



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 06:50 AM GMT

PDB ID : 2YIU  
Title : X-RAY STRUCTURE OF THE DIMERIC CYTOCHROME BC1 COMPLEX  
FROM THE SOIL BACTERIUM PARACOCCLUS DENITRIFICANS AT 2.7  
ANGSTROM RESOLUTION  
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wig, B.; Hunte, C.  
Deposited on : 2011-05-16  
Resolution : 2.70 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

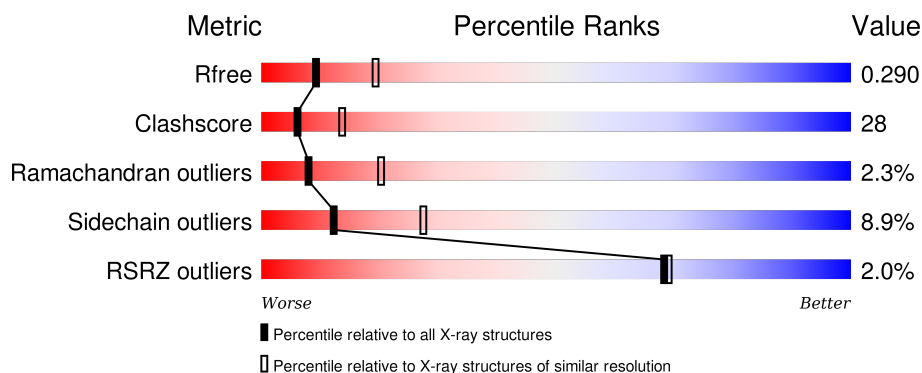
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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	450	<div> <div>62%</div> <div>28%</div> <div>5%</div> <div>5%</div> </div>
1	D	450	<div> <div>60%</div> <div>30%</div> <div>5%</div> <div>5%</div> </div>
2	B	263	<div>2%</div> <div> <div>41%</div> <div>30%</div> <div>8%</div> <div>22%</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	190	<div><div></div><div>7%</div><div>49%</div><div>37%</div><div>5% • 8%</div></div>

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 12990 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 CYTOCHROME B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	428	Total	C	N	O	S	0	0	0
			3439	2332	538	551	18			
1	D	428	Total	C	N	O	S	0	0	0
			3439	2332	538	551	18			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	441	HIS	-	EXPRESSION TAG	UNP P05418
A	442	HIS	-	EXPRESSION TAG	UNP P05418
A	443	HIS	-	EXPRESSION TAG	UNP P05418
A	444	HIS	-	EXPRESSION TAG	UNP P05418
A	445	HIS	-	EXPRESSION TAG	UNP P05418
A	446	HIS	-	EXPRESSION TAG	UNP P05418
A	447	HIS	-	EXPRESSION TAG	UNP P05418
A	448	HIS	-	EXPRESSION TAG	UNP P05418
A	449	HIS	-	EXPRESSION TAG	UNP P05418
A	450	HIS	-	EXPRESSION TAG	UNP P05418
D	441	HIS	-	EXPRESSION TAG	UNP P05418
D	442	HIS	-	EXPRESSION TAG	UNP P05418
D	443	HIS	-	EXPRESSION TAG	UNP P05418
D	444	HIS	-	EXPRESSION TAG	UNP P05418
D	445	HIS	-	EXPRESSION TAG	UNP P05418
D	446	HIS	-	EXPRESSION TAG	UNP P05418
D	447	HIS	-	EXPRESSION TAG	UNP P05418
D	448	HIS	-	EXPRESSION TAG	UNP P05418
D	449	HIS	-	EXPRESSION TAG	UNP P05418
D	450	HIS	-	EXPRESSION TAG	UNP P05418

