/1	0/0/0/0
2	HEM	F	1402	1,5	-	0/6/54/54	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 (76) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1402	HEM	C3B-C2B	-4.09	1.35	1.40
2	F	1402	HEM	C3C-C2C	-3.96	1.35	1.40
2	C	1402	HEM	C3B-C2B	-3.96	1.35	1.40
2	E	1402	HEM	C3B-C2B	-3.63	1.35	1.40
2	F	1402	HEM	C3B-C2B	-3.35	1.35	1.40
2	D	1402	HEM	C3B-C2B	-3.32	1.36	1.40
2	B	1402	HEM	C3B-C2B	-2.92	1.36	1.40
2	C	1402	HEM	C3C-C2C	-2.80	1.36	1.40
2	D	1402	HEM	C3C-C2C	-2.41	1.37	1.40
2	B	1402	HEM	C3C-C2C	-2.23	1.37	1.40
2	C	1402	HEM	C4D-ND	2.00	1.39	1.36
3	F	1403	BCD	O31-C31	2.06	1.47	1.43
2	F	1402	HEM	C1D-ND	2.08	1.40	1.36
3	D	1403	BCD	O42-C13	2.11	1.47	1.41
2	E	1402	HEM	CMA-C3A	2.14	1.56	1.51
2	D	1402	HEM	C4B-NB	2.15	1.40	1.36
2	E	1402	HEM	C1C-NC	2.18	1.39	1.36
2	E	1402	HEM	C1A-NA	2.20	1.40	1.36
3	F	1403	BCD	O51-C11	2.22	1.47	1.41
2	C	1402	HEM	CMB-C2B	2.26	1.56	1.51
2	B	1402	HEM	C4A-NA	2.27	1.41	1.36
2	D	1402	HEM	CAD-C3D	2.29	1.56	1.52
2	C	1402	HEM	CMD-C2D	2.30	1.56	1.51
2	A	1402	HEM	C4C-NC	2.30	1.39	1.36
3	A	1403	BCD	O52-C12	2.33	1.47	1.41
2	E	1402	HEM	C1D-ND	2.34	1.41	1.36
3	B	1403	BCD	O25-C25	2.36	1.48	1.43
2	B	1402	HEM	CMA-C3A	2.36	1.56	1.51
3	B	1403	BCD	O56-C16	2.37	1.47	1.41
2	B	1402	HEM	C1C-NC	2.39	1.39	1.36
3	C	1403	BCD	C33-C23	2.40	1.58	1.52
2	A	1402	HEM	C1C-NC	2.44	1.39	1.36
2	E	1402	HEM	CMC-C2C	2.46	1.56	1.51
2	E	1402	HEM	CAA-C2A	2.61	1.56	1.52
2	A	1402	HEM	CMD-C2D	2.64	1.57	1.51
2	F	1402	HEM	CMD-C2D	2.65	1.57	1.51
2	E	1402	HEM	C1B-NB	2.77	1.40	1.36
2	C	1402	HEM	C3B-CAB	2.79	1.53	1.47
2	D	1402	HEM	CAA-C2A	2.93	1.57	1.52
2	F	1402	HEM	CMB-C2B	2.96	1.57	1.51
2	B	1402	HEM	CAA-C2A	3.05	1.57	1.52
2	E	1402	HEM	CMD-C2D	3.05	1.57	1.51
2	B	1402	HEM	CMC-C2C	3.07	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1402	HEM	C1B-NB	3.11	1.40	1.36
2	B	1402	HEM	CMD-C2D	3.15	1.58	1.51
2	D	1402	HEM	CMC-C2C	3.19	1.58	1.51
2	E	1402	HEM	CMB-C2B	3.23	1.58	1.51
2	F	1402	HEM	C4D-ND	3.23	1.40	1.36
2	A	1402	HEM	C4D-ND	3.24	1.40	1.36
2	A	1402	HEM	C3B-CAB	3.25	1.54	1.47
2	A	1402	HEM	CMC-C2C	3.39	1.58	1.51
2	F	1402	HEM	C3B-CAB	3.42	1.54	1.47
2	B	1402	HEM	CMB-C2B	3.45	1.58	1.51
2	D	1402	HEM	CMD-C2D	3.47	1.58	1.51
2	B	1402	HEM	C3B-CAB	3.48	1.54	1.47
2	D	1402	HEM	CMB-C2B	3.53	1.59	1.51
2	E	1402	HEM	C3B-CAB	3.54	1.54	1.47
2	A	1402	HEM	CMB-C2B	3.82	1.59	1.51
2	D	1402	HEM	C3C-CAC	3.82	1.55	1.47
2	D	1402	HEM	C3B-CAB	3.83	1.55	1.47
3	B	1403	BCD	O52-C12	3.87	1.51	1.41
3	C	1403	BCD	O52-C12	4.06	1.51	1.41
2	B	1402	HEM	C4D-ND	4.19	1.41	1.36
2	E	1402	HEM	C4D-ND	4.27	1.41	1.36
2	F	1402	HEM	C3C-CAC	4.39	1.56	1.47
2	C	1402	HEM	C3C-CAC	4.50	1.56	1.47
2	A	1402	HEM	C3C-CAC	4.77	1.57	1.47
2	D	1402	HEM	C3D-C2D	4.85	1.52	1.37
2	B	1402	HEM	C3D-C2D	4.95	1.52	1.37
2	B	1402	HEM	C3C-CAC	4.96	1.57	1.47
2	F	1402	HEM	C3D-C2D	5.01	1.52	1.37
