



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 04:00 PM GMT

PDB ID : 4DVQ  
Title : Structure of human aldosterone synthase, CYP11B2, in complex with deoxycorticosterone  
Authors : Strushkevich, N.; Shen, L.; Tempel, W.; Arrowsmith, C.; Edwards, A.; Usanov, S.A.; Park, H.-W.  
Deposited on : 2012-02-23  
Resolution : 2.49 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

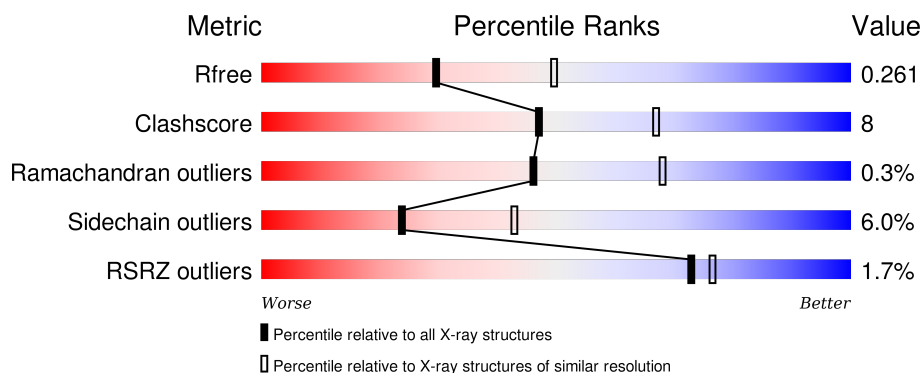
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.49 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	483	<div> <div></div> <div>80%14% . .</div> </div>
1	B	483	<div> <div>%</div> <div>79%16% . .</div> </div>
1	C	483	<div> <div></div> <div>80%13% . .</div> </div>
1	D	483	<div> <div></div> <div>78%16% . .</div> </div>
1	E	483	<div> <div></div> <div>80%15% . .</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	483	<div><div><div>%</div><div><div></div><div>76%</div><div>20%</div><div></div></div><div></div></div></div>
1	G	483	<div><div><div>2%</div><div><div></div><div>79%</div><div>15%</div><div></div></div><div></div></div></div>
1	H	483	<div><div><div>%</div><div><div></div><div>79%</div><div>16%</div><div></div></div><div></div></div></div>
1	I	483	<div><div><div>5%</div><div><div></div><div>75%</div><div>19%</div><div></div></div><div></div></div></div>
1	J	483	<div><div><div>5%</div><div><div></div><div>78%</div><div>16%</div><div></div></div><div></div></div></div>
1	K	483	<div><div><div>%</div><div><div></div><div>73%</div><div>20%</div><div></div></div><div></div></div></div>
1	L	483	<div><div><div>3%</div><div><div></div><div>76%</div><div>16%</div><div></div></div><div></div></div></div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 46194 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 P450 11B2, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	463	Total	C	N	O	S	0	0	0
			3758	2431	662	645	20			
1	B	463	Total	C	N	O	S	0	0	0
			3758	2431	662	645	20			
1	C	462	Total	C	N	O	S	0	0	0
			3750	2425	661	644	20			
1	D	462	Total	C	N	O	S	0	0	0
			3750	2425	661	644	20			
1	E	470	Total	C	N	O	S	0	0	0
			3826	2469	683	654	20			
1	F	469	Total	C	N	O	S	0	0	0
			3818	2465	681	652	20			
1	G	462	Total	C	N	O	S	0	0	0
			3750	2425	661	644	20			
1	H	462	Total	C	N	O	S	0	0	0
			3750	2425	661	644	20			
1	I	462	Total	C	N	O	S	0	0	0
			3750	2425	661	644	20			
1	J	462	Total	C	N	O	S	0	0	0
			3750	2425	661	644	20			
1	K	460	Total	C	N	O	S	0	0	0
			3734	2415	659	640	20			
1	L	454	Total	C	N	O	S	0	0	0
			3691	2387	650	634	20			

There are 156 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	MET	-	EXPRESSION TAG	UNP P19099
A	28	ALA	-	EXPRESSION TAG	UNP P19099
A	29	LYS	-	EXPRESSION TAG	UNP P19099
A	30	LYS	-	EXPRESSION TAG	UNP P19099
A	31	THR	-	EXPRESSION TAG	UNP P19099

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Chain	Residue	Modelled	Actual	Comment	Reference
A	32	SER	-	EXPRESSION TAG	UNP P19099
A	33	SER	-	EXPRESSION TAG	UNP P19099
A	504	HIS	-	EXPRESSION TAG	UNP P19099
A	505	HIS	-	EXPRESSION TAG	UNP P19099
A	506	HIS	-	EXPRESSION TAG	UNP P19099
A	507	HIS	-	EXPRESSION TAG	UNP P19099
A	508	HIS	-	EXPRESSION TAG	UNP P19099
A	509	HIS	-	EXPRESSION TAG	UNP P19099
B	27	MET	-	EXPRESSION TAG	UNP P19099
B	28	ALA	-	EXPRESSION TAG	UNP P19099
B	29	LYS	-	EXPRESSION TAG	UNP P19099
B	30	LYS	-	EXPRESSION TAG	UNP P19099
B	31	THR	-	EXPRESSION TAG	UNP P19099
B	32	SER	-	EXPRESSION TAG	UNP P19099
B	33	SER	-	EXPRESSION TAG	UNP P19099
B	504	HIS	-	EXPRESSION TAG	UNP P19099
B	505	HIS	-	EXPRESSION TAG	UNP P19099
B	506	HIS	-	EXPRESSION TAG	UNP P19099
B	507	HIS	-	EXPRESSION TAG	UNP P19099
B	508	HIS	-	EXPRESSION TAG	UNP P19099
B	509	HIS	-	EXPRESSION TAG	UNP P19099
C	27	MET	-	EXPRESSION TAG	UNP P19099
C	28	ALA	-	EXPRESSION TAG	UNP P19099
C	29	LYS	-	EXPRESSION TAG	UNP P19099
C	30	LYS	-	EXPRESSION TAG	UNP P19099
C	31	THR	-	EXPRESSION TAG	UNP P19099
C	32	SER	-	EXPRESSION TAG	UNP P19099
C	33	SER	-	EXPRESSION TAG	UNP P19099
C	504	HIS	-	EXPRESSION TAG	UNP P19099
C	505	HIS	-	EXPRESSION TAG	UNP P19099
C	506	HIS	-	EXPRESSION TAG	UNP P19099
C	507	HIS	-	EXPRESSION TAG	UNP P19099
C	508	HIS	-	EXPRESSION TAG	UNP P19099
C	509	HIS	-	EXPRESSION TAG	UNP P19099
D	27	MET	-	EXPRESSION TAG	UNP P19099
D	28	ALA	-	EXPRESSION TAG	UNP P19099
D	29	LYS	-	EXPRESSION TAG	UNP P19099
D	30	LYS	-	EXPRESSION TAG	UNP P19099
D	31	THR	-	EXPRESSION TAG	UNP P19099
D	32	SER	-	EXPRESSION TAG	UNP P19099
D	33	SER	-	EXPRESSION TAG	UNP P19099
D	504	HIS	-	EXPRESSION TAG	UNP P19099

