Full wwPDB NMR Structure Validation Report (i)

Feb 26, 2022 – 06:23 PM EST

PDB ID	:	2AX5
Title	:	Solution Structure of Urm1 from Saccharomyces Cerevisiae
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Deposited on	:	2005-09-03

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

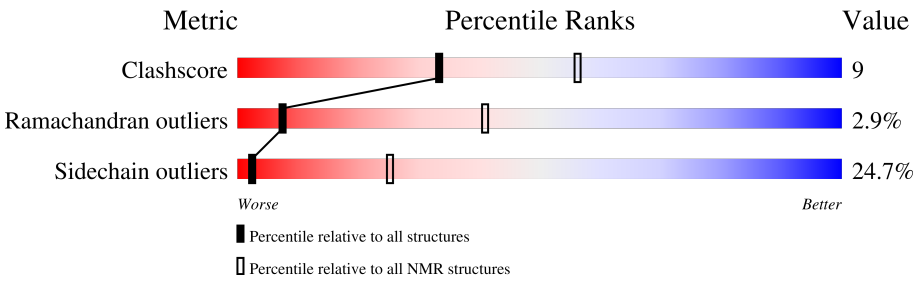
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

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	107	58% 30% 5% 7%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 4 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:2-A:95 (94)	0.44	4

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 6 clusters and 1 single-model cluster was found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1541 atoms, of which 767 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Hypothetical 11.0 kDa protein in FAA3-MAS3 intergenic region.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	99	1541	490	767	124	157	3	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	LEU	-	expression tag	UNP P40554
A	101	GLU	-	expression tag	UNP P40554
A	102	HIS	-	expression tag	UNP P40554
A	103	HIS	-	expression tag	UNP P40554
A	104	HIS	-	expression tag	UNP P40554
A	105	HIS	-	expression tag	UNP P40554
A	106	HIS	-	expression tag	UNP P40554
A	107	HIS	-	expression tag	UNP P40554

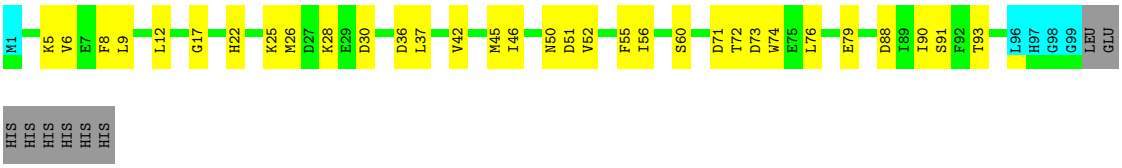
4 Residue-property plots (i)

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 11.0 kDa protein in FAA3-MAS3 intergenic region

Chain A: 58% 30% 5% 7%



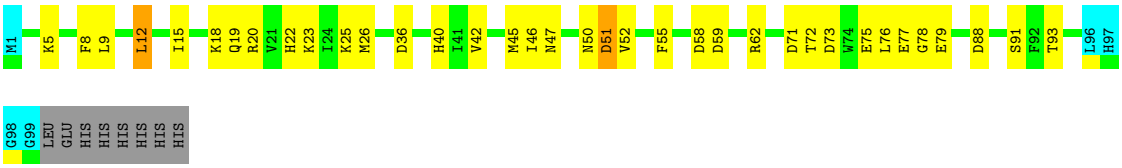
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Hypothetical 11.0 kDa protein in FAA3-MAS3 intergenic region

