



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 09:07 PM BST

PDB ID : 2I96
Title : Solution structure of the oxidized microsomal human cytochrome b5
Authors : Nunez-Quintana, M.; Truan, G.; Van Heijenoort, C.
Deposited on : 2006-09-05

This is a Full wwPDB NMR Structure Validation 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/NMRValidationReportHelp>
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:

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : rb-20027457
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

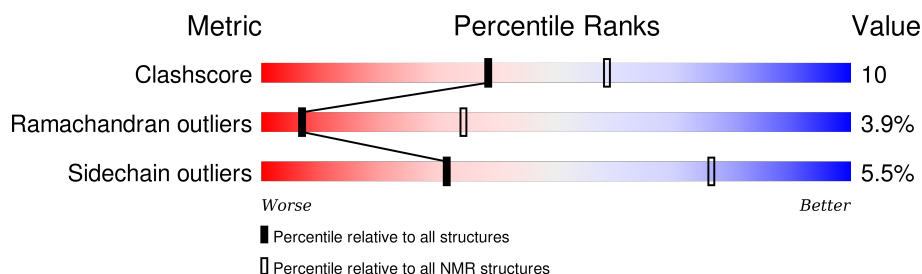
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 89%.

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)	NMR archive (#Entries)
Clashscore	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	108	<div> <div></div> <div>56%</div> <div>19%</div> <div>25%</div> </div>

2 Ensemble composition and analysis

This entry contains 20 models. Model 9 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:29-A:109 (81)	0.58	9

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 5 clusters and 7 single-model clusters were found.

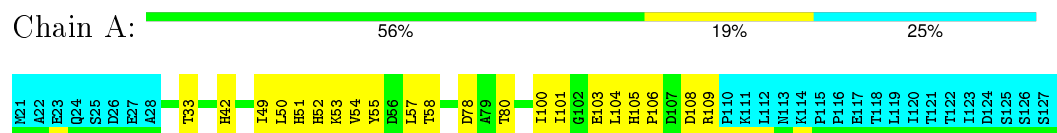
Cluster number	Models
1	1, 4, 9, 15, 16
2	5, 18
3	7, 13
4	2, 3
5	8, 14
Single-model clusters	6; 10; 11; 12; 17; 19; 20

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: Cytochrome b5

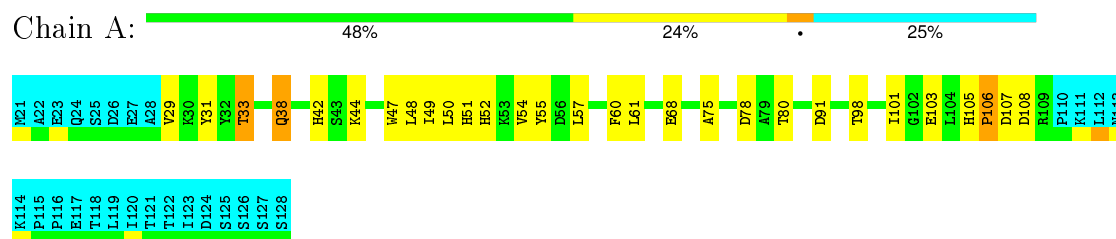


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

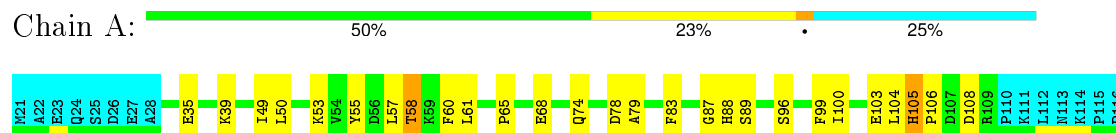
4.2.1 Score per residue for model 1

- Molecule 1: Cytochrome b5



4.2.2 Score per residue for model 2

- Molecule 1: Cytochrome b5



E117
T118
L119
I120
T121
T122
I123
D124
S125
S126
S127
S128

4.2.3 Score per residue for model 3

- Molecule 1: Cytochrome b5

Chain A: 

W21 A22 E23 Q24 S25 D26 E27 A28 Y31 Y32 T33 H42 I49 K53 V54 Y55 D78 A79 T80 E84 S96 S97 T98 F99 I100 E103 L104 H105 P106 D107 D108 R109 P110 K111 L112 M113 K114 P115 P116 E117 T118 L119 I120 T121 T122 I123 D124 S125 S126 S127 S128

4.2.4 Score per residue for model 4

- Molecule 1: Cytochrome b5

Chain A: 

