



Full wwPDB NMR Structure Validation Report ⓘ

Apr 27, 2016 – 02:40 AM BST

PDB ID : 2M56
Title : The structure of the complex of cytochrome P450cam and its electron donor
putidaredoxin determined by paramagnetic NMR spectroscopy
Authors : Hiruma, Y.; Hass, M.A.S.; Ubbink, M.
Deposited on : 2013-02-14

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

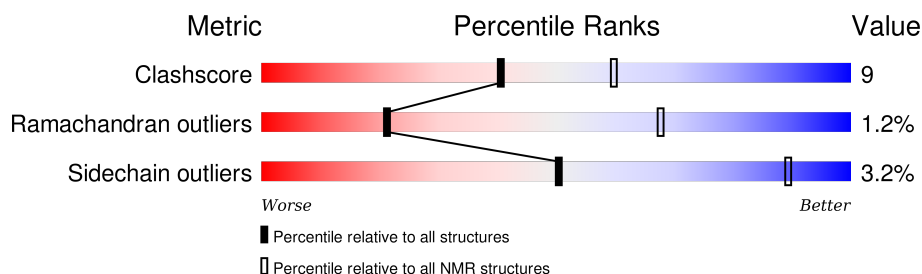
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 8%.

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	404	
2	B	106	

2 Ensemble composition and analysis

This entry contains 10 models. Model 4 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:11-A:414 (404)	0.00	4
2	B:1-B:106 (106)	0.00	6

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 2 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 5, 6, 7, 8
2	9, 10

3 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7977 atoms, of which 3925 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Camphor 5-monooxygenase.

Mol	Chain	Residues	Atoms						Trace
1	A	404	Total	C	H	N	O	S	0
			6355	2029	3155	559	594	18	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	276	GLN	GLU	SEE REMARK 999	UNP P00183

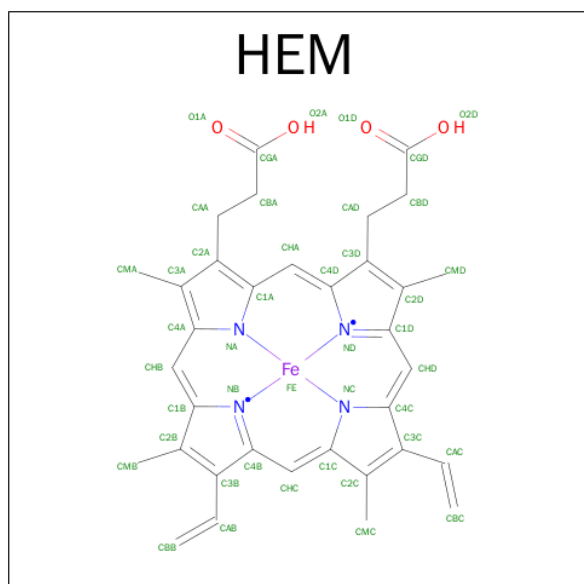
- Molecule 2 is a protein called Putidaredoxin.

Mol	Chain	Residues	Atoms						Trace
2	B	106	Total	C	H	N	O	S	0
			1564	488	770	136	162	8	

There is a discrepancy between the modelled and reference sequences:

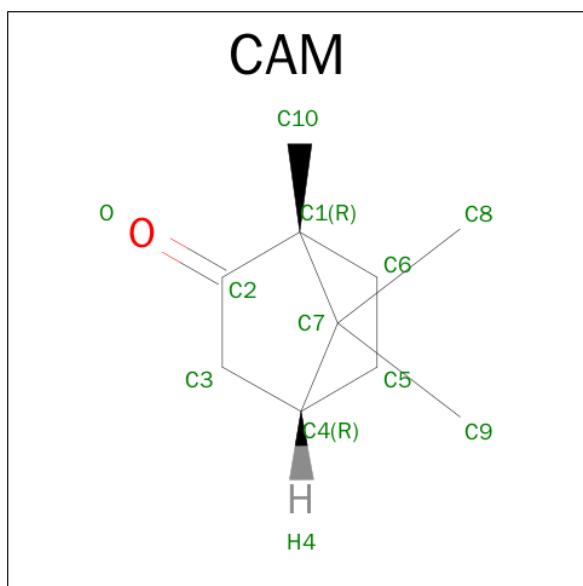
Chain	Residue	Modelled	Actual	Comment	Reference
B	73	SER	CYS	ENGINEERED MUTATION	UNP P00259

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



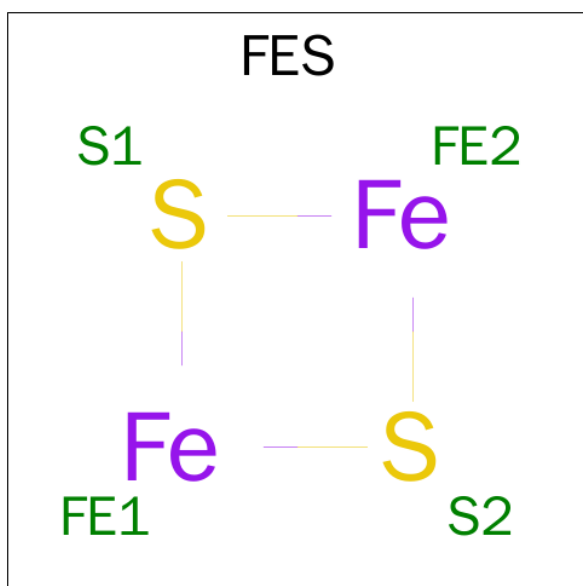
Mol	Chain	Residues	Atoms				
3	A	1	Total	C	Fe	N	O
			43	34	1	4	4

- Molecule 4 is CAMPHOR (three-letter code: CAM) (formula: $C_{10}H_{16}O$).