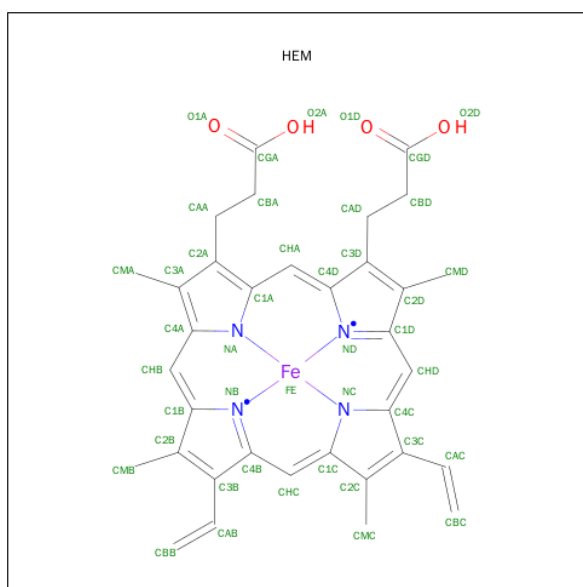
- Molecule 2 is a protein called CYTOCHROME C1, HEME PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	206	Total	C	N	O	S	0	0	0
			1594	1020	264	301	9			
2	E	206	Total	C	N	O	S	0	0	0
			1594	1020	264	301	9			

- Molecule 3 is a protein called UBIQUINOL-CYTOCHROME C REDUCTASE IRON-SULFUR SUBUNIT.

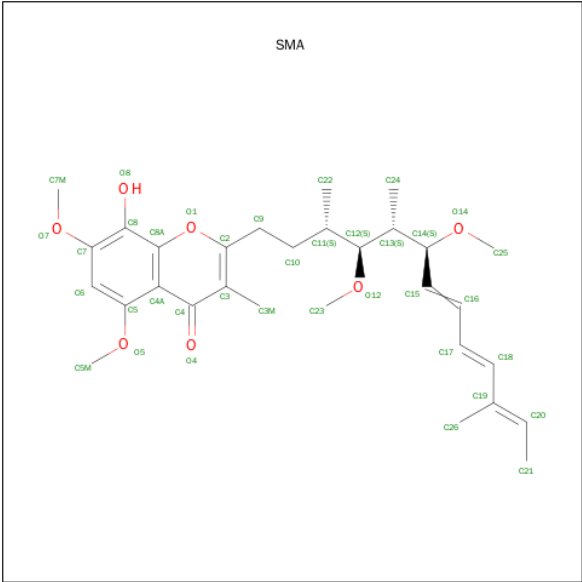
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	174	Total	C	N	O	S	0	0	0
			1289	804	230	248	7			
3	F	174	Total	C	N	O	S	0	0	0
			1289	804	230	248	7			

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



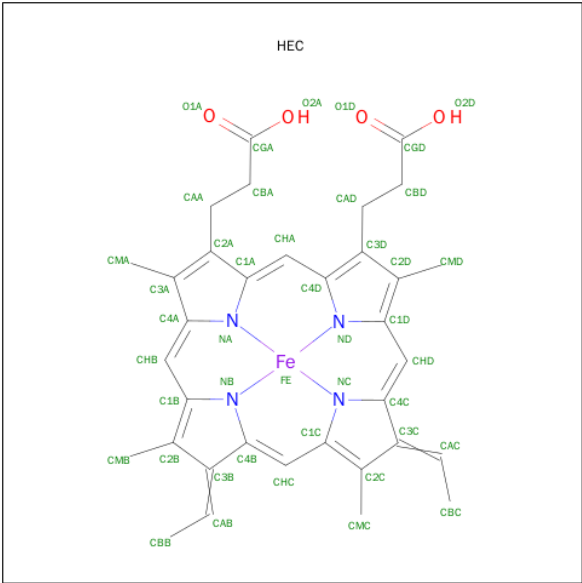
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
4	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
4	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
4	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 5 is STIGMATELLIN A (three-letter code: SMA) (formula:  $C_{30}H_{42}O_7$ ).