W21 A22 E23 Q24 S25 D26 E27 A28 Y31 Y32 T33 E36 L48 I49 L50 H51 H52 K53 V54 Y55 D56 L57 T58 K59 E69 D78 S89 T90 D91 I100 E103 L104 H105 P106 D107 D108 R109 P110 K111 L112 M113 N113 K114 P115 P116 E117 T118 L119 I120 T121 T122 D124

S125
S126
S127
S128

4.2.5 Score per residue for model 5

- Molecule 1: Cytochrome b5

Chain A: 

W21 A22 E23 Q24 S25 D26 E27 A28 L34 I37 H42 W47 L48 I49 L50 H51 H52 K53 V54 Y55 D56 L57 T58 K59 D78 T98 F99 I100 I101 L104 H105 P106 D107 D108 R109 P110 K111 L112 M113 K114 P115 P116 E117 T118 L119 I120 T121 T122 I123 D124 S125 S126 S127

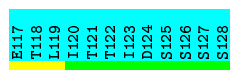
S128

4.2.6 Score per residue for model 6

- Molecule 1: Cytochrome b5

Chain A: 

W21 A22 E23 Q24 S25 D26 E27 A28 V29 T33 L34 E35 E36 I37 Q38 S45 L48 I49 L50 H51 H52 K53 V54 Y55 D56 L57 T58 K59 P65 D78 E84 D91 S96 F99 I100 I101 G102 E103 L104 H105 P106 D107 D108 R109 P110 K111 L112 M113 K114 P115 P116



