



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 12:22 PM GMT

PDB ID : 3R1B  
Title : Open crystal structure of cytochrome P450 2B4 covalently bound to the mechanism-based inactivator tert-butylphenylacetylene  
Authors : Gay, S.C.; Zhang, H.; Stout, C.D.; Hollenberg, P.F.; Halpert, J.R.  
Deposited on : 2011-03-09  
Resolution : 3.00 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

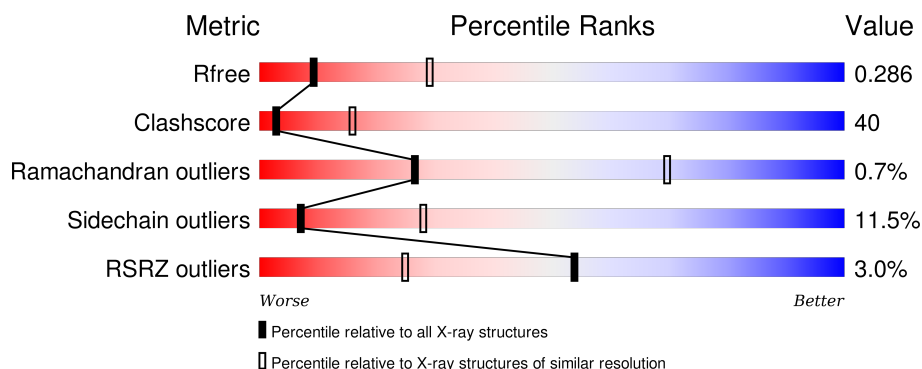
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	476	<div> <div>58%</div> <div>34%</div> <div>6%</div> <div>•</div> </div>
1	B	476	<div> <div>2%</div> <div>53%</div> <div>38%</div> <div>7%</div> <div>•</div> </div>
1	C	476	<div> <div>5%</div> <div>49%</div> <div>39%</div> <div>8%</div> <div>•</div> </div>
1	D	476	<div> <div>4%</div> <div>42%</div> <div>46%</div> <div>9%</div> <div>•</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	HEM	D	500	-	-	X	-
3	TB2	A	501	-	-	X	-
3	TB2	C	501	-	-	X	-
3	TB2	D	501	-	-	X	X
4	SUC	B	602	-	-	X	-
4	SUC	D	604	-	-	X	-
5	CM5	A	608	-	-	-	X
5	CM5	D	610	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14499 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 2B4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	465	Total	C	N	O	S	2	0	0
			3583	2294	619	659	11			
1	B	465	Total	C	N	O	S	2	0	0
			3589	2308	615	656	10			
1	C	456	Total	C	N	O	S	1	0	0
			3406	2171	589	638	8			
1	D	464	Total	C	N	O	S	0	0	0
			3445	2199	598	640	8			

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	ALA	GLU	ENGINEERED MUTATION	UNP P00178
A	?	-	PHE	DELETION	UNP P00178
A	?	-	SER	DELETION	UNP P00178
A	?	-	LEU	DELETION	UNP P00178
A	?	-	LEU	DELETION	UNP P00178
A	?	-	LEU	DELETION	UNP P00178
A	?	-	LEU	DELETION	UNP P00178
A	?	-	LEU	DELETION	UNP P00178
A	?	-	ALA	DELETION	UNP P00178
A	?	-	PHE	DELETION	UNP P00178
A	?	-	LEU	DELETION	UNP P00178
A	?	-	ALA	DELETION	UNP P00178
A	?	-	GLY	DELETION	UNP P00178
A	?	-	LEU	DELETION	UNP P00178
A	?	-	LEU	DELETION	UNP P00178
A	?	-	LEU	DELETION	UNP P00178
A	?	-	LEU	DELETION	UNP P00178
A	?	-	LEU	DELETION	UNP P00178
A	?	-	PHE	DELETION	UNP P00178
A	?	-	ARG	DELETION	UNP P00178
A	22	LYS	GLY	ENGINEERED MUTATION	UNP P00178

