Full wwPDB NMR Structure Validation Report (i)

Dec 10, 2022 – 07:13 PM EST

PDB ID	:	1D1R
Title	:	NMR SOLUTION STRUCTURE OF THE PRODUCT OF THE E. COLI YCIH GENE.
Authors	:	Cort, J.R.; Koonin, E.V.; Bash, P.A.; Kennedy, M.A.
Deposited on	:	1999-09-20

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
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

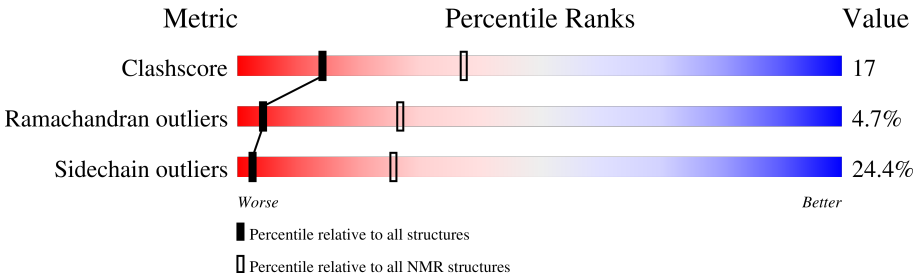
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.31.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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	116	35% 25% • 9% 28%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 18 is the overall representative, medoid model (most similar to other models). The authors have identified model 4 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:31-A:40, A:46-A:107 (72)	0.58	18

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, 8, 9, 16, 17, 18, 19, 20
2	6, 7, 10, 11, 12, 13, 14, 15

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1260 atoms, of which 657 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called HYPOTHETICAL 11.4 KD PROTEIN YCIH IN PYRF-OSMB INTERGENIC REGION.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	83	1260	373	657	111	115	4	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	110	LEU	-	expression tag	UNP P08245
A	111	GLU	-	expression tag	UNP P08245
A	112	HIS	-	expression tag	UNP P08245
A	113	HIS	-	expression tag	UNP P08245
A	114	HIS	-	expression tag	UNP P08245
A	115	HIS	-	expression tag	UNP P08245
A	116	HIS	-	expression tag	UNP P08245
A	117	HIS	-	expression tag	UNP P08245

4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide 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: HYPOTHETICAL 11.4 KD PROTEIN YCIH IN PYRF-OSMB INTERGENIC REGION

Chain A: 35% 25% • 9% 28%

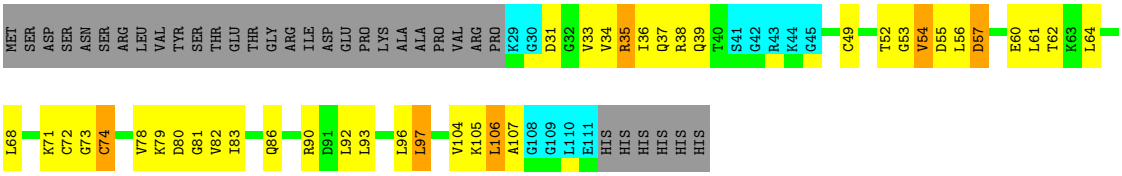
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: HYPOTHETICAL 11.4 KD PROTEIN YCIH IN PYRF-OSMB INTERGENIC REGION

Chain A: 28% 29% 5% 9% 28%



4.2.2 Score per residue for model 2

• Molecule 1: HYPOTHETICAL 11.4 KD PROTEIN YCIH IN PYRF-OSMB INTERGENIC REGION

Chain A: 31% 26% • • 9% 28%

MET SER ASP SER ASN SER ARG LEU VAL TYR SER THR GLU THR GLY ARG ILE ASP GLU PRO LYS ALA ALA PRO VAL ARG PRO K29 G30 V33 V34 R35 I36 Q37 R38 Q39 T40 S41 G42 R43 K44 G45 V48 C49 L50 V54 D55 L56 D57 D58 A59 E60 L61 L64 A65

L68 C72 G73 C74 G75 G76 A77 V78 K79 D80 Q86 R90 D91 L92 L93 K94 S95 L96 L97 K100 K103 V104 K105 L106 A107 G108 G109 L110 E111 HIS HIS HIS HIS HIS

4.2.3 Score per residue for model 3

• Molecule 1: HYPOTHETICAL 11.4 KD PROTEIN YCIH IN PYRF-OSMB INTERGENIC REGION

Chain A: 34% 26% • 9% 28%

MET SER ASP SER ASN SER ARG LEU VAL TYR SER THR GLU THR GLY ARG ILE ASP GLU PRO LYS ALA ALA PRO VAL ARG PRO K29 G30 D31 G32 V33 V34 R35 I36 Q37 R38 Q39 T40 S41 G42 R43 K44 G45 C49 L50 V54 D55 L56 D57 D58 L61 T62 K63 L68 K69

K70 V78 I83 E84 I85 Q86 Q87 R90 L93 K94 S95 L96 L97 K103 V104 K105 L106 A107 G108 G109 L110 E111 HIS HIS HIS HIS HIS

4.2.4 Score per residue for model 4

• Molecule 1: HYPOTHETICAL 11.4 KD PROTEIN YCIH IN PYRF-OSMB INTERGENIC REGION

Chain A: 34% 23% 5% 9% 28%

MET SER ASP SER ASN SER ARG LEU VAL TYR SER THR GLU THR GLY ARG ILE ASP GLU PRO LYS ALA ALA PRO VAL ARG PRO K29 G30 D31 G32 V33 V34 R35 I36 Q37 R38 Q39 T40 S41 G42 R43 K44 G45 C49 L56 D57 D58 K63 L64 L68 K71 C72 G73 C74

