



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 03:35 am GMT

PDB ID : 1M56  
Title : Structure of cytochrome c oxidase from Rhodobactor sphaeroides (Wild Type)  
Authors : Svensson-Ek, M.; Abramson, J.; Larsson, G.; Tornroth, S.; Brezezinski, P.; Iwata, S.  
Deposited on : 2002-07-08  
Resolution : 2.30 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.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

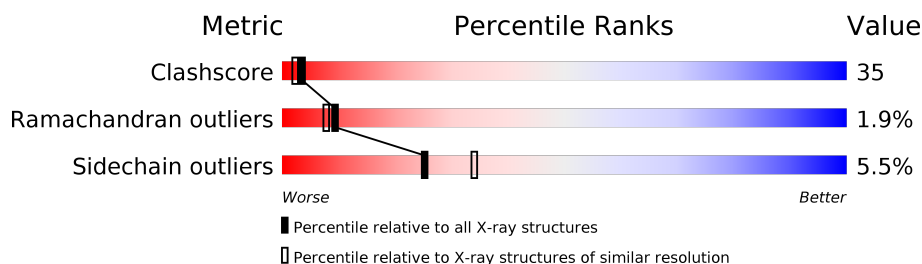
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)


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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	566	
1	G	566	
2	B	264	
2	H	264	
3	C	266	
3	I	266	
4	D	51	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
4	J	51	

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
8	HEA	A	1001	X	-	-	-
8	HEA	A	1002	X	-	-	-
8	HEA	G	1001	X	-	-	-
8	HEA	G	1002	X	-	-	-
9	PEH	C	2013	-	-	X	-
9	PEH	D	2011	-	-	X	-
9	PEH	I	3010	-	-	X	-
9	PEH	I	3013	-	-	X	-

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 18934 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 C OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	547	Total	C	N	O	S	0	0	0
			4322	2892	684	715	31			
1	G	547	Total	C	N	O	S	0	0	0
			4322	2892	684	715	31			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	436	ILE	SER	SEE REMARK 999	UNP P33517
A	437	TYR	THR	SEE REMARK 999	UNP P33517
A	438	PHE	SER	SEE REMARK 999	UNP P33517
A	439	TRP	GLY	SEE REMARK 999	UNP P33517
A	518	THR	SER	SEE REMARK 999	UNP P33517
A	520	THR	SER	SEE REMARK 999	UNP P33517
A	521	ARG	-	SEE REMARK 999	UNP P33517
G	436	ILE	SER	SEE REMARK 999	UNP P33517
G	437	TYR	THR	SEE REMARK 999	UNP P33517
G	438	PHE	SER	SEE REMARK 999	UNP P33517
G	439	TRP	GLY	SEE REMARK 999	UNP P33517
G	518	THR	SER	SEE REMARK 999	UNP P33517
G	520	THR	SER	SEE REMARK 999	UNP P33517
G	521	ARG	-	SEE REMARK 999	UNP P33517

- Molecule 2 is a protein called CYTOCHROME C OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	260	Total	C	N	O	S	0	0	0
			2046	1334	332	374	6			
2	H	260	Total	C	N	O	S	0	0	0
			2046	1334	332	374	6			

- Molecule 3 is a protein called CYTOCHROME C OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	265	Total	C	N	O	S	0	0	0
			2139	1448	342	337	12			
3	I	265	Total	C	N	O	S	0	0	0
			2139	1448	342	337	12			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	30	PHE	ASN	SEE REMARK 999	UNP P84153
C	92	MET	ILE	SEE REMARK 999	UNP P84153
C	244	ILE	MET	SEE REMARK 999	UNP P84153
I	30	PHE	ASN	SEE REMARK 999	UNP P84153
I	92	MET	ILE	SEE REMARK 999	UNP P84153
I	244	ILE	MET	SEE REMARK 999	UNP P84153

- Molecule 4 is a protein called CYTOCHROME C OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	42	Total	C	N	O	S	0	0	0
			311	203	52	54	2			
4	J	42	Total	C	N	O	S	0	0	0
			311	203	52	54	2			