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Chain	Residue	Modelled	Actual	Comment	Reference
A	23	LYS	HIS	ENGINEERED MUTATION	UNP P00178
A	24	THR	PRO	ENGINEERED MUTATION	UNP P00178
A	25	SER	LYS	ENGINEERED MUTATION	UNP P00178
A	26	SER	ALA	ENGINEERED MUTATION	UNP P00178
A	27	LYS	HIS	ENGINEERED MUTATION	UNP P00178
A	29	LYS	ARG	ENGINEERED MUTATION	UNP P00178
A	221	SER	PRO	CONFLICT	UNP P00178
A	226	TYR	HIS	ENGINEERED MUTATION	UNP P00178
A	492	HIS	-	EXPRESSION TAG	UNP P00178
A	493	HIS	-	EXPRESSION TAG	UNP P00178
A	494	HIS	-	EXPRESSION TAG	UNP P00178
A	495	HIS	-	EXPRESSION TAG	UNP P00178
B	21	ALA	GLU	ENGINEERED MUTATION	UNP P00178
B	?	-	PHE	DELETION	UNP P00178
B	?	-	SER	DELETION	UNP P00178
B	?	-	LEU	DELETION	UNP P00178
B	?	-	LEU	DELETION	UNP P00178
B	?	-	LEU	DELETION	UNP P00178
B	?	-	LEU	DELETION	UNP P00178
B	?	-	LEU	DELETION	UNP P00178
B	?	-	ALA	DELETION	UNP P00178
B	?	-	PHE	DELETION	UNP P00178
B	?	-	LEU	DELETION	UNP P00178
B	?	-	ALA	DELETION	UNP P00178
B	?	-	GLY	DELETION	UNP P00178
B	?	-	LEU	DELETION	UNP P00178
B	?	-	LEU	DELETION	UNP P00178
B	?	-	LEU	DELETION	UNP P00178
B	?	-	LEU	DELETION	UNP P00178
B	?	-	LEU	DELETION	UNP P00178
B	?	-	PHE	DELETION	UNP P00178
B	?	-	ARG	DELETION	UNP P00178
B	22	LYS	GLY	ENGINEERED MUTATION	UNP P00178
B	23	LYS	HIS	ENGINEERED MUTATION	UNP P00178
B	24	THR	PRO	ENGINEERED MUTATION	UNP P00178
B	25	SER	LYS	ENGINEERED MUTATION	UNP P00178
B	26	SER	ALA	ENGINEERED MUTATION	UNP P00178
B	27	LYS	HIS	ENGINEERED MUTATION	UNP P00178
B	29	LYS	ARG	ENGINEERED MUTATION	UNP P00178
B	221	SER	PRO	CONFLICT	UNP P00178
B	226	TYR	HIS	ENGINEERED MUTATION	UNP P00178
B	492	HIS	-	EXPRESSION TAG	UNP P00178

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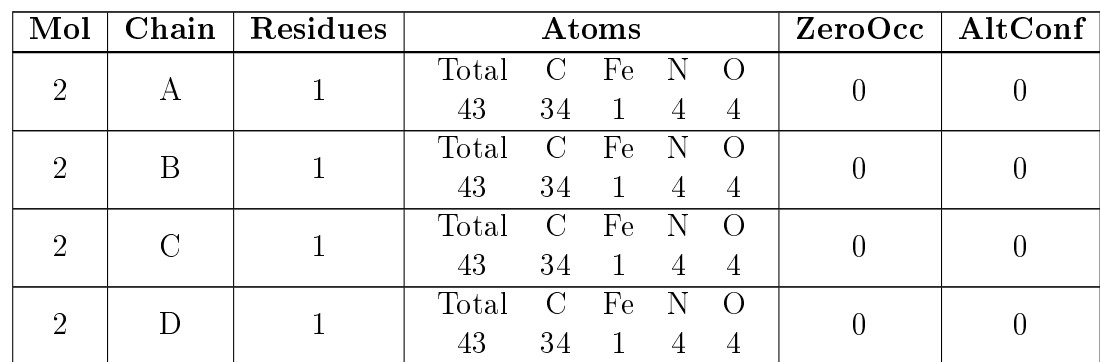
Chain	Residue	Modelled	Actual	Comment	Reference
B	493	HIS	-	EXPRESSION TAG	UNP P00178
B	494	HIS	-	EXPRESSION TAG	UNP P00178
B	495	HIS	-	EXPRESSION TAG	UNP P00178
C	21	ALA	GLU	ENGINEERED MUTATION	UNP P00178
C	?	-	PHE	DELETION	UNP P00178
C	?	-	SER	DELETION	UNP P00178
C	?	-	LEU	DELETION	UNP P00178
C	?	-	LEU	DELETION	UNP P00178
C	?	-	LEU	DELETION	UNP P00178
C	?	-	LEU	DELETION	UNP P00178
C	?	-	LEU	DELETION	UNP P00178
C	?	-	ALA	DELETION	UNP P00178
C	?	-	PHE	DELETION	UNP P00178
C	?	-	LEU	DELETION	UNP P00178
C	?	-	ALA	DELETION	UNP P00178
C	?	-	GLY	DELETION	UNP P00178
C	?	-	LEU	DELETION	UNP P00178
C	?	-	LEU	DELETION	UNP P00178
C	?	-	LEU	DELETION	UNP P00178
C	?	-	LEU	DELETION	UNP P00178
C	?	-	LEU	DELETION	UNP P00178
C	?	-	PHE	DELETION	UNP P00178
C	?	-	ARG	DELETION	UNP P00178
C	22	LYS	GLY	ENGINEERED MUTATION	UNP P00178
C	23	LYS	HIS	ENGINEERED MUTATION	UNP P00178
C	24	THR	PRO	ENGINEERED MUTATION	UNP P00178
C	25	SER	LYS	ENGINEERED MUTATION	UNP P00178
C	26	SER	ALA	ENGINEERED MUTATION	UNP P00178
C	27	LYS	HIS	ENGINEERED MUTATION	UNP P00178
C	29	LYS	ARG	ENGINEERED MUTATION	UNP P00178
C	221	SER	PRO	CONFLICT	UNP P00178
C	226	TYR	HIS	ENGINEERED MUTATION	UNP P00178
C	492	HIS	-	EXPRESSION TAG	UNP P00178
C	493	HIS	-	EXPRESSION TAG	UNP P00178
C	494	HIS	-	EXPRESSION TAG	UNP P00178
C	495	HIS	-	EXPRESSION TAG	UNP P00178
D	21	ALA	GLU	ENGINEERED MUTATION	UNP P00178
D	?	-	PHE	DELETION	UNP P00178
D	?	-	SER	DELETION	UNP P00178
D	?	-	LEU	DELETION	UNP P00178
D	?	-	LEU	DELETION	UNP P00178
D	?	-	LEU	DELETION	UNP P00178

