



Full wwPDB NMR Structure Validation Report ⓘ

Nov 2, 2021 – 02:47 PM EDT

PDB ID : 2NS5
Title : The conserved N-terminal domain of Par-3 adopts a novel PB1-like structure required for Par-3 oligomerization and apical membrane localization
Authors : Feng, W.; Wu, H.; Chan, L.-N.; Zhang, M.
Deposited on : 2006-11-03

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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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 : 2.23.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

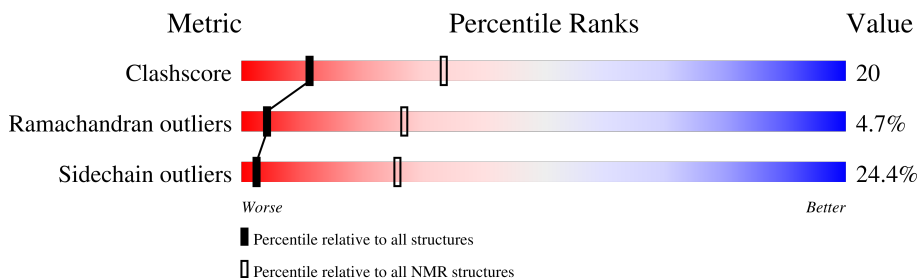
1 Overall quality at a glance

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	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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	85	54% 42% ..

2 Ensemble composition and analysis

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: *minimized average structure*.

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:18-A:100 (83)	0.27	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 3 clusters and 1 single-model cluster was found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1344 atoms, of which 665 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Partitioning-defective 3 homolog.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	85	1344	424	665	121	130	4	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	SER	-	expression tag	UNP Q9Z340
A	17	GLU	-	expression tag	UNP Q9Z340
A	18	PHE	-	expression tag	UNP Q9Z340
A	30	ASP	VAL	engineered mutation	UNP Q9Z340

4 Residue-property plots

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: Partitioning-defective 3 homolog

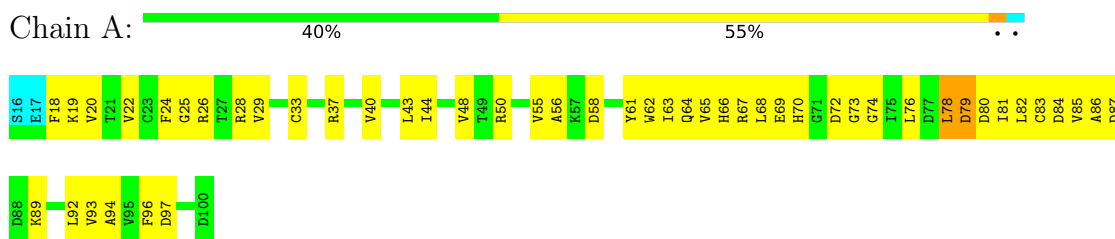


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

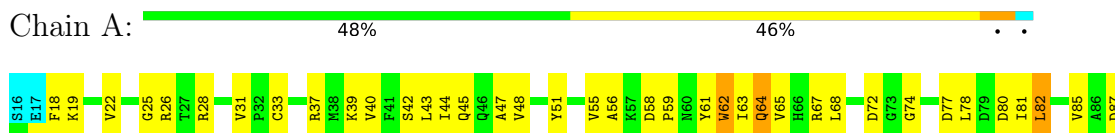
4.2.1 Score per residue for model 1

- Molecule 1: Partitioning-defective 3 homolog



4.2.2 Score per residue for model 2

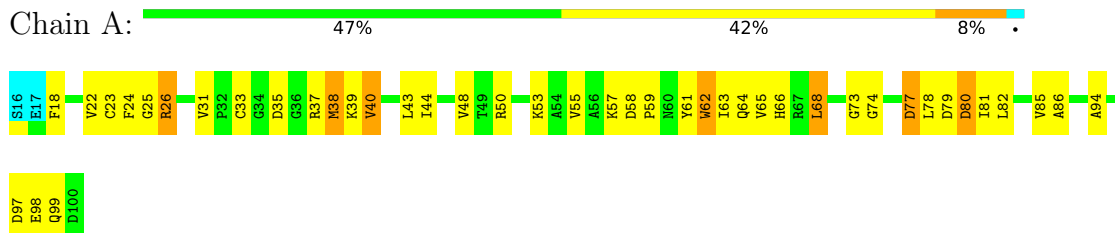
- Molecule 1: Partitioning-defective 3 homolog