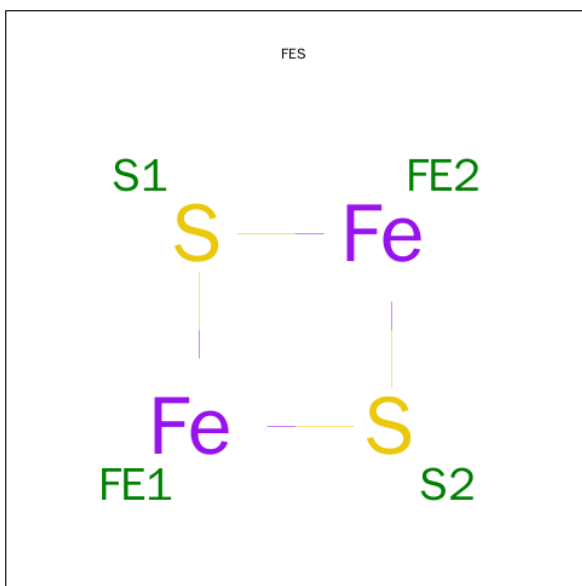
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O		0	0
			37	30	7			
5	D	1	Total	C	O		0	0
			37	30	7			

- Molecule 6 is HEME C (three-letter code: HEC) (formula: C<sub>34</sub>H<sub>34</sub>FeN<sub>4</sub>O<sub>4</sub>).



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

- Molecule 7 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula:  $\text{Fe}_2\text{S}_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	Fe	S	0	0
			4	2	2		
7	F	1	Total	Fe	S	0	0
			4	2	2		

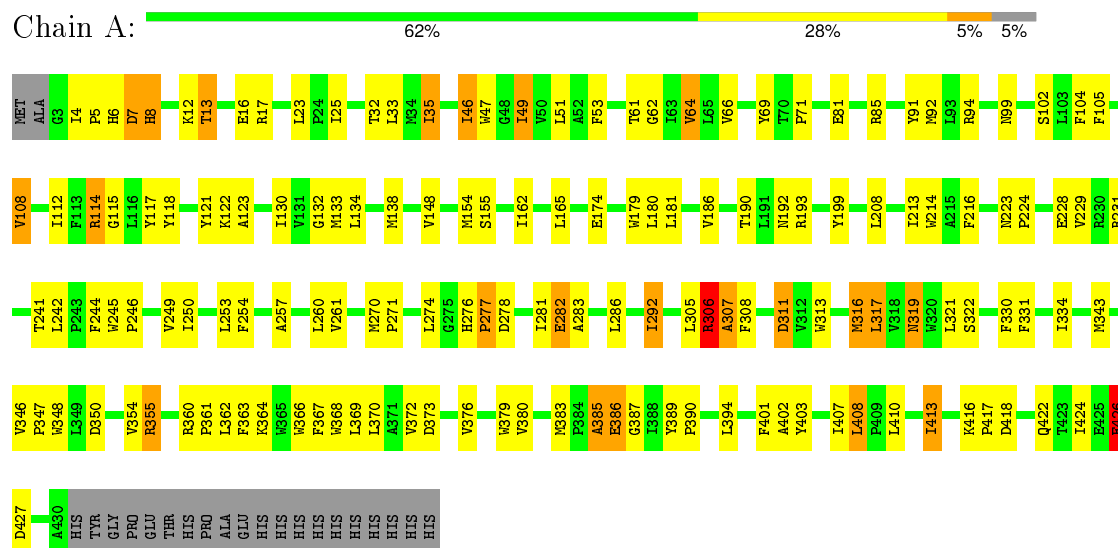
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	3	Total	O	0	0
			3	3		
8	B	1	Total	O	0	0
			1	1		
8	D	1	Total	O	0	0
			1	1		
8	F	1	Total	O	0	0
			1	1		

