



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 08:10 am GMT

PDB ID : 4BF4
Title : PikC D50N mutant in complex with the engineered cycloalkane substrate mimic bearing a terminal N,N-dimethylamino group
Authors : Podust, L.M.
Deposited on : 2013-03-14
Resolution : 2.70 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

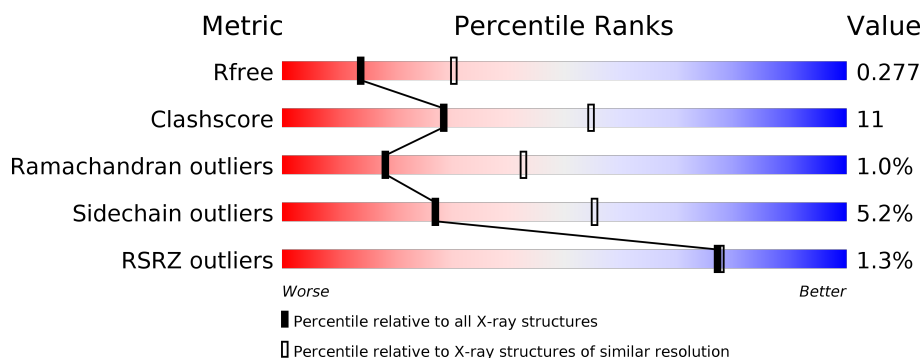
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	100719	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (2.70-2.70)

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 $\leq 5\%$. 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	436	
1	B	436	
1	C	436	
1	D	436	
1	E	436	
1	F	436	

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Mol	Chain	Length	Quality of chain
1	G	436	
1	H	436	
1	I	436	
1	J	436	
1	K	436	
1	L	436	
1	M	436	
1	N	436	
1	O	436	
1	P	436	

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	SO4	A	1408	-	-	X	-
3	SO4	H	1408	-	-	-	X
3	SO4	I	1408	-	-	-	X
3	SO4	O	1409	-	-	-	X
4	17Q	C	1410	-	-	-	X
4	17Q	G	1410	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 50342 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 HYDROXYLASE PIKC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	396	Total	C	N	O	S	0	0	0
			3031	1912	545	561	13			
1	B	397	Total	C	N	O	S	0	2	0
			3069	1939	553	564	13			
1	C	396	Total	C	N	O	S	0	1	0
			3063	1937	549	564	13			
1	D	397	Total	C	N	O	S	0	2	0
			3076	1942	552	569	13			
1	E	397	Total	C	N	O	S	0	1	0
			3068	1938	550	567	13			
1	F	396	Total	C	N	O	S	0	4	0
			3075	1944	552	566	13			
1	G	396	Total	C	N	O	S	0	4	0
			3093	1952	557	571	13			
1	H	396	Total	C	N	O	S	0	1	0
			3057	1935	549	560	13			
1	I	396	Total	C	N	O	S	0	2	0
			3066	1939	550	564	13			
1	J	397	Total	C	N	O	S	0	1	0
			3060	1934	551	562	13			
1	K	397	Total	C	N	O	S	0	2	0
			3076	1944	551	568	13			
1	L	397	Total	C	N	O	S	0	2	0
			3065	1938	551	563	13			
1	M	397	Total	C	N	O	S	0	1	0
			3065	1936	551	565	13			
1	N	397	Total	C	N	O	S	0	1	0
			3064	1938	550	563	13			
1	O	397	Total	C	N	O	S	0	0	0
			3052	1931	548	560	13			
1	P	396	Total	C	N	O	S	0	1	0
			3058	1932	548	565	13			

There are 336 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP O87605
A	-18	GLY	-	EXPRESSION TAG	UNP O87605
A	-17	SER	-	EXPRESSION TAG	UNP O87605
A	-16	SER	-	EXPRESSION TAG	UNP O87605
A	-15	HIS	-	EXPRESSION TAG	UNP O87605
A	-14	HIS	-	EXPRESSION TAG	UNP O87605
A	-13	HIS	-	EXPRESSION TAG	UNP O87605
A	-12	HIS	-	EXPRESSION TAG	UNP O87605
A	-11	HIS	-	EXPRESSION TAG	UNP O87605
A	-10	HIS	-	EXPRESSION TAG	UNP O87605
A	-9	SER	-	EXPRESSION TAG	UNP O87605
A	-8	SER	-	EXPRESSION TAG	UNP O87605
A	-7	GLY	-	EXPRESSION TAG	UNP O87605
A	-6	LEU	-	EXPRESSION TAG	UNP O87605
A	-5	VAL	-	EXPRESSION TAG	UNP O87605
A	-4	PRO	-	EXPRESSION TAG	UNP O87605
A	-3	ARG	-	EXPRESSION TAG	UNP O87605
A	-2	GLY	-	EXPRESSION TAG	UNP O87605
A	-1	SER	-	EXPRESSION TAG	UNP O87605
A	0	HIS	-	EXPRESSION TAG	UNP O87605
A	50	ASN	ASP	ENGINEERED MUTATION	UNP O87605
B	-19	MET	-	EXPRESSION TAG	UNP O87605
B	-18	GLY	-	EXPRESSION TAG	UNP O87605
B	-17	SER	-	EXPRESSION TAG	UNP O87605
B	-16	SER	-	EXPRESSION TAG	UNP O87605
B	-15	HIS	-	EXPRESSION TAG	UNP O87605
B	-14	HIS	-	EXPRESSION TAG	UNP O87605
B	-13	HIS	-	EXPRESSION TAG	UNP O87605
B	-12	HIS	-	EXPRESSION TAG	UNP O87605
B	-11	HIS	-	EXPRESSION TAG	UNP O87605
B	-10	HIS	-	EXPRESSION TAG	UNP O87605
B	-9	SER	-	EXPRESSION TAG	UNP O87605
B	-8	SER	-	EXPRESSION TAG	UNP O87605
B	-7	GLY	-	EXPRESSION TAG	UNP O87605
B	-6	LEU	-	EXPRESSION TAG	UNP O87605
B	-5	VAL	-	EXPRESSION TAG	UNP O87605
B	-4	PRO	-	EXPRESSION TAG	UNP O87605
B	-3	ARG	-	EXPRESSION TAG	UNP O87605
B	-2	GLY	-	EXPRESSION TAG	UNP O87605
B	-1	SER	-	EXPRESSION TAG	UNP O87605
B	0	HIS	-	EXPRESSION TAG	UNP O87605
B	50	ASN	ASP	ENGINEERED MUTATION	UNP O87605

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-19	MET	-	EXPRESSION TAG	UNP O87605
C	-18	GLY	-	EXPRESSION TAG	UNP O87605
C	-17	SER	-	EXPRESSION TAG	UNP O87605
C	-16	SER	-	EXPRESSION TAG	UNP O87605
C	-15	HIS	-	EXPRESSION TAG	UNP O87605
C	-14	HIS	-	EXPRESSION TAG	UNP O87605
C	-13	HIS	-	EXPRESSION TAG	UNP O87605
C	-12	HIS	-	EXPRESSION TAG	UNP O87605
C	-11	HIS	-	EXPRESSION TAG	UNP O87605
C	-10	HIS	-	EXPRESSION TAG	UNP O87605
C	-9	SER	-	EXPRESSION TAG	UNP O87605
C	-8	SER	-	EXPRESSION TAG	UNP O87605
C	-7	GLY	-	EXPRESSION TAG	UNP O87605
C	-6	LEU	-	EXPRESSION TAG	UNP O87605
C	-5	VAL	-	EXPRESSION TAG	UNP O87605
C	-4	PRO	-	EXPRESSION TAG	UNP O87605
C	-3	ARG	-	EXPRESSION TAG	UNP O87605
C	-2	GLY	-	EXPRESSION TAG	UNP O87605
C	-1	SER	-	EXPRESSION TAG	UNP O87605
C	0	HIS	-	EXPRESSION TAG	UNP O87605
C	50	ASN	ASP	ENGINEERED MUTATION	UNP O87605
D	-19	MET	-	EXPRESSION TAG	UNP O87605
D	-18	GLY	-	EXPRESSION TAG	UNP O87605
D	-17	SER	-	EXPRESSION TAG	UNP O87605
D	-16	SER	-	EXPRESSION TAG	UNP O87605
D	-15	HIS	-	EXPRESSION TAG	UNP O87605
D	-14	HIS	-	EXPRESSION TAG	UNP O87605
D	-13	HIS	-	EXPRESSION TAG	UNP O87605
D	-12	HIS	-	EXPRESSION TAG	UNP O87605
D	-11	HIS	-	EXPRESSION TAG	UNP O87605
D	-10	HIS	-	EXPRESSION TAG	UNP O87605
D	-9	SER	-	EXPRESSION TAG	UNP O87605
D	-8	SER	-	EXPRESSION TAG	UNP O87605
D	-7	GLY	-	EXPRESSION TAG	UNP O87605
D	-6	LEU	-	EXPRESSION TAG	UNP O87605
D	-5	VAL	-	EXPRESSION TAG	UNP O87605
D	-4	PRO	-	EXPRESSION TAG	UNP O87605
D	-3	ARG	-	EXPRESSION TAG	UNP O87605
D	-2	GLY	-	EXPRESSION TAG	UNP O87605
D	-1	SER	-	EXPRESSION TAG	UNP O87605
D	0	HIS	-	EXPRESSION TAG	UNP O87605
D	50	ASN	ASP	ENGINEERED MUTATION	UNP O87605