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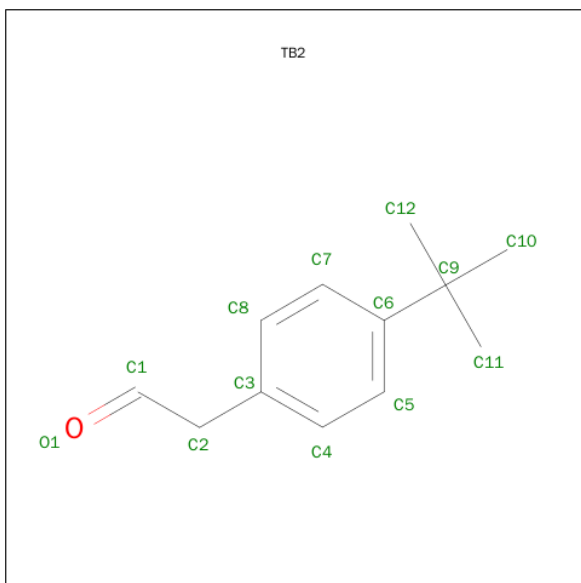
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Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	LEU	DELETION	UNP P00178
D	?	-	LEU	DELETION	UNP P00178
D	?	-	ALA	DELETION	UNP P00178
D	?	-	PHE	DELETION	UNP P00178
D	?	-	LEU	DELETION	UNP P00178
D	?	-	ALA	DELETION	UNP P00178
D	?	-	GLY	DELETION	UNP P00178
D	?	-	LEU	DELETION	UNP P00178
D	?	-	LEU	DELETION	UNP P00178
D	?	-	LEU	DELETION	UNP P00178
D	?	-	LEU	DELETION	UNP P00178
D	?	-	LEU	DELETION	UNP P00178
D	?	-	PHE	DELETION	UNP P00178
D	?	-	ARG	DELETION	UNP P00178
D	22	LYS	GLY	ENGINEERED MUTATION	UNP P00178
D	23	LYS	HIS	ENGINEERED MUTATION	UNP P00178
D	24	THR	PRO	ENGINEERED MUTATION	UNP P00178
D	25	SER	LYS	ENGINEERED MUTATION	UNP P00178
D	26	SER	ALA	ENGINEERED MUTATION	UNP P00178
D	27	LYS	HIS	ENGINEERED MUTATION	UNP P00178
D	29	LYS	ARG	ENGINEERED MUTATION	UNP P00178
D	221	SER	PRO	CONFLICT	UNP P00178
D	226	TYR	HIS	ENGINEERED MUTATION	UNP P00178
D	492	HIS	-	EXPRESSION TAG	UNP P00178
D	493	HIS	-	EXPRESSION TAG	UNP P00178
D	494	HIS	-	EXPRESSION TAG	UNP P00178
D	495	HIS	-	EXPRESSION TAG	UNP P00178

