



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 05:28 AM GMT

PDB ID : 2QJY  
Title : Crystal structure of rhodobacter sphaeroides double mutant with stigmatellin and UQ2  
Authors : Esser, L.; Xia, D.  
Deposited on : 2007-07-09  
Resolution : 2.40 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

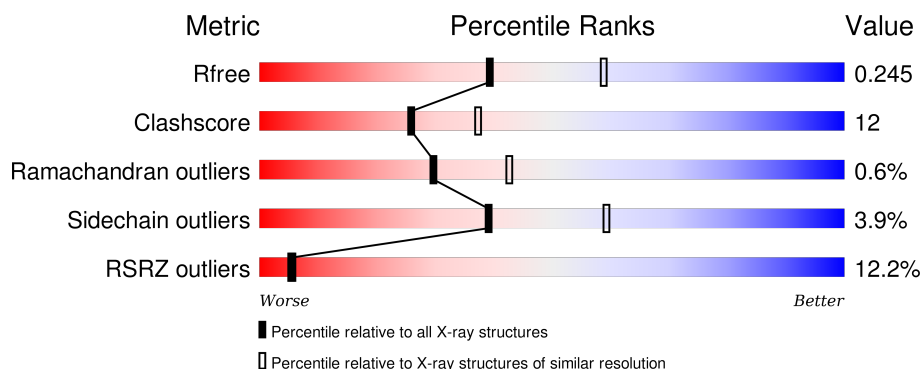
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	445	<div> <div>2%</div> <div>77%</div> <div>17%</div> <div>• •</div> </div>
1	D	445	<div> <div>3%</div> <div>77%</div> <div>18%</div> <div>• •</div> </div>
1	G	445	<div> <div>7%</div> <div>75%</div> <div>20%</div> <div>• •</div> </div>
1	J	445	<div> <div>8%</div> <div>73%</div> <div>21%</div> <div>• •</div> </div>
1	M	445	<div> <div>11%</div> <div>72%</div> <div>23%</div> <div>• •</div> </div>

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Mol	Chain	Length	Quality of chain
1	P	445	
2	B	269	
2	E	269	
2	H	269	
2	K	269	
2	N	269	
2	Q	269	
3	C	187	
3	F	187	
3	I	187	
3	L	187	
3	O	187	
3	R	187	

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
10	LOP	D	1022	-	-	-	X
10	LOP	G	1023	-	-	-	X
10	LOP	J	1024	-	-	-	X
10	LOP	P	1026	-	-	-	X
11	UQ2	A	1101	-	-	-	X
11	UQ2	D	1102	-	-	-	X
11	UQ2	G	1103	-	-	-	X
11	UQ2	J	1104	-	-	-	X
11	UQ2	M	1105	-	-	-	X
11	UQ2	P	1106	-	-	-	X

## 2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 42656 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
			3440	2322	548	555	15			
1	D	428	Total	C	N	O	S	0	0	0
			3440	2322	548	555	15			
1	G	428	Total	C	N	O	S	0	0	0
			3440	2322	548	555	15			
1	J	428	Total	C	N	O	S	0	0	0
			3440	2322	548	555	15			
1	M	428	Total	C	N	O	S	0	0	0
			3440	2322	548	555	15			
1	P	428	Total	C	N	O	S	0	0	0
			3440	2322	548	555	15			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	287	ARG	SER	ENGINEERED	UNP Q02761
D	287	ARG	SER	ENGINEERED	UNP Q02761
G	287	ARG	SER	ENGINEERED	UNP Q02761
J	287	ARG	SER	ENGINEERED	UNP Q02761
M	287	ARG	SER	ENGINEERED	UNP Q02761
P	287	ARG	SER	ENGINEERED	UNP Q02761

- Molecule 2 is a protein called Cytochrome c1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	256	Total	C	N	O	S	0	0	0
			1953	1240	326	374	13			
2	E	256	Total	C	N	O	S	0	0	0
			1953	1240	326	374	13			
2	H	256	Total	C	N	O	S	0	0	0
			1953	1240	326	374	13			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	K	256	Total 1953	C 1240	N 326	O 374	S 13	0	0	0
2	N	256	Total 1953	C 1240	N 326	O 374	S 13	0	0	0
2	Q	256	Total 1953	C 1240	N 326	O 374	S 13	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	264	HIS	-	EXPRESSION TAG	UNP Q3IY11
B	265	HIS	-	EXPRESSION TAG	UNP Q3IY11
B	266	HIS	-	EXPRESSION TAG	UNP Q3IY11
B	267	HIS	-	EXPRESSION TAG	UNP Q3IY11
B	268	HIS	-	EXPRESSION TAG	UNP Q3IY11
B	269	HIS	-	EXPRESSION TAG	UNP Q3IY11
E	264	HIS	-	EXPRESSION TAG	UNP Q3IY11
E	265	HIS	-	EXPRESSION TAG	UNP Q3IY11
E	266	HIS	-	EXPRESSION TAG	UNP Q3IY11
E	267	HIS	-	EXPRESSION TAG	UNP Q3IY11
E	268	HIS	-	EXPRESSION TAG	UNP Q3IY11
E	269	HIS	-	EXPRESSION TAG	UNP Q3IY11
H	264	HIS	-	EXPRESSION TAG	UNP Q3IY11
H	265	HIS	-	EXPRESSION TAG	UNP Q3IY11
H	266	HIS	-	EXPRESSION TAG	UNP Q3IY11
H	267	HIS	-	EXPRESSION TAG	UNP Q3IY11
H	268	HIS	-	EXPRESSION TAG	UNP Q3IY11
H	269	HIS	-	EXPRESSION TAG	UNP Q3IY11
K	264	HIS	-	EXPRESSION TAG	UNP Q3IY11
K	265	HIS	-	EXPRESSION TAG	UNP Q3IY11
K	266	HIS	-	EXPRESSION TAG	UNP Q3IY11
K	267	HIS	-	EXPRESSION TAG	UNP Q3IY11
K	268	HIS	-	EXPRESSION TAG	UNP Q3IY11
K	269	HIS	-	EXPRESSION TAG	UNP Q3IY11
N	264	HIS	-	EXPRESSION TAG	UNP Q3IY11
N	265	HIS	-	EXPRESSION TAG	UNP Q3IY11
N	266	HIS	-	EXPRESSION TAG	UNP Q3IY11
N	267	HIS	-	EXPRESSION TAG	UNP Q3IY11
N	268	HIS	-	EXPRESSION TAG	UNP Q3IY11
N	269	HIS	-	EXPRESSION TAG	UNP Q3IY11
Q	264	HIS	-	EXPRESSION TAG	UNP Q3IY11
Q	265	HIS	-	EXPRESSION TAG	UNP Q3IY11

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	266	HIS	-	EXPRESSION TAG	UNP Q3IY11
Q	267	HIS	-	EXPRESSION TAG	UNP Q3IY11
Q	268	HIS	-	EXPRESSION TAG	UNP Q3IY11
Q	269	HIS	-	EXPRESSION TAG	UNP Q3IY11

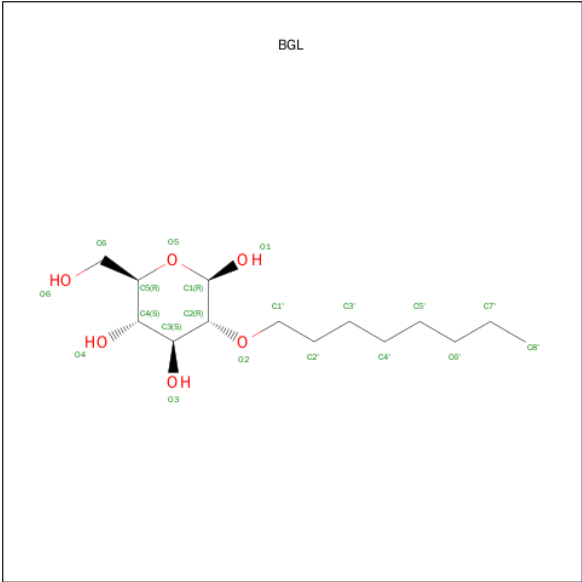
- Molecule 3 is a protein called Ubiquinol-cytochrome c reductase iron-sulfur subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	179	Total	C	N	O	S	0	0	0
			1340	843	237	254	6			
3	F	179	Total	C	N	O	S	0	0	0
			1340	843	237	254	6			
3	I	179	Total	C	N	O	S	0	0	0
			1340	843	237	254	6			
3	L	179	Total	C	N	O	S	0	0	0
			1340	843	237	254	6			
3	O	179	Total	C	N	O	S	0	0	0
			1340	843	237	254	6			
3	R	179	Total	C	N	O	S	0	0	0
			1340	843	237	254	6			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	135	SER	VAL	ENGINEERED	UNP Q02762
F	135	SER	VAL	ENGINEERED	UNP Q02762
I	135	SER	VAL	ENGINEERED	UNP Q02762
L	135	SER	VAL	ENGINEERED	UNP Q02762
O	135	SER	VAL	ENGINEERED	UNP Q02762
R	135	SER	VAL	ENGINEERED	UNP Q02762