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-19	MET	-	EXPRESSION TAG	UNP O87605
E	-18	GLY	-	EXPRESSION TAG	UNP O87605
E	-17	SER	-	EXPRESSION TAG	UNP O87605
E	-16	SER	-	EXPRESSION TAG	UNP O87605
E	-15	HIS	-	EXPRESSION TAG	UNP O87605
E	-14	HIS	-	EXPRESSION TAG	UNP O87605
E	-13	HIS	-	EXPRESSION TAG	UNP O87605
E	-12	HIS	-	EXPRESSION TAG	UNP O87605
E	-11	HIS	-	EXPRESSION TAG	UNP O87605
E	-10	HIS	-	EXPRESSION TAG	UNP O87605
E	-9	SER	-	EXPRESSION TAG	UNP O87605
E	-8	SER	-	EXPRESSION TAG	UNP O87605
E	-7	GLY	-	EXPRESSION TAG	UNP O87605
E	-6	LEU	-	EXPRESSION TAG	UNP O87605
E	-5	VAL	-	EXPRESSION TAG	UNP O87605
E	-4	PRO	-	EXPRESSION TAG	UNP O87605
E	-3	ARG	-	EXPRESSION TAG	UNP O87605
E	-2	GLY	-	EXPRESSION TAG	UNP O87605
E	-1	SER	-	EXPRESSION TAG	UNP O87605
E	0	HIS	-	EXPRESSION TAG	UNP O87605
E	50	ASN	ASP	ENGINEERED MUTATION	UNP O87605
F	-19	MET	-	EXPRESSION TAG	UNP O87605
F	-18	GLY	-	EXPRESSION TAG	UNP O87605
F	-17	SER	-	EXPRESSION TAG	UNP O87605
F	-16	SER	-	EXPRESSION TAG	UNP O87605
F	-15	HIS	-	EXPRESSION TAG	UNP O87605
F	-14	HIS	-	EXPRESSION TAG	UNP O87605
F	-13	HIS	-	EXPRESSION TAG	UNP O87605
F	-12	HIS	-	EXPRESSION TAG	UNP O87605
F	-11	HIS	-	EXPRESSION TAG	UNP O87605
F	-10	HIS	-	EXPRESSION TAG	UNP O87605
F	-9	SER	-	EXPRESSION TAG	UNP O87605
F	-8	SER	-	EXPRESSION TAG	UNP O87605
F	-7	GLY	-	EXPRESSION TAG	UNP O87605
F	-6	LEU	-	EXPRESSION TAG	UNP O87605
F	-5	VAL	-	EXPRESSION TAG	UNP O87605
F	-4	PRO	-	EXPRESSION TAG	UNP O87605
F	-3	ARG	-	EXPRESSION TAG	UNP O87605
F	-2	GLY	-	EXPRESSION TAG	UNP O87605
F	-1	SER	-	EXPRESSION TAG	UNP O87605
F	0	HIS	-	EXPRESSION TAG	UNP O87605
F	50	ASN	ASP	ENGINEERED MUTATION	UNP O87605

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-19	MET	-	EXPRESSION TAG	UNP O87605
G	-18	GLY	-	EXPRESSION TAG	UNP O87605
G	-17	SER	-	EXPRESSION TAG	UNP O87605
G	-16	SER	-	EXPRESSION TAG	UNP O87605
G	-15	HIS	-	EXPRESSION TAG	UNP O87605
G	-14	HIS	-	EXPRESSION TAG	UNP O87605
G	-13	HIS	-	EXPRESSION TAG	UNP O87605
G	-12	HIS	-	EXPRESSION TAG	UNP O87605
G	-11	HIS	-	EXPRESSION TAG	UNP O87605
G	-10	HIS	-	EXPRESSION TAG	UNP O87605
G	-9	SER	-	EXPRESSION TAG	UNP O87605
G	-8	SER	-	EXPRESSION TAG	UNP O87605
G	-7	GLY	-	EXPRESSION TAG	UNP O87605
G	-6	LEU	-	EXPRESSION TAG	UNP O87605
G	-5	VAL	-	EXPRESSION TAG	UNP O87605
G	-4	PRO	-	EXPRESSION TAG	UNP O87605
G	-3	ARG	-	EXPRESSION TAG	UNP O87605
G	-2	GLY	-	EXPRESSION TAG	UNP O87605
G	-1	SER	-	EXPRESSION TAG	UNP O87605
G	0	HIS	-	EXPRESSION TAG	UNP O87605
G	50	ASN	ASP	ENGINEERED MUTATION	UNP O87605
H	-19	MET	-	EXPRESSION TAG	UNP O87605
H	-18	GLY	-	EXPRESSION TAG	UNP O87605
H	-17	SER	-	EXPRESSION TAG	UNP O87605
H	-16	SER	-	EXPRESSION TAG	UNP O87605
H	-15	HIS	-	EXPRESSION TAG	UNP O87605
H	-14	HIS	-	EXPRESSION TAG	UNP O87605
H	-13	HIS	-	EXPRESSION TAG	UNP O87605
H	-12	HIS	-	EXPRESSION TAG	UNP O87605
H	-11	HIS	-	EXPRESSION TAG	UNP O87605
H	-10	HIS	-	EXPRESSION TAG	UNP O87605
H	-9	SER	-	EXPRESSION TAG	UNP O87605
H	-8	SER	-	EXPRESSION TAG	UNP O87605
H	-7	GLY	-	EXPRESSION TAG	UNP O87605
H	-6	LEU	-	EXPRESSION TAG	UNP O87605
H	-5	VAL	-	EXPRESSION TAG	UNP O87605
H	-4	PRO	-	EXPRESSION TAG	UNP O87605
H	-3	ARG	-	EXPRESSION TAG	UNP O87605
H	-2	GLY	-	EXPRESSION TAG	UNP O87605
H	-1	SER	-	EXPRESSION TAG	UNP O87605
H	0	HIS	-	EXPRESSION TAG	UNP O87605
H	50	ASN	ASP	ENGINEERED MUTATION	UNP O87605

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-19	MET	-	EXPRESSION TAG	UNP O87605
I	-18	GLY	-	EXPRESSION TAG	UNP O87605
I	-17	SER	-	EXPRESSION TAG	UNP O87605
I	-16	SER	-	EXPRESSION TAG	UNP O87605
I	-15	HIS	-	EXPRESSION TAG	UNP O87605
I	-14	HIS	-	EXPRESSION TAG	UNP O87605
I	-13	HIS	-	EXPRESSION TAG	UNP O87605
I	-12	HIS	-	EXPRESSION TAG	UNP O87605
I	-11	HIS	-	EXPRESSION TAG	UNP O87605
I	-10	HIS	-	EXPRESSION TAG	UNP O87605
I	-9	SER	-	EXPRESSION TAG	UNP O87605
I	-8	SER	-	EXPRESSION TAG	UNP O87605
I	-7	GLY	-	EXPRESSION TAG	UNP O87605
I	-6	LEU	-	EXPRESSION TAG	UNP O87605
I	-5	VAL	-	EXPRESSION TAG	UNP O87605
I	-4	PRO	-	EXPRESSION TAG	UNP O87605
I	-3	ARG	-	EXPRESSION TAG	UNP O87605
I	-2	GLY	-	EXPRESSION TAG	UNP O87605
I	-1	SER	-	EXPRESSION TAG	UNP O87605
I	0	HIS	-	EXPRESSION TAG	UNP O87605
I	50	ASN	ASP	ENGINEERED MUTATION	UNP O87605
J	-19	MET	-	EXPRESSION TAG	UNP O87605
J	-18	GLY	-	EXPRESSION TAG	UNP O87605
J	-17	SER	-	EXPRESSION TAG	UNP O87605
J	-16	SER	-	EXPRESSION TAG	UNP O87605
J	-15	HIS	-	EXPRESSION TAG	UNP O87605
J	-14	HIS	-	EXPRESSION TAG	UNP O87605
J	-13	HIS	-	EXPRESSION TAG	UNP O87605
J	-12	HIS	-	EXPRESSION TAG	UNP O87605
J	-11	HIS	-	EXPRESSION TAG	UNP O87605
J	-10	HIS	-	EXPRESSION TAG	UNP O87605
J	-9	SER	-	EXPRESSION TAG	UNP O87605
J	-8	SER	-	EXPRESSION TAG	UNP O87605
J	-7	GLY	-	EXPRESSION TAG	UNP O87605
J	-6	LEU	-	EXPRESSION TAG	UNP O87605
J	-5	VAL	-	EXPRESSION TAG	UNP O87605
J	-4	PRO	-	EXPRESSION TAG	UNP O87605
J	-3	ARG	-	EXPRESSION TAG	UNP O87605
J	-2	GLY	-	EXPRESSION TAG	UNP O87605
J	-1	SER	-	EXPRESSION TAG	UNP O87605
J	0	HIS	-	EXPRESSION TAG	UNP O87605
J	50	ASN	ASP	ENGINEERED MUTATION	UNP O87605