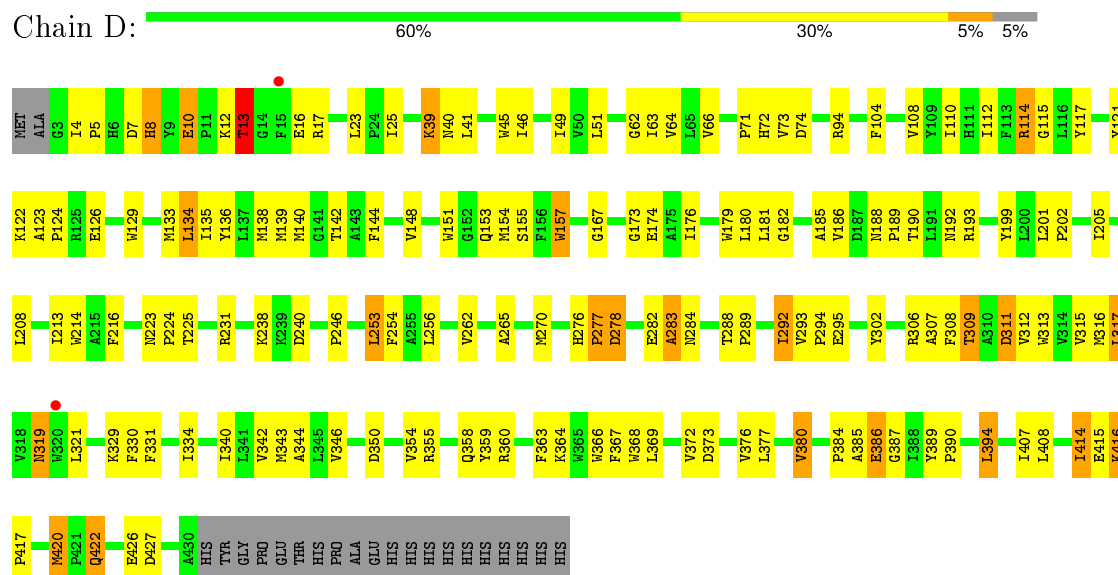
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 ( $\text{RSRZ} > 2$ ). 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: CYTOCHROME B