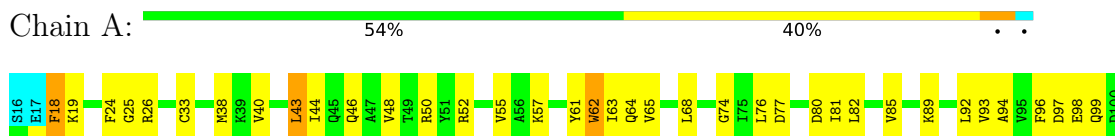
4.2.3 Score per residue for model 3

- Molecule 1: Partitioning-defective 3 homolog



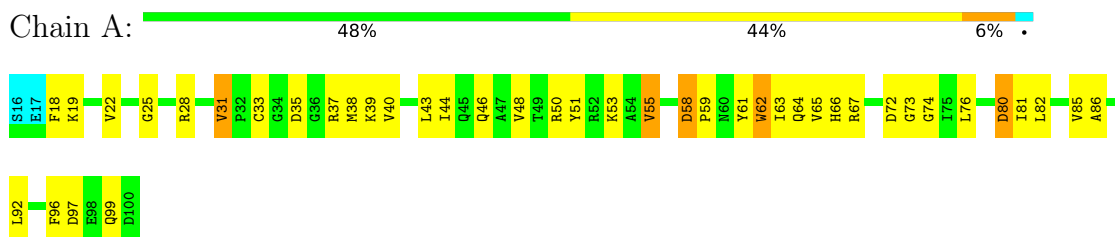
4.2.4 Score per residue for model 4 (medoid)

- Molecule 1: Partitioning-defective 3 homolog



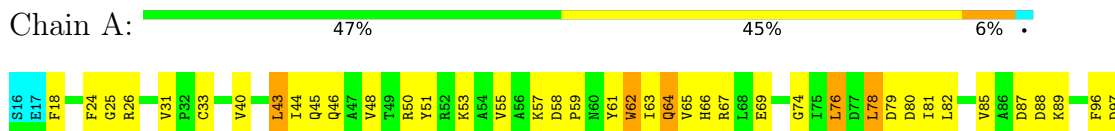
4.2.5 Score per residue for model 5

- Molecule 1: Partitioning-defective 3 homolog



4.2.6 Score per residue for model 6

- Molecule 1: Partitioning-defective 3 homolog



E98
Q99
D100

4.2.7 Score per residue for model 7

- Molecule 1: Partitioning-defective 3 homolog

Chain A:  49% 41% 7%

S16 E17 F18 V22 C23 F24 G25 R26 T27 R28 V29 D30 C33 V40 F41 F44 I44 A47 V48 V55 M60 Y61 W62 I63 O64 V65 L68 G71 D72 G73 G74 L75 L76 D77 L78 D79 D80 I81 L82 C83 D84 V85 A86 K89 R91 L92 V93 A94 V95 F96

D97 E98 Q99 D100

4.2.8 Score per residue for model 8

- Molecule 1: Partitioning-defective 3 homolog

Chain A:  47% 45% 6%

S16 E17 F18 K19 V20 T21 V22 C23 G25 R28 C33 V40 F41 S42 L43 I44 V48 Y51 V55 D58 P59 M60 Y61 W62 I63 O64 R66 L68 G71 D72 G73 G74 I75 L76 D77 L78 D79 D80 I81 L82 V85 D88 K89 V93 A94

D97 E98 Q99 D100

4.2.9 Score per residue for model 9

- Molecule 1: Partitioning-defective 3 homolog

Chain A:  54% 36% 7%

S16 E17 F18 K19 F24 G25 R26 T27 R28 V29 D30 V31 V40 L43 I44 A47 V48 T49 R50 D58 Y61 W62 I63 O64 V65 H66 R67 L68 G73 G74 I75 L76 D77 L78 D79 D80 I81 L82 V85 K89 A94 D97 E98 Q99 D100

4.2.10 Score per residue for model 10

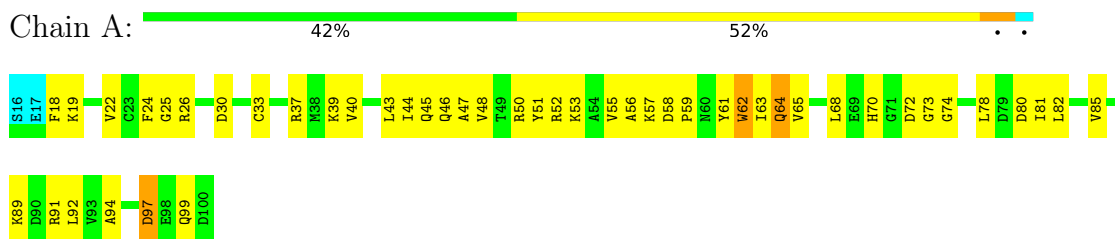
- Molecule 1: Partitioning-defective 3 homolog

Chain A:  55% 34% 8%

S16 E17 F18 V22 C23 F24 G25 C33 G34 D35 K38 R39 V40 I44 O45 Q46 A47 V48 T49 R50 Y51 V55 A56 K57 P58 D59 P59 I60 W62 I63 O64 V65 H66 R67 G74 I75 L76 D77 L78 D80 V85 A86 L92 V93 A94 D97 D100