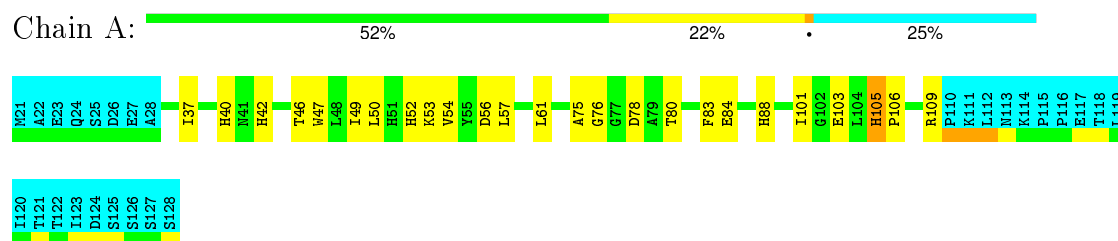
4.2.7 Score per residue for model 7

- Molecule 1: Cytochrome b5



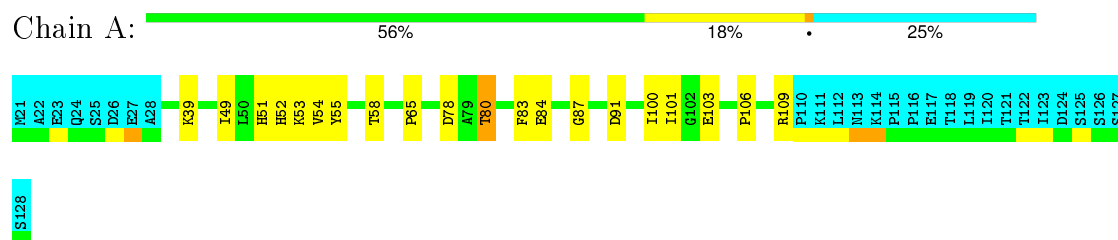
4.2.8 Score per residue for model 8

- Molecule 1: Cytochrome b5



4.2.9 Score per residue for model 9 (medoid)

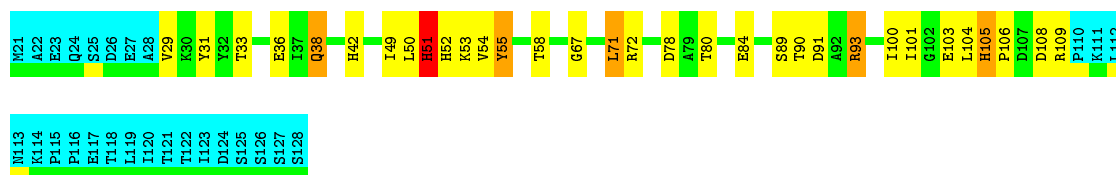
- Molecule 1: Cytochrome b5



4.2.10 Score per residue for model 10

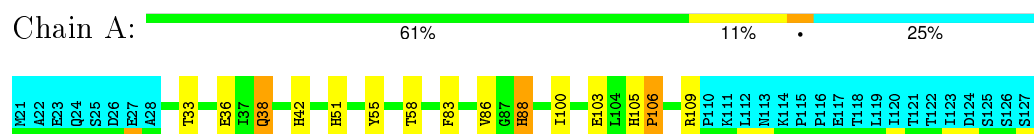
- Molecule 1: Cytochrome b5





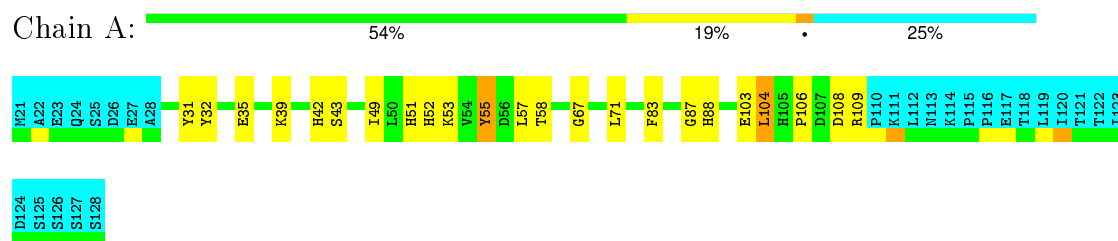
4.2.11 Score per residue for model 11

- Molecule 1: Cytochrome b5



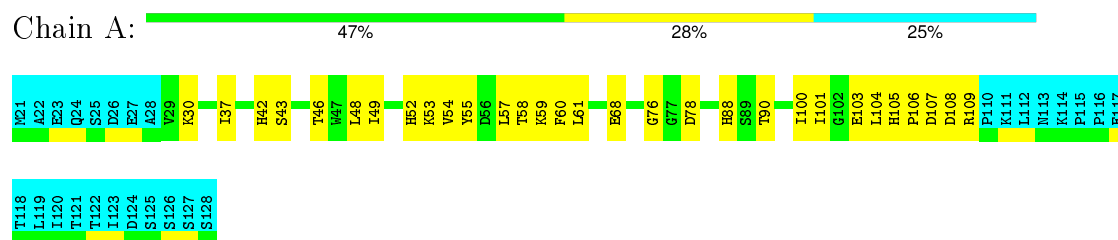
4.2.12 Score per residue for model 12

- Molecule 1: Cytochrome b5



4.2.13 Score per residue for model 13

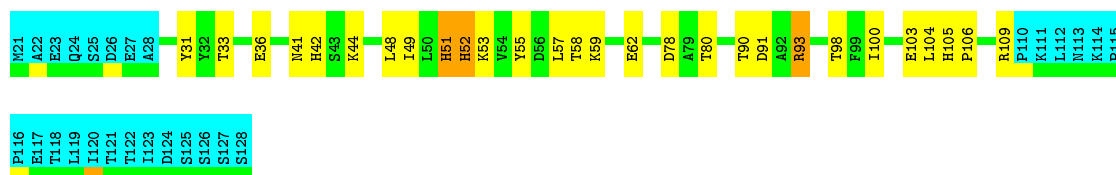
- Molecule 1: Cytochrome b5



4.2.14 Score per residue for model 14

- Molecule 1: Cytochrome b5

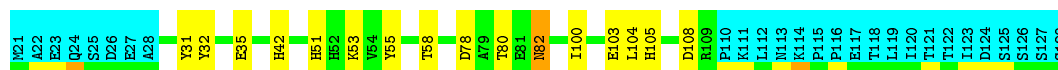




4.2.15 Score per residue for model 15

- Molecule 1: Cytochrome b5

Chain A: 60% 14% 25%



4.2.16 Score per residue for model 16

- Molecule 1: Cytochrome b5

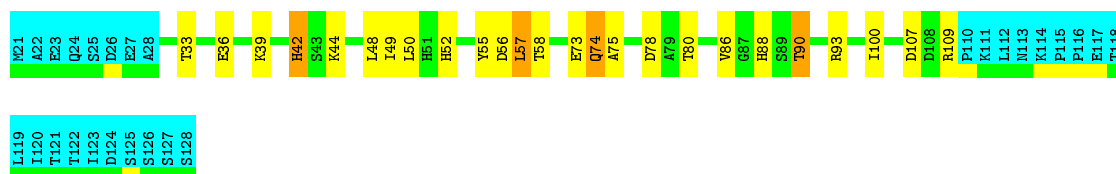
Chain A: 53% 21% 25%



4.2.17 Score per residue for model 17

- Molecule 1: Cytochrome b5

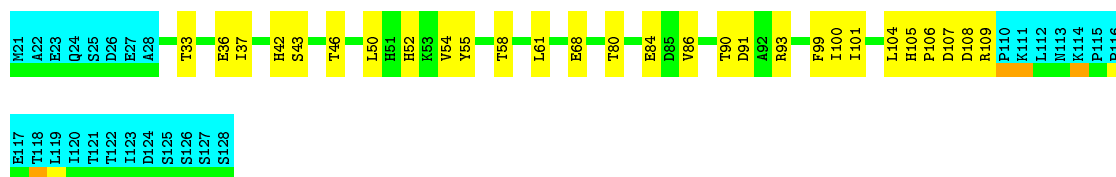
Chain A: 52% 19% 25%



4.2.18 Score per residue for model 18

- Molecule 1: Cytochrome b5

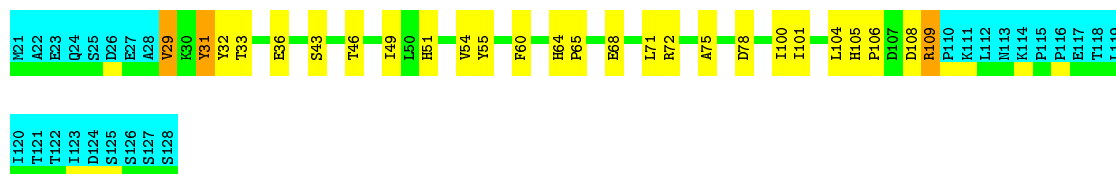
Chain A: 49% 26% 25%