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-19	MET	-	EXPRESSION TAG	UNP O87605
K	-18	GLY	-	EXPRESSION TAG	UNP O87605
K	-17	SER	-	EXPRESSION TAG	UNP O87605
K	-16	SER	-	EXPRESSION TAG	UNP O87605
K	-15	HIS	-	EXPRESSION TAG	UNP O87605
K	-14	HIS	-	EXPRESSION TAG	UNP O87605
K	-13	HIS	-	EXPRESSION TAG	UNP O87605
K	-12	HIS	-	EXPRESSION TAG	UNP O87605
K	-11	HIS	-	EXPRESSION TAG	UNP O87605
K	-10	HIS	-	EXPRESSION TAG	UNP O87605
K	-9	SER	-	EXPRESSION TAG	UNP O87605
K	-8	SER	-	EXPRESSION TAG	UNP O87605
K	-7	GLY	-	EXPRESSION TAG	UNP O87605
K	-6	LEU	-	EXPRESSION TAG	UNP O87605
K	-5	VAL	-	EXPRESSION TAG	UNP O87605
K	-4	PRO	-	EXPRESSION TAG	UNP O87605
K	-3	ARG	-	EXPRESSION TAG	UNP O87605
K	-2	GLY	-	EXPRESSION TAG	UNP O87605
K	-1	SER	-	EXPRESSION TAG	UNP O87605
K	0	HIS	-	EXPRESSION TAG	UNP O87605
K	50	ASN	ASP	ENGINEERED MUTATION	UNP O87605
L	-19	MET	-	EXPRESSION TAG	UNP O87605
L	-18	GLY	-	EXPRESSION TAG	UNP O87605
L	-17	SER	-	EXPRESSION TAG	UNP O87605
L	-16	SER	-	EXPRESSION TAG	UNP O87605
L	-15	HIS	-	EXPRESSION TAG	UNP O87605
L	-14	HIS	-	EXPRESSION TAG	UNP O87605
L	-13	HIS	-	EXPRESSION TAG	UNP O87605
L	-12	HIS	-	EXPRESSION TAG	UNP O87605
L	-11	HIS	-	EXPRESSION TAG	UNP O87605
L	-10	HIS	-	EXPRESSION TAG	UNP O87605
L	-9	SER	-	EXPRESSION TAG	UNP O87605
L	-8	SER	-	EXPRESSION TAG	UNP O87605
L	-7	GLY	-	EXPRESSION TAG	UNP O87605
L	-6	LEU	-	EXPRESSION TAG	UNP O87605
L	-5	VAL	-	EXPRESSION TAG	UNP O87605
L	-4	PRO	-	EXPRESSION TAG	UNP O87605
L	-3	ARG	-	EXPRESSION TAG	UNP O87605
L	-2	GLY	-	EXPRESSION TAG	UNP O87605
L	-1	SER	-	EXPRESSION TAG	UNP O87605
L	0	HIS	-	EXPRESSION TAG	UNP O87605
L	50	ASN	ASP	ENGINEERED MUTATION	UNP O87605

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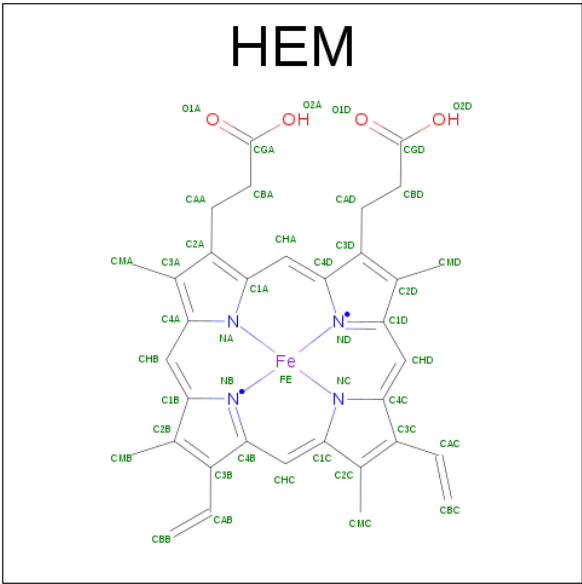
Chain	Residue	Modelled	Actual	Comment	Reference
M	-19	MET	-	EXPRESSION TAG	UNP O87605
M	-18	GLY	-	EXPRESSION TAG	UNP O87605
M	-17	SER	-	EXPRESSION TAG	UNP O87605
M	-16	SER	-	EXPRESSION TAG	UNP O87605
M	-15	HIS	-	EXPRESSION TAG	UNP O87605
M	-14	HIS	-	EXPRESSION TAG	UNP O87605
M	-13	HIS	-	EXPRESSION TAG	UNP O87605
M	-12	HIS	-	EXPRESSION TAG	UNP O87605
M	-11	HIS	-	EXPRESSION TAG	UNP O87605
M	-10	HIS	-	EXPRESSION TAG	UNP O87605
M	-9	SER	-	EXPRESSION TAG	UNP O87605
M	-8	SER	-	EXPRESSION TAG	UNP O87605
M	-7	GLY	-	EXPRESSION TAG	UNP O87605
M	-6	LEU	-	EXPRESSION TAG	UNP O87605
M	-5	VAL	-	EXPRESSION TAG	UNP O87605
M	-4	PRO	-	EXPRESSION TAG	UNP O87605
M	-3	ARG	-	EXPRESSION TAG	UNP O87605
M	-2	GLY	-	EXPRESSION TAG	UNP O87605
M	-1	SER	-	EXPRESSION TAG	UNP O87605
M	0	HIS	-	EXPRESSION TAG	UNP O87605
M	50	ASN	ASP	ENGINEERED MUTATION	UNP O87605
N	-19	MET	-	EXPRESSION TAG	UNP O87605
N	-18	GLY	-	EXPRESSION TAG	UNP O87605
N	-17	SER	-	EXPRESSION TAG	UNP O87605
N	-16	SER	-	EXPRESSION TAG	UNP O87605
N	-15	HIS	-	EXPRESSION TAG	UNP O87605
N	-14	HIS	-	EXPRESSION TAG	UNP O87605
N	-13	HIS	-	EXPRESSION TAG	UNP O87605
N	-12	HIS	-	EXPRESSION TAG	UNP O87605
N	-11	HIS	-	EXPRESSION TAG	UNP O87605
N	-10	HIS	-	EXPRESSION TAG	UNP O87605
N	-9	SER	-	EXPRESSION TAG	UNP O87605
N	-8	SER	-	EXPRESSION TAG	UNP O87605
N	-7	GLY	-	EXPRESSION TAG	UNP O87605
N	-6	LEU	-	EXPRESSION TAG	UNP O87605
N	-5	VAL	-	EXPRESSION TAG	UNP O87605
N	-4	PRO	-	EXPRESSION TAG	UNP O87605
N	-3	ARG	-	EXPRESSION TAG	UNP O87605
N	-2	GLY	-	EXPRESSION TAG	UNP O87605
N	-1	SER	-	EXPRESSION TAG	UNP O87605
N	0	HIS	-	EXPRESSION TAG	UNP O87605
N	50	ASN	ASP	ENGINEERED MUTATION	UNP O87605

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Chain	Residue	Modelled	Actual	Comment	Reference
O	-19	MET	-	EXPRESSION TAG	UNP O87605
O	-18	GLY	-	EXPRESSION TAG	UNP O87605
O	-17	SER	-	EXPRESSION TAG	UNP O87605
O	-16	SER	-	EXPRESSION TAG	UNP O87605
O	-15	HIS	-	EXPRESSION TAG	UNP O87605
O	-14	HIS	-	EXPRESSION TAG	UNP O87605
O	-13	HIS	-	EXPRESSION TAG	UNP O87605
O	-12	HIS	-	EXPRESSION TAG	UNP O87605
O	-11	HIS	-	EXPRESSION TAG	UNP O87605
O	-10	HIS	-	EXPRESSION TAG	UNP O87605
O	-9	SER	-	EXPRESSION TAG	UNP O87605
O	-8	SER	-	EXPRESSION TAG	UNP O87605
O	-7	GLY	-	EXPRESSION TAG	UNP O87605
O	-6	LEU	-	EXPRESSION TAG	UNP O87605
O	-5	VAL	-	EXPRESSION TAG	UNP O87605
O	-4	PRO	-	EXPRESSION TAG	UNP O87605
O	-3	ARG	-	EXPRESSION TAG	UNP O87605
O	-2	GLY	-	EXPRESSION TAG	UNP O87605
O	-1	SER	-	EXPRESSION TAG	UNP O87605
O	0	HIS	-	EXPRESSION TAG	UNP O87605
O	50	ASN	ASP	ENGINEERED MUTATION	UNP O87605
P	-19	MET	-	EXPRESSION TAG	UNP O87605
P	-18	GLY	-	EXPRESSION TAG	UNP O87605
P	-17	SER	-	EXPRESSION TAG	UNP O87605
P	-16	SER	-	EXPRESSION TAG	UNP O87605
P	-15	HIS	-	EXPRESSION TAG	UNP O87605
P	-14	HIS	-	EXPRESSION TAG	UNP O87605
P	-13	HIS	-	EXPRESSION TAG	UNP O87605
P	-12	HIS	-	EXPRESSION TAG	UNP O87605
P	-11	HIS	-	EXPRESSION TAG	UNP O87605
P	-10	HIS	-	EXPRESSION TAG	UNP O87605
P	-9	SER	-	EXPRESSION TAG	UNP O87605
P	-8	SER	-	EXPRESSION TAG	UNP O87605
P	-7	GLY	-	EXPRESSION TAG	UNP O87605
P	-6	LEU	-	EXPRESSION TAG	UNP O87605
P	-5	VAL	-	EXPRESSION TAG	UNP O87605
P	-4	PRO	-	EXPRESSION TAG	UNP O87605
P	-3	ARG	-	EXPRESSION TAG	UNP O87605
P	-2	GLY	-	EXPRESSION TAG	UNP O87605
P	-1	SER	-	EXPRESSION TAG	UNP O87605
P	0	HIS	-	EXPRESSION TAG	UNP O87605
P	50	ASN	ASP	ENGINEERED MUTATION	UNP O87605