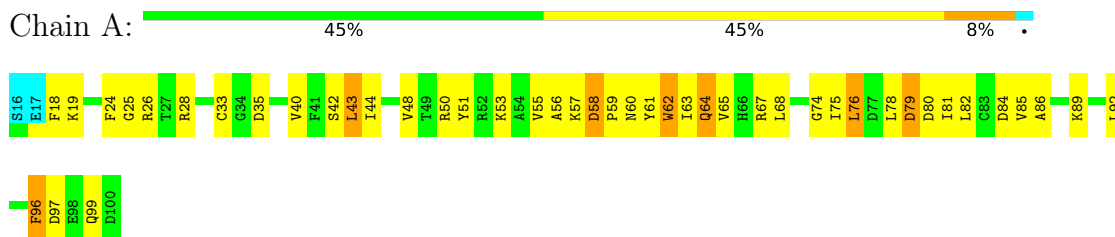
4.2.11 Score per residue for model 11

- Molecule 1: Partitioning-defective 3 homolog



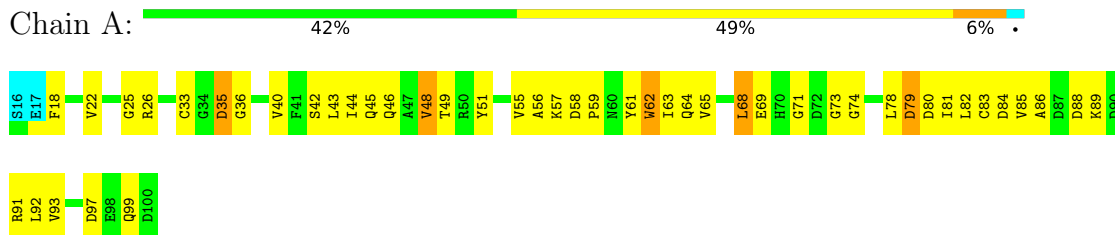
4.2.12 Score per residue for model 12

- Molecule 1: Partitioning-defective 3 homolog



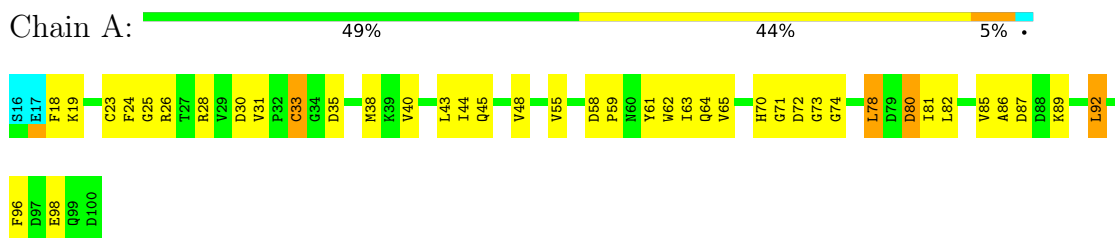
4.2.13 Score per residue for model 13

- Molecule 1: Partitioning-defective 3 homolog



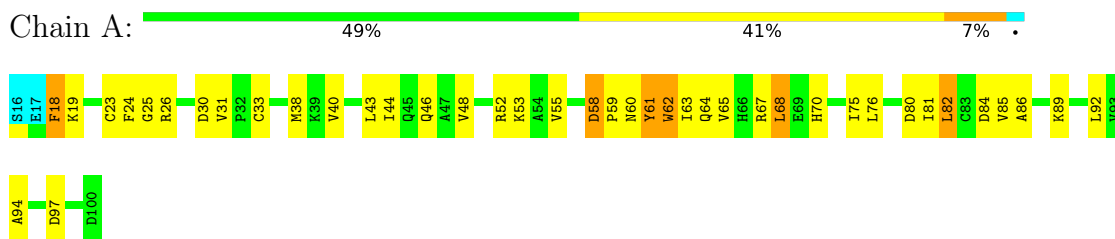
4.2.14 Score per residue for model 14

- Molecule 1: Partitioning-defective 3 homolog



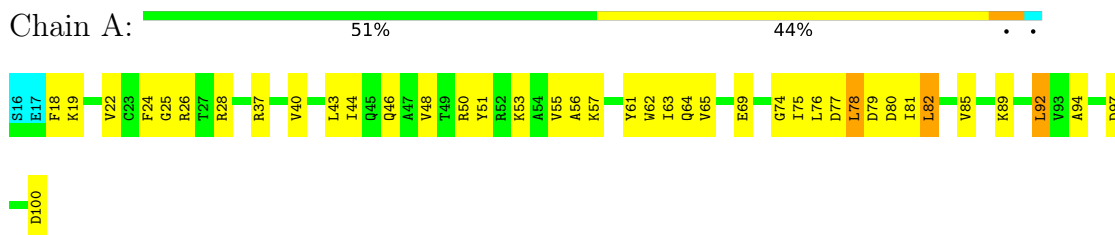
4.2.15 Score per residue for model 15

- Molecule 1: Partitioning-defective 3 homolog



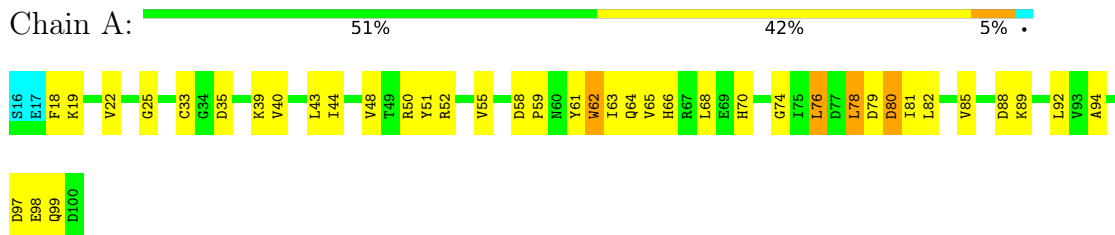
4.2.16 Score per residue for model 16

- Molecule 1: Partitioning-defective 3 homolog