2	D	1402	HEM	C4D-ND	5.21	1.42	1.36
2	E	1402	HEM	C3C-CAC	5.31	1.58	1.47
2	C	1402	HEM	C3D-C2D	5.46	1.53	1.37
2	E	1402	HEM	C3D-C2D	5.59	1.54	1.37
2	A	1402	HEM	C3D-C2D	5.67	1.54	1.37

All (375) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1403	BCD	O54-C54-C44	-10.73	87.79	109.75
3	E	1403	BCD	O55-C55-C45	-9.67	89.97	109.75
3	E	1403	BCD	C15-O44-C44	-9.11	95.79	118.00
3	C	1403	BCD	O53-C53-C43	-8.72	91.90	109.75
3	F	1403	BCD	C37-C47-C57	-8.69	92.44	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1403	BCD	C36-C46-C56	-8.27	93.32	110.88
3	A	1403	BCD	C14-O43-C43	-8.00	98.50	118.00
3	B	1403	BCD	C36-C46-C56	-7.47	95.01	110.88
3	E	1403	BCD	C12-O41-C41	-7.41	99.95	118.00
3	E	1403	BCD	C16-O45-C45	-7.33	100.15	118.00
3	B	1403	BCD	C33-C43-C53	-6.67	96.72	110.88
3	B	1403	BCD	C13-C23-C33	-6.29	98.28	109.98
3	C	1403	BCD	C13-O42-C42	-6.29	102.68	118.00
3	C	1403	BCD	C15-O44-C44	-6.01	103.35	118.00
3	B	1403	BCD	O53-C53-C43	-5.85	97.79	109.75
3	E	1403	BCD	O53-C13-C23	-5.59	99.52	110.30
3	E	1403	BCD	C17-O57-C57	-5.55	103.26	113.72
3	F	1403	BCD	O51-C51-C61	-5.52	93.17	106.41
3	C	1403	BCD	O54-C54-C44	-5.51	98.47	109.75
3	D	1403	BCD	C27-C37-C47	-5.47	98.27	109.61
3	C	1403	BCD	C17-O57-C57	-5.46	103.43	113.72
3	B	1403	BCD	O27-C27-C37	-5.45	98.49	110.36
3	A	1403	BCD	C13-O42-C42	-5.43	104.76	118.00
3	B	1403	BCD	O41-C12-C22	-5.40	95.95	108.11
3	B	1403	BCD	C15-O44-C44	-5.38	104.89	118.00
3	E	1403	BCD	C35-C45-C55	-5.29	99.65	110.88
3	B	1403	BCD	C12-O41-C41	-5.24	105.23	118.00
2	A	1402	HEM	C1D-C2D-C3D	-5.05	103.48	107.00
3	F	1403	BCD	C12-O41-C41	-4.97	105.89	118.00
3	B	1403	BCD	C32-C42-C52	-4.96	100.36	110.88
3	E	1403	BCD	C37-C47-C57	-4.94	100.39	110.88
3	B	1403	BCD	O53-C13-C23	-4.93	100.78	110.30
3	F	1403	BCD	C14-O54-C54	-4.91	104.47	113.72
3	F	1403	BCD	O56-C56-C46	-4.90	99.72	109.75
3	A	1403	BCD	O44-C44-C34	-4.82	95.59	107.19
3	F	1403	BCD	C16-C26-C36	-4.73	101.19	109.98
2	C	1402	HEM	C1D-C2D-C3D	-4.63	103.78	107.00
3	E	1403	BCD	O23-C23-C13	-4.61	100.39	110.03
3	F	1403	BCD	C26-C36-C46	-4.58	100.11	109.61
3	B	1403	BCD	C15-C25-C35	-4.55	101.53	109.98
3	D	1403	BCD	C17-C27-C37	-4.51	101.60	109.98
3	B	1403	BCD	O52-C52-C42	-4.49	100.57	109.75
3	E	1403	BCD	C32-C42-C52	-4.41	101.52	110.88
3	A	1403	BCD	O22-C22-C32	-4.38	100.83	110.36
2	E	1402	HEM	CAD-CBD-CGD	-4.21	105.46	112.66
3	A	1403	BCD	O42-C13-O53	-4.15	100.62	110.70
3	C	1403	BCD	O57-C17-C27	-4.14	102.31	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1403	BCD	C16-O45-C45	-4.04	108.14	118.00
3	C	1403	BCD	C16-O45-C45	-4.03	108.17	118.00
3	F	1403	BCD	C16-O56-C56	-4.03	106.12	113.72
3	D	1403	BCD	C26-C36-C46	-4.03	101.25	109.61
3	E	1403	BCD	O57-C57-C47	-4.00	101.57	109.75
2	B	1402	HEM	CBA-CAA-C2A	-3.99	104.85	112.48
3	A	1403	BCD	O35-C35-C45	-3.98	100.81	109.87