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



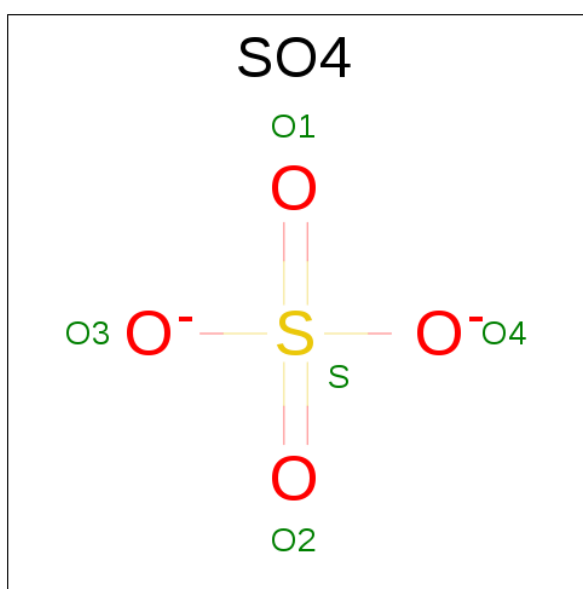
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	G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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	M	1	Total	C	Fe	N	O	
			43	34	1	4	4	
2	N	1	Total	C	Fe	N	O	
			43	34	1	4	4	
2	O	1	Total	C	Fe	N	O	
			43	34	1	4	4	
2	P	1	Total	C	Fe	N	O	
			43	34	1	4	4	

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



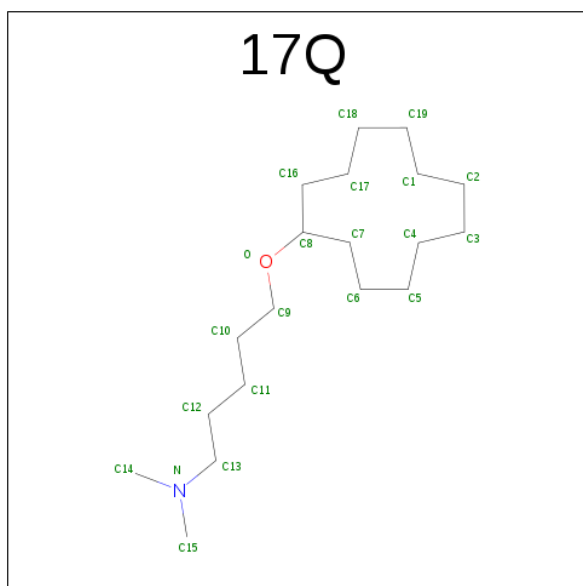
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	O S		
			5 4 1		0	0
3	B	1	Total	O S		
			5 4 1		0	0
3	B	1	Total	O S		
			5 4 1		0	0
3	D	1	Total	O S		
			5 4 1		0	0
3	F	1	Total	O S		
			5 4 1		0	0
3	H	1	Total	O S		
			5 4 1		0	0
3	H	1	Total	O S		
			5 4 1		0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	I	1	Total	O	S	0	0
			5	4	1		
3	I	1	Total	O	S	0	0
			5	4	1		
3	J	1	Total	O	S	0	0
			5	4	1		
3	O	1	Total	O	S	0	0
			5	4	1		
3	O	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is 1.7.6 5-CYCLODODECYLOXY-N,N-DIMETHYL-PENTAN-1-AMINE (three-letter code: 17Q) (formula: C₁₉H₃₉NO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	N	O	0	0
			21	19	1	1		
4	G	1	Total	C	N	O	0	0
			21	19	1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	35	Total	O	0	0
			35	35		
5	B	32	Total	O	0	0
			32	32		

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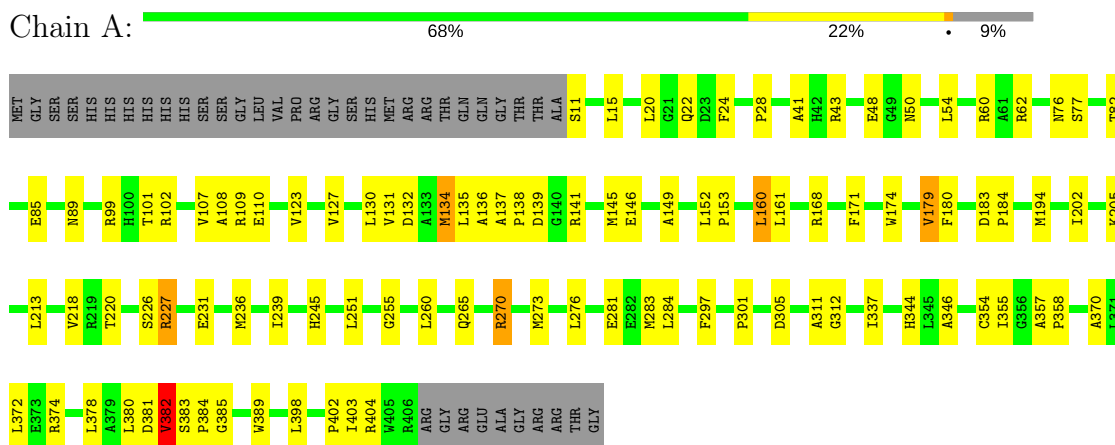
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	43	Total 43	O 43	0	0
5	D	46	Total 46	O 46	0	0
5	E	37	Total 37	O 37	0	0
5	F	39	Total 39	O 39	0	0
5	G	57	Total 57	O 57	0	0
5	H	35	Total 35	O 35	0	0
5	I	39	Total 39	O 39	0	0
5	J	34	Total 34	O 34	0	0
5	K	28	Total 28	O 28	0	0
5	L	21	Total 21	O 21	0	0
5	M	16	Total 16	O 16	0	0
5	N	15	Total 15	O 15	0	0
5	O	20	Total 20	O 20	0	0
5	P	17	Total 17	O 17	0	0

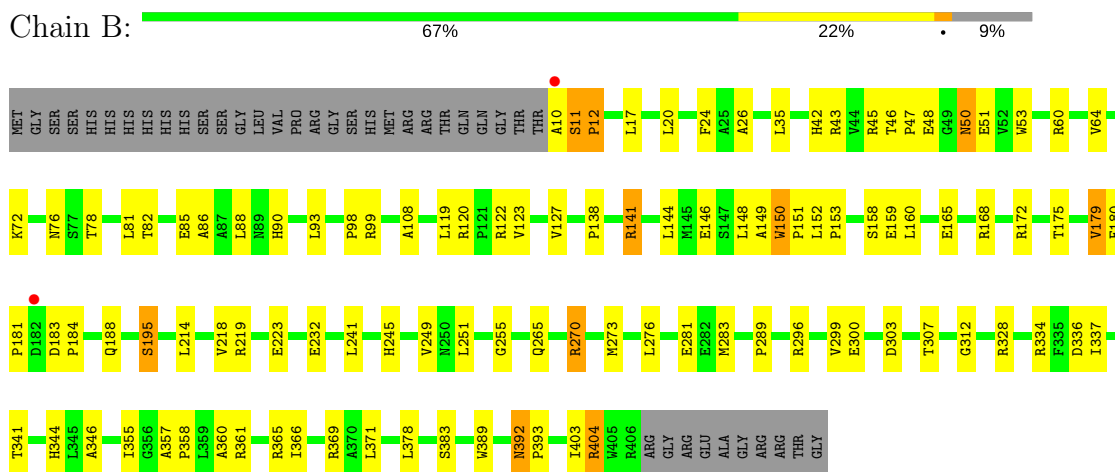
3 Residue-property plots

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

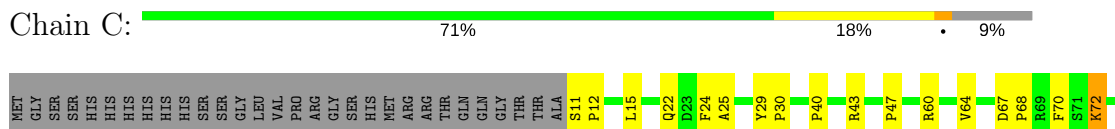
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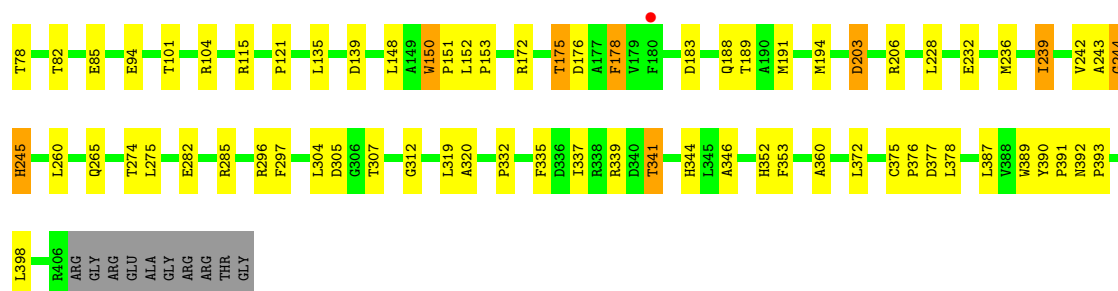


• Molecule 1: CYTOCHROME P450 HYDROXYLASE PIKC



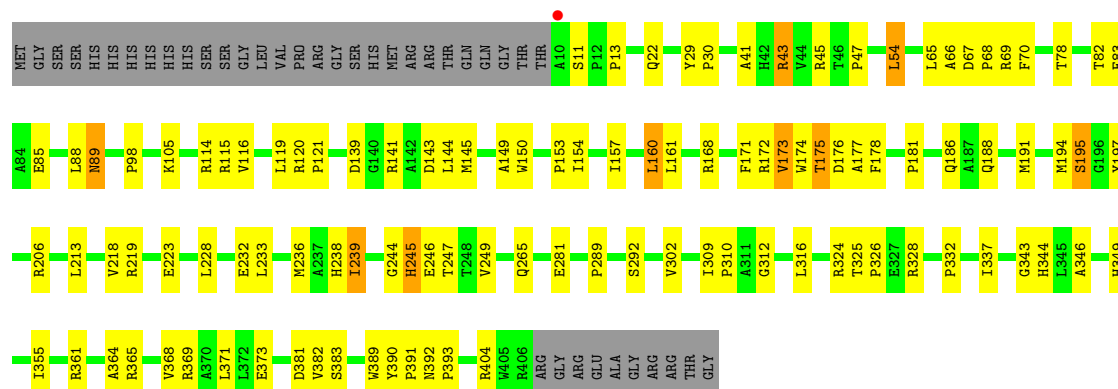
• Molecule 1: CYTOCHROME P450 HYDROXYLASE PIKC