4.2.19 Score per residue for model 19

- Molecule 1: Cytochrome b5

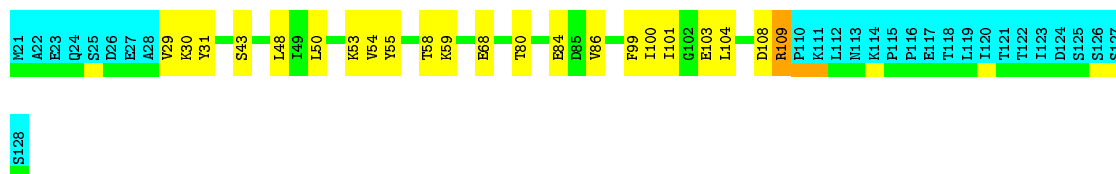
Chain A: 51% 21% 25%



4.2.20 Score per residue for model 20

- Molecule 1: Cytochrome b5

Chain A: 55% 19% 25%



5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
CNS	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	BMRB entry 6921
Number of chemical shift lists	1
Total number of shifts	1267
Number of shifts mapped to atoms	1267
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	89%

No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality

6.1 Standard geometry

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

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 (average) 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	0.38±0.06	0±0/681 (0.0±0.1%)	0.58±0.02	0±0/921 (0.0±0.0%)
All	All	0.39	3/13620 (0.0%)	0.58	0/18420 (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	Planarity
1	A	0.0±0.0	0.2±0.5
All	All	0	4

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	55	TYR	CE1-CZ	7.09	1.47	1.38	12	1
1	A	55	TYR	CE2-CZ	-5.41	1.31	1.38	12	1
1	A	31	TYR	CE2-CZ	-5.03	1.32	1.38	15	1

There are no bond-angle outliers.

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	55	TYR	Sidechain	2
1	A	32	TYR	Sidechain	1
1	A	31	TYR	Sidechain	1

6.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	664	628	623	13±4
2	A	43	30	30	1±1
All	All	14140	13160	13060	262