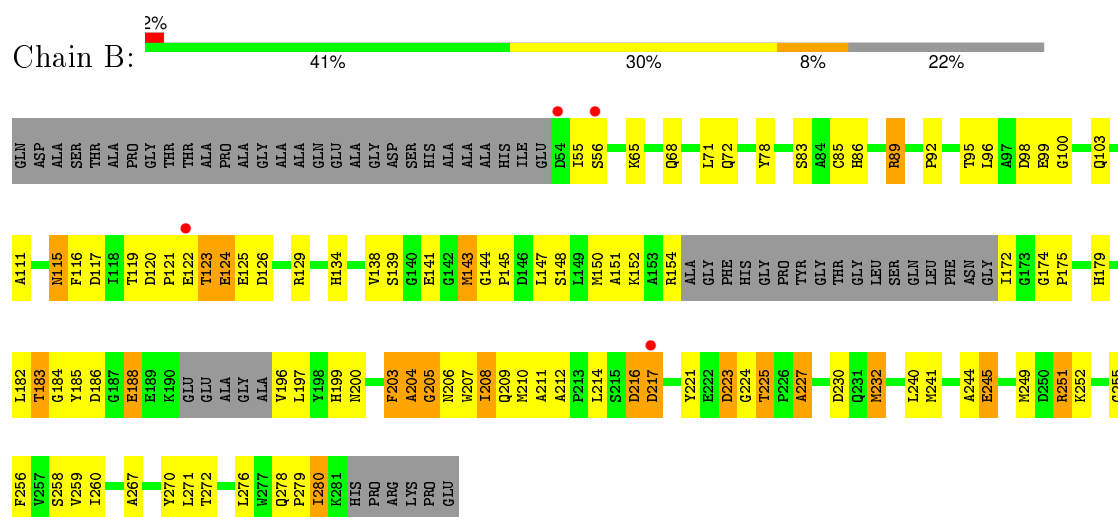


#### • Molecule 1: CYTOCHROME B

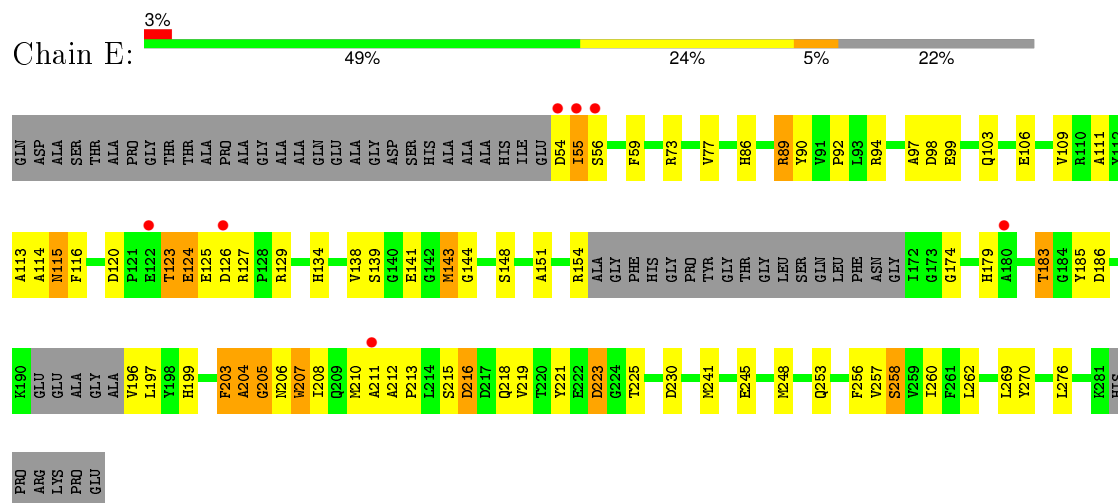


#### • Molecule 2: CYTOCHROME C1, HEME PROTEIN

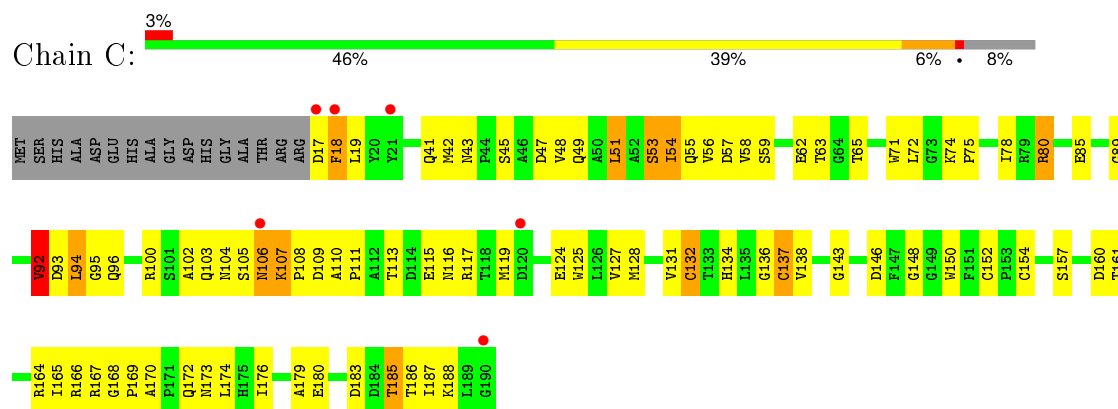




• Molecule 2: CYTOCHROME C1, HEME PROTEIN



• Molecule 3: UBIQUINOL-CYTOCHROME C REDUCTASE IRON-SULFUR SUBUNIT



• Molecule 3: UBIQUINOL-CYTOCHROME C REDUCTASE IRON-SULFUR SUBUNIT





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.30Å 164.91Å 100.61Å 90.00° 103.18° 90.00°	Depositor
Resolution (Å)	97.96 – 2.70 47.02 – 2.70	Depositor EDS
% Data completeness (in resolution range)	94.3 (97.96-2.70) 94.4 (47.02-2.70)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.07 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, $R_{free}$	0.238 , 0.290 0.239 , 0.290	Depositor DCC
$R_{free}$ test set	3535 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	32.2	Xtriage
Anisotropy	0.353	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 53.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	3 of 70028 reflections (0.004%)	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	12990	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 54.17 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.7952e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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 [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, FES, SMA, HEC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.79	0/3573	0.87	5/4904 (0.1%)
1	D	0.71	1/3573 (0.0%)	0.78	4/4904 (0.1%)
2	B	0.71	0/1634	0.86	1/2223 (0.0%)
2	E	0.63	0/1634	0.73	0/2223
3	C	0.70	0/1317	0.87	1/1796 (0.1%)
3	F	0.63	0/1317	0.80	1/1796 (0.1%)
All	All	0.72	1/13048 (0.0%)	0.82	12/17846 (0.1%)

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
3	C	0	1
3	F	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	157	TRP	CB-CG	-5.04	1.41	1.50