Mol	Chain	Residues	Atoms		
4	A	1	Total	C	O
			11	10	1

- Molecule 5 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



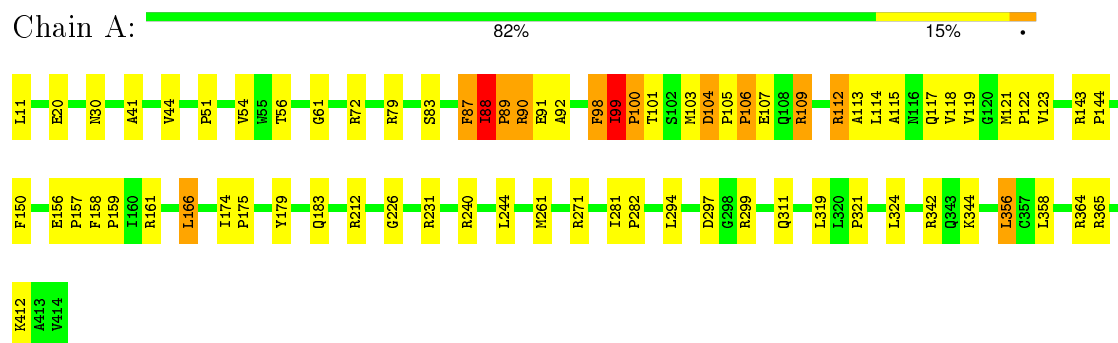
Mol	Chain	Residues	Atoms		
5	B	1	Total	Fe	S
			4	2	2

4 Residue-property plots [i](#)

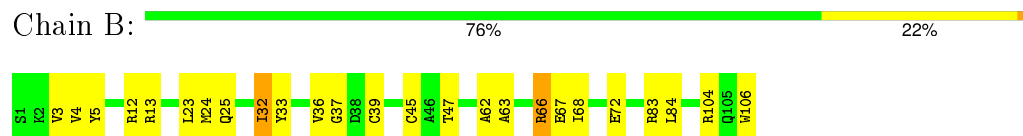
4.1 Average score per residue in the NMR ensemble

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: Camphor 5-monooxygenase



- Molecule 2: Putidaredoxin

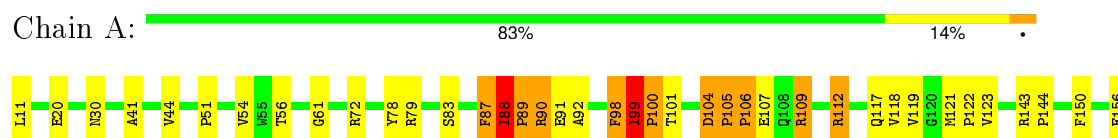


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

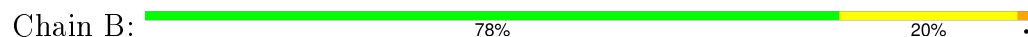
4.2.1 Score per residue for model 1

- Molecule 1: Camphor 5-monooxygenase



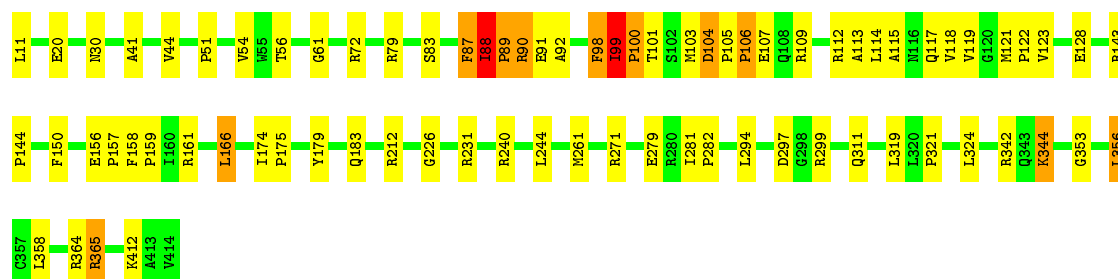
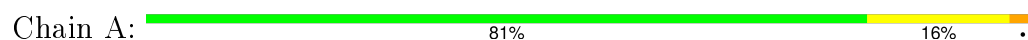


- Molecule 2: Putidaredoxin

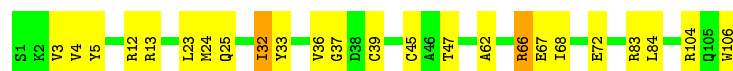
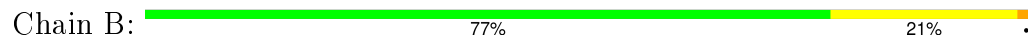