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 10.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:38:GLN:HE21	1:A:38:GLN:HA	0.77	1.39	6	1
1:A:49:ILE:HB	1:A:78:ASP:H	0.77	1.38	3	1
1:A:44:LYS:HE2	1:A:44:LYS:HA	0.75	1.57	14	1
1:A:53:LYS:HE2	1:A:100:ILE:HG21	0.75	1.58	10	1
1:A:53:LYS:HE3	1:A:100:ILE:HG21	0.74	1.59	5	2
1:A:38:GLN:HA	1:A:38:GLN:HE21	0.72	1.45	10	3
1:A:104:LEU:HB3	1:A:108:ASP:HB2	0.68	1.63	2	4
1:A:80:THR:HA	1:A:83:PHE:HB3	0.68	1.65	8	1
1:A:55:TYR:CE2	1:A:100:ILE:HG12	0.68	2.23	18	17
1:A:33:THR:O	1:A:36:GLU:HG2	0.68	1.89	6	7
1:A:29:VAL:HG12	1:A:31:TYR:CE1	0.67	2.24	19	1
1:A:48:LEU:HD22	1:A:57:LEU:HD21	0.64	1.70	14	4
1:A:50:LEU:O	1:A:80:THR:HB	0.62	1.95	1	5
1:A:53:LYS:HD3	1:A:103:GLU:CG	0.60	2.26	13	2
1:A:54:VAL:HG13	1:A:101:ILE:HG13	0.60	1.73	19	12
1:A:49:ILE:HD13	1:A:104:LEU:HD11	0.60	1.73	12	1
1:A:67:GLY:O	1:A:71:LEU:HG	0.59	1.97	12	1
1:A:104:LEU:HG	1:A:108:ASP:HB2	0.59	1.75	7	2
1:A:40:HIS:CE1	1:A:47:TRP:HB2	0.59	2.32	8	1
1:A:71:LEU:HD13	1:A:72:ARG:N	0.59	2.13	10	1
1:A:90:THR:O	1:A:93:ARG:HG2	0.59	1.98	17	3
1:A:105:HIS:CD2	1:A:106:PRO:HD2	0.58	2.32	4	7
1:A:96:SER:HA	1:A:99:PHE:HD2	0.58	1.58	6	3
1:A:57:LEU:O	1:A:59:LYS:N	0.58	2.37	5	5
1:A:57:LEU:O	1:A:61:LEU:HG	0.58	1.99	8	2
1:A:31:TYR:HB3	1:A:105:HIS:HA	0.57	1.76	3	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:53:LYS:HG2	1:A:103:GLU:HG2	0.57	1.75	20	5
1:A:105:HIS:CG	1:A:106:PRO:HD2	0.56	2.35	5	8
2:A:129:HEM:HBD1	2:A:129:HEM:HHA	0.56	1.75	5	1
1:A:83:PHE:HA	1:A:87:GLY:HA2	0.55	1.77	16	1
1:A:49:ILE:HB	1:A:78:ASP:HA	0.55	1.79	8	7
1:A:31:TYR:CD1	1:A:103:GLU:HB2	0.55	2.36	12	1
1:A:52:HIS:CE1	1:A:109:ARG:HA	0.55	2.36	17	1
1:A:83:PHE:HD1	1:A:88:HIS:HD1	0.54	1.44	12	2
1:A:49:ILE:O	1:A:78:ASP:HA	0.54	2.02	4	6
1:A:80:THR:O	1:A:84:GLU:HG2	0.54	2.03	8	6
1:A:37:ILE:HD13	1:A:47:TRP:CE3	0.54	2.38	5	2
1:A:74:GLN:HB3	1:A:79:ALA:HB1	0.54	1.79	2	1
1:A:53:LYS:HD3	1:A:103:GLU:HG3	0.53	1.81	13	3
1:A:48:LEU:CD2	1:A:55:TYR:HB2	0.53	2.34	17	6
1:A:50:LEU:HB2	1:A:55:TYR:CE1	0.53	2.39	17	6
1:A:105:HIS:HB3	1:A:108:ASP:OD1	0.52	2.04	5	1
1:A:48:LEU:HG	1:A:50:LEU:CD2	0.52	2.34	6	2
1:A:42:HIS:CE1	1:A:44:LYS:HB3	0.52	2.39	17	1
1:A:49:ILE:C	1:A:50:LEU:HD22	0.52	2.25	6	1
1:A:89:SER:HB3	1:A:91:ASP:OD2	0.52	2.05	10	1
1:A:104:LEU:HB3	1:A:109:ARG:HA	0.52	1.80	7	1
1:A:33:THR:OG1	1:A:36:GLU:HG3	0.52	2.04	16	1
1:A:53:LYS:HD3	1:A:103:GLU:HG2	0.52	1.81	9	2
1:A:55:TYR:CZ	1:A:100:ILE:HG12	0.51	2.40	15	2
1:A:33:THR:HB	1:A:35:GLU:CD	0.51	2.26	6	1
1:A:69:GLU:O	1:A:72:ARG:HG2	0.51	2.06	16	1
1:A:80:THR:HA	1:A:83:PHE:CB	0.50	2.35	8	1
1:A:89:SER:OG	2:A:129:HEM:HAA2	0.50	2.07	2	1
1:A:33:THR:HA	1:A:105:HIS:HB2	0.50	1.82	3	2
1:A:37:ILE:HD12	1:A:104:LEU:HD11	0.50	1.84	18	1
1:A:48:LEU:HD13	2:A:129:HEM:HMC1	0.50	1.82	13	1
1:A:57:LEU:HD21	2:A:129:HEM:HAB	0.49	1.81	17	2
1:A:57:LEU:HA	1:A:60:PHE:CD2	0.49	2.41	1	1
1:A:50:LEU:HD23	1:A:55:TYR:CD1	0.49	2.42	6	1
1:A:29:VAL:HB	1:A:31:TYR:CE1	0.49	2.42	20	1
1:A:104:LEU:HG	1:A:108:ASP:CB	0.49	2.38	3	2
1:A:54:VAL:HG13	1:A:101:ILE:CG1	0.49	2.37	19	1
1:A:74:GLN:HG3	2:A:129:HEM:CBC	0.49	2.38	16	1
1:A:104:LEU:O	1:A:109:ARG:HB2	0.49	2.07	16	1
1:A:69:GLU:H	1:A:69:GLU:CD	0.49	2.11	4	1
1:A:48:LEU:HG	1:A:50:LEU:HD21	0.48	1.83	6	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:57:LEU:HA	1:A:60:PHE:HD2	0.48	1.68	1	1
1:A:55:TYR:CG	2:A:129:HEM:HBB1	0.48	2.43	3	1
1:A:89:SER:HB3	2:A:129:HEM:O2A	0.48	2.09	7	1
1:A:49:ILE:HB	1:A:78:ASP:N	0.48	2.17	3	1