- Molecule 5 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	2	Total	Cu	0	0
			2	2		
5	G	1	Total	Cu	0	0
			1	1		
5	B	2	Total	Cu	0	0
			2	2		
5	A	1	Total	Cu	0	0
			1	1		

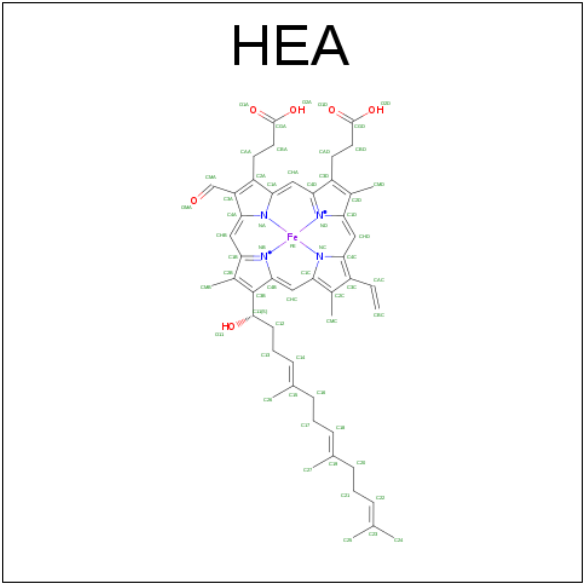
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	1	Total	Mg	0	0
			1	1		
6	A	1	Total	Mg	0	0
			1	1		

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

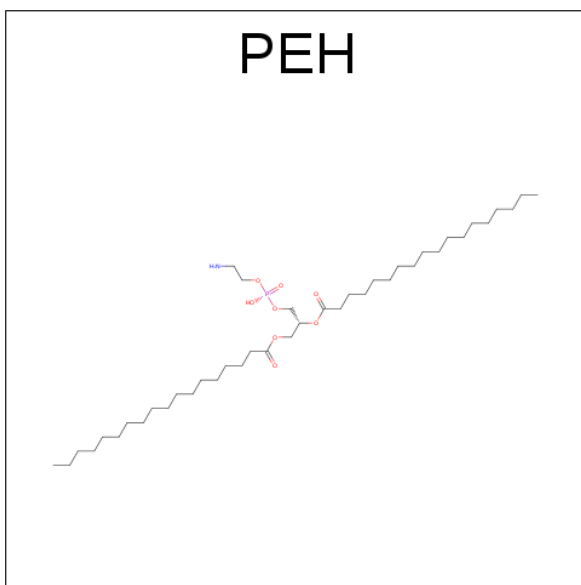
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	G	1	Total	Ca	0	0
			1	1		
7	A	1	Total	Ca	0	0
			1	1		

- Molecule 8 is HEME-A (three-letter code: HEA) (formula: C<sub>49</sub>H<sub>56</sub>FeN<sub>4</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
8	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
8	G	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
8	G	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		

- Molecule 9 is DI-STEAROYL-3-SN-PHOSPHATIDYLETHANOLAMINE (three-letter code: PEH) (formula: C<sub>41</sub>H<sub>82</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	C	1	Total	C	N	O	P	0	0
			51	41	1	8	1		
9	A	1	Total	C	N	O	P	0	0
			51	41	1	8	1		
9	C	1	Total	C	N	O	P	0	0
			51	41	1	8	1		
9	D	1	Total	C	N	O	P	0	0
			51	41	1	8	1		
9	A	1	Total	C	N	O	P	0	0
			51	41	1	8	1		
9	C	1	Total	C	N	O	P	0	0
			51	41	1	8	1		
9	I	1	Total	C	N	O	P	0	0
			51	41	1	8	1		
9	G	1	Total	C	N	O	P	0	0
			51	41	1	8	1		
9	I	1	Total	C	N	O	P	0	0
			51	41	1	8	1		
9	J	1	Total	C	N	O	P	0	0
			51	41	1	8	1		
9	G	1	Total	C	N	O	P	0	0
			51	41	1	8	1		
9	I	1	Total	C	N	O	P	0	0
			51	41	1	8	1		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	101	Total 101	O 101	0	0
10	B	68	Total 68	O 68	0	0
10	C	39	Total 39	O 39	0	0
10	D	12	Total 12	O 12	0	0
10	G	106	Total 106	O 106	0	0
10	H	64	Total 64	O 64	0	0
10	I	38	Total 38	O 38	0	0
10	J	8	Total 8	O 8	0	0