2	B	1402	HEM	C1D-C2D-C3D	-3.94	104.25	107.00
3	B	1403	BCD	O66-C66-C56	-3.90	98.21	111.34
3	D	1403	BCD	C14-O54-C54	-3.79	106.58	113.72
2	D	1402	HEM	CBD-CAD-C3D	-3.78	105.25	112.47
3	D	1403	BCD	O52-C52-C62	-3.76	97.40	106.41
3	A	1403	BCD	O47-C47-C37	-3.73	98.22	107.19
3	B	1403	BCD	C13-O42-C42	-3.65	109.11	118.00
3	A	1403	BCD	C37-C47-C57	-3.64	103.15	110.88
3	F	1403	BCD	C27-C37-C47	-3.63	102.08	109.61
3	C	1403	BCD	O34-C34-C44	-3.61	101.65	109.87
2	A	1402	HEM	CBD-CAD-C3D	-3.60	105.60	112.47
3	D	1403	BCD	C11-O47-C47	-3.57	109.31	118.00
3	B	1403	BCD	C67-C57-C47	-3.55	103.56	113.24
3	F	1403	BCD	C17-O46-C46	-3.54	109.38	118.00
3	C	1403	BCD	C36-C46-C56	-3.51	103.42	110.88
3	C	1403	BCD	C16-C26-C36	-3.44	103.58	109.98
2	F	1402	HEM	C1D-C2D-C3D	-3.44	104.60	107.00
3	C	1403	BCD	O56-C16-C26	-3.39	103.75	110.30
2	E	1402	HEM	C1D-C2D-C3D	-3.38	104.64	107.00
3	A	1403	BCD	C34-C44-C54	-3.38	103.70	110.88
3	E	1403	BCD	C15-O55-C55	-3.38	107.35	113.72
3	D	1403	BCD	C32-C42-C52	-3.38	103.70	110.88
3	E	1403	BCD	C16-C26-C36	-3.38	103.70	109.98
3	F	1403	BCD	O67-C67-C57	-3.37	100.01	111.34
3	E	1403	BCD	C33-C43-C53	-3.36	103.75	110.88
2	A	1402	HEM	CBA-CAA-C2A	-3.35	106.07	112.48
3	E	1403	BCD	O44-C15-O55	-3.35	102.55	110.70
3	F	1403	BCD	O46-C17-O57	-3.31	102.65	110.70
2	D	1402	HEM	CAD-CBD-CGD	-3.29	107.03	112.66
2	F	1402	HEM	CAA-CBA-CGA	-3.29	107.05	112.66
3	C	1403	BCD	C35-C45-C55	-3.27	103.94	110.88
3	D	1403	BCD	C17-O46-C46	-3.26	110.05	118.00
2	F	1402	HEM	CBD-CAD-C3D	-3.25	106.26	112.47
3	B	1403	BCD	O21-C21-C11	-3.25	103.23	110.03
3	B	1403	BCD	O34-C34-C44	-3.24	102.50	109.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1403	BCD	C31-C41-C51	-3.22	104.05	110.88
3	E	1403	BCD	C36-C46-C56	-3.21	104.07	110.88
2	D	1402	HEM	C1D-C2D-C3D	-3.20	104.77	107.00
3	A	1403	BCD	O53-C53-C43	-3.19	103.23	109.75
3	D	1403	BCD	O54-C54-C64	-3.19	98.78	106.41
3	E	1403	BCD	O56-C16-C26	-3.18	104.16	110.30
3	F	1403	BCD	C36-C46-C56	-3.17	104.15	110.88
3	B	1403	BCD	C22-C32-C42	-3.14	103.09	109.61
3	F	1403	BCD	O55-C15-C25	-3.13	104.25	110.30
3	C	1403	BCD	C32-C42-C52	-3.13	104.24	110.88
3	B	1403	BCD	C16-O45-C45	-3.11	110.43	118.00
2	E	1402	HEM	CBD-CAD-C3D	-3.08	106.59	112.47
3	D	1403	BCD	O31-C31-C21	-3.03	103.76	110.36
3	E	1403	BCD	C24-C34-C44	-3.03	103.32	109.61
3	F	1403	BCD	O54-C14-C24	-3.02	104.47	110.30
3	E	1403	BCD	O43-C14-O54	-2.98	103.45	110.70
3	F	1403	BCD	O61-C61-C51	-2.96	101.38	111.34
3	B	1403	BCD	O55-C55-C45	-2.92	103.78	109.75
2	D	1402	HEM	CMA-C3A-C4A	-2.88	124.04	128.46
3	F	1403	BCD	O62-C62-C52	-2.87	101.70	111.34
3	D	1403	BCD	C14-O43-C43	-2.83	111.10	118.00
3	A	1403	BCD	C11-O51-C51	-2.81	108.42	113.72
2	B	1402	HEM	CBD-CAD-C3D	-2.78	107.16	112.47
2	D	1402	HEM	CAA-CBA-CGA	-2.76	107.95	112.66
3	B	1403	BCD	O55-C15-C25	-2.75	104.98	110.30