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



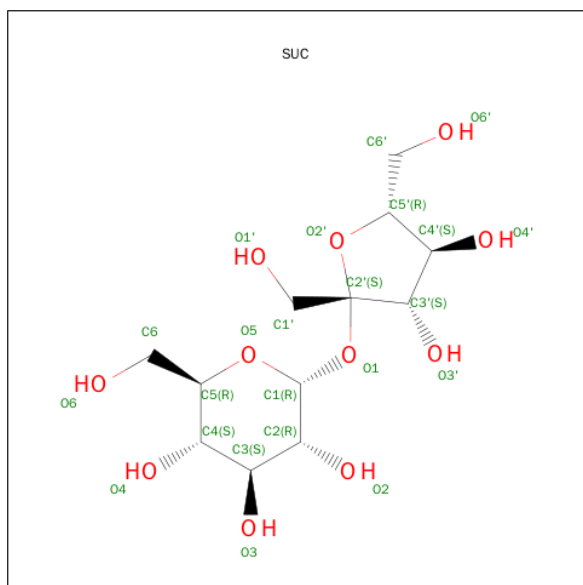
- Molecule 3 is (4-TERT-BUTYLPHENYL)ACETALDEHYDE (three-letter code: TB2) (formula: C<sub>12</sub>H<sub>16</sub>O).





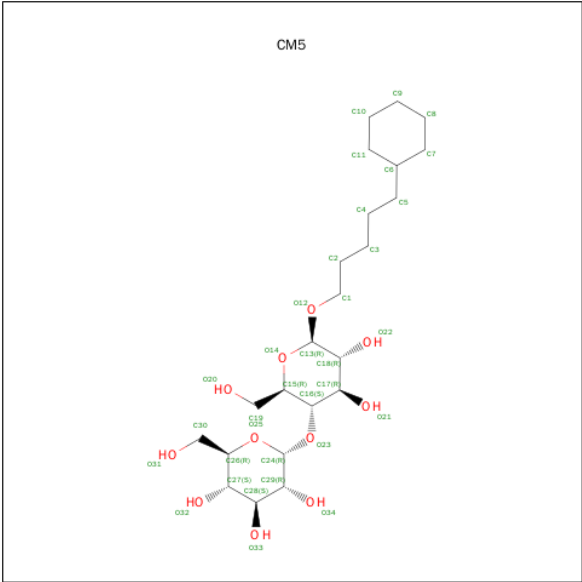
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	12	1		
3	B	1	Total	C	O	0	0
			13	12	1		
3	C	1	Total	C	O	0	0
			13	12	1		
3	D	1	Total	C	O	0	0
			13	12	1		

- Molecule 4 is SUGAR (SUCROSE) (three-letter code: SUC) (formula:  $C_{12}H_{22}O_{11}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			23	12	11		
4	B	1	Total	C	O	0	0
			23	12	11		
4	C	1	Total	C	O	0	0
			23	12	11		
4	D	1	Total	C	O	0	0
			23	12	11		

- Molecule 5 is 5-CYCLOHEXYL-1-PENTYL-BETA-D-MALTOSIDE (three-letter code: CM5) (formula:  $C_{23}H_{42}O_{11}$ ).

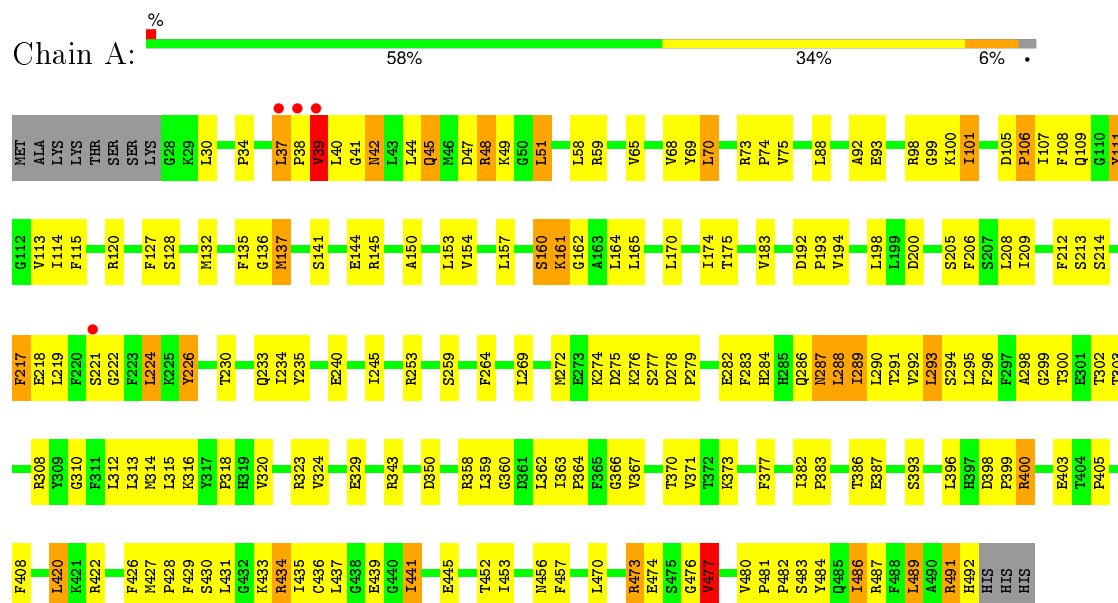


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			24	18	6		
5	B	1	Total	C	O	0	0
			34	23	11		
5	B	1	Total	C	O	0	0
			34	23	11		
5	A	1	Total	C	O	0	0
			34	23	11		
5	D	1	Total	C	O	0	0
			34	23	11		