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Chain	Residue	Modelled	Actual	Comment	Reference
D	505	HIS	-	EXPRESSION TAG	UNP P19099
D	506	HIS	-	EXPRESSION TAG	UNP P19099
D	507	HIS	-	EXPRESSION TAG	UNP P19099
D	508	HIS	-	EXPRESSION TAG	UNP P19099
D	509	HIS	-	EXPRESSION TAG	UNP P19099
E	27	MET	-	EXPRESSION TAG	UNP P19099
E	28	ALA	-	EXPRESSION TAG	UNP P19099
E	29	LYS	-	EXPRESSION TAG	UNP P19099
E	30	LYS	-	EXPRESSION TAG	UNP P19099
E	31	THR	-	EXPRESSION TAG	UNP P19099
E	32	SER	-	EXPRESSION TAG	UNP P19099
E	33	SER	-	EXPRESSION TAG	UNP P19099
E	504	HIS	-	EXPRESSION TAG	UNP P19099
E	505	HIS	-	EXPRESSION TAG	UNP P19099
E	506	HIS	-	EXPRESSION TAG	UNP P19099
E	507	HIS	-	EXPRESSION TAG	UNP P19099
E	508	HIS	-	EXPRESSION TAG	UNP P19099
E	509	HIS	-	EXPRESSION TAG	UNP P19099
F	27	MET	-	EXPRESSION TAG	UNP P19099
F	28	ALA	-	EXPRESSION TAG	UNP P19099
F	29	LYS	-	EXPRESSION TAG	UNP P19099
F	30	LYS	-	EXPRESSION TAG	UNP P19099
F	31	THR	-	EXPRESSION TAG	UNP P19099
F	32	SER	-	EXPRESSION TAG	UNP P19099
F	33	SER	-	EXPRESSION TAG	UNP P19099
F	504	HIS	-	EXPRESSION TAG	UNP P19099
F	505	HIS	-	EXPRESSION TAG	UNP P19099
F	506	HIS	-	EXPRESSION TAG	UNP P19099
F	507	HIS	-	EXPRESSION TAG	UNP P19099
F	508	HIS	-	EXPRESSION TAG	UNP P19099
F	509	HIS	-	EXPRESSION TAG	UNP P19099
G	27	MET	-	EXPRESSION TAG	UNP P19099
G	28	ALA	-	EXPRESSION TAG	UNP P19099
G	29	LYS	-	EXPRESSION TAG	UNP P19099
G	30	LYS	-	EXPRESSION TAG	UNP P19099
G	31	THR	-	EXPRESSION TAG	UNP P19099
G	32	SER	-	EXPRESSION TAG	UNP P19099
G	33	SER	-	EXPRESSION TAG	UNP P19099
G	504	HIS	-	EXPRESSION TAG	UNP P19099
G	505	HIS	-	EXPRESSION TAG	UNP P19099
G	506	HIS	-	EXPRESSION TAG	UNP P19099
G	507	HIS	-	EXPRESSION TAG	UNP P19099

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Chain	Residue	Modelled	Actual	Comment	Reference
G	508	HIS	-	EXPRESSION TAG	UNP P19099
G	509	HIS	-	EXPRESSION TAG	UNP P19099
H	27	MET	-	EXPRESSION TAG	UNP P19099
H	28	ALA	-	EXPRESSION TAG	UNP P19099
H	29	LYS	-	EXPRESSION TAG	UNP P19099
H	30	LYS	-	EXPRESSION TAG	UNP P19099
H	31	THR	-	EXPRESSION TAG	UNP P19099
H	32	SER	-	EXPRESSION TAG	UNP P19099
H	33	SER	-	EXPRESSION TAG	UNP P19099
H	504	HIS	-	EXPRESSION TAG	UNP P19099
H	505	HIS	-	EXPRESSION TAG	UNP P19099
H	506	HIS	-	EXPRESSION TAG	UNP P19099
H	507	HIS	-	EXPRESSION TAG	UNP P19099
H	508	HIS	-	EXPRESSION TAG	UNP P19099
H	509	HIS	-	EXPRESSION TAG	UNP P19099
I	27	MET	-	EXPRESSION TAG	UNP P19099
I	28	ALA	-	EXPRESSION TAG	UNP P19099
I	29	LYS	-	EXPRESSION TAG	UNP P19099
I	30	LYS	-	EXPRESSION TAG	UNP P19099
I	31	THR	-	EXPRESSION TAG	UNP P19099
I	32	SER	-	EXPRESSION TAG	UNP P19099
I	33	SER	-	EXPRESSION TAG	UNP P19099
I	504	HIS	-	EXPRESSION TAG	UNP P19099
I	505	HIS	-	EXPRESSION TAG	UNP P19099
I	506	HIS	-	EXPRESSION TAG	UNP P19099
I	507	HIS	-	EXPRESSION TAG	UNP P19099
I	508	HIS	-	EXPRESSION TAG	UNP P19099
I	509	HIS	-	EXPRESSION TAG	UNP P19099
J	27	MET	-	EXPRESSION TAG	UNP P19099
J	28	ALA	-	EXPRESSION TAG	UNP P19099
J	29	LYS	-	EXPRESSION TAG	UNP P19099
J	30	LYS	-	EXPRESSION TAG	UNP P19099
J	31	THR	-	EXPRESSION TAG	UNP P19099
J	32	SER	-	EXPRESSION TAG	UNP P19099
J	33	SER	-	EXPRESSION TAG	UNP P19099
J	504	HIS	-	EXPRESSION TAG	UNP P19099
J	505	HIS	-	EXPRESSION TAG	UNP P19099
J	506	HIS	-	EXPRESSION TAG	UNP P19099
J	507	HIS	-	EXPRESSION TAG	UNP P19099
J	508	HIS	-	EXPRESSION TAG	UNP P19099
J	509	HIS	-	EXPRESSION TAG	UNP P19099
K	27	MET	-	EXPRESSION TAG	UNP P19099