3	A	1403	BCD	C17-O46-C46	-2.75	111.31	118.00
3	A	1403	BCD	O45-C16-O56	-2.74	104.06	110.70
3	B	1403	BCD	C16-O56-C56	-2.72	108.59	113.72
3	E	1403	BCD	C25-C35-C45	-2.72	103.97	109.61
3	F	1403	BCD	C15-O44-C44	-2.72	111.38	118.00
3	C	1403	BCD	C33-C43-C53	-2.71	105.11	110.88
3	E	1403	BCD	C11-O51-C51	-2.71	108.61	113.72
3	D	1403	BCD	C15-O44-C44	-2.69	111.43	118.00
3	B	1403	BCD	O43-C14-O54	-2.68	104.19	110.70
3	C	1403	BCD	O56-C56-C46	-2.66	104.31	109.75
3	E	1403	BCD	O61-C61-C51	-2.66	102.40	111.34
3	B	1403	BCD	C24-C34-C44	-2.64	104.12	109.61
2	A	1402	HEM	CAD-CBD-CGD	-2.63	108.17	112.66
3	A	1403	BCD	C17-C27-C37	-2.63	105.10	109.98
3	C	1403	BCD	O52-C52-C42	-2.58	104.47	109.75
3	F	1403	BCD	C25-C35-C45	-2.56	104.29	109.61
3	D	1403	BCD	C11-C21-C31	-2.53	105.28	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1403	BCD	O31-C31-C41	-2.52	104.14	109.87
3	B	1403	BCD	C11-O51-C51	-2.51	108.99	113.72
2	E	1402	HEM	CAA-CBA-CGA	-2.50	108.39	112.66
3	D	1403	BCD	C33-C43-C53	-2.50	105.57	110.88
3	D	1403	BCD	C12-O41-C41	-2.48	111.94	118.00
3	C	1403	BCD	C37-C47-C57	-2.48	105.62	110.88
2	F	1402	HEM	CAD-CBD-CGD	-2.47	108.44	112.66
3	E	1403	BCD	O65-C65-C55	-2.47	103.04	111.34
3	F	1403	BCD	C33-C43-C53	-2.42	105.73	110.88
3	B	1403	BCD	O51-C51-C41	-2.41	104.81	109.75
3	D	1403	BCD	C35-C45-C55	-2.40	105.77	110.88
3	A	1403	BCD	C13-C23-C33	-2.39	105.53	109.98
2	E	1402	HEM	CMD-C2D-C1D	-2.38	124.80	128.46
2	A	1402	HEM	CMA-C3A-C4A	-2.38	124.80	128.46
3	B	1403	BCD	O67-C67-C57	-2.37	103.36	111.34
3	F	1403	BCD	O33-C33-C23	-2.34	105.26	110.36
3	D	1403	BCD	C14-C24-C34	-2.34	105.63	109.98
3	C	1403	BCD	C14-O43-C43	-2.34	112.30	118.00
3	C	1403	BCD	O26-C26-C16	-2.34	105.14	110.03
3	F	1403	BCD	C11-O51-C51	-2.33	109.33	113.72
3	B	1403	BCD	C27-C37-C47	-2.32	104.80	109.61
3	F	1403	BCD	O21-C21-C31	-2.32	105.31	110.36
3	B	1403	BCD	O47-C47-C57	-2.31	103.66	109.34
3	F	1403	BCD	O34-C34-C44	-2.31	104.61	109.87
3	E	1403	BCD	O51-C11-C21	-2.28	105.90	110.30
3	F	1403	BCD	C12-C22-C32	-2.28	105.75	109.98
2	C	1402	HEM	CAA-CBA-CGA	-2.26	108.80	112.66
2	C	1402	HEM	CAD-CBD-CGD	-2.26	108.80	112.66
3	A	1403	BCD	O52-C52-C42	-2.25	105.14	109.75
3	E	1403	BCD	C21-C31-C41	-2.25	104.95	109.61
3	B	1403	BCD	O54-C54-C44	-2.25	105.16	109.75
2	B	1402	HEM	CAA-CBA-CGA	-2.24	108.84	112.66
3	F	1403	BCD	O27-C27-C37	-2.24	105.49	110.36
3	A	1403	BCD	O45-C45-C35	-2.23	101.82	107.19
3	C	1403	BCD	O23-C23-C13	-2.20	105.42	110.03
3	F	1403	BCD	C35-C45-C55	-2.20	106.20	110.88
3	A	1403	BCD	O43-C43-C53	-2.18	103.98	109.34
3	F	1403	BCD	O57-C57-C67	-2.17	101.22	106.41
3	E	1403	BCD	O56-C56-C46	-2.15	105.34	109.75
3	C	1403	BCD	O31-C31-C21	-2.15	105.67	110.36
3	A	1403	BCD	O21-C21-C11	-2.14	105.55	110.03
3	F	1403	BCD	O51-C11-C21	-2.12	106.20	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1403	BCD	O41-C41-C51	-2.12	104.13	109.34