G75 G76 D80 Q86 Q87 D88 K89 R90 L93 K94 S95 L96 L97 K100 G101 M102 K103 V104 K105 L106 A107 G108 G109 L110 E111 HIS HIS HIS HIS HIS

4.2.5 Score per residue for model 5

• Molecule 1: HYPOTHETICAL 11.4 KD PROTEIN YCIH IN PYRF-OSMB INTERGENIC REGION

Chain A: 40% 19% • 9% 28%

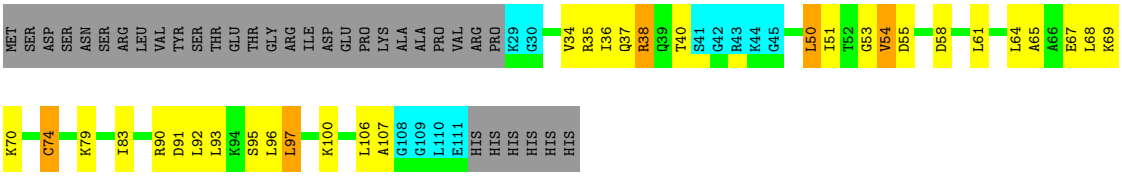
MET SER ASP SER ASN SER ARG LEU VAL TYR SER THR GLU THR GLY ARG ILE ASP GLU PRO LYS ALA ALA PRO VAL ARG PRO K29 G30 D31 R35 I36 Q37 R38 S41 G42 R43 K44 G45 C49 V54 L61 A65 L68 K69 K70 K71 C74 G75 G76 G81

V82 R90 L93 L96 L97 K100 G101 M102 K105 L106 A107 G108 G109 L110 E111 HIS HIS HIS HIS HIS

4.2.6 Score per residue for model 6

• Molecule 1: HYPOTHETICAL 11.4 KD PROTEIN YCIH IN PYRF-OSMB INTERGENIC REGION

Chain A: 34% 23% • 9% 28%



4.2.7 Score per residue for model 7

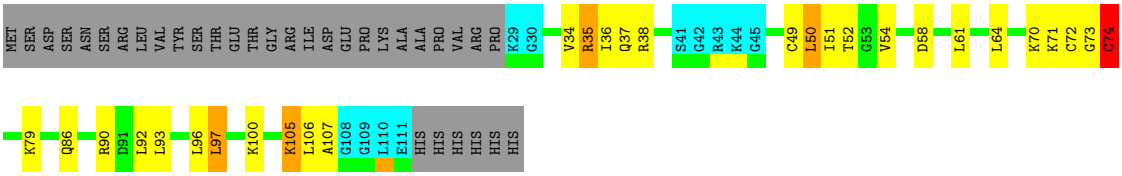
• Molecule 1: HYPOTHETICAL 11.4 KD PROTEIN YCIH IN PYRF-OSMB INTERGENIC REGION

Chain A: 34% 20% 8% 9% 28%

4.2.8 Score per residue for model 8

• Molecule 1: HYPOTHETICAL 11.4 KD PROTEIN YCIH IN PYRF-OSMB INTERGENIC REGION

Chain A: 37% 21% • • 9% 28%



4.2.9 Score per residue for model 9

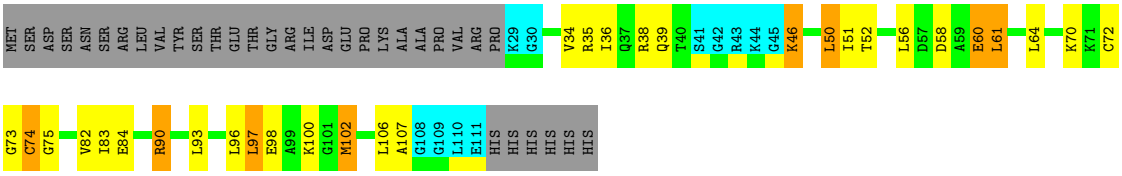
• Molecule 1: HYPOTHETICAL 11.4 KD PROTEIN YCIH IN PYRF-OSMB INTERGENIC REGION