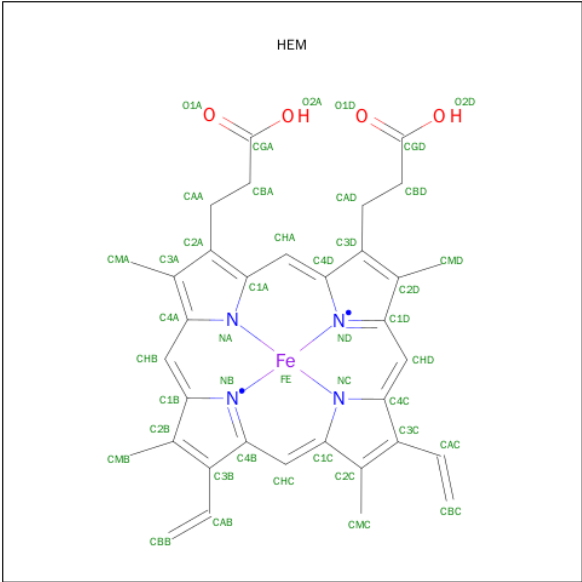
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Chain	Residue	Modelled	Actual	Comment	Reference
K	28	ALA	-	EXPRESSION TAG	UNP P19099
K	29	LYS	-	EXPRESSION TAG	UNP P19099
K	30	LYS	-	EXPRESSION TAG	UNP P19099
K	31	THR	-	EXPRESSION TAG	UNP P19099
K	32	SER	-	EXPRESSION TAG	UNP P19099
K	33	SER	-	EXPRESSION TAG	UNP P19099
K	504	HIS	-	EXPRESSION TAG	UNP P19099
K	505	HIS	-	EXPRESSION TAG	UNP P19099
K	506	HIS	-	EXPRESSION TAG	UNP P19099
K	507	HIS	-	EXPRESSION TAG	UNP P19099
K	508	HIS	-	EXPRESSION TAG	UNP P19099
K	509	HIS	-	EXPRESSION TAG	UNP P19099
L	27	MET	-	EXPRESSION TAG	UNP P19099
L	28	ALA	-	EXPRESSION TAG	UNP P19099
L	29	LYS	-	EXPRESSION TAG	UNP P19099
L	30	LYS	-	EXPRESSION TAG	UNP P19099
L	31	THR	-	EXPRESSION TAG	UNP P19099
L	32	SER	-	EXPRESSION TAG	UNP P19099
L	33	SER	-	EXPRESSION TAG	UNP P19099
L	504	HIS	-	EXPRESSION TAG	UNP P19099
L	505	HIS	-	EXPRESSION TAG	UNP P19099
L	506	HIS	-	EXPRESSION TAG	UNP P19099
L	507	HIS	-	EXPRESSION TAG	UNP P19099
L	508	HIS	-	EXPRESSION TAG	UNP P19099
L	509	HIS	-	EXPRESSION TAG	UNP P19099

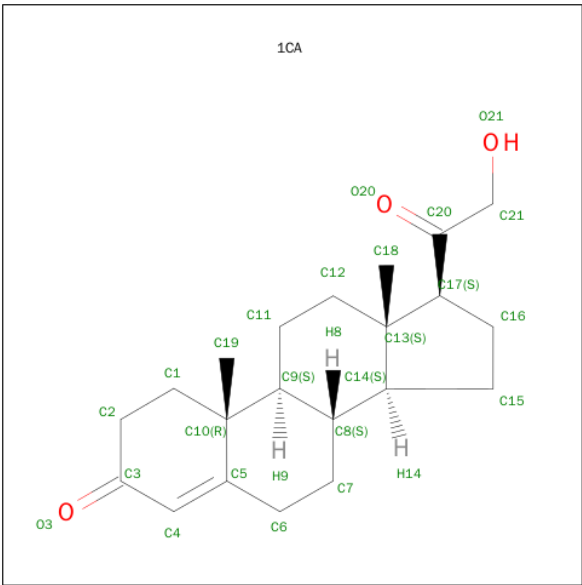
- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).





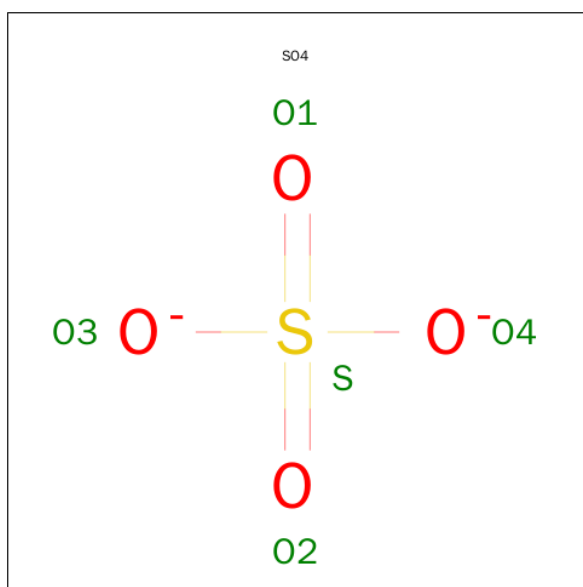
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	G	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	H	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	I	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	J	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	K	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	L	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is DESOXYCORTICOSTERONE (three-letter code: 1CA) (formula: C<sub>21</sub>H<sub>30</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			24	21	3		
3	B	1	Total	C	O	0	0
			24	21	3		
3	C	1	Total	C	O	0	0
			24	21	3		
3	D	1	Total	C	O	0	0
			24	21	3		
3	E	1	Total	C	O	0	0
			24	21	3		
3	F	1	Total	C	O	0	0
			24	21	3		
3	G	1	Total	C	O	0	0
			24	21	3		
3	H	1	Total	C	O	0	0
			24	21	3		
3	I	1	Total	C	O	0	0
			24	21	3		
3	J	1	Total	C	O	0	0
			24	21	3		
3	K	1	Total	C	O	0	0
			24	21	3		
3	L	1	Total	C	O	0	0
			24	21	3		

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	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	E	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	K	1	Total	O	S	0	0
			5	4	1		
4	L	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	31	Total	O	0	0
			31	31		
5	B	14	Total	O	0	0
			14	14		
5	C	31	Total	O	0	0
			31	31		

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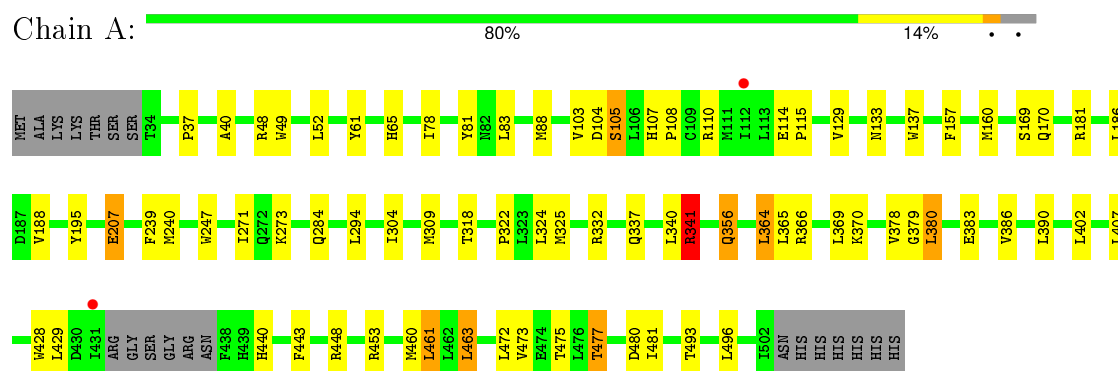
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	34	Total 34	O 34	0	0
5	E	30	Total 30	O 30	0	0
5	F	33	Total 33	O 33	0	0
5	G	18	Total 18	O 18	0	0
5	H	25	Total 25	O 25	0	0
5	I	6	Total 6	O 6	0	0
5	J	6	Total 6	O 6	0	0
5	K	13	Total 13	O 13	0	0
5	L	19	Total 19	O 19	0	0