3	D	1403	BCD	O45-C16-O56	-2.10	105.60	110.70
2	F	1402	HEM	CBA-CAA-C2A	-2.10	108.47	112.48
3	B	1403	BCD	O26-C26-C16	-2.10	105.64	110.03
3	C	1403	BCD	O67-C67-C57	-2.10	104.28	111.34
2	A	1402	HEM	CAA-CBA-CGA	-2.09	109.10	112.66
3	E	1403	BCD	O24-C24-C34	-2.09	105.82	110.36
3	E	1403	BCD	C66-C56-C46	-2.08	107.56	113.24
3	A	1403	BCD	O56-C56-C46	-2.07	105.51	109.75
3	D	1403	BCD	C24-C34-C44	-2.05	105.36	109.61
3	C	1403	BCD	C13-O53-C53	-2.05	109.86	113.72
3	A	1403	BCD	C26-C36-C46	-2.04	105.37	109.61
3	A	1403	BCD	C16-O45-C45	-2.03	113.05	118.00
2	A	1402	HEM	C3C-C4C-NC	-2.02	107.14	110.94
2	C	1402	HEM	C3C-C4C-NC	-2.00	107.17	110.94
3	C	1403	BCD	O47-C47-C37	2.00	112.01	107.19
3	F	1403	BCD	C62-C52-C42	2.00	118.70	113.24
3	A	1403	BCD	C13-O53-C53	2.01	117.49	113.72
3	D	1403	BCD	C13-C23-C33	2.01	113.71	109.98
3	B	1403	BCD	O42-C42-C52	2.01	114.29	109.34
3	C	1403	BCD	O21-C21-C31	2.01	114.73	110.36
3	C	1403	BCD	C17-O46-C46	2.02	122.92	118.00
3	D	1403	BCD	O63-C63-C53	2.02	118.15	111.34
3	F	1403	BCD	O44-C44-C54	2.06	114.40	109.34
3	D	1403	BCD	O45-C16-C26	2.06	112.75	108.11
3	D	1403	BCD	O47-C47-C57	2.06	114.41	109.34
3	E	1403	BCD	O21-C21-C31	2.07	114.86	110.36
3	B	1403	BCD	O44-C44-C54	2.08	114.46	109.34
3	B	1403	BCD	O46-C17-O57	2.09	115.78	110.70
2	A	1402	HEM	CMC-C2C-C3C	2.10	128.78	124.89
3	A	1403	BCD	C16-O56-C56	2.10	117.67	113.72
3	F	1403	BCD	O56-C56-C66	2.10	111.44	106.41
3	F	1403	BCD	C67-C57-C47	2.12	119.00	113.24
3	A	1403	BCD	C15-O55-C55	2.12	117.71	113.72
3	E	1403	BCD	O43-C43-C53	2.15	114.62	109.34
3	F	1403	BCD	O52-C12-C22	2.15	114.44	110.30
2	A	1402	HEM	CMD-C2D-C3D	2.16	129.01	124.94
3	D	1403	BCD	O56-C16-C26	2.16	114.47	110.30
3	A	1403	BCD	O44-C15-C25	2.16	112.99	108.11
3	D	1403	BCD	O44-C44-C34	2.18	112.43	107.19
3	B	1403	BCD	O51-C51-C61	2.21	111.70	106.41
3	A	1403	BCD	O55-C15-C25	2.22	114.58	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1403	BCD	O56-C56-C66	2.22	111.74	106.41
3	B	1403	BCD	O31-C31-C41	2.23	114.94	109.87
3	B	1403	BCD	O51-C11-C21	2.24	114.61	110.30
3	F	1403	BCD	O45-C16-C26	2.24	113.16	108.11
3	C	1403	BCD	O31-C31-C41	2.25	114.98	109.87
3	F	1403	BCD	O41-C41-C51	2.25	114.87	109.34
3	E	1403	BCD	O46-C17-C27	2.25	113.19	108.11
3	C	1403	BCD	O47-C11-O51	2.26	116.17	110.70
3	C	1403	BCD	C62-C52-C42	2.26	119.41	113.24
3	C	1403	BCD	O45-C45-C35	2.28	112.67	107.19
3	F	1403	BCD	O25-C25-C35	2.28	115.31	110.36
3	B	1403	BCD	C25-C35-C45	2.29	114.34	109.61
3	A	1403	BCD	O47-C47-C57	2.30	114.99	109.34
3	B	1403	BCD	O36-C36-C46	2.30	115.10	109.87
3	C	1403	BCD	O23-C23-C33	2.31	115.37	110.36
3	A	1403	BCD	O57-C57-C67	2.31	111.94	106.41
3	C	1403	BCD	O35-C35-C45	2.31	115.13	109.87
3	F	1403	BCD	O65-C65-C55	2.33	119.18	111.34
2	F	1402	HEM	CMD-C2D-C3D	2.33	129.33	124.94