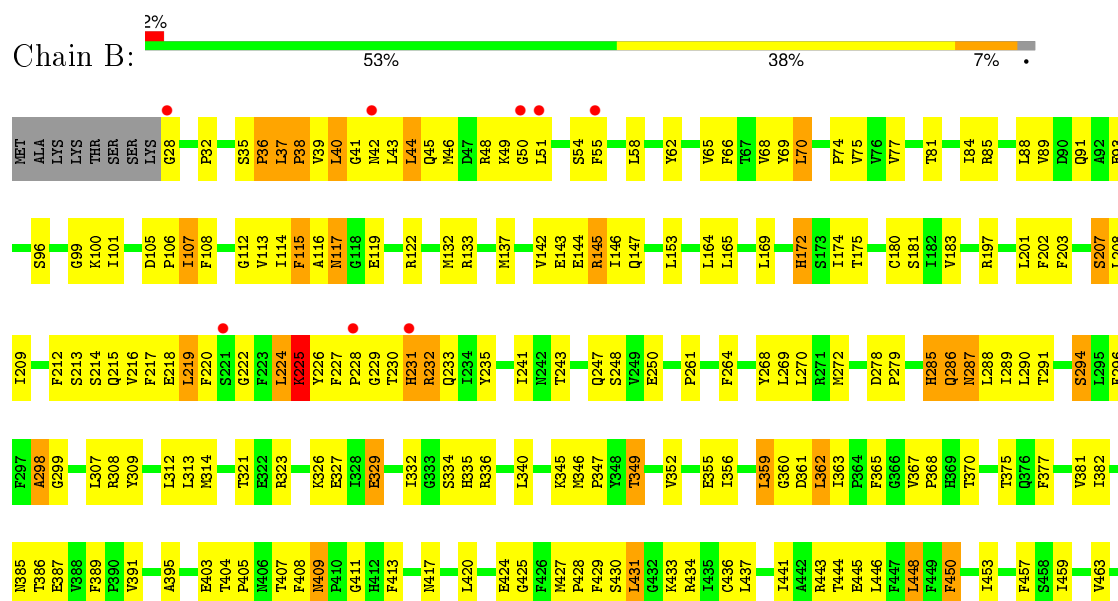
### 3 Residue-property plots

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 ( $RSRZ > 2$ ). 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 2B4