1:A:105:HIS:HB3	1:A:107:ASP:OD1	0.48	2.09	4	1
1:A:57:LEU:HD12	1:A:60:PHE:HD2	0.48	1.69	2	1
1:A:51:HIS:O	1:A:52:HIS:HB2	0.48	2.09	10	4
1:A:104:LEU:HB2	1:A:109:ARG:HA	0.47	1.85	6	1
1:A:46:THR:HG23	1:A:75:ALA:HB2	0.47	1.87	8	1
1:A:46:THR:HG21	1:A:61:LEU:HD21	0.47	1.87	13	1
1:A:103:GLU:OE1	1:A:109:ARG:HD2	0.47	2.10	11	1
1:A:34:LEU:HB2	1:A:108:ASP:OD2	0.47	2.10	5	1
1:A:37:ILE:HG22	1:A:37:ILE:O	0.47	2.09	8	1
1:A:65:PRO:HB2	2:A:129:HEM:HBD2	0.46	1.87	9	1
1:A:57:LEU:HD11	2:A:129:HEM:HAB	0.46	1.87	16	3
1:A:52:HIS:O	1:A:104:LEU:HG	0.46	2.11	14	1
1:A:58:THR:O	1:A:61:LEU:HG	0.46	2.10	2	1
1:A:37:ILE:HD12	1:A:54:VAL:HG21	0.46	1.87	16	1
1:A:31:TYR:HD1	1:A:103:GLU:HB2	0.46	1.71	12	1
1:A:90:THR:HG23	1:A:93:ARG:HD3	0.46	1.86	7	1
1:A:105:HIS:HB2	1:A:106:PRO:HD2	0.46	1.86	6	1
1:A:29:VAL:HG13	1:A:31:TYR:CE1	0.46	2.46	10	1
1:A:91:ASP:HB3	2:A:129:HEM:O2A	0.45	2.11	4	1
1:A:78:ASP:OD1	1:A:80:THR:HG22	0.45	2.12	14	1
1:A:83:PHE:O	1:A:87:GLY:HA2	0.45	2.12	2	2
1:A:35:GLU:O	1:A:39:LYS:HG3	0.45	2.12	12	1
1:A:30:LYS:N	1:A:30:LYS:HD2	0.45	2.27	13	1
1:A:32:TYR:O	1:A:104:LEU:HA	0.45	2.12	19	2
1:A:105:HIS:C	1:A:107:ASP:H	0.44	2.16	1	1
1:A:38:GLN:NE2	1:A:38:GLN:HA	0.44	2.18	6	1
1:A:38:GLN:CA	1:A:38:GLN:HE21	0.44	2.19	6	1
1:A:48:LEU:HD21	1:A:55:TYR:HB2	0.44	1.88	17	1
1:A:73:GLU:O	1:A:74:GLN:HB2	0.44	2.12	17	1
1:A:35:GLU:O	1:A:39:LYS:HB2	0.44	2.13	2	1
1:A:104:LEU:HB3	1:A:108:ASP:HB3	0.44	1.88	18	1
1:A:65:PRO:HG2	2:A:129:HEM:HAA2	0.44	1.90	7	1
1:A:47:TRP:O	1:A:75:ALA:HB1	0.44	2.13	1	1
1:A:57:LEU:HB2	1:A:73:GLU:OE1	0.44	2.12	17	1
1:A:55:TYR:HA	1:A:99:PHE:O	0.44	2.12	20	2
1:A:105:HIS:HB3	1:A:107:ASP:OD2	0.43	2.13	1	2
1:A:58:THR:O	1:A:59:LYS:HB2	0.43	2.13	20	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:29:VAL:HG21	1:A:103:GLU:HG3	0.43	1.89	1	1
1:A:50:LEU:O	1:A:51:HIS:HB2	0.43	2.13	7	2
2:A:129:HEM:HBD1	2:A:129:HEM:HMD2	0.43	1.90	15	1
1:A:71:LEU:C	1:A:71:LEU:HD22	0.43	2.34	10	1
1:A:46:THR:HB	1:A:61:LEU:HD21	0.43	1.90	18	1
1:A:68:GLU:O	1:A:71:LEU:HB2	0.43	2.14	19	1
1:A:78:ASP:HB3	1:A:80:THR:HG22	0.43	1.91	15	1
1:A:82:ASN:N	1:A:82:ASN:HD22	0.43	2.12	15	1
1:A:52:HIS:NE2	1:A:109:ARG:HA	0.42	2.29	17	1
1:A:37:ILE:HD13	1:A:47:TRP:CZ3	0.42	2.49	5	1
1:A:64:HIS:CE1	1:A:71:LEU:HD21	0.42	2.50	7	1
1:A:57:LEU:HB3	1:A:60:PHE:HB3	0.42	1.91	13	1
1:A:104:LEU:CB	1:A:108:ASP:HB2	0.42	2.44	10	1
1:A:73:GLU:HB3	1:A:75:ALA:HB2	0.42	1.91	17	1
1:A:73:GLU:O	1:A:73:GLU:HG2	0.41	2.14	17	1
1:A:37:ILE:O	1:A:76:GLY:HA2	0.41	2.14	13	1
1:A:57:LEU:HD12	1:A:60:PHE:CD2	0.41	2.50	2	1
1:A:55:TYR:CD2	2:A:129:HEM:HBB1	0.41	2.50	17	1
1:A:53:LYS:HA	1:A:103:GLU:HG2	0.41	1.92	10	1
1:A:29:VAL:HB	1:A:31:TYR:CZ	0.41	2.51	20	1
1:A:53:LYS:HG2	1:A:103:GLU:CG	0.41	2.45	8	1
1:A:46:THR:HG23	1:A:75:ALA:CB	0.41	2.45	8	1
1:A:57:LEU:HD22	1:A:60:PHE:CD2	0.41	2.51	13	1
1:A:31:TYR:CG	1:A:106:PRO:HD3	0.41	2.50	14	1
1:A:50:LEU:HB2	1:A:55:TYR:HE1	0.40	1.76	18	1
1:A:31:TYR:CB	1:A:105:HIS:HA	0.40	2.46	4	1
1:A:48:LEU:HD23	1:A:48:LEU:N	0.40	2.31	20	1
1:A:29:VAL:HG11	1:A:103:GLU:HG3	0.40	1.93	6	1
1:A:60:PHE:CE2	1:A:64:HIS:HB2	0.40	2.51	19	1
1:A:57:LEU:O	1:A:60:PHE:N	0.40	2.54	16	1
1:A:90:THR:O	1:A:93:ARG:HB3	0.40	2.16	10	1
1:A:72:ARG:HA	1:A:75:ALA:HB3	0.40	1.94	19	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. 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	81/108 (75%)	67±3 (83±4%)	11±3 (13±3%)	3±1 (4±2%)	7	34
All	All	1620/2160 (75%)	1344 (83%)	213 (13%)	63 (4%)	7	34