3	A	1403	BCD	C12-C22-C32	2.34	114.33	109.98
3	D	1403	BCD	O34-C34-C24	2.35	115.47	110.36
3	F	1403	BCD	O44-C44-C34	2.35	112.86	107.19
2	D	1402	HEM	CMB-C2B-C3B	2.35	129.26	124.89
3	E	1403	BCD	O33-C33-C43	2.36	115.24	109.87
3	C	1403	BCD	C12-C22-C32	2.37	114.38	109.98
3	C	1403	BCD	O54-C54-C64	2.39	112.13	106.41
3	C	1403	BCD	O51-C51-C61	2.40	112.16	106.41
3	A	1403	BCD	O44-C44-C54	2.40	115.25	109.34
3	D	1403	BCD	O43-C43-C53	2.40	115.26	109.34
3	C	1403	BCD	O27-C27-C17	2.41	115.06	110.03
3	A	1403	BCD	O33-C33-C43	2.43	115.41	109.87
3	F	1403	BCD	O31-C31-C21	2.44	115.67	110.36
3	B	1403	BCD	O32-C32-C42	2.44	115.43	109.87
3	B	1403	BCD	O54-C54-C64	2.47	112.32	106.41
3	D	1403	BCD	O22-C22-C12	2.47	115.20	110.03
3	C	1403	BCD	C63-C53-C43	2.53	120.14	113.24
3	A	1403	BCD	O23-C23-C13	2.54	115.34	110.03
3	E	1403	BCD	C14-C24-C34	2.57	114.75	109.98
2	D	1402	HEM	CMD-C2D-C3D	2.57	129.78	124.94
3	A	1403	BCD	C62-C52-C42	2.57	120.25	113.24
3	F	1403	BCD	O35-C35-C25	2.58	115.97	110.36
2	A	1402	HEM	CMB-C2B-C3B	2.61	129.73	124.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1403	BCD	O46-C17-O57	2.61	117.03	110.70
3	D	1403	BCD	O25-C25-C15	2.63	115.53	110.03
3	C	1403	BCD	O46-C46-C36	2.63	113.53	107.19
3	C	1403	BCD	C13-C23-C33	2.64	114.88	109.98
3	F	1403	BCD	O36-C36-C26	2.64	116.09	110.36
3	D	1403	BCD	O41-C12-C22	2.64	114.06	108.11
3	A	1403	BCD	C11-O47-C47	2.66	124.48	118.00
3	D	1403	BCD	O32-C32-C42	2.66	115.93	109.87
3	B	1403	BCD	C13-O53-C53	2.67	118.74	113.72
3	C	1403	BCD	O53-C13-C23	2.68	115.47	110.30
3	E	1403	BCD	O45-C16-O56	2.69	117.23	110.70
2	B	1402	HEM	C4C-C3C-C2C	2.70	108.78	106.90
3	F	1403	BCD	O55-C55-C65	2.74	112.97	106.41
3	B	1403	BCD	O45-C45-C35	2.74	113.79	107.19
3	F	1403	BCD	O46-C46-C36	2.76	113.83	107.19
3	B	1403	BCD	O47-C47-C37	2.77	113.85	107.19
3	D	1403	BCD	O44-C44-C54	2.77	116.15	109.34
3	E	1403	BCD	O54-C14-C24	2.78	115.65	110.30
3	C	1403	BCD	C11-C21-C31	2.79	115.17	109.98
2	B	1402	HEM	CMD-C2D-C3D	2.83	130.28	124.94
2	D	1402	HEM	C4C-C3C-C2C	2.84	108.88	106.90
3	C	1403	BCD	O26-C26-C36	2.84	116.54	110.36
3	A	1403	BCD	O52-C12-C22	2.84	115.78	110.30
3	D	1403	BCD	O46-C17-C27	2.87	114.58	108.11
3	F	1403	BCD	O23-C23-C13	2.88	116.05	110.03
3	F	1403	BCD	O47-C47-C57	2.88	116.44	109.34
3	D	1403	BCD	O26-C26-C16	2.92	116.13	110.03
3	B	1403	BCD	O55-C55-C65	2.94	113.46	106.41
2	E	1402	HEM	CMD-C2D-C3D	2.97	130.55	124.94
3	A	1403	BCD	O32-C32-C42	2.99	116.68	109.87
3	C	1403	BCD	C67-C57-C47	3.00	121.42	113.24
3	B	1403	BCD	O34-C34-C24	3.01	116.92	110.36
2	C	1402	HEM	CMB-C2B-C3B	3.03	130.52	124.89
3	A	1403	BCD	O62-C62-C52	3.05	121.61	111.34
3	D	1403	BCD	O53-C13-C23	3.05	116.18	110.30
3	D	1403	BCD	O45-C45-C55	3.05	116.86	109.34
3	B	1403	BCD	O43-C43-C53	3.06	116.86	109.34
3	F	1403	BCD	O33-C33-C43	3.06	116.83	109.87