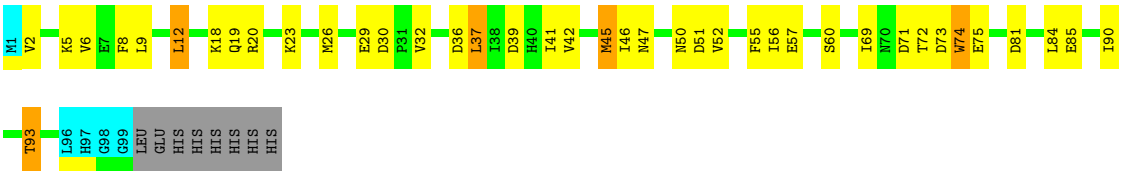
Chain A: 54% 32% • 5% 7%



4.2.2 Score per residue for model 2

• Molecule 1: Hypothetical 11.0 kDa protein in FAA3-MAS3 intergenic region

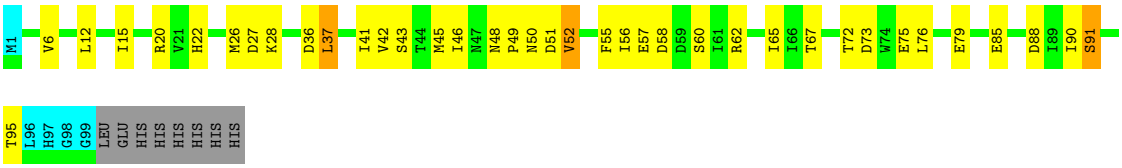
Chain A: 50% 33% 5% 5% 7%



4.2.3 Score per residue for model 3

- Molecule 1: Hypothetical 11.0 kDa protein in FAA3-MAS3 intergenic region

Chain A: 52% 33% • 5% 7%



4.2.4 Score per residue for model 4 (medoid)

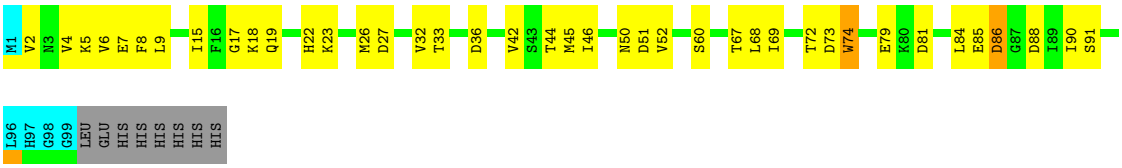
- Molecule 1: Hypothetical 11.0 kDa protein in FAA3-MAS3 intergenic region

Chain A: 56% 28% • 5% 7%

4.2.5 Score per residue for model 5

- Molecule 1: Hypothetical 11.0 kDa protein in FAA3-MAS3 intergenic region

Chain A: 50% 36% • 5% 7%



4.2.6 Score per residue for model 6

- Molecule 1: Hypothetical 11.0 kDa protein in FAA3-MAS3 intergenic region

Chain A: 60% 25% • 5% 7%

M1 V4 K5 V6 E7 L12 G17 K25 M26 D27 K28 D36 L37 V42 M45 I46 N47 N48 P49 N50 D51 V52 S53 I54 F55 S60 I69 N70 D73 W74 E75 L76 D88 I89 I90 S91 S94 T95 L96 H97 G98 G99 LEU GLU HIS HIS HIS HIS HIS HIS HIS

4.2.7 Score per residue for model 7

• Molecule 1: Hypothetical 11.0 kDa protein in FAA3-MAS3 intergenic region

Chain A: 54% 28% 6% 5% 7%

M1 V4 K5 V6 E7 F8 L9 L12 F16 G17 K18 Q19 R20 K25 M26 D27 K28 D36 L37 I38 D39 V42 I46 N50 D51 V52 S53 I54 F55 I56 I61 R62 P63 G64 I65 I69 D73 W74 E75 L76 I90 S91 F92 T93 S94 T95 L96 H97 G98 G99 LEU GLU HIS HIS HIS HIS HIS HIS HIS

4.2.8 Score per residue for model 8

• Molecule 1: Hypothetical 11.0 kDa protein in FAA3-MAS3 intergenic region

Chain A: 48% 37% • 5% 7%

M1 V6 E7 F8 L9 I15 F16 G17 K18 K25 M26 D27 K28 D36 L37 I38 D39 H40 I41 V42 M45 I46 N47 N48 P49 N50 D51 V52 S53 I54 F55 I56 E57 D58 D59 S60 I61 R62 T67 D71 T72 D73 W74 E75 L76 E77 G78 E79 K80 D81 E85 I90 S91 F92 T93 L96 H97 G98 G99 LEU GLU HIS HIS HIS HIS HIS HIS HIS