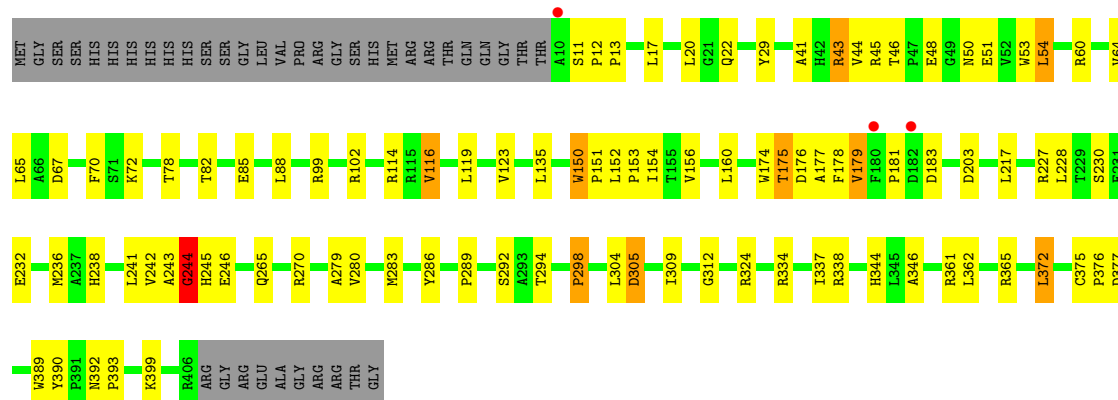
• Molecule 1: CYTOCHROME P450 HYDROXYLASE PIKC

Chain D: 66% 23% 9%



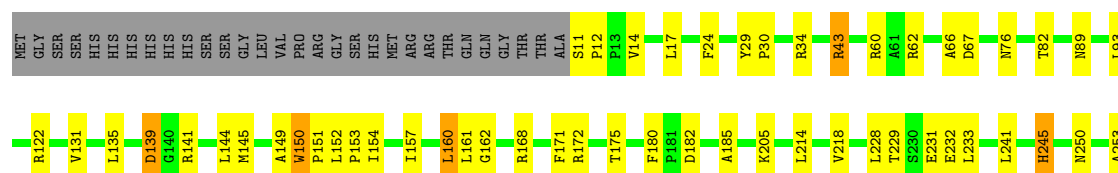
• Molecule 1: CYTOCHROME P450 HYDROXYLASE PIKC

Chain E: 69% 19% 9%



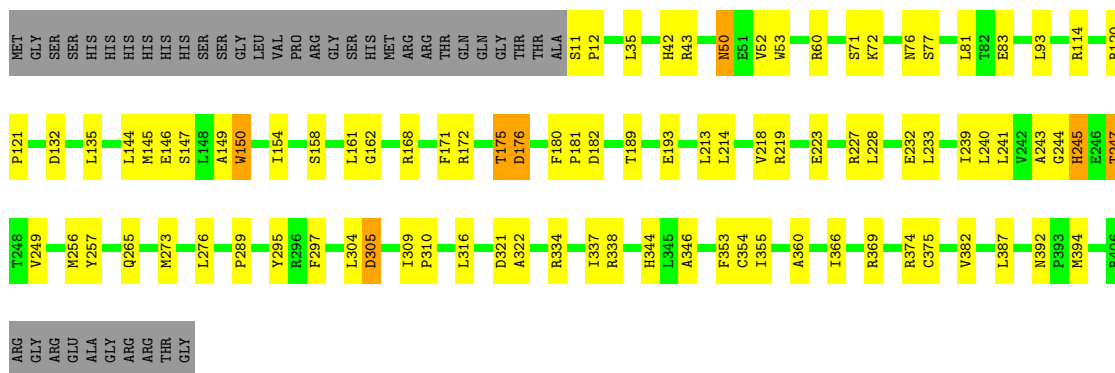
• Molecule 1: CYTOCHROME P450 HYDROXYLASE PIKC

Chain F: 71% 18% 9%



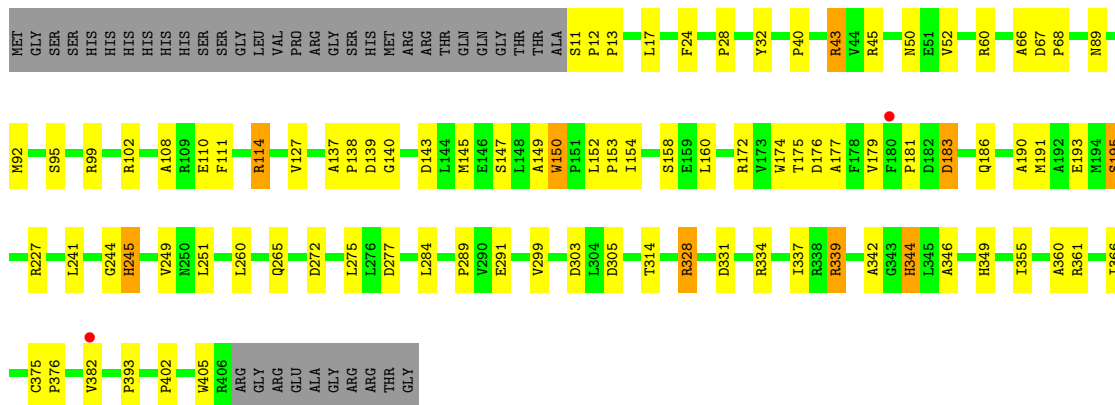
- Molecule 1: CYTOCHROME P450 HYDROXYLASE PIKC

Chain G: 70% 19% 9%



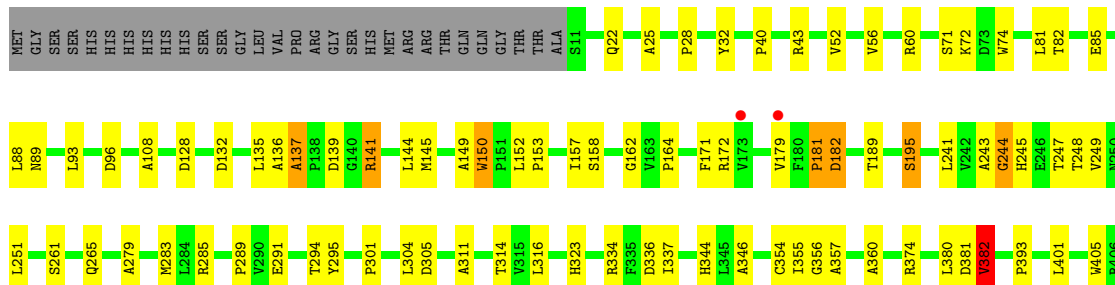
- Molecule 1: CYTOCHROME P450 HYDROXYLASE PIKC

Chain H:  70% 19% 9%



- Molecule 1: CYTOCHROME P450 HYDROXYLASE PIKC

Chain I:  71% 18% 9%



ARG
GLY
ARG
GLU
ALA
GLY
ARG
THR
GLY

• Molecule 1: CYTOCHROME P450 HYDROXYLASE PIKC

Chain J:  72% 18% 9%

MET GLY SER HIS HIS HIS HIS SER SER GLY VAL PRO ARG GLY SER HIS MET MET ARG ARG THR GLN GLN THR THR THR A10 S11 R34 A41 H42 H43 E48 L54 G57 R60 A61 T79 E85 N91 N92 L93 G244 H245 M113 R114 R115 L118

R122 I126 D139 M145 L148 A149 W150 P151 L152 P153 T155 E159 L160 L161 E165 P166 R172 T175 D183 P184 S195 G196 Y197 L201 I202 L214 V218 R219 E223 L233 H238 I239 L240 N241 V242 A243 L244 H245 M113 R114 R115 L118

Q265 L269 L276 E281 E282 M283 L284 P289 Y295 P298 D305 G312 L316 V317 D321 D331 R334 L337 R338 H344 L345 A346 H352 F353 A360 L371 C375 P376 D377 L378 D381 Y390 P391 R404 W405 R406 ARG GLY

ARG GLU ALA ARG ARG ARG THR GLY

• Molecule 1: CYTOCHROME P450 HYDROXYLASE PIKC

Chain K:  68% 22% 9%

MET GLY SER HIS HIS HIS HIS SER SER LEU VAL PRO ARG GLY SER HIS MET MET ARG ARG THR GLN GLN THR THR A10 S11 P12 Q22 P40 R43 V44 E48 W53 L54 R60 V64 L65 A66 D73 W74 P75 R75 E83 N89 S95

R99 H100 T101 R104 Q124 M134 L135 A136 A137 R141 M145 L148 A149 W150 P151 L152 P153 I154 T155 V156 I157 L160 L161 T175 D176 A177 F178 A187 A190 S204 Q208 L214 V218 D224 R227 L234 L241 G244 H245 E246

T247 T248 L260 P263 L266 A267 R270 M273 L276 G278 A279 V280 E281 M283 Y295 P301 L304 D305 P310 A311 G312 D313 T314 V315 L316 T325 P326 E327 R328 F329 R334 R339 H344 H349 L359 A360 E363 A364 R365 I366

