Full wwPDB NMR Structure Validation Report (i)

Mar 7, 2022 – 06:51 AM EST

PDB ID	:	2YT7
Title	:	Solution structure of the PDZ domain of Amyloid beta A4 precursor protein-binding family A member 3
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Deposited on	:	2007-04-05

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
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:

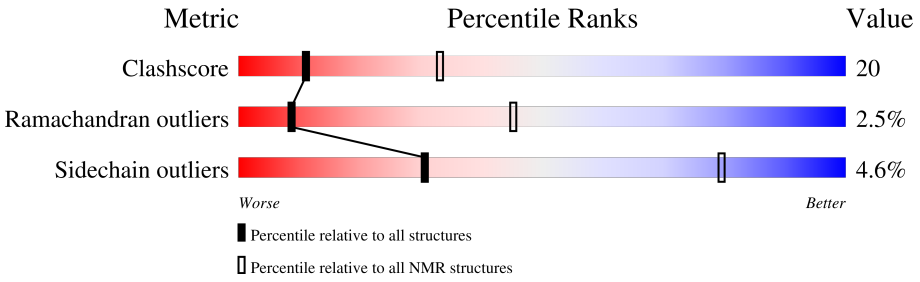
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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	101	55% 21% • 23%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 15 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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:11-A:29, A:38-A:96 (78)	0.22	15

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 and 2 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1437 atoms, of which 725 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Amyloid beta A4 precursor protein-binding family A member 3.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	101	1437	436	725	133	140	3	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP O96018
A	2	SER	-	expression tag	UNP O96018
A	3	SER	-	expression tag	UNP O96018
A	4	GLY	-	expression tag	UNP O96018
A	5	SER	-	expression tag	UNP O96018
A	6	SER	-	expression tag	UNP O96018
A	7	GLY	-	expression tag	UNP O96018

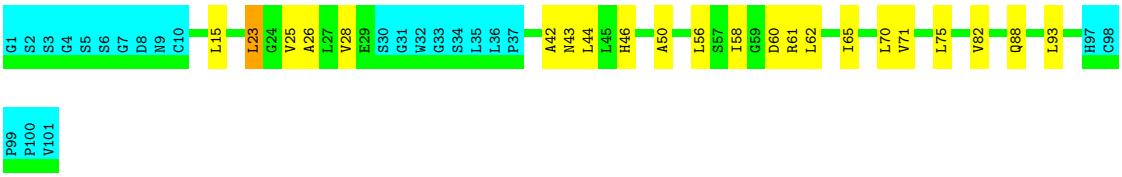
4 Residue-property plots (i)

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: Amyloid beta A4 precursor protein-binding family A member 3

Chain A: 55% 21% • 23%



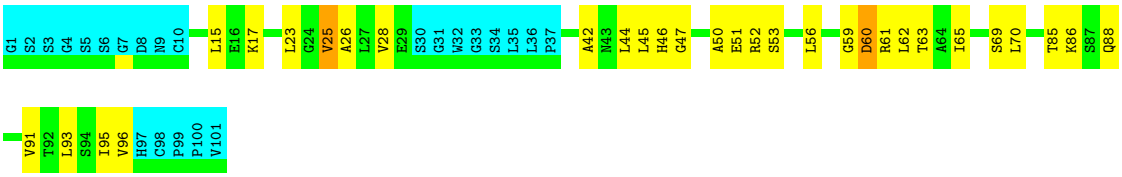
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Amyloid beta A4 precursor protein-binding family A member 3

