wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 12:21 PM GMT

PDB ID	:	3QU8
Title	:	Crystal structure of a human cytochrome P450 2B6 (Y226H/K262R) in complex with the inhibitor 4-(4-Nitrobenzyl)pyridine.
Authors	:	Shah, M.B.; Pascual, J.; Stout, C.D.; Halpert, J.R.
Deposited on	:	2011-02-23
Resolution	:	2.80 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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

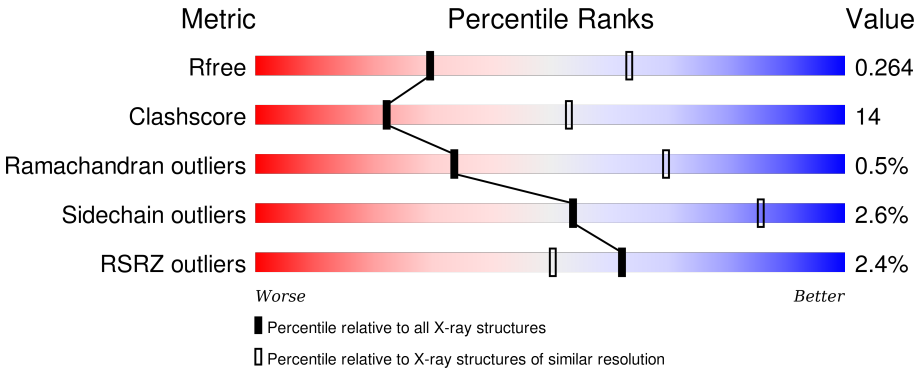
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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.



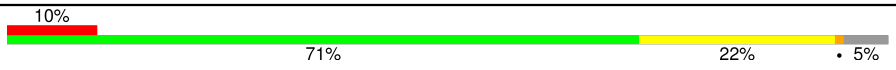
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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 >=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 <=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	76% 18%
1	B	476	% 77% 17%
1	C	476	76% 19%
1	D	476	% 76% 20%
1	E	476	% 73% 22%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	476	

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
3	3QU	A	501	-	-	-	X
3	3QU	B	501	-	-	-	X
3	3QU	D	501	-	-	-	X
3	3QU	E	501	-	-	-	X
4	CM5	B	602	-	-	-	X
4	CM5	C	603	-	-	-	X
4	CM5	D	604	X	-	-	-
4	CM5	D	607	-	-	-	X
4	CM5	F	606	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 22964 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 2B6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	462	Total	C	N	O	S	0	0	0
			3732	2416	641	658	17			
1	B	459	Total	C	N	O	S	0	0	0
			3713	2403	639	655	16			
1	C	462	Total	C	N	O	S	0	0	0
			3724	2408	642	658	16			
1	D	458	Total	C	N	O	S	0	0	0
			3693	2389	635	653	16			
1	E	459	Total	C	N	O	S	0	0	0
			3717	2406	640	655	16			
1	F	453	Total	C	N	O	S	0	0	0
			3649	2359	625	649	16			

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	GLU	ENGINEERED MUTATION	UNP P20813
A	22	LYS	ARG	ENGINEERED MUTATION	UNP P20813
A	23	LYS	HIS	ENGINEERED MUTATION	UNP P20813
A	24	THR	PRO	ENGINEERED MUTATION	UNP P20813
A	25	SER	ASN	ENGINEERED MUTATION	UNP P20813
A	26	SER	THR	ENGINEERED MUTATION	UNP P20813
A	27	LYS	HIS	ENGINEERED MUTATION	UNP P20813
A	28	GLY	ASP	ENGINEERED MUTATION	UNP P20813
A	29	LYS	ARG	ENGINEERED MUTATION	UNP P20813
A	226	HIS	TYR	ENGINEERED MUTATION	UNP P20813
A	262	ARG	LYS	ENGINEERED MUTATION	UNP P20813
A	492	HIS	-	EXPRESSION TAG	UNP P20813
A	493	HIS	-	EXPRESSION TAG	UNP P20813
A	494	HIS	-	EXPRESSION TAG	UNP P20813
A	495	HIS	-	EXPRESSION TAG	UNP P20813
B	2	ALA	GLU	ENGINEERED MUTATION	UNP P20813
B	22	LYS	ARG	ENGINEERED MUTATION	UNP P20813

Continued on next page...

Continued from previous page...