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	355	ARG	NE-CZ-NH2	-7.83	116.39	120.30
1	A	355	ARG	NE-CZ-NH1	7.54	124.07	120.30
3	C	137	CYS	CA-CB-SG	-6.08	103.06	114.00
3	F	69	VAL	CB-CA-C	-5.88	100.22	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	306	ARG	NE-CZ-NH2	-5.87	117.37	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	17	ASP	Peptide
3	F	107	LYS	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	3439	0	3402	165	0
1	D	3439	0	3402	158	0
2	B	1594	0	1530	135	0
2	E	1594	0	1530	93	0
3	C	1289	0	1231	97	0
3	F	1289	0	1231	85	0
4	A	86	0	60	19	0
4	D	86	0	60	18	0
5	A	37	0	42	2	0
5	D	37	0	41	2	0
6	B	43	0	30	5	0
6	E	43	0	30	4	0
7	C	4	0	0	1	0
7	F	4	0	0	1	0
8	A	3	0	0	1	0
8	B	1	0	0	0	0
8	D	1	0	0	0	0
8	F	1	0	0	0	0
All	All	12990	0	12589	720	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 28.

The worst 5 of 720 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:123:THR:CG2	2:E:125:GLU:H	1.37	1.37
2:B:99:GLU:HA	2:B:103:GLN:NE2	1.43	1.33
2:E:205:GLY:HA2	2:E:206:ASN:OD1	1.26	1.30
2:B:123:THR:HG22	2:B:124:GLU:N	1.32	1.22
3:F:183:ASP:OD1	3:F:186:THR:HB	1.46	1.16

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	426/450 (95%)	394 (92%)	26 (6%)	6 (1%)	14	35
1	D	426/450 (95%)	399 (94%)	21 (5%)	6 (1%)	14	35
2	B	200/263 (76%)	173 (86%)	20 (10%)	7 (4%)	4	10
2	E	200/263 (76%)	181 (90%)	14 (7%)	5 (2%)	7	18
3	C	172/190 (90%)	155 (90%)	12 (7%)	5 (3%)	6	14
3	F	172/190 (90%)	145 (84%)	20 (12%)	7 (4%)	3	7
All	All	1596/1806 (88%)	1447 (91%)	113 (7%)	36 (2%)	8	20

5 of 36 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	13	THR
1	A	386	GLU
2	B	124	GLU
2	B	204	ALA
3	C	53	SER

### 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	351/376 (93%)	320 (91%)	31 (9%)	12	28
1	D	351/376 (93%)	320 (91%)	31 (9%)	12	28
2	B	166/205 (81%)	148 (89%)	18 (11%)	8	18
2	E	166/205 (81%)	154 (93%)	12 (7%)	18	41
3	C	131/146 (90%)	118 (90%)	13 (10%)	10	22
3	F	131/146 (90%)	121 (92%)	10 (8%)	16	37
All	All	1296/1454 (89%)	1181 (91%)	115 (9%)	12	27

5 of 115 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	56	VAL
1	D	10	GLU
3	F	51	LEU
3	C	63	THR
3	C	113	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	49	GLN
1	D	20	HIS
3	F	43	ASN
3	C	116	ASN
1	D	8	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 ⓘ

10 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	$\# Z  > 2$
4	HEM	A	500	1	30,50,50	2.64	8 (26%)	24,82,82	2.68	12 (50%)
4	HEM	A	501	1	30,50,50	2.44	11 (36%)	24,82,82	2.40	10 (41%)
5	SMA	A	502	-	35,38,38	1.46	7 (20%)	40,52,52	2.44	20 (50%)
6	HEC	B	500	2	24,50,50	2.43	3 (12%)	19,82,82	3.49	8 (42%)
7	FES	C	500	3	0,4,4	0.00	-	0,4,4	0.00	-
4	HEM	D	500	1	30,50,50	2.53	8 (26%)	24,82,82	2.76	14 (58%)
4	HEM	D	501	1	30,50,50	2.26	8 (26%)	24,82,82	2.38	9 (37%)
5	SMA	D	502	-	35,38,38	1.27	4 (11%)	40,52,52	2.00	17 (42%)
6	HEC	E	500	2	24,50,50	2.44	3 (12%)	19,82,82	3.50	8 (42%)
7	FES	F	500	3	0,4,4	0.00	-	0,4,4	0.00	-