4.2.2 Score per residue for model 2

- Molecule 1: Camphor 5-monooxygenase

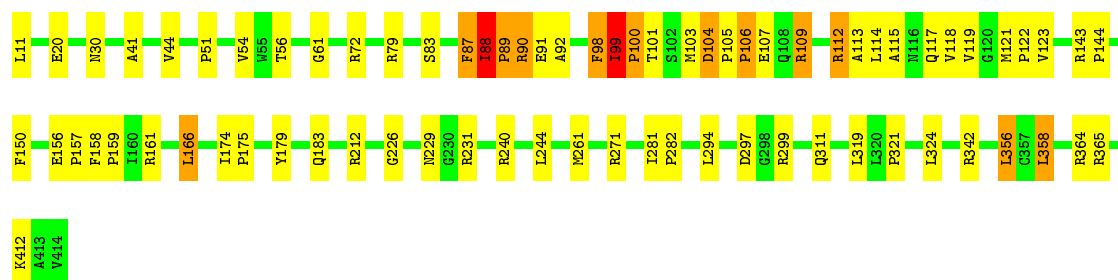
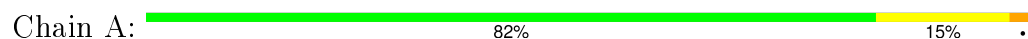


- Molecule 2: Putidaredoxin




4.2.3 Score per residue for model 3

- Molecule 1: Camphor 5-monooxygenase




- Molecule 2: Putidaredoxin

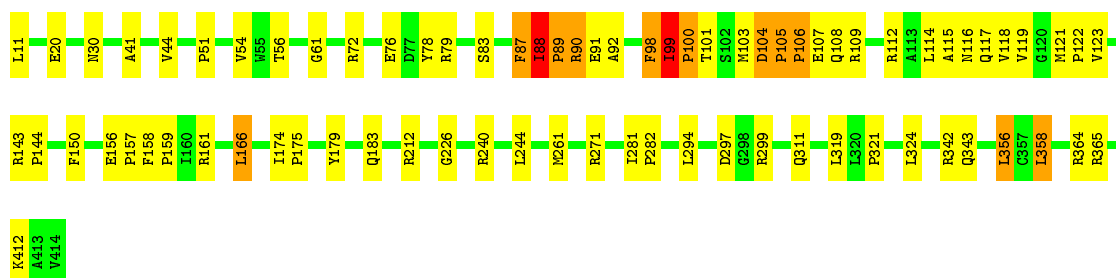
Chain B:  76% 23% .




4.2.4 Score per residue for model 4 (medoid)

- Molecule 1: Camphor 5-monooxygenase

Chain A:  81% 16% .




- Molecule 2: Putidaredoxin

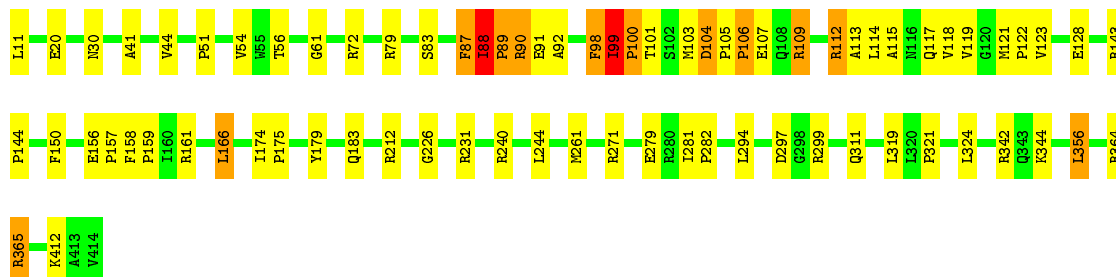
Chain B:  77% 21% .




4.2.5 Score per residue for model 5

- Molecule 1: Camphor 5-monooxygenase

Chain A:  81% 15% .



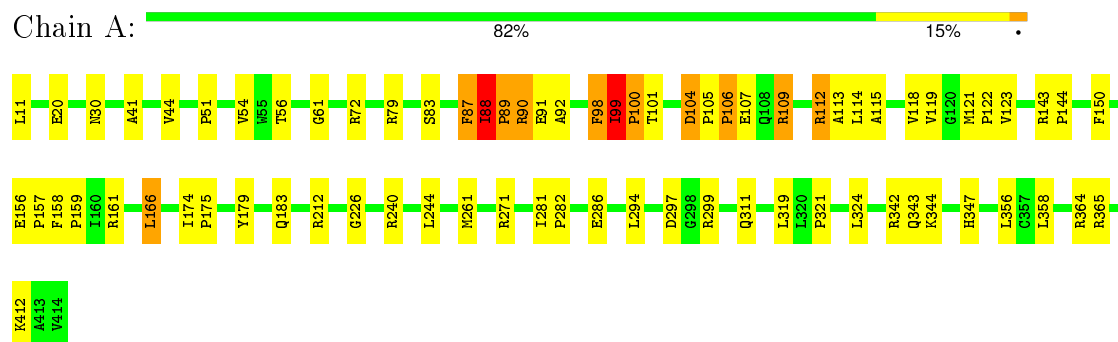
- Molecule 2: Putidaredoxin

Chain B:  79% 19% .