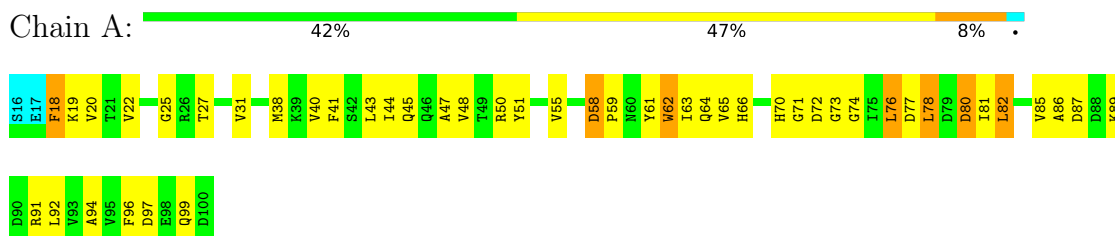
4.2.17 Score per residue for model 17

- Molecule 1: Partitioning-defective 3 homolog



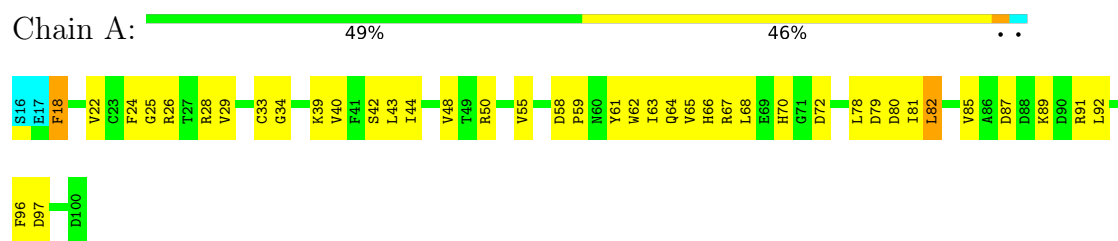
4.2.18 Score per residue for model 18

- Molecule 1: Partitioning-defective 3 homolog



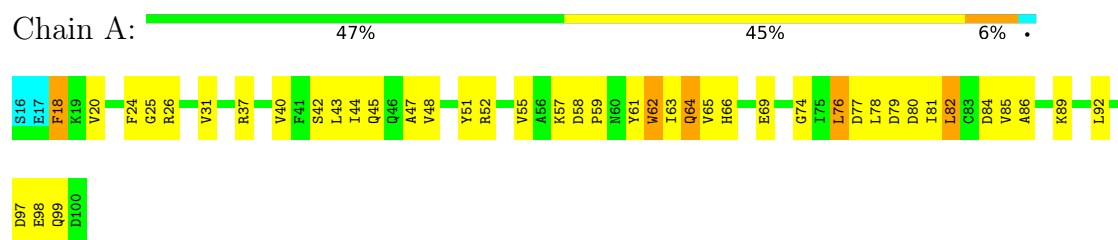
4.2.19 Score per residue for model 19

- Molecule 1: Partitioning-defective 3 homolog



4.2.20 Score per residue for model 20

- Molecule 1: Partitioning-defective 3 homolog



5 Refinement protocol and experimental data overview

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

Of the 200 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	664	654	652	27±2
All	All	13280	13080	13040	532

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 20.

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:LEU:HD13	1:A:82:LEU:HD11	0.90	1.40	3	4
1:A:43:LEU:HD13	1:A:82:LEU:HD21	0.90	1.43	20	3
1:A:22:VAL:HG12	1:A:94:ALA:HB2	0.88	1.46	7	6
1:A:44:ILE:CG2	1:A:65:VAL:HG11	0.86	2.01	15	19
1:A:40:VAL:HG23	1:A:80:ASP:O	0.82	1.74	11	19
1:A:44:ILE:O	1:A:48:VAL:HG23	0.81	1.75	5	17
1:A:61:TYR:CZ	1:A:63:ILE:HD11	0.79	2.12	11	20
1:A:76:LEU:HD11	1:A:92:LEU:HD22	0.78	1.54	20	5
1:A:44:ILE:HD13	1:A:68:LEU:HD23	0.78	1.55	8	2
1:A:44:ILE:HG23	1:A:65:VAL:HG11	0.78	1.54	14	7
1:A:20:VAL:HG11	1:A:86:ALA:HB1	0.77	1.56	1	1
1:A:22:VAL:CG1	1:A:94:ALA:HB2	0.76	2.10	7	9
1:A:43:LEU:CD1	1:A:82:LEU:HD11	0.76	2.10	19	2
1:A:81:ILE:O	1:A:85:VAL:HG12	0.76	1.79	6	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:82:LEU:HD13	1:A:86:ALA:HB3	0.76	1.56	15	3
1:A:43:LEU:HD22	1:A:82:LEU:HD11	0.76	1.57	2	1
1:A:48:VAL:HG21	1:A:65:VAL:HG21	0.74	1.60	17	16
1:A:81:ILE:O	1:A:85:VAL:HG22	0.73	1.83	11	8
1:A:44:ILE:HD12	1:A:78:LEU:HD23	0.73	1.59	14	5
1:A:43:LEU:HD13	1:A:82:LEU:HD22	0.70	1.62	17	2
1:A:44:ILE:HG12	1:A:68:LEU:HD11	0.70	1.62	7	8
1:A:22:VAL:HG13	1:A:68:LEU:HD11	0.68	1.65	8	2
1:A:51:TYR:O	1:A:55:VAL:HG22	0.68	1.88	20	3
1:A:43:LEU:CD1	1:A:82:LEU:HD21	0.68	2.19	15	2
1:A:43:LEU:HG	1:A:82:LEU:HD11	0.68	1.65	12	1
1:A:76:LEU:CD1	1:A:92:LEU:HD22	0.67	2.20	7	3
1:A:44:ILE:HG21	1:A:65:VAL:HG11	0.65	1.68	15	10
1:A:43:LEU:O	1:A:43:LEU:HD13	0.64	1.93	9	2
1:A:18:PHE:CE2	1:A:82:LEU:HD12	0.63	2.28	8	2
1:A:44:ILE:HD12	1:A:78:LEU:CD2	0.63	2.23	16	6
1:A:37:ARG:O	1:A:37:ARG:CG	0.62	2.48	2	1
1:A:18:PHE:CE1	1:A:82:LEU:HD12	0.62	2.29	9	4
1:A:61:TYR:OH	1:A:63:ILE:HD11	0.61	1.95	5	15
1:A:63:ILE:HG23	1:A:96:PHE:CD2	0.60	2.31	2	3
1:A:76:LEU:HB3	1:A:85:VAL:HG21	0.59	1.73	17	2
1:A:40:VAL:CG2	1:A:85:VAL:HG21	0.59	2.27	11	2
1:A:55:VAL:HG22	1:A:55:VAL:O	0.59	1.97	12	14
1:A:55:VAL:HG13	1:A:57:LYS:HD2	0.59	1.74	12	1
1:A:82:LEU:CD1	1:A:86:ALA:HB3	0.58	2.27	18	3
1:A:51:TYR:O	1:A:55:VAL:HG12	0.58	1.98	10	8
1:A:31:VAL:HG11	1:A:43:LEU:HG	0.58	1.76	3	3
1:A:38:MET:O	1:A:82:LEU:HD23	0.58	1.99	3	1
1:A:43:LEU:HD22	1:A:82:LEU:HD13	0.58	1.75	5	3
1:A:43:LEU:CD2	1:A:82:LEU:HD13	0.57	2.29	5	1
1:A:24:PHE:CE2	1:A:48:VAL:HG22	0.57	2.35	8	2
1:A:20:VAL:HG21	1:A:43:LEU:HD21	0.57	1.77	20	2
1:A:20:VAL:CG2	1:A:43:LEU:HD11	0.57	2.29	20	2
1:A:69:GLU:O	1:A:93:VAL:HG22	0.56	2.01	1	1
1:A:70:HIS:HA	1:A:92:LEU:HD23	0.56	1.76	18	4
1:A:65:VAL:HG13	1:A:65:VAL:O	0.56	2.00	6	1
1:A:74:GLY:O	1:A:76:LEU:HD23	0.56	2.01	17	1
1:A:76:LEU:HD23	1:A:85:VAL:CG2	0.56	2.30	9	4
1:A:55:VAL:HG23	1:A:57:LYS:HG3	0.56	1.77	4	1
1:A:39:LYS:HE2	1:A:81:ILE:HD11	0.55	1.78	3	1
1:A:40:VAL:HA	1:A:43:LEU:HD23	0.55	1.78	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:82:LEU:HG	1:A:86:ALA:HB3	0.54	1.78	7	1
1:A:43:LEU:HD12	1:A:82:LEU:HD21	0.54	1.77	19	1
1:A:44:ILE:CG2	1:A:65:VAL:HG21	0.54	2.33	6	1
1:A:31:VAL:HG21	1:A:47:ALA:HB2	0.54	1.80	18	3
1:A:43:LEU:HD13	1:A:82:LEU:CD2	0.54	2.33	17	2
1:A:70:HIS:CE1	1:A:92:LEU:HD21	0.53	2.38	17	4
1:A:52:ARG:CZ	1:A:63:ILE:HD12	0.53	2.33	15	1
1:A:85:VAL:O	1:A:85:VAL:HG22	0.53	2.04	6	1
1:A:31:VAL:HG11	1:A:43:LEU:HD12	0.53	1.81	14	1
1:A:44:ILE:CD1	1:A:68:LEU:HD23	0.52	2.33	8	2
1:A:55:VAL:O	1:A:56:ALA:HB3	0.52	2.05	16	5
1:A:67:ARG:NH1	1:A:75:ILE:HD13	0.52	2.19	12	1
1:A:22:VAL:O	1:A:29:VAL:HG22	0.52	2.05	19	1
1:A:62:TRP:CD1	1:A:99:GLN:CB	0.51	2.93	13	2
1:A:82:LEU:HD13	1:A:86:ALA:CB	0.51	2.34	18	1
1:A:20:VAL:HG21	1:A:43:LEU:HD11	0.51	1.83	1	1
1:A:55:VAL:HG11	1:A:57:LYS:HD2	0.51	1.83	13	4
1:A:22:VAL:O	1:A:29:VAL:HG12	0.51	2.05	1	1
1:A:81:ILE:O	1:A:85:VAL:HG23	0.51	2.06	1	1
1:A:18:PHE:HE2	1:A:82:LEU:HD12	0.51	1.65	8	1
1:A:40:VAL:O	1:A:44:ILE:HG13	0.50	2.06	5	19
1:A:43:LEU:HD13	1:A:82:LEU:HD13	0.50	1.84	6	1
1:A:43:LEU:HD12	1:A:44:ILE:N	0.50	2.21	5	1
1:A:68:LEU:HD23	1:A:94:ALA:HA	0.50	1.83	2	1
1:A:61:TYR:CE1	1:A:63:ILE:HD11	0.50	2.42	15	3
1:A:55:VAL:HG21	1:A:57:LYS:HD2	0.50	1.82	16	1
1:A:24:PHE:HA	1:A:94:ALA:HB3	0.49	1.84	4	2
1:A:33:CYS:SG	1:A:82:LEU:HD22	0.49	2.47	14	2
1:A:22:VAL:HG12	1:A:94:ALA:CB	0.49	2.28	7	1
1:A:31:VAL:HG11	1:A:43:LEU:CD2	0.49	2.38	9	1
1:A:76:LEU:HD23	1:A:85:VAL:CG1	0.49	2.38	1	1
1:A:76:LEU:HD23	1:A:85:VAL:HG22	0.49	1.85	9	1
1:A:31:VAL:HG11	1:A:43:LEU:CD1	0.49	2.37	14	1
1:A:76:LEU:CD2	1:A:85:VAL:HG22	0.48	2.38	9	2
1:A:40:VAL:CG2	1:A:79:ASP:N	0.48	2.76	3	1
1:A:69:GLU:O	1:A:93:VAL:HG12	0.48	2.09	13	1
1:A:27:THR:HG21	1:A:51:TYR:CD1	0.47	2.45	18	1
1:A:24:PHE:HE2	1:A:48:VAL:HG22	0.47	1.69	14	1
1:A:40:VAL:HG23	1:A:78:LEU:C	0.47	2.29	3	1
1:A:40:VAL:HG12	1:A:44:ILE:CD1	0.47	2.39	5	1
1:A:62:TRP:CZ3	1:A:64:GLN:CG	0.47	2.98	11	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:92:LEU:HD12	1:A:92:LEU:N	0.47	2.25	14	1
1:A:61:TYR:CZ	1:A:63:ILE:CD1	0.47	2.98	6	7
1:A:40:VAL:O	1:A:43:LEU:HG	0.47	2.09	5	1
1:A:55:VAL:HG11	1:A:57:LYS:CD	0.46	2.40	3	1
1:A:43:LEU:HD22	1:A:82:LEU:CD1	0.46	2.41	13	1
1:A:22:VAL:HG23	1:A:31:VAL:HG21	0.46	1.87	5	1
1:A:22:VAL:CG1	1:A:24:PHE:CE1	0.46	2.99	8	1
1:A:48:VAL:HG21	1:A:65:VAL:CG2	0.46	2.39	13	1
1:A:39:LYS:HA	1:A:81:ILE:HD13	0.46	1.87	3	1
1:A:81:ILE:CG2	1:A:82:LEU:N	0.46	2.79	13	17
1:A:68:LEU:HD13	1:A:93:VAL:O	0.45	2.12	8	1
1:A:76:LEU:HD13	1:A:92:LEU:HD22	0.45	1.87	16	1
1:A:62:TRP:CD1	1:A:99:GLN:HB2	0.45	2.46	3	12
1:A:44:ILE:CG1	1:A:68:LEU:HD11	0.45	2.37	7	1
1:A:31:VAL:HG11	1:A:43:LEU:HD22	0.45	1.87	9	1
1:A:70:HIS:CE1	1:A:92:LEU:CD2	0.45	3.00	15	2
1:A:81:ILE:HG22	1:A:83:CYS:H	0.45	1.72	7	1
1:A:18:PHE:CD1	1:A:82:LEU:HD21	0.45	2.46	13	1
1:A:82:LEU:O	1:A:86:ALA:N	0.45	2.50	3	2
1:A:62:TRP:CZ3	1:A:64:GLN:HB2	0.44	2.46	10	2
1:A:22:VAL:HG23	1:A:31:VAL:CG2	0.44	2.42	5	1
1:A:85:VAL:HG23	1:A:86:ALA:N	0.44	2.27	14	4
1:A:18:PHE:CD2	1:A:82:LEU:HD21	0.44	2.48	4	1
1:A:24:PHE:CE1	1:A:47:ALA:HB1	0.44	2.47	7	3
1:A:75:ILE:HG22	1:A:76:LEU:N	0.44	2.28	15	4
1:A:24:PHE:CD1	1:A:94:ALA:CB	0.44	3.01	4	1
1:A:44:ILE:CG2	1:A:65:VAL:CG2	0.44	2.96	6	1
1:A:85:VAL:HG13	1:A:86:ALA:N	0.44	2.28	10	4
1:A:76:LEU:HD23	1:A:85:VAL:HB	0.43	1.89	18	2
1:A:61:TYR:CE2	1:A:63:ILE:HG12	0.43	2.48	13	9
1:A:48:VAL:HG23	1:A:65:VAL:CG2	0.43	2.42	10	1
1:A:55:VAL:HG13	1:A:57:LYS:CD	0.43	2.43	12	1
1:A:24:PHE:O	1:A:26:ARG:N	0.43	2.52	20	11
1:A:63:ILE:HG23	1:A:96:PHE:HD2	0.43	1.74	5	5
1:A:44:ILE:HG22	1:A:65:VAL:HG11	0.43	1.89	6	1
1:A:36:GLY:HA2	1:A:82:LEU:HD23	0.43	1.90	13	1
1:A:58:ASP:CB	1:A:59:PRO:CD	0.43	2.97	15	10
1:A:62:TRP:CH2	1:A:64:GLN:HB2	0.43	2.48	12	7
1:A:58:ASP:CB	1:A:59:PRO:HD2	0.43	2.44	8	5
1:A:55:VAL:O	1:A:55:VAL:HG22	0.42	2.14	13	1
1:A:55:VAL:HG23	1:A:57:LYS:CG	0.42	2.44	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:67:ARG:NH1	1:A:75:ILE:HG21	0.42	2.29	8	1
1:A:77:ASP:OD1	1:A:78:LEU:HD12	0.42	2.14	10	1
1:A:48:VAL:CG1	1:A:49:THR:N	0.42	2.82	9	3
1:A:40:VAL:HG12	1:A:44:ILE:HD11	0.42	1.92	5	1
1:A:39:LYS:HG2	1:A:81:ILE:HD13	0.42	1.92	5	1
1:A:68:LEU:HD11	1:A:94:ALA:HB2	0.42	1.91	9	2
1:A:20:VAL:CG2	1:A:43:LEU:HD21	0.42	2.44	20	1
1:A:43:LEU:CD1	1:A:82:LEU:HD22	0.42	2.45	6	1
1:A:43:LEU:HG	1:A:82:LEU:HD21	0.42	1.92	9	1
1:A:81:ILE:HG22	1:A:82:LEU:N	0.41	2.30	15	6
1:A:43:LEU:C	1:A:43:LEU:HD12	0.41	2.34	8	1
1:A:96:PHE:CD1	1:A:96:PHE:N	0.41	2.88	12	1
1:A:55:VAL:HG23	1:A:57:LYS:HB2	0.41	1.90	20	1
1:A:44:ILE:HG23	1:A:65:VAL:HG21	0.41	1.91	6	1
1:A:43:LEU:CG	1:A:82:LEU:HD11	0.41	2.40	12	1
1:A:57:LYS:HD3	1:A:61:TYR:CZ	0.41	2.50	4	2
1:A:23:CYS:O	1:A:94:ALA:HB3	0.41	2.15	10	1
1:A:63:ILE:HA	1:A:97:ASP:O	0.41	2.15	11	1
1:A:40:VAL:HG22	1:A:85:VAL:HG11	0.41	1.93	4	1
1:A:55:VAL:CG1	1:A:57:LYS:CD	0.41	2.99	3	1
1:A:75:ILE:CG2	1:A:76:LEU:N	0.41	2.83	15	2
1:A:40:VAL:HG11	1:A:77:ASP:O	0.41	2.15	10	1
1:A:55:VAL:O	1:A:55:VAL:CG2	0.41	2.68	12	1
1:A:40:VAL:HG23	1:A:79:ASP:N	0.41	2.31	3	1
1:A:37:ARG:O	1:A:37:ARG:HG3	0.41	2.14	2	1
1:A:21:THR:CG2	1:A:28:ARG:CG	0.41	2.99	8	1
1:A:40:VAL:HG13	1:A:80:ASP:O	0.41	2.15	3	1
1:A:41:PHE:CD2	1:A:78:LEU:HB3	0.41	2.51	18	1
1:A:41:PHE:HD1	1:A:78:LEU:HD22	0.40	1.76	7	1
1:A:68:LEU:CD1	1:A:94:ALA:HB2	0.40	2.47	9	1
1:A:76:LEU:HD23	1:A:85:VAL:HG21	0.40	1.92	12	1
1:A:69:GLU:HA	1:A:76:LEU:HD12	0.40	1.93	1	1
1:A:91:ARG:O	1:A:92:LEU:HD23	0.40	2.15	7	1
1:A:44:ILE:CG2	1:A:65:VAL:CG1	0.40	3.00	10	1
1:A:52:ARG:HD3	1:A:63:ILE:HD12	0.40	1.94	11	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	82/85 (96%)	67±2 (82±3%)	11±3 (13±3%)	4±1 (5±2%)	4	27
All	All	1640/1700 (96%)	1348 (82%)	215 (13%)	77 (5%)	4	27

All 12 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	25	GLY	20
1	A	74	GLY	17
1	A	66	HIS	10
1	A	73	GLY	10
1	A	79	ASP	9
1	A	71	GLY	5
1	A	77	ASP	1
1	A	72	ASP	1
1	A	56	ALA	1
1	A	35	ASP	1
1	A	60	ASN	1
1	A	34	GLY	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	72/74 (97%)	54±2 (76±3%)	18±2 (24±3%)	2	26
All	All	1440/1480 (97%)	1089 (76%)	351 (24%)	2	26

All 51 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	62	TRP	20
1	A	18	PHE	19
1	A	64	GLN	19
1	A	97	ASP	19
1	A	89	LYS	16
1	A	33	CYS	15
1	A	78	LEU	15
1	A	19	LYS	13
1	A	50	ARG	12
1	A	28	ARG	9
1	A	67	ARG	8
1	A	77	ASP	8
1	A	82	LEU	8
1	A	80	ASP	8
1	A	46	GLN	8
1	A	79	ASP	7
1	A	45	GLN	7
1	A	35	ASP	7
1	A	38	MET	7
1	A	53	LYS	7
1	A	37	ARG	6
1	A	58	ASP	6
1	A	72	ASP	6
1	A	87	ASP	6
1	A	42	SER	6
1	A	98	GLU	6
1	A	92	LEU	6
1	A	76	LEU	6
1	A	84	ASP	5
1	A	26	ARG	5
1	A	43	LEU	5
1	A	96	PHE	5
1	A	30	ASP	5
1	A	91	ARG	5
1	A	39	LYS	4
1	A	68	LEU	4
1	A	88	ASP	4
1	A	83	CYS	3
1	A	23	CYS	3
1	A	52	ARG	3
1	A	69	GLU	3
1	A	100	ASP	3
1	A	60	ASN	3

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Mol	Chain	Res	Type	Models (Total)
1	A	48	VAL	3
1	A	99	GLN	2
1	A	40	VAL	1
1	A	93	VAL	1
1	A	31	VAL	1
1	A	55	VAL	1
1	A	22	VAL	1
1	A	61	TYR	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

No chemical shift data were provided