Full wwPDB NMR Structure Validation Report (i)

Apr 26, 2016 – 03:43 PM BST

PDB ID	:	1A2I
Title	:	SOLUTION STRUCTURE OF DESULFOVIBRIO VULGARIS (HILDENBOROUGH) FERROCYTOCHROME C3, NMR, 20 STRUCTURES
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Deposited on	:	1998-01-05

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 (i) symbol.

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

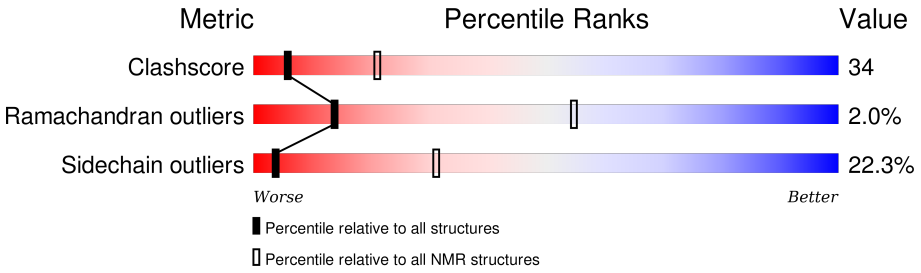
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	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 (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 46%.

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	107	46% 31% 5% 19%

2 Ensemble composition and analysis

This entry contains 20 models. Model 5 is the overall representative, medoid model (most similar to other models).

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:4-A:36, A:43-A:55, A:62-A:87, A:93-A:107 (87)	0.11	5

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 3 clusters. No single-model clusters were found.

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

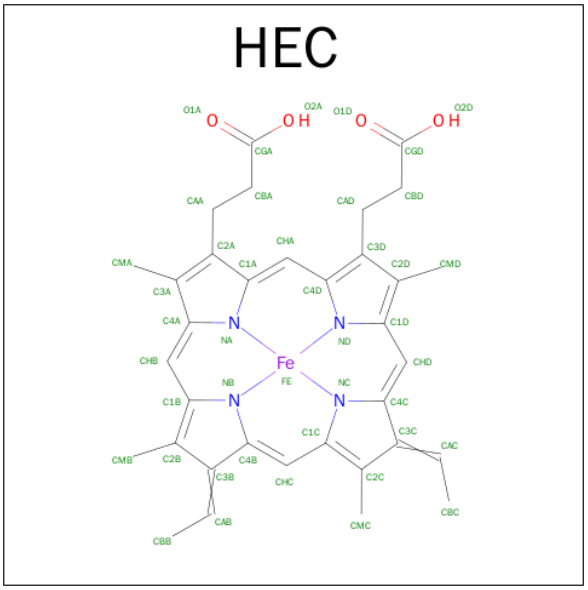
3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1880 atoms, of which 898 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called CYTOCHROME C3.

Mol	Chain	Residues	Atoms						Trace
1	A	107	Total	C	H	N	O	S	0
			1580	495	770	152	152	11	

- Molecule 2 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



Mol	Chain	Residues	Atoms					
2	A	1	Total	C	Fe	H	N	O
			75	34	1	32	4	4
2	A	1	Total	C	Fe	H	N	O
			75	34	1	32	4	4
2	A	1	Total	C	Fe	H	N	O
			75	34	1	32	4	4
2	A	1	Total	C	Fe	H	N	O
			75	34	1	32	4	4

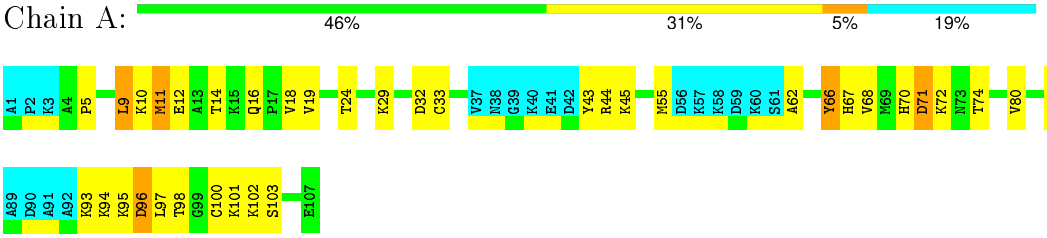
4 Residue-property plots

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 C3

Chain A:



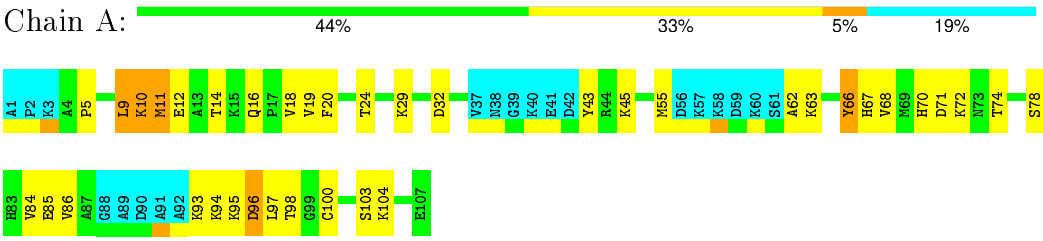
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: CYTOCHROME C3

Chain A:



4.2.2 Score per residue for model 2

- Molecule 1: CYTOCHROME C3

Chain A:

4.2.3 Score per residue for model 3

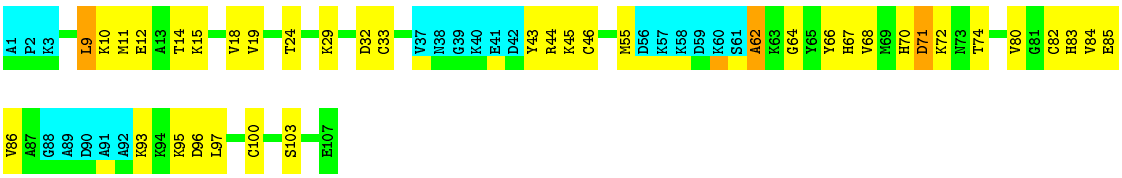
- Molecule 1: CYTOCHROME C3

Chain A:

4.2.4 Score per residue for model 4

- Molecule 1: CYTOCHROME C3

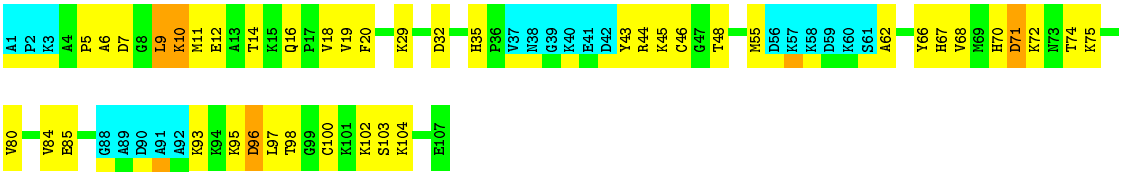
Chain A:



4.2.5 Score per residue for model 5 (medoid)

- Molecule 1: CYTOCHROME C3

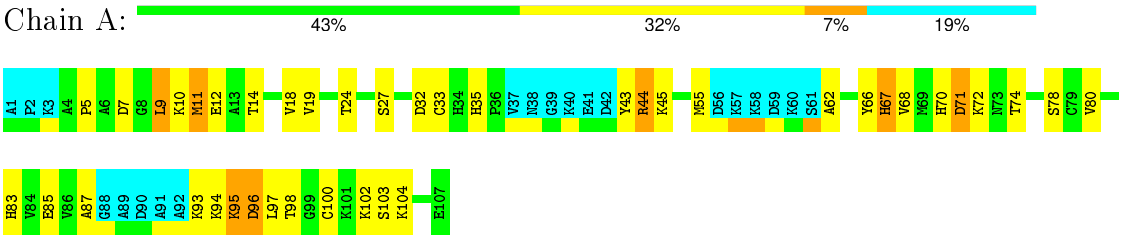
Chain A:



4.2.6 Score per residue for model 6

- Molecule 1: CYTOCHROME C3

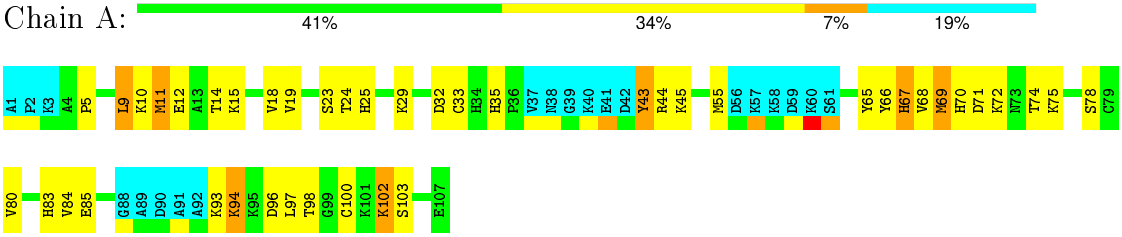
Chain A:



4.2.7 Score per residue for model 7

- Molecule 1: CYTOCHROME C3

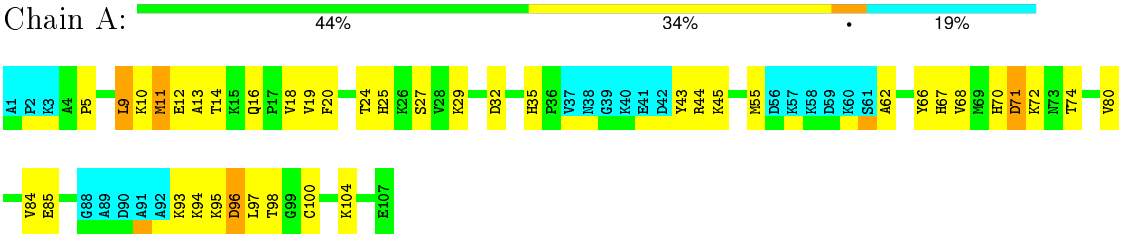
Chain A:



4.2.8 Score per residue for model 8

- Molecule 1: CYTOCHROME C3

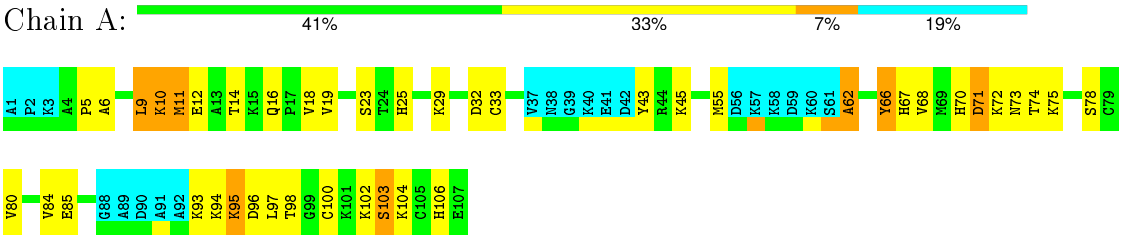
Chain A:



4.2.9 Score per residue for model 9

- Molecule 1: CYTOCHROME C3

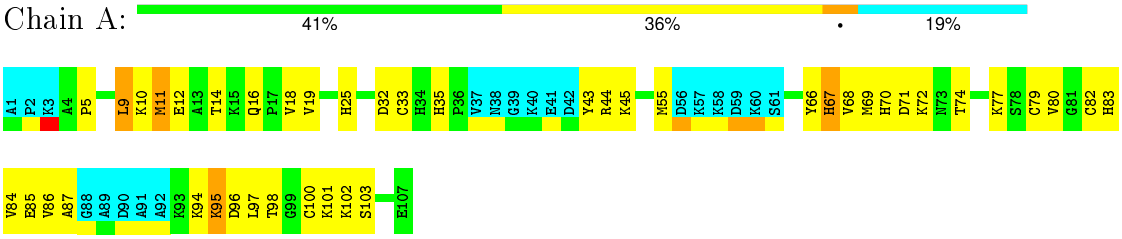
Chain A:



4.2.10 Score per residue for model 10

• Molecule 1: CYTOCHROME C3

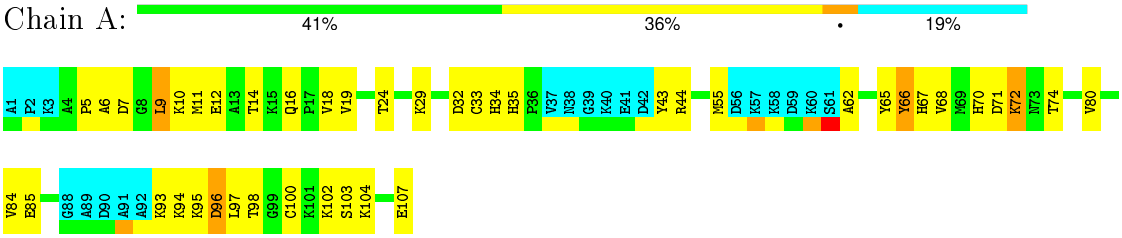
Chain A:



4.2.11 Score per residue for model 11

• Molecule 1: CYTOCHROME C3

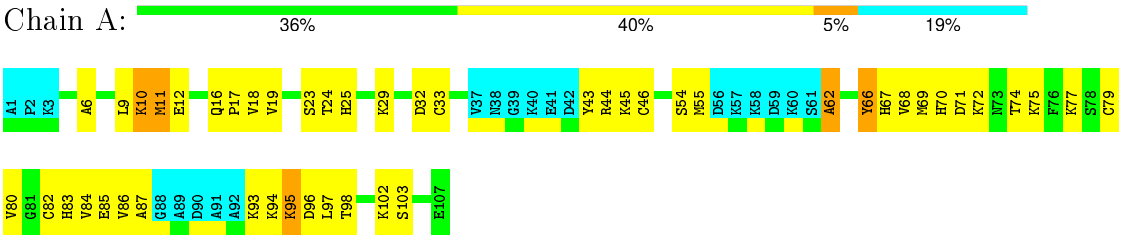
Chain A:



4.2.12 Score per residue for model 12

• Molecule 1: CYTOCHROME C3

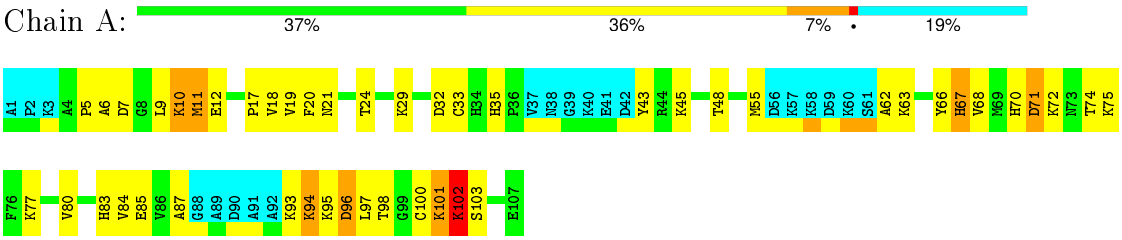
Chain A:



4.2.13 Score per residue for model 13

• Molecule 1: CYTOCHROME C3

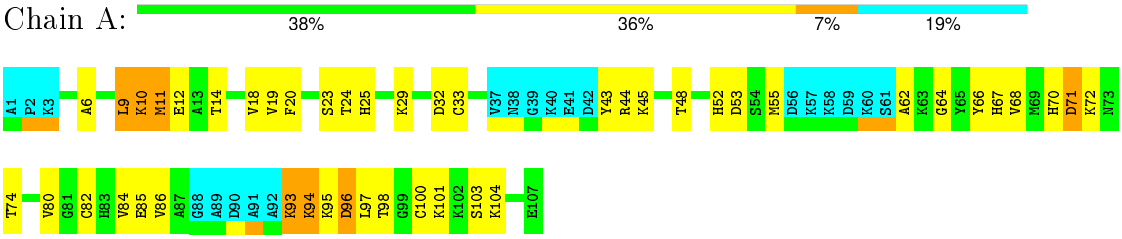
Chain A:



4.2.14 Score per residue for model 14

• Molecule 1: CYTOCHROME C3

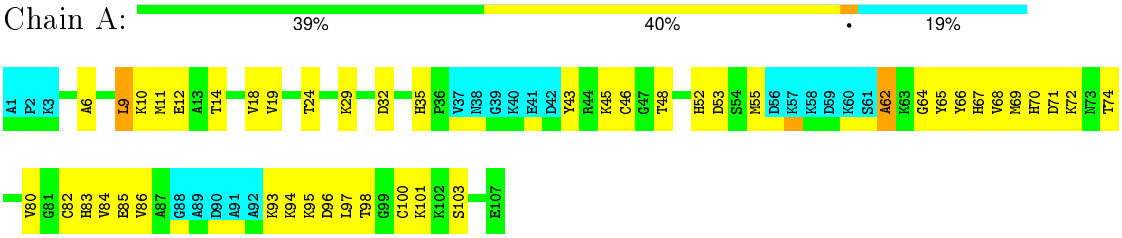
Chain A:



4.2.15 Score per residue for model 15

• Molecule 1: CYTOCHROME C3

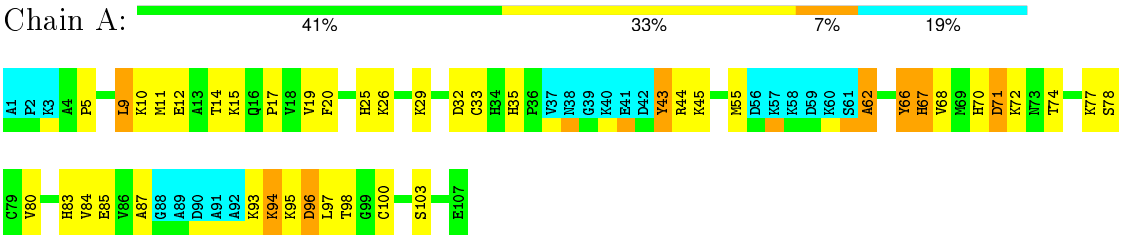
Chain A:



4.2.16 Score per residue for model 16

• Molecule 1: CYTOCHROME C3

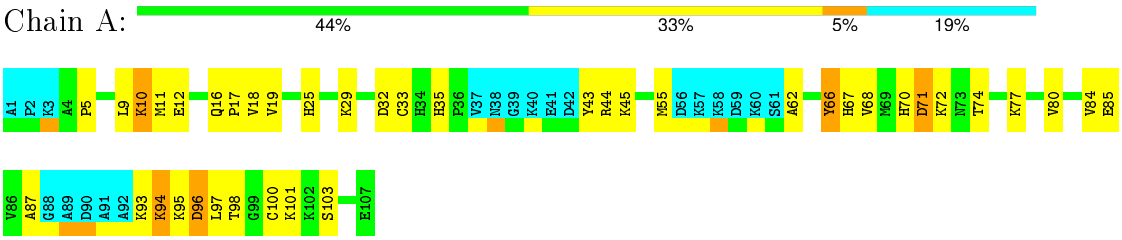
Chain A:



4.2.17 Score per residue for model 17

• Molecule 1: CYTOCHROME C3

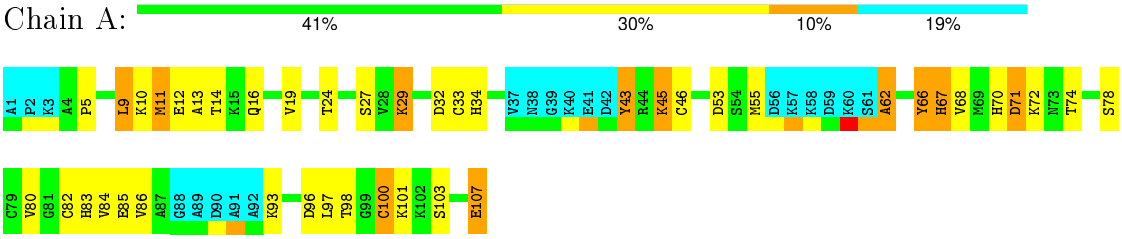
Chain A:



4.2.18 Score per residue for model 18

• Molecule 1: CYTOCHROME C3

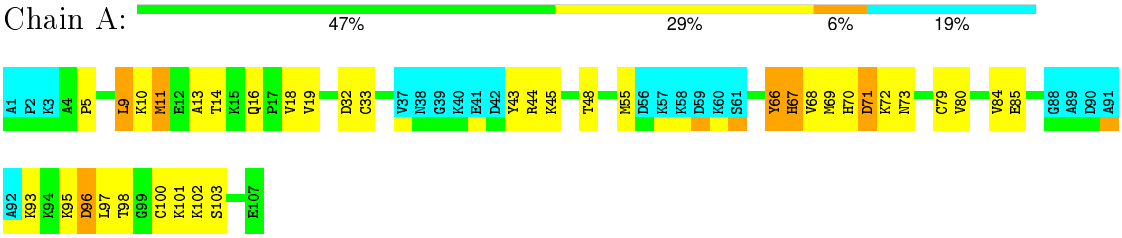
Chain A:



4.2.19 Score per residue for model 19

• Molecule 1: CYTOCHROME C3

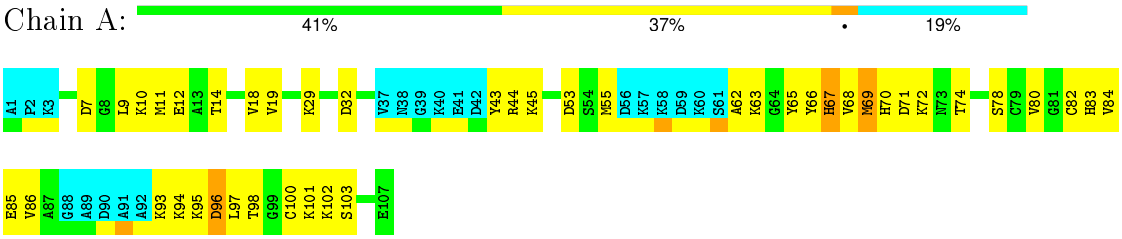
Chain A:



4.2.20 Score per residue for model 20

• Molecule 1: CYTOCHROME C3

Chain A:



5 Refinement protocol and experimental data overview

The models were refined using the following method: *RESTRAINED MOLECULAR DYNAMICS WITH SIMULATED ANNEALING*.

Of the 600 calculated structures, 20 were deposited, based on the following criterion: *LEAST RESTRAINT VIOLATION*.

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

Software name	Classification	Version
DYANA	refinement	1.4
DYANA	structure solution	

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 5625
Number of chemical shift lists	5
Total number of shifts	742
Number of shifts mapped to atoms	662
Number of unparsed shifts	0
Number of shifts with mapping errors	80
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	46%

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: HEC

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	668	634	650	41±4
2	A	172	128	120	39±4
All	All	16800	15240	15400	1110

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 34.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:43:TYR:CE2	2:A:108:HEC:HMB3	1.06	1.86	3	15
2:A:109:HEC:CGD	2:A:109:HEC:HMD1	0.91	1.95	10	13
1:A:80:VAL:O	1:A:84:VAL:HG23	0.90	1.65	11	19
2:A:110:HEC:HBC3	2:A:110:HEC:HMC1	0.88	1.46	15	11
2:A:110:HEC:HMC1	2:A:110:HEC:HBC3	0.88	1.46	20	9
1:A:9:LEU:HD11	2:A:108:HEC:HBD1	0.86	1.48	18	13
1:A:11:MET:SD	2:A:111:HEC:HMD1	0.84	2.13	11	3
2:A:108:HEC:HMC1	2:A:108:HEC:HBC3	0.83	1.49	15	10
2:A:108:HEC:HBC3	2:A:108:HEC:HMC1	0.83	1.49	8	10
2:A:109:HEC:HMD1	2:A:109:HEC:CGD	0.83	2.03	14	2
1:A:18:VAL:HG21	2:A:111:HEC:C2D	0.81	2.06	6	12