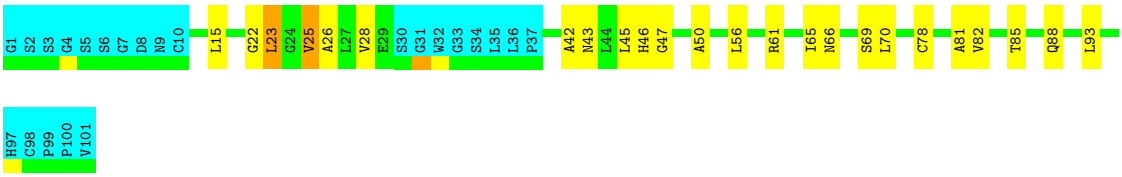
Chain A: 47% 29% • 23%



4.2.2 Score per residue for model 2

• Molecule 1: Amyloid beta A4 precursor protein-binding family A member 3

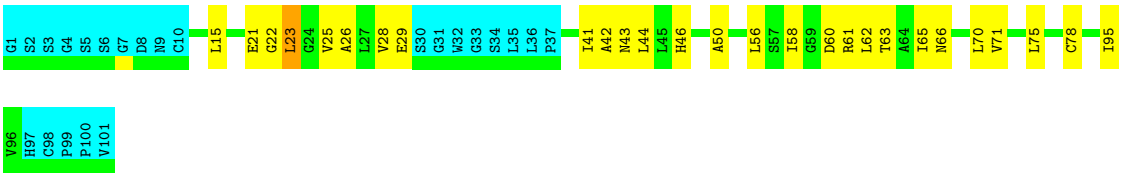
Chain A: 53% 22% • 23%



4.2.3 Score per residue for model 3

- Molecule 1: Amyloid beta A4 precursor protein-binding family A member 3

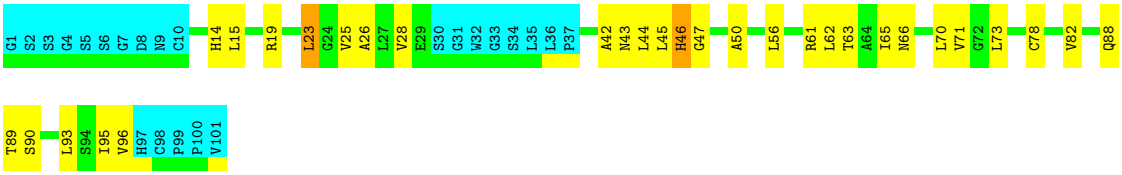
Chain A: 50% 26% • 23%



4.2.4 Score per residue for model 4

- Molecule 1: Amyloid beta A4 precursor protein-binding family A member 3

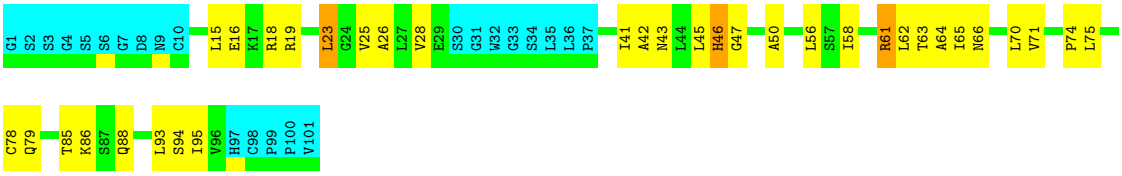
Chain A: 47% 29% • 23%



4.2.5 Score per residue for model 5

- Molecule 1: Amyloid beta A4 precursor protein-binding family A member 3

Chain A: 43% 32% • 23%



4.2.6 Score per residue for model 6

- Molecule 1: Amyloid beta A4 precursor protein-binding family A member 3

Chain A: 52% 22% • 23%

G1 S2 S3 G4 S5 S6 G7 D8 N9 C10 R11 E12 V13 R18 R19 L23 A26 L27 V28 E29 S30 G31 W32 G33 S34 L35 L36 P37 I41 A42 N43 H46 L56 S57 I58 R61 L62 I65 V71 L75 Q88 T89 L93 S94 I95 V96 H97 C98

P99 P100 V101

4.2.7 Score per residue for model 7

- Molecule 1: Amyloid beta A4 precursor protein-binding family A member 3

Chain A: 50% 25% • 23%

G1 S2 S3 G4 S5 S6 G7 D8 N9 C10 L15 E16 K17 L23 G24 V25 A26 L27 V28 E29 S30 G31 W32 G33 S34 L35 L36 P37 A42 N43 L44 L45 H46 G47 A50 S57 I58 G59 D60 R61 L62 T63 A64 I65 N66 L70 C78 V82 Q88 I95

V96 H97 C98 P99 P100 V101

4.2.8 Score per residue for model 8

- Molecule 1: Amyloid beta A4 precursor protein-binding family A member 3

Chain A: 61% 15% • 23%

G1 S2 S3 G4 S5 S6 G7 D8 N9 C10 R18 R19 L23 A26 L27 V28 E29 S30 G31 W32 G33 S34 L35 L36 P37 A42 H46 L56 L62 I65 L70 L73 V82 Q88 T89 L93 H97 C98 P99 P100 V101

4.2.9 Score per residue for model 9

- Molecule 1: Amyloid beta A4 precursor protein-binding family A member 3

Chain A: 50% 25% • 23%

G1 S2 S3 G4 S5 S6 G7 D8 N9 C10 R11 E12 V13 H14 L15 R18 R19 L23 A26 L27 V28 E29 S30 G31 W32 G33 S34 L35 L36 P37 I41 A42 N43 H46 A50 E51 R52 S53 L56 G59 D60 R61 L62 T63 A64 I65 S69 P74 L75

V82 L93 H97 C98 P99 P100 V101

4.2.10 Score per residue for model 10

- Molecule 1: Amyloid beta A4 precursor protein-binding family A member 3

Chain A: 54% 21% • 23%

G1 S2 S3 G4 S5 S6 G7 D8 N9 C10 R11 E12 V13 H14 L15 R18 R19 L23 A26 L27 V28 E29 S30 G31 W32 G33 S34 L35 L36 P37 I41 A42 N43 L44 L45 H46 A50 L56 S57 I58 G59 D60 R61 L62 L75 Q88 L93 H97 C98 P99

P100 V101

4.2.11 Score per residue for model 11

- Molecule 1: Amyloid beta A4 precursor protein-binding family A member 3

Chain A: 51% 23% • 23%

G1 S2 S3 G4 S5 S6 G7 D8 N9 C10 G22 L23 G24 V25 A26 L27 V28 E29 S30 G31 W32 G33 S34 L35 L36 P37 I41 A42 N43 L44 L45 H46 A50 L56 S57 I58 R61 L62 I65 N66 V71 L75 Q79 V82 R83 E84 T85 Q88

L93 H97 C98 P99 P100 V101

4.2.12 Score per residue for model 12

- Molecule 1: Amyloid beta A4 precursor protein-binding family A member 3

Chain A: 49% 26% • 23%

G1 S2 S3 G4 S5 S6 G7 D8 N9 C10 R11 E12 V13 H14 L15 E16 K17 L23 G24 V25 A26 L27 V28 E29 S30 G31 W32 G33 S34 L35 L36 P37 A42 N43 L44 L45 H46 G47 G48 P49 L56 S57 I58 G59 D60 R61 L62 I65 L70 V71 G72 L73 P74 L75

V82 V91 T92 L93 V96 H97 C98 P99 P100 V101

4.2.13 Score per residue for model 13

- Molecule 1: Amyloid beta A4 precursor protein-binding family A member 3

Chain A: 50% 26% • 23%

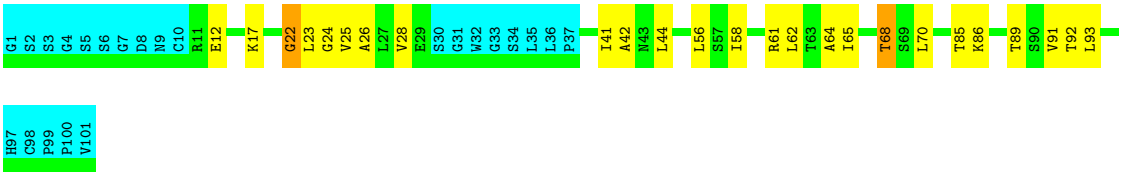
G1 S2 S3 G4 S5 S6 G7 D8 N9 C10 L15 R18 R19 G20 E21 G22 L23 G24 V25 A26 L27 V28 E29 S30 G31 W32 G33 S34 L35 L36 P37 A42 N43 L44 L45 H46 G47 A50 L56 R61 A64 T68 V71 V82 T85 K86 S87 Q88

V91 T92 L93 S94 I95 V96 H97 C98 P99 P100 V101

4.2.14 Score per residue for model 14

• Molecule 1: Amyloid beta A4 precursor protein-binding family A member 3

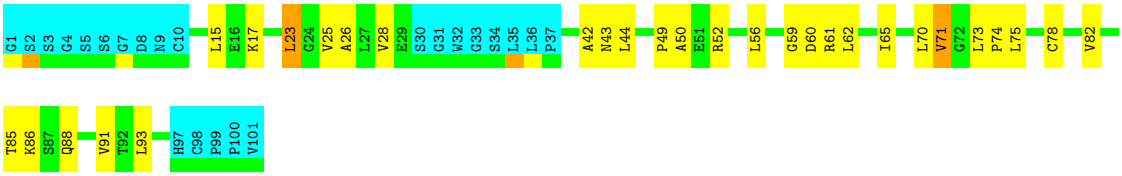
Chain A: 52% 23% • 23%



4.2.15 Score per residue for model 15 (medoid)

• Molecule 1: Amyloid beta A4 precursor protein-binding family A member 3

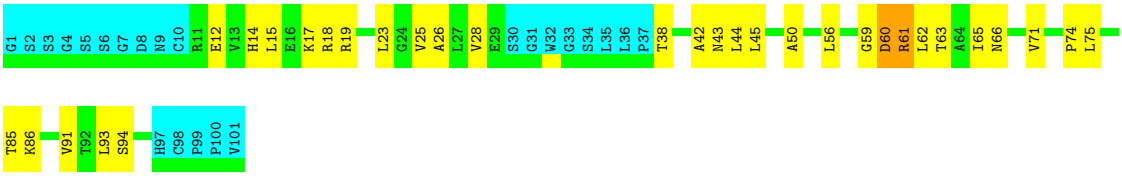
Chain A: 48% 28% • 23%



4.2.16 Score per residue for model 16

• Molecule 1: Amyloid beta A4 precursor protein-binding family A member 3

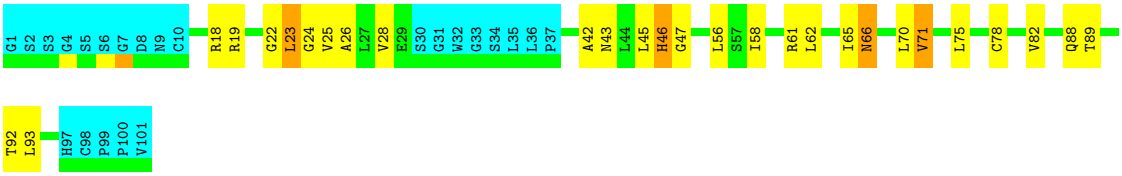
Chain A: 46% 30% • 23%



4.2.17 Score per residue for model 17

• Molecule 1: Amyloid beta A4 precursor protein-binding family A member 3

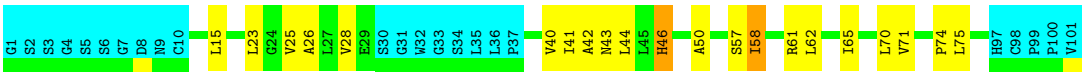
Chain A: 50% 24% • 23%



4.2.18 Score per residue for model 18

• Molecule 1: Amyloid beta A4 precursor protein-binding family A member 3

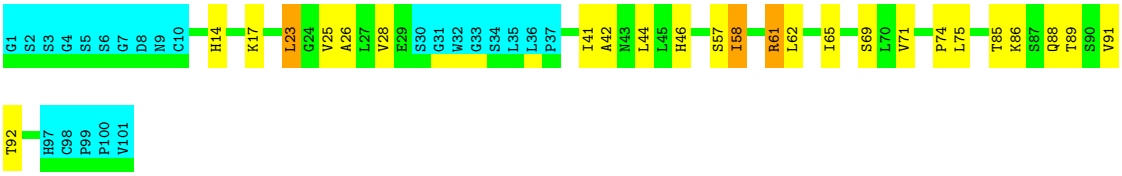
Chain A: 56% 19% • 23%



4.2.19 Score per residue for model 19

• Molecule 1: Amyloid beta A4 precursor protein-binding family A member 3

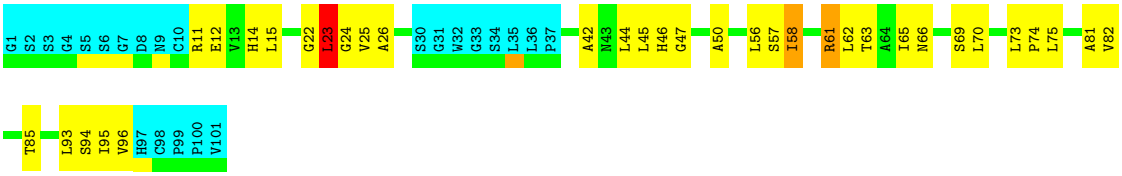
Chain A: 52% 22% • 23%



4.2.20 Score per residue for model 20

• Molecule 1: Amyloid beta A4 precursor protein-binding family A member 3

Chain A: 43% 32% • • 23%



5 Refinement protocol and experimental data overview (i)

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the least restraint violations,structures with the lowest energy,target function*.

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

Software name	Classification	Version
CYANA	structure solution	2.0.17
CYANA	refinement	2.0.17

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	560	591	591	23±5
All	All	11200	11820	11820	469

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:56:LEU:HD13	1:A:93:LEU:HD12	1.02	1.32	10	16
1:A:25:VAL:HG12	1:A:44:LEU:HD22	0.77	1.56	12	9
1:A:56:LEU:HD13	1:A:93:LEU:CD1	0.77	2.09	5	6
1:A:65:ILE:HG22	1:A:66:ASN:ND2	0.75	1.97	11	3
1:A:56:LEU:CD1	1:A:93:LEU:HD12	0.74	2.13	5	8
1:A:41:ILE:O	1:A:58:ILE:HG23	0.72	1.83	5	6
1:A:62:LEU:HD11	1:A:65:ILE:CG1	0.71	2.15	9	11
1:A:15:LEU:HD22	1:A:49:PRO:O	0.69	1.87	12	2
1:A:28:VAL:HG22	1:A:42:ALA:HB2	0.67	1.66	1	7
1:A:71:VAL:O	1:A:71:VAL:HG13	0.67	1.88	13	6
1:A:62:LEU:C	1:A:62:LEU:HD23	0.66	2.11	9	7
1:A:41:ILE:HG21	1:A:44:LEU:HD21	0.66	1.67	3	3
1:A:25:VAL:HG12	1:A:44:LEU:CD2	0.65	2.22	12	1
1:A:70:LEU:HA	1:A:73:LEU:HD12	0.65	1.67	4	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:65:ILE:HG22	1:A:66:ASN:OD1	0.65	1.91	16	1
1:A:23:LEU:CD2	1:A:50:ALA:HB2	0.64	2.22	10	5
1:A:50:ALA:O	1:A:56:LEU:HD12	0.64	1.93	11	5
1:A:65:ILE:HD12	1:A:70:LEU:HD11	0.63	1.68	8	4
1:A:61:ARG:NH2	1:A:71:VAL:HG23	0.63	2.09	12	2
1:A:28:VAL:CG2	1:A:42:ALA:HB2	0.62	2.24	1	9
1:A:64:ALA:HB1	1:A:68:THR:O	0.61	1.95	14	2
1:A:62:LEU:HD11	1:A:65:ILE:HG13	0.61	1.72	12	4
1:A:29:GLU:HG3	1:A:75:LEU:HD22	0.60	1.73	6	1
1:A:17:LYS:CE	1:A:91:VAL:CG2	0.60	2.80	19	6
1:A:61:ARG:CZ	1:A:63:THR:CG2	0.60	2.80	20	1
1:A:45:LEU:C	1:A:45:LEU:HD13	0.59	2.17	1	2
1:A:62:LEU:HD21	1:A:70:LEU:HD12	0.59	1.74	1	3
1:A:28:VAL:HG13	1:A:42:ALA:HB2	0.59	1.73	19	11
1:A:61:ARG:NH1	1:A:63:THR:HG22	0.59	2.11	3	3
1:A:58:ILE:HD12	1:A:58:ILE:H	0.59	1.58	7	5
1:A:41:ILE:CG2	1:A:44:LEU:HD21	0.59	2.28	3	2
1:A:70:LEU:HD13	1:A:78:CYS:SG	0.58	2.38	5	4
1:A:15:LEU:HD13	1:A:50:ALA:HA	0.58	1.74	16	11
1:A:66:ASN:HD22	1:A:66:ASN:N	0.58	1.96	17	1
1:A:61:ARG:HH22	1:A:71:VAL:HG13	0.57	1.59	4	1
1:A:62:LEU:CD2	1:A:70:LEU:HD12	0.57	2.30	15	5
1:A:65:ILE:HD11	1:A:70:LEU:HD11	0.56	1.77	3	1
1:A:65:ILE:HG22	1:A:66:ASN:HD22	0.56	1.60	3	2
1:A:61:ARG:HH11	1:A:63:THR:HG22	0.56	1.59	7	2
1:A:28:VAL:CG1	1:A:42:ALA:HB2	0.55	2.32	14	11
1:A:26:ALA:HB3	1:A:43:ASN:O	0.55	2.01	16	14
1:A:23:LEU:HD13	1:A:82:VAL:HG23	0.55	1.78	17	6
1:A:61:ARG:O	1:A:95:ILE:HG22	0.55	2.02	3	3
1:A:65:ILE:CD1	1:A:70:LEU:HD11	0.55	2.31	3	2
1:A:38:THR:HG22	1:A:61:ARG:NH2	0.55	2.16	16	1
1:A:12:GLU:CG	1:A:14:HIS:NE2	0.55	2.70	16	1
1:A:58:ILE:N	1:A:58:ILE:HD13	0.54	2.17	17	1
1:A:23:LEU:O	1:A:23:LEU:HD23	0.54	2.03	17	14
1:A:19:ARG:N	1:A:89:THR:HG22	0.54	2.18	6	4
1:A:81:ALA:O	1:A:85:THR:HG23	0.53	2.02	2	2
1:A:23:LEU:CD1	1:A:82:VAL:HG23	0.53	2.34	17	5
1:A:23:LEU:HD13	1:A:25:VAL:HG21	0.53	1.81	19	7
1:A:66:ASN:ND2	1:A:85:THR:HG22	0.51	2.21	5	1
1:A:79:GLN:OE1	1:A:79:GLN:N	0.50	2.44	5	1
1:A:95:ILE:HD12	1:A:96:VAL:C	0.50	2.26	20	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:12:GLU:HG3	1:A:14:HIS:CD2	0.50	2.41	16	1
1:A:15:LEU:HD13	1:A:50:ALA:CB	0.50	2.36	20	1
1:A:41:ILE:HG21	1:A:44:LEU:CD2	0.50	2.36	3	1
1:A:12:GLU:CD	1:A:14:HIS:CE1	0.50	2.86	9	1
1:A:45:LEU:HD23	1:A:45:LEU:C	0.49	2.28	16	4
1:A:62:LEU:HD23	1:A:63:THR:N	0.49	2.21	16	2
1:A:66:ASN:ND2	1:A:88:GLN:OE1	0.49	2.45	2	1
1:A:26:ALA:O	1:A:42:ALA:N	0.49	2.45	18	19
1:A:95:ILE:CD1	1:A:96:VAL:O	0.49	2.60	1	2
1:A:95:ILE:HD12	1:A:96:VAL:N	0.49	2.22	20	3
1:A:62:LEU:HD22	1:A:70:LEU:HD12	0.49	1.82	7	2
1:A:22:GLY:O	1:A:24:GLY:N	0.49	2.45	11	4
1:A:28:VAL:HA	1:A:75:LEU:HD13	0.49	1.84	17	2
1:A:64:ALA:CB	1:A:68:THR:O	0.48	2.61	13	2
1:A:95:ILE:HD12	1:A:96:VAL:O	0.48	2.08	1	2
1:A:61:ARG:HH22	1:A:71:VAL:HG23	0.48	1.68	19	2
1:A:85:THR:O	1:A:88:GLN:N	0.48	2.46	5	5
1:A:15:LEU:HD13	1:A:50:ALA:CA	0.48	2.38	20	2
1:A:23:LEU:HD23	1:A:23:LEU:O	0.48	2.08	14	3
1:A:45:LEU:O	1:A:47:GLY:N	0.48	2.47	5	9
1:A:75:LEU:HD11	1:A:79:GLN:NE2	0.48	2.24	5	1
1:A:78:CYS:O	1:A:82:VAL:HG12	0.47	2.08	4	4
1:A:11:ARG:N	1:A:95:ILE:O	0.47	2.47	20	1
1:A:88:GLN:N	1:A:88:GLN:CD	0.47	2.67	10	4
1:A:12:GLU:HG2	1:A:14:HIS:CE1	0.47	2.45	20	3
1:A:41:ILE:CG2	1:A:44:LEU:CD2	0.47	2.93	3	1
1:A:41:ILE:HD12	1:A:60:ASP:HB2	0.47	1.87	9	1
1:A:66:ASN:ND2	1:A:85:THR:CG2	0.47	2.77	5	1
1:A:17:LYS:CE	1:A:91:VAL:HG21	0.46	2.40	12	2
1:A:45:LEU:C	1:A:45:LEU:CD1	0.46	2.83	1	1
1:A:62:LEU:HD11	1:A:65:ILE:CD1	0.46	2.39	12	2
1:A:62:LEU:HD12	1:A:93:LEU:HD22	0.46	1.86	14	1
1:A:17:LYS:N	1:A:89:THR:O	0.46	2.48	14	1
1:A:95:ILE:HD12	1:A:95:ILE:C	0.46	2.31	20	2
1:A:60:ASP:OD1	1:A:60:ASP:N	0.46	2.49	12	1
1:A:71:VAL:O	1:A:71:VAL:CG1	0.46	2.63	11	1
1:A:65:ILE:O	1:A:66:ASN:ND2	0.46	2.49	3	2
1:A:87:SER:OG	1:A:88:GLN:NE2	0.46	2.49	13	1
1:A:22:GLY:O	1:A:23:LEU:C	0.45	2.55	11	5
1:A:29:GLU:HG2	1:A:75:LEU:HD22	0.45	1.88	10	1
1:A:79:GLN:O	1:A:83:ARG:CD	0.45	2.64	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:85:THR:O	1:A:86:LYS:C	0.45	2.55	16	7
1:A:18:ARG:O	1:A:19:ARG:C	0.45	2.54	8	8
1:A:74:PRO:O	1:A:75:LEU:C	0.45	2.55	19	7
1:A:65:ILE:CG2	1:A:66:ASN:OD1	0.45	2.62	16	1
1:A:65:ILE:O	1:A:66:ASN:CG	0.45	2.54	20	3
1:A:66:ASN:N	1:A:66:ASN:ND2	0.45	2.64	17	1
1:A:29:GLU:CG	1:A:75:LEU:HD22	0.45	2.42	10	1
1:A:18:ARG:O	1:A:21:GLU:CB	0.45	2.65	13	1
1:A:51:GLU:O	1:A:53:SER:N	0.44	2.51	1	2
1:A:64:ALA:N	1:A:94:SER:OG	0.44	2.51	5	1
1:A:25:VAL:HG23	1:A:82:VAL:HG21	0.44	1.88	17	4
1:A:15:LEU:C	1:A:16:GLU:CD	0.44	2.76	5	1
1:A:57:SER:O	1:A:58:ILE:C	0.44	2.56	20	4
1:A:23:LEU:HD13	1:A:82:VAL:CG2	0.44	2.42	8	2
1:A:17:LYS:HE3	1:A:91:VAL:CG2	0.44	2.43	12	1
1:A:59:GLY:O	1:A:60:ASP:C	0.44	2.55	9	6
1:A:62:LEU:CD1	1:A:65:ILE:HD11	0.44	2.42	12	1
1:A:88:GLN:NE2	1:A:90:SER:O	0.44	2.50	4	1
1:A:62:LEU:HD11	1:A:65:ILE:HD11	0.44	1.89	6	2
1:A:23:LEU:HD11	1:A:91:VAL:HG11	0.44	1.89	13	1
1:A:28:VAL:HG22	1:A:40:VAL:O	0.44	2.12	18	1
1:A:14:HIS:N	1:A:14:HIS:CD2	0.44	2.85	4	1
1:A:11:ARG:CD	1:A:13:VAL:CG2	0.44	2.96	6	1
1:A:11:ARG:HD2	1:A:13:VAL:CG2	0.44	2.43	6	2
1:A:17:LYS:HE2	1:A:91:VAL:CG2	0.44	2.43	16	2
1:A:61:ARG:NH1	1:A:96:VAL:N	0.43	2.65	20	1
1:A:23:LEU:HD21	1:A:50:ALA:HB2	0.43	1.89	10	1
1:A:65:ILE:HD12	1:A:70:LEU:CD1	0.43	2.42	14	1
1:A:95:ILE:C	1:A:95:ILE:HD12	0.43	2.33	6	3
1:A:23:LEU:CD2	1:A:23:LEU:O	0.43	2.66	7	1
1:A:61:ARG:HD2	1:A:96:VAL:HG23	0.43	1.90	7	1
1:A:62:LEU:CD1	1:A:93:LEU:HD22	0.43	2.43	14	1
1:A:29:GLU:O	1:A:29:GLU:CD	0.43	2.56	7	1
1:A:15:LEU:HD22	1:A:50:ALA:HA	0.43	1.90	18	3
1:A:22:GLY:C	1:A:24:GLY:N	0.43	2.72	20	2
1:A:43:ASN:O	1:A:44:LEU:HD23	0.43	2.14	15	1
1:A:61:ARG:NH1	1:A:62:LEU:O	0.42	2.51	12	1
1:A:16:GLU:CD	1:A:16:GLU:N	0.42	2.73	5	1
1:A:43:ASN:HA	1:A:58:ILE:HD12	0.42	1.90	17	1
1:A:23:LEU:O	1:A:23:LEU:CD2	0.42	2.67	6	3
1:A:14:HIS:CD2	1:A:92:THR:HG23	0.42	2.50	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:17:LYS:HE2	1:A:91:VAL:HG21	0.42	1.91	12	1
1:A:28:VAL:C	1:A:75:LEU:HD13	0.42	2.36	11	1
1:A:15:LEU:C	1:A:16:GLU:OE2	0.41	2.58	5	1
1:A:23:LEU:HD12	1:A:85:THR:OG1	0.41	2.15	11	1
1:A:51:GLU:C	1:A:53:SER:N	0.41	2.74	1	2
1:A:29:GLU:CD	1:A:75:LEU:HD22	0.41	2.36	3	1
1:A:62:LEU:HD23	1:A:62:LEU:C	0.41	2.36	10	1
1:A:62:LEU:C	1:A:62:LEU:CD2	0.41	2.83	9	1
1:A:52:ARG:HB2	1:A:52:ARG:CZ	0.41	2.46	15	1
1:A:12:GLU:OE2	1:A:92:THR:HG22	0.41	2.16	14	1
1:A:12:GLU:HG2	1:A:14:HIS:NE2	0.41	2.31	16	1
1:A:88:GLN:O	1:A:88:GLN:CG	0.40	2.69	11	1
1:A:88:GLN:OE1	1:A:88:GLN:CA	0.40	2.69	13	1
1:A:23:LEU:HD13	1:A:25:VAL:CG2	0.40	2.44	19	1
1:A:21:GLU:O	1:A:22:GLY:C	0.40	2.59	3	1
1:A:66:ASN:ND2	1:A:92:THR:H	0.40	2.14	17	1
1:A:62:LEU:HD11	1:A:65:ILE:HG12	0.40	1.93	18	1
1:A:17:LYS:CG	1:A:88:GLN:O	0.40	2.70	7	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	78/101 (77%)	67±2 (85±2%)	9±2 (12±3%)	2±1 (2±1%)	9	45
All	All	1560/2020 (77%)	1333 (85%)	188 (12%)	39 (2%)	9	45

All 9 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	46	HIS	17
1	A	71	VAL	6
1	A	69	SER	4
1	A	23	LEU	3

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Mol	Chain	Res	Type	Models (Total)
1	A	58	ILE	3
1	A	52	ARG	2
1	A	60	ASP	2
1	A	22	GLY	1
1	A	41	ILE	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	59/77 (77%)	56±1 (95±2%)	3±1 (5±2%)	31	79
All	All	1180/1540 (77%)	1126 (95%)	54 (5%)	31	79

All 15 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	61	ARG	16
1	A	23	LEU	10
1	A	46	HIS	6
1	A	28	VAL	4
1	A	60	ASP	4
1	A	94	SER	3
1	A	25	VAL	2
1	A	11	ARG	2
1	A	56	LEU	1
1	A	83	ARG	1
1	A	62	LEU	1
1	A	68	THR	1
1	A	66	ASN	1
1	A	69	SER	1
1	A	89	THR	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