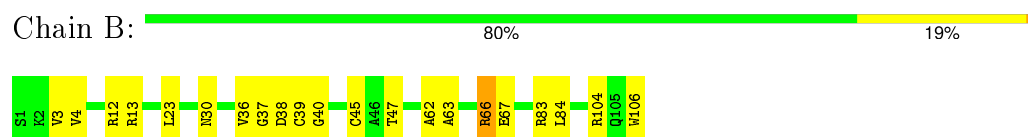


4.2.6 Score per residue for model 6

- Molecule 1: Camphor 5-monooxygenase

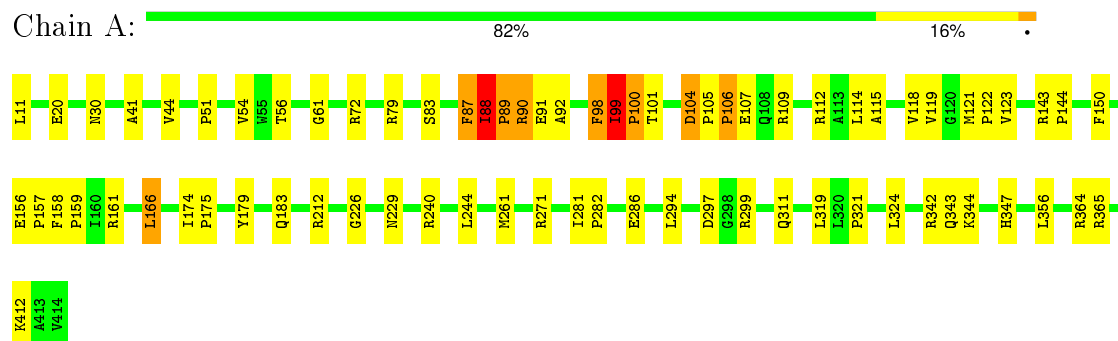


- Molecule 2: Putidaredoxin

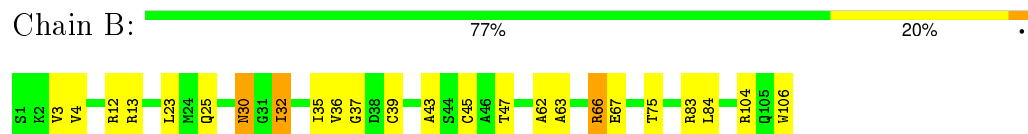


4.2.7 Score per residue for model 7

- Molecule 1: Camphor 5-monooxygenase

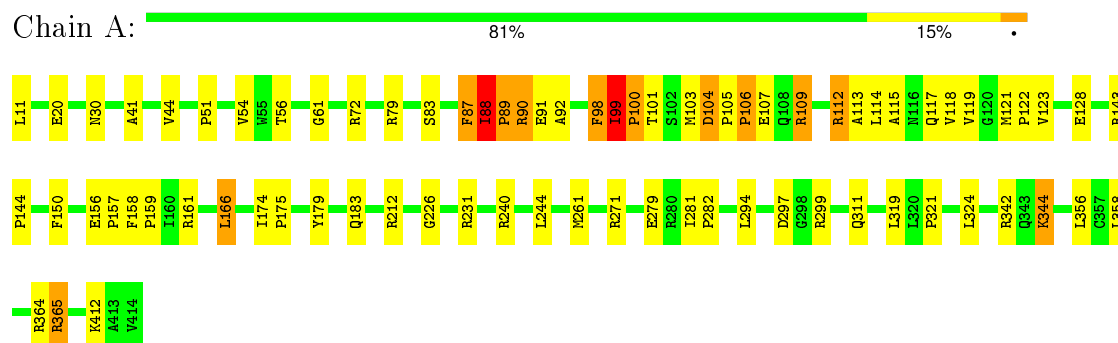


- Molecule 2: Putidaredoxin

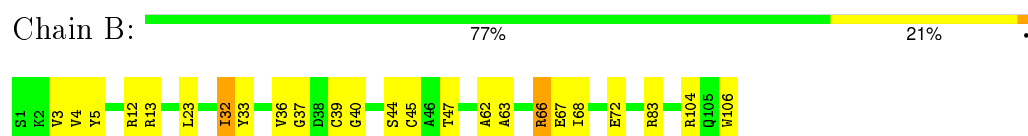


4.2.8 Score per residue for model 8

- Molecule 1: Camphor 5-monooxygenase

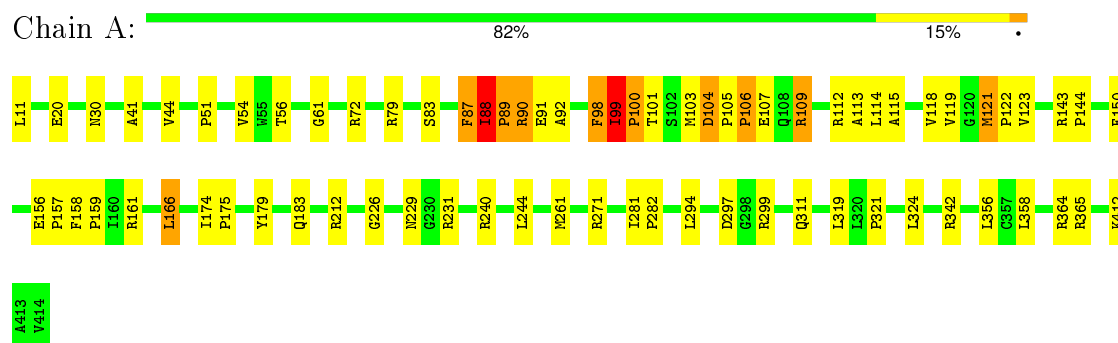


- Molecule 2: Putidaredoxin

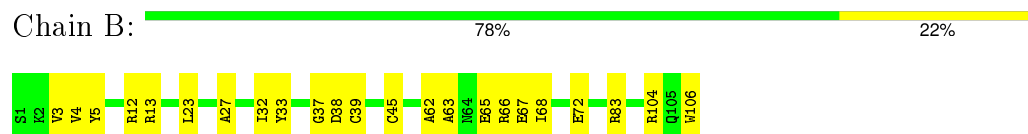


4.2.9 Score per residue for model 9

- Molecule 1: Camphor 5-monooxygenase

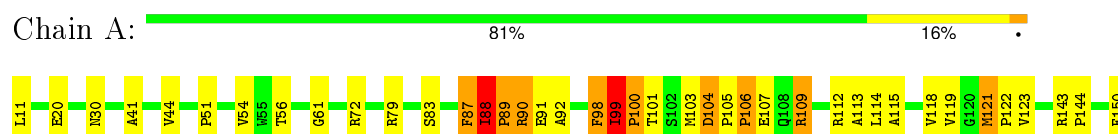


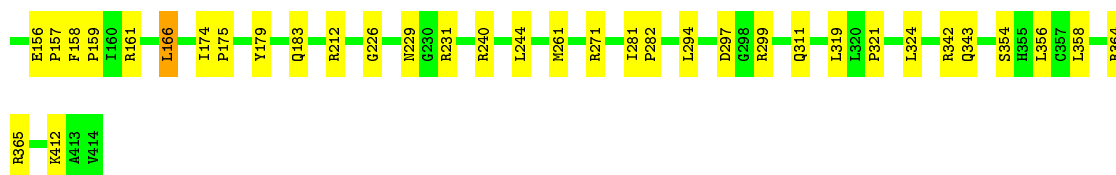
- Molecule 2: Putidaredoxin



4.2.10 Score per residue for model 10

- Molecule 1: Camphor 5-monooxygenase





- Molecule 2: Putidaredoxin

Chain B: 74% 26%



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 10 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
X-PLOR NIH	structure solution	
X-PLOR NIH	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)	2m56_cs.str
Number of chemical shift lists	1
Total number of shifts	494
Number of shifts mapped to atoms	494
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	8%

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

6 Model quality i

6.1 Standard geometry i

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