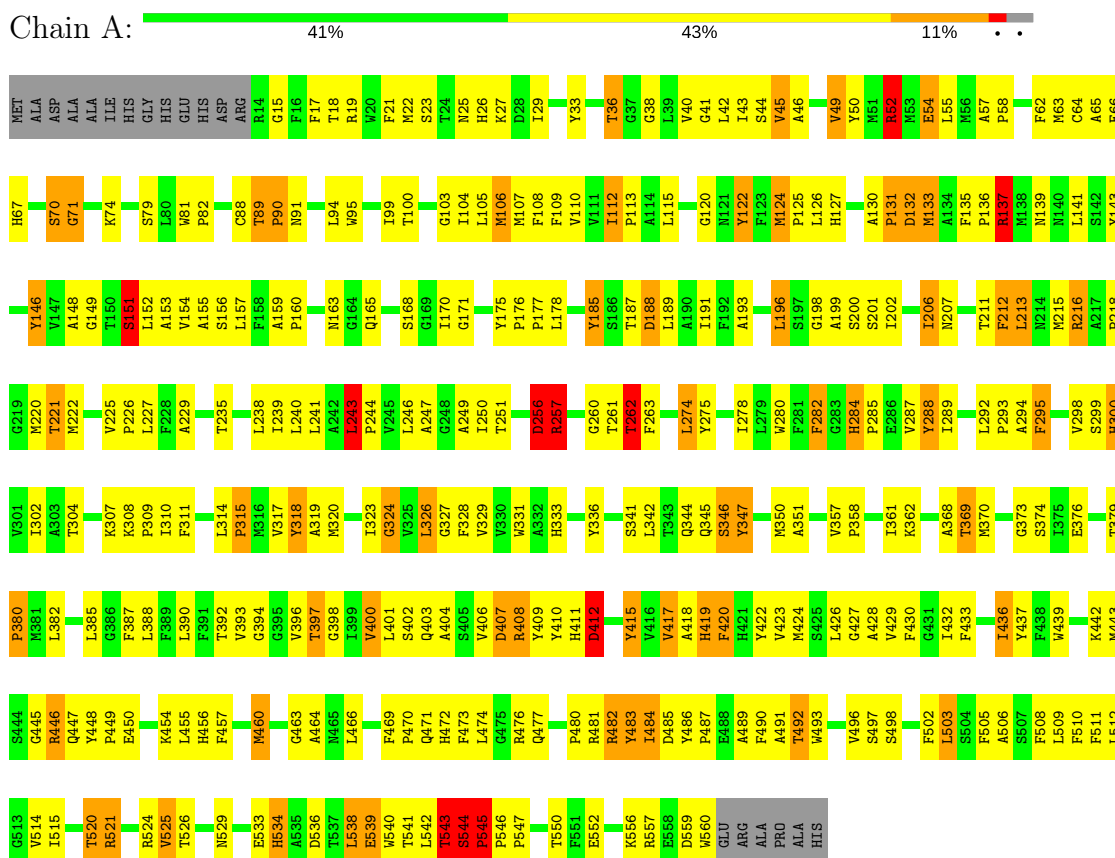


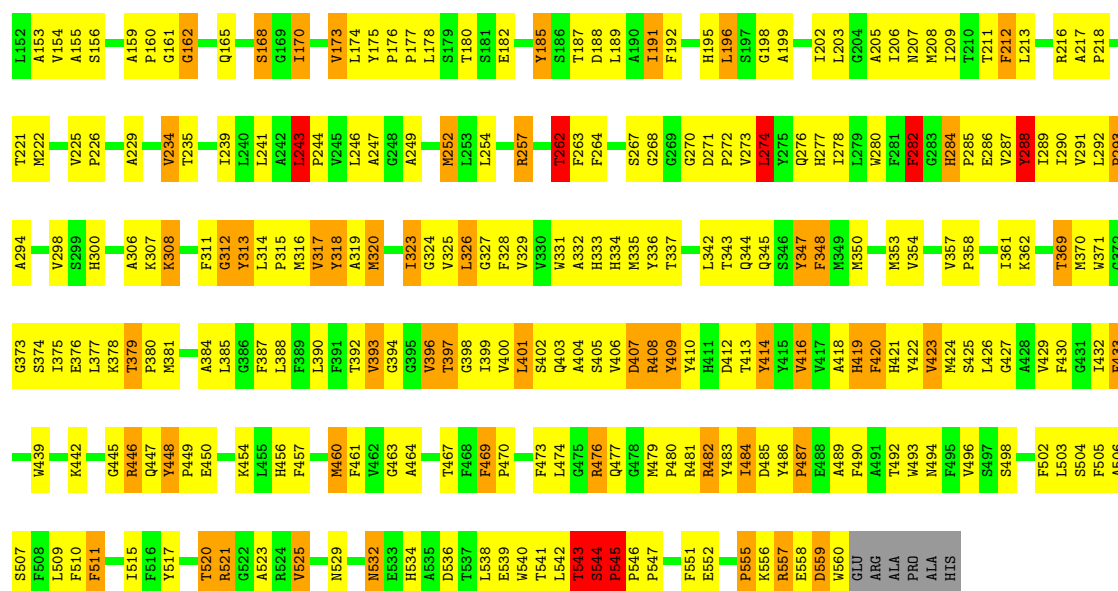
### 3 Residue-property plots

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

Note EDS was not executed.