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
4	HEM	A	500	1	-	0/10/54/54	0/0/8/8
4	HEM	A	501	1	-	0/10/54/54	0/0/8/8
5	SMA	A	502	-	-	0/33/34/34	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	HEC	B	500	2	-	2/6/54/54	0/0/8/8
7	FES	C	500	3	-	0/0/4/4	0/1/1/1
4	HEM	D	500	1	-	0/10/54/54	0/0/8/8
4	HEM	D	501	1	-	0/10/54/54	0/0/8/8
5	SMA	D	502	-	-	0/33/34/34	0/2/2/2
6	HEC	E	500	2	-	0/6/54/54	0/0/8/8
7	FES	F	500	3	-	0/0/4/4	0/1/1/1

The worst 5 of 52 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	500	HEM	C3B-C4B	-9.95	1.43	1.51
4	A	501	HEM	C3B-C4B	-9.58	1.43	1.51
4	D	500	HEM	C3B-C4B	-9.55	1.43	1.51
4	D	501	HEM	C3B-C4B	-8.36	1.44	1.51
6	E	500	HEC	C3B-C2B	-7.36	1.33	1.40

The worst 5 of 98 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	500	HEC	CBB-CAB-C3B	-9.37	106.53	127.35
6	B	500	HEC	CBB-CAB-C3B	-8.34	108.82	127.35
6	B	500	HEC	CBC-CAC-C3C	-7.73	110.18	127.35
6	E	500	HEC	CBC-CAC-C3C	-7.08	111.62	127.35
4	D	500	HEM	C3B-CAB-CBB	-5.71	115.69	124.46

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	500	HEC	C3A-C2A-CAA-CBA
6	B	500	HEC	C1A-C2A-CAA-CBA

There are no ring outliers.

10 monomers are involved in 52 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	500	HEM	15	0
4	A	501	HEM	4	0
5	A	502	SMA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	500	HEC	5	0
7	C	500	FES	1	0
4	D	500	HEM	13	0
4	D	501	HEM	5	0
5	D	502	SMA	2	0
6	E	500	HEC	4	0
7	F	500	FES	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 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, 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	428/450 (95%)	-0.22	0 <span>100</span> <span>100</span>	9, 21, 41, 61	0
1	D	428/450 (95%)	-0.25	2 (0%) <span>91</span> <span>93</span>	9, 22, 44, 61	0
2	B	206/263 (78%)	0.11	4 (1%) <span>70</span> <span>70</span>	18, 33, 54, 69	0
2	E	206/263 (78%)	0.14	7 (3%) <span>49</span> <span>49</span>	18, 35, 55, 71	0
3	C	174/190 (91%)	0.12	6 (3%) <span>49</span> <span>49</span>	12, 31, 46, 54	0
3	F	174/190 (91%)	0.39	13 (7%) <span>17</span> <span>15</span>	13, 38, 59, 62	0
All	All	1616/1806 (89%)	-0.04	32 (1%) <span>68</span> <span>69</span>	9, 27, 52, 71	0

The worst 5 of 32 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	190	GLY	5.9
2	E	54	ASP	5.6
3	C	21	TYR	4.2
2	E	122	GLU	3.9
2	B	122	GLU	3.9

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	SMA	A	502	37/37	0.97	0.16	0.42	12,17,33,36	0
4	HEM	D	500	43/43	0.98	0.17	0.39	12,16,23,25	0
5	SMA	D	502	37/37	0.98	0.15	0.30	6,14,37,41	0
4	HEM	A	501	43/43	0.98	0.16	0.28	9,14,16,18	0
6	HEC	E	500	43/43	0.97	0.17	0.03	24,29,34,36	0
7	FES	F	500	4/4	0.99	0.13	-0.10	16,20,22,23	0
4	HEM	A	500	43/43	0.98	0.15	-0.16	9,14,22,25	0
4	HEM	D	501	43/43	0.98	0.14	-0.25	7,17,26,27	0
6	HEC	B	500	43/43	0.97	0.15	-0.58	19,26,37,42	0
7	FES	C	500	4/4	0.99	0.11	-1.23	22,26,26,28	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.