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:9:LEU:HD13	1:A:9:LEU:O	0.81	1.76	19	8
1:A:24:THR:HG21	2:A:110:HEC:CGA	0.80	2.06	13	3
1:A:9:LEU:O	1:A:9:LEU:HD13	0.80	1.77	17	12
1:A:10:LYS:HB2	1:A:19:VAL:HG22	0.79	1.54	4	17
1:A:10:LYS:HB3	1:A:19:VAL:HG22	0.77	1.54	17	3
1:A:18:VAL:HG21	2:A:111:HEC:C1D	0.77	2.09	6	16
1:A:74:THR:HG22	2:A:109:HEC:O1A	0.76	1.80	7	7
1:A:104:LYS:HB3	2:A:110:HEC:HMA3	0.75	1.58	9	2
1:A:24:THR:HG21	2:A:110:HEC:HBA1	0.74	1.57	8	6
1:A:97:LEU:O	2:A:111:HEC:HMC1	0.74	1.83	4	18
1:A:43:TYR:CZ	2:A:108:HEC:HMB3	0.74	2.18	18	8
1:A:74:THR:HG22	2:A:109:HEC:O2A	0.72	1.82	16	8
1:A:100:CYS:SG	2:A:111:HEC:HMB1	0.69	2.27	10	19
2:A:110:HEC:CBC	2:A:110:HEC:HMC1	0.69	2.17	6	11
1:A:9:LEU:HD22	1:A:9:LEU:C	0.69	2.07	14	8
2:A:110:HEC:HMC1	2:A:110:HEC:CBC	0.68	2.17	20	9
1:A:9:LEU:C	1:A:9:LEU:HD22	0.68	2.08	2	5
1:A:68:VAL:HG12	2:A:109:HEC:C3A	0.67	2.19	5	20
2:A:111:HEC:HBC3	2:A:111:HEC:HMC1	0.66	1.67	3	8
2:A:111:HEC:HMC1	2:A:111:HEC:HBC3	0.65	1.67	14	12
1:A:20:PHE:CE1	1:A:25:HIS:CE1	0.64	2.86	8	2
1:A:9:LEU:HD11	2:A:108:HEC:CBD	0.63	2.22	18	8
1:A:72:LYS:HD3	1:A:84:VAL:HG21	0.62	1.71	11	7
1:A:66:TYR:O	1:A:66:TYR:CD1	0.61	2.54	13	10
1:A:66:TYR:CD1	1:A:66:TYR:O	0.60	2.54	14	10
2:A:109:HEC:HMB1	2:A:109:HEC:HBB3	0.60	1.73	14	13
2:A:110:HEC:HBB3	2:A:110:HEC:HMB1	0.60	1.72	6	9
2:A:109:HEC:HBB3	2:A:109:HEC:HMB1	0.60	1.73	11	7
1:A:72:LYS:HE2	1:A:84:VAL:HG21	0.60	1.72	7	1
1:A:24:THR:HG21	2:A:110:HEC:O1A	0.60	1.95	1	3
1:A:11:MET:CE	2:A:108:HEC:CGD	0.58	2.81	18	10
1:A:10:LYS:CB	1:A:19:VAL:HG22	0.58	2.28	12	8
1:A:18:VAL:HG11	2:A:111:HEC:HMD3	0.57	1.77	6	4
2:A:110:HEC:HMB1	2:A:110:HEC:HBB3	0.57	1.76	11	11
1:A:45:LYS:O	2:A:109:HEC:HMC3	0.57	2.00	18	1
1:A:107:GLU:OXT	1:A:107:GLU:HG3	0.57	2.00	18	1
2:A:109:HEC:O2D	2:A:109:HEC:HMD1	0.56	2.00	3	2
1:A:93:LYS:O	1:A:97:LEU:N	0.56	2.39	17	19
1:A:24:THR:HG21	2:A:110:HEC:HBA2	0.56	1.78	15	2
1:A:33:CYS:SG	2:A:110:HEC:HMC2	0.56	2.41	13	15
2:A:108:HEC:CBC	2:A:108:HEC:HMC1	0.56	2.27	8	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:14:THR:HG23	2:A:111:HEC:O2D	0.55	2.00	7	3
1:A:69:MET:HG2	2:A:111:HEC:HMD2	0.54	1.77	7	2
1:A:72:LYS:CE	1:A:84:VAL:HG21	0.54	2.32	7	2
2:A:108:HEC:HMC1	2:A:108:HEC:CBC	0.53	2.30	14	10
1:A:14:THR:HG23	2:A:111:HEC:O1D	0.53	2.02	10	2
1:A:67:HIS:CE1	1:A:71:ASP:OD2	0.53	2.61	19	1
1:A:12:GLU:O	1:A:12:GLU:CG	0.53	2.57	12	1
1:A:12:GLU:CG	1:A:12:GLU:O	0.53	2.55	13	1
2:A:108:HEC:HBB3	2:A:108:HEC:HMB1	0.52	1.80	1	10
1:A:52:HIS:CE1	1:A:62:ALA:O	0.52	2.63	14	2
2:A:108:HEC:HMB1	2:A:108:HEC:HBB3	0.52	1.80	12	10
1:A:9:LEU:HD22	1:A:10:LYS:N	0.52	2.19	2	5
1:A:32:ASP:OD1	2:A:110:HEC:CBC	0.52	2.58	19	20
1:A:68:VAL:CG1	2:A:109:HEC:C3A	0.51	2.87	5	20
2:A:109:HEC:CBD	2:A:109:HEC:HMD1	0.51	2.34	13	13
1:A:66:TYR:CG	1:A:66:TYR:O	0.51	2.62	11	12
1:A:11:MET:HE3	2:A:108:HEC:CGD	0.51	2.35	18	5
1:A:9:LEU:C	1:A:9:LEU:HD13	0.51	2.25	13	1
1:A:66:TYR:O	1:A:66:TYR:CG	0.51	2.63	8	8
1:A:11:MET:HE2	2:A:111:HEC:HMD1	0.51	1.81	10	5
1:A:96:ASP:O	1:A:104:LYS:CG	0.51	2.59	8	5
1:A:43:TYR:N	1:A:43:TYR:CD1	0.51	2.77	16	2
1:A:13:ALA:HB3	2:A:111:HEC:O1D	0.51	2.06	18	3
1:A:74:THR:CG2	2:A:109:HEC:O2A	0.50	2.59	6	7
1:A:67:HIS:O	1:A:71:ASP:CB	0.50	2.59	1	19
1:A:83:HIS:CE1	2:A:111:HEC:HBC1	0.50	2.40	7	10
1:A:74:THR:CG2	2:A:109:HEC:O1A	0.50	2.60	2	4
2:A:108:HEC:HBC1	2:A:110:HEC:C1C	0.50	2.36	9	20
1:A:100:CYS:SG	2:A:111:HEC:CMB	0.50	3.00	10	1
1:A:11:MET:O	2:A:111:HEC:CGD	0.50	2.59	15	3
1:A:14:THR:HG23	2:A:111:HEC:CGD	0.49	2.38	8	2
1:A:74:THR:HB	2:A:109:HEC:CGA	0.49	2.38	10	16
2:A:109:HEC:HMD1	2:A:109:HEC:CBD	0.49	2.37	16	7
1:A:72:LYS:CD	1:A:84:VAL:HG21	0.49	2.37	11	2
1:A:11:MET:HE3	2:A:108:HEC:O1D	0.49	2.06	6	3
1:A:24:THR:HG21	2:A:110:HEC:O2A	0.49	2.07	13	1
1:A:20:PHE:CE2	2:A:108:HEC:CHD	0.49	2.96	14	1
1:A:97:LEU:O	2:A:111:HEC:CMC	0.48	2.60	5	6
1:A:11:MET:CE	2:A:108:HEC:O2D	0.48	2.61	2	4
1:A:18:VAL:CG1	2:A:111:HEC:HMD3	0.48	2.38	6	1
1:A:67:HIS:CE1	1:A:74:THR:HG22	0.48	2.43	1	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:108:HEC:HMA3	2:A:108:HEC:HBA2	0.48	1.85	3	3
1:A:74:THR:CB	2:A:109:HEC:CGA	0.48	2.91	10	16
1:A:11:MET:CE	2:A:108:HEC:O1D	0.48	2.62	6	2
1:A:9:LEU:O	1:A:9:LEU:CD1	0.48	2.59	13	1
1:A:82:CYS:O	1:A:86:VAL:HG23	0.47	2.09	4	8
1:A:67:HIS:CE1	1:A:71:ASP:CG	0.47	2.87	11	3
1:A:96:ASP:O	1:A:97:LEU:HD23	0.47	2.09	17	10
1:A:98:THR:HA	2:A:111:HEC:HMC2	0.47	1.87	7	18
1:A:67:HIS:NE2	2:A:109:HEC:O2A	0.47	2.48	15	11
1:A:72:LYS:HD2	1:A:84:VAL:HG21	0.47	1.87	9	1
1:A:67:HIS:CG	1:A:67:HIS:O	0.47	2.67	7	1
1:A:66:TYR:CD1	1:A:66:TYR:C	0.46	2.88	19	9
2:A:108:HEC:HBA2	2:A:108:HEC:HMA3	0.46	1.86	5	1
1:A:80:VAL:HG22	2:A:111:HEC:HMC2	0.46	1.87	5	6
2:A:108:HEC:CBD	2:A:108:HEC:HMD1	0.46	2.40	19	10
2:A:108:HEC:HBD2	2:A:108:HEC:HMD1	0.46	1.87	13	7
1:A:14:THR:N	2:A:111:HEC:O2D	0.46	2.49	16	5
1:A:65:TYR:O	1:A:69:MET:CG	0.46	2.63	15	1
1:A:67:HIS:NE2	2:A:109:HEC:O1A	0.46	2.49	7	8
2:A:110:HEC:CBC	2:A:110:HEC:CMC	0.46	2.92	6	1
2:A:110:HEC:CMC	2:A:110:HEC:CBC	0.46	2.92	9	3
1:A:9:LEU:CD2	1:A:9:LEU:C	0.46	2.81	14	7
1:A:67:HIS:ND1	1:A:71:ASP:CG	0.46	2.70	11	3
1:A:11:MET:HE2	2:A:108:HEC:O2D	0.46	2.11	13	1
1:A:52:HIS:ND1	1:A:62:ALA:O	0.46	2.49	14	2
1:A:9:LEU:HD13	1:A:20:PHE:HB3	0.45	1.88	5	4
1:A:66:TYR:C	1:A:66:TYR:CD1	0.45	2.89	18	8
2:A:109:HEC:HBD2	2:A:109:HEC:HMD1	0.45	1.89	4	3
1:A:11:MET:CB	2:A:111:HEC:O2D	0.45	2.64	12	2
1:A:18:VAL:CG2	2:A:111:HEC:C2D	0.45	2.88	6	2
2:A:108:HEC:HMD1	2:A:108:HEC:CBD	0.45	2.41	2	10
1:A:14:THR:N	2:A:111:HEC:O1D	0.45	2.49	3	5
1:A:9:LEU:C	1:A:9:LEU:CD2	0.45	2.82	2	3
1:A:94:LYS:CG	1:A:98:THR:OG1	0.45	2.64	8	2
1:A:11:MET:HE3	2:A:108:HEC:O2D	0.45	2.11	19	3
1:A:12:GLU:CD	1:A:12:GLU:O	0.45	2.55	17	13
1:A:70:HIS:O	1:A:71:ASP:C	0.45	2.54	9	20
1:A:72:LYS:O	1:A:74:THR:N	0.45	2.50	10	6
2:A:109:HEC:HMD1	2:A:109:HEC:O2D	0.45	2.10	20	1
1:A:10:LYS:NZ	1:A:19:VAL:CG2	0.45	2.79	6	2
2:A:109:HEC:O1D	2:A:109:HEC:HMD1	0.45	2.10	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:80:VAL:HG13	1:A:98:THR:HB	0.45	1.89	20	4
1:A:46:CYS:SG	2:A:108:HEC:HMD3	0.44	2.53	4	4
2:A:111:HEC:HBA1	2:A:111:HEC:HMA2	0.44	1.89	15	1
2:A:108:HEC:HMD1	2:A:108:HEC:HBD2	0.44	1.89	14	7
1:A:17:PRO:O	1:A:18:VAL:CG2	0.44	2.66	17	3
1:A:74:THR:HA	2:A:109:HEC:CGA	0.44	2.42	9	3
1:A:20:PHE:O	1:A:21:ASN:ND2	0.44	2.51	13	1
1:A:11:MET:HE2	2:A:108:HEC:CGD	0.44	2.42	20	2
2:A:109:HEC:HMD1	2:A:109:HEC:O1D	0.43	2.10	12	3
1:A:24:THR:HG21	2:A:110:HEC:CBA	0.43	2.42	7	4
1:A:32:ASP:CG	2:A:110:HEC:CBC	0.43	2.87	11	11
1:A:25:HIS:CG	2:A:108:HEC:HBC2	0.43	2.48	9	2
1:A:43:TYR:HB3	2:A:108:HEC:C3A	0.43	2.44	6	16
2:A:110:HEC:C2A	2:A:110:HEC:O2A	0.43	2.66	20	1
1:A:25:HIS:CD2	2:A:108:HEC:HBC2	0.43	2.47	9	7
1:A:5:PRO:HD3	2:A:108:HEC:C4A	0.43	2.43	16	4
1:A:67:HIS:HE2	2:A:109:HEC:CBA	0.43	2.27	18	1
1:A:44:ARG:HG3	2:A:109:HEC:CMC	0.43	2.44	6	1
2:A:110:HEC:O2A	2:A:110:HEC:C2A	0.43	2.67	13	1
1:A:13:ALA:N	2:A:111:HEC:O1D	0.43	2.50	8	1
1:A:101:LYS:O	1:A:102:LYS:CB	0.43	2.67	13	1
1:A:67:HIS:HE2	2:A:109:HEC:CGA	0.42	2.27	18	1
2:A:111:HEC:HMA2	2:A:111:HEC:HBA1	0.42	1.91	13	3
1:A:5:PRO:HG3	2:A:108:HEC:C2A	0.42	2.45	8	11
1:A:67:HIS:NE2	1:A:74:THR:HG22	0.42	2.29	11	1
1:A:11:MET:SD	2:A:111:HEC:CMD	0.42	3.05	18	1
1:A:103:SER:N	1:A:106:HIS:O	0.42	2.49	9	1
1:A:11:MET:SD	1:A:65:TYR:OH	0.42	2.77	11	2
2:A:109:HEC:HMD1	2:A:109:HEC:HBD2	0.42	1.92	5	1
1:A:12:GLU:O	1:A:12:GLU:CD	0.42	2.57	16	6
1:A:9:LEU:HD13	1:A:9:LEU:C	0.42	2.34	17	1
1:A:18:VAL:CB	2:A:111:HEC:HMD3	0.41	2.45	6	1
1:A:20:PHE:C	1:A:21:ASN:ND2	0.41	2.73	13	1
2:A:108:HEC:HBC1	2:A:110:HEC:CHC	0.41	2.45	2	4
1:A:11:MET:HE2	2:A:108:HEC:O1D	0.41	2.15	16	1
1:A:68:VAL:HG12	2:A:109:HEC:CMA	0.41	2.44	5	2
2:A:108:HEC:CBA	2:A:108:HEC:HHA	0.41	2.45	19	2
1:A:17:PRO:O	1:A:18:VAL:HG23	0.41	2.15	13	2
1:A:46:CYS:HA	2:A:109:HEC:CHC	0.41	2.46	18	1
1:A:94:LYS:O	1:A:98:THR:OG1	0.41	2.38	7	1
1:A:74:THR:HB	2:A:109:HEC:CBA	0.41	2.46	3	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:80:VAL:O	1:A:84:VAL:CG2	0.41	2.59	14	1
1:A:11:MET:O	1:A:17:PRO:HA	0.41	2.16	16	1
1:A:97:LEU:O	2:A:111:HEC:HBC3	0.41	2.15	2	1
1:A:11:MET:CG	1:A:11:MET:O	0.41	2.69	19	1
1:A:11:MET:SD	2:A:108:HEC:O2D	0.40	2.79	19	2
1:A:46:CYS:SG	2:A:108:HEC:CMD	0.40	3.10	4	2
1:A:97:LEU:HD11	2:A:110:HEC:HBD1	0.40	1.92	10	2
1:A:69:MET:SD	1:A:79:CYS:SG	0.40	3.20	19	3
1:A:11:MET:SD	2:A:108:HEC:O1D	0.40	2.79	6	1
1:A:24:THR:CG2	2:A:110:HEC:O2A	0.40	2.69	6	1
2:A:110:HEC:HMA2	2:A:110:HEC:O1A	0.40	2.16	17	1
1:A:11:MET:O	2:A:111:HEC:O1D	0.40	2.39	11	1
1:A:10:LYS:HA	1:A:18:VAL:O	0.40	2.15	13	1
1:A:24:THR:CG2	2:A:110:HEC:O1A	0.40	2.69	14	1
1:A:71:ASP:O	1:A:78:SER:CB	0.40	2.69	20	1
1:A:11:MET:O	1:A:17:PRO:CB	0.40	2.69	13	1
1:A:43:TYR:HB3	2:A:108:HEC:C4A	0.40	2.46	16	1
1:A:65:TYR:O	1:A:69:MET:SD	0.40	2.80	7	1
1:A:73:ASN:OD1	1:A:73:ASN:O	0.40	2.40	19	1
2:A:109:HEC:HBD2	2:A:109:HEC:CMD	0.40	2.47	4	1
1:A:65:TYR:OH	2:A:111:HEC:O1D	0.40	2.40	11	1
1:A:34:HIS:O	1:A:35:HIS:C	0.40	2.59	11	1
1:A:29:LYS:O	1:A:32:ASP:CB	0.40	2.69	18	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	86/107 (80%)	70±1 (82±1%)	14±2 (17±2%)	2±1 (2±1%)	14	55
All	All	1720/2140 (80%)	1402 (82%)	284 (17%)	34 (2%)	14	55

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	62	ALA	16
1	A	6	ALA	9
1	A	64	GLY	3
1	A	43	TYR	3
1	A	102	LYS	2
1	A	73	ASN	1

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	74/88 (84%)	58±2 (78±3%)	17±2 (22±3%)	4 31
All	All	1480/1760 (84%)	1150 (78%)	330 (22%)	4 31

All 35 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	96	ASP	20
1	A	55	MET	20
1	A	85	GLU	20
1	A	103	SER	19
1	A	45	LYS	19
1	A	29	LYS	17
1	A	95	LYS	17
1	A	11	MET	16
1	A	9	LEU	16
1	A	44	ARG	14
1	A	94	LYS	14
1	A	72	LYS	12
1	A	71	ASP	12
1	A	16	GLN	11
1	A	102	LYS	10
1	A	101	LYS	10
1	A	66	TYR	10
1	A	10	LYS	8
1	A	67	HIS	8
1	A	78	SER	7

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Mol	Chain	Res	Type	Models (Total)
1	A	23	SER	6
1	A	77	LYS	6
1	A	75	LYS	5
1	A	7	ASP	5
1	A	48	THR	5
1	A	63	LYS	4
1	A	53	ASP	4
1	A	27	SER	3
1	A	15	LYS	3
1	A	107	GLU	2
1	A	69	MET	2
1	A	26	LYS	2
1	A	54	SER	1
1	A	93	LYS	1
1	A	100	CYS	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

4 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
2	HEC	A	108	1	24,50,50	1.76±0.02	2±0 (8±0%)
2	HEC	A	109	1	24,50,50	1.81±0.01	2±0 (8±0%)
2	HEC	A	110	1	24,50,50	1.73±0.01	2±0 (8±0%)
2	HEC	A	111	1	24,50,50	1.79±0.01	2±0 (8±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	HEC	A	108	1	19,82,82	2.33±0.00	2±0 (10±0%)
2	HEC	A	109	1	19,82,82	2.33±0.00	2±0 (10±0%)
2	HEC	A	110	1	19,82,82	2.33±0.00	2±0 (10±0%)
2	HEC	A	111	1	19,82,82	2.33±0.00	2±0 (10±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	HEC	A	108	1	-	0±0,6,54,54	0±0,0,8,8
2	HEC	A	109	1	-	0±0,6,54,54	0±0,0,8,8
2	HEC	A	110	1	-	0±0,6,54,54	0±0,0,8,8
2	HEC	A	111	1	-	0±0,6,54,54	0±0,0,8,8

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
2	A	109	HEC	C3C-C2C	5.23	1.35	1.40	19	20
2	A	111	HEC	C3B-C2B	5.23	1.35	1.40	9	20
2	A	109	HEC	C3B-C2B	5.21	1.35	1.40	4	20
2	A	108	HEC	C3C-C2C	5.21	1.35	1.40	1	20
2	A	110	HEC	C3C-C2C	5.20	1.35	1.40	1	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	A	108	HEC	C3B-C2B	5.20	1.35	1.40	8	20
2	A	111	HEC	C3C-C2C	5.20	1.35	1.40	7	20
2	A	110	HEC	C3B-C2B	5.18	1.35	1.40	16	20

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(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	A	111	HEC	CBC-CAC-C3C	6.13	113.94	127.34	16	20
2	A	108	HEC	CBC-CAC-C3C	6.13	113.94	127.34	17	20
2	A	108	HEC	CBB-CAB-C3B	6.13	113.95	127.34	2	20
2	A	111	HEC	CBB-CAB-C3B	6.13	113.94	127.34	11	20
2	A	110	HEC	CBC-CAC-C3C	6.13	113.95	127.34	15	20
2	A	110	HEC	CBB-CAB-C3B	6.12	113.95	127.34	4	20
2	A	109	HEC	CBB-CAB-C3B	6.12	113.95	127.34	13	20
2	A	109	HEC	CBC-CAC-C3C	6.12	113.95	127.34	14	20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 46% for the well-defined parts and 47% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 5625

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	662
Number of shifts mapped to atoms	662
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	100

7.1.2 Chemical shift referencing

No chemical shift referencing corrections were calculated (not enough data).

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 46%, i.e. 478 atoms were assigned a chemical shift out of a possible 1036. 0 out of 9 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	170/429 (40%)	170/171 (99%)	0/174 (0%)	0/84 (0%)
Sidechain	286/502 (57%)	286/301 (95%)	0/180 (0%)	0/21 (0%)
Aromatic	22/105 (21%)	22/58 (38%)	0/38 (0%)	0/9 (0%)
Overall	478/1036 (46%)	478/530 (90%)	0/392 (0%)	0/114 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 47%, i.e. 587 atoms were assigned a chemical shift out of a possible 1255. 0 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	208/527 (39%)	208/210 (99%)	0/214 (0%)	0/103 (0%)
Sidechain	357/623 (57%)	357/372 (96%)	0/224 (0%)	0/27 (0%)
Aromatic	22/105 (21%)	22/58 (38%)	0/38 (0%)	0/9 (0%)
Overall	587/1255 (47%)	587/640 (92%)	0/476 (0%)	0/139 (0%)

7.1.4 Statistically unusual chemical shifts (i)

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	83	HIS	HB2	19.82	4.91 – 1.31	46.4
1	A	106	HIS	HB3	18.45	5.00 – 1.10	39.5
1	A	52	HIS	HB3	16.11	5.00 – 1.10	33.5
1	A	83	HIS	HB3	14.51	5.00 – 1.10	29.4
1	A	34	HIS	HB3	13.97	5.00 – 1.10	28.0
1	A	35	HIS	HB2	11.37	4.91 – 1.31	22.9
1	A	22	HIS	HB2	10.68	4.91 – 1.31	21.0
1	A	25	HIS	HB3	10.57	5.00 – 1.10	19.3
1	A	25	HIS	HB2	9.58	4.91 – 1.31	18.0
1	A	52	HIS	HB2	9.38	4.91 – 1.31	17.4
1	A	22	HIS	HB3	9.24	5.00 – 1.10	15.9
1	A	70	HIS	HB2	8.71	4.91 – 1.31	15.6
1	A	4	ALA	HA	-2.52	6.46 – 2.06	-15.4
1	A	5	PRO	HD2	-1.84	5.45 – 1.85	-15.2
1	A	70	HIS	HB3	8.86	5.00 – 1.10	14.9
1	A	5	PRO	HD3	-1.84	5.52 – 1.72	-14.4
1	A	52	HIS	HA	10.85	6.81 – 2.41	14.2
1	A	35	HIS	HB3	8.28	5.00 – 1.10	13.4
1	A	79	CYS	HA	-2.78	7.47 – 1.87	-13.3
1	A	68	VAL	HG13	4.27	2.13 – -0.47	13.2
1	A	68	VAL	HG12	4.27	2.13 – -0.47	13.2
1	A	68	VAL	HG11	4.27	2.13 – -0.47	13.2
1	A	106	HIS	HB2	7.48	4.91 – 1.31	12.1
1	A	33	CYS	HB3	-2.75	5.25 – 0.55	-12.0
1	A	16	GLN	HG3	5.50	3.75 – 0.85	11.0
1	A	97	LEU	HD21	-2.28	2.14 – -0.66	-10.8
1	A	97	LEU	HD22	-2.28	2.14 – -0.66	-10.8
1	A	97	LEU	HD23	-2.28	2.14 – -0.66	-10.8
1	A	69	MET	HB3	-1.58	3.70 – 0.30	-10.5
1	A	18	VAL	HG23	-2.07	2.20 – -0.60	-10.2
1	A	18	VAL	HG22	-2.07	2.20 – -0.60	-10.2

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Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	18	VAL	HG21	-2.07	2.20 – -0.60	-10.2
1	A	35	HIS	HA	9.10	6.81 – 2.41	10.2
1	A	22	HIS	HA	8.86	6.81 – 2.41	9.7
1	A	82	CYS	HB3	-1.58	5.25 – 0.55	-9.5
1	A	106	HIS	HA	8.66	6.81 – 2.41	9.2
1	A	18	VAL	HB	-0.88	3.59 – 0.39	-9.0
1	A	34	HIS	HB2	6.10	4.91 – 1.31	8.3
1	A	18	VAL	HG12	-1.31	2.13 – -0.47	-8.2
1	A	18	VAL	HG13	-1.31	2.13 – -0.47	-8.2
1	A	18	VAL	HG11	-1.31	2.13 – -0.47	-8.2
1	A	36	PRO	HD2	6.59	5.45 – 1.85	8.2
1	A	2	PRO	HG2	-0.42	3.48 – 0.38	-7.6
1	A	62	ALA	HB2	-0.47	2.61 – 0.11	-7.3
1	A	62	ALA	HB1	-0.47	2.61 – 0.11	-7.3
1	A	62	ALA	HB3	-0.47	2.61 – 0.11	-7.3
1	A	63	LYS	HD3	3.26	2.75 – 0.45	7.2
1	A	2	PRO	HB2	-0.45	3.82 – 0.32	-7.2
1	A	36	PRO	HD3	6.30	5.52 – 1.72	7.1
1	A	68	VAL	HG23	2.77	2.20 – -0.60	7.0
1	A	68	VAL	HG22	2.77	2.20 – -0.60	7.0
1	A	68	VAL	HG21	2.77	2.20 – -0.60	7.0
1	A	77	LYS	HB3	-0.06	3.10 – 0.40	-6.7
1	A	63	LYS	HD2	3.14	2.76 – 0.46	6.7
1	A	41	GLU	HG2	3.67	3.33 – 1.23	6.6
1	A	20	PHE	HD2	5.08	8.56 – 5.56	-6.6
1	A	100	CYS	HB3	-0.15	5.25 – 0.55	-6.5
1	A	77	LYS	HB2	0.17	3.03 – 0.53	-6.4
1	A	66	TYR	HD2	8.87	8.44 – 5.44	6.4
1	A	66	TYR	HD1	8.87	8.44 – 5.44	6.4
1	A	25	HIS	HA	7.44	6.81 – 2.41	6.4
1	A	52	HIS	H	12.61	11.68 – 4.78	6.3
1	A	82	CYS	HB2	0.13	5.20 – 0.70	-6.3
1	A	36	PRO	HA	6.46	6.05 – 2.75	6.2
1	A	23	SER	H	11.94	11.23 – 5.33	6.2
1	A	63	LYS	HA	6.95	6.46 – 2.06	6.1
1	A	46	CYS	HB3	0.04	5.25 – 0.55	-6.1
1	A	46	CYS	HA	1.27	7.47 – 1.87	-6.1
1	A	16	GLN	HB2	3.56	3.30 – 0.80	6.0
1	A	36	PRO	HG2	3.80	3.48 – 0.38	6.0
1	A	42	ASP	HB2	4.34	4.07 – 1.37	6.0
1	A	5	PRO	HG2	3.78	3.48 – 0.38	6.0
1	A	43	TYR	HE1	5.36	7.86 – 5.56	-5.9

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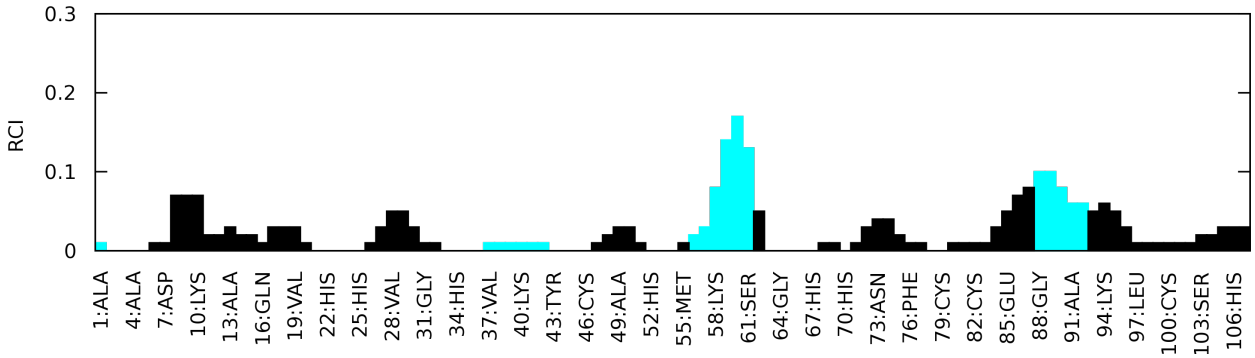
Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	43	TYR	HE2	5.36	7.86 – 5.56	-5.9
1	A	34	HIS	HA	7.14	6.81 – 2.41	5.8
1	A	20	PHE	HB3	0.79	4.85 – 1.05	-5.7
1	A	104	LYS	HB2	0.36	3.03 – 0.53	-5.7
1	A	65	TYR	HB2	4.95	4.76 – 1.06	5.5
1	A	69	MET	HB2	0.17	3.73 – 0.33	-5.5
1	A	66	TYR	HB3	4.92	4.75 – 0.95	5.4
1	A	79	CYS	HB2	0.50	5.20 – 0.70	-5.4
1	A	76	PHE	HZ	9.29	9.11 – 4.91	5.4
1	A	7	ASP	HA	6.28	6.15 – 3.05	5.4
1	A	76	PHE	HE1	8.82	8.69 – 5.49	5.4
1	A	76	PHE	HE2	8.82	8.69 – 5.49	5.4
1	A	78	SER	HA	2.27	6.53 – 2.43	-5.4
1	A	79	CYS	H	4.79	11.75 – 5.05	-5.4
1	A	2	PRO	HD3	1.58	5.52 – 1.72	-5.4
1	A	67	HIS	HB3	5.13	5.00 – 1.10	5.3
1	A	97	LEU	HB3	3.46	3.34 – -0.26	5.3
1	A	22	HIS	H	11.89	11.68 – 4.78	5.3
1	A	70	HIS	HA	6.92	6.81 – 2.41	5.3
1	A	41	GLU	HG3	3.36	3.31 – 1.21	5.2
1	A	104	LYS	HD3	0.41	2.75 – 0.45	-5.2
1	A	11	MET	HE1	-0.59	4.28 – -0.52	-5.1
1	A	11	MET	HE2	-0.59	4.28 – -0.52	-5.1
1	A	11	MET	HE3	-0.59	4.28 – -0.52	-5.1
1	A	35	HIS	H	11.72	11.68 – 4.78	5.1
1	A	41	GLU	HB3	3.11	3.10 – 0.90	5.0
1	A	47	GLY	HA2	5.88	5.87 – 2.07	5.0

7.1.5 Random Coil Index (RCI) plots

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:



7.2 Chemical shift list 2

File name: BMRB entry 5625

Chemical shift list name: *assigned_chem_shift_list_2*

7.2.1 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	20
Number of shifts mapped to atoms	0
Number of unparsed shifts	0
Number of shifts with mapping errors	20
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- Chain not found in structure. All 20 occurences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	1	HEC	HBD2	0.34	0.01	2
UNMAPPED	1	HEC	HAD1	0.13	0.01	2
UNMAPPED	1	HEC	HBD1	1.41	0.01	2
UNMAPPED	1	HEC	HAA1	6.09	0.01	2
UNMAPPED	1	HEC	HAA2	3.99	0.01	2
UNMAPPED	1	HEC	HMC	9.96	0.01	1
UNMAPPED	1	HEC	HMA	29.11	0.01	1
UNMAPPED	1	HEC	HHC	12.37	0.01	1
UNMAPPED	1	HEC	HAD2	-4.07	0.01	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	1	HEC	HBC	-2.28	0.01	1
UNMAPPED	1	HEC	HMD	17.97	0.01	1
UNMAPPED	1	HEC	HHB	-3.6	0.01	1
UNMAPPED	1	HEC	HAB	2.83	0.01	1
UNMAPPED	1	HEC	HBA1	2.72	0.01	2
UNMAPPED	1	HEC	HBB	0.64	0.01	1
UNMAPPED	1	HEC	HBA2	2.48	0.01	2
UNMAPPED	1	HEC	HHA	11.56	0.01	1
UNMAPPED	1	HEC	HAC	-3.26	0.01	1
UNMAPPED	1	HEC	HMB	18.3	0.01	1
UNMAPPED	1	HEC	HHD	-6.37	0.01	1

7.2.2 Chemical shift referencing

No chemical shift referencing corrections were calculated (not enough data).

7.2.3 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 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 1036. 0 out of 9 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	0/429 (0%)	0/171 (0%)	0/174 (0%)	0/84 (0%)
Sidechain	0/502 (0%)	0/301 (0%)	0/180 (0%)	0/21 (0%)
Aromatic	0/105 (0%)	0/58 (0%)	0/38 (0%)	0/9 (0%)
Overall	0/1036 (0%)	0/530 (0%)	0/392 (0%)	0/114 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 1255. 0 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	0/527 (0%)	0/210 (0%)	0/214 (0%)	0/103 (0%)
Sidechain	0/623 (0%)	0/372 (0%)	0/224 (0%)	0/27 (0%)
Aromatic	0/105 (0%)	0/58 (0%)	0/38 (0%)	0/9 (0%)
Overall	0/1255 (0%)	0/640 (0%)	0/476 (0%)	0/139 (0%)

7.2.4 Statistically unusual chemical shifts

There are no statistically unusual chemical shifts.

7.2.5 Random Coil Index (RCI) plots

No *random coil index* (RCI) plot could be generated from the current chemical shift list (assigned_chem_shift_list_2). RCI is only applicable to proteins.

7.3 Chemical shift list 3

File name: BMRB entry 5625

Chemical shift list name: *assigned_chem_shift_list_3*

7.3.1 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	20
Number of shifts mapped to atoms	0
Number of unparsed shifts	0
Number of shifts with mapping errors	20
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- Chain not found in structure. All 20 occurences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	1	HEC	HBD2	-0.94	0.01	2
UNMAPPED	1	HEC	HAD1	1.36	0.01	2
UNMAPPED	1	HEC	HBD1	-0.94	0.01	2
UNMAPPED	1	HEC	HAA1	12.4	0.01	2
UNMAPPED	1	HEC	HAA2	6.45	0.01	2
UNMAPPED	1	HEC	HMC	21.91	0.01	1
UNMAPPED	1	HEC	HMA	21.95	0.01	1
UNMAPPED	1	HEC	HHC	3.43	0.01	1
UNMAPPED	1	HEC	HAD2	-1.26	0.01	2
UNMAPPED	1	HEC	HBC	2.22	0.01	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	1	HEC	HMD	5.08	0.01	1
UNMAPPED	1	HEC	HHB	0.85	0.01	1
UNMAPPED	1	HEC	HAB	-1.67	0.01	1
UNMAPPED	1	HEC	HBA1	-0.45	0.01	2
UNMAPPED	1	HEC	HBB	-3.25	0.01	1
UNMAPPED	1	HEC	HBA2	0.99	0.01	2
UNMAPPED	1	HEC	HHA	2.0	0.01	1
UNMAPPED	1	HEC	HAC	2.08	0.01	1
UNMAPPED	1	HEC	HMB	4.36	0.01	1
UNMAPPED	1	HEC	HHD	0.97	0.01	1

7.3.2 Chemical shift referencing (i)

No chemical shift referencing corrections were calculated (not enough data).

7.3.3 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 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 1036. 0 out of 9 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	0/429 (0%)	0/171 (0%)	0/174 (0%)	0/84 (0%)
Sidechain	0/502 (0%)	0/301 (0%)	0/180 (0%)	0/21 (0%)
Aromatic	0/105 (0%)	0/58 (0%)	0/38 (0%)	0/9 (0%)
Overall	0/1036 (0%)	0/530 (0%)	0/392 (0%)	0/114 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 1255. 0 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	0/527 (0%)	0/210 (0%)	0/214 (0%)	0/103 (0%)
Sidechain	0/623 (0%)	0/372 (0%)	0/224 (0%)	0/27 (0%)
Aromatic	0/105 (0%)	0/58 (0%)	0/38 (0%)	0/9 (0%)
Overall	0/1255 (0%)	0/640 (0%)	0/476 (0%)	0/139 (0%)

7.3.4 Statistically unusual chemical shifts

There are no statistically unusual chemical shifts.

7.3.5 Random Coil Index (RCI) plots

No *random coil index* (RCI) plot could be generated from the current chemical shift list (assigned_chem_shift_list_3). RCI is only applicable to proteins.

7.4 Chemical shift list 4

File name: BMRB entry 5625

Chemical shift list name: *assigned_chem_shift_list_4*

7.4.1 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	20
Number of shifts mapped to atoms	0
Number of unparsed shifts	0
Number of shifts with mapping errors	20
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- Chain not found in structure. All 20 occurences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	1	HEC	HBD2	-1.27	0.01	2
UNMAPPED	1	HEC	HAD1	17.13	0.01	2
UNMAPPED	1	HEC	HBD1	-0.01	0.01	2
UNMAPPED	1	HEC	HAA1	-2.66	0.01	2
UNMAPPED	1	HEC	HAA2	6.59	0.01	2
UNMAPPED	1	HEC	HMC	9.97	0.01	1
UNMAPPED	1	HEC	HMA	-3.93	0.01	1
UNMAPPED	1	HEC	HHC	-2.41	0.01	1
UNMAPPED	1	HEC	HAD2	16.96	0.01	2
UNMAPPED	1	HEC	HBC	-0.81	0.01	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	1	HEC	HMD	20.46	0.01	1
UNMAPPED	1	HEC	HHB	8.94	0.01	1
UNMAPPED	1	HEC	HAB	-0.9	0.01	1
UNMAPPED	1	HEC	HBA1	0.59	0.01	2
UNMAPPED	1	HEC	HBB	-2.3	0.01	1
UNMAPPED	1	HEC	HBA2	-3.77	0.01	2
UNMAPPED	1	HEC	HHA	-0.66	0.01	1
UNMAPPED	1	HEC	HAC	-0.75	0.01	1
UNMAPPED	1	HEC	HMB	13.65	0.01	1
UNMAPPED	1	HEC	HHD	10.28	0.01	1

7.4.2 Chemical shift referencing (i)

No chemical shift referencing corrections were calculated (not enough data).

7.4.3 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 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 1036. 0 out of 9 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	0/429 (0%)	0/171 (0%)	0/174 (0%)	0/84 (0%)
Sidechain	0/502 (0%)	0/301 (0%)	0/180 (0%)	0/21 (0%)
Aromatic	0/105 (0%)	0/58 (0%)	0/38 (0%)	0/9 (0%)
Overall	0/1036 (0%)	0/530 (0%)	0/392 (0%)	0/114 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 1255. 0 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	0/527 (0%)	0/210 (0%)	0/214 (0%)	0/103 (0%)
Sidechain	0/623 (0%)	0/372 (0%)	0/224 (0%)	0/27 (0%)
Aromatic	0/105 (0%)	0/58 (0%)	0/38 (0%)	0/9 (0%)
Overall	0/1255 (0%)	0/640 (0%)	0/476 (0%)	0/139 (0%)

7.4.4 Statistically unusual chemical shifts

There are no statistically unusual chemical shifts.

7.4.5 Random Coil Index (RCI) plots

No *random coil index* (RCI) plot could be generated from the current chemical shift list (assigned_chem_shift_list_4). RCI is only applicable to proteins.

7.5 Chemical shift list 5

File name: BMRB entry 5625

Chemical shift list name: *assigned_chem_shift_list_5*

7.5.1 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	20
Number of shifts mapped to atoms	0
Number of unparsed shifts	0
Number of shifts with mapping errors	20
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- Chain not found in structure. All 20 occurences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	1	HEC	HBD2	0.49	0.01	2
UNMAPPED	1	HEC	HAD1	-3.49	0.01	2
UNMAPPED	1	HEC	HBD1	1.32	0.01	2
UNMAPPED	1	HEC	HAA1	9.1	0.01	2
UNMAPPED	1	HEC	HAA2	5.56	0.01	2
UNMAPPED	1	HEC	HMC	9.92	0.01	1
UNMAPPED	1	HEC	HMA	29.52	0.01	1
UNMAPPED	1	HEC	HHC	12.59	0.01	1
UNMAPPED	1	HEC	HAD2	-0.21	0.01	2
UNMAPPED	1	HEC	HBC	-0.69	0.01	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	1	HEC	HMD	17.07	0.01	1
UNMAPPED	1	HEC	HHB	-0.32	0.01	1
UNMAPPED	1	HEC	HAB	1.44	0.01	1
UNMAPPED	1	HEC	HBA1	3.46	0.01	2
UNMAPPED	1	HEC	HBB	0.98	0.01	1
UNMAPPED	1	HEC	HBA2	3.11	0.01	2
UNMAPPED	1	HEC	HHA	11.98	0.01	1
UNMAPPED	1	HEC	HAC	1.62	0.01	1
UNMAPPED	1	HEC	HMB	18.06	0.01	1
UNMAPPED	1	HEC	HHD	-3.72	0.01	1

7.5.2 Chemical shift referencing (i)

No chemical shift referencing corrections were calculated (not enough data).

7.5.3 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 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 1036. 0 out of 9 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	0/429 (0%)	0/171 (0%)	0/174 (0%)	0/84 (0%)
Sidechain	0/502 (0%)	0/301 (0%)	0/180 (0%)	0/21 (0%)
Aromatic	0/105 (0%)	0/58 (0%)	0/38 (0%)	0/9 (0%)
Overall	0/1036 (0%)	0/530 (0%)	0/392 (0%)	0/114 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 1255. 0 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	0/527 (0%)	0/210 (0%)	0/214 (0%)	0/103 (0%)
Sidechain	0/623 (0%)	0/372 (0%)	0/224 (0%)	0/27 (0%)
Aromatic	0/105 (0%)	0/58 (0%)	0/38 (0%)	0/9 (0%)
Overall	0/1255 (0%)	0/640 (0%)	0/476 (0%)	0/139 (0%)

7.5.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

7.5.5 Random Coil Index (RCI) plots (i)

No *random coil index* (RCI) plot could be generated from the current chemical shift list (assigned_chem_shift_list_5). RCI is only applicable to proteins.