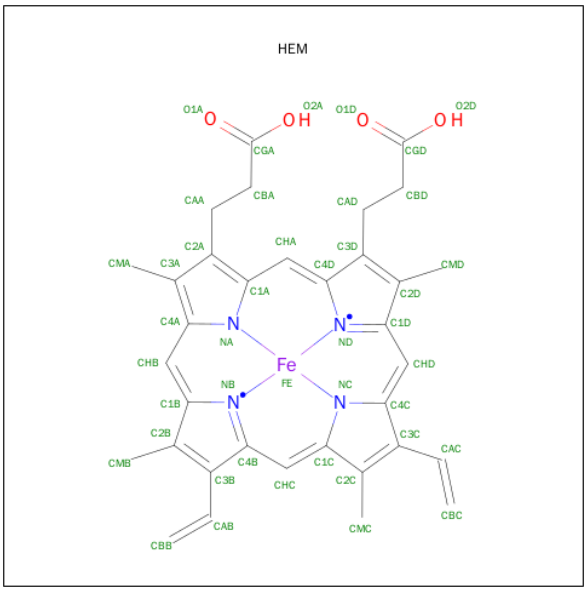
Chain	Residue	Modelled	Actual	Comment	Reference
B	23	LYS	HIS	ENGINEERED MUTATION	UNP P20813
B	24	THR	PRO	ENGINEERED MUTATION	UNP P20813
B	25	SER	ASN	ENGINEERED MUTATION	UNP P20813
B	26	SER	THR	ENGINEERED MUTATION	UNP P20813
B	27	LYS	HIS	ENGINEERED MUTATION	UNP P20813
B	28	GLY	ASP	ENGINEERED MUTATION	UNP P20813
B	29	LYS	ARG	ENGINEERED MUTATION	UNP P20813
B	226	HIS	TYR	ENGINEERED MUTATION	UNP P20813
B	262	ARG	LYS	ENGINEERED MUTATION	UNP P20813
B	492	HIS	-	EXPRESSION TAG	UNP P20813
B	493	HIS	-	EXPRESSION TAG	UNP P20813
B	494	HIS	-	EXPRESSION TAG	UNP P20813
B	495	HIS	-	EXPRESSION TAG	UNP P20813
C	2	ALA	GLU	ENGINEERED MUTATION	UNP P20813
C	22	LYS	ARG	ENGINEERED MUTATION	UNP P20813
C	23	LYS	HIS	ENGINEERED MUTATION	UNP P20813
C	24	THR	PRO	ENGINEERED MUTATION	UNP P20813
C	25	SER	ASN	ENGINEERED MUTATION	UNP P20813
C	26	SER	THR	ENGINEERED MUTATION	UNP P20813
C	27	LYS	HIS	ENGINEERED MUTATION	UNP P20813
C	28	GLY	ASP	ENGINEERED MUTATION	UNP P20813
C	29	LYS	ARG	ENGINEERED MUTATION	UNP P20813
C	226	HIS	TYR	ENGINEERED MUTATION	UNP P20813
C	262	ARG	LYS	ENGINEERED MUTATION	UNP P20813
C	492	HIS	-	EXPRESSION TAG	UNP P20813
C	493	HIS	-	EXPRESSION TAG	UNP P20813
C	494	HIS	-	EXPRESSION TAG	UNP P20813
C	495	HIS	-	EXPRESSION TAG	UNP P20813
D	2	ALA	GLU	ENGINEERED MUTATION	UNP P20813
D	22	LYS	ARG	ENGINEERED MUTATION	UNP P20813
D	23	LYS	HIS	ENGINEERED MUTATION	UNP P20813
D	24	THR	PRO	ENGINEERED MUTATION	UNP P20813
D	25	SER	ASN	ENGINEERED MUTATION	UNP P20813
D	26	SER	THR	ENGINEERED MUTATION	UNP P20813
D	27	LYS	HIS	ENGINEERED MUTATION	UNP P20813
D	28	GLY	ASP	ENGINEERED MUTATION	UNP P20813
D	29	LYS	ARG	ENGINEERED MUTATION	UNP P20813
D	226	HIS	TYR	ENGINEERED MUTATION	UNP P20813
D	262	ARG	LYS	ENGINEERED MUTATION	UNP P20813
D	492	HIS	-	EXPRESSION TAG	UNP P20813
D	493	HIS	-	EXPRESSION TAG	UNP P20813
D	494	HIS	-	EXPRESSION TAG	UNP P20813

Continued on next page...

Continued from previous page...

