



wwPDB X-ray Structure Validation Summary 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 wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at 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.

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

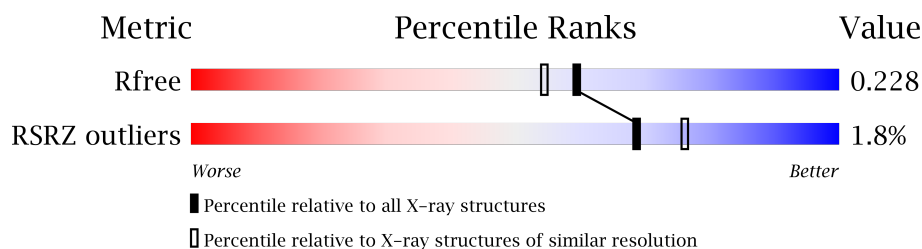
1 Overall quality at a glance

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:

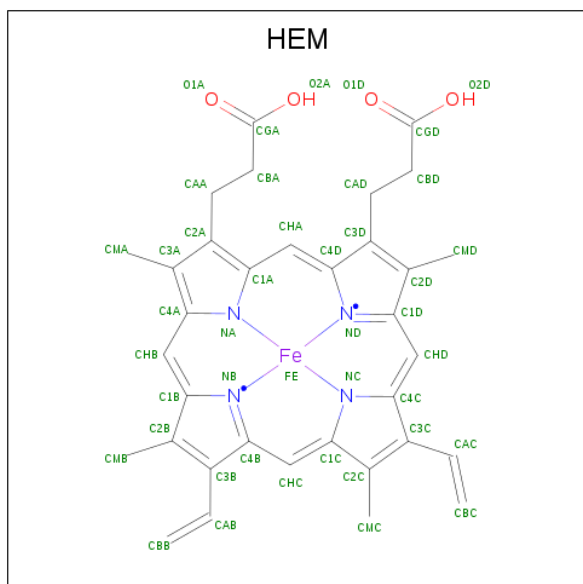
Chain	Residue	Modelled	Actual	Comment	Reference
A	402	HIS	-	expression tag	UNP A0R4Q6
A	403	HIS	-	expression tag	UNP A0R4Q6
A	404	HIS	-	expression tag	UNP A0R4Q6
A	405	HIS	-	expression tag	UNP A0R4Q6
A	406	HIS	-	expression tag	UNP A0R4Q6
A	407	HIS	-	expression tag	UNP A0R4Q6
B	402	HIS	-	expression tag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



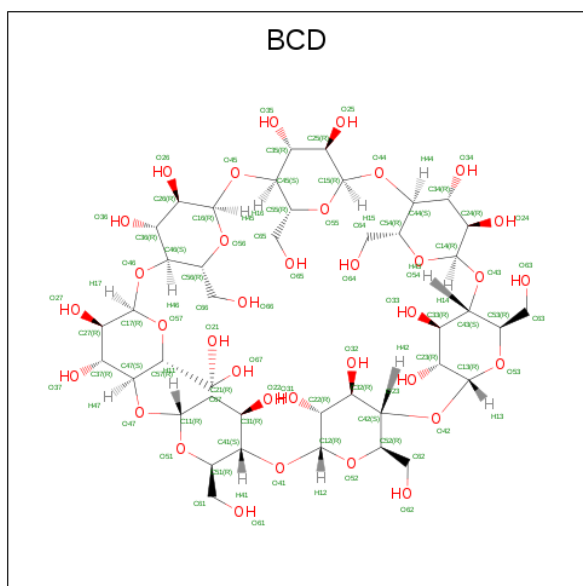
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	
			43	34	1	4	4	
							0	0

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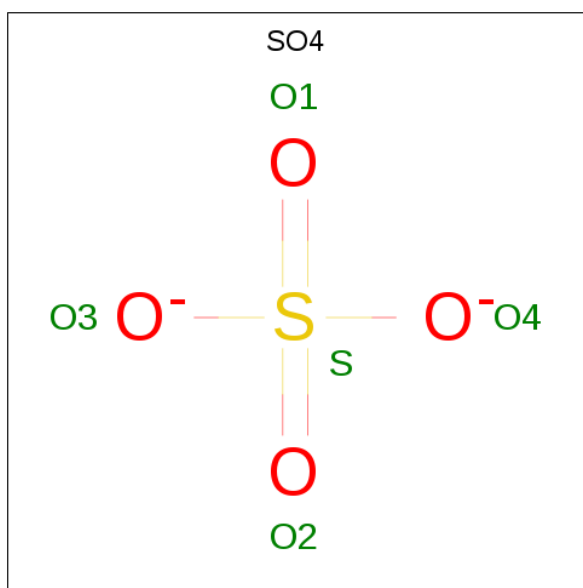
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is 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	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: O₄S).



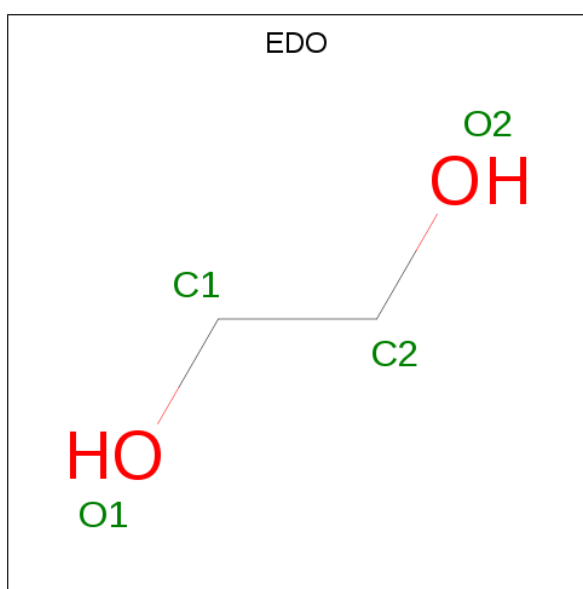
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	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: $C_2H_6O_2$).



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

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3 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	22.0	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 33.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	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 ²)	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.*

¹Intensities estimated from amplitudes.

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

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

The worst 5 of 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

The worst 5 of 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

5 of 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

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 [i](#)

5.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	402/407 (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

The worst 5 of 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

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 ⓘ

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å 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.