R369 C375 P384 L387 V388 W389 Y390 P391 L398 I403 R404 W405 R406 ARG GLY ARG ARG GLU ALA GLY ARG ARG GLY

• Molecule 1: CYTOCHROME P450 HYDROXYLASE PIKC

Chain L:  69% 21% 9%

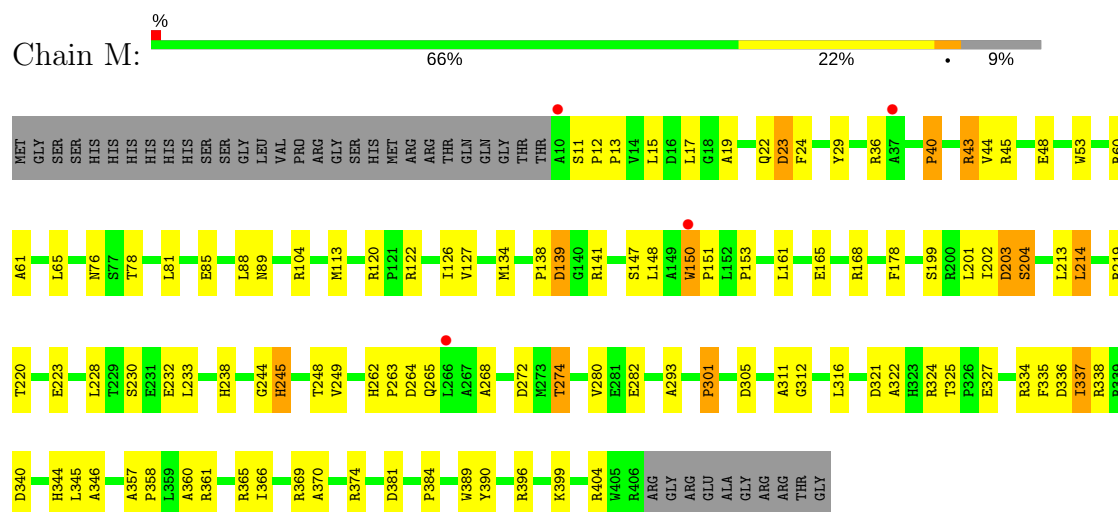
MET GLY SER HIS HIS HIS HIS SER SER LEU VAL PRO ARG GLY SER HIS MET MET ARG ARG THR GLN GLN THR THR A10 V14 A25 P28 Y29 Y32 P40 R43 N50 V56 G57 Y58 D59 R60 D67 P68 R69 Q208 L213 D224 T78 T79

N89 M92 L93 E94 S95 H100 R104 E110 F111 V116 D139 L144 S147 L148 W149 A149 P151 L152 P153 I154 P164 E165 P166 T175 T179 F180 P181 D182 D183 Q186 T189 S195 I202 D203 S204 R205 R206 G207 R208 L213 D224

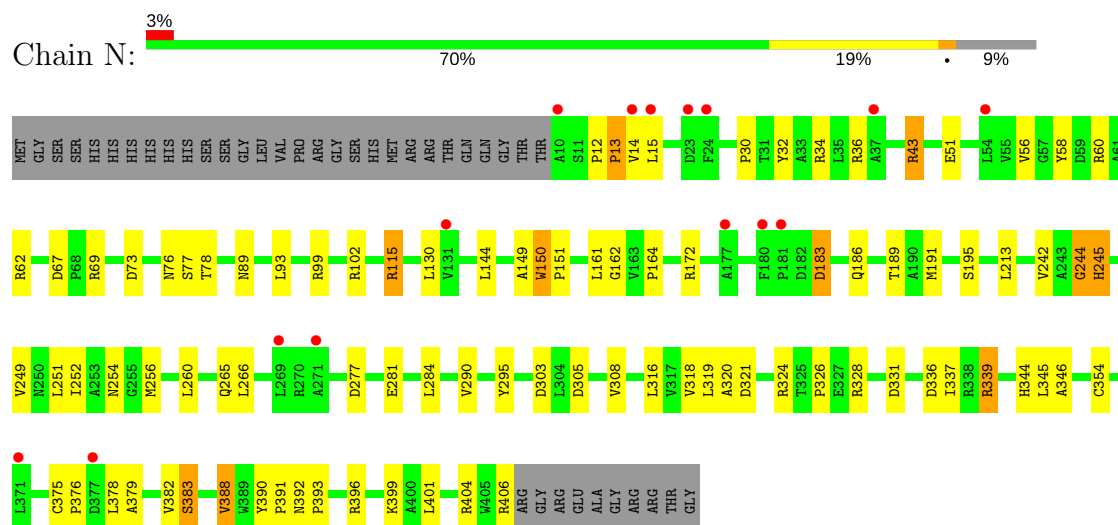
R227 L233 A243 G244 H245 P263 Q265 L266 L269 E281 E282 R285 Y286 E291 P298 V299 E300 F301 D303 L304 D305 G306 T307 V308 I309 P310 A311 A320 R324 R328 R339 D340 T341 A342 G343 H344 L345 A346 R361 L362 R369 A370 L371

C375 P376 D381 S383 P384 Y390 P391 N392 P393 R396 L401 L406 ARG GLY ARG ARG GLU ALA GLY ARG ARG THR GLY

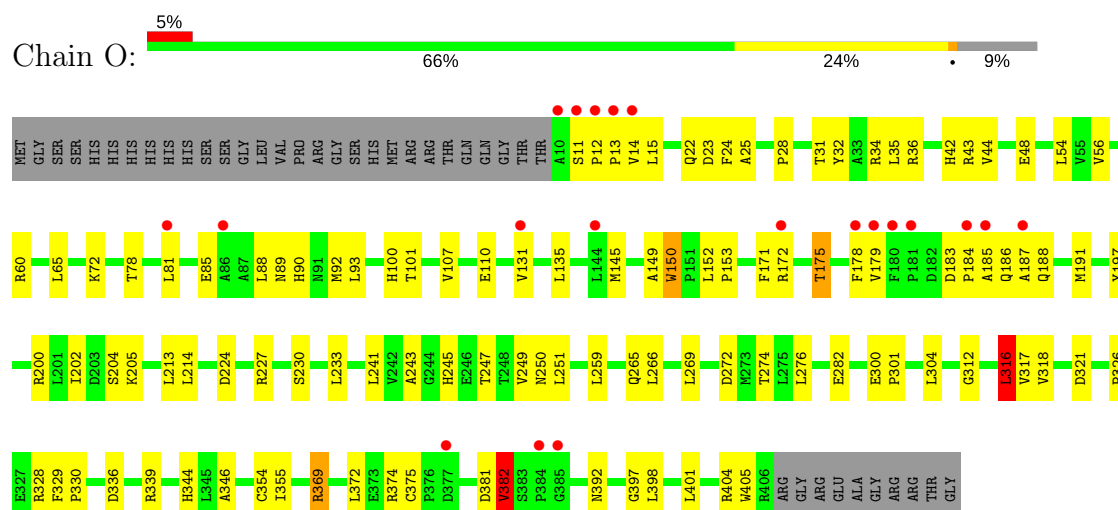
• Molecule 1: CYTOCHROME P450 HYDROXYLASE PIKC



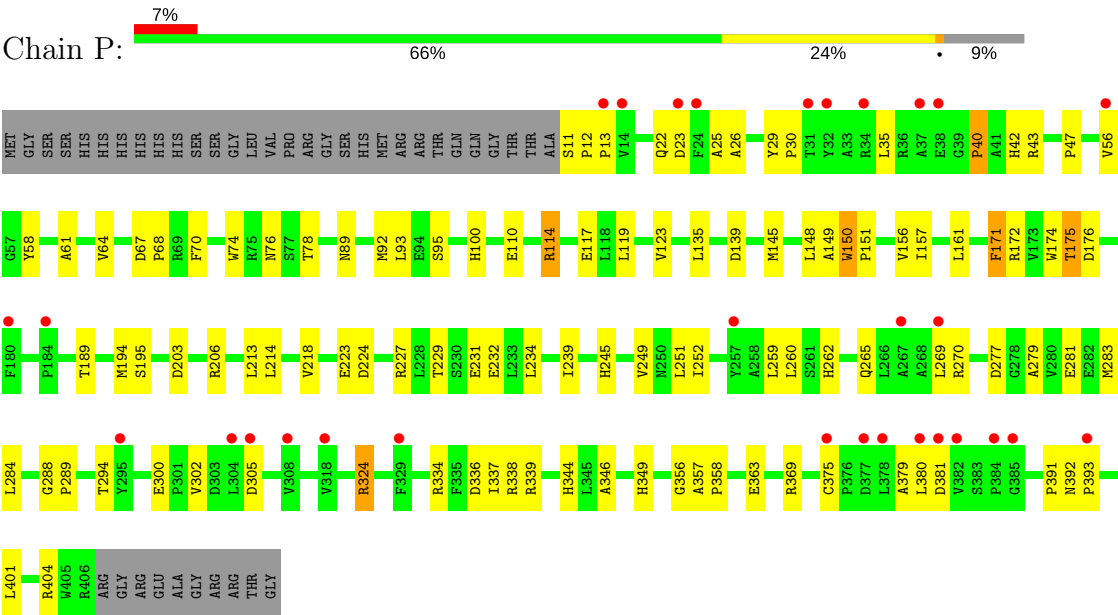
• Molecule 1: CYTOCHROME P450 HYDROXYLASE PIKC



• Molecule 1: CYTOCHROME P450 HYDROXYLASE PIKC



● Molecule 1: CYTOCHROME P450 HYDROXYLASE PIKC



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	110.27Å 130.11Å 134.90Å 66.48° 70.25° 72.23°	Depositor
Resolution (Å)	119.84 – 2.70 91.88 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.3 (119.84-2.70) 85.8 (91.88-2.70)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.196 , 0.279 0.199 , 0.277	Depositor DCC
R_{free} test set	8479 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	44.7	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.030 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	50342	wwPDB-VP
Average B, all atoms (Å ²)	46.0	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 23.21 % 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 4.8815e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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, SO4, 17Q