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	1.10±0.00	1±0/3279 (0.0±0.0%)	1.24±0.00	10±0/4454 (0.2±0.0%)
2	B	1.08±0.00	0±0/805 (0.0±0.0%)	1.21±0.00	0±0/1093 (0.0±0.0%)
All	All	1.10	10/40840 (0.0%)	1.24	97/55470 (0.2%)

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	10.6±0.5
2	B	0.0±0.0	2.8±0.4
All	All	0	134

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	99	ILE	N-CA	5.80	1.57	1.46	1	10

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
1	A	107	GLU	N-CA-CB	-7.45	97.20	110.60	2	10
1	A	105	PRO	N-CA-C	7.21	130.85	112.10	1	10
1	A	88	ILE	CA-CB-CG1	-6.39	98.85	111.00	1	10
1	A	89	PRO	N-CA-C	-6.20	95.98	112.10	1	10
1	A	104	ASP	CB-CA-C	6.16	122.73	110.40	1	10
1	A	104	ASP	CA-CB-CG	-5.37	101.59	113.40	1	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	99	ILE	N-CA-C	5.26	125.22	111.00	1	10
1	A	87	PHE	N-CA-CB	-5.19	101.27	110.60	1	10
1	A	103	MET	N-CA-CB	-5.12	101.38	110.60	2	7
1	A	98	PHE	N-CA-CB	-5.10	101.42	110.60	1	10

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	79	ARG	Sidechain	10
1	A	112	ARG	Sidechain	10
1	A	342	ARG	Sidechain	10
1	A	365	ARG	Sidechain	10
1	A	109	ARG	Sidechain	10
1	A	212	ARG	Sidechain	10
1	A	299	ARG	Sidechain	10
2	B	83	ARG	Sidechain	10
1	A	72	ARG	Sidechain	10
1	A	364	ARG	Sidechain	10
2	B	66	ARG	Sidechain	10
1	A	271	ARG	Sidechain	10
2	B	104	ARG	Sidechain	8
1	A	231	ARG	Sidechain	6

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	3200	3155	3152	63±4
2	B	794	770	771	13±2
3	A	43	0	30	8±3
5	B	4	0	0	2±0
All	All	40520	39250	39687	731