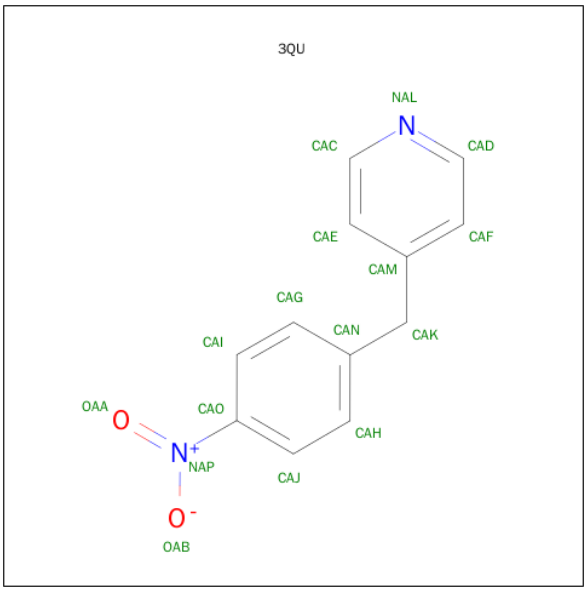
Chain	Residue	Modelled	Actual	Comment	Reference
D	495	HIS	-	EXPRESSION TAG	UNP P20813
E	2	ALA	GLU	ENGINEERED MUTATION	UNP P20813
E	22	LYS	ARG	ENGINEERED MUTATION	UNP P20813
E	23	LYS	HIS	ENGINEERED MUTATION	UNP P20813
E	24	THR	PRO	ENGINEERED MUTATION	UNP P20813
E	25	SER	ASN	ENGINEERED MUTATION	UNP P20813
E	26	SER	THR	ENGINEERED MUTATION	UNP P20813
E	27	LYS	HIS	ENGINEERED MUTATION	UNP P20813
E	28	GLY	ASP	ENGINEERED MUTATION	UNP P20813
E	29	LYS	ARG	ENGINEERED MUTATION	UNP P20813
E	226	HIS	TYR	ENGINEERED MUTATION	UNP P20813
E	262	ARG	LYS	ENGINEERED MUTATION	UNP P20813
E	492	HIS	-	EXPRESSION TAG	UNP P20813
E	493	HIS	-	EXPRESSION TAG	UNP P20813
E	494	HIS	-	EXPRESSION TAG	UNP P20813
E	495	HIS	-	EXPRESSION TAG	UNP P20813
F	2	ALA	GLU	ENGINEERED MUTATION	UNP P20813
F	22	LYS	ARG	ENGINEERED MUTATION	UNP P20813
F	23	LYS	HIS	ENGINEERED MUTATION	UNP P20813
F	24	THR	PRO	ENGINEERED MUTATION	UNP P20813
F	25	SER	ASN	ENGINEERED MUTATION	UNP P20813
F	26	SER	THR	ENGINEERED MUTATION	UNP P20813
F	27	LYS	HIS	ENGINEERED MUTATION	UNP P20813
F	28	GLY	ASP	ENGINEERED MUTATION	UNP P20813
F	29	LYS	ARG	ENGINEERED MUTATION	UNP P20813
F	226	HIS	TYR	ENGINEERED MUTATION	UNP P20813
F	262	ARG	LYS	ENGINEERED MUTATION	UNP P20813
F	492	HIS	-	EXPRESSION TAG	UNP P20813
F	493	HIS	-	EXPRESSION TAG	UNP P20813
F	494	HIS	-	EXPRESSION TAG	UNP P20813
F	495	HIS	-	EXPRESSION TAG	UNP P20813

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



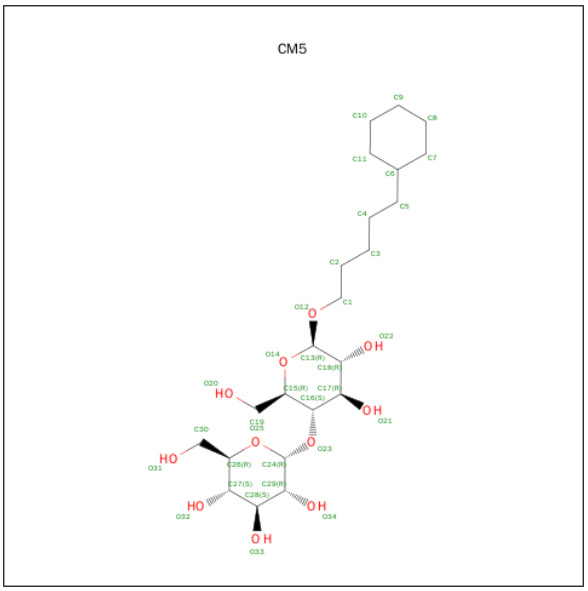
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is 4-(4-NITROBENZYL)PYRIDINE (three-letter code: 3QU) (formula: $C_{12}H_{10}N_2O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N 7 6 1	0	0
3	B	1	Total C N O 16 12 2 2	0	0
3	C	1	Total C N 7 6 1	0	0
3	D	1	Total C N 13 12 1	0	0
3	E	1	Total C N 13 12 1	0	0

- Molecule 4 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
4	A	1	Total C O 34 23 11	0	0
4	B	1	Total C O 34 23 11	0	0
4	B	1	Total C O 34 23 11	0	0
4	C	1	Total C O 34 23 11	0	0
4	D	1	Total C O 34 23 11	0	0
4	D	1	Total C O 34 23 11	0	0
4	E	1	Total C O 34 23 11	0	0
4	F	1	Total C O 34 23 11	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	25	Total O 25 25	0	0
5	B	23	Total O 23 23	0	0
5	C	29	Total O 29 29	0	0
5	D	38	Total O 38 38	0	0

Continued on next page...