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	0.61	0/3100	0.75	0/4234
1	B	0.60	0/3142	0.72	0/4292
1	C	0.62	0/3136	0.75	1/4283 (0.0%)
1	D	0.63	0/3149	0.75	1/4301 (0.0%)
1	E	0.66	0/3141	0.77	1/4290 (0.0%)
1	F	0.59	0/3149	0.71	0/4303
1	G	0.61	0/3166	0.71	0/4324
1	H	0.62	0/3130	0.74	0/4275
1	I	0.57	0/3139	0.72	0/4288
1	J	0.58	0/3133	0.69	0/4280
1	K	0.55	0/3149	0.70	0/4301
1	L	0.54	0/3138	0.70	0/4287
1	M	0.54	0/3138	0.68	0/4286
1	N	0.48	0/3137	0.63	0/4285
1	O	0.51	0/3125	0.67	1/4269 (0.0%)
1	P	0.47	0/3131	0.64	0/4276
All	All	0.58	0/50203	0.71	4/68574 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1
1	I	0	1
All	All	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	15	LEU	CB-CG-CD2	-5.29	102.01	111.00
1	E	54	LEU	CA-CB-CG	5.09	127.00	115.30
1	D	65	LEU	CA-CB-CG	5.05	126.92	115.30
1	O	316	LEU	CA-CB-CG	5.00	126.80	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	244	GLY	Peptide
1	I	179	VAL	Peptide

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	3031	0	2990	67	0
1	B	3069	0	3026	93	0
1	C	3063	0	3024	71	0
1	D	3076	0	3027	78	0
1	E	3068	0	3022	63	0
1	F	3075	0	3019	70	0
1	G	3093	0	3049	78	0
1	H	3057	0	3020	57	0
1	I	3066	0	3020	65	0
1	J	3060	0	3016	61	0
1	K	3076	0	3032	60	0
1	L	3065	0	3014	61	0
1	M	3065	0	3014	68	0
1	N	3064	0	3025	63	0
1	O	3052	0	3008	70	0
1	P	3058	0	3006	60	0
2	A	43	0	30	1	0
2	B	43	0	30	6	0
2	C	43	0	30	6	0
2	D	43	0	30	8	0
2	E	43	0	30	5	0
2	F	43	0	30	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	43	0	30	6	0
2	H	43	0	30	7	0
2	I	43	0	30	5	0
2	J	43	0	30	4	0
2	K	43	0	30	3	0
2	L	43	0	30	4	0
2	M	43	0	30	5	0
2	N	43	0	30	7	0
2	O	43	0	30	4	0
2	P	43	0	30	5	0
3	A	5	0	0	2	0
3	B	10	0	0	0	0
3	D	5	0	0	0	0
3	F	5	0	0	1	0
3	H	10	0	0	1	0
3	I	10	0	0	0	0
3	J	5	0	0	0	0
3	O	10	0	0	1	0
4	C	21	0	39	6	0
4	G	21	0	39	5	0
5	A	35	0	0	0	0
5	B	32	0	0	0	0
5	C	43	0	0	3	0
5	D	46	0	0	3	0
5	E	37	0	0	1	0
5	F	39	0	0	2	0
5	G	57	0	0	2	0
5	H	35	0	0	4	0
5	I	39	0	0	0	0
5	J	34	0	0	1	0
5	K	28	0	0	1	0
5	L	21	0	0	0	0
5	M	16	0	0	0	0
5	N	15	0	0	0	0
5	O	20	0	0	0	0
5	P	17	0	0	1	0
All	All	50342	0	48870	1084	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 11.

The worst 5 of 1084 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:O:227:ARG:NH1	1:O:227:ARG:HB3	1.69	1.07
1:I:128:ASP:HA	1:I:374:ARG:HH12	1.21	1.06
1:G:171:PHE:O	1:G:175:THR:HG22	1.56	1.05
1:N:390:TYR:HE1	1:N:399:LYS:HG3	1.20	1.04
1:F:171:PHE:O	1:F:175:THR:HG22	1.59	1.02

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	394/436 (90%)	370 (94%)	20 (5%)	4 (1%)	18	43
1	B	397/436 (91%)	367 (92%)	29 (7%)	1 (0%)	44	73
1	C	395/436 (91%)	370 (94%)	23 (6%)	2 (0%)	32	60
1	D	397/436 (91%)	366 (92%)	28 (7%)	3 (1%)	22	49
1	E	396/436 (91%)	367 (93%)	26 (7%)	3 (1%)	22	49
1	F	398/436 (91%)	362 (91%)	30 (8%)	6 (2%)	12	30
1	G	398/436 (91%)	373 (94%)	22 (6%)	3 (1%)	22	49
1	H	395/436 (91%)	368 (93%)	26 (7%)	1 (0%)	44	73
1	I	396/436 (91%)	363 (92%)	29 (7%)	4 (1%)	18	43
1	J	396/436 (91%)	370 (93%)	24 (6%)	2 (0%)	32	60
1	K	397/436 (91%)	362 (91%)	30 (8%)	5 (1%)	14	35
1	L	397/436 (91%)	357 (90%)	33 (8%)	7 (2%)	10	25
1	M	396/436 (91%)	367 (93%)	22 (6%)	7 (2%)	10	25
1	N	396/436 (91%)	355 (90%)	37 (9%)	4 (1%)	18	43
1	O	395/436 (91%)	343 (87%)	47 (12%)	5 (1%)	14	35
1	P	395/436 (91%)	356 (90%)	35 (9%)	4 (1%)	18	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	6338/6976 (91%)	5816 (92%)	461 (7%)	61 (1%)	18	43

5 of 61 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	382	VAL
1	E	179	VAL
1	E	305	ASP
1	F	245[A]	HIS
1	F	245[B]	HIS

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	312/355 (88%)	293 (94%)	19 (6%)	22	47
1	B	316/355 (89%)	298 (94%)	18 (6%)	24	51
1	C	317/355 (89%)	300 (95%)	17 (5%)	26	54
1	D	318/355 (90%)	300 (94%)	18 (6%)	24	51
1	E	317/355 (89%)	304 (96%)	13 (4%)	35	66
1	F	317/355 (89%)	307 (97%)	10 (3%)	44	75
1	G	321/355 (90%)	307 (96%)	14 (4%)	33	63
1	H	315/355 (89%)	298 (95%)	17 (5%)	26	54
1	I	316/355 (89%)	302 (96%)	14 (4%)	33	63
1	J	315/355 (89%)	301 (96%)	14 (4%)	33	63
1	K	318/355 (90%)	302 (95%)	16 (5%)	28	57
1	L	314/355 (88%)	289 (92%)	25 (8%)	14	32
1	M	315/355 (89%)	295 (94%)	20 (6%)	21	46
1	N	316/355 (89%)	304 (96%)	12 (4%)	38	68
1	O	313/355 (88%)	295 (94%)	18 (6%)	23	50
1	P	315/355 (89%)	296 (94%)	19 (6%)	22	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	5055/5680 (89%)	4791 (95%)	264 (5%)	27 55

5 of 264 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	241	LEU
1	J	139	ASP
1	O	382	VAL
1	H	303	ASP
1	I	189	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 74 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	245	HIS
1	I	238	HIS
1	O	265	GLN
1	G	265	GLN
1	H	245	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](#)

30 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	1407	1	28,50,50	2.13	6 (21%)	17,82,82	1.62	4 (23%)
3	SO4	A	1408	-	4,4,4	0.33	0	6,6,6	0.50	0
2	HEM	B	1407	1	28,50,50	2.06	6 (21%)	17,82,82	2.06	5 (29%)
3	SO4	B	1408	-	4,4,4	0.34	0	6,6,6	0.31	0
3	SO4	B	1409	-	4,4,4	0.34	0	6,6,6	0.24	0
2	HEM	C	1407	1	28,50,50	2.28	6 (21%)	17,82,82	2.30	5 (29%)
4	17Q	C	1410	-	21,21,21	0.30	0	21,23,23	0.98	2 (9%)
2	HEM	D	1407	1	28,50,50	2.03	5 (17%)	17,82,82	1.64	3 (17%)
3	SO4	D	1408	-	4,4,4	0.75	0	6,6,6	0.78	0
2	HEM	E	1407	1	28,50,50	2.06	8 (28%)	17,82,82	2.19	5 (29%)
2	HEM	F	1407	1	28,50,50	2.23	9 (32%)	17,82,82	1.93	4 (23%)
3	SO4	F	1408	-	4,4,4	0.59	0	6,6,6	0.49	0
2	HEM	G	1407	1	28,50,50	2.22	8 (28%)	17,82,82	1.74	2 (11%)
4	17Q	G	1410	-	21,21,21	0.47	0	21,23,23	0.68	0
2	HEM	H	1407	1	28,50,50	2.17	7 (25%)	17,82,82	1.51	2 (11%)
3	SO4	H	1408	-	4,4,4	0.56	0	6,6,6	0.50	0
3	SO4	H	1409	-	4,4,4	0.37	0	6,6,6	0.30	0
2	HEM	I	1407	1	28,50,50	2.14	7 (25%)	17,82,82	2.11	4 (23%)
3	SO4	I	1408	-	4,4,4	0.76	0	6,6,6	0.74	0
3	SO4	I	1409	-	4,4,4	0.31	0	6,6,6	0.37	0
2	HEM	J	1407	1	28,50,50	2.17	6 (21%)	17,82,82	1.52	3 (17%)
3	SO4	J	1408	-	4,4,4	0.68	0	6,6,6	0.46	0
2	HEM	K	1407	1	28,50,50	2.18	6 (21%)	17,82,82	1.58	4 (23%)
2	HEM	L	1407	1	28,50,50	2.10	6 (21%)	17,82,82	1.77	4 (23%)
2	HEM	M	1407	1	28,50,50	2.27	8 (28%)	17,82,82	1.54	4 (23%)
2	HEM	N	1407	1	28,50,50	2.20	6 (21%)	17,82,82	1.40	2 (11%)
2	HEM	O	1407	1	28,50,50	2.19	8 (28%)	17,82,82	1.83	4 (23%)
3	SO4	O	1408	-	4,4,4	0.63	0	6,6,6	0.57	0
3	SO4	O	1409	-	4,4,4	0.55	0	6,6,6	0.85	0
2	HEM	P	1407	1	28,50,50	2.20	6 (21%)	17,82,82	1.54	3 (17%)