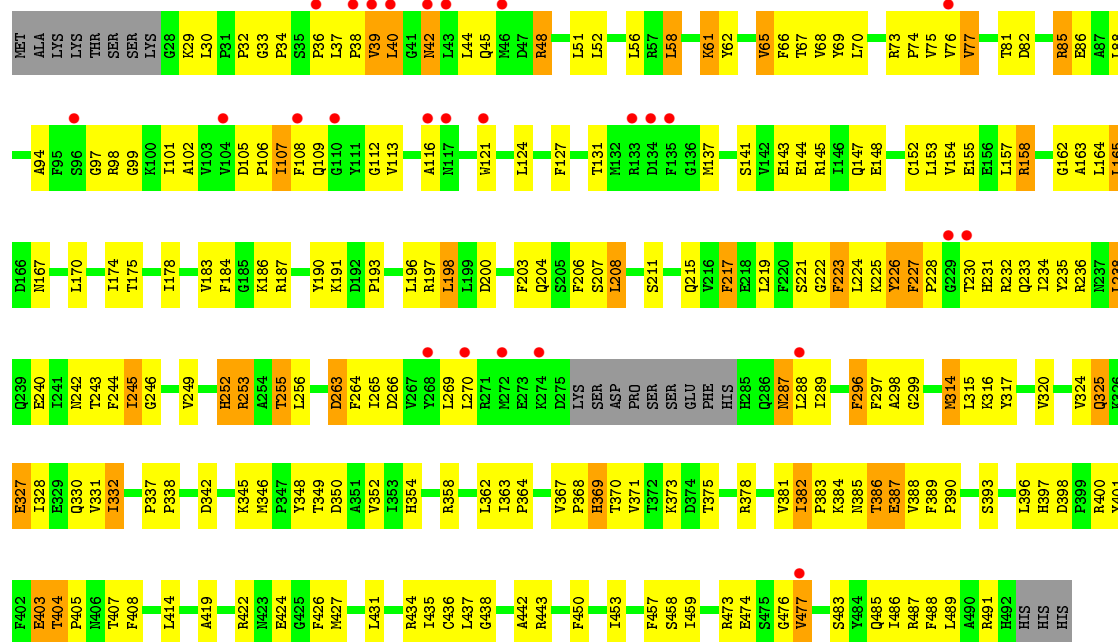


#### • Molecule 1: Cytochrome P450 2B4

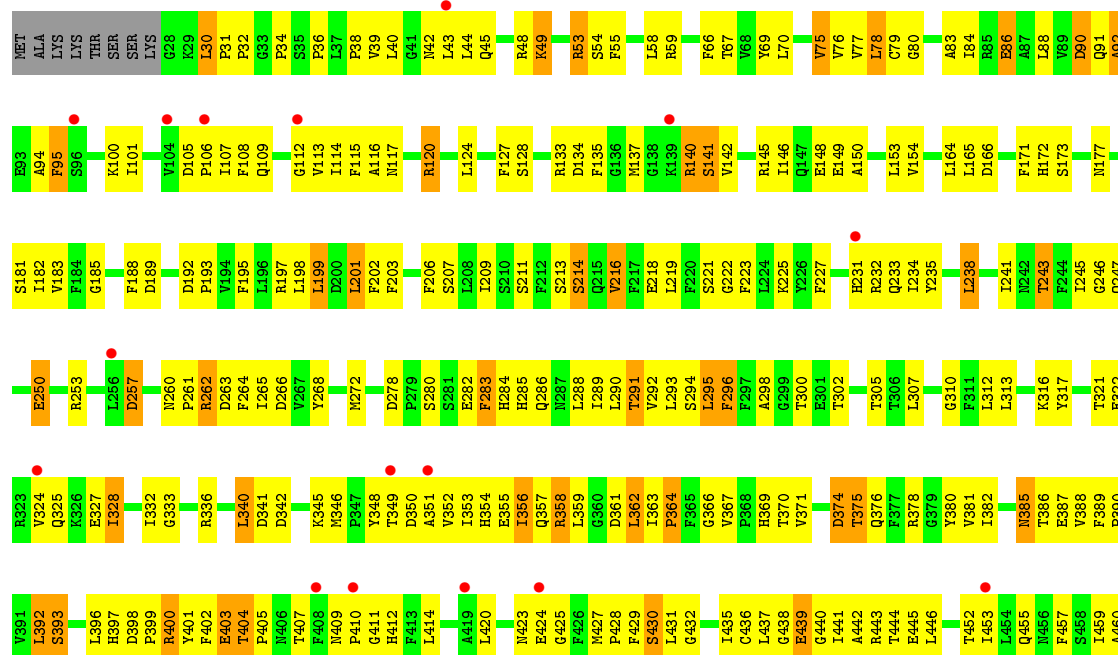


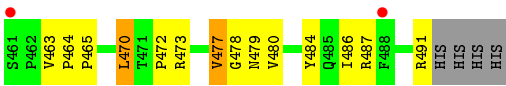


• Molecule 1: Cytochrome P450 2B4



• Molecule 1: Cytochrome P450 2B4





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	193.92Å 153.69Å 129.66Å 90.00° 122.22° 90.00°	Depositor
Resolution (Å)	53.43 – 3.00 53.44 – 3.00	Depositor EDS
% Data completeness (in resolution range)	94.8 (53.43-3.00) 99.3 (53.44-3.00)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.82 (at 3.01Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.6.4_486)	Depositor
R, $R_{free}$	0.242 , 0.288 0.245 , 0.286	Depositor DCC
$R_{free}$ test set	3237 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	92.5	Xtriage
Anisotropy	0.236	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 93.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 63927 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	14499	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.28% 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: HEM, CM5, TB2, SUC

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	0.31	1/3672 (0.0%)	0.56	6/4995 (0.1%)
1	B	0.35	0/3679	0.69	14/5003 (0.3%)
1	C	0.31	0/3484	0.67	5/4749 (0.1%)
1	D	0.32	0/3527	0.70	9/4814 (0.2%)
All	All	0.32	1/14362 (0.0%)	0.66	34/19561 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	161	LYS	CA-CB	-5.92	1.41	1.53