Continued from previous page...

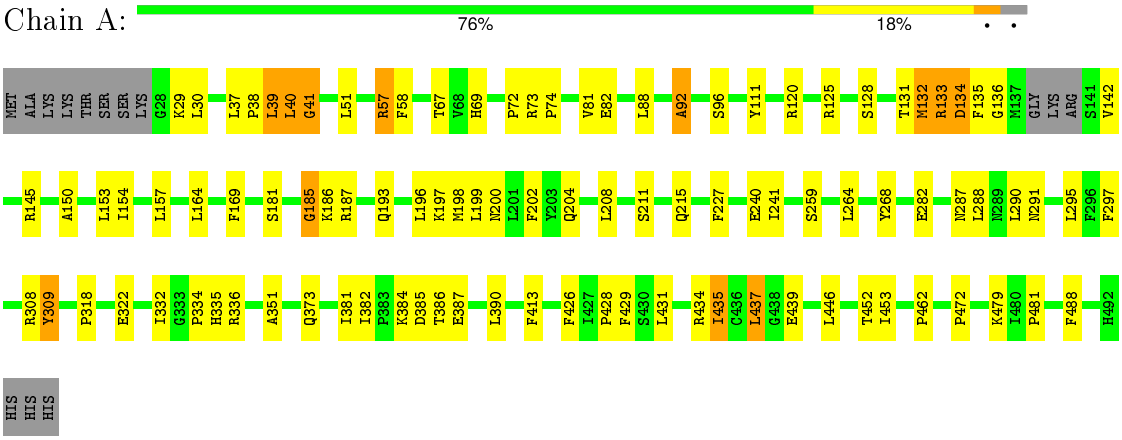
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	23	Total O 23 23	0	0
5	F	12	Total O 12 12	0	0

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.

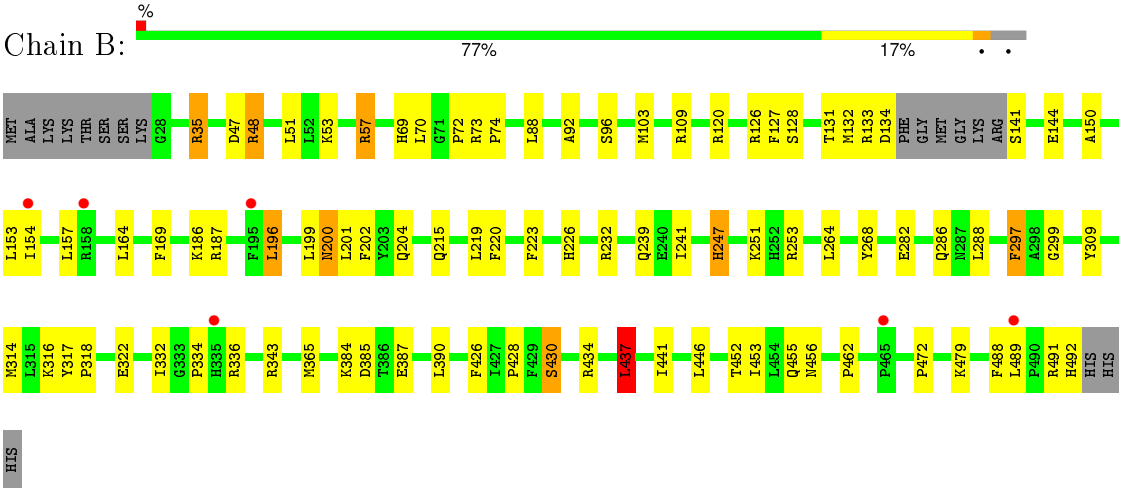
- Molecule 1: Cytochrome P450 2B6

Chain A:



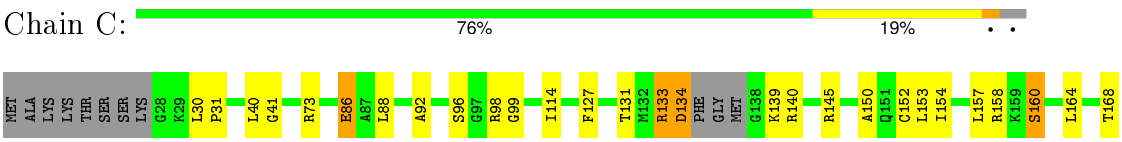
- Molecule 1: Cytochrome P450 2B6

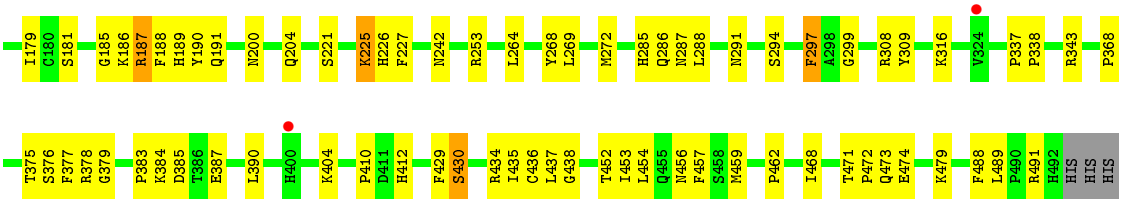
Chain B:



- Molecule 1: Cytochrome P450 2B6

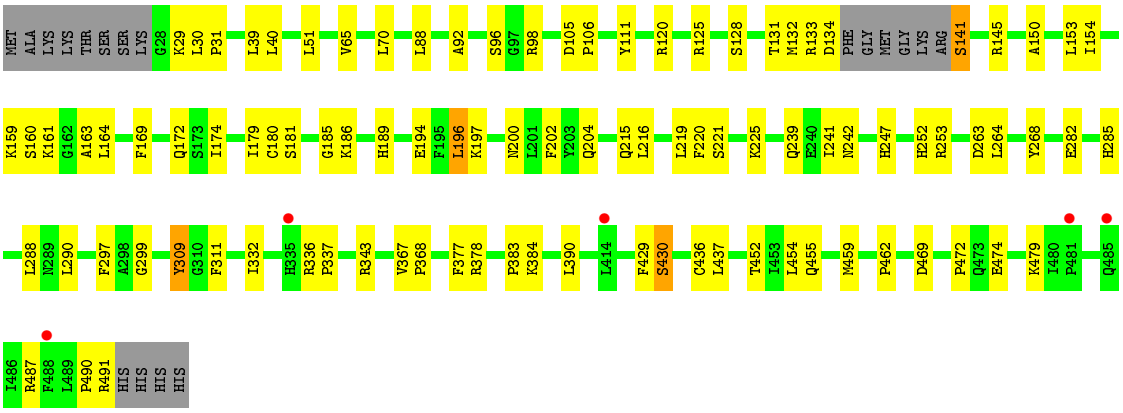
Chain C:





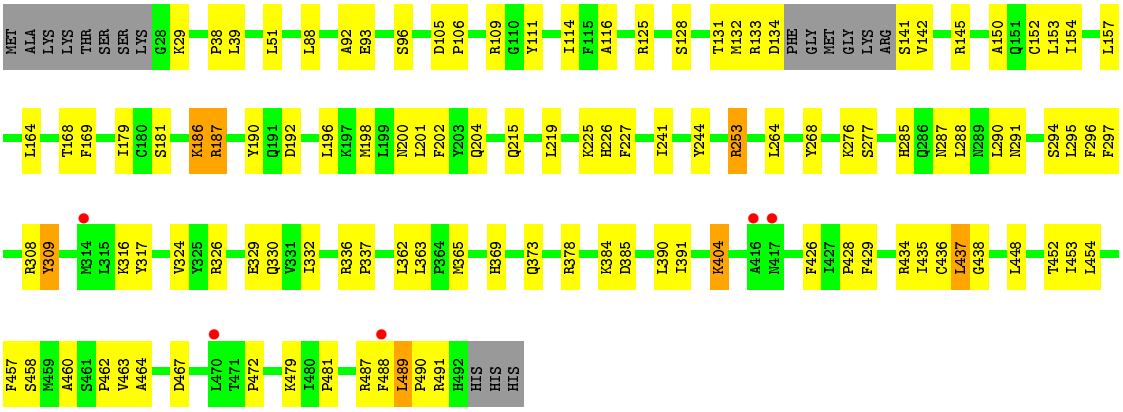
• Molecule 1: Cytochrome P450 2B6

Chain D:



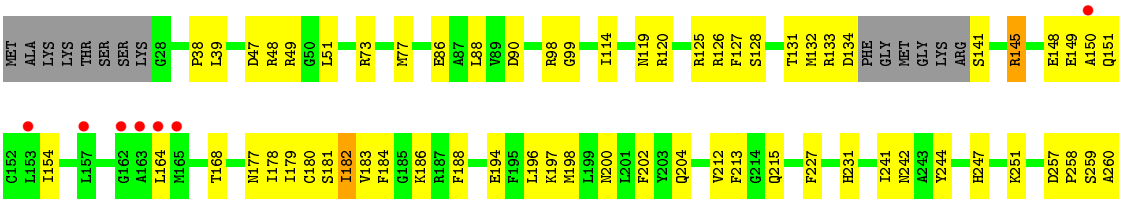
• Molecule 1: Cytochrome P450 2B6

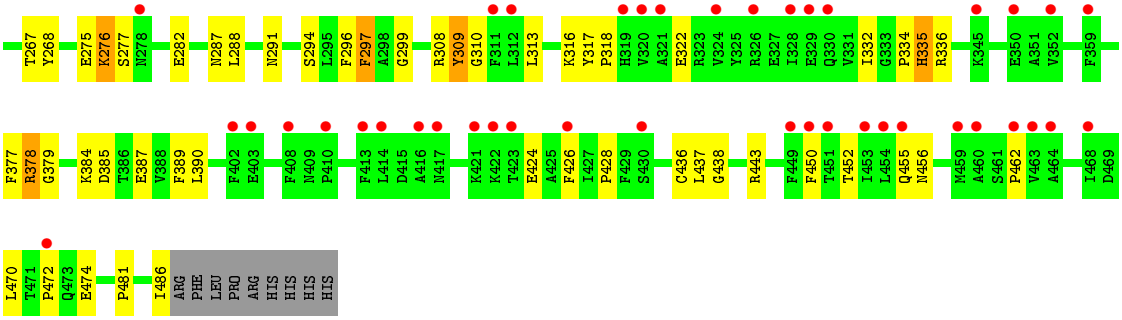
Chain E:



• Molecule 1: Cytochrome P450 2B6

Chain F:




T267 Y268 E275 K276 S277 N278 E282 N287 L288 N291 S294 L295 F296 F297 A298 G299 R308 Y309 G310 F311 L312 L313 K316 Y317 P318 H319 V320 A321 E322 R323 V324 Y325 R326 E327 I328 E329 Q330 V331 I332 G333 P334 H335 R336 K345 E350 A351 V352 F359
F377 R378 G379 K384 D385 T386 E387 V388 F389 L390 F402 E403 F408 N409 P410 F413 L414 D415 A416 N417 K421 K422 T423 E424 A425 F426 I427 P428 F429 S430 C436 L437 G438 R443 F449 P450 T451 T452 I453 L454 Q455 N456 N459 A460 S461 P462 V463 A464 I468 D469
L470 T471 P472 Q473 E474 P481 I486 ARG PHE LEU PRO ARG HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	101.88Å 101.88Å 299.51Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.51 – 2.80 50.22 – 2.80	Depositor EDS
% Data completeness (in resolution range)	88.9 (50.51-2.80) 88.9 (50.22-2.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.31 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.218 , 0.259 0.226 , 0.264	Depositor DCC
R_{free} test set	3810 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	54.6	Xtriage
Anisotropy	0.164	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 49.4	EDS
Estimated twinning fraction	0.043 for -h,-k,l 0.149 for h,-h-k,-l 0.048 for -k,-h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Outliers	0 of 76006 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	22964	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.91% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, CM5, 3QU

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	0.84	0/3833	0.75	1/5185 (0.0%)
1	B	0.83	0/3813	0.78	4/5158 (0.1%)
1	C	0.90	2/3822 (0.1%)	0.76	1/5167 (0.0%)
1	D	0.83	0/3791	0.78	2/5129 (0.0%)
1	E	0.82	0/3817	0.75	0/5162
1	F	0.95	1/3745 (0.0%)	0.78	0/5067
All	All	0.86	3/22821 (0.0%)	0.77	8/30868 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	450	PHE	CE2-CZ	5.42	1.47	1.37
1	C	152	CYS	CB-SG	-5.35	1.73	1.81
1	C	86	GLU	CG-CD	5.07	1.59	1.51

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	474	GLU	CB-CA-C	-5.88	98.64	110.40
1	A	185	GLY	N-CA-C	5.46	126.76	113.10
1	C	343	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	B	343	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	B	103	MET	CG-SD-CE	-5.40	91.57	100.20

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	3732	0	3712	103	0
1	B	3713	0	3702	93	0
1	C	3724	0	3711	83	0
1	D	3693	0	3682	97	0
1	E	3717	0	3713	117	0
1	F	3649	0	3635	100	0
2	A	43	0	30	10	0
2	B	43	0	30	4	0
2	C	43	0	30	9	0
2	D	43	0	30	12	0
2	E	43	0	30	9	0
2	F	43	0	30	18	0
3	A	7	0	4	0	0
3	B	16	0	10	0	0
3	C	7	0	4	0	0
3	D	13	0	10	0	0
3	E	13	0	10	1	0
4	A	34	0	35	1	0
4	B	68	0	77	34	0
4	C	34	0	40	5	0
4	D	68	0	78	12	0
4	E	34	0	40	3	0
4	F	34	0	38	5	0
5	A	25	0	0	1	0
5	B	23	0	0	12	0
5	C	29	0	0	2	0
5	D	38	0	0	5	0
5	E	23	0	0	5	0
5	F	12	0	0	5	0
All	All	22964	0	22681	629	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 14.