4.2.9 Score per residue for model 9

• Molecule 1: Hypothetical 11.0 kDa protein in FAA3-MAS3 intergenic region

Chain A: 44% 41% • 5% 7%

M1 V4 K5 V6 E7 F8 L9 L12 G17 K18 Q19 R20 V21 H22 K23 I24 K25 M26 D27 K28 E29 D30 P31 V32 T33 V34 G35 D36 L37 I38 D39 H40 I41 V42 S43 T44 M45 I46 N47 N48 P49 N50 D51 V52 F55 I56 E57 S60 I65 I66 T67 L68 I69 N70 D71 T72 D73 W74 E79 Y82 D88 I89 I90 S91 F92 T93 L96 H97 G98 G99 LEU GLU HIS HIS HIS HIS HIS HIS HIS

4.2.10 Score per residue for model 10

• Molecule 1: Hypothetical 11.0 kDa protein in FAA3-MAS3 intergenic region

Chain A: 58% 27% • 5% 7%

M1 V4 K5 L12 G17 K18 H22 K25 M26 D27 K28 E29 D30 T33 D36 L37 V42 I46 N47 N48 P49 N50 D51 V52 R62 I66 T72 D73 L76 E77 G78 E79 E85 F92 T93 S94 T95 L96 H97 G98 G99 LEU GLU HIS HIS

HIS HIS HIS HIS

4.2.11 Score per residue for model 11

• Molecule 1: Hypothetical 11.0 kDa protein in FAA3-MAS3 intergenic region

Chain A: 57% 29% • 5% 7%

M1 K5 F8 L9 L12 F16 Q19 H22 K25 K28 E29 D30 T33 D36 L37 I38 D39 V42 M45 I46 N50 D51 V52 F55 I61 I65 I69 N70 D71 T72 D73 L76 E85 D88 I89 I90 S91 F92 L96

H97 G98 G99 LEU GLU HIS HIS HIS HIS HIS HIS

4.2.12 Score per residue for model 12

• Molecule 1: Hypothetical 11.0 kDa protein in FAA3-MAS3 intergenic region

Chain A: 54% 32% • 5% 7%

M1 V4 K5 V6 E7 F8 L9 L12 F16 G17 I24 K25 M26 D27 K28 E29 D30 P31 V32 D36 L37 I38 D39 H40 I41 V42 M45 I46 N50 D51 V52 F55 D58 D59 S60 I65 D73 L76 L84 D88 I89 I90 S91 F92 T93

L96 H97 G98 G99 LEU GLU HIS HIS HIS HIS HIS HIS

4.2.13 Score per residue for model 13

• Molecule 1: Hypothetical 11.0 kDa protein in FAA3-MAS3 intergenic region

Chain A: 56% 31% • 5% 7%

M1 K5 V6 E7 F8 L9 G17 K18 Q19 R20 V21 H22 K25 M26 D27 K28 E29 D30 D36 L37 I38 D39 V42 I46 N47 N48 P49 N50 D51 V52 I56 D59 S60 I61 R62 I69 N70 D71 T72 E79 Y82 I90 S91 F92 T93 L96 H97

G98 G99 LEU GLU HIS HIS HIS HIS HIS

4.2.14 Score per residue for model 14

• Molecule 1: Hypothetical 11.0 kDa protein in FAA3-MAS3 intergenic region

Chain A: 55% 31% • 5% 7%

M1 V2 F8 L12 I15 F16 G17 R20 V21 H22 K23 M26 D27 K28 E29 D30 T33 V34 L37 I38 V42 M45 I46 N50 D51 V52 F55 R62 T67 D71 T72 D73 W74 E75 L76 E79 D86 G87 D88 F92 T93 S94 T95

L96 H97 G98 G99 LEU GLU HIS HIS HIS HIS HIS HIS

4.2.15 Score per residue for model 15

• Molecule 1: Hypothetical 11.0 kDa protein in FAA3-MAS3 intergenic region

Chain A: 55% 32% • 5% 7%

M1 K5 V6 E7 F8 L9 L12 G17 K18 Q19 H22 K25 M26 D27 K28 E29 D30 D36 L37 V42 M45 I46 N50 D51 V52 S53 I54 F55 D71 T72 D73 W74 E75 L76 D88 I89 I90 T93 S94 T95 L96 H97 G98 G99 LEU GLU HIS HIS

HIS HIS HIS HIS

4.2.16 Score per residue for model 16

• Molecule 1: Hypothetical 11.0 kDa protein in FAA3-MAS3 intergenic region

Chain A: 59% 25% • • 5% 7%

M1 V2 N3 V4 E7 F8 L9 L12 G17 R20 V21 H22 M26 L37 I41 V42 I46 D51 V52 F55 I56 E57 D58 D59 S60 I61 R62 P63 D71 T72 D73 W74 E75 L76 E79 D86 I90 T93 L96 H97 G98 G99 LEU GLU

HIS HIS HIS HIS HIS HIS

4.2.17 Score per residue for model 17

• Molecule 1: Hypothetical 11.0 kDa protein in FAA3-MAS3 intergenic region

Chain A: 56% 31% • 5% 7%

M1 E7 G17 K18 Q19 R20 V21 H22 K25 M26 D27 K28 E29 D30 T33 D36 L37 I41 V42 S43 T44 M45 I46 N50 D51 V52 I56 E57 D71 T72 D73 L76 E79 E85 D88 I89 I90 S91 F92 T93 S94 T95 L96 H97 G98 G99 LEU

GLU HIS HIS HIS HIS HIS

4.2.18 Score per residue for model 18

• Molecule 1: Hypothetical 11.0 kDa protein in FAA3-MAS3 intergenic region

Chain A: 54% 30% • 5% 7%

M1 V2 K5 V6 L12 F16 G17 H22 K23 I24 K25 M26 E29 D30 L37 I38 D39 V42 M45 I46 N50 D51 V52 I56 D59 T67 N70 D71 T72 D73 W74 E75 L76 E79 D86 G87 D88 I89 I90 S91 F92 T93 L96 H97

G98 G99 LEU GLU HIS HIS HIS HIS HIS HIS

4.2.19 Score per residue for model 19

• Molecule 1: Hypothetical 11.0 kDa protein in FAA3-MAS3 intergenic region

Chain A: 58% 29% • 5% 7%

M1 K5 V6 L9 L12 I15 F16 G17 I24 K25 M26 D30 L37 I41 V42 M45 I46 N50 D51 V52 S53 I54 F55 D58 D59 S60 I61 R62 I65 T72 D73 W74 E75 L76 D88 I89 I90 T93 S94 T95 L96 H97 G98 G99 LEU

GLU HIS HIS HIS HIS HIS HIS

4.2.20 Score per residue for model 20

• Molecule 1: Hypothetical 11.0 kDa protein in FAA3-MAS3 intergenic region

Chain A: 50% 36% • 5% 7%

M1 V4 K5 V6 E7 F8 L9 G17 K18 Q19 R20 V21 H22 K23 I24 K25 M26 D27 K28 E29 D30 P31 V32 D36 L37 V42 S43 T44 M45 I46 N47 N50 D51 V52 I56 E57 D58 D59 G64 T67 T72 D73 W74 E75 L76 E77 E85 I90 S91

F92 T93 S94 T95 L96 H97 G98 G99 LEU GLU HIS HIS HIS HIS HIS HIS

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *distance geometry, simulated annealing, molecular dynamics, torsion angle dynamics*.

Of the 150 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CNS	structure solution	1.1
CNS	refinement	1.1

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.

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 (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	740	731	729	13±3
All	All	14800	14620	14580	266

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:24:ILE:HD11	1:A:41:ILE:HD12	0.82	1.49	12	1
1:A:4:VAL:HG21	1:A:37:LEU:HD21	0.76	1.56	20	5
1:A:46:ILE:HG21	1:A:52:VAL:HG23	0.74	1.59	13	16
1:A:46:ILE:CG2	1:A:52:VAL:HG23	0.73	2.14	17	16
1:A:12:LEU:HD21	1:A:55:PHE:CE1	0.72	2.20	12	8
1:A:8:PHE:C	1:A:9:LEU:HD22	0.70	2.07	20	4
1:A:42:VAL:HG13	1:A:52:VAL:HG11	0.70	1.61	3	4
1:A:42:VAL:HG21	1:A:56:ILE:HD11	0.70	1.63	16	2
1:A:6:VAL:HG12	1:A:90:ILE:HB	0.68	1.65	20	14
1:A:24:ILE:CD1	1:A:41:ILE:HD12	0.68	2.19	12	1
1:A:42:VAL:HG13	1:A:52:VAL:HG21	0.66	1.68	20	10
1:A:42:VAL:HG21	1:A:56:ILE:HG13	0.65	1.68	17	6
1:A:69:ILE:HD11	1:A:74:TRP:CD1	0.64	2.28	7	2
1:A:42:VAL:HG13	1:A:52:VAL:CG1	0.63	2.22	7	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:24:ILE:HG13	1:A:41:ILE:HD11	0.62	1.71	19	1
1:A:4:VAL:CG1	1:A:90:ILE:HD13	0.62	2.25	12	1
1:A:42:VAL:HG13	1:A:52:VAL:CG2	0.62	2.25	16	14
1:A:42:VAL:HG21	1:A:56:ILE:CD1	0.61	2.26	13	4
1:A:55:PHE:CZ	1:A:65:ILE:HG21	0.61	2.30	9	1
1:A:12:LEU:HD21	1:A:55:PHE:CD1	0.60	2.31	7	2
1:A:46:ILE:HG22	1:A:52:VAL:HG22	0.59	1.73	7	2
1:A:73:ASP:HB2	1:A:76:LEU:HD12	0.59	1.74	14	4
1:A:16:PHE:CZ	1:A:46:ILE:HD11	0.58	2.33	11	1
1:A:38:ILE:HD11	1:A:74:TRP:CH2	0.58	2.33	7	1
1:A:38:ILE:HA	1:A:41:ILE:HD12	0.58	1.75	8	2
1:A:66:ILE:HD11	1:A:95:THR:HG23	0.58	1.75	10	1
1:A:12:LEU:HD21	1:A:55:PHE:CZ	0.57	2.35	6	1
1:A:12:LEU:HD11	1:A:55:PHE:CE1	0.57	2.34	14	2
1:A:68:LEU:HD13	1:A:72:THR:O	0.57	2.00	5	1
1:A:69:ILE:HG23	1:A:90:ILE:CD1	0.56	2.30	11	1
1:A:2:VAL:HG23	1:A:86:ASP:HA	0.56	1.77	14	4
1:A:34:VAL:O	1:A:38:ILE:HD12	0.56	2.00	9	2
1:A:8:PHE:C	1:A:9:LEU:HD12	0.55	2.22	13	7
1:A:32:VAL:CG1	1:A:84:LEU:HD12	0.54	2.32	5	2
1:A:4:VAL:CG2	1:A:37:LEU:HD21	0.54	2.31	20	3
1:A:55:PHE:CE1	1:A:65:ILE:HD13	0.54	2.38	11	2
1:A:61:ILE:HG22	1:A:65:ILE:HD12	0.53	1.80	11	1
1:A:88:ASP:C	1:A:89:ILE:HD12	0.53	2.24	18	2
1:A:54:ILE:HD12	1:A:55:PHE:N	0.53	2.19	15	1
1:A:46:ILE:CG2	1:A:52:VAL:HG22	0.53	2.33	3	4
1:A:89:ILE:HD12	1:A:89:ILE:N	0.53	2.19	17	2
1:A:9:LEU:HB2	1:A:93:THR:HG23	0.52	1.80	4	2
1:A:55:PHE:CD1	1:A:65:ILE:HD13	0.52	2.39	7	1
1:A:9:LEU:CB	1:A:93:THR:HG23	0.52	2.35	19	1
1:A:4:VAL:HG11	1:A:90:ILE:HD12	0.51	1.81	5	1
1:A:24:ILE:HB	1:A:37:LEU:HD21	0.51	1.83	12	2
1:A:67:THR:CG2	1:A:74:TRP:CE3	0.51	2.94	8	1
1:A:69:ILE:HG23	1:A:90:ILE:HD12	0.50	1.83	11	1
1:A:67:THR:HG23	1:A:91:SER:O	0.49	2.07	3	1
1:A:16:PHE:CE1	1:A:46:ILE:HD11	0.49	2.42	18	2
1:A:55:PHE:HE1	1:A:65:ILE:HG21	0.49	1.66	4	1
1:A:12:LEU:HD12	1:A:94:SER:OG	0.49	2.08	6	1
1:A:4:VAL:HG21	1:A:37:LEU:CD2	0.48	2.36	20	1
1:A:69:ILE:HG21	1:A:82:TYR:CE1	0.48	2.44	9	1
1:A:42:VAL:CG1	1:A:52:VAL:HG11	0.48	2.38	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:32:VAL:HG12	1:A:84:LEU:HD12	0.48	1.85	5	1
1:A:9:LEU:HD13	1:A:93:THR:CG2	0.48	2.38	8	1
1:A:15:ILE:CG2	1:A:51:ASP:HB3	0.48	2.39	3	5
1:A:67:THR:HG22	1:A:74:TRP:CE3	0.48	2.44	8	1
1:A:56:ILE:HG23	1:A:60:SER:C	0.48	2.29	13	1
1:A:8:PHE:O	1:A:9:LEU:HD12	0.48	2.09	15	1
1:A:42:VAL:HG21	1:A:56:ILE:CG1	0.47	2.39	17	1
1:A:9:LEU:HB2	1:A:93:THR:HG22	0.47	1.86	2	2
1:A:37:LEU:CD1	1:A:41:ILE:HD11	0.47	2.39	3	1
1:A:52:VAL:HG12	1:A:56:ILE:HB	0.47	1.86	3	3
1:A:42:VAL:HG21	1:A:56:ILE:HD12	0.47	1.87	13	1
1:A:42:VAL:O	1:A:42:VAL:HG12	0.47	2.10	3	18
1:A:4:VAL:HG13	1:A:88:ASP:OD1	0.47	2.10	5	1
1:A:90:ILE:N	1:A:90:ILE:HD12	0.47	2.25	16	1
1:A:24:ILE:HG13	1:A:37:LEU:HD11	0.47	1.86	12	1
1:A:67:THR:HG23	1:A:74:TRP:CG	0.47	2.45	20	2
1:A:12:LEU:HD21	1:A:55:PHE:CE2	0.46	2.44	9	1
1:A:2:VAL:O	1:A:2:VAL:HG23	0.46	2.10	2	1
1:A:8:PHE:CD2	1:A:12:LEU:HD13	0.46	2.44	14	1
1:A:67:THR:HG22	1:A:92:PHE:CE2	0.46	2.46	9	1
1:A:12:LEU:HD11	1:A:65:ILE:HD12	0.46	1.86	3	1
1:A:8:PHE:CD1	1:A:12:LEU:HD22	0.46	2.45	2	1
1:A:41:ILE:HG23	1:A:45:MET:SD	0.46	2.51	2	2
1:A:46:ILE:HG21	1:A:52:VAL:CG2	0.45	2.37	6	1
1:A:69:ILE:HG21	1:A:82:TYR:CZ	0.45	2.46	13	1
1:A:41:ILE:HG22	1:A:46:ILE:HD12	0.45	1.88	16	1
1:A:29:GLU:HG2	1:A:32:VAL:HG22	0.45	1.87	2	1
1:A:2:VAL:O	1:A:2:VAL:HG13	0.45	2.11	18	2
1:A:61:ILE:CG2	1:A:65:ILE:HD12	0.44	2.41	11	3
1:A:67:THR:HA	1:A:91:SER:O	0.44	2.13	20	1
1:A:4:VAL:CG1	1:A:90:ILE:HD12	0.44	2.42	5	1
1:A:15:ILE:HD13	1:A:54:ILE:HD11	0.44	1.87	8	1
1:A:4:VAL:HG22	1:A:24:ILE:O	0.44	2.13	9	1
1:A:69:ILE:HG23	1:A:74:TRP:CD1	0.44	2.47	2	1
1:A:89:ILE:N	1:A:89:ILE:CD1	0.44	2.81	17	1
1:A:9:LEU:HD22	1:A:9:LEU:N	0.44	2.28	20	1
1:A:16:PHE:CE1	1:A:41:ILE:HD11	0.43	2.48	12	1
1:A:73:ASP:HB2	1:A:76:LEU:HD23	0.43	1.90	16	1
1:A:29:GLU:O	1:A:32:VAL:HG23	0.43	2.14	20	1
1:A:7:GLU:OE1	1:A:9:LEU:HD11	0.43	2.14	8	1
1:A:74:TRP:CZ3	1:A:79:GLU:HG2	0.42	2.49	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:6:VAL:HG12	1:A:90:ILE:O	0.42	2.14	13	1
1:A:69:ILE:HD11	1:A:74:TRP:HD1	0.42	1.74	6	1
1:A:38:ILE:O	1:A:42:VAL:HG23	0.42	2.14	13	1
1:A:8:PHE:CD1	1:A:92:PHE:HB2	0.41	2.50	11	1
1:A:23:LYS:O	1:A:24:ILE:HD13	0.41	2.15	18	1
1:A:4:VAL:HG21	1:A:37:LEU:HG	0.41	1.92	6	1
1:A:28:LYS:HB3	1:A:32:VAL:HG21	0.41	1.92	20	1
1:A:37:LEU:HD23	1:A:84:LEU:CD1	0.41	2.45	2	1
1:A:38:ILE:HD11	1:A:92:PHE:HZ	0.41	1.75	12	1
1:A:24:ILE:HD12	1:A:24:ILE:N	0.41	2.30	20	1
1:A:32:VAL:HG12	1:A:36:ASP:HB2	0.41	1.93	9	1
1:A:41:ILE:O	1:A:46:ILE:HD12	0.41	2.15	17	1
1:A:48:ASN:O	1:A:50:ASN:N	0.41	2.54	6	1
1:A:41:ILE:HG22	1:A:46:ILE:CD1	0.41	2.46	9	1
1:A:15:ILE:CG2	1:A:51:ASP:CB	0.40	2.99	3	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	94/107 (88%)	75±2 (80±2%)	16±2 (17±2%)	3±1 (3±1%)	7	41
All	All	1880/2140 (88%)	1502 (80%)	324 (17%)	54 (3%)	7	41

All 13 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	50	ASN	16
1	A	17	GLY	15
1	A	79	GLU	5
1	A	28	LYS	4
1	A	78	GLY	2
1	A	49	PRO	2
1	A	64	GLY	2

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Mol	Chain	Res	Type	Models (Total)
1	A	86	ASP	2
1	A	63	PRO	2
1	A	58	ASP	1
1	A	47	ASN	1
1	A	27	ASP	1
1	A	52	VAL	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	86/97 (89%)	65±4 (75±4%)	21±4 (25±4%)	2 25
All	All	1720/1940 (89%)	1295 (75%)	425 (25%)	2 25

All 52 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	26	MET	18
1	A	37	LEU	17
1	A	45	MET	16
1	A	36	ASP	15
1	A	73	ASP	15
1	A	76	LEU	14
1	A	93	THR	14
1	A	22	HIS	13
1	A	25	LYS	13
1	A	72	THR	13
1	A	30	ASP	13
1	A	5	LYS	12
1	A	51	ASP	12
1	A	88	ASP	12
1	A	91	SER	12
1	A	71	ASP	11
1	A	28	LYS	11
1	A	18	LYS	10
1	A	20	ARG	10

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Mol	Chain	Res	Type	Models (Total)
1	A	60	SER	10
1	A	12	LEU	9
1	A	39	ASP	9
1	A	74	TRP	9
1	A	62	ARG	8
1	A	85	GLU	8
1	A	79	GLU	8
1	A	95	THR	8
1	A	19	GLN	7
1	A	57	GLU	7
1	A	29	GLU	7
1	A	94	SER	6
1	A	23	LYS	5
1	A	47	ASN	5
1	A	58	ASP	5
1	A	75	GLU	5
1	A	48	ASN	5
1	A	52	VAL	5
1	A	53	SER	5
1	A	7	GLU	5
1	A	33	THR	5
1	A	50	ASN	5
1	A	59	ASP	4
1	A	27	ASP	4
1	A	77	GLU	3
1	A	81	ASP	3
1	A	43	SER	3
1	A	92	PHE	3
1	A	44	THR	2
1	A	67	THR	2
1	A	70	ASN	2
1	A	40	HIS	1
1	A	80	LYS	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