Chain A: 37% 23% • 9% 28%

4.2.10 Score per residue for model 10

• Molecule 1: HYPOTHETICAL 11.4 KD PROTEIN YCIH IN PYRF-OSMB INTERGENIC REGION

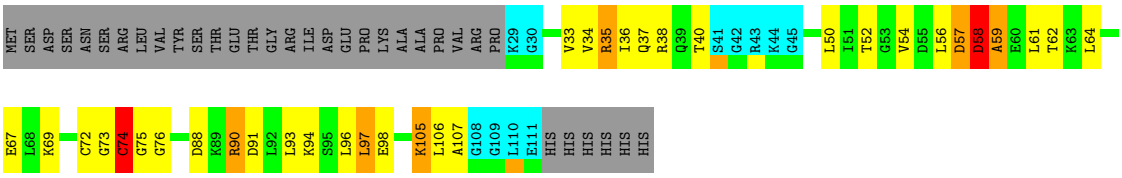
Chain A: 35% 20% 7% 9% 28%



4.2.11 Score per residue for model 11

• Molecule 1: HYPOTHETICAL 11.4 KD PROTEIN YCIH IN PYRF-OSMB INTERGENIC REGION

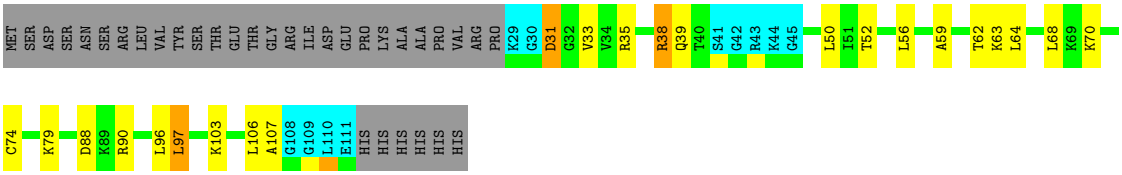
Chain A: 32% 23% 5% • 9% 28%



4.2.12 Score per residue for model 12

• Molecule 1: HYPOTHETICAL 11.4 KD PROTEIN YCIH IN PYRF-OSMB INTERGENIC REGION

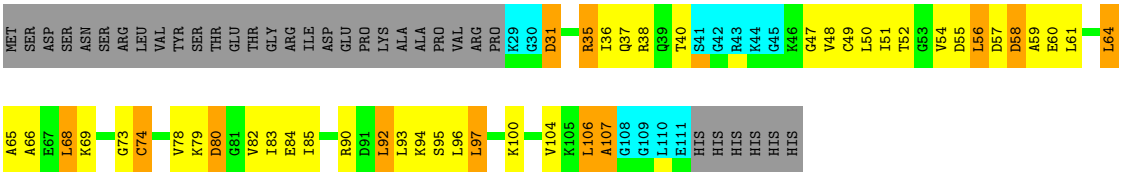
Chain A: 42% 17% • 9% 28%



4.2.13 Score per residue for model 13

• Molecule 1: HYPOTHETICAL 11.4 KD PROTEIN YCIH IN PYRF-OSMB INTERGENIC REGION

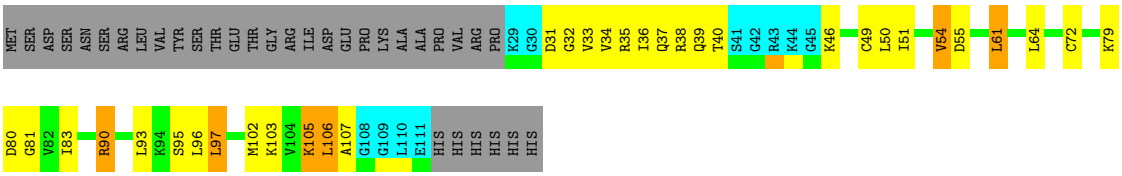
Chain A: 23% 28% 10% 9% 28%



4.2.14 Score per residue for model 14

• Molecule 1: HYPOTHETICAL 11.4 KD PROTEIN YCIH IN PYRF-OSMB INTERGENIC REGION

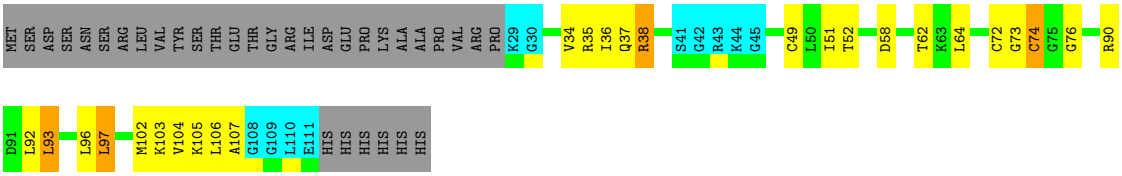
Chain A: 34% 23% 5% 9% 28%



4.2.15 Score per residue for model 15

• Molecule 1: HYPOTHETICAL 11.4 KD PROTEIN YCIH IN PYRF-OSMB INTERGENIC REGION

Chain A: 40% 19% • 9% 28%



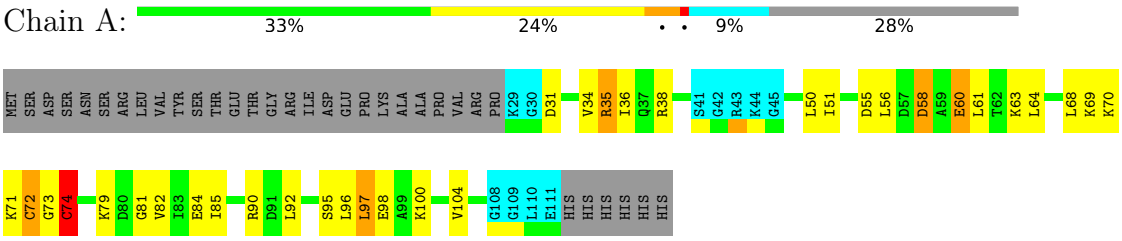
4.2.16 Score per residue for model 16

• Molecule 1: HYPOTHETICAL 11.4 KD PROTEIN YCIH IN PYRF-OSMB INTERGENIC REGION

Chain A: 34% 24% • 9% 28%