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 9.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:358:LEU:CD1	3:A:501:HEM:HBD2	1.21	1.65	8	3
1:A:358:LEU:HD11	3:A:501:HEM:HBD2	1.00	1.06	8	1
1:A:99:ILE:HD11	1:A:240:ARG:CZ	0.95	1.90	6	10
1:A:100:PRO:O	3:A:501:HEM:O2D	0.95	1.85	6	10
1:A:100:PRO:O	3:A:501:HEM:CGD	0.89	2.20	6	10
1:A:358:LEU:CD1	3:A:501:HEM:CBD	0.83	2.53	8	2
1:A:99:ILE:HD11	1:A:240:ARG:NE	0.83	1.87	6	10
1:A:358:LEU:HD13	3:A:501:HEM:HBD2	0.82	1.48	10	1
2:B:36:VAL:HG11	2:B:106:TRP:CZ2	0.81	2.11	8	1
1:A:112:ARG:NH1	3:A:501:HEM:CBD	0.77	2.47	5	2
1:A:112:ARG:NH1	3:A:501:HEM:O1D	0.77	2.18	5	2
1:A:99:ILE:HG13	1:A:240:ARG:HB3	0.72	1.58	6	10
1:A:113:ALA:HB2	2:B:106:TRP:CD2	0.70	2.21	5	2
2:B:45:CYS:HG	5:B:201:FES:FE1	0.70	1.02	7	10
1:A:100:PRO:HG2	3:A:501:HEM:HAD1	0.67	1.67	3	10
1:A:112:ARG:HH11	3:A:501:HEM:CBD	0.63	2.03	5	1
1:A:158:PHE:HB3	1:A:159:PRO:HD3	0.63	1.69	6	10
1:A:121:MET:N	1:A:122:PRO:HD2	0.62	2.08	6	10
1:A:358:LEU:HD12	3:A:501:HEM:HBD2	0.61	1.68	8	1
1:A:113:ALA:HB1	2:B:106:TRP:CD1	0.61	2.30	9	2
2:B:5:TYR:CG	2:B:32:ILE:HD13	0.60	2.32	9	7
1:A:114:LEU:HD11	1:A:226:GLY:HA3	0.58	1.75	4	9
1:A:356:LEU:HD12	2:B:39:CYS:O	0.58	1.98	5	1
1:A:112:ARG:NH1	3:A:501:HEM:CGD	0.58	2.66	5	1
1:A:113:ALA:HB2	2:B:106:TRP:CG	0.57	2.33	8	3
2:B:3:VAL:HG11	2:B:23:LEU:HD22	0.57	1.77	4	10
1:A:100:PRO:O	3:A:501:HEM:O1D	0.57	2.21	6	10
1:A:294:LEU:N	1:A:294:LEU:HD23	0.57	2.13	6	4
1:A:294:LEU:HD23	1:A:294:LEU:N	0.57	2.13	1	6
1:A:112:ARG:HH11	3:A:501:HEM:CGD	0.57	2.12	5	1
1:A:89:PRO:HD2	1:A:92:ALA:HB3	0.56	1.78	6	10
1:A:104:ASP:O	1:A:106:PRO:HD2	0.56	2.01	6	10
1:A:353:GLY:O	1:A:356:LEU:HD12	0.56	2.01	2	1
1:A:358:LEU:HD12	3:A:501:HEM:CBD	0.56	2.27	8	1
1:A:89:PRO:O	1:A:90:ARG:C	0.55	2.44	6	10
1:A:89:PRO:O	1:A:91:GLU:N	0.55	2.40	6	10
1:A:112:ARG:NH1	3:A:501:HEM:HBD2	0.55	2.17	5	1
2:B:67:GLU:HG3	2:B:84:LEU:HD12	0.54	1.79	2	6
1:A:112:ARG:CZ	1:A:358:LEU:HD11	0.54	2.32	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:83:SER:HB3	1:A:101:THR:O	0.54	2.03	6	10
1:A:319:LEU:O	1:A:321:PRO:HD3	0.54	2.02	6	10
1:A:98:PHE:HB3	1:A:244:LEU:HB2	0.54	1.78	6	10
1:A:356:LEU:HD13	2:B:39:CYS:O	0.54	2.03	2	5
1:A:100:PRO:CD	1:A:244:LEU:CD2	0.53	2.86	6	10
1:A:89:PRO:HG2	1:A:92:ALA:CB	0.53	2.32	6	10
2:B:37:GLY:HA2	5:B:201:FES:S2	0.53	2.44	2	10
1:A:89:PRO:HG2	1:A:92:ALA:HB2	0.53	1.80	6	10
2:B:27:ALA:HA	2:B:32:ILE:HD12	0.53	1.80	10	3
1:A:294:LEU:H	1:A:294:LEU:HD23	0.53	1.62	6	6
1:A:294:LEU:HD23	1:A:294:LEU:H	0.53	1.62	1	4
1:A:100:PRO:HD2	1:A:101:THR:OG1	0.52	2.04	2	10
1:A:99:ILE:HG13	1:A:240:ARG:CB	0.52	2.34	6	10
2:B:36:VAL:HB	2:B:47:THR:HB	0.52	1.82	6	8
1:A:100:PRO:HB2	3:A:501:HEM:CGD	0.52	2.34	3	10
1:A:166:LEU:HD23	1:A:166:LEU:C	0.52	2.25	6	3
1:A:166:LEU:C	1:A:166:LEU:HD23	0.52	2.25	1	7
1:A:100:PRO:CD	1:A:244:LEU:HD22	0.51	2.35	6	10
1:A:98:PHE:O	1:A:99:ILE:HG12	0.51	2.05	6	10
1:A:297:ASP:OD2	3:A:501:HEM:O2A	0.51	2.28	6	10
1:A:112:ARG:HH11	3:A:501:HEM:HBD2	0.51	1.63	5	1
1:A:121:MET:N	1:A:122:PRO:CD	0.51	2.73	6	10
1:A:321:PRO:HG2	1:A:324:LEU:HD22	0.51	1.82	6	10