The worst 5 of 629 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)
4:B:608:CM5:C16	4:B:608:CM5:O23	1.64	1.42
4:B:608:CM5:H17	4:B:608:CM5:C24	1.61	1.28
1:A:381:ILE:HG21	1:B:239:GLN:CG	1.65	1.25
1:A:136:GLY:HA2	1:A:142:VAL:CG2	1.65	1.24
1:B:232:ARG:HH12	4:B:602:CM5:C19	1.48	1.24

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	458/476 (96%)	436 (95%)	18 (4%)	4 (1%)	21	55
1	B	455/476 (96%)	431 (95%)	21 (5%)	3 (1%)	26	62
1	C	456/476 (96%)	424 (93%)	30 (7%)	2 (0%)	39	74
1	D	454/476 (95%)	424 (93%)	28 (6%)	2 (0%)	39	74
1	E	455/476 (96%)	433 (95%)	22 (5%)	0	100	100
1	F	449/476 (94%)	417 (93%)	29 (6%)	3 (1%)	26	62
All	All	2727/2856 (96%)	2565 (94%)	148 (5%)	14 (0%)	34	69

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	430	SER
1	F	276	LYS
1	F	378	ARG
1	B	430	SER
1	C	190	TYR

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	404/418 (97%)	392 (97%)	12 (3%)	48 82
1	B	403/418 (96%)	391 (97%)	12 (3%)	48 82
1	C	402/418 (96%)	393 (98%)	9 (2%)	60 89
1	D	400/418 (96%)	394 (98%)	6 (2%)	72 93
1	E	404/418 (97%)	390 (96%)	14 (4%)	43 77
1	F	396/418 (95%)	387 (98%)	9 (2%)	58 88
All	All	2409/2508 (96%)	2347 (97%)	62 (3%)	54 86

5 of 62 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	187	ARG
1	D	189	HIS
1	F	186	LYS
1	C	309	TYR
1	D	196	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	231	HIS
1	E	286	GLN
1	C	285	HIS
1	B	455	GLN
1	E	226	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

19 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	1,3	30,50,50	2.21	8 (26%)	24,82,82	2.30	9 (37%)
3	3QU	A	501	2	7,7,17	0.25	0	8,8,22	1.22	0
4	CM5	A	601	-	36,36,36	4.16	16 (44%)	49,49,49	5.57	27 (55%)
2	HEM	B	500	1,3	30,50,50	1.76	8 (26%)	24,82,82	2.93	13 (54%)
3	3QU	B	501	2	15,17,17	0.43	0	20,22,22	1.73	5 (25%)
4	CM5	B	602	-	36,36,36	2.83	9 (25%)	49,49,49	5.06	24 (48%)
4	CM5	B	608	-	36,36,36	3.17	14 (38%)	49,49,49	5.96	26 (53%)
2	HEM	C	500	1,3	30,50,50	3.54	14 (46%)	24,82,82	2.71	9 (37%)
3	3QU	C	501	2	7,7,17	0.26	0	8,8,22	1.21	0
4	CM5	C	603	-	36,36,36	3.38	13 (36%)	49,49,49	5.39	23 (46%)
2	HEM	D	500	1,3	30,50,50	2.21	8 (26%)	24,82,82	2.31	9 (37%)
3	3QU	D	501	2	14,14,17	0.33	0	17,17,22	0.86	0
4	CM5	D	604	-	36,36,36	4.09	16 (44%)	49,49,49	6.37	25 (51%)
4	CM5	D	607	-	36,36,36	3.52	13 (36%)	49,49,49	5.06	26 (53%)
2	HEM	E	500	1,3	30,50,50	2.21	8 (26%)	24,82,82	2.31	9 (37%)
3	3QU	E	501	2	14,14,17	0.79	0	17,17,22	0.90	1 (5%)
4	CM5	E	605	-	36,36,36	3.49	14 (38%)	49,49,49	3.19	22 (44%)
2	HEM	F	500	1	30,50,50	2.21	8 (26%)	24,82,82	2.31	9 (37%)
4	CM5	F	606	-	36,36,36	3.00	13 (36%)	49,49,49	4.70	25 (51%)

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	1,3	-	0/10/54/54	0/0/8/8
3	3QU	A	501	2	-	0/0/0/8	0/1/1/2
4	CM5	A	601	-	-	0/17/65/65	0/3/3/3
2	HEM	B	500	1,3	-	0/10/54/54	0/0/8/8
3	3QU	B	501	2	-	0/8/8/8	0/2/2/2
4	CM5	B	602	-	-	0/17/65/65	0/3/3/3
4	CM5	B	608	-	-	0/17/65/65	0/3/3/3
2	HEM	C	500	1,3	-	0/10/54/54	0/0/8/8
3	3QU	C	501	2	-	0/0/0/8	0/1/1/2
4	CM5	C	603	-	-	0/17/65/65	0/3/3/3
2	HEM	D	500	1,3	-	0/10/54/54	0/0/8/8
3	3QU	D	501	2	-	0/4/4/8	0/2/2/2
4	CM5	D	604	-	1/1/11/11	0/17/65/65	0/3/3/3
4	CM5	D	607	-	-	0/17/65/65	0/3/3/3
2	HEM	E	500	1,3	-	0/10/54/54	0/0/8/8
3	3QU	E	501	2	-	0/4/4/8	0/2/2/2
4	CM5	E	605	-	-	0/17/65/65	0/3/3/3
2	HEM	F	500	1	-	0/10/54/54	0/0/8/8
4	CM5	F	606	-	-	0/17/65/65	0/3/3/3