All 19 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	58	THR	14
1	A	106	PRO	10
1	A	51	HIS	7
1	A	68	GLU	6
1	A	43	SER	4
1	A	52	HIS	3
1	A	86	VAL	3
1	A	65	PRO	3
1	A	88	HIS	2
1	A	91	ASP	2
1	A	87	GLY	1
1	A	107	ASP	1
1	A	76	GLY	1
1	A	109	ARG	1
1	A	45	SER	1
1	A	93	ARG	1
1	A	105	HIS	1
1	A	46	THR	1
1	A	67	GLY	1

6.3.2 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 PDB entries followed by that with respect to all NMR entries. 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	72/97 (74%)	68±2 (95±3%)	4±2 (5±3%)	31	76
All	All	1440/1940 (74%)	1361 (95%)	79 (5%)	31	76

All 39 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	42	HIS	13
1	A	105	HIS	7
1	A	98	THR	5
1	A	109	ARG	4
1	A	38	GLN	4
1	A	88	HIS	3
1	A	91	ASP	3
1	A	51	HIS	3
1	A	56	ASP	2
1	A	104	LEU	2
1	A	57	LEU	2
1	A	90	THR	2
1	A	33	THR	2
1	A	39	LYS	2
1	A	43	SER	1
1	A	30	LYS	1
1	A	108	ASP	1
1	A	71	LEU	1
1	A	80	THR	1
1	A	35	GLU	1
1	A	55	TYR	1
1	A	44	LYS	1
1	A	48	LEU	1
1	A	41	ASN	1
1	A	86	VAL	1
1	A	53	LYS	1
1	A	78	ASP	1
1	A	84	GLU	1
1	A	74	GLN	1
1	A	82	ASN	1
1	A	52	HIS	1
1	A	89	SER	1
1	A	69	GLU	1
1	A	62	GLU	1
1	A	29	VAL	1
1	A	36	GLU	1
1	A	107	ASP	1
1	A	93	ARG	1
1	A	81	GLU	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds 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 is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	HEM	A	129	1	24,50,50	0.95±0.03	0±0 (0±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of 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 angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	HEM	A	129	1	16,82,82	2.74±0.07	2±0 (12±0%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	129	1	-	0±0,6,54,54	0±0,0,8,8