3	C	1403	BCD	O41-C12-O52	3.07	118.14	110.70
3	C	1403	BCD	O22-C22-C12	3.11	116.54	110.03
3	A	1403	BCD	C11-C21-C31	3.12	115.78	109.98
3	C	1403	BCD	C14-C24-C34	3.12	115.79	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1403	BCD	O43-C14-C24	3.14	115.18	108.11
3	E	1403	BCD	C64-C54-C44	3.14	121.80	113.24
3	E	1403	BCD	C13-C23-C33	3.16	115.85	109.98
3	A	1403	BCD	O47-C11-O51	3.18	118.42	110.70
3	A	1403	BCD	O36-C36-C26	3.19	117.30	110.36
3	E	1403	BCD	O41-C12-C22	3.22	115.36	108.11
3	B	1403	BCD	O25-C25-C15	3.28	116.88	110.03
3	E	1403	BCD	O45-C45-C35	3.28	115.09	107.19
2	E	1402	HEM	CMB-C2B-C3B	3.29	130.99	124.89
3	B	1403	BCD	C66-C56-C46	3.35	122.36	113.24
3	F	1403	BCD	O47-C47-C37	3.37	115.31	107.19
3	F	1403	BCD	O26-C26-C36	3.45	117.86	110.36
3	E	1403	BCD	O46-C46-C56	3.46	117.85	109.34
3	E	1403	BCD	O45-C16-C26	3.46	115.91	108.11
2	C	1402	HEM	C4C-C3C-C2C	3.50	109.34	106.90
3	C	1403	BCD	O55-C55-C65	3.51	114.81	106.41
3	A	1403	BCD	O56-C16-C26	3.51	117.07	110.30
3	E	1403	BCD	O26-C26-C36	3.58	118.15	110.36
3	B	1403	BCD	O41-C12-O52	3.59	119.41	110.70
3	A	1403	BCD	C66-C56-C46	3.61	123.07	113.24
2	A	1402	HEM	C4C-C3C-C2C	3.71	109.49	106.90
3	A	1403	BCD	O25-C25-C15	3.73	117.82	110.03
3	E	1403	BCD	C17-C27-C37	3.88	117.20	109.98
3	E	1403	BCD	O52-C52-C62	3.89	115.73	106.41
3	D	1403	BCD	C62-C52-C42	3.91	123.90	113.24
3	B	1403	BCD	O54-C14-C24	3.94	117.90	110.30
3	B	1403	BCD	C16-C26-C36	3.96	117.34	109.98
3	D	1403	BCD	O47-C47-C37	3.97	116.75	107.19
3	A	1403	BCD	C63-C53-C43	3.99	124.13	113.24
3	B	1403	BCD	O56-C16-C26	4.00	118.00	110.30
3	C	1403	BCD	O44-C44-C54	4.00	119.19	109.34
2	F	1402	HEM	C4C-C3C-C2C	4.00	109.69	106.90
3	D	1403	BCD	O23-C23-C13	4.02	118.44	110.03
3	C	1403	BCD	O54-C14-C24	4.04	118.09	110.30
3	F	1403	BCD	O47-C11-C21	4.06	117.25	108.11
3	E	1403	BCD	O46-C46-C36	4.12	117.10	107.19
3	B	1403	BCD	C63-C53-C43	4.12	124.48	113.24
3	A	1403	BCD	O51-C51-C61	4.16	116.38	106.41
3	F	1403	BCD	C17-C27-C37	4.17	117.72	109.98
3	D	1403	BCD	O42-C42-C52	4.25	119.79	109.34
3	F	1403	BCD	O27-C27-C17	4.25	118.92	110.03
3	F	1403	BCD	O41-C12-C22	4.30	117.79	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1403	BCD	O44-C15-C25	4.35	117.92	108.11
3	B	1403	BCD	O44-C15-C25	4.36	117.94	108.11
3	B	1403	BCD	O33-C33-C23	4.39	119.92	110.36
3	F	1403	BCD	O43-C14-C24	4.41	118.04	108.11
3	C	1403	BCD	O53-C53-C63	4.41	116.98	106.41
3	E	1403	BCD	C65-C55-C45	4.45	125.39	113.24
3	B	1403	BCD	O46-C46-C36	4.52	118.08	107.19
3	C	1403	BCD	O52-C12-C22	4.53	119.04	110.30
3	D	1403	BCD	C16-O56-C56	4.57	122.33	113.72
3	E	1403	BCD	O57-C57-C67	4.62	117.47	106.41
3	B	1403	BCD	O42-C13-C23	4.67	118.64	108.11
3	C	1403	BCD	O41-C41-C31	4.72	118.54	107.19
3	E	1403	BCD	O41-C41-C31	4.72	118.56	107.19
3	D	1403	BCD	C13-O53-C53	4.74	122.64	113.72
3	A	1403	BCD	O42-C13-C23	4.82	118.97	108.11