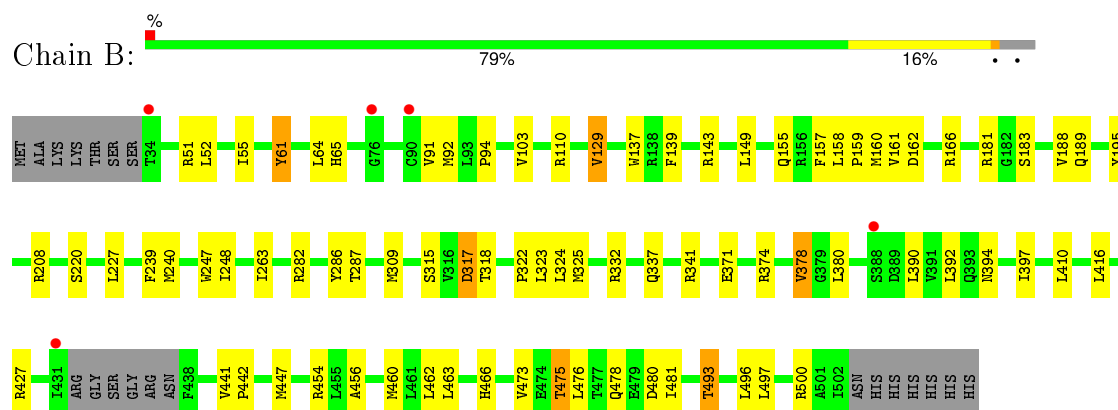
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

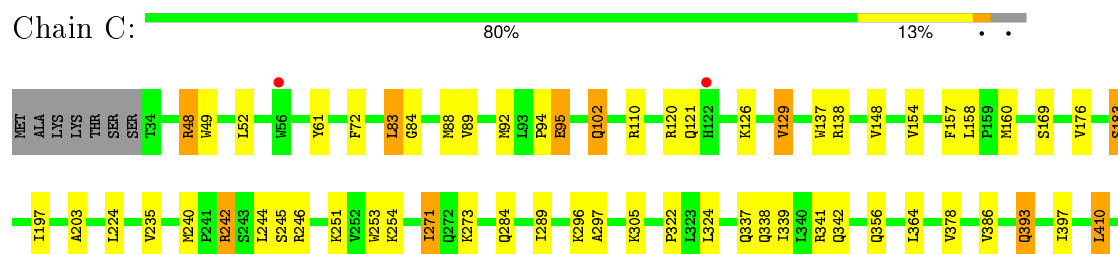
- Molecule 1: Cytochrome P450 11B2, mitochondrial



- Molecule 1: Cytochrome P450 11B2, mitochondrial



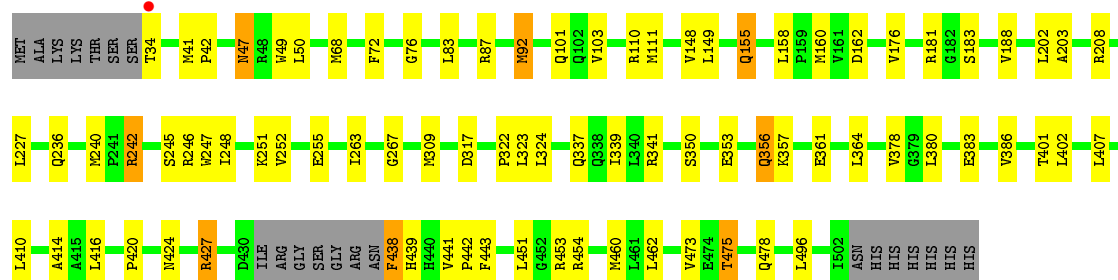
- Molecule 1: Cytochrome P450 11B2, mitochondrial





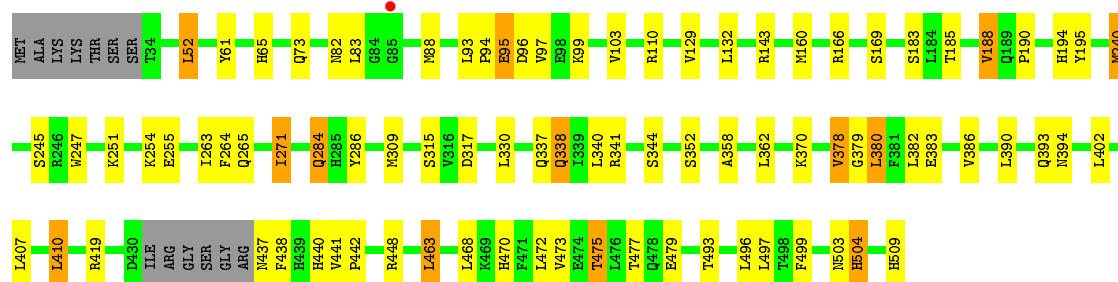
- Molecule 1: Cytochrome P450 11B2, mitochondrial

Chain D: 78% 16% . .



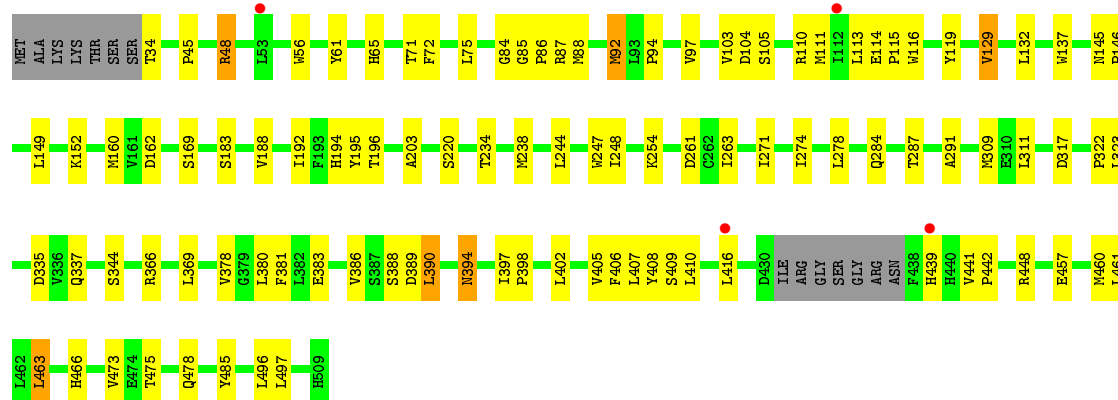
- Molecule 1: Cytochrome P450 11B2, mitochondrial

Chain E: 80% 15% . .



- Molecule 1: Cytochrome P450 11B2, mitochondrial

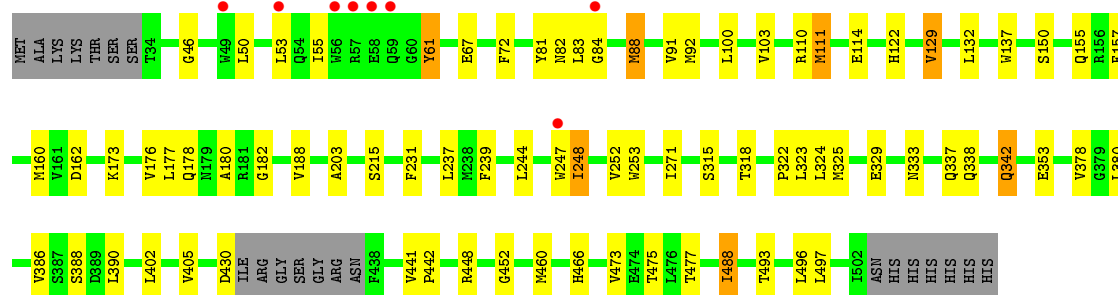
Chain F: 76% 20% . .