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	A	129	HEM	CBD-CAD-C3D	7.64	125.88	112.47	10	20
2	A	129	HEM	CBA-CAA-C2A	7.24	125.22	112.49	2	20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 89% for the well-defined parts and 87% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 6921

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1267
Number of shifts mapped to atoms	1267
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	30

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	103	-0.72 ± 0.26	Should be applied
$^{13}\text{C}_\beta$	97	-0.08 ± 0.13	None needed (< 0.5 ppm)
$^{13}\text{C}'$	99	-0.36 ± 0.14	None needed (< 0.5 ppm)
^{15}N	96	0.89 ± 0.30	Should be applied

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 89%, i.e. 904 atoms were assigned a chemical shift out of a possible 1018. 11 out of 11 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	395/401 (99%)	158/160 (99%)	160/162 (99%)	77/79 (97%)
Sidechain	434/500 (87%)	268/292 (92%)	162/189 (86%)	4/19 (21%)

Continued on next page...

Continued from previous page...

	Total	¹H	¹³C	¹⁵N
Aromatic	75/117 (64%)	39/61 (64%)	35/43 (81%)	1/13 (8%)
Overall	904/1018 (89%)	465/513 (91%)	357/394 (91%)	82/111 (74%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 87%, i.e. 1143 atoms were assigned a chemical shift out of a possible 1321. 13 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	495/530 (93%)	197/211 (93%)	202/216 (94%)	96/103 (93%)
Sidechain	573/674 (85%)	355/395 (90%)	212/256 (83%)	6/23 (26%)
Aromatic	75/117 (64%)	39/61 (64%)	35/43 (81%)	1/13 (8%)
Overall	1143/1321 (87%)	591/667 (89%)	449/515 (87%)	103/139 (74%)

7.1.4 Statistically unusual chemical shifts ⓘ

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	65	PRO	HB3	-3.19	3.81 – 0.21	-14.5
1	A	71	LEU	HD21	-2.44	2.14 – -0.66	-11.3
1	A	71	LEU	HD22	-2.44	2.14 – -0.66	-11.3
1	A	71	LEU	HD23	-2.44	2.14 – -0.66	-11.3
1	A	50	LEU	HG	-1.95	3.16 – -0.14	-10.5
1	A	71	LEU	HD13	3.38	2.16 – -0.64	9.3
1	A	71	LEU	HD12	3.38	2.16 – -0.64	9.3
1	A	71	LEU	HD11	3.38	2.16 – -0.64	9.3
1	A	65	PRO	HD3	0.69	5.52 – 1.72	-7.7
1	A	86	VAL	HB	4.32	3.59 – 0.39	7.3
1	A	65	PRO	HG3	-0.32	3.56 – 0.26	-6.7
1	A	101	ILE	HD11	-1.17	2.13 – -0.77	-6.4
1	A	101	ILE	HD12	-1.17	2.13 – -0.77	-6.4
1	A	101	ILE	HD13	-1.17	2.13 – -0.77	-6.4
1	A	86	VAL	HG12	2.48	2.13 – -0.47	6.4
1	A	86	VAL	HG11	2.48	2.13 – -0.47	6.4
1	A	86	VAL	HG13	2.48	2.13 – -0.47	6.4
1	A	57	LEU	HG	-0.48	3.16 – -0.14	-6.0
1	A	48	LEU	HG	-0.46	3.16 – -0.14	-6.0
1	A	89	SER	H	11.68	11.23 – 5.33	5.8
1	A	66	GLY	HA2	6.15	5.87 – 2.07	5.7
1	A	23	GLU	CG	29.35	42.24 – 29.94	-5.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	93	ARG	HG2	3.05	2.92 – 0.22	5.5
1	A	67	GLY	HA3	5.98	5.80 – 2.00	5.5
1	A	106	PRO	HD3	1.55	5.52 – 1.72	-5.4
1	A	50	LEU	HD22	-0.78	2.14 – -0.66	-5.4
1	A	50	LEU	HD21	-0.78	2.14 – -0.66	-5.4
1	A	50	LEU	HD23	-0.78	2.14 – -0.66	-5.4
1	A	83	PHE	HB3	0.99	4.85 – 1.05	-5.2
1	A	88	HIS	CB	19.61	40.69 – 19.69	-5.0

7.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:

