



# Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 06:10 PM BST

PDB ID : 1SR3  
Title : Solution structure of the heme chaperone CcmE of Escherichia coli  
Authors : Enggist, E.; Thony-Meyer, L.; Guntert, P.; Pervushin, K.  
Deposited on : 2004-03-22

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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 : unknown  
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

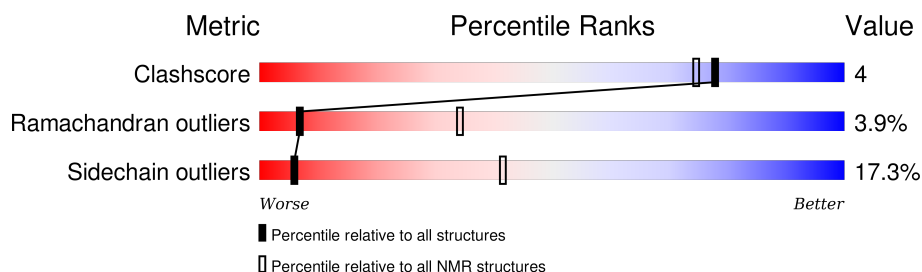
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment was not calculated.

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  $\geq 3$ , 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	136	<div> <div></div> <div>52%</div> <div>10%</div> <div>21%</div> <div>16%</div> </div>

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 8 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:36-A:47, A:53-A:73, A:78-A:129 (85)	0.32	8

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. No single-model clusters were found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1777 atoms, of which 884 are hydrogens and 0 are deuteriums.

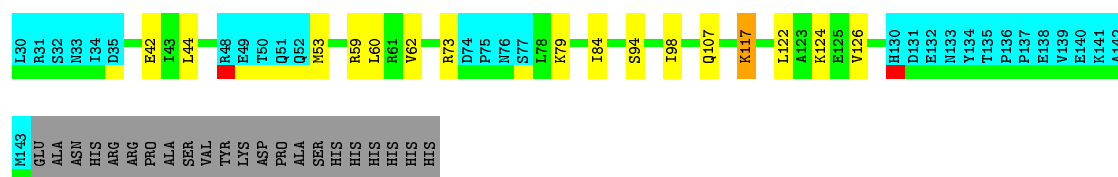
- Molecule 1 is a protein called APO-CCME.

Mol	Chain	Residues	Atoms						Trace
1	A	114	Total	C	H	N	O	S	0
			1777	562	884	152	175	4	

There are 6 discrepancies between the modelled and reference sequences:

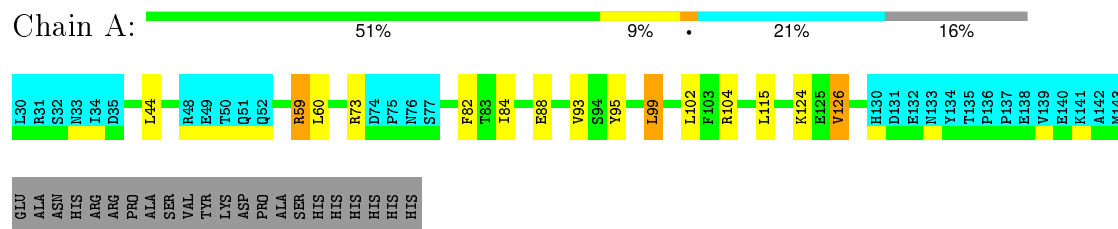
Chain	Residue	Modelled	Actual	Comment	Reference
A	160	HIS	-	INSERTION	UNP P69490
A	161	HIS	-	INSERTION	UNP P69490
A	162	HIS	-	INSERTION	UNP P69490
A	163	HIS	-	INSERTION	UNP P69490
A	164	HIS	-	INSERTION	UNP P69490
A	165	HIS	-	INSERTION	UNP P69490





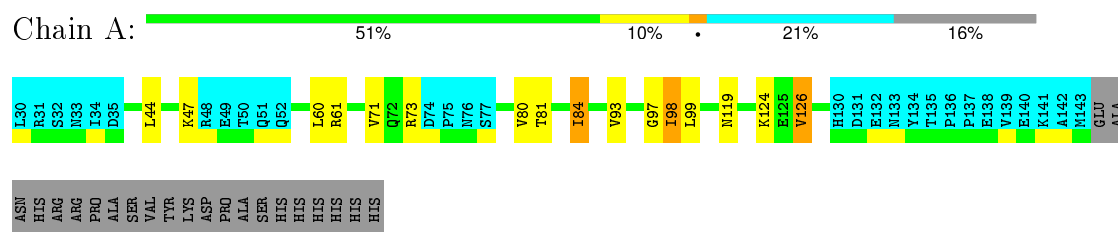
#### 4.2.3 Score per residue for model 3

- Molecule 1: APO-CCME



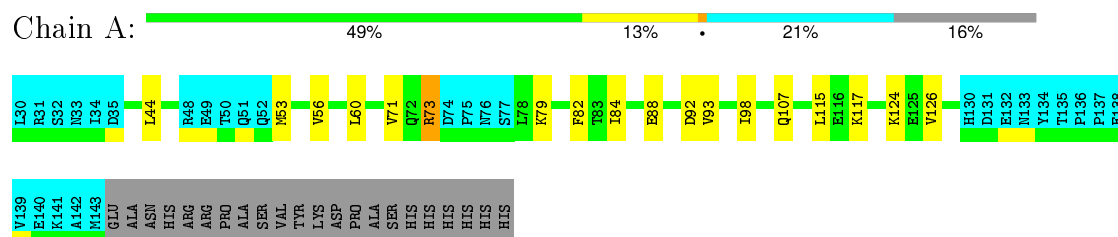
#### 4.2.4 Score per residue for model 4

- Molecule 1: APO-CCME



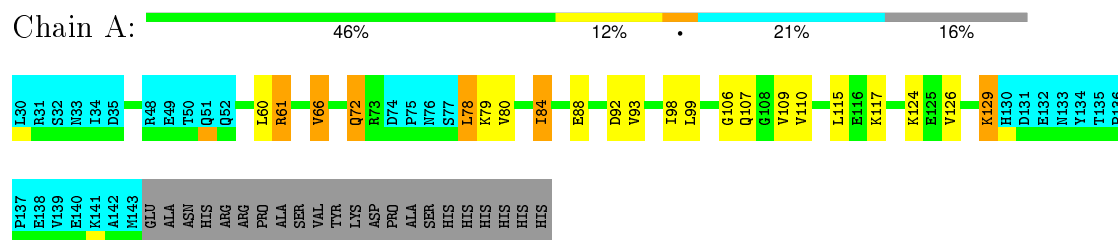
#### 4.2.5 Score per residue for model 5

- Molecule 1: APO-CCME



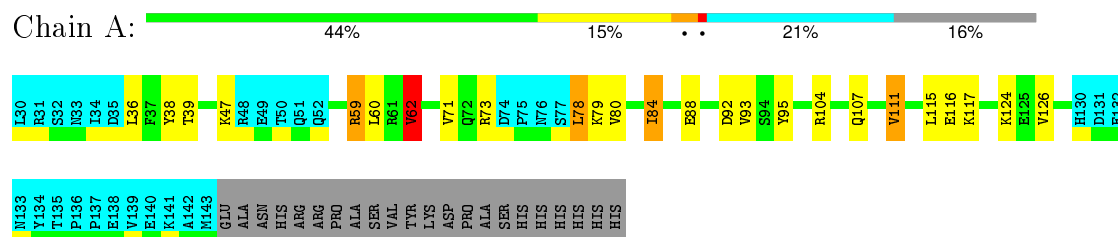
#### 4.2.6 Score per residue for model 6

- Molecule 1: APO-CCME



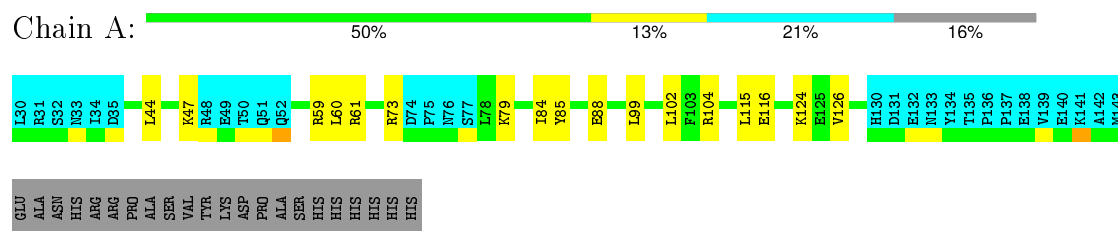
#### 4.2.7 Score per residue for model 7

- Molecule 1: APO-CCME



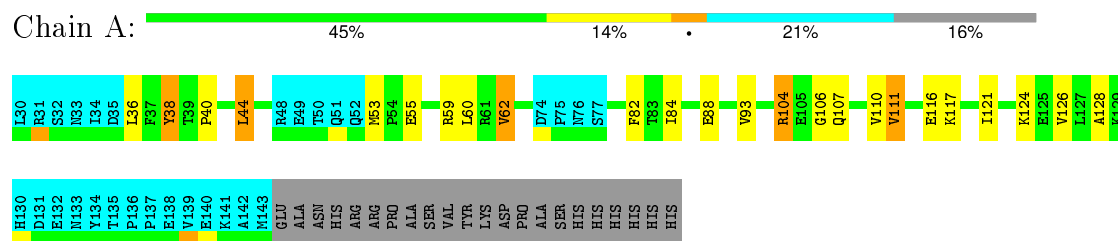
#### 4.2.8 Score per residue for model 8 (medoid)

- Molecule 1: APO-CCME



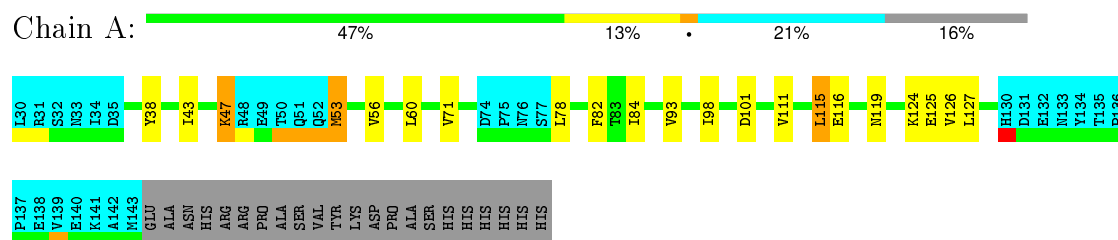
#### 4.2.9 Score per residue for model 9

- Molecule 1: APO-CCME



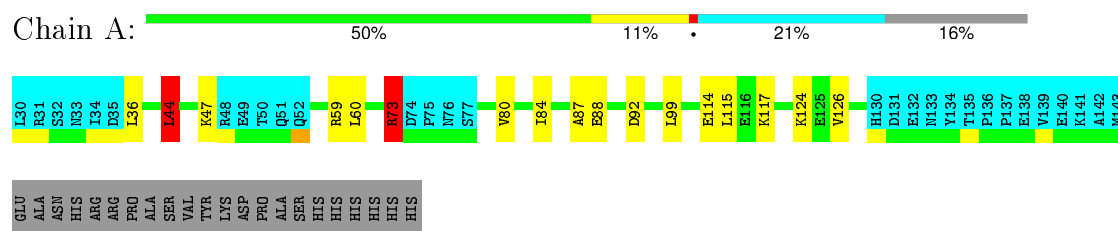
#### 4.2.10 Score per residue for model 10

- Molecule 1: APO-CCME



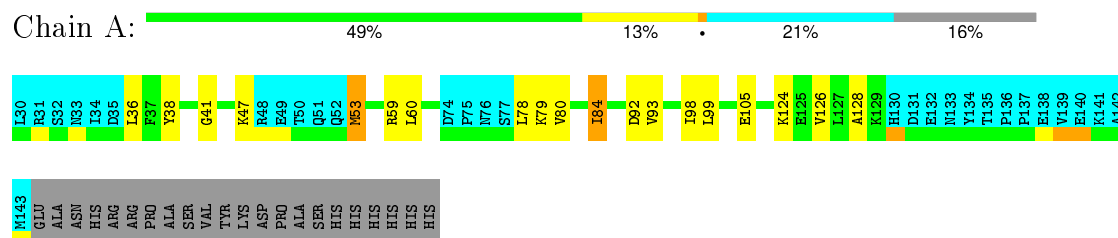
#### 4.2.11 Score per residue for model 11

- Molecule 1: APO-CCME



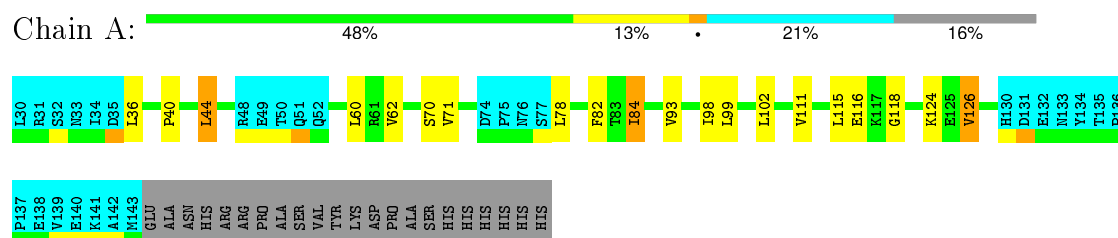
#### 4.2.12 Score per residue for model 12

- Molecule 1: APO-CCME



#### 4.2.13 Score per residue for model 13

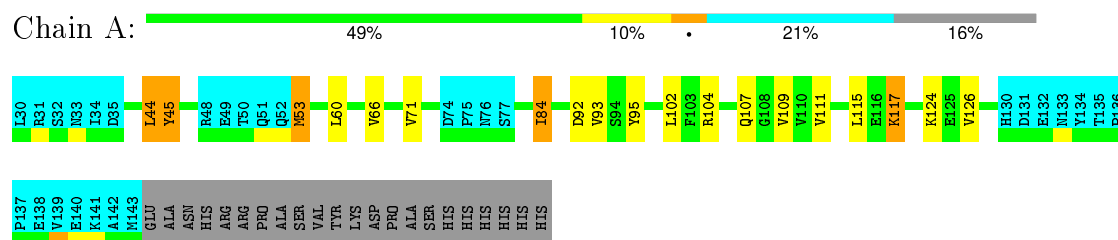
- Molecule 1: APO-CCME





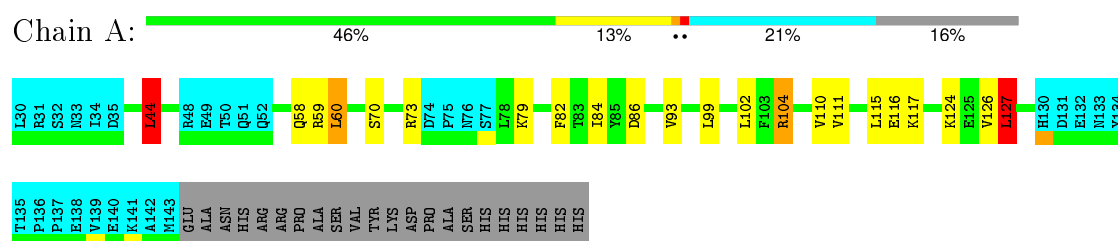
## 4.2.14 Score per residue for model 14

- Molecule 1: APO-CCME



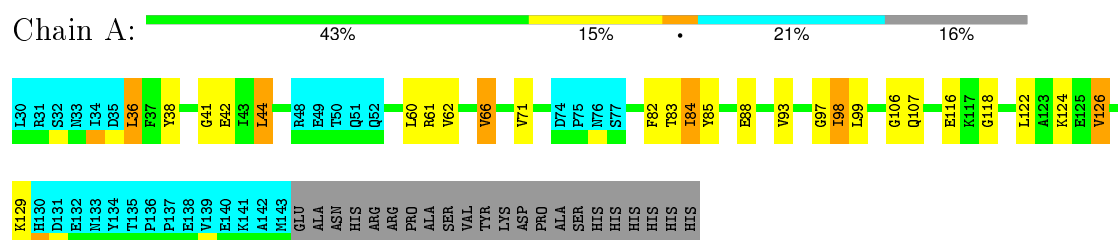
## 4.2.15 Score per residue for model 15

- Molecule 1: APO-CCME



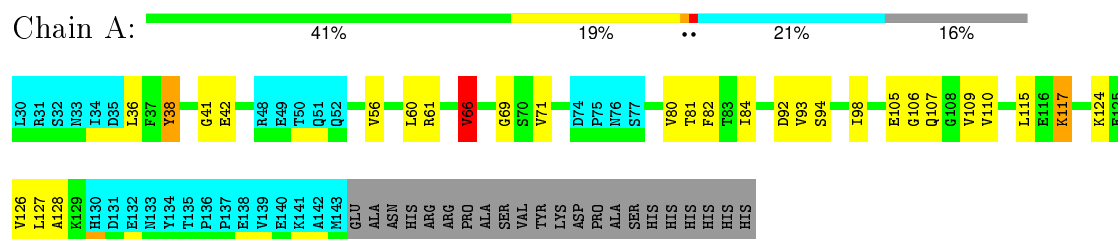
## 4.2.16 Score per residue for model 16

- Molecule 1: APO-CCME



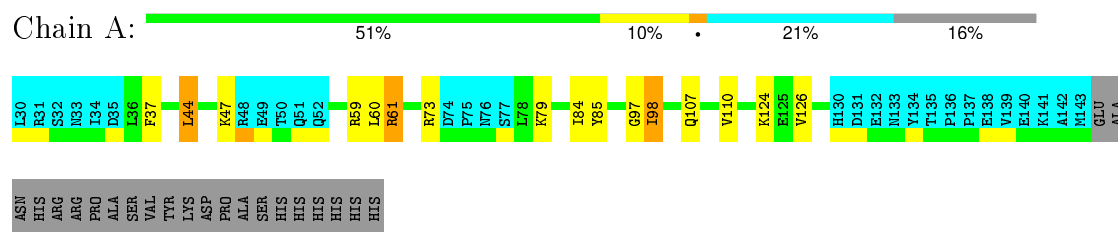
## 4.2.17 Score per residue for model 17

- Molecule 1: APO-CCME



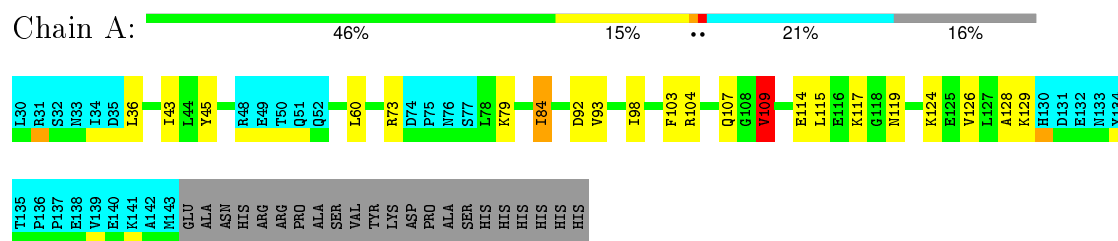
#### 4.2.18 Score per residue for model 18

- Molecule 1: APO-CCME



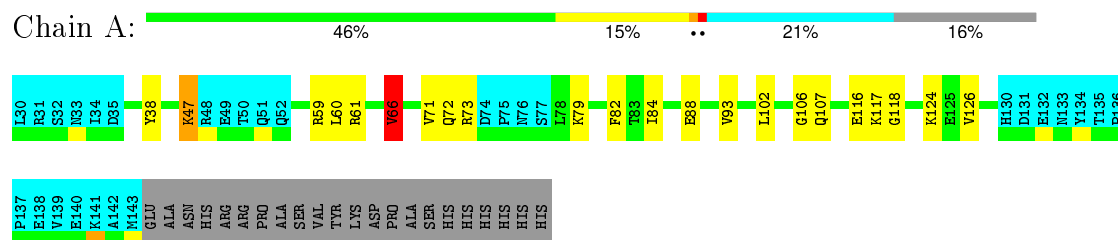
#### 4.2.19 Score per residue for model 19

- Molecule 1: APO-CCME



#### 4.2.20 Score per residue for model 20

- Molecule 1: APO-CCME



## 5 Refinement protocol and experimental data overview

Of the 20 calculated structures, 20 were deposited, based on the following criterion: *all calculated structures submitted*.

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

Software name	Classification	Version
DYANA	refinement	
CANDID	structure solution	

No chemical shift data was provided. 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

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	0.62±0.01	0±0/667 (0.0±0.0%)	1.17±0.04	1±1/900 (0.1±0.1%)
All	All	0.62	0/13340 (0.0%)	1.17	25/18000 (0.1%)

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	1.5±1.2
All	All	0	30

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
1	A	62	VAL	CA-CB-CG1	11.77	128.55	110.90	7	5
1	A	109	VAL	CA-CB-CG1	7.92	122.78	110.90	19	1
1	A	66	VAL	CA-CB-CG1	7.80	122.60	110.90	20	2
1	A	44	LEU	CB-CG-CD1	7.53	123.80	111.00	11	2
1	A	111	VAL	CA-CB-CG2	6.83	121.14	110.90	14	2
1	A	61	ARG	NE-CZ-NH2	-6.34	117.13	120.30	4	2
1	A	44	LEU	CB-CG-CD2	6.26	121.65	111.00	16	1
1	A	110	VAL	CA-CB-CG1	6.17	120.15	110.90	9	2
1	A	59	ARG	NE-CZ-NH2	-5.70	117.45	120.30	20	2
1	A	95	TYR	CB-CG-CD2	-5.25	117.85	121.00	7	1
1	A	45	TYR	CB-CG-CD2	-5.23	117.86	121.00	14	1
1	A	61	ARG	NE-CZ-NH1	5.22	122.91	120.30	6	1
1	A	59	ARG	NE-CZ-NH1	5.21	122.91	120.30	8	1
1	A	95	TYR	CB-CG-CD1	-5.18	117.89	121.00	3	1
1	A	127	LEU	CB-CG-CD2	5.15	119.75	111.00	15	1

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	47	LYS	Peptide	6
1	A	104	ARG	Sidechain	5
1	A	61	ARG	Sidechain	4
1	A	59	ARG	Sidechain	3
1	A	85	TYR	Sidechain	3
1	A	38	TYR	Sidechain	3
1	A	73	ARG	Sidechain	2
1	A	95	TYR	Sidechain	1
1	A	45	TYR	Sidechain	1
1	A	62	VAL	Peptide	1
1	A	106	GLY	Peptide	1

## 6.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in 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	655	669	669	5±3
All	All	13100	13380	13380	96

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 4.

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:ILE:HG22	1:A:119:ASN:HD21	0.69	1.48	19	1
1:A:44:LEU:H	1:A:44:LEU:HD13	0.68	1.47	15	1
1:A:66:VAL:HG13	1:A:106:GLY:H	0.66	1.50	16	4
1:A:110:VAL:HG22	1:A:127:LEU:HB2	0.66	1.66	15	1
1:A:44:LEU:HD22	1:A:44:LEU:H	0.65	1.49	9	1
1:A:82:PHE:CE1	1:A:93:VAL:HG21	0.60	2.31	3	7
1:A:84:ILE:HD11	1:A:93:VAL:HG11	0.59	1.74	16	3
1:A:44:LEU:HD12	1:A:45:TYR:CE1	0.59	2.32	14	1
1:A:103:PHE:CD2	1:A:109:VAL:HG21	0.59	2.32	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:111:VAL:CG1	1:A:121:ILE:HG21	0.59	2.28	9	1
1:A:36:LEU:HD11	1:A:38:TYR:CE1	0.58	2.33	16	1
1:A:99:LEU:CD2	1:A:126:VAL:HG11	0.54	2.31	13	4
1:A:38:TYR:CE2	1:A:47:LYS:HD3	0.53	2.39	20	1
1:A:56:VAL:HG11	1:A:117:LYS:HE3	0.53	1.80	17	1
1:A:66:VAL:HG13	1:A:106:GLY:N	0.53	2.15	16	2
1:A:78:LEU:HD22	1:A:78:LEU:H	0.53	1.62	6	1
1:A:36:LEU:C	1:A:36:LEU:HD12	0.52	2.25	17	2
1:A:82:PHE:CD1	1:A:93:VAL:CG2	0.52	2.92	10	8
1:A:36:LEU:HD13	1:A:38:TYR:CE1	0.52	2.40	17	1
1:A:110:VAL:HG23	1:A:129:LYS:HE2	0.52	1.81	6	1
1:A:43:ILE:HG22	1:A:119:ASN:HD22	0.51	1.63	10	1
1:A:44:LEU:CD1	1:A:44:LEU:H	0.51	2.17	15	1
1:A:80:VAL:HG21	1:A:99:LEU:HD22	0.51	1.82	6	1
1:A:62:VAL:HG12	1:A:111:VAL:HG12	0.51	1.82	9	1
1:A:43:ILE:HG22	1:A:119:ASN:ND2	0.50	2.19	19	2
1:A:43:ILE:CG2	1:A:119:ASN:HD21	0.50	2.18	19	1
1:A:56:VAL:HA	1:A:115:LEU:HD23	0.49	1.84	5	1
1:A:40:PRO:O	1:A:44:LEU:HD21	0.49	2.07	9	2
1:A:71:VAL:HG22	1:A:73:ARG:HG2	0.48	1.85	5	1
1:A:84:ILE:HD11	1:A:93:VAL:HG21	0.48	1.86	6	3
1:A:44:LEU:HD23	1:A:44:LEU:N	0.48	2.23	13	2
1:A:84:ILE:HD11	1:A:93:VAL:CG2	0.47	2.40	6	5
1:A:44:LEU:HD13	1:A:44:LEU:H	0.47	1.69	11	1
1:A:84:ILE:HD11	1:A:93:VAL:CG1	0.47	2.39	13	1
1:A:44:LEU:HD13	1:A:44:LEU:N	0.46	2.23	15	1
1:A:62:VAL:HG13	1:A:111:VAL:HG12	0.46	1.88	7	1
1:A:82:PHE:CZ	1:A:93:VAL:HG21	0.45	2.46	13	6
1:A:38:TYR:CE2	1:A:47:LYS:HD2	0.45	2.46	10	1
1:A:72:GLN:O	1:A:80:VAL:HG23	0.45	2.10	6	1
1:A:38:TYR:C	1:A:62:VAL:HG23	0.45	2.32	9	1
1:A:39:THR:HA	1:A:62:VAL:HG23	0.45	1.88	7	1
1:A:125:GLU:HG3	1:A:127:LEU:HD21	0.45	1.89	10	1
1:A:111:VAL:HG11	1:A:121:ILE:HG21	0.44	1.89	9	1
1:A:44:LEU:CD1	1:A:44:LEU:N	0.44	2.81	15	1
1:A:44:LEU:N	1:A:44:LEU:HD23	0.44	2.26	1	1
1:A:107:GLN:OE1	1:A:128:ALA:HB1	0.44	2.13	9	1
1:A:103:PHE:CE2	1:A:109:VAL:HG21	0.43	2.48	19	1
1:A:116:GLU:HG2	1:A:122:LEU:HD21	0.43	1.89	16	1
1:A:58:GLN:HG3	1:A:60:LEU:HD12	0.43	1.89	15	1
1:A:94:SER:OG	1:A:122:LEU:HD13	0.42	2.14	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:44:LEU:N	1:A:44:LEU:CD1	0.42	2.83	11	1
1:A:82:PHE:CD1	1:A:93:VAL:HG21	0.42	2.49	9	2
1:A:93:VAL:HG11	1:A:111:VAL:HG21	0.42	1.91	15	1
1:A:38:TYR:CE2	1:A:47:LYS:CD	0.42	3.03	12	1
1:A:44:LEU:HD22	1:A:44:LEU:N	0.42	2.24	9	1
1:A:82:PHE:CE1	1:A:93:VAL:CG2	0.41	3.04	10	1
1:A:56:VAL:HA	1:A:115:LEU:HD13	0.41	1.91	10	1
1:A:44:LEU:N	1:A:44:LEU:HD13	0.40	2.31	11	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	85/136 (62%)	69±2 (82±3%)	12±2 (15±2%)	3±1 (4±2%)	<b>7</b>	34
All	All	1700/2720 (62%)	1387 (82%)	247 (15%)	66 (4%)	<b>7</b>	34

All 17 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	126	VAL	20
1	A	71	VAL	6
1	A	99	LEU	5
1	A	73	ARG	5
1	A	53	MET	4
1	A	117	LYS	4
1	A	98	ILE	4
1	A	41	GLY	3
1	A	97	GLY	3
1	A	118	GLY	3
1	A	78	LEU	2
1	A	129	LYS	2
1	A	86	ASP	1
1	A	69	GLY	1

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Mol	Chain	Res	Type	Models (Total)
1	A	87	ALA	1
1	A	47	LYS	1
1	A	37	PHE	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	70/117 (60%)	58±2 (83±3%)	12±2 (17±3%)	6	41
All	All	1400/2340 (60%)	1158 (83%)	242 (17%)	6	41

All 42 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	60	LEU	20
1	A	124	LYS	20
1	A	84	ILE	20
1	A	44	LEU	13
1	A	115	LEU	12
1	A	107	GLN	11
1	A	79	LYS	10
1	A	88	GLU	10
1	A	117	LYS	10
1	A	98	ILE	10
1	A	92	ASP	8
1	A	59	ARG	8
1	A	116	GLU	7
1	A	36	LEU	6
1	A	102	LEU	6
1	A	73	ARG	6
1	A	80	VAL	6
1	A	53	MET	5
1	A	66	VAL	5
1	A	78	LEU	4
1	A	111	VAL	4
1	A	104	ARG	4

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Mol	Chain	Res	Type	Models (Total)
1	A	109	VAL	4
1	A	81	THR	3
1	A	71	VAL	3
1	A	42	GLU	3
1	A	61	ARG	3
1	A	101	ASP	2
1	A	105	GLU	2
1	A	72	GLN	2
1	A	114	GLU	2
1	A	70	SER	2
1	A	55	GLU	2
1	A	127	LEU	1
1	A	62	VAL	1
1	A	47	LYS	1
1	A	39	THR	1
1	A	94	SER	1
1	A	83	THR	1
1	A	129	LYS	1
1	A	110	VAL	1
1	A	119	ASN	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 ⓘ

There are no ligands in this entry.

## 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

No chemical shift data were provided