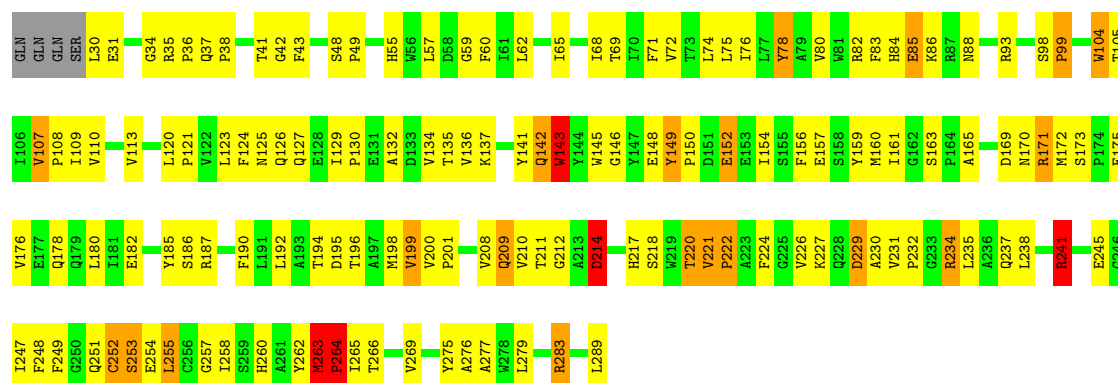
#### • Molecule 1: CYTOCHROME C OXIDASE





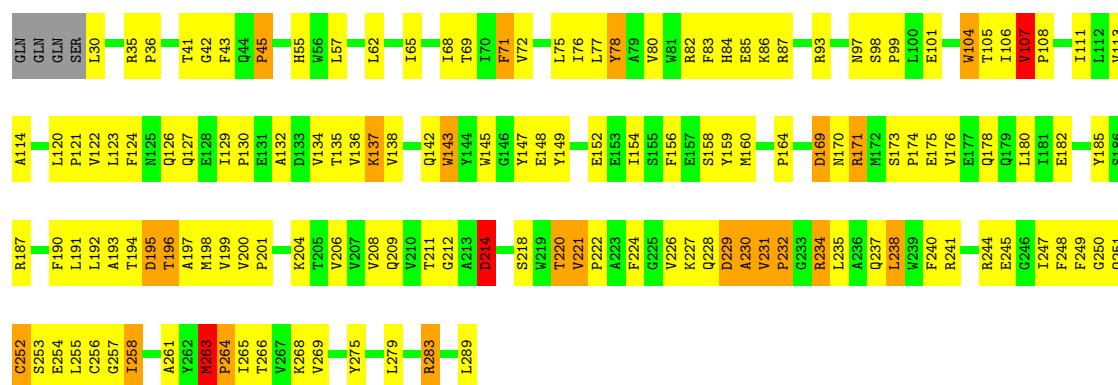
## • Molecule 2: CYTOCHROME C OXIDASE

Chain B: 44% 45% 8% ..

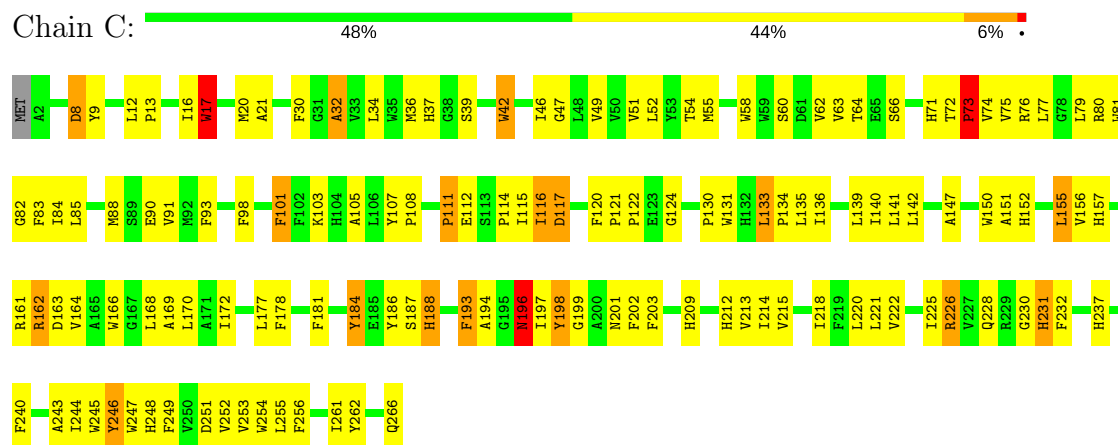


## • Molecule 2: CYTOCHROME C OXIDASE

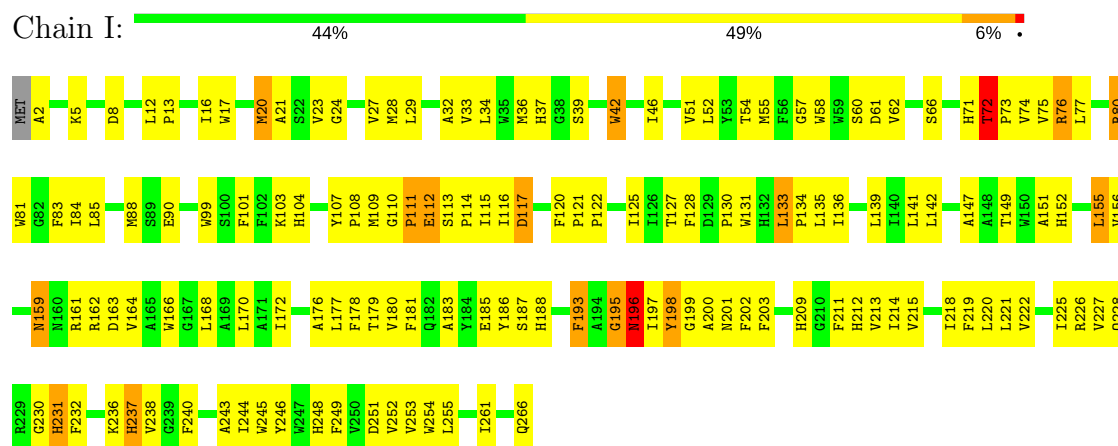
Chain H: 45% 44% 8% ..



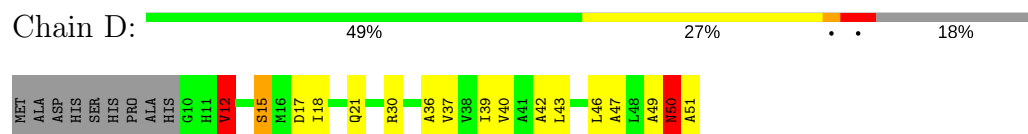
## • Molecule 3: CYTOCHROME C OXIDASE



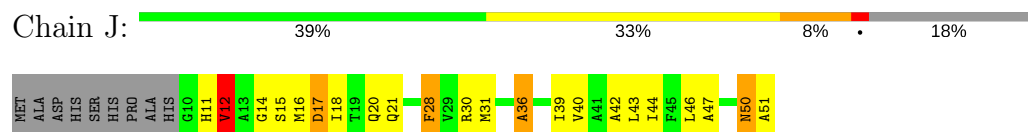
• Molecule 3: CYTOCHROME C OXIDASE



• Molecule 4: CYTOCHROME C OXIDASE



• Molecule 4: CYTOCHROME C OXIDASE



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	340.36 Å   340.36 Å   89.67 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	40.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (40.00-2.30)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.236 , 0.275	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	18934	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, PEH, CA, CU, HEA

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	0.70	2/4482 (0.0%)	1.91	106/6114 (1.7%)
1	G	0.71	1/4482 (0.0%)	1.86	97/6114 (1.6%)
2	B	0.57	0/2105	1.73	38/2879 (1.3%)
2	H	0.58	0/2105	1.67	36/2879 (1.3%)
3	C	0.53	0/2232	1.43	22/3054 (0.7%)
3	I	0.55	0/2232	1.49	22/3054 (0.7%)
4	D	0.52	0/316	1.66	6/428 (1.4%)
4	J	0.53	0/316	1.61	6/428 (1.4%)
All	All	0.63	3/18270 (0.0%)	1.74	333/24950 (1.3%)

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	A	0	12
1	G	0	15
2	B	0	6
2	H	0	5
3	C	0	3
3	I	0	2
4	D	0	1
All	All	0	44

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	543	THR	C-O	5.96	1.34	1.23
1	G	544	SER	N-CA	-5.23	1.35	1.46
1	A	544	SER	N-CA	-5.20	1.35	1.46

The worst 5 of 333 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	543	THR	C-N-CA	21.14	174.56	121.70
1	A	257	ARG	NE-CZ-NH1	-20.04	110.28	120.30
2	B	171	ARG	NE-CZ-NH1	16.88	128.74	120.30
1	A	521	ARG	NE-CZ-NH2	-16.71	111.94	120.30
2	B	234	ARG	NE-CZ-NH2	-16.71	111.95	120.30

There are no chirality outliers.

5 of 44 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	108	PHE	Mainchain
1	A	112	ILE	Mainchain
1	A	157	LEU	Mainchain
1	A	202	ILE	Mainchain
1	A	257	ARG	Mainchain

## 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	4322	0	4238	314	0
1	G	4322	0	4238	339	0
2	B	2046	0	2011	126	0
2	H	2046	0	2011	143	0
3	C	2139	0	2056	155	0
3	I	2139	0	2056	153	0
4	D	311	0	319	25	0
4	J	311	0	319	42	0
5	A	1	0	0	0	0
5	B	2	0	0	0	0
5	G	1	0	0	0	0
5	H	2	0	0	0	0
6	A	1	0	0	0	0
6	G	1	0	0	0	0
7	A	1	0	0	0	0
7	G	1	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	120	0	108	26	0
8	G	120	0	108	18	0
9	A	102	0	162	34	0
9	C	153	0	243	48	0
9	D	51	0	81	21	0
9	G	102	0	162	29	0
9	I	153	0	243	51	0
9	J	51	0	81	16	0
10	A	101	0	0	7	0
10	B	68	0	0	3	0
10	C	39	0	0	5	0
10	D	12	0	0	0	0
10	G	106	0	0	9	0
10	H	64	0	0	6	0
10	I	38	0	0	4	0
10	J	8	0	0	2	0
All	All	18934	0	18436	1291	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 35.

The worst 5 of 1291 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)
3:I:8:ASP:HB3	3:I:72:THR:HG21	1.27	1.12
1:A:520:THR:HG22	1:A:521:ARG:HG2	1.32	1.12
9:I:3013:PEH:O14	9:I:3013:PEH:H121	1.51	1.11
9:I:3013:PEH:C3H	9:I:3013:PEH:H2D2	1.78	1.11
9:C:2013:PEH:H121	9:C:2013:PEH:O14	1.48	1.06

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	545/566 (96%)	479 (88%)	54 (10%)	12 (2%)	8	6
1	G	545/566 (96%)	466 (86%)	67 (12%)	12 (2%)	8	6
2	B	258/264 (98%)	222 (86%)	32 (12%)	4 (2%)	11	10
2	H	258/264 (98%)	220 (85%)	33 (13%)	5 (2%)	9	8
3	C	263/266 (99%)	229 (87%)	30 (11%)	4 (2%)	12	11
3	I	263/266 (99%)	234 (89%)	25 (10%)	4 (2%)	12	11
4	D	40/51 (78%)	37 (92%)	2 (5%)	1 (2%)	6	5
4	J	40/51 (78%)	32 (80%)	7 (18%)	1 (2%)	6	5
All	All	2212/2294 (96%)	1919 (87%)	250 (11%)	43 (2%)	9	8

5 of 43 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	544	SER
3	C	111	PRO
1	G	327	GLY
1	G	544	SER
2	H	264	PRO

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	446/459 (97%)	422 (95%)	24 (5%)	26	35
1	G	446/459 (97%)	410 (92%)	36 (8%)	14	17
2	B	216/220 (98%)	204 (94%)	12 (6%)	25	33
2	H	216/220 (98%)	209 (97%)	7 (3%)	44	60
3	C	215/216 (100%)	207 (96%)	8 (4%)	39	53
3	I	215/216 (100%)	206 (96%)	9 (4%)	34	47

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	30/37 (81%)	28 (93%)	2 (7%)	19	24
4	J	30/37 (81%)	29 (97%)	1 (3%)	43	59
All	All	1814/1864 (97%)	1715 (94%)	99 (6%)	25	34

5 of 99 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	15	SER
1	G	122	TYR
3	I	111	PRO
1	G	23	SER
1	G	55	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	201	ASN
1	G	26	HIS
3	I	212	HIS
3	C	212	HIS
3	C	231	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 10 are monoatomic - leaving 16 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
8	HEA	A	1001	1	44,67,67	1.62	7 (15%)	37,103,103	2.41	15 (40%)
8	HEA	A	1002	1	44,67,67	1.71	6 (13%)	37,103,103	1.95	12 (32%)
9	PEH	A	2009	-	50,50,50	1.50	2 (4%)	52,55,55	1.07	4 (7%)
9	PEH	A	2012	-	50,50,50	1.56	3 (6%)	52,55,55	1.09	5 (9%)
9	PEH	C	2008	-	50,50,50	1.55	2 (4%)	52,55,55	1.23	4 (7%)
9	PEH	C	2010	-	50,50,50	1.58	2 (4%)	52,55,55	1.04	4 (7%)
9	PEH	C	2013	-	50,50,50	1.56	2 (4%)	52,55,55	1.16	3 (5%)
9	PEH	D	2011	-	50,50,50	1.51	2 (4%)	52,55,55	1.29	4 (7%)
8	HEA	G	1001	1	44,67,67	1.49	6 (13%)	37,103,103	2.44	19 (51%)
8	HEA	G	1002	1	44,67,67	1.86	6 (13%)	37,103,103	2.26	14 (37%)
9	PEH	G	3009	-	50,50,50	1.52	2 (4%)	52,55,55	1.06	1 (1%)
9	PEH	G	3012	-	50,50,50	1.55	3 (6%)	52,55,55	1.14	5 (9%)
9	PEH	I	3008	-	50,50,50	1.52	2 (4%)	52,55,55	1.20	4 (7%)
9	PEH	I	3010	-	50,50,50	1.58	2 (4%)	52,55,55	1.01	4 (7%)
9	PEH	I	3013	-	50,50,50	1.52	3 (6%)	52,55,55	1.10	4 (7%)
9	PEH	J	3011	-	50,50,50	1.51	2 (4%)	52,55,55	1.32	4 (7%)

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
8	HEA	A	1001	1	3/3/7/16	0/24/76/76	0/0/8/8
8	HEA	A	1002	1	3/3/7/16	0/24/76/76	0/0/8/8
9	PEH	A	2009	-	-	0/54/54/54	0/0/0/0
9	PEH	A	2012	-	-	0/54/54/54	0/0/0/0
9	PEH	C	2008	-	-	0/54/54/54	0/0/0/0
9	PEH	C	2010	-	-	0/54/54/54	0/0/0/0
9	PEH	C	2013	-	-	1/54/54/54	0/0/0/0
9	PEH	D	2011	-	-	0/54/54/54	0/0/0/0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	HEA	G	1001	1	3/3/7/16	0/24/76/76	0/0/8/8
8	HEA	G	1002	1	3/3/7/16	0/24/76/76	0/0/8/8
9	PEH	G	3009	-	-	0/54/54/54	0/0/0/0
9	PEH	G	3012	-	-	0/54/54/54	0/0/0/0
9	PEH	I	3008	-	-	0/54/54/54	0/0/0/0
9	PEH	I	3010	-	-	0/54/54/54	0/0/0/0
9	PEH	I	3013	-	-	1/54/54/54	0/0/0/0
9	PEH	J	3011	-	-	0/54/54/54	0/0/0/0

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	G	1002	HEA	C3A-C2A	-6.71	1.31	1.40
8	A	1002	HEA	C3A-C2A	-5.71	1.32	1.40
8	G	1002	HEA	C3C-C2C	-4.77	1.34	1.40
8	A	1001	HEA	C3C-CAC	-4.55	1.38	1.47
8	A	1002	HEA	C3C-CAC	-4.50	1.38	1.47

The worst 5 of 106 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1001	HEA	C13-C14-C15	-6.68	110.89	127.68
9	J	3011	PEH	C2-O21-C21	-5.72	104.36	117.88
9	G	3009	PEH	C3-C2-C1	-5.19	100.15	111.86
8	G	1001	HEA	C13-C14-C15	-5.18	114.68	127.68
8	A	1002	HEA	C17-C18-C19	-4.91	115.34	127.68

5 of 12 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	G	1001	HEA	ND
8	G	1001	HEA	NA
8	G	1001	HEA	NB
8	G	1002	HEA	ND
8	G	1002	HEA	NA

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	I	3013	PEH	P-O12-C11-C12
9	C	2013	PEH	P-O12-C11-C12

There are no ring outliers.

16 monomers are involved in 226 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	1001	HEA	17	0
8	A	1002	HEA	9	0
9	A	2009	PEH	20	0
9	A	2012	PEH	14	0
9	C	2008	PEH	7	0
9	C	2010	PEH	20	0
9	C	2013	PEH	21	0
9	D	2011	PEH	21	0
8	G	1001	HEA	11	0
8	G	1002	HEA	7	0
9	G	3009	PEH	17	0
9	G	3012	PEH	12	0
9	I	3008	PEH	9	0
9	I	3010	PEH	21	0
9	I	3013	PEH	22	0
9	J	3011	PEH	16	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

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.