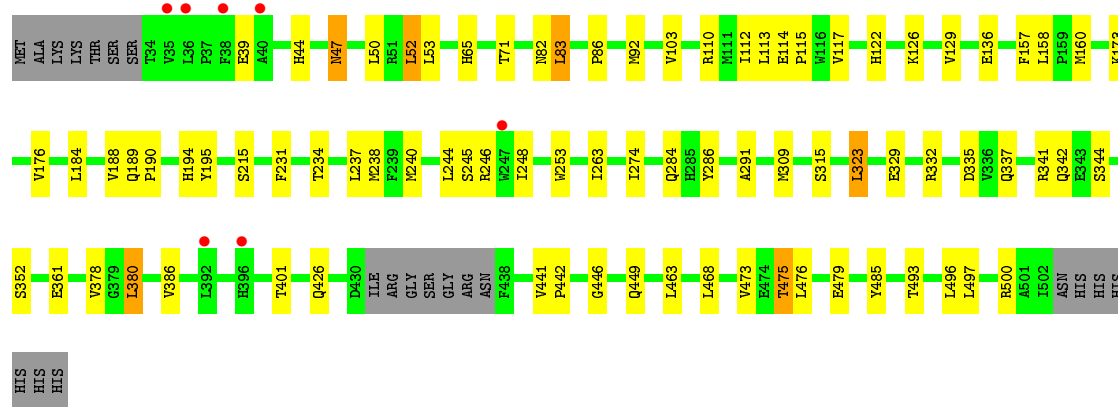
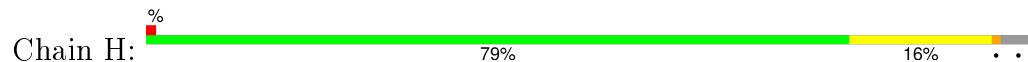
- Molecule 1: Cytochrome P450 11B2, mitochondrial

Chain G: 79% 15% . .

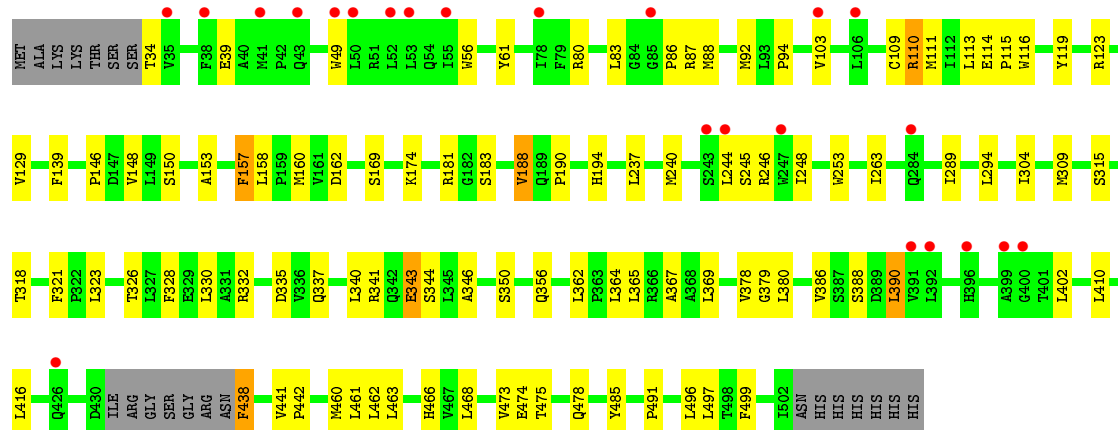
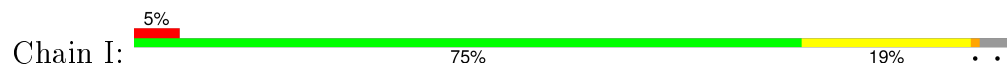




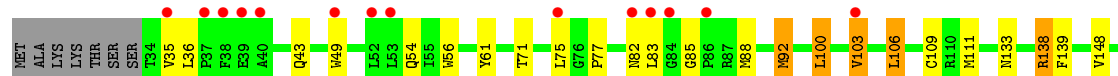
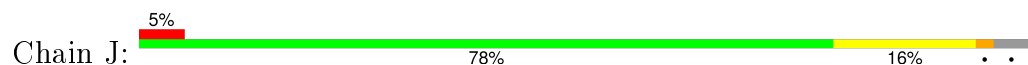
- Molecule 1: Cytochrome P450 11B2, mitochondrial