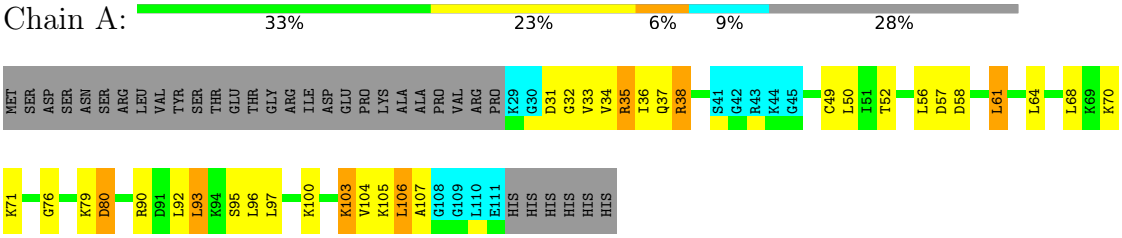
4.2.17 Score per residue for model 17

• Molecule 1: HYPOTHETICAL 11.4 KD PROTEIN YCIH IN PYRF-OSMB INTERGENIC REGION



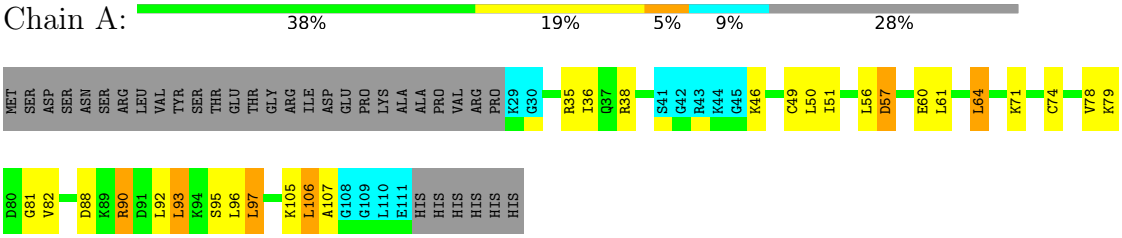
4.2.18 Score per residue for model 18 (medoid)

• Molecule 1: HYPOTHETICAL 11.4 KD PROTEIN YCIH IN PYRF-OSMB INTERGENIC REGION



4.2.19 Score per residue for model 19

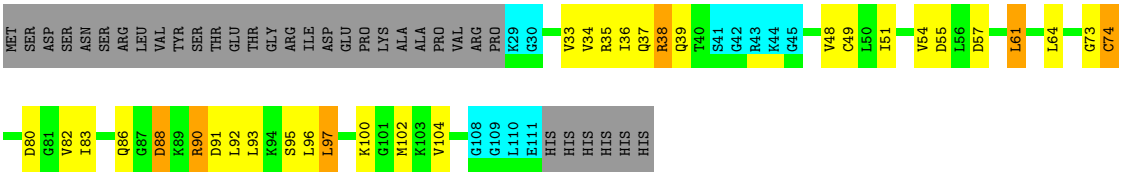
• Molecule 1: HYPOTHETICAL 11.4 KD PROTEIN YCIH IN PYRF-OSMB INTERGENIC REGION



4.2.20 Score per residue for model 20

• Molecule 1: HYPOTHETICAL 11.4 KD PROTEIN YCIH IN PYRF-OSMB INTERGENIC REGION

Chain A: 34% 22% 5% 9% 28%



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *DISTANCE GEOMETRY SIMULATED ANNEALING*.

Of the 25 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
X-PLOR	refinement	3.1
Felix	structure solution	97
VNMR	structure solution	6.1A

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

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

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	3.0±0.0
All	All	0	60

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	35	ARG	Sidechain	20
1	A	38	ARG	Sidechain	20
1	A	90	ARG	Sidechain	20

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	531	582	582	19±6
All	All	10620	11640	11640	389

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 17.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:ILE:HG21	1:A:93:LEU:HD13	1.05	1.24	20	9
1:A:96:LEU:HD12	1:A:97:LEU:N	0.90	1.81	15	12
1:A:52:THR:HG23	1:A:81:GLY:O	0.87	1.69	1	1
1:A:33:VAL:HG13	1:A:103:LYS:O	0.87	1.70	4	2
1:A:33:VAL:HG23	1:A:103:LYS:O	0.84	1.72	16	1
1:A:34:VAL:O	1:A:104:VAL:HG23	0.82	1.74	7	4
1:A:36:ILE:HD11	1:A:97:LEU:HD23	0.81	1.49	6	4
1:A:97:LEU:HD13	1:A:104:VAL:CG2	0.81	2.05	20	2
1:A:82:VAL:O	1:A:83:ILE:HD13	0.80	1.77	13	1
1:A:97:LEU:HD22	1:A:104:VAL:HG22	0.80	1.50	3	2
1:A:36:ILE:CG2	1:A:93:LEU:HD13	0.79	2.05	20	10
1:A:37:GLN:HB3	1:A:107:ALA:HB3	0.77	1.57	14	8
1:A:97:LEU:HD23	1:A:104:VAL:HG13	0.76	1.57	18	2
1:A:96:LEU:HD23	1:A:97:LEU:N	0.76	1.96	17	6
1:A:94:LYS:HD2	1:A:106:LEU:HD21	0.76	1.58	2	1
1:A:97:LEU:HD13	1:A:104:VAL:HG13	0.75	1.57	1	1
1:A:51:ILE:N	1:A:51:ILE:HD12	0.75	1.96	10	1
1:A:34:VAL:HG13	1:A:54:VAL:HG22	0.74	1.57	6	2
1:A:37:GLN:CB	1:A:107:ALA:HB3	0.74	2.12	11	4
1:A:36:ILE:HD11	1:A:97:LEU:HD13	0.74	1.60	3	2
1:A:34:VAL:HG22	1:A:54:VAL:HG22	0.74	1.59	1	3
1:A:78:VAL:HG22	1:A:83:ILE:HG12	0.73	1.57	1	1
1:A:36:ILE:HG21	1:A:93:LEU:HG	0.73	1.59	13	3
1:A:36:ILE:HG23	1:A:51:ILE:HG13	0.73	1.61	10	4
1:A:61:LEU:HD23	1:A:83:ILE:HD11	0.73	1.59	14	1
1:A:90:ARG:HA	1:A:93:LEU:HD12	0.73	1.57	5	5
1:A:34:VAL:HB	1:A:97:LEU:HD21	0.72	1.61	16	4
1:A:59:ALA:O	1:A:62:THR:HG22	0.71	1.85	12	1
1:A:50:LEU:HD12	1:A:84:GLU:HG3	0.71	1.61	3	1
1:A:97:LEU:HD13	1:A:104:VAL:HG22	0.69	1.64	1	1
1:A:37:GLN:HB3	1:A:107:ALA:HB2	0.69	1.65	13	1
1:A:73:GLY:O	1:A:74:CYS:CB	0.67	2.42	1	8
1:A:97:LEU:HD23	1:A:104:VAL:HG22	0.67	1.65	18	2
1:A:58:ASP:O	1:A:59:ALA:HB3	0.67	1.90	13	2
1:A:36:ILE:HD11	1:A:97:LEU:HD12	0.67	1.64	20	2
1:A:50:LEU:O	1:A:51:ILE:HD13	0.67	1.88	8	3
1:A:36:ILE:CD1	1:A:97:LEU:HD22	0.67	2.19	2	1
1:A:97:LEU:HD13	1:A:104:VAL:CG1	0.67	2.19	1	1
1:A:97:LEU:CD2	1:A:104:VAL:HG13	0.66	2.19	18	2
1:A:65:ALA:HA	1:A:68:LEU:HD12	0.66	1.67	5	2
1:A:97:LEU:CD2	1:A:104:VAL:HG22	0.66	2.20	3	2
1:A:97:LEU:HD13	1:A:104:VAL:CB	0.66	2.21	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:ILE:HG21	1:A:93:LEU:CD1	0.65	2.14	20	1
1:A:33:VAL:O	1:A:33:VAL:HG23	0.64	1.93	12	5
1:A:106:LEU:O	1:A:107:ALA:HB3	0.63	1.93	10	4
1:A:34:VAL:HG13	1:A:54:VAL:CG2	0.63	2.23	9	2
1:A:54:VAL:HB	1:A:61:LEU:HD21	0.63	1.70	2	3
1:A:97:LEU:HD13	1:A:104:VAL:HB	0.63	1.71	20	1
1:A:106:LEU:O	1:A:107:ALA:HB2	0.62	1.94	13	1
1:A:97:LEU:CD1	1:A:104:VAL:HG13	0.62	2.23	1	1
1:A:51:ILE:HB	1:A:83:ILE:HD12	0.62	1.70	9	2
1:A:96:LEU:HD23	1:A:96:LEU:C	0.62	2.14	3	3
1:A:36:ILE:HD12	1:A:104:VAL:CG2	0.62	2.24	17	3
1:A:33:VAL:HG12	1:A:103:LYS:HB3	0.61	1.71	2	2
1:A:97:LEU:HD22	1:A:104:VAL:HB	0.61	1.70	17	3
1:A:93:LEU:HD13	1:A:96:LEU:HD21	0.61	1.71	1	2
1:A:36:ILE:HG21	1:A:93:LEU:HB3	0.61	1.71	9	3
1:A:54:VAL:HG13	1:A:54:VAL:O	0.60	1.95	14	1
1:A:36:ILE:HD12	1:A:104:VAL:HG21	0.60	1.73	17	1
1:A:33:VAL:HG12	1:A:103:LYS:CB	0.59	2.27	14	3
1:A:36:ILE:HG21	1:A:93:LEU:HD22	0.59	1.74	4	4
1:A:96:LEU:HD12	1:A:96:LEU:C	0.59	2.17	10	8
1:A:97:LEU:HD23	1:A:104:VAL:CG2	0.58	2.29	2	2
1:A:64:LEU:O	1:A:68:LEU:HD12	0.58	1.99	13	1
1:A:93:LEU:HA	1:A:96:LEU:HD21	0.58	1.76	1	11
1:A:97:LEU:HD23	1:A:104:VAL:CG1	0.57	2.28	2	2
1:A:34:VAL:HB	1:A:97:LEU:HD11	0.57	1.75	1	3
1:A:64:LEU:O	1:A:64:LEU:HD13	0.56	2.00	19	1
1:A:36:ILE:CD1	1:A:104:VAL:HG21	0.56	2.31	17	2
1:A:51:ILE:N	1:A:51:ILE:CD1	0.56	2.68	10	1
1:A:36:ILE:HG23	1:A:51:ILE:CG1	0.56	2.31	10	1
1:A:36:ILE:CD1	1:A:97:LEU:HD12	0.56	2.29	20	1
1:A:56:LEU:HD12	1:A:60:GLU:CB	0.56	2.29	17	1
1:A:34:VAL:HG21	1:A:97:LEU:HD11	0.56	1.78	18	1
1:A:58:ASP:O	1:A:59:ALA:CB	0.55	2.53	13	2
1:A:39:GLN:HB2	1:A:50:LEU:HD13	0.55	1.78	9	1
1:A:96:LEU:CD1	1:A:97:LEU:N	0.55	2.68	18	7
1:A:36:ILE:HG21	1:A:93:LEU:CG	0.55	2.30	13	1
1:A:36:ILE:HG23	1:A:51:ILE:HG12	0.54	1.78	19	1
1:A:72:CYS:SG	1:A:85:ILE:HD12	0.54	2.43	17	1
1:A:36:ILE:HG12	1:A:93:LEU:HD22	0.54	1.79	18	4
1:A:94:LYS:CG	1:A:106:LEU:HD11	0.53	2.33	7	1
1:A:34:VAL:HG23	1:A:102:MET:CE	0.53	2.34	10	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:97:LEU:HD13	1:A:104:VAL:HG23	0.53	1.77	20	1
1:A:50:LEU:C	1:A:51:ILE:HD13	0.53	2.24	6	3
1:A:68:LEU:CD2	1:A:96:LEU:HD22	0.53	2.34	1	1
1:A:93:LEU:HD23	1:A:96:LEU:HD21	0.52	1.79	5	1
1:A:96:LEU:C	1:A:96:LEU:HD23	0.52	2.24	6	1
1:A:54:VAL:HG11	1:A:61:LEU:HD21	0.52	1.81	14	1
1:A:54:VAL:CG1	1:A:56:LEU:HD12	0.52	2.34	3	1
1:A:72:CYS:SG	1:A:85:ILE:HG23	0.52	2.45	16	1
1:A:97:LEU:HD22	1:A:104:VAL:CG2	0.52	2.34	1	1
1:A:39:GLN:O	1:A:48:VAL:HG22	0.52	2.04	20	1
1:A:33:VAL:HG12	1:A:103:LYS:HB2	0.52	1.80	18	1
1:A:37:GLN:CD	1:A:107:ALA:HB3	0.51	2.26	18	2
1:A:37:GLN:HA	1:A:107:ALA:HB2	0.51	1.82	7	2
1:A:78:VAL:HG22	1:A:83:ILE:HG23	0.51	1.82	3	1
1:A:78:VAL:O	1:A:78:VAL:HG23	0.51	2.06	19	1
1:A:36:ILE:HD11	1:A:97:LEU:HD22	0.51	1.82	2	1
1:A:65:ALA:HB1	1:A:78:VAL:HG22	0.51	1.82	13	1
1:A:36:ILE:HD11	1:A:97:LEU:CD1	0.51	2.34	20	1
1:A:33:VAL:O	1:A:33:VAL:HG13	0.51	2.05	16	1
1:A:82:VAL:C	1:A:83:ILE:HD13	0.51	2.26	13	1
1:A:106:LEU:O	1:A:107:ALA:CB	0.50	2.59	13	2
1:A:34:VAL:CG2	1:A:97:LEU:HD11	0.50	2.35	18	1
1:A:36:ILE:HG21	1:A:93:LEU:CB	0.50	2.37	9	3
1:A:54:VAL:CG1	1:A:61:LEU:HD21	0.49	2.37	14	2
1:A:56:LEU:HB2	1:A:61:LEU:HD11	0.49	1.82	2	1
1:A:92:LEU:HD23	1:A:92:LEU:C	0.49	2.28	6	1
1:A:53:GLY:O	1:A:55:ASP:N	0.49	2.46	1	2
1:A:54:VAL:CB	1:A:61:LEU:HD21	0.49	2.37	2	1
1:A:39:GLN:CB	1:A:50:LEU:HD13	0.49	2.38	9	1
1:A:39:GLN:HB2	1:A:50:LEU:CD1	0.48	2.38	14	1
1:A:73:GLY:O	1:A:74:CYS:HB3	0.48	2.08	20	1
1:A:57:ASP:O	1:A:61:LEU:HD12	0.48	2.08	18	1
1:A:34:VAL:CB	1:A:97:LEU:HD11	0.48	2.38	18	2
1:A:90:ARG:HB3	1:A:106:LEU:HD21	0.48	1.85	19	1
1:A:78:VAL:HG12	1:A:79:LYS:N	0.48	2.24	1	1
1:A:32:GLY:CA	1:A:56:LEU:HD21	0.47	2.39	4	1
1:A:79:LYS:O	1:A:81:GLY:N	0.47	2.47	14	1
1:A:97:LEU:HD12	1:A:104:VAL:HB	0.47	1.86	16	1
1:A:54:VAL:HG11	1:A:61:LEU:HG	0.47	1.85	3	1
1:A:105:LYS:O	1:A:107:ALA:N	0.47	2.47	8	6
1:A:34:VAL:HG12	1:A:35:ARG:N	0.47	2.25	18	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:ILE:HG12	1:A:93:LEU:HD12	0.46	1.86	1	1
1:A:97:LEU:HB3	1:A:104:VAL:CG2	0.46	2.40	3	1
1:A:51:ILE:N	1:A:51:ILE:HD13	0.46	2.24	9	2
1:A:88:ASP:O	1:A:89:LYS:CG	0.46	2.63	16	1
1:A:36:ILE:HG23	1:A:51:ILE:HD12	0.46	1.88	9	1
1:A:97:LEU:CD1	1:A:104:VAL:HG22	0.46	2.36	1	1
1:A:36:ILE:CG2	1:A:93:LEU:HD22	0.46	2.41	3	2
1:A:68:LEU:N	1:A:68:LEU:CD2	0.46	2.79	4	1
1:A:73:GLY:O	1:A:74:CYS:HB2	0.45	2.11	7	6
1:A:97:LEU:HB3	1:A:104:VAL:CG1	0.45	2.41	13	1
1:A:50:LEU:C	1:A:51:ILE:HD12	0.45	2.30	10	1
1:A:47:GLY:O	1:A:48:VAL:CG1	0.45	2.65	13	1
1:A:37:GLN:OE1	1:A:107:ALA:HB3	0.45	2.12	9	1
1:A:31:ASP:N	1:A:31:ASP:OD1	0.45	2.49	12	1
1:A:56:LEU:HD12	1:A:60:GLU:HB2	0.45	1.87	17	1
1:A:57:ASP:O	1:A:58:ASP:O	0.45	2.35	11	1
1:A:33:VAL:O	1:A:33:VAL:CG2	0.45	2.65	20	3
1:A:94:LYS:HG3	1:A:106:LEU:HD11	0.45	1.89	7	1
1:A:65:ALA:HB1	1:A:78:VAL:HG11	0.45	1.89	2	1
1:A:81:GLY:O	1:A:82:VAL:HG23	0.45	2.11	5	2
1:A:56:LEU:HD13	1:A:60:GLU:HB3	0.45	1.89	19	1
1:A:68:LEU:N	1:A:68:LEU:HD22	0.44	2.27	4	1
1:A:56:LEU:HD22	1:A:60:GLU:OE2	0.44	2.11	7	1
1:A:56:LEU:HB2	1:A:61:LEU:CD1	0.44	2.42	2	1
1:A:32:GLY:O	1:A:33:VAL:HG13	0.44	2.11	14	1
1:A:54:VAL:O	1:A:56:LEU:N	0.44	2.50	13	1
1:A:83:ILE:N	1:A:83:ILE:HD13	0.44	2.27	10	1
1:A:96:LEU:C	1:A:96:LEU:CD2	0.44	2.84	3	1
1:A:36:ILE:CD1	1:A:97:LEU:CD1	0.43	2.94	20	1
1:A:73:GLY:O	1:A:74:CYS:SG	0.43	2.77	8	2
1:A:61:LEU:CD2	1:A:83:ILE:HD11	0.43	2.39	14	2
1:A:94:LYS:CG	1:A:106:LEU:CD1	0.43	2.97	7	1
1:A:106:LEU:N	1:A:106:LEU:HD22	0.43	2.28	10	1
1:A:90:ARG:HG3	1:A:91:ASP:N	0.43	2.28	11	1
1:A:36:ILE:CD1	1:A:104:VAL:CG2	0.43	2.96	13	2
1:A:80:ASP:N	1:A:80:ASP:OD1	0.43	2.52	13	1
1:A:49:CYS:SG	1:A:51:ILE:HD11	0.43	2.54	15	1
1:A:35:ARG:O	1:A:51:ILE:HG23	0.43	2.14	7	1
1:A:84:GLU:O	1:A:85:ILE:HD13	0.43	2.14	13	1
1:A:97:LEU:CG	1:A:104:VAL:HB	0.43	2.44	13	1
1:A:68:LEU:HD21	1:A:96:LEU:CD1	0.43	2.43	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:105:LYS:O	1:A:106:LEU:C	0.43	2.57	18	5
1:A:81:GLY:O	1:A:82:VAL:CG2	0.43	2.67	19	2
1:A:90:ARG:CG	1:A:91:ASP:N	0.43	2.81	11	1
1:A:97:LEU:CD1	1:A:102:MET:HB2	0.42	2.44	7	2
1:A:39:GLN:OE1	1:A:50:LEU:HD13	0.42	2.13	7	1
1:A:60:GLU:O	1:A:61:LEU:C	0.42	2.57	10	1
1:A:76:GLY:O	1:A:77:ALA:HB2	0.42	2.15	2	1
1:A:106:LEU:C	1:A:106:LEU:HD23	0.42	2.35	14	1
1:A:32:GLY:HA3	1:A:56:LEU:HD21	0.42	1.92	18	1
1:A:85:ILE:HG22	1:A:86:GLN:N	0.42	2.29	7	1
1:A:96:LEU:CD1	1:A:97:LEU:HD22	0.42	2.45	13	1
1:A:54:VAL:O	1:A:54:VAL:CG1	0.42	2.66	14	1
1:A:82:VAL:HG12	1:A:83:ILE:N	0.42	2.30	20	1
1:A:68:LEU:O	1:A:72:CYS:SG	0.42	2.78	1	1
1:A:92:LEU:HD23	1:A:96:LEU:HD23	0.42	1.92	2	1
1:A:79:LYS:N	1:A:82:VAL:O	0.42	2.53	1	1
1:A:37:GLN:HA	1:A:107:ALA:CB	0.42	2.44	2	1
1:A:106:LEU:N	1:A:106:LEU:CD2	0.42	2.83	10	1
1:A:95:SER:O	1:A:96:LEU:C	0.41	2.57	18	2
1:A:65:ALA:O	1:A:66:ALA:C	0.41	2.57	13	1
1:A:34:VAL:HG11	1:A:97:LEU:HD21	0.41	1.91	8	1
1:A:96:LEU:C	1:A:96:LEU:CD1	0.41	2.88	10	1
1:A:97:LEU:CD1	1:A:104:VAL:HG23	0.41	2.45	20	1
1:A:38:ARG:O	1:A:38:ARG:CG	0.41	2.68	2	1
1:A:90:ARG:HE	1:A:106:LEU:HD12	0.41	1.75	10	1
1:A:97:LEU:CD2	1:A:104:VAL:HB	0.41	2.46	4	1
1:A:53:GLY:O	1:A:54:VAL:C	0.41	2.59	9	1
1:A:73:GLY:C	1:A:74:CYS:SG	0.41	2.99	15	1
1:A:106:LEU:O	1:A:107:ALA:C	0.41	2.58	6	1
1:A:82:VAL:O	1:A:82:VAL:HG12	0.41	2.13	10	1
1:A:36:ILE:HD12	1:A:97:LEU:HD22	0.41	1.92	18	1
1:A:63:LYS:O	1:A:64:LEU:C	0.41	2.59	4	1
1:A:100:LYS:N	1:A:100:LYS:HD2	0.41	2.30	9	1
1:A:34:VAL:HG23	1:A:102:MET:HE3	0.41	1.93	14	1
1:A:97:LEU:HD22	1:A:97:LEU:HA	0.41	1.77	16	1
1:A:64:LEU:O	1:A:64:LEU:CD1	0.41	2.68	19	1
1:A:56:LEU:HD11	1:A:102:MET:SD	0.41	2.55	9	1
1:A:39:GLN:CB	1:A:50:LEU:CD1	0.41	2.99	14	1
1:A:81:GLY:C	1:A:82:VAL:CG2	0.40	2.88	17	1
1:A:36:ILE:HD11	1:A:97:LEU:CD2	0.40	2.34	6	1
1:A:56:LEU:O	1:A:57:ASP:C	0.40	2.59	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:32:GLY:C	1:A:33:VAL:CG2	0.40	2.90	3	1
1:A:92:LEU:O	1:A:92:LEU:HD23	0.40	2.16	13	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	72/116 (62%)	57±2 (80±3%)	11±3 (16±4%)	3±1 (5±2%)	4 27
All	All	1440/2320 (62%)	1148 (80%)	225 (16%)	67 (5%)	4 27

All 16 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	74	CYS	16
1	A	106	LEU	12
1	A	58	ASP	7
1	A	76	GLY	6
1	A	54	VAL	4
1	A	80	ASP	4
1	A	88	ASP	3
1	A	57	ASP	3
1	A	31	ASP	3
1	A	46	LYS	2
1	A	75	GLY	2
1	A	77	ALA	1
1	A	87	GLY	1
1	A	59	ALA	1
1	A	55	ASP	1
1	A	107	ALA	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	57/93 (61%)	43±3 (76±6%)	14±3 (24±6%)	2 26
All	All	1140/1860 (61%)	862 (76%)	278 (24%)	2 26

All 45 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	97	LEU	17
1	A	64	LEU	16
1	A	61	LEU	15
1	A	49	CYS	12
1	A	50	LEU	11
1	A	58	ASP	10
1	A	100	LYS	10
1	A	72	CYS	9
1	A	70	LYS	9
1	A	79	LYS	9
1	A	52	THR	9
1	A	92	LEU	8
1	A	71	LYS	7
1	A	68	LEU	7
1	A	95	SER	7
1	A	57	ASP	6
1	A	86	GLN	6
1	A	40	THR	6
1	A	38	ARG	6
1	A	31	ASP	5
1	A	60	GLU	5
1	A	62	THR	5
1	A	80	ASP	5
1	A	105	LYS	5
1	A	93	LEU	5
1	A	69	LYS	5
1	A	102	MET	5
1	A	74	CYS	5
1	A	56	LEU	5

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Mol	Chain	Res	Type	Models (Total)
1	A	37	GLN	4
1	A	39	GLN	4
1	A	106	LEU	4
1	A	98	GLU	4
1	A	88	ASP	4
1	A	35	ARG	3
1	A	63	LYS	3
1	A	103	LYS	3
1	A	67	GLU	3
1	A	91	ASP	3
1	A	94	LYS	3
1	A	55	ASP	3
1	A	90	ARG	2
1	A	84	GLU	2
1	A	46	LYS	2
1	A	48	VAL	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

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 (i)

No chemical shift data were provided