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	37	LEU	N-CA-C	-5.98	94.85	111.00
1	D	328	ILE	CB-CA-C	-5.98	99.64	111.60
1	D	378	ARG	N-CA-C	5.97	127.12	111.00
1	B	335	HIS	N-CA-C	5.95	127.07	111.00
1	C	255	THR	N-CA-CB	-5.93	99.03	110.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	3583	0	3434	226	0
1	B	3589	0	3460	209	0
1	C	3406	0	3187	300	0
1	D	3445	0	3216	382	0
2	A	43	0	30	17	0
2	B	43	0	30	14	0
2	C	43	0	30	12	0
2	D	43	0	30	25	0
3	A	13	0	15	8	0
3	B	13	0	15	5	0
3	C	13	0	15	6	0
3	D	13	0	15	14	0
4	A	23	0	22	6	0
4	B	23	0	22	12	0
4	C	23	0	22	5	0
4	D	23	0	22	11	0
5	A	58	0	73	5	0
5	B	68	0	84	5	0
5	D	34	0	42	3	0
All	All	14499	0	13764	1119	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 40.

The worst 5 of 1119 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:D:30:LEU:HD12	1:D:31:PRO:CD	1.18	1.61
1:A:298:ALA:HB1	3:A:501:TB2:C8	1.39	1.52
1:D:30:LEU:CD1	1:D:31:PRO:HD2	1.39	1.51
1:D:298:ALA:HB2	3:D:501:TB2:C7	1.52	1.37
1:C:233:GLN:NE2	1:C:236:ARG:HD3	1.43	1.34

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	463/476 (97%)	440 (95%)	18 (4%)	5 (1%)	17	58
1	B	463/476 (97%)	426 (92%)	36 (8%)	1 (0%)	52	88
1	C	452/476 (95%)	423 (94%)	27 (6%)	2 (0%)	39	80
1	D	462/476 (97%)	415 (90%)	43 (9%)	4 (1%)	21	64
All	All	1840/1904 (97%)	1704 (93%)	124 (7%)	12 (1%)	26	70

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	39	VAL
1	A	45	GLN
1	D	430	SER
1	A	136	GLY
1	B	36	PRO

### 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	375/421 (89%)	338 (90%)	37 (10%)	10	35
1	B	377/421 (90%)	336 (89%)	41 (11%)	8	30
1	C	343/421 (82%)	299 (87%)	44 (13%)	5	23
1	D	345/421 (82%)	301 (87%)	44 (13%)	5	23
All	All	1440/1684 (86%)	1274 (88%)	166 (12%)	7	28

5 of 166 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	473	ARG
1	C	198	LEU
1	D	356	ILE

*Continued on next page...*

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Mol	Chain	Res	Type
1	B	489	LEU
1	C	65	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	231	HIS
1	C	287	ASN
1	D	242	ASN
1	C	215	GLN
1	D	237	ASN

### 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](#)

17 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	500	1	30,50,50	2.07	10 (33%)	24,82,82	2.35	13 (54%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	TB2	A	501	1	13,13,13	0.56	0	17,18,18	0.82	0
4	SUC	A	601	-	24,24,24	1.07	2 (8%)	36,36,36	1.76	12 (33%)
5	CM5	A	605	-	25,25,36	0.43	0	32,32,49	0.85	1 (3%)
5	CM5	A	608	-	36,36,36	0.43	0	49,49,49	1.21	3 (6%)
2	HEM	B	500	1	30,50,50	2.04	8 (26%)	24,82,82	2.31	12 (50%)
3	TB2	B	501	1	13,13,13	0.57	0	17,18,18	0.75	0
4	SUC	B	602	-	24,24,24	1.04	2 (8%)	36,36,36	1.80	13 (36%)
5	CM5	B	606	-	36,36,36	0.40	0	49,49,49	1.01	3 (6%)
5	CM5	B	607	-	36,36,36	0.40	0	49,49,49	0.83	1 (2%)
2	HEM	C	500	1	30,50,50	2.12	8 (26%)	24,82,82	2.32	10 (41%)
3	TB2	C	501	1	13,13,13	0.57	0	17,18,18	0.87	0
4	SUC	C	603	-	24,24,24	1.08	2 (8%)	36,36,36	2.00	12 (33%)
2	HEM	D	500	1	30,50,50	2.20	9 (30%)	24,82,82	2.34	10 (41%)
3	TB2	D	501	1	13,13,13	0.64	0	17,18,18	0.84	1 (5%)
4	SUC	D	604	-	24,24,24	1.05	1 (4%)	36,36,36	1.86	13 (36%)
5	CM5	D	610	-	36,36,36	0.39	0	49,49,49	0.77	1 (2%)