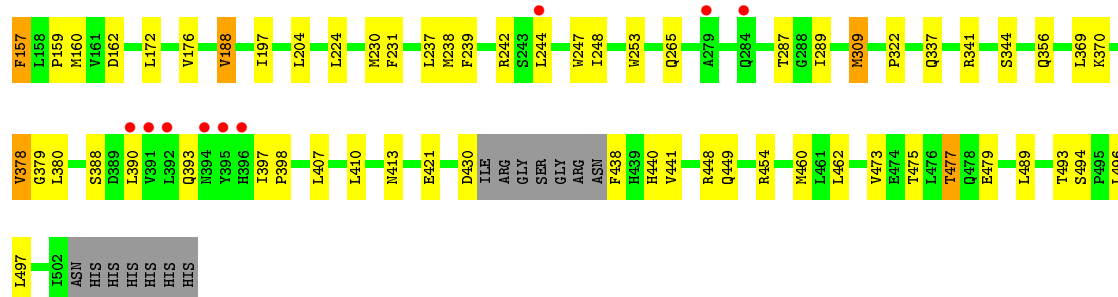


- Molecule 1: Cytochrome P450 11B2, mitochondrial

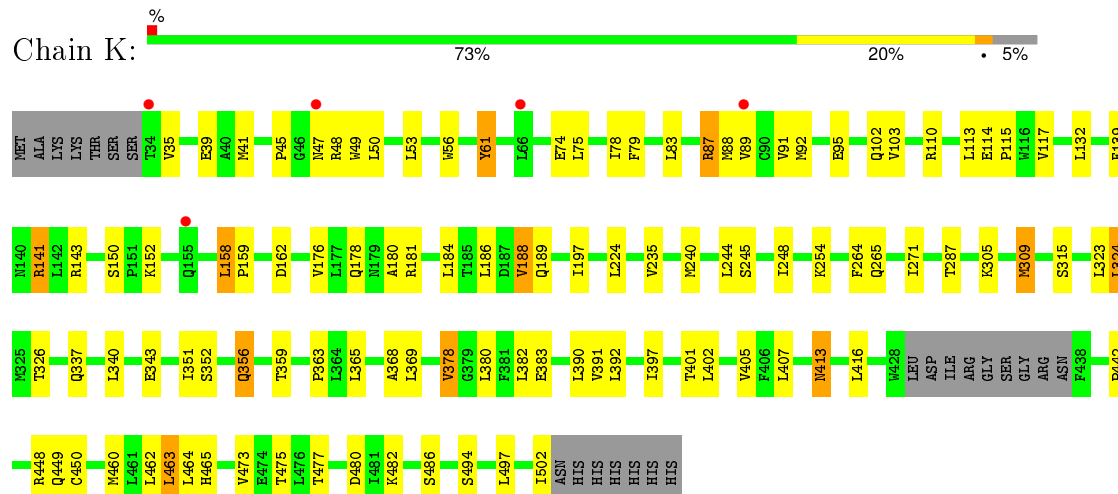


- Molecule 1: Cytochrome P450 11B2, mitochondrial

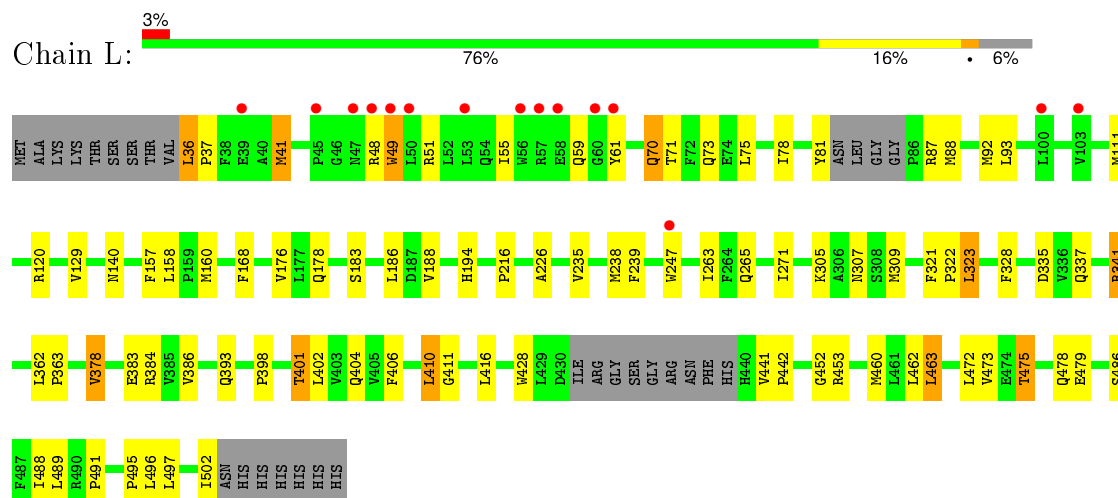




- Molecule 1: Cytochrome P450 11B2, mitochondrial



- Molecule 1: Cytochrome P450 11B2, mitochondrial





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	130.35Å 199.63Å 150.15Å 90.00° 112.18° 90.00°	Depositor
Resolution (Å)	48.07 – 2.49 48.07 – 2.49	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.07-2.49) 99.2 (48.07-2.49)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.19 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.204 , 0.263 0.205 , 0.261	Depositor DCC
$R_{free}$ test set	12313 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	51.7	Xtriage
Anisotropy	0.001	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 28.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	3 of 245705 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	46194	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	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 42.03 % 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 2.1639e-04. 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, 1CA, SO4

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	0.68	3/3858 (0.1%)	0.69	2/5235 (0.0%)
1	B	0.63	1/3858 (0.0%)	0.66	0/5235
1	C	0.67	2/3850 (0.1%)	0.68	0/5224
1	D	0.67	2/3850 (0.1%)	0.68	0/5224
1	E	0.67	1/3932 (0.0%)	0.68	0/5336
1	F	0.66	1/3924 (0.0%)	0.66	0/5325
1	G	0.62	0/3850	0.65	0/5224
1	H	0.64	0/3850	0.67	0/5224
1	I	0.62	2/3850 (0.1%)	0.63	0/5224
1	J	0.61	3/3850 (0.1%)	0.62	1/5224 (0.0%)
1	K	0.62	1/3834 (0.0%)	0.64	0/5202
1	L	0.63	3/3788 (0.1%)	0.65	0/5137
All	All	0.64	19/46294 (0.0%)	0.66	3/62814 (0.0%)

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	247	TRP	CD2-CE2	5.77	1.48	1.41
1	A	247	TRP	CD2-CE2	5.71	1.48	1.41
1	E	247	TRP	CD2-CE2	5.57	1.48	1.41
1	L	428	TRP	CD2-CE2	5.45	1.47	1.41
1	J	56	TRP	CD2-CE2	5.34	1.47	1.41

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	341	ARG	NE-CZ-NH1	-5.13	117.74	120.30
1	J	454	ARG	NE-CZ-NH1	5.07	122.84	120.30
1	A	104	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

There are no planarity outliers.

## 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	3758	0	3796	48	0
1	B	3758	0	3796	55	0
1	C	3750	0	3785	51	0
1	D	3750	0	3785	52	0
1	E	3826	0	3839	54	0
1	F	3818	0	3833	67	0
1	G	3750	0	3785	57	0
1	H	3750	0	3785	52	0
1	I	3750	0	3785	62	0
1	J	3750	0	3785	51	0
1	K	3734	0	3770	80	0
1	L	3691	0	3730	55	0
2	A	43	0	30	6	0
2	B	43	0	30	4	0
2	C	43	0	30	4	0
2	D	43	0	30	2	0
2	E	43	0	30	7	0
2	F	43	0	30	4	0
2	G	43	0	30	5	0
2	H	43	0	30	2	0
2	I	43	0	30	4	0
2	J	43	0	30	0	0
2	K	43	0	30	3	0
2	L	43	0	30	9	0
3	A	24	0	30	0	0
3	B	24	0	30	0	0
3	C	24	0	30	1	0
3	D	24	0	30	0	0
3	E	24	0	30	0	0
3	F	24	0	30	0	0
3	G	24	0	30	0	0
3	H	24	0	30	0	0
3	I	24	0	30	1	0
3	J	24	0	30	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	K	24	0	30	0	0
3	L	24	0	30	1	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
4	E	5	0	0	0	0
4	F	5	0	0	0	0
4	G	5	0	0	0	0
4	K	5	0	0	0	0
4	L	5	0	0	0	0
5	A	31	0	0	0	0
5	B	14	0	0	1	0
5	C	31	0	0	0	0
5	D	34	0	0	1	0
5	E	30	0	0	0	0
5	F	33	0	0	2	0
5	G	18	0	0	0	0
5	H	25	0	0	0	0
5	I	6	0	0	0	0
5	J	6	0	0	0	0
5	K	13	0	0	1	0
5	L	19	0	0	0	0
All	All	46194	0	46194	691	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 8.

The worst 5 of 691 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)
1:I:475:THR:CG2	1:I:497:LEU:HD23	1.87	1.04
1:J:369:LEU:HD22	1:J:460:MET:HE2	1.38	1.03
1:G:337:GLN:HE22	1:G:473:VAL:H	1.04	1.01
1:H:475:THR:HG22	1:H:496:LEU:O	1.62	0.99
1:F:475:THR:HG22	1:F:496:LEU:O	1.61	0.98

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	459/483 (95%)	444 (97%)	14 (3%)	1 (0%)	52	75
1	B	459/483 (95%)	437 (95%)	21 (5%)	1 (0%)	52	75
1	C	458/483 (95%)	444 (97%)	13 (3%)	1 (0%)	52	75
1	D	458/483 (95%)	435 (95%)	23 (5%)	0	100	100
1	E	466/483 (96%)	445 (96%)	16 (3%)	5 (1%)	17	31
1	F	465/483 (96%)	449 (97%)	15 (3%)	1 (0%)	52	75
1	G	458/483 (95%)	439 (96%)	19 (4%)	0	100	100
1	H	458/483 (95%)	439 (96%)	18 (4%)	1 (0%)	52	75
1	I	458/483 (95%)	429 (94%)	29 (6%)	0	100	100
1	J	458/483 (95%)	435 (95%)	18 (4%)	5 (1%)	17	31
1	K	456/483 (94%)	433 (95%)	21 (5%)	2 (0%)	39	61
1	L	448/483 (93%)	434 (97%)	13 (3%)	1 (0%)	52	75
All	All	5501/5796 (95%)	5263 (96%)	220 (4%)	18 (0%)	46	68

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	504	HIS
1	B	427	ARG
1	F	48	ARG
1	J	477	THR
1	A	477	THR

### 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	408/425 (96%)	390 (96%)	18 (4%)	35	60
1	B	408/425 (96%)	389 (95%)	19 (5%)	32	56
1	C	407/425 (96%)	382 (94%)	25 (6%)	23	42
1	D	407/425 (96%)	385 (95%)	22 (5%)	27	49
1	E	415/425 (98%)	385 (93%)	30 (7%)	18	33
1	F	414/425 (97%)	390 (94%)	24 (6%)	25	45
1	G	407/425 (96%)	387 (95%)	20 (5%)	31	55
1	H	407/425 (96%)	380 (93%)	27 (7%)	21	38
1	I	407/425 (96%)	385 (95%)	22 (5%)	27	49
1	J	407/425 (96%)	384 (94%)	23 (6%)	25	46
1	K	405/425 (95%)	374 (92%)	31 (8%)	16	30
1	L	401/425 (94%)	370 (92%)	31 (8%)	16	30
All	All	4893/5100 (96%)	4601 (94%)	292 (6%)	24	43

5 of 292 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	390	LEU
1	H	103	VAL
1	L	92	MET
1	F	457	GLU
1	G	247	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 109 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	59	GLN
1	G	101	GLN
1	K	470	HIS
1	F	65	HIS
1	F	337	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 ⓘ

33 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	601	1	30,50,50	2.27	7 (23%)	24,82,82	2.71	12 (50%)
3	1CA	A	602	-	27,27,27	0.82	1 (3%)	42,43,43	1.31	6 (14%)
4	SO4	A	603	-	4,4,4	0.41	0	6,6,6	0.37	0
2	HEM	B	601	1	30,50,50	2.25	6 (20%)	24,82,82	2.43	8 (33%)
3	1CA	B	602	-	27,27,27	0.73	0	42,43,43	1.17	5 (11%)
4	SO4	B	603	-	4,4,4	0.44	0	6,6,6	0.35	0
2	HEM	C	601	1	30,50,50	2.72	5 (16%)	24,82,82	2.39	8 (33%)
3	1CA	C	602	-	27,27,27	1.01	3 (11%)	42,43,43	1.64	12 (28%)
4	SO4	C	603	-	4,4,4	0.45	0	6,6,6	0.24	0
2	HEM	D	601	1	30,50,50	2.45	5 (16%)	24,82,82	2.38	9 (37%)
3	1CA	D	602	-	27,27,27	0.85	0	42,43,43	1.38	7 (16%)
4	SO4	D	603	-	4,4,4	0.47	0	6,6,6	0.19	0
2	HEM	E	601	1	30,50,50	2.08	6 (20%)	24,82,82	2.27	7 (29%)
3	1CA	E	602	-	27,27,27	0.81	0	42,43,43	1.50	9 (21%)
4	SO4	E	603	-	4,4,4	0.46	0	6,6,6	0.41	0
2	HEM	F	601	1	30,50,50	2.22	6 (20%)	24,82,82	2.43	10 (41%)
3	1CA	F	602	-	27,27,27	1.01	1 (3%)	42,43,43	1.27	7 (16%)
4	SO4	F	603	-	4,4,4	0.42	0	6,6,6	0.24	0
2	HEM	G	601	1	30,50,50	2.23	7 (23%)	24,82,82	2.37	11 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	1CA	G	602	-	27,27,27	0.89	0	42,43,43	1.23	3 (7%)
4	SO4	G	603	-	4,4,4	0.37	0	6,6,6	0.59	0
2	HEM	H	601	1	30,50,50	1.97	6 (20%)	24,82,82	2.40	9 (37%)
3	1CA	H	602	-	27,27,27	0.84	1 (3%)	42,43,43	1.14	5 (11%)
2	HEM	I	601	1	30,50,50	2.05	5 (16%)	24,82,82	2.25	9 (37%)
3	1CA	I	602	-	27,27,27	0.83	0	42,43,43	1.52	8 (19%)
2	HEM	J	601	1	30,50,50	2.31	9 (30%)	24,82,82	2.29	10 (41%)
3	1CA	J	602	-	27,27,27	0.84	1 (3%)	42,43,43	1.39	7 (16%)
2	HEM	K	601	1	30,50,50	2.23	8 (26%)	24,82,82	2.32	9 (37%)
3	1CA	K	602	-	27,27,27	0.61	0	42,43,43	1.52	8 (19%)
4	SO4	K	603	-	4,4,4	0.38	0	6,6,6	0.49	0
2	HEM	L	601	1	30,50,50	2.24	5 (16%)	24,82,82	2.44	9 (37%)
3	1CA	L	602	-	27,27,27	0.66	0	42,43,43	1.29	2 (4%)
4	SO4	L	603	-	4,4,4	0.38	0	6,6,6	0.28	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	601	1	-	0/10/54/54	0/0/8/8
3	1CA	A	602	-	-	0/6/64/64	0/4/4/4
4	SO4	A	603	-	-	0/0/0/0	0/0/0/0
2	HEM	B	601	1	-	0/10/54/54	0/0/8/8
3	1CA	B	602	-	-	0/6/64/64	0/4/4/4
4	SO4	B	603	-	-	0/0/0/0	0/0/0/0
2	HEM	C	601	1	-	0/10/54/54	0/0/8/8
3	1CA	C	602	-	-	0/6/64/64	0/4/4/4
4	SO4	C	603	-	-	0/0/0/0	0/0/0/0
2	HEM	D	601	1	-	0/10/54/54	0/0/8/8
3	1CA	D	602	-	-	0/6/64/64	0/4/4/4
4	SO4	D	603	-	-	0/0/0/0	0/0/0/0
2	HEM	E	601	1	-	0/10/54/54	0/0/8/8
3	1CA	E	602	-	-	0/6/64/64	0/4/4/4
4	SO4	E	603	-	-	0/0/0/0	0/0/0/0
2	HEM	F	601	1	-	0/10/54/54	0/0/8/8
3	1CA	F	602	-	-	0/6/64/64	0/4/4/4
4	SO4	F	603	-	-	0/0/0/0	0/0/0/0
2	HEM	G	601	1	-	0/10/54/54	0/0/8/8