3	D	1403	BCD	O42-C13-C23	4.83	118.99	108.11
3	E	1403	BCD	O42-C42-C32	4.93	119.06	107.19
3	B	1403	BCD	O42-C42-C32	4.95	119.11	107.19
3	E	1403	BCD	O43-C14-C24	5.12	119.65	108.11
3	F	1403	BCD	O22-C22-C12	5.15	120.80	110.03
3	B	1403	BCD	O41-C41-C31	5.24	119.81	107.19
3	E	1403	BCD	O55-C15-C25	5.42	120.75	110.30
3	C	1403	BCD	O42-C42-C52	5.44	122.72	109.34
3	E	1403	BCD	O53-C53-C43	5.45	120.90	109.75
3	A	1403	BCD	O46-C46-C56	5.52	122.91	109.34
3	B	1403	BCD	O52-C52-C62	5.57	119.76	106.41
3	F	1403	BCD	O46-C17-C27	5.65	120.83	108.11
3	B	1403	BCD	O52-C12-C22	5.91	121.70	110.30
3	C	1403	BCD	O43-C43-C33	5.98	121.58	107.19
3	E	1403	BCD	O47-C47-C37	6.02	121.68	107.19
3	C	1403	BCD	O42-C13-C23	6.07	121.78	108.11
3	A	1403	BCD	O54-C14-C24	6.21	122.27	110.30
3	C	1403	BCD	O46-C17-C27	6.42	122.58	108.11
3	E	1403	BCD	O45-C45-C55	6.66	125.74	109.34

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

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Mol	Chain	Res	Type	Atom
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.

No monomer is involved in short contacts.

## 4.7 Other polymers [i](#)

There are no such residues in this entry.

## 4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 5 Fit of model and data ⓘ

### 5.1 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%)	-0.33	8 (1%) 65 73	12, 22, 44, 60	0
1	B	404/407 (99%)	-0.32	6 (1%) 74 80	12, 22, 44, 64	0
1	C	402/407 (98%)	-0.30	7 (1%) 70 77	12, 22, 43, 57	0
1	D	402/407 (98%)	-0.28	6 (1%) 74 80	12, 22, 43, 61	0
1	E	402/407 (98%)	-0.30	8 (1%) 65 73	12, 22, 43, 56	0
1	F	402/407 (98%)	-0.30	8 (1%) 65 73	12, 22, 44, 55	0
All	All	2414/2442 (98%)	-0.31	43 (1%) 69 76	12, 22, 44, 64	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	165	GLY	5.4
1	F	170	VAL	4.7
1	C	170	VAL	4.3
1	D	167	SER	4.2
1	B	165	GLY	4.1
1	D	168	SER	4.0
1	A	165	GLY	3.9
1	B	167	SER	3.9
1	E	170	VAL	3.8
1	B	168	SER	3.8
1	C	165	GLY	3.6
1	B	170	VAL	3.5
1	D	166	LEU	3.4
1	A	170	VAL	3.4
1	C	168	SER	3.3
1	F	165	GLY	3.2
1	D	170	VAL	3.1
1	A	169	HIS	2.9
1	E	168	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	F	168	SER	2.7
1	F	166	LEU	2.7
1	A	168	SER	2.7
1	F	401	ALA	2.6
1	E	167	SER	2.5
1	A	166	LEU	2.5
1	B	166	LEU	2.5
1	A	167	SER	2.5
1	F	167	SER	2.4
1	E	169	HIS	2.4
1	F	402	HIS	2.4
1	A	402	HIS	2.3
1	B	169	HIS	2.3
1	C	169	HIS	2.3
1	C	401	ALA	2.3
1	D	165	GLY	2.3
1	E	164	CYS	2.2
1	A	164[A]	CYS	2.2
1	C	167	SER	2.2
1	E	2	THR	2.2
1	F	2	THR	2.2
1	E	166	LEU	2.2
1	D	164[A]	CYS	2.2
1	C	402	HIS	2.0

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

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

## 5.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.4 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

## 5.5 Other polymers ⓘ

There are no such residues in this entry.