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	500	1	-	0/10/54/54	0/0/8/8
3	TB2	A	501	1	-	0/9/9/9	0/1/1/1
4	SUC	A	601	-	-	0/12/51/51	0/2/2/2
5	CM5	A	605	-	-	0/13/41/65	0/2/2/3
5	CM5	A	608	-	-	0/17/65/65	0/3/3/3
2	HEM	B	500	1	-	0/10/54/54	0/0/8/8
3	TB2	B	501	1	-	0/9/9/9	0/1/1/1
4	SUC	B	602	-	-	0/12/51/51	0/2/2/2
5	CM5	B	606	-	-	0/17/65/65	0/3/3/3
5	CM5	B	607	-	-	0/17/65/65	0/3/3/3
2	HEM	C	500	1	-	0/10/54/54	0/0/8/8
3	TB2	C	501	1	-	0/9/9/9	0/1/1/1
4	SUC	C	603	-	-	0/12/51/51	0/2/2/2
2	HEM	D	500	1	-	0/10/54/54	0/0/8/8
3	TB2	D	501	1	-	0/9/9/9	0/1/1/1
4	SUC	D	604	-	-	0/12/51/51	0/2/2/2
5	CM5	D	610	-	-	0/17/65/65	0/3/3/3

The worst 5 of 42 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	500	HEM	C3B-C4B	-7.33	1.45	1.51
2	B	500	HEM	C3B-C4B	-6.52	1.46	1.51
2	A	500	HEM	C3B-C4B	-6.45	1.46	1.51
2	C	500	HEM	C3B-C4B	-6.35	1.46	1.51
2	C	500	HEM	C3D-C4D	-5.26	1.44	1.51

The worst 5 of 105 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	603	SUC	C2'-O1-C1	-3.88	107.29	117.53
2	D	500	HEM	C3C-CAC-CBC	-3.23	119.50	124.46
4	D	604	SUC	C2'-O1-C1	-3.14	109.24	117.53
2	A	500	HEM	CAA-C2A-C1A	-3.12	123.62	127.01
2	A	500	HEM	C3C-CAC-CBC	-2.58	120.50	124.46

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

16 monomers are involved in 148 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	HEM	17	0
3	A	501	TB2	8	0
4	A	601	SUC	6	0
5	A	605	CM5	5	0
2	B	500	HEM	14	0
3	B	501	TB2	5	0
4	B	602	SUC	12	0
5	B	606	CM5	2	0
5	B	607	CM5	3	0
2	C	500	HEM	12	0
3	C	501	TB2	6	0
4	C	603	SUC	5	0
2	D	500	HEM	25	0
3	D	501	TB2	14	0
4	D	604	SUC	11	0
5	D	610	CM5	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	465/476 (97%)	-0.19	4 (0%)	85 64	49, 79, 130, 196	2 (0%)
1	B	465/476 (97%)	-0.11	8 (1%)	73 45	54, 88, 160, 184	2 (0%)
1	C	456/476 (95%)	0.10	26 (5%)	27 10	56, 97, 181, 211	1 (0%)
1	D	464/476 (97%)	0.09	18 (3%)	43 18	60, 127, 166, 206	0
All	All	1850/1904 (97%)	-0.03	56 (3%)	54 25	49, 95, 166, 211	5 (0%)

The worst 5 of 56 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	50	GLY	11.0
1	A	38	PRO	6.8
1	C	39	VAL	6.4
1	A	39	VAL	6.1
1	C	43	LEU	5.3

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

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

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	CM5	A	608	34/34	0.76	0.43	3.54	61,125,148,155	0
5	CM5	D	610	34/34	0.79	0.34	2.58	89,144,167,172	0
3	TB2	D	501	13/13	0.87	0.51	2.31	98,106,114,116	0
5	CM5	B	607	34/34	0.77	0.31	1.78	59,122,134,136	0
5	CM5	A	605	24/34	0.89	0.30	1.24	65,96,109,115	0
2	HEM	B	500	43/43	0.98	0.28	1.18	46,60,72,85	0
3	TB2	B	501	13/13	0.95	0.30	0.95	53,65,74,76	0
3	TB2	A	501	13/13	0.97	0.29	0.93	50,61,66,68	0
2	HEM	A	500	43/43	0.98	0.27	0.74	40,54,64,71	0
3	TB2	C	501	13/13	0.96	0.33	0.54	71,79,85,88	0
2	HEM	D	500	43/43	0.93	0.29	0.45	94,103,118,127	0
4	SUC	C	603	23/23	0.82	0.21	0.38	82,101,110,120	0
2	HEM	C	500	43/43	0.97	0.27	0.19	66,83,95,108	0
5	CM5	B	606	34/34	0.88	0.24	-0.10	68,114,133,137	0
4	SUC	D	604	23/23	0.86	0.18	-0.66	140,147,153,155	0
4	SUC	B	602	23/23	0.91	0.15	-1.03	78,89,98,100	0
4	SUC	A	601	23/23	0.86	0.17	-1.39	54,81,93,98	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.