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	1CA	G	602	-	-	0/6/64/64	0/4/4/4
4	SO4	G	603	-	-	0/0/0/0	0/0/0/0
2	HEM	H	601	1	-	0/10/54/54	0/0/8/8
3	1CA	H	602	-	-	0/6/64/64	0/4/4/4
2	HEM	I	601	1	-	0/10/54/54	0/0/8/8
3	1CA	I	602	-	-	0/6/64/64	0/4/4/4
2	HEM	J	601	1	-	0/10/54/54	0/0/8/8
3	1CA	J	602	-	-	0/6/64/64	0/4/4/4
2	HEM	K	601	1	-	0/10/54/54	0/0/8/8
3	1CA	K	602	-	-	0/6/64/64	0/4/4/4
4	SO4	K	603	-	-	0/0/0/0	0/0/0/0
2	HEM	L	601	1	-	0/10/54/54	0/0/8/8
3	1CA	L	602	-	-	0/6/64/64	0/4/4/4
4	SO4	L	603	-	-	0/0/0/0	0/0/0/0

The worst 5 of 82 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	HEM	C3B-C4B	-10.75	1.42	1.51
2	D	601	HEM	C3B-C4B	-10.05	1.42	1.51
2	A	601	HEM	C3B-C4B	-9.11	1.43	1.51
2	B	601	HEM	C3B-C4B	-8.67	1.44	1.51
2	K	601	HEM	C3B-C4B	-7.96	1.44	1.51

The worst 5 of 190 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	HEM	C3C-CAC-CBC	-5.60	115.87	124.46
2	B	601	HEM	C3C-CAC-CBC	-4.70	117.24	124.46
2	H	601	HEM	C3C-CAC-CBC	-4.52	117.52	124.46
2	L	601	HEM	C3C-CAC-CBC	-4.51	117.54	124.46
2	A	601	HEM	C3B-CAB-CBB	-4.30	117.86	124.46

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 53 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	HEM	6	0
2	B	601	HEM	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	601	HEM	4	0
3	C	602	1CA	1	0
2	D	601	HEM	2	0
2	E	601	HEM	7	0
2	F	601	HEM	4	0
2	G	601	HEM	5	0
2	H	601	HEM	2	0
2	I	601	HEM	4	0
3	I	602	1CA	1	0
2	K	601	HEM	3	0
2	L	601	HEM	9	0
3	L	602	1CA	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 ⓘ

### 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	463/483 (95%)	-0.20	2 (0%) 93 93	26, 42, 64, 113	0
1	B	463/483 (95%)	-0.07	5 (1%) 82 84	32, 50, 76, 107	0
1	C	462/483 (95%)	-0.23	2 (0%) 93 93	26, 43, 68, 95	0
1	D	462/483 (95%)	-0.26	1 (0%) 95 96	26, 44, 69, 88	0
1	E	470/483 (97%)	-0.21	1 (0%) 95 96	28, 44, 66, 97	0
1	F	469/483 (97%)	-0.09	4 (0%) 85 88	29, 47, 80, 123	0
1	G	462/483 (95%)	-0.12	8 (1%) 73 76	32, 50, 91, 147	0
1	H	462/483 (95%)	-0.13	7 (1%) 76 79	31, 48, 78, 106	0
1	I	462/483 (95%)	0.20	23 (4%) 32 37	35, 60, 101, 121	0
1	J	462/483 (95%)	0.13	23 (4%) 32 37	37, 59, 101, 119	0
1	K	460/483 (95%)	-0.01	5 (1%) 82 84	38, 60, 85, 112	0
1	L	454/483 (93%)	-0.00	15 (3%) 50 55	36, 55, 95, 154	0
All	All	5551/5796 (95%)	-0.08	96 (1%) 73 76	26, 50, 84, 154	0

The worst 5 of 96 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	431	ILE	4.8
1	I	53	LEU	4.4
1	L	49	TRP	4.4
1	L	58	GLU	4.3
1	I	391	VAL	4.2

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

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

## 6.3 Carbohydrates

There are no carbohydrates in this entry.

## 6.4 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, 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
3	1CA	A	602	24/24	0.98	0.18	1.20	29,35,38,38	0
3	1CA	L	602	24/24	0.96	0.18	1.07	42,46,52,57	0
2	HEM	I	601	43/43	0.97	0.17	0.45	36,46,57,62	0
3	1CA	F	602	24/24	0.97	0.17	0.45	35,38,43,49	0
3	1CA	K	602	24/24	0.94	0.16	0.44	43,45,52,55	0
3	1CA	B	602	24/24	0.95	0.17	0.40	34,36,39,44	0
2	HEM	C	601	43/43	0.98	0.15	0.29	25,30,35,38	0
2	HEM	J	601	43/43	0.96	0.16	0.21	35,41,53,57	0
2	HEM	E	601	43/43	0.98	0.15	0.20	25,29,41,42	0
3	1CA	I	602	24/24	0.96	0.16	0.14	41,45,52,59	0
2	HEM	G	601	43/43	0.98	0.16	0.11	32,35,39,43	0
2	HEM	H	601	43/43	0.98	0.14	0.10	30,35,38,41	0
3	1CA	J	602	24/24	0.95	0.15	-0.00	42,46,52,57	0
3	1CA	E	602	24/24	0.97	0.14	-0.03	31,33,39,40	0
2	HEM	D	601	43/43	0.98	0.14	-0.15	27,31,39,44	0
2	HEM	K	601	43/43	0.97	0.14	-0.21	36,45,52,55	0
3	1CA	H	602	24/24	0.97	0.14	-0.31	33,36,39,40	0
2	HEM	L	601	43/43	0.98	0.15	-0.37	38,45,51,56	0
3	1CA	C	602	24/24	0.97	0.14	-0.45	32,35,39,41	0
2	HEM	A	601	43/43	0.99	0.14	-0.50	25,29,34,38	0
2	HEM	F	601	43/43	0.98	0.15	-0.57	30,33,39,41	0
2	HEM	B	601	43/43	0.98	0.15	-0.64	30,35,47,51	0
3	1CA	G	602	24/24	0.97	0.14	-0.78	34,38,39,41	0
3	1CA	D	602	24/24	0.98	0.12	-1.65	30,34,38,43	0
4	SO4	E	603	5/5	0.97	0.12	-	59,61,70,71	0
4	SO4	L	603	5/5	0.94	0.11	-	60,66,69,75	0
4	SO4	B	603	5/5	0.95	0.11	-	74,74,76,80	0
4	SO4	A	603	5/5	0.98	0.07	-	55,55,56,58	0
4	SO4	C	603	5/5	0.95	0.12	-	72,73,76,77	0
4	SO4	F	603	5/5	0.97	0.10	-	63,65,70,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	SO4	K	603	5/5	0.97	0.09	-	64,71,73,75	0
4	SO4	D	603	5/5	0.96	0.08	-	67,76,78,81	0
4	SO4	G	603	5/5	0.97	0.12	-	58,63,64,64	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.