1:A:89:PRO:CD	1:A:92:ALA:HB3	0.50	2.36	6	10
1:A:56:THR:O	1:A:61:GLY:HA2	0.50	2.07	6	10
2:B:27:ALA:HA	2:B:32:ILE:HD13	0.49	1.83	1	1
1:A:150:PHE:CZ	1:A:261:MET:HG3	0.49	2.43	6	10
1:A:118:VAL:HA	1:A:123:VAL:HG21	0.48	1.85	1	10
1:A:112:ARG:CG	1:A:358:LEU:HD11	0.48	2.39	3	1
2:B:24:MET:SD	5:B:201:FES:S2	0.48	3.11	5	4
1:A:358:LEU:HD11	3:A:501:HEM:CBD	0.48	2.02	8	1
1:A:143:ARG:HB3	1:A:144:PRO:HD3	0.48	1.85	6	10
1:A:113:ALA:HB2	2:B:106:TRP:CE3	0.47	2.45	2	1
1:A:118:VAL:C	1:A:123:VAL:HG21	0.47	2.31	9	10
1:A:179:TYR:O	1:A:183:GLN:HG2	0.47	2.10	6	10
1:A:87:PHE:O	1:A:88:ILE:HG13	0.47	2.10	6	10
2:B:32:ILE:CG2	2:B:35:ILE:HD12	0.47	2.40	7	2
1:A:115:ALA:O	1:A:119:VAL:HG22	0.46	2.10	10	9
1:A:99:ILE:CG2	1:A:99:ILE:O	0.46	2.63	9	6
1:A:99:ILE:O	1:A:99:ILE:CG2	0.46	2.63	3	4
1:A:116:ASN:HA	1:A:358:LEU:CD2	0.46	2.41	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:294:LEU:N	1:A:294:LEU:CD2	0.46	2.79	6	5
1:A:90:ARG:O	1:A:90:ARG:HG2	0.46	2.11	6	4
1:A:294:LEU:CD2	1:A:294:LEU:N	0.46	2.79	1	5
1:A:90:ARG:HG2	1:A:90:ARG:O	0.46	2.11	3	6
2:B:24:MET:CE	5:B:201:FES:S2	0.45	3.05	3	1
2:B:43:ALA:HB3	2:B:66:ARG:HD3	0.45	1.88	7	1
1:A:356:LEU:HD22	2:B:39:CYS:C	0.45	2.31	1	1
1:A:156:GLU:N	1:A:157:PRO:HD2	0.45	2.27	6	10
2:B:39:CYS:SG	2:B:45:CYS:SG	0.45	3.15	2	8
1:A:344:LYS:HD3	1:A:344:LYS:N	0.45	2.27	1	2
1:A:78:TYR:CD1	1:A:105:PRO:HD2	0.44	2.48	4	2
1:A:112:ARG:HB2	2:B:106:TRP:CZ3	0.44	2.47	8	1
1:A:344:LYS:N	1:A:344:LYS:HD3	0.44	2.27	2	1
1:A:281:ILE:N	1:A:282:PRO:CD	0.43	2.81	1	10
2:B:15:LEU:HD11	2:B:32:ILE:HD11	0.43	1.88	1	1
1:A:98:PHE:O	1:A:99:ILE:CG1	0.43	2.66	6	10
1:A:89:PRO:O	1:A:89:PRO:CD	0.43	2.65	6	6
1:A:11:LEU:HD22	1:A:11:LEU:N	0.43	2.28	6	7
1:A:11:LEU:N	1:A:11:LEU:HD22	0.43	2.28	1	3
1:A:89:PRO:CD	1:A:89:PRO:O	0.43	2.65	4	4
1:A:358:LEU:HD12	3:A:501:HEM:C3D	0.43	2.48	8	1
2:B:106:TRP:HA	2:B:106:TRP:CE3	0.43	2.47	4	1
1:A:412:LYS:HG3	1:A:412:LYS:O	0.43	2.13	6	9
1:A:412:LYS:O	1:A:412:LYS:HG3	0.43	2.13	1	1
1:A:356:LEU:HD22	2:B:39:CYS:O	0.43	2.14	2	1
2:B:30:ASN:HB3	2:B:32:ILE:CD1	0.43	2.44	7	1
2:B:4:VAL:HG11	2:B:12:ARG:CZ	0.43	2.44	1	10
1:A:118:VAL:HG23	1:A:119:VAL:HG13	0.42	1.90	1	1
1:A:354:SER:HA	2:B:44:SER:HB3	0.42	1.90	10	1
1:A:356:LEU:HD22	2:B:40:GLY:CA	0.42	2.44	6	2
1:A:118:VAL:CA	1:A:123:VAL:HG21	0.42	2.44	6	9
2:B:68:ILE:O	2:B:72:GLU:HG3	0.42	2.15	8	8
1:A:174:ILE:N	1:A:175:PRO:CD	0.42	2.83	6	10
1:A:344:LYS:HE2	1:A:344:LYS:HB2	0.41	1.71	5	1
2:B:5:TYR:CD1	2:B:32:ILE:CD1	0.41	3.04	3	3
1:A:41:ALA:O	1:A:44:VAL:HG22	0.41	2.16	6	10
1:A:51:PRO:HG2	1:A:54:VAL:HG12	0.41	1.91	6	10
1:A:113:ALA:CB	2:B:106:TRP:CG	0.41	3.03	3	1
1:A:100:PRO:HD3	1:A:244:LEU:HD22	0.41	1.92	6	10
1:A:158:PHE:CB	1:A:159:PRO:HD3	0.41	2.45	6	10
1:A:281:ILE:N	1:A:282:PRO:HD2	0.41	2.31	1	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:112:ARG:HG2	1:A:358:LEU:HD11	0.41	1.92	6	1
2:B:63:ALA:HB1	2:B:67:GLU:HB3	0.41	1.93	1	9
1:A:100:PRO:HD3	1:A:244:LEU:CD2	0.40	2.45	6	5
1:A:157:PRO:O	1:A:161:ARG:HB2	0.40	2.17	6	10
1:A:356:LEU:HD23	1:A:356:LEU:HA	0.40	1.68	5	1