- Molecule 4 is beta-octyl glucopyranoside (three-letter code: BGL) (formula: C<sub>14</sub>H<sub>28</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			20	14	6		
4	E	1	Total	C	O	0	0
			20	14	6		
4	G	1	Total	C	O	0	0
			20	14	6		
4	K	1	Total	C	O	0	0
			20	14	6		
4	N	1	Total	C	O	0	0
			20	14	6		
4	P	1	Total	C	O	0	0
			20	14	6		

- Molecule 5 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	1	Total	Sr	0	0
			1	1		
5	Q	1	Total	Sr	0	0
			1	1		
5	K	1	Total	Sr	0	0
			1	1		
5	E	1	Total	Sr	0	0
			1	1		
5	H	1	Total	Sr	0	0
			1	1		
5	B	1	Total	Sr	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Sr	0	0
			1	1		
5	N	1	Total	Sr	0	0
			1	1		
5	M	1	Total	Sr	0	0
			1	1		

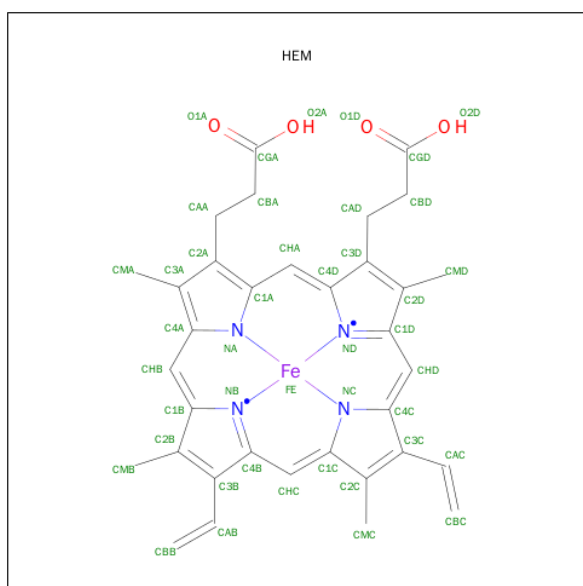
- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	R	1	Total	Cl	0	0
			1	1		
6	I	1	Total	Cl	0	0
			1	1		

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	R	1	Total	Na	0	0
			1	1		

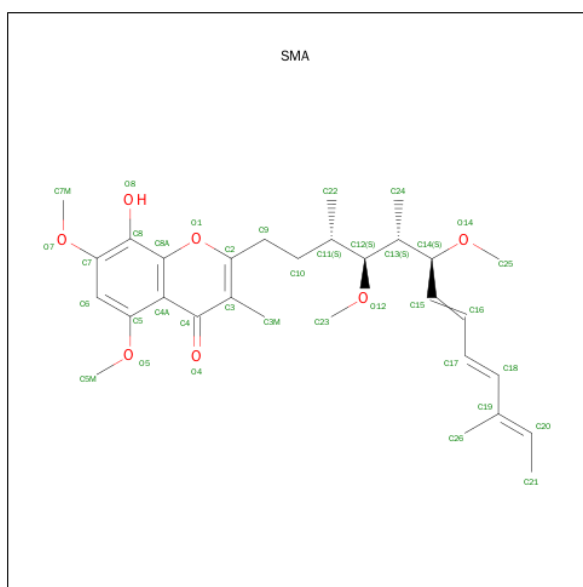
- Molecule 8 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).





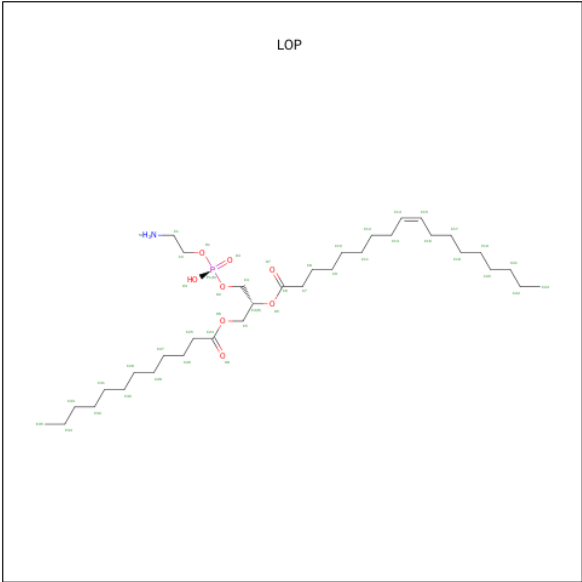
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	G	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	G	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	H	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	J	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	J	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	K	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	M	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	M	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	N	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	P	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	P	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	Q	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 9 is STIGMATELLIN A (three-letter code: SMA) (formula: C<sub>30</sub>H<sub>42</sub>O<sub>7</sub>).



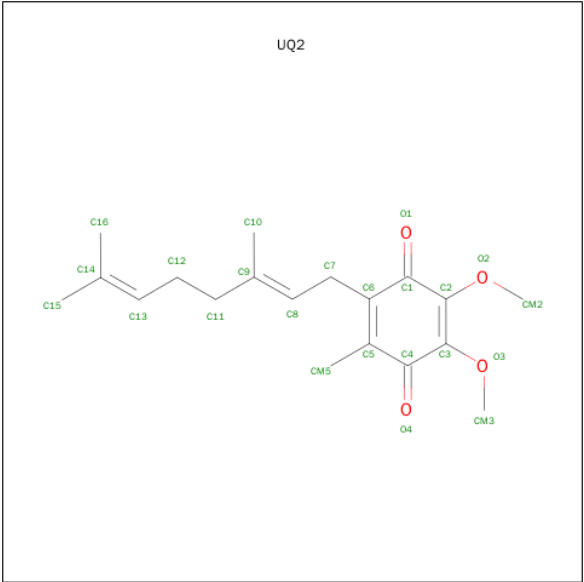
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			37	30	7		
9	D	1	Total	C	O	0	0
			37	30	7		
9	G	1	Total	C	O	0	0
			37	30	7		
9	J	1	Total	C	O	0	0
			37	30	7		
9	M	1	Total	C	O	0	0
			37	30	7		
9	P	1	Total	C	O	0	0
			37	30	7		

- Molecule 10 is (1R)-2-{[(R)-(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(DODECANOYLOXY)METHYL]ETHYL (9Z)-OCTADEC-9-ENOATE (three-letter code: LOP) (formula: C<sub>35</sub>H<sub>68</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	A	1	Total	C	N	O	P	0	0
			45	35	1	8	1		
10	D	1	Total	C	N	O	P	0	0
			45	35	1	8	1		
10	G	1	Total	C	N	O	P	0	0
			45	35	1	8	1		
10	J	1	Total	C	N	O	P	0	0
			45	35	1	8	1		
10	M	1	Total	C	N	O	P	0	0
			45	35	1	8	1		
10	P	1	Total	C	N	O	P	0	0
			45	35	1	8	1		

- Molecule 11 is UBIQUINONE-2 (three-letter code: UQ2) (formula: C<sub>19</sub>H<sub>26</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	C	O	0	0
			23	19	4		
11	D	1	Total	C	O	0	0
			23	19	4		
11	G	1	Total	C	O	0	0
			23	19	4		
11	J	1	Total	C	O	0	0
			23	19	4		
11	M	1	Total	C	O	0	0
			23	19	4		
11	P	1	Total	C	O	0	0
			23	19	4		

- Molecule 12 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	C	1	Total	Fe	S	0	0
			4	2	2		
12	F	1	Total	Fe	S	0	0
			4	2	2		
12	I	1	Total	Fe	S	0	0
			4	2	2		
12	L	1	Total	Fe	S	0	0
			4	2	2		
12	O	1	Total	Fe	S	0	0
			4	2	2		
12	R	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	73	Total	O	0	0
			73	73		
13	B	19	Total	O	0	0
			19	19		
13	C	47	Total	O	0	0
			47	47		
13	D	64	Total	O	0	0
			64	64		
13	E	14	Total	O	0	0
			14	14		
13	F	36	Total	O	0	0
			36	36		

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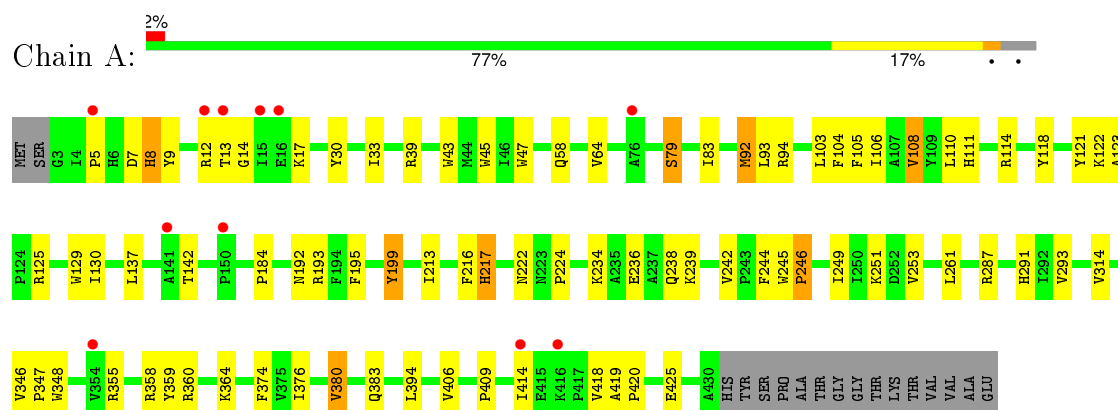
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	G	68	Total 68	O 68	0	0
13	H	35	Total 35	O 35	0	0
13	I	42	Total 42	O 42	0	0
13	J	55	Total 55	O 55	0	0
13	K	17	Total 17	O 17	0	0
13	L	42	Total 42	O 42	0	0
13	M	34	Total 34	O 34	0	0
13	N	11	Total 11	O 11	0	0
13	O	41	Total 41	O 41	0	0
13	P	60	Total 60	O 60	0	0
13	Q	16	Total 16	O 16	0	0
13	R	24	Total 24	O 24	0	0

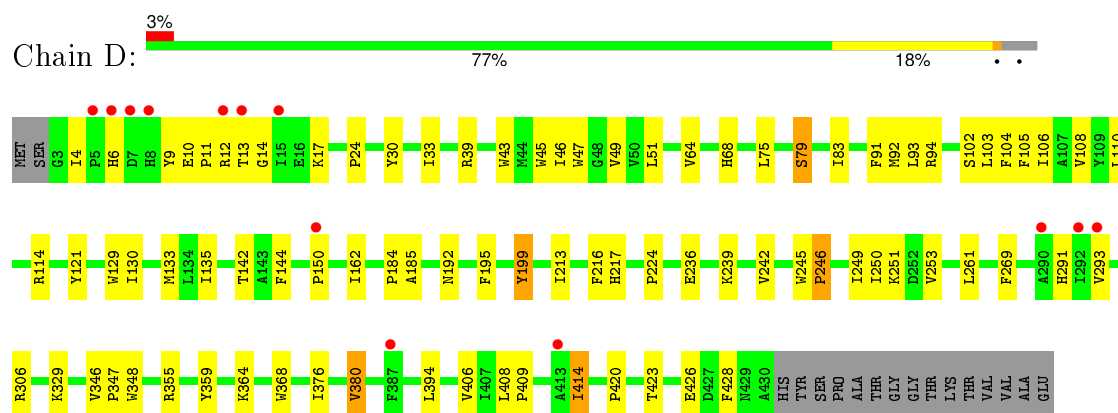
### 3 Residue-property plots [i](#)

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

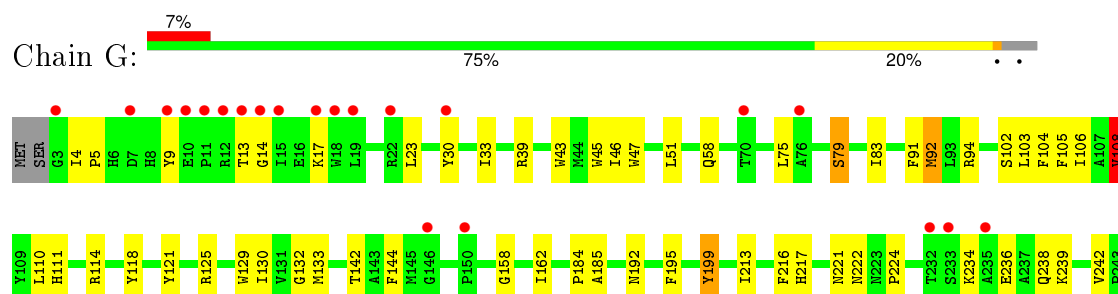
#### • Molecule 1: Cytochrome b

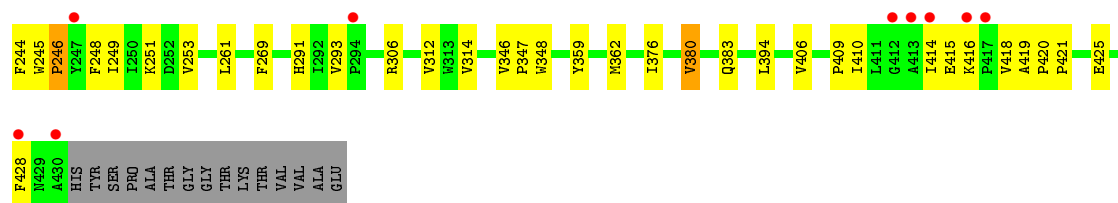


#### • Molecule 1: Cytochrome b

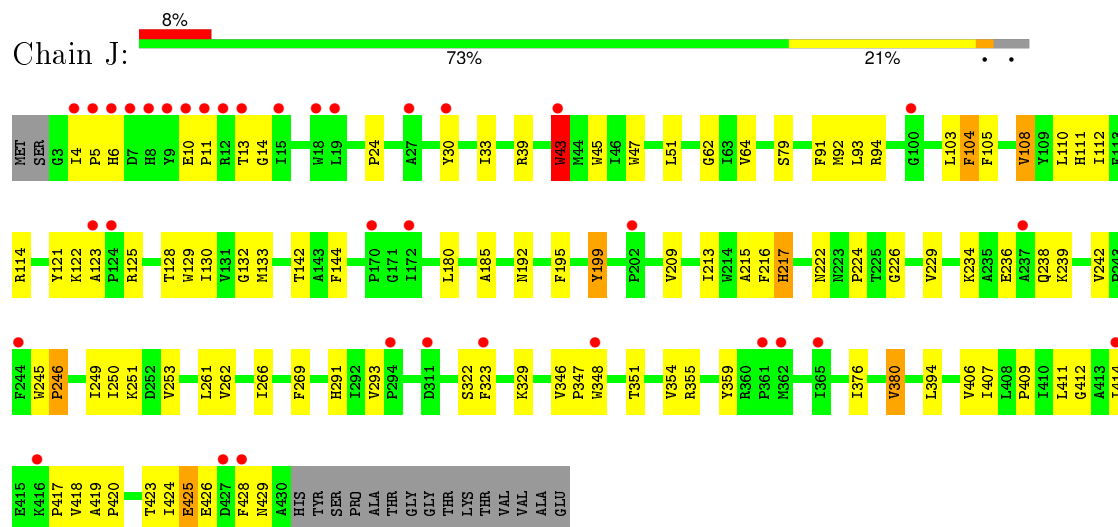


#### • Molecule 1: Cytochrome b

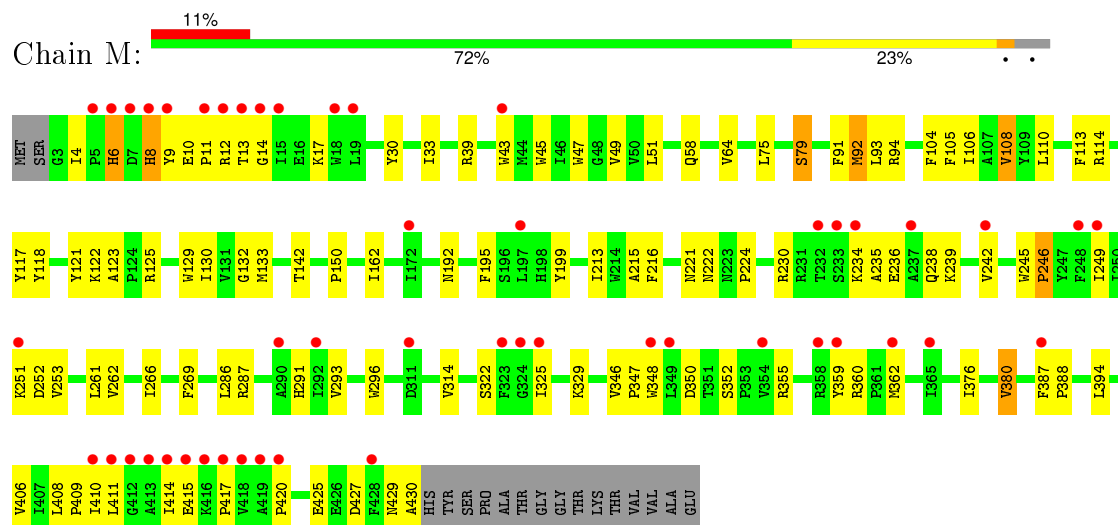




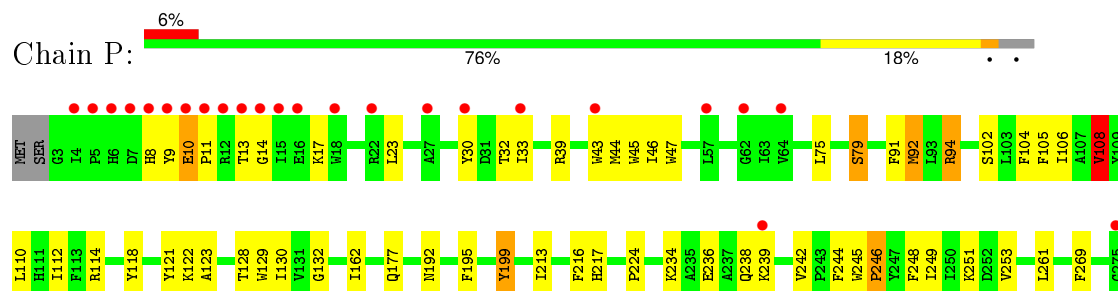
• Molecule 1: Cytochrome b



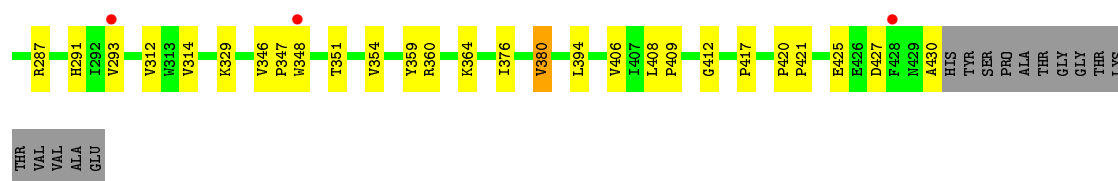
• Molecule 1: Cytochrome b



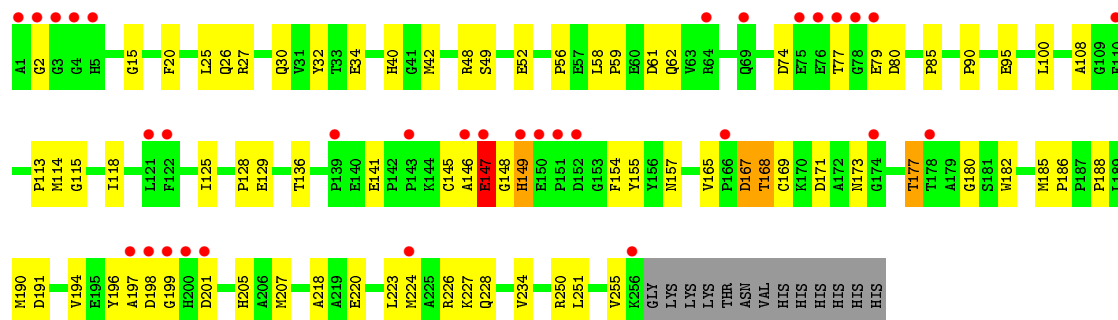
• Molecule 1: Cytochrome b



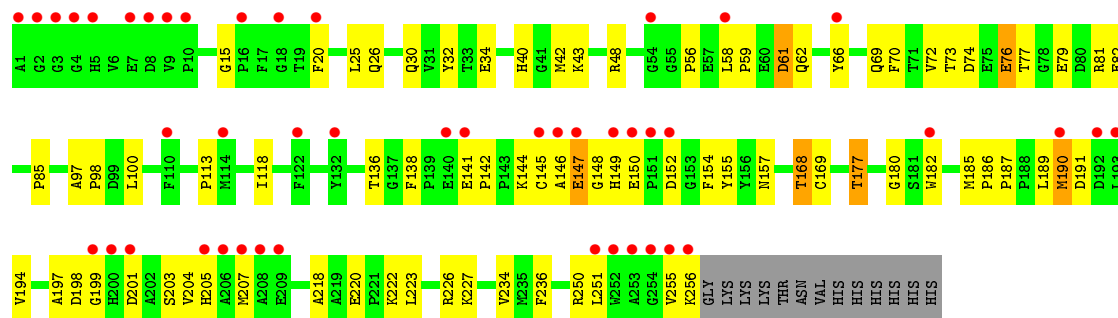




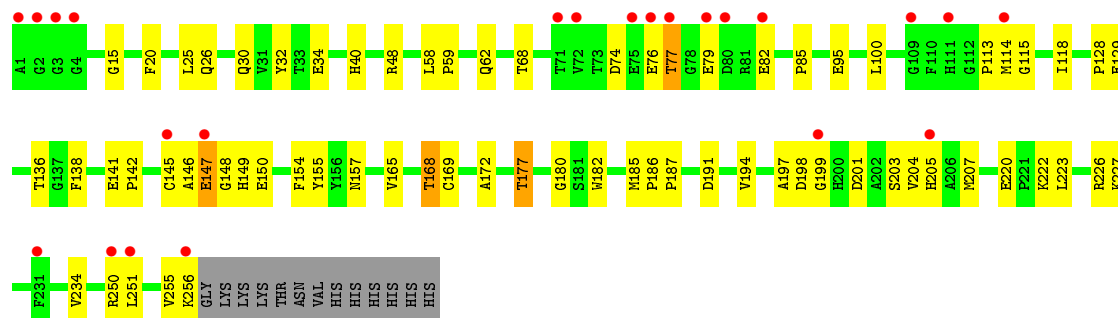
• Molecule 2: Cytochrome c1



• Molecule 2: Cytochrome c1

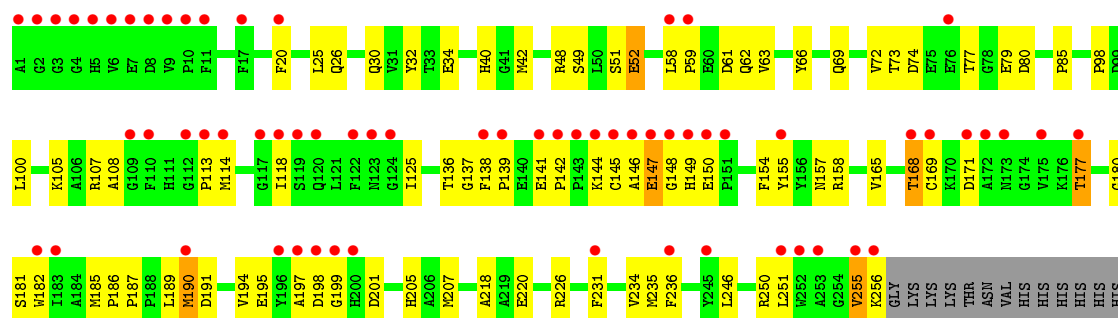


• Molecule 2: Cytochrome c1

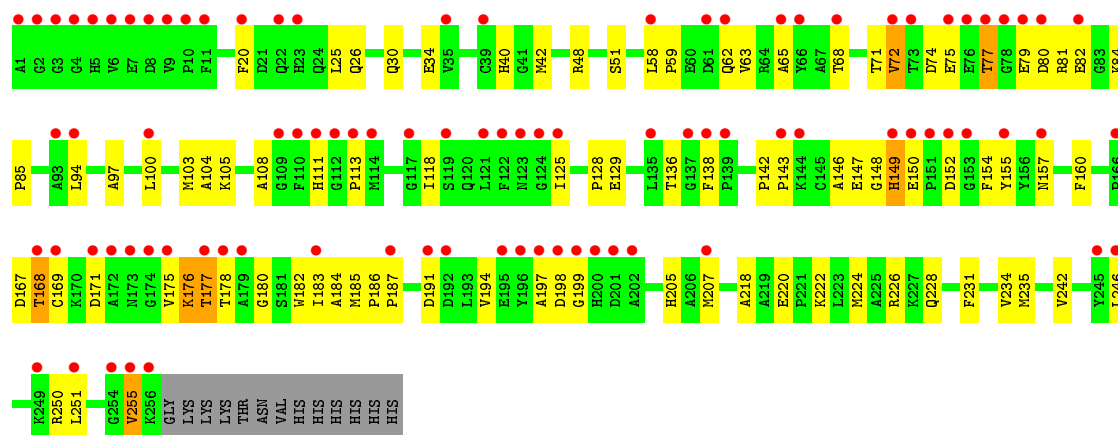


• Molecule 2: Cytochrome c1

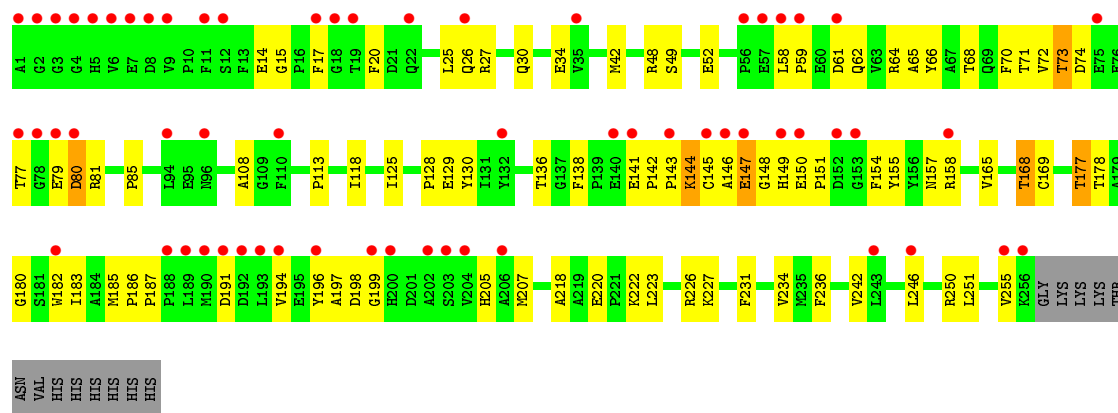




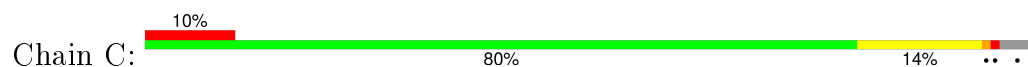
• Molecule 2: Cytochrome c1

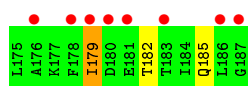


• Molecule 2: Cytochrome c1

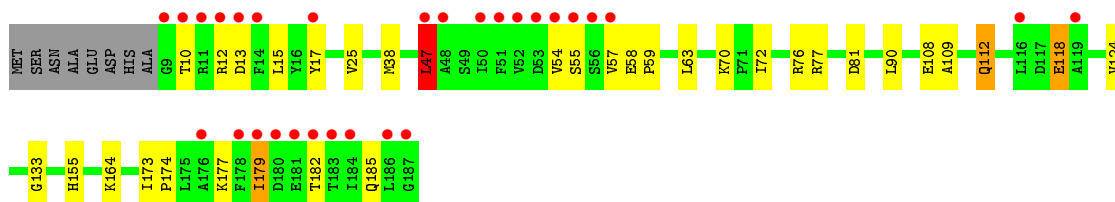
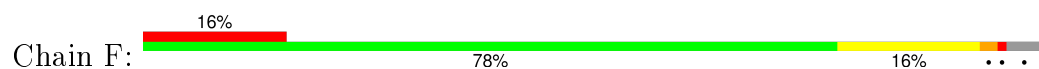


• Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit

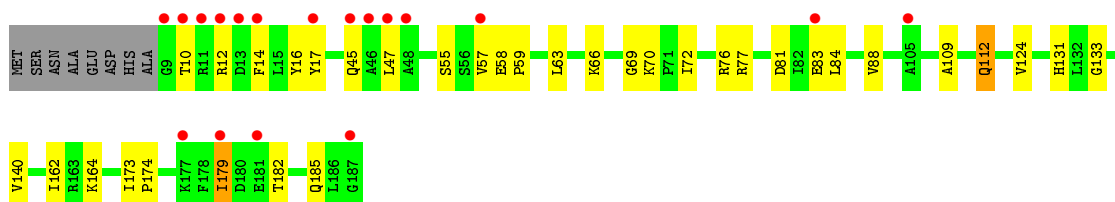
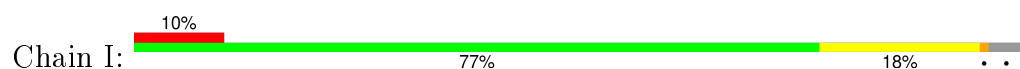




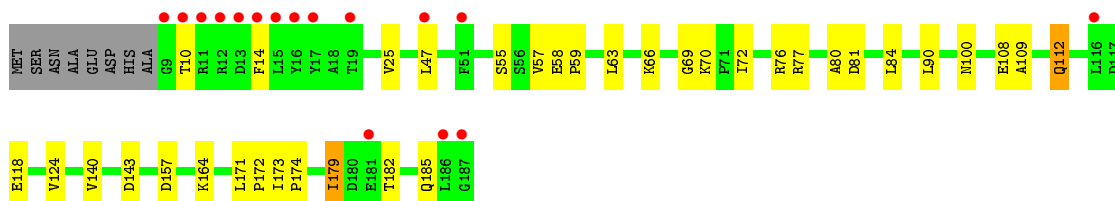
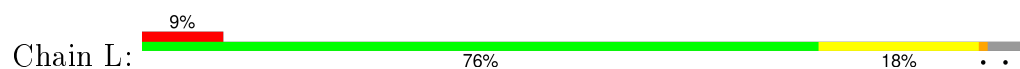
- Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit



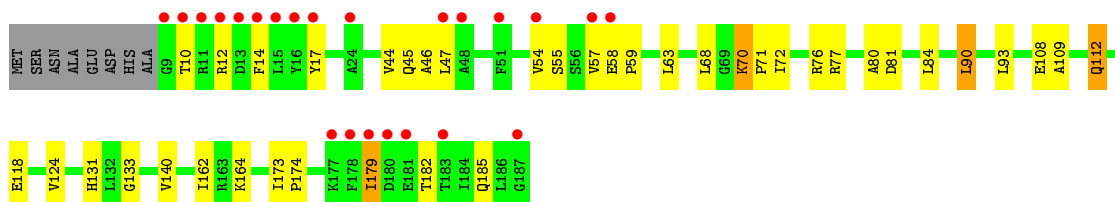
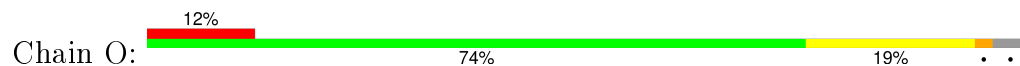
- Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit



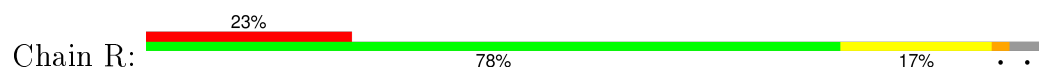
- Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit

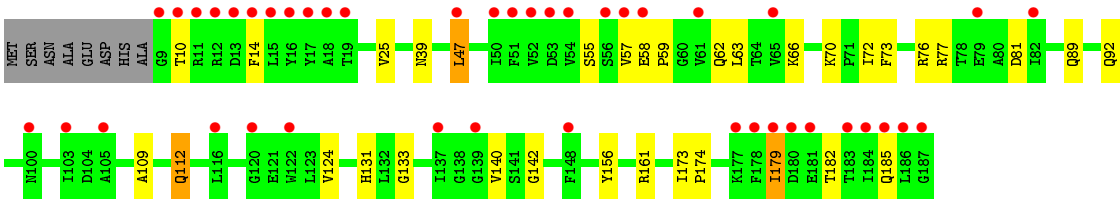


- Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit



- Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	351.89Å 147.04Å 161.31Å 90.00° 104.25° 90.00°	Depositor
Resolution (Å)	18.00 – 2.40 47.10 – 2.35	Depositor EDS
% Data completeness (in resolution range)	93.7 (18.00-2.40) 91.9 (47.10-2.35)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.48 (at 2.34Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.226 , 0.251 0.229 , 0.245	Depositor DCC
$R_{free}$ test set	4928 reflections (1.74%)	DCC
Wilson B-factor (Å <sup>2</sup> )	51.5	Xtriage
Anisotropy	0.289	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 60.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 574713 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	42656	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.94% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: CL, SR, BGL, LOP, FES, NA, HEM, UQ2, SMA

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	0.39	0/3570	0.66	0/4897
1	D	0.39	0/3570	0.66	0/4897
1	G	0.38	0/3570	0.66	1/4897 (0.0%)
1	J	0.40	0/3570	0.66	0/4897
1	M	0.38	0/3570	0.65	0/4897
1	P	0.38	0/3570	0.65	1/4897 (0.0%)
2	B	0.37	0/2010	0.67	0/2733
2	E	0.36	0/2010	0.68	0/2733
2	H	0.37	0/2010	0.68	0/2733
2	K	0.36	0/2010	0.67	0/2733
2	N	0.36	0/2010	0.67	0/2733
2	Q	0.35	0/2010	0.66	0/2733
3	C	0.38	0/1370	0.74	1/1866 (0.1%)
3	F	0.39	0/1370	0.74	2/1866 (0.1%)
3	I	0.39	0/1370	0.76	1/1866 (0.1%)
3	L	0.38	0/1370	0.72	1/1866 (0.1%)
3	O	0.38	0/1370	0.72	1/1866 (0.1%)
3	R	0.38	0/1370	0.73	2/1866 (0.1%)
All	All	0.38	0/41700	0.68	10/56976 (0.0%)

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
2	B	0	1
2	E	0	1
2	H	0	1
2	K	0	1
All	All	0	4

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	47	LEU	CA-CB-CG	7.62	132.83	115.30
3	R	47	LEU	CA-CB-CG	7.10	131.63	115.30
3	C	47	LEU	CA-CB-CG	6.99	131.38	115.30
3	L	47	LEU	CA-CB-CG	6.49	130.22	115.30
1	P	108	VAL	CB-CA-C	-5.59	100.78	111.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	32	TYR	Sidechain
2	E	32	TYR	Sidechain
2	H	32	TYR	Sidechain
2	K	32	TYR	Sidechain

## 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	3440	0	3428	70	0
1	D	3440	0	3428	81	0
1	G	3440	0	3428	91	0
1	J	3440	0	3428	96	0
1	M	3440	0	3428	95	0
1	P	3440	0	3428	78	0
2	B	1953	0	1848	65	0
2	E	1953	0	1848	89	0
2	H	1953	0	1848	71	0
2	K	1953	0	1848	70	0
2	N	1953	0	1848	81	0
2	Q	1953	0	1848	78	0
3	C	1340	0	1303	26	0
3	F	1340	0	1303	27	0
3	I	1340	0	1303	27	0
3	L	1340	0	1303	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	O	1340	0	1303	27	0
3	R	1340	0	1303	26	0
4	B	20	0	28	1	0
4	E	20	0	28	3	0
4	G	20	0	28	2	0
4	K	20	0	28	2	0
4	N	20	0	28	1	0
4	P	20	0	28	2	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	E	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
5	K	1	0	0	0	0
5	M	1	0	0	0	0
5	N	1	0	0	0	0
5	Q	1	0	0	0	0
6	I	1	0	0	0	0
6	R	1	0	0	0	0
7	R	1	0	0	0	0
8	A	86	0	60	7	0
8	B	43	0	30	1	0
8	D	86	0	60	8	0
8	E	43	0	30	1	0
8	G	86	0	60	9	0
8	H	43	0	30	1	0
8	J	86	0	60	15	0
8	K	43	0	30	2	0
8	M	86	0	60	8	0
8	N	43	0	30	3	0
8	P	86	0	60	7	0
8	Q	43	0	30	2	0
9	A	37	0	42	0	0
9	D	37	0	42	0	0
9	G	37	0	42	0	0
9	J	37	0	42	1	0
9	M	37	0	42	0	0
9	P	37	0	42	1	0
10	A	45	0	67	6	0
10	D	45	0	67	1	0
10	G	45	0	67	3	0
10	J	45	0	67	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	M	45	0	67	3	0
10	P	45	0	67	2	0
11	A	23	0	26	2	0
11	D	23	0	26	2	0
11	G	23	0	26	3	0
11	J	23	0	26	1	0
11	M	23	0	26	2	0
11	P	23	0	26	4	0
12	C	4	0	0	0	0
12	F	4	0	0	0	0
12	I	4	0	0	0	0
12	L	4	0	0	0	0
12	O	4	0	0	0	0
12	R	4	0	0	0	0
13	A	73	0	0	1	0
13	B	19	0	0	2	0
13	C	47	0	0	0	0
13	D	64	0	0	4	0
13	E	14	0	0	1	0
13	F	36	0	0	0	0
13	G	68	0	0	2	0
13	H	35	0	0	3	0
13	I	42	0	0	0	0
13	J	55	0	0	3	0
13	K	17	0	0	0	0
13	L	42	0	0	1	0
13	M	34	0	0	1	0
13	N	11	0	0	1	0
13	O	41	0	0	1	0
13	P	60	0	0	1	0
13	Q	16	0	0	1	0
13	R	24	0	0	2	0
All	All	42656	0	40992	1025	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 12.

The worst 5 of 1025 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:Q:144:LYS:HZ3	2:Q:144:LYS:HA	1.06	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:139:PRO:HG3	2:K:158:ARG:HH11	1.14	1.12
2:N:77:THR:HG22	2:N:79:GLU:H	1.25	1.02
2:Q:144:LYS:NZ	2:Q:144:LYS:HA	1.75	1.01
2:B:250:ARG:HD3	3:C:12:ARG:HG2	1.41	1.01

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	426/445 (96%)	412 (97%)	14 (3%)	0	100	100
1	D	426/445 (96%)	413 (97%)	13 (3%)	0	100	100
1	G	426/445 (96%)	412 (97%)	14 (3%)	0	100	100
1	J	426/445 (96%)	407 (96%)	18 (4%)	1 (0%)	52	69
1	M	426/445 (96%)	407 (96%)	19 (4%)	0	100	100
1	P	426/445 (96%)	408 (96%)	18 (4%)	0	100	100
2	B	254/269 (94%)	233 (92%)	18 (7%)	3 (1%)	16	23
2	E	254/269 (94%)	231 (91%)	20 (8%)	3 (1%)	16	23
2	H	254/269 (94%)	233 (92%)	18 (7%)	3 (1%)	16	23
2	K	254/269 (94%)	231 (91%)	18 (7%)	5 (2%)	9	11
2	N	254/269 (94%)	229 (90%)	20 (8%)	5 (2%)	9	11
2	Q	254/269 (94%)	231 (91%)	21 (8%)	2 (1%)	24	35
3	C	177/187 (95%)	163 (92%)	13 (7%)	1 (1%)	30	43
3	F	177/187 (95%)	161 (91%)	15 (8%)	1 (1%)	30	43
3	I	177/187 (95%)	162 (92%)	12 (7%)	3 (2%)	11	14
3	L	177/187 (95%)	161 (91%)	14 (8%)	2 (1%)	17	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	O	177/187 (95%)	162 (92%)	12 (7%)	3 (2%)	11	14
3	R	177/187 (95%)	161 (91%)	15 (8%)	1 (1%)	30	43
All	All	5142/5406 (95%)	4817 (94%)	292 (6%)	33 (1%)	30	43

5 of 33 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	147	GLU
2	E	147	GLU
2	E	190	MET
2	H	77	THR
2	H	147	GLU

### 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	353/366 (96%)	338 (96%)	15 (4%)	36	56
1	D	353/366 (96%)	345 (98%)	8 (2%)	58	78
1	G	353/366 (96%)	343 (97%)	10 (3%)	51	72
1	J	353/366 (96%)	342 (97%)	11 (3%)	47	69
1	M	353/366 (96%)	340 (96%)	13 (4%)	41	62
1	P	353/366 (96%)	341 (97%)	12 (3%)	44	65
2	B	203/215 (94%)	191 (94%)	12 (6%)	24	38
2	E	203/215 (94%)	193 (95%)	10 (5%)	31	48
2	H	203/215 (94%)	197 (97%)	6 (3%)	48	70
2	K	203/215 (94%)	192 (95%)	11 (5%)	27	43
2	N	203/215 (94%)	194 (96%)	9 (4%)	35	53
2	Q	203/215 (94%)	193 (95%)	10 (5%)	31	48
3	C	138/144 (96%)	133 (96%)	5 (4%)	42	63
3	F	138/144 (96%)	131 (95%)	7 (5%)	29	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	I	138/144 (96%)	132 (96%)	6 (4%)	35	55
3	L	138/144 (96%)	133 (96%)	5 (4%)	42	63
3	O	138/144 (96%)	131 (95%)	7 (5%)	29	46
3	R	138/144 (96%)	133 (96%)	5 (4%)	42	63
All	All	4164/4350 (96%)	4002 (96%)	162 (4%)	39	59

5 of 162 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	I	47	LEU
2	K	52	GLU
2	Q	73	THR
3	I	83	GLU
1	J	104	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 73 such sidechains are listed below:

Mol	Chain	Res	Type
3	I	112	GLN
2	K	62	GLN
2	Q	149	HIS
1	J	221	ASN
2	K	228	GLN

### 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 ⓘ

Of 60 ligands modelled in this entry, 12 are monoatomic - leaving 48 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$
9	SMA	A	1001	-	35,38,38	1.89	5 (14%)	40,52,52	1.94	7 (17%)
10	LOP	A	1021	-	43,44,44	0.63	0	44,49,49	1.17	6 (13%)
11	UQ2	A	1101	-	23,23,23	1.48	5 (21%)	28,31,31	1.15	2 (7%)
8	HEM	A	501	1	30,50,50	2.80	10 (33%)	24,82,82	3.19	8 (33%)
8	HEM	A	502	1	30,50,50	2.92	9 (30%)	24,82,82	3.27	8 (33%)
4	BGL	B	1041	-	19,20,20	0.70	0	23,25,25	0.88	1 (4%)
8	HEM	B	301	2	30,50,50	3.12	12 (40%)	24,82,82	3.40	8 (33%)
12	FES	C	200	3	0,4,4	0.00	-	0,4,4	0.00	-
9	SMA	D	1002	-	35,38,38	1.82	6 (17%)	40,52,52	1.92	9 (22%)
10	LOP	D	1022	-	43,44,44	0.72	0	44,49,49	1.18	4 (9%)
11	UQ2	D	1102	-	23,23,23	1.33	6 (26%)	28,31,31	1.18	3 (10%)
8	HEM	D	501	1	30,50,50	2.69	10 (33%)	24,82,82	3.16	8 (33%)
8	HEM	D	502	1	30,50,50	2.78	12 (40%)	24,82,82	3.30	9 (37%)
4	BGL	E	1042	-	19,20,20	0.69	0	23,25,25	0.95	1 (4%)
8	HEM	E	301	2	30,50,50	2.96	12 (40%)	24,82,82	3.34	8 (33%)
12	FES	F	200	3	0,4,4	0.00	-	0,4,4	0.00	-
9	SMA	G	1003	-	35,38,38	1.87	5 (14%)	40,52,52	1.82	9 (22%)
10	LOP	G	1023	-	43,44,44	0.72	0	44,49,49	1.17	4 (9%)
4	BGL	G	1043	-	19,20,20	0.88	1 (5%)	23,25,25	0.79	0
11	UQ2	G	1103	-	23,23,23	1.38	5 (21%)	28,31,31	1.07	2 (7%)
8	HEM	G	501	1	30,50,50	2.77	11 (36%)	24,82,82	3.25	8 (33%)
8	HEM	G	502	1	30,50,50	3.11	9 (30%)	24,82,82	3.39	8 (33%)
8	HEM	H	301	2	30,50,50	2.76	10 (33%)	24,82,82	3.40	8 (33%)
12	FES	I	200	3	0,4,4	0.00	-	0,4,4	0.00	-
9	SMA	J	1004	-	35,38,38	1.80	5 (14%)	40,52,52	1.84	7 (17%)
10	LOP	J	1024	-	43,44,44	0.66	0	44,49,49	1.26	6 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
11	UQ2	J	1104	-	23,23,23	1.23	2 (8%)	28,31,31	1.07	1 (3%)
8	HEM	J	501	1	30,50,50	2.86	11 (36%)	24,82,82	3.32	8 (33%)
8	HEM	J	502	1	30,50,50	3.03	11 (36%)	24,82,82	3.44	8 (33%)
4	BGL	K	1044	-	19,20,20	0.84	1 (5%)	23,25,25	1.07	2 (8%)
8	HEM	K	301	2	30,50,50	2.73	11 (36%)	24,82,82	3.39	8 (33%)
12	FES	L	200	3	0,4,4	0.00	-	0,4,4	0.00	-
9	SMA	M	1005	-	35,38,38	1.92	5 (14%)	40,52,52	1.88	8 (20%)
10	LOP	M	1025	-	43,44,44	0.69	0	44,49,49	1.15	3 (6%)
11	UQ2	M	1105	-	23,23,23	1.45	5 (21%)	28,31,31	1.15	2 (7%)
8	HEM	M	501	1	30,50,50	2.83	12 (40%)	24,82,82	3.25	8 (33%)
8	HEM	M	502	1	30,50,50	2.90	10 (33%)	24,82,82	3.26	8 (33%)
4	BGL	N	1045	-	19,20,20	0.94	1 (5%)	23,25,25	0.78	0
8	HEM	N	301	2	30,50,50	2.98	11 (36%)	24,82,82	3.37	8 (33%)
12	FES	O	200	3	0,4,4	0.00	-	0,4,4	0.00	-
9	SMA	P	1006	-	35,38,38	1.85	6 (17%)	40,52,52	2.11	11 (27%)
10	LOP	P	1026	-	43,44,44	0.62	0	44,49,49	1.19	5 (11%)
4	BGL	P	1046	-	19,20,20	0.86	0	23,25,25	0.92	1 (4%)
11	UQ2	P	1106	-	23,23,23	1.52	6 (26%)	28,31,31	1.21	4 (14%)
8	HEM	P	501	1	30,50,50	2.74	11 (36%)	24,82,82	3.25	8 (33%)
8	HEM	P	502	1	30,50,50	2.82	11 (36%)	24,82,82	3.19	8 (33%)
8	HEM	Q	301	2	30,50,50	2.93	13 (43%)	24,82,82	3.34	8 (33%)
12	FES	R	200	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
9	SMA	A	1001	-	-	0/33/34/34	0/2/2/2
10	LOP	A	1021	-	-	0/48/48/48	0/0/0/0
11	UQ2	A	1101	-	-	0/15/39/39	0/1/1/1
8	HEM	A	501	1	-	0/10/54/54	0/0/8/8
8	HEM	A	502	1	-	0/10/54/54	0/0/8/8
4	BGL	B	1041	-	-	0/11/31/31	0/1/1/1
8	HEM	B	301	2	-	0/10/54/54	0/0/8/8
12	FES	C	200	3	-	0/0/4/4	0/1/1/1
9	SMA	D	1002	-	-	0/33/34/34	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	LOP	D	1022	-	-	0/48/48/48	0/0/0/0
11	UQ2	D	1102	-	-	0/15/39/39	0/1/1/1
8	HEM	D	501	1	-	0/10/54/54	0/0/8/8
8	HEM	D	502	1	-	0/10/54/54	0/0/8/8
4	BGL	E	1042	-	-	0/11/31/31	0/1/1/1
8	HEM	E	301	2	-	0/10/54/54	0/0/8/8
12	FES	F	200	3	-	0/0/4/4	0/1/1/1
9	SMA	G	1003	-	-	0/33/34/34	0/2/2/2
10	LOP	G	1023	-	-	0/48/48/48	0/0/0/0
4	BGL	G	1043	-	-	0/11/31/31	0/1/1/1
11	UQ2	G	1103	-	-	0/15/39/39	0/1/1/1
8	HEM	G	501	1	-	0/10/54/54	0/0/8/8
8	HEM	G	502	1	-	0/10/54/54	0/0/8/8
8	HEM	H	301	2	-	0/10/54/54	0/0/8/8
12	FES	I	200	3	-	0/0/4/4	0/1/1/1
9	SMA	J	1004	-	-	0/33/34/34	0/2/2/2
10	LOP	J	1024	-	-	0/48/48/48	0/0/0/0
11	UQ2	J	1104	-	-	0/15/39/39	0/1/1/1
8	HEM	J	501	1	-	0/10/54/54	0/0/8/8
8	HEM	J	502	1	-	0/10/54/54	0/0/8/8
4	BGL	K	1044	-	-	0/11/31/31	0/1/1/1
8	HEM	K	301	2	-	0/10/54/54	0/0/8/8
12	FES	L	200	3	-	0/0/4/4	0/1/1/1
9	SMA	M	1005	-	-	0/33/34/34	0/2/2/2
10	LOP	M	1025	-	-	0/48/48/48	0/0/0/0
11	UQ2	M	1105	-	-	0/15/39/39	0/1/1/1
8	HEM	M	501	1	-	0/10/54/54	0/0/8/8
8	HEM	M	502	1	-	0/10/54/54	0/0/8/8
4	BGL	N	1045	-	-	0/11/31/31	0/1/1/1
8	HEM	N	301	2	-	0/10/54/54	0/0/8/8
12	FES	O	200	3	-	0/0/4/4	0/1/1/1
9	SMA	P	1006	-	-	0/33/34/34	0/2/2/2
10	LOP	P	1026	-	-	0/48/48/48	0/0/0/0
4	BGL	P	1046	-	-	0/11/31/31	0/1/1/1
11	UQ2	P	1106	-	-	0/15/39/39	0/1/1/1
8	HEM	P	501	1	-	0/10/54/54	0/0/8/8
8	HEM	P	502	1	-	0/10/54/54	0/0/8/8
8	HEM	Q	301	2	-	0/10/54/54	0/0/8/8
12	FES	R	200	3	-	0/0/4/4	0/1/1/1

The worst 5 of 260 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	G	502	HEM	C3B-C4B	-9.05	1.43	1.51
8	J	502	HEM	C3C-CAC	-7.90	1.36	1.51
8	P	502	HEM	C3B-C4B	-7.47	1.45	1.51
8	A	502	HEM	C3B-C4B	-7.29	1.45	1.51
8	B	301	HEM	C3B-C4B	-7.26	1.45	1.51

The worst 5 of 243 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	J	502	HEM	C3C-CAC-CBC	-10.52	108.32	124.46
8	G	502	HEM	C3C-CAC-CBC	-9.91	109.25	124.46
8	K	301	HEM	C3B-CAB-CBB	-9.51	109.86	124.46
8	H	301	HEM	C3B-CAB-CBB	-9.51	109.87	124.46
8	E	301	HEM	C3B-CAB-CBB	-9.40	110.04	124.46

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

38 monomers are involved in 107 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	1021	LOP	6	0
11	A	1101	UQ2	2	0
8	A	501	HEM	3	0
8	A	502	HEM	4	0
4	B	1041	BGL	1	0
8	B	301	HEM	1	0
10	D	1022	LOP	1	0
11	D	1102	UQ2	2	0
8	D	501	HEM	5	0
8	D	502	HEM	3	0
4	E	1042	BGL	3	0
8	E	301	HEM	1	0
10	G	1023	LOP	3	0
4	G	1043	BGL	2	0
11	G	1103	UQ2	3	0
8	G	501	HEM	4	0
8	G	502	HEM	5	0
8	H	301	HEM	1	0
9	J	1004	SMA	1	0
10	J	1024	LOP	1	0
11	J	1104	UQ2	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	J	501	HEM	9	0
8	J	502	HEM	6	0
4	K	1044	BGL	2	0
8	K	301	HEM	2	0
10	M	1025	LOP	3	0
11	M	1105	UQ2	2	0
8	M	501	HEM	3	0
8	M	502	HEM	5	0
4	N	1045	BGL	1	0
8	N	301	HEM	3	0
9	P	1006	SMA	1	0
10	P	1026	LOP	2	0
4	P	1046	BGL	2	0
11	P	1106	UQ2	4	0
8	P	501	HEM	4	0
8	P	502	HEM	3	0
8	Q	301	HEM	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	428/445 (96%)	0.48	11 (2%) 59 58	35, 53, 90, 117	0
1	D	428/445 (96%)	0.40	13 (3%) 54 53	35, 53, 93, 124	0
1	G	428/445 (96%)	0.65	30 (7%) 19 19	35, 56, 100, 124	0
1	J	428/445 (96%)	0.71	35 (8%) 14 14	36, 62, 101, 125	0
1	M	428/445 (96%)	0.77	49 (11%) 7 7	38, 67, 107, 130	0
1	P	428/445 (96%)	0.56	27 (6%) 23 24	35, 56, 100, 127	0
2	B	256/269 (95%)	0.85	33 (12%) 5 5	47, 78, 112, 134	0
2	E	256/269 (95%)	0.99	46 (17%) 2 2	50, 80, 117, 133	0
2	H	256/269 (95%)	0.64	23 (8%) 12 11	40, 72, 113, 135	0
2	K	256/269 (95%)	1.39	65 (25%) 1 1	49, 87, 120, 136	0
2	N	256/269 (95%)	1.81	91 (35%) 0 0	59, 95, 121, 135	0
2	Q	256/269 (95%)	1.23	61 (23%) 1 1	51, 87, 119, 134	0
3	C	179/187 (95%)	0.75	19 (10%) 8 8	37, 59, 101, 139	0
3	F	179/187 (95%)	0.77	29 (16%) 3 2	38, 63, 102, 140	0
3	I	179/187 (95%)	0.61	18 (10%) 9 8	41, 58, 105, 139	0
3	L	179/187 (95%)	0.61	16 (8%) 12 12	37, 59, 104, 139	0
3	O	179/187 (95%)	0.82	23 (12%) 5 5	34, 64, 108, 138	0
3	R	179/187 (95%)	1.17	43 (24%) 1 1	46, 70, 108, 138	0
All	All	5178/5406 (95%)	0.80	632 (12%) 5 5	34, 66, 112, 140	0

The worst 5 of 632 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	9	GLY	18.8
2	Q	2	GLY	18.7
2	E	3	GLY	18.1

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Mol	Chain	Res	Type	RSRZ
3	I	9	GLY	18.1
2	K	3	GLY	16.2

## 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
11	UQ2	A	1101	23/23	0.66	0.42	11.67	102,105,108,109	0
11	UQ2	D	1102	23/23	0.64	0.37	7.62	92,98,107,107	0
11	UQ2	G	1103	23/23	0.69	0.38	6.84	109,116,117,118	0
11	UQ2	M	1105	23/23	0.64	0.44	6.23	112,123,125,125	0
11	UQ2	J	1104	23/23	0.53	0.49	5.86	107,115,116,117	0
10	LOP	J	1024	45/45	0.82	0.36	5.73	93,113,125,126	0
11	UQ2	P	1106	23/23	0.70	0.32	3.73	101,104,107,108	0
10	LOP	P	1026	45/45	0.83	0.28	2.87	69,95,99,100	0
10	LOP	G	1023	45/45	0.77	0.27	2.84	88,102,112,113	0
10	LOP	D	1022	45/45	0.87	0.25	2.34	63,88,98,102	0
4	BGL	G	1043	20/20	0.78	0.27	1.75	89,91,101,101	0
10	LOP	M	1025	45/45	0.80	0.28	1.55	89,114,123,123	0
10	LOP	A	1021	45/45	0.89	0.22	1.50	72,86,94,99	0
12	FES	L	200	4/4	0.99	0.20	1.32	40,41,41,42	0
4	BGL	P	1046	20/20	0.88	0.26	1.29	87,93,95,95	0
9	SMA	J	1004	37/37	0.95	0.24	1.12	40,49,79,85	0
8	HEM	A	502	43/43	0.98	0.25	1.11	32,37,49,49	0
8	HEM	B	301	43/43	0.95	0.20	0.79	51,56,70,73	0
9	SMA	P	1006	37/37	0.95	0.21	0.76	34,45,76,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
9	SMA	D	1002	37/37	0.94	0.22	0.73	39,44,76,78	0
8	HEM	P	502	43/43	0.98	0.24	0.73	35,40,49,53	0
8	HEM	G	502	43/43	0.98	0.23	0.68	32,36,45,49	0
4	BGL	B	1041	20/20	0.80	0.23	0.50	87,97,101,102	0
9	SMA	G	1003	37/37	0.96	0.22	0.48	35,43,60,65	0
8	HEM	J	502	43/43	0.98	0.22	0.48	37,41,54,57	0
8	HEM	H	301	43/43	0.96	0.17	0.41	33,42,47,50	0
4	BGL	N	1045	20/20	0.71	0.31	0.40	107,111,113,114	0
8	HEM	D	502	43/43	0.97	0.22	0.38	32,37,49,58	0
4	BGL	E	1042	20/20	0.90	0.20	0.37	80,85,102,102	0
12	FES	F	200	4/4	0.99	0.18	0.36	43,43,44,45	0
9	SMA	M	1005	37/37	0.96	0.20	0.36	56,66,73,73	0
8	HEM	M	502	43/43	0.98	0.21	0.29	47,49,59,63	0
8	HEM	J	501	43/43	0.95	0.18	0.26	67,75,79,81	0
8	HEM	M	501	43/43	0.97	0.17	0.23	63,69,75,78	0
12	FES	O	200	4/4	0.98	0.18	0.17	42,43,43,43	0
12	FES	C	200	4/4	0.99	0.18	0.12	41,42,42,43	0
9	SMA	A	1001	37/37	0.95	0.21	0.11	38,47,54,56	0
6	CL	I	2004	1/1	0.93	0.16	0.10	67,67,67,67	0
8	HEM	A	501	43/43	0.98	0.18	0.01	43,47,51,53	0
8	HEM	G	501	43/43	0.97	0.17	-0.03	50,59,62,62	0
8	HEM	E	301	43/43	0.96	0.17	-0.07	53,62,73,76	0
8	HEM	D	501	43/43	0.97	0.15	-0.09	40,48,53,55	0
8	HEM	K	301	43/43	0.96	0.17	-0.20	49,55,67,69	0
4	BGL	K	1044	20/20	0.86	0.20	-0.25	95,99,101,101	0
8	HEM	N	301	43/43	0.94	0.20	-0.26	65,72,79,84	0
8	HEM	P	501	43/43	0.98	0.16	-0.42	48,54,57,57	0
12	FES	I	200	4/4	0.97	0.17	-0.49	47,48,48,48	0
12	FES	R	200	4/4	0.98	0.15	-0.60	55,57,58,58	0
8	HEM	Q	301	43/43	0.96	0.15	-0.83	56,65,73,78	0
6	CL	R	2005	1/1	0.94	0.09	-1.46	67,67,67,67	0
7	NA	R	2001	1/1	0.95	0.10	-1.46	62,62,62,62	0
5	SR	H	1013	1/1	0.89	0.08	-2.18	113,113,113,113	0
5	SR	Q	1016	1/1	0.70	0.08	-2.60	137,137,137,137	0
5	SR	E	1012	1/1	0.79	0.04	-2.65	138,138,138,138	0
5	SR	B	1011	1/1	0.79	0.04	-2.66	132,132,132,132	0
5	SR	K	1014	1/1	0.77	0.11	-2.92	145,145,145,145	0
5	SR	N	1015	1/1	0.94	0.06	-4.08	153,153,153,153	0
5	SR	G	1018	1/1	0.80	0.19	-	98,98,98,98	0
5	SR	M	1019	1/1	0.85	0.08	-	154,154,154,154	0
5	SR	A	1017	1/1	0.94	0.17	-	114,114,114,114	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.