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	1407	1	-	0/6/54/54	0/0/8/8
3	SO4	A	1408	-	-	0/0/0/0	0/0/0/0
2	HEM	B	1407	1	-	0/6/54/54	0/0/8/8
3	SO4	B	1408	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1409	-	-	0/0/0/0	0/0/0/0
2	HEM	C	1407	1	-	0/6/54/54	0/0/8/8
4	17Q	C	1410	-	-	0/23/23/23	1/1/1/1
2	HEM	D	1407	1	-	0/6/54/54	0/0/8/8
3	SO4	D	1408	-	-	0/0/0/0	0/0/0/0
2	HEM	E	1407	1	-	0/6/54/54	0/0/8/8
2	HEM	F	1407	1	-	0/6/54/54	0/0/8/8
3	SO4	F	1408	-	-	0/0/0/0	0/0/0/0
2	HEM	G	1407	1	-	0/6/54/54	0/0/8/8
4	17Q	G	1410	-	-	0/23/23/23	1/1/1/1
2	HEM	H	1407	1	-	0/6/54/54	0/0/8/8
3	SO4	H	1408	-	-	0/0/0/0	0/0/0/0
3	SO4	H	1409	-	-	0/0/0/0	0/0/0/0
2	HEM	I	1407	1	-	0/6/54/54	0/0/8/8
3	SO4	I	1408	-	-	0/0/0/0	0/0/0/0
3	SO4	I	1409	-	-	0/0/0/0	0/0/0/0
2	HEM	J	1407	1	-	0/6/54/54	0/0/8/8
3	SO4	J	1408	-	-	0/0/0/0	0/0/0/0
2	HEM	K	1407	1	-	0/6/54/54	0/0/8/8
2	HEM	L	1407	1	-	0/6/54/54	0/0/8/8
2	HEM	M	1407	1	-	0/6/54/54	0/0/8/8
2	HEM	N	1407	1	-	0/6/54/54	0/0/8/8
2	HEM	O	1407	1	-	0/6/54/54	0/0/8/8
3	SO4	O	1408	-	-	0/0/0/0	0/0/0/0
3	SO4	O	1409	-	-	0/0/0/0	0/0/0/0
2	HEM	P	1407	1	-	0/6/54/54	0/0/8/8

The worst 5 of 108 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1407	HEM	C3C-C2C	-5.72	1.32	1.40
2	P	1407	HEM	C3B-C2B	-5.68	1.32	1.40
2	J	1407	HEM	C3B-C2B	-5.35	1.33	1.40
2	L	1407	HEM	C3C-C2C	-5.31	1.33	1.40
2	M	1407	HEM	C3C-C2C	-5.26	1.33	1.40

The worst 5 of 60 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1407	HEM	C1D-C2D-C3D	-5.57	103.12	107.00
2	E	1407	HEM	C1D-C2D-C3D	-4.97	103.54	107.00
2	F	1407	HEM	CBD-CAD-C3D	-4.77	103.36	112.47
2	I	1407	HEM	CBD-CAD-C3D	-4.71	103.48	112.47
2	I	1407	HEM	C1D-C2D-C3D	-4.68	103.74	107.00

There are no chirality outliers.

There are no torsion outliers.

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	1410	17Q	C1-C16-C17-C18-C19-C2-C3-C4-C5-C6-C7-C8
4	G	1410	17Q	C1-C16-C17-C18-C19-C2-C3-C4-C5-C6-C7-C8

22 monomers are involved in 94 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1407	HEM	1	0
3	A	1408	SO4	2	0
2	B	1407	HEM	6	0
2	C	1407	HEM	6	0
4	C	1410	17Q	6	0
2	D	1407	HEM	8	0
2	E	1407	HEM	5	0
2	F	1407	HEM	3	0
3	F	1408	SO4	1	0
2	G	1407	HEM	6	0
4	G	1410	17Q	5	0
2	H	1407	HEM	7	0
3	H	1409	SO4	1	0
2	I	1407	HEM	5	0
2	J	1407	HEM	4	0
2	K	1407	HEM	3	0
2	L	1407	HEM	4	0
2	M	1407	HEM	5	0
2	N	1407	HEM	7	0
2	O	1407	HEM	4	0
3	O	1409	SO4	1	0
2	P	1407	HEM	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, 95th 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	396/436 (90%)	-0.57	0 100 100	17, 33, 55, 71	0
1	B	397/436 (91%)	-0.48	2 (0%) 90 92	20, 35, 57, 76	0
1	C	396/436 (90%)	-0.54	1 (0%) 93 94	16, 33, 55, 73	0
1	D	397/436 (91%)	-0.49	1 (0%) 93 94	18, 32, 55, 81	0
1	E	397/436 (91%)	-0.48	3 (0%) 86 86	16, 33, 55, 73	0
1	F	396/436 (90%)	-0.48	0 100 100	16, 39, 66, 84	0
1	G	396/436 (90%)	-0.54	0 100 100	19, 35, 52, 61	0
1	H	396/436 (90%)	-0.46	2 (0%) 90 92	18, 35, 61, 87	0
1	I	396/436 (90%)	-0.46	2 (0%) 90 92	20, 39, 66, 79	0
1	J	397/436 (91%)	-0.43	2 (0%) 90 92	21, 42, 68, 91	0
1	K	397/436 (91%)	-0.33	1 (0%) 93 94	25, 46, 72, 90	0
1	L	397/436 (91%)	-0.27	2 (0%) 90 92	21, 50, 86, 99	0
1	M	397/436 (91%)	-0.17	4 (1%) 82 82	30, 53, 85, 91	0
1	N	397/436 (91%)	0.07	15 (3%) 41 39	34, 72, 116, 158	0
1	O	397/436 (91%)	0.04	20 (5%) 30 28	28, 57, 105, 133	0
1	P	396/436 (90%)	0.27	30 (7%) 15 12	29, 78, 129, 155	0
All	All	6345/6976 (90%)	-0.33	85 (1%) 77 78	16, 41, 91, 158	0

The worst 5 of 85 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	184	PRO	8.5
1	O	179	VAL	6.5
1	O	180	PHE	6.1
1	O	10	ALA	5.4
1	P	385	GLY	5.0

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, 95th 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
4	17Q	C	1410	21/21	0.87	0.28	7.51	53,57,60,60	0
4	17Q	G	1410	21/21	0.91	0.26	4.55	39,49,55,55	0
3	SO4	I	1408	5/5	0.95	0.24	4.25	39,41,42,43	0
3	SO4	H	1408	5/5	0.96	0.18	4.07	42,42,44,45	0
3	SO4	O	1409	5/5	0.96	0.18	3.96	39,39,40,40	0
3	SO4	D	1408	5/5	0.92	0.16	1.52	37,37,39,40	0
2	HEM	F	1407	43/43	0.98	0.14	0.26	17,22,24,26	0
2	HEM	I	1407	43/43	0.97	0.14	0.07	23,25,29,31	0
2	HEM	H	1407	43/43	0.98	0.14	0.05	15,19,21,22	0
2	HEM	P	1407	43/43	0.96	0.17	0.04	36,46,51,54	0
2	HEM	J	1407	43/43	0.98	0.15	-0.06	26,28,31,32	0
2	HEM	O	1407	43/43	0.97	0.14	-0.22	29,33,38,41	0
2	HEM	E	1407	43/43	0.97	0.13	-0.32	13,18,21,23	0
2	HEM	G	1407	43/43	0.97	0.13	-0.35	17,23,24,28	0
2	HEM	K	1407	43/43	0.98	0.13	-0.41	21,25,27,29	0
2	HEM	C	1407	43/43	0.98	0.12	-0.46	12,14,19,24	0
2	HEM	L	1407	43/43	0.97	0.13	-0.50	19,24,27,31	0
2	HEM	B	1407	43/43	0.98	0.12	-0.56	19,25,27,29	0
2	HEM	D	1407	43/43	0.98	0.12	-0.58	13,18,22,23	0
2	HEM	M	1407	43/43	0.98	0.12	-0.76	18,23,26,31	0
2	HEM	A	1407	43/43	0.98	0.12	-0.80	14,20,24,28	0
2	HEM	N	1407	43/43	0.98	0.13	-1.04	29,33,44,49	0
3	SO4	H	1409	5/5	0.96	0.13	-	38,39,40,40	0
3	SO4	B	1408	5/5	0.96	0.15	-	61,62,63,63	0
3	SO4	O	1408	5/5	0.97	0.18	-	41,41,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	SO4	A	1408	5/5	0.95	0.10	-	41,42,43,43	0
3	SO4	F	1408	5/5	0.96	0.15	-	38,39,40,41	0
3	SO4	I	1409	5/5	0.99	0.06	-	53,54,55,55	0
3	SO4	J	1408	5/5	0.95	0.21	-	41,42,42,43	0
3	SO4	B	1409	5/5	0.98	0.12	-	49,49,51,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.