The worst 5 of 162 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	603	CM5	O23-C24	-13.84	1.04	1.41
4	A	601	CM5	O21-C17	-13.35	1.11	1.43
2	C	500	HEM	C3B-C4B	-12.54	1.40	1.51
4	E	605	CM5	O23-C24	-11.46	1.10	1.41
4	D	604	CM5	C29-C28	-10.94	1.23	1.52

The worst 5 of 262 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	606	CM5	O12-C13-C18	-21.08	81.43	108.04
4	C	603	CM5	O33-C28-C27	-18.06	69.67	110.34
4	A	601	CM5	O33-C28-C29	-17.48	70.97	110.34
4	B	608	CM5	O14-C15-C19	-17.00	63.38	106.36
4	B	608	CM5	O14-C13-O12	-16.41	70.54	110.05

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	D	604	CM5	C16

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 122 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	HEM	10	0
4	A	601	CM5	1	0
2	B	500	HEM	4	0
4	B	602	CM5	14	0
4	B	608	CM5	20	0
2	C	500	HEM	9	0
4	C	603	CM5	5	0
2	D	500	HEM	12	0
4	D	604	CM5	4	0
4	D	607	CM5	8	0
2	E	500	HEM	9	0
3	E	501	3QU	1	0
4	E	605	CM5	3	0
2	F	500	HEM	18	0
4	F	606	CM5	5	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^{th} 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^2)	Q<0.9
1	A	462/476 (97%)	0.01	0 100 100	26, 51, 74, 82	0
1	B	459/476 (96%)	0.06	6 (1%) 79 71	28, 51, 74, 82	0
1	C	462/476 (97%)	0.04	2 (0%) 93 90	24, 50, 74, 79	0
1	D	458/476 (96%)	0.02	5 (1%) 82 74	24, 51, 74, 82	0
1	E	459/476 (96%)	0.02	5 (1%) 82 74	26, 51, 74, 87	0
1	F	453/476 (95%)	0.44	48 (10%) 8 4	24, 51, 74, 79	0
All	All	2753/2856 (96%)	0.10	66 (2%) 62 50	24, 51, 74, 87	0

The worst 5 of 66 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	463	VAL	6.9
1	F	416	ALA	5.4
1	F	460	ALA	5.1
1	F	422	LYS	4.9
1	F	153	LEU	4.6

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^{th} 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^2)	Q<0.9
3	3QU	A	501	7/16	0.92	0.29	9.59	47,50,51,52	0
3	3QU	D	501	13/16	0.93	0.25	4.88	47,49,54,54	0
4	CM5	F	606	34/34	0.78	0.33	3.83	45,62,74,76	0
3	3QU	B	501	16/16	0.94	0.27	3.23	47,51,60,66	0
4	CM5	B	602	34/34	0.78	0.30	3.20	61,72,84,85	0
4	CM5	C	603	34/34	0.81	0.27	2.45	54,63,70,71	0
4	CM5	D	607	34/34	0.80	0.23	2.43	72,97,101,103	0
3	3QU	E	501	13/16	0.96	0.24	2.25	55,57,60,63	0
3	3QU	C	501	7/16	0.93	0.25	1.54	47,50,51,52	0
4	CM5	A	601	34/34	0.92	0.24	1.45	53,60,73,74	0
4	CM5	B	608	34/34	0.81	0.23	1.30	46,84,100,100	0
4	CM5	E	605	34/34	0.86	0.26	1.22	66,73,91,92	0
2	HEM	A	500	43/43	0.97	0.21	0.62	25,31,39,43	0
2	HEM	E	500	43/43	0.97	0.20	0.51	17,28,36,40	0
4	CM5	D	604	34/34	0.89	0.20	0.32	58,67,77,79	0
2	HEM	F	500	43/43	0.95	0.22	-0.04	53,65,66,67	0
2	HEM	D	500	43/43	0.97	0.18	-0.11	23,33,38,39	0
2	HEM	B	500	43/43	0.98	0.18	-0.40	15,20,29,31	0
2	HEM	C	500	43/43	0.98	0.15	-0.94	21,27,36,46	0

6.5 Other polymers

There are no such residues in this entry.