6.3 Torsion angles [i](#)

6.3.1 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 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	402/404 (100%)	381±0 (95±0%)	16±0 (4±0%)	5±0 (1±0%)	21	68
2	B	104/106 (98%)	99±0 (95±0%)	4±0 (4±0%)	1±0 (1±0%)	24	71
All	All	5060/5100 (99%)	4800 (95%)	200 (4%)	60 (1%)	21	68

All 6 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	99	ILE	10
1	A	100	PRO	10
2	B	62	ALA	10
1	A	88	ILE	10
1	A	106	PRO	10
1	A	90	ARG	10

6.3.2 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 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	349/349 (100%)	339±1 (97±0%)	10±1 (3±0%)	55	91
2	B	89/89 (100%)	84±1 (95±1%)	5±1 (5±1%)	33	78
All	All	4380/4380 (100%)	4238 (97%)	142 (3%)	50	89

All 30 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	30	ASN	10
1	A	20	GLU	10
1	A	311	GLN	10
2	B	13	ARG	10
1	A	166	LEU	10
1	A	356	LEU	8
2	B	33	TYR	8
2	B	66	ARG	7
1	A	109	ARG	7
2	B	32	ILE	6
1	A	117	GLN	6
2	B	25	GLN	5
1	A	358	LEU	5
1	A	229	ASN	4
1	A	343	GLN	4
1	A	344	LYS	4
1	A	365	ARG	3
1	A	128	GLU	3
1	A	286	GLU	3
1	A	279	GLU	3
2	B	30	ASN	3
1	A	121	MET	2
2	B	44	SER	2
1	A	347	HIS	2
2	B	38	ASP	2
2	B	106	TRP	1
1	A	108	GLN	1
2	B	65	GLU	1
1	A	76	GLU	1
2	B	75	THR	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.6 Ligand geometry ⓘ

3 ligands are 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
3	HEM	A	501	1	24,50,50	1.91±0.00	0±0 (0±0%)
4	CAM	A	502	-	12,12,12	0.50±0.00	0±0 (0±0%)
5	FES	B	201	2	0,4,4	0.00±0.00	-

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
3	HEM	A	501	1	16,82,82	2.44±0.00	1±0 (6±0%)
4	CAM	A	502	-	21,21,21	2.81±0.00	2±0 (9±0%)
5	FES	B	201	2	0,4,4	0.00±0.00	-

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
3	HEM	A	501	1	-	0±0,6,54,54	0±0,0,8,8
4	CAM	A	502	-	-	0±0,0,31,31	0±0,0,2,2
5	FES	B	201	2	-	0±0,0,4,4	0±0,1,1,1

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
4	A	502	CAM	C7-C1-C2	7.07	109.56	100.46	6	10
3	A	501	HEM	CBD-CAD-C3D	5.52	122.15	112.47	3	10
4	A	502	CAM	C3-C2-C1	5.08	96.54	107.77	6	10

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 [i](#)

The completeness of assignment taking into account all chemical shift lists is 8% for the well-defined parts and 8% for the entire structure.

7.1 Chemical shift list 1

File name: 2m56_cs.str

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping [i](#)

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	494
Number of shifts mapped to atoms	494
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	0	—	—
$^{13}\text{C}_\beta$	0	—	—
$^{13}\text{C}'$	0	—	—
^{15}N	247	-0.01 \pm 0.28	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 8%, i.e. 493 atoms were assigned a chemical shift out of a possible 6237. 0 out of 86 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	493/2482 (20%)	246/986 (25%)	0/1020 (0%)	247/476 (52%)
Sidechain	0/3311 (0%)	0/1944 (0%)	0/1218 (0%)	0/149 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	0/444 (0%)	0/239 (0%)	0/184 (0%)	0/21 (0%)
Overall	493/6237 (8%)	246/3169 (8%)	0/2422 (0%)	247/646 (38%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 8%, i.e. 493 atoms were assigned a chemical shift out of a possible 6237. 0 out of 86 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	493/2482 (20%)	246/986 (25%)	0/1020 (0%)	247/476 (52%)
Sidechain	0/3311 (0%)	0/1944 (0%)	0/1218 (0%)	0/149 (0%)
Aromatic	0/444 (0%)	0/239 (0%)	0/184 (0%)	0/21 (0%)
Overall	493/6237 (8%)	246/3169 (8%)	0/2422 (0%)	247/646 (38%)

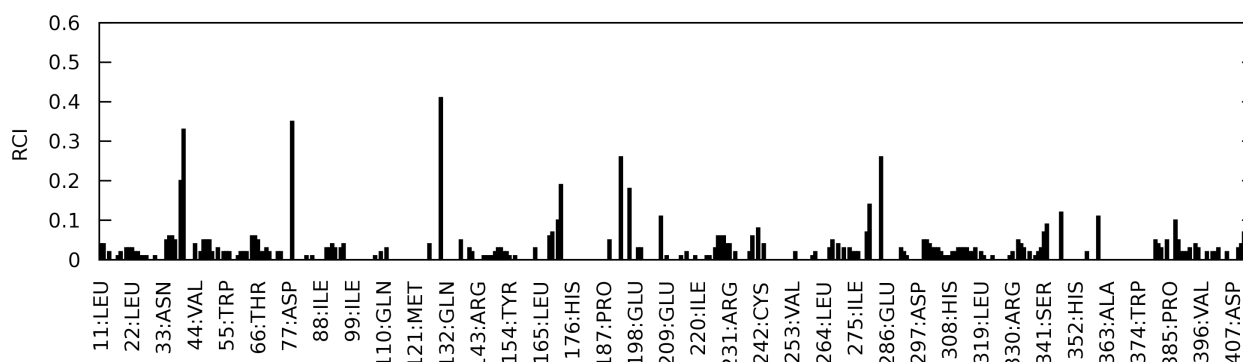
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

The images below report *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:



Random coil index (RCI) for chain B:

