Full wwPDB NMR Structure Validation Report (i)

Feb 27, 2022 – 06:39 PM EST

PDB ID	:	2DKM
Title	:	Solution structures of the fn3 domain of human collagen alpha-1(XX) chain
Authors	:	Sato, M.; Saito, K.; Koshiba, S.; Inoue, M.; Kigawa, T.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2006-04-12

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:

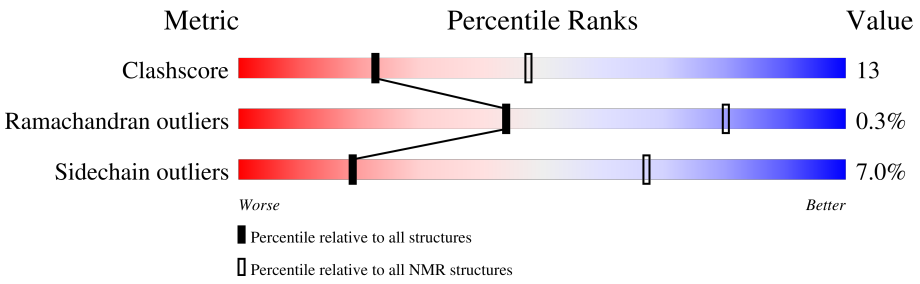
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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	104	66% 13% 20%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 20 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:9-A:45, A:54-A:99 (83)	0.27	20

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1512 atoms, of which 750 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Collagen alpha-1(XX) chain.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	104	1512	465	750	143	153	1	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	cloning artifact	UNP Q9P218
A	2	SER	-	cloning artifact	UNP Q9P218
A	3	SER	-	cloning artifact	UNP Q9P218
A	4	GLY	-	cloning artifact	UNP Q9P218
A	5	SER	-	cloning artifact	UNP Q9P218
A	6	SER	-	cloning artifact	UNP Q9P218
A	7	GLY	-	cloning artifact	UNP Q9P218
A	99	SER	-	cloning artifact	UNP Q9P218
A	100	GLY	-	cloning artifact	UNP Q9P218
A	101	PRO	-	cloning artifact	UNP Q9P218
A	102	SER	-	cloning artifact	UNP Q9P218
A	103	SER	-	cloning artifact	UNP Q9P218
A	104	GLY	-	cloning artifact	UNP Q9P218

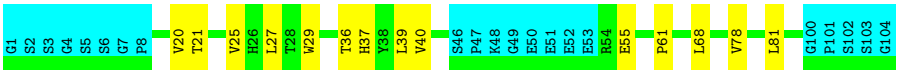
4 Residue-property plots (i)

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: Collagen alpha-1(XX) chain

Chain A: 66% 13% 20%



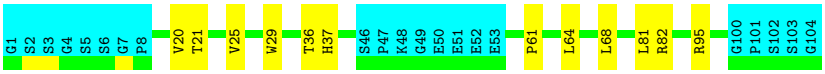
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Collagen alpha-1(XX) chain

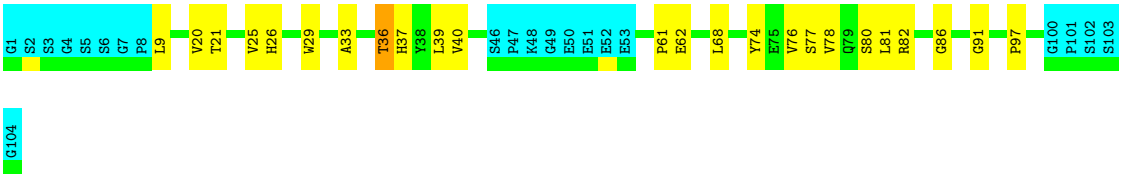
Chain A: 68% 12% 20%



4.2.2 Score per residue for model 2

• Molecule 1: Collagen alpha-1(XX) chain

Chain A: 57% 22% • 20%



4.2.3 Score per residue for model 3

- Molecule 1: Collagen alpha-1(XX) chain

Chain A: 56% 18% 6% 20%

G1 S2 S3 G4 S5 S6 G7 P8 L9 R13 A14 L17 V20 T21 P22 L27 T28 W29 Q30 T36 H37 Y38 L39 V40 S46 P47 K48 G49 E50 E51 E52 E53 R54 E55 V58 G59 R60 P61 V78 Q79 S80 L81 R82 G83 S87 E88 G100 P101 S102 S103

G104

4.2.4 Score per residue for model 4

- Molecule 1: Collagen alpha-1(XX) chain

Chain A: 61% 17% • 20%

G1 S2 S3 G4 S5 S6 G7 P8 P12 L15 T16 L17 A18 A19 V20 T21 P22 V25 W29 T36 H37 Y38 L39 S43 S46 P47 K48 G49 E50 E51 E52 E53 R54 E55 P61 L68 V78 Q79 S80 L81 S87 E88 G100 P101 S102 S103 G104

4.2.5 Score per residue for model 5

- Molecule 1: Collagen alpha-1(XX) chain

Chain A: 56% 21% • 20%

G1 S2 S3 G4 S5 S6 G7 P8 L15 T16 L17 A18 A19 V20 T21 P22 L27 T28 W29 S32 A33 G34 A35 T36 L39 V40 S46 P47 K48 G49 E50 E51 E52 E53 R60 P61 E62 D73 Q79 S80 L81 S87 E88 I92 R95 G100 P101 S102

S103 G104

4.2.6 Score per residue for model 6

- Molecule 1: Collagen alpha-1(XX) chain

Chain A: 58% 20% • 20%

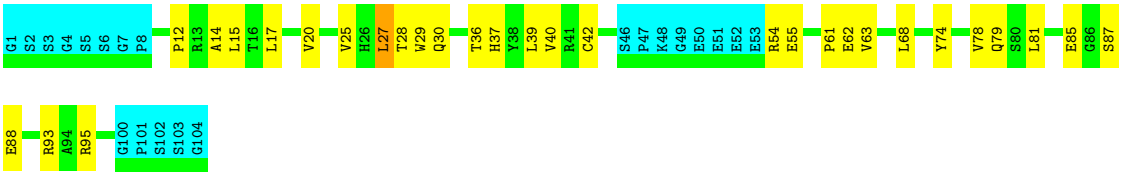
G1 S2 S3 G4 S5 S6 G7 P8 P12 R13 A14 L15 T16 L17 V20 V25 H26 L27 T28 W29 T36 H37 Y38 L39 V40 S46 P47 K48 G49 E50 E51 E52 E53 Q57 P61 D66 G67 L68 D73 L81 S87 I92 S99 G100 P101 S102 S103

G104

4.2.7 Score per residue for model 7

- Molecule 1: Collagen alpha-1(XX) chain

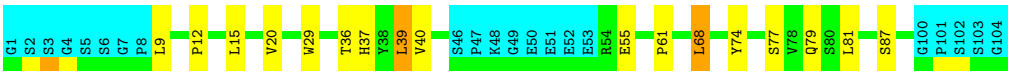
Chain A: 51% 28% • 20%



4.2.8 Score per residue for model 8

- Molecule 1: Collagen alpha-1(XX) chain

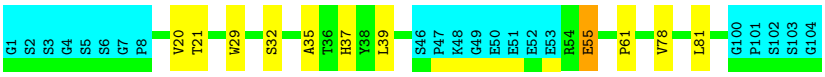
Chain A: 63% 14% • 20%



4.2.9 Score per residue for model 9

- Molecule 1: Collagen alpha-1(XX) chain

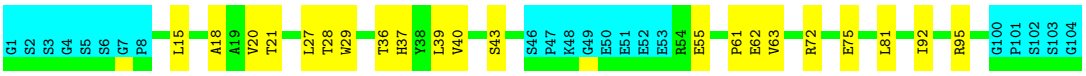
Chain A: 69% 10% • 20%



4.2.10 Score per residue for model 10

- Molecule 1: Collagen alpha-1(XX) chain

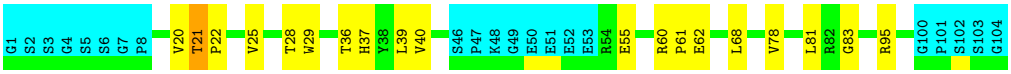
Chain A: 60% 20% 20%



4.2.11 Score per residue for model 11

- Molecule 1: Collagen alpha-1(XX) chain

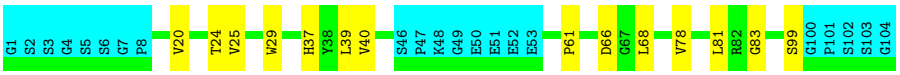
Chain A: 62% 17% • 20%



4.2.12 Score per residue for model 12

- Molecule 1: Collagen alpha-1(XX) chain

Chain A:



4.2.13 Score per residue for model 13

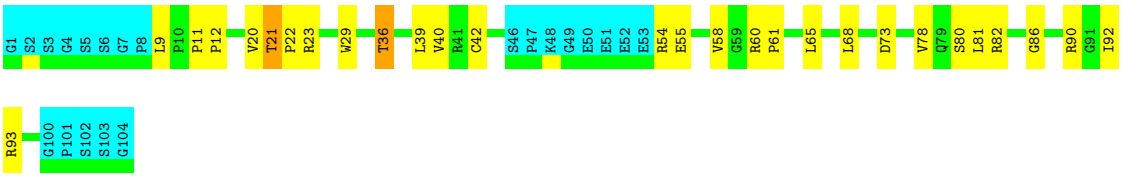
- Molecule 1: Collagen alpha-1(XX) chain

Chain A:

4.2.14 Score per residue for model 14

- Molecule 1: Collagen alpha-1(XX) chain

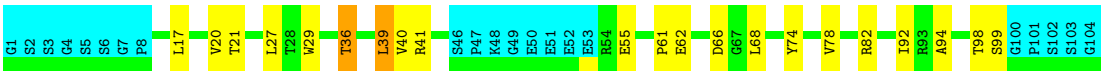
Chain A:



4.2.15 Score per residue for model 15

- Molecule 1: Collagen alpha-1(XX) chain

Chain A:



4.2.16 Score per residue for model 16

- Molecule 1: Collagen alpha-1(XX) chain

Chain A: 59% 20% • 20%

G1 S2 S3 G4 S5 S6 G7 P8 P12 R13 A14 L15 V20 V25 W29 T36 H37 Y38 L39 S46 P47 K48 G49 E50 E51 E52 E53 Q57 P61 L68 V76 S77 V78 Q79 S80 L81 E88 G91 I92 R93 G100 P101 S102 S103 G104

4.2.17 Score per residue for model 17

- Molecule 1: Collagen alpha-1(XX) chain

Chain A: 62% 16% • 20%

G1 S2 S3 G4 S5 S6 G7 P8 L9 V20 T21 P22 V25 W29 A35 Y38 L39 S46 P47 K48 G49 E50 E51 E52 E53 R54 E55 R60 P61 D66 G67 L68 R72 V78 R95 G100 P101 S102 S103 G104

4.2.18 Score per residue for model 18

- Molecule 1: Collagen alpha-1(XX) chain

Chain A: 59% 18% • 20%

G1 S2 S3 G4 S5 S6 G7 P8 L9 R13 V20 T21 P22 V25 W29 A35 T36 H37 Y38 L39 V40 S46 P47 K48 G49 E50 E51 E52 E53 R54 E55 V58 G59 R60 P61 L64 L68 V78 Q79 S80 L81 R95 G100 P101 S102 S103 G104

4.2.19 Score per residue for model 19

- Molecule 1: Collagen alpha-1(XX) chain

Chain A: 56% 22% • 20%

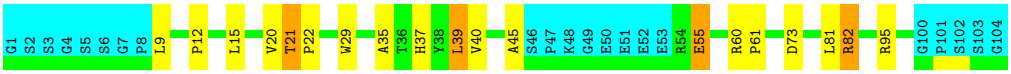
G1 S2 S3 G4 S5 S6 G7 P8 L9 A14 V20 T21 V25 H26 L27 T28 W29 Q30 A35 T36 H37 Y38 L39 V40 R41 C42 S46 P47 K48 G49 E50 E51 E52 E53 P61 L64 L65 V78 Q79 S80 L81 S87 E88 A89 R90 R95 T96 G100 P101

S102 S103 G104

4.2.20 Score per residue for model 20 (medoid)

- Molecule 1: Collagen alpha-1(XX) chain

Chain A: 62% 14% • 20%


G1
S2
S3
G4
S5
S6
G7
P8
L9
P12
L15
V20
T21
P22
W29
A35
T36
H37
Y38
L39
V40
A45
S46
P47
K48
G49
E50
E51
E52
E53
R54
E55
R60
P61
D73
L81
R82
R95
G100
P101
S102
S103
G104

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: *target function, structures with the least restraint violations*.

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	630	639	637	16±4
All	All	12600	12780	12740	319

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 13.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:27:LEU:HD13	1:A:28:THR:N	0.76	1.96	7	5
1:A:9:LEU:HD11	1:A:35:ALA:HB2	0.75	1.55	19	3
1:A:36:THR:HG23	1:A:37:HIS:ND1	0.70	2.02	16	5
1:A:15:LEU:O	1:A:92:ILE:HD12	0.69	1.87	5	2
1:A:25:VAL:HG23	1:A:68:LEU:CD1	0.68	2.19	17	10
1:A:68:LEU:HD13	1:A:74:TYR:CE2	0.68	2.24	8	1
1:A:39:LEU:HD13	1:A:40:VAL:N	0.67	2.04	18	13
1:A:25:VAL:HG23	1:A:68:LEU:HD13	0.67	1.64	4	5
1:A:36:THR:HG23	1:A:37:HIS:CE1	0.66	2.25	16	3
1:A:32:SER:CB	1:A:35:ALA:HB3	0.66	2.21	5	1
1:A:45:ALA:HB3	1:A:73:ASP:CG	0.66	2.11	20	1
1:A:29:TRP:CE2	1:A:78:VAL:HG11	0.65	2.26	17	6
1:A:39:LEU:HD21	1:A:55:GLU:CG	0.65	2.22	17	3
1:A:74:TYR:HB2	1:A:94:ALA:HB3	0.64	1.68	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:27:LEU:HD11	1:A:92:ILE:HG21	0.64	1.69	10	1
1:A:39:LEU:C	1:A:39:LEU:HD13	0.62	2.14	5	1
1:A:68:LEU:CD1	1:A:74:TYR:CE2	0.61	2.83	8	1
1:A:95:ARG:O	1:A:96:THR:HG23	0.61	1.95	19	1
1:A:39:LEU:HD21	1:A:55:GLU:HG2	0.60	1.73	20	1
1:A:27:LEU:HD13	1:A:28:THR:H	0.59	1.56	7	2
1:A:20:VAL:HG13	1:A:20:VAL:O	0.59	1.97	5	3
1:A:32:SER:HB3	1:A:35:ALA:HB3	0.59	1.73	13	1
1:A:20:VAL:O	1:A:20:VAL:HG13	0.58	1.99	15	16
1:A:12:PRO:HB2	1:A:15:LEU:HD11	0.57	1.74	20	5
1:A:68:LEU:HD22	1:A:74:TYR:CZ	0.57	2.35	7	3
1:A:9:LEU:HD21	1:A:80:SER:O	0.56	2.01	3	3
1:A:42:CYS:SG	1:A:65:LEU:HD13	0.56	2.41	19	1
1:A:9:LEU:HD23	1:A:9:LEU:H	0.56	1.60	18	1
1:A:39:LEU:HD13	1:A:39:LEU:C	0.55	2.21	18	9
1:A:36:THR:HG22	1:A:82:ARG:HA	0.55	1.79	14	3
1:A:29:TRP:CD2	1:A:61:PRO:O	0.55	2.60	6	20
1:A:29:TRP:CE2	1:A:61:PRO:O	0.55	2.60	3	20
1:A:39:LEU:C	1:A:39:LEU:CD1	0.55	2.75	5	5
1:A:39:LEU:HB2	1:A:81:LEU:HD21	0.54	1.79	5	4
1:A:39:LEU:HD11	1:A:55:GLU:HG3	0.54	1.79	17	2
1:A:68:LEU:CD1	1:A:74:TYR:CD2	0.54	2.91	8	1
1:A:29:TRP:CZ3	1:A:78:VAL:HG21	0.53	2.38	7	11
1:A:29:TRP:CE3	1:A:78:VAL:HG21	0.53	2.38	11	4
1:A:37:HIS:CD2	1:A:81:LEU:HB2	0.53	2.39	19	15
1:A:32:SER:OG	1:A:35:ALA:HB3	0.52	2.04	9	1
1:A:45:ALA:HB3	1:A:73:ASP:OD1	0.51	2.05	20	1
1:A:68:LEU:HD22	1:A:74:TYR:CE2	0.51	2.40	7	1
1:A:39:LEU:HD12	1:A:57:GLN:HG3	0.50	1.82	16	1
1:A:25:VAL:O	1:A:64:LEU:HD12	0.50	2.07	1	3
1:A:39:LEU:HD21	1:A:55:GLU:HG3	0.50	1.82	4	4
1:A:88:GLU:OE1	1:A:90:ARG:CZ	0.50	2.60	19	1
1:A:79:GLN:NE2	1:A:87:SER:O	0.50	2.45	8	3
1:A:95:ARG:O	1:A:96:THR:CG2	0.50	2.60	19	1
1:A:15:LEU:HD23	1:A:29:TRP:HB3	0.49	1.84	5	2
1:A:60:ARG:CZ	1:A:62:GLU:OE2	0.49	2.60	5	1
1:A:39:LEU:HD12	1:A:57:GLN:CG	0.49	2.37	16	1
1:A:39:LEU:HD22	1:A:57:GLN:HG3	0.49	1.84	6	1
1:A:17:LEU:CD1	1:A:19:ALA:C	0.49	2.81	5	1
1:A:88:GLU:OE1	1:A:90:ARG:NE	0.49	2.46	19	1
1:A:9:LEU:HD13	1:A:35:ALA:HB2	0.48	1.85	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:18:ALA:HB2	1:A:28:THR:HG23	0.48	1.85	10	1
1:A:40:VAL:HG11	1:A:63:VAL:HG21	0.47	1.86	7	2
1:A:82:ARG:CD	1:A:82:ARG:O	0.47	2.62	20	1
1:A:9:LEU:CD1	1:A:35:ALA:HB2	0.47	2.39	18	1
1:A:29:TRP:CE2	1:A:61:PRO:HA	0.47	2.45	17	7
1:A:62:GLU:OE1	1:A:62:GLU:N	0.47	2.47	15	1
1:A:65:LEU:HB2	1:A:68:LEU:HD11	0.47	1.85	14	1
1:A:76:VAL:O	1:A:91:GLY:CA	0.47	2.63	16	2
1:A:43:SER:O	1:A:75:GLU:N	0.47	2.48	10	1
1:A:9:LEU:HD23	1:A:87:SER:HB2	0.47	1.86	8	1
1:A:9:LEU:CD1	1:A:33:ALA:O	0.46	2.62	2	1
1:A:38:TYR:CD1	1:A:38:TYR:N	0.46	2.84	6	2
1:A:92:ILE:CG1	1:A:93:ARG:N	0.46	2.79	14	2
1:A:27:LEU:HD21	1:A:92:ILE:HG22	0.46	1.88	15	1
1:A:39:LEU:HB2	1:A:81:LEU:HD11	0.46	1.86	3	1
1:A:58:VAL:HG23	1:A:60:ARG:O	0.46	2.11	14	3
1:A:78:VAL:HG12	1:A:79:GLN:N	0.46	2.26	16	1
1:A:37:HIS:NE2	1:A:81:LEU:CB	0.46	2.79	10	3
1:A:25:VAL:CG2	1:A:68:LEU:HD13	0.45	2.39	4	2
1:A:98:THR:O	1:A:99:SER:C	0.45	2.55	15	1
1:A:68:LEU:CD2	1:A:68:LEU:N	0.45	2.80	8	1
1:A:37:HIS:CE1	1:A:81:LEU:HB3	0.45	2.46	12	1
1:A:17:LEU:HD12	1:A:27:LEU:CD2	0.45	2.41	6	1
1:A:25:VAL:HG23	1:A:68:LEU:HD12	0.45	1.88	12	2
1:A:55:GLU:OE1	1:A:55:GLU:N	0.45	2.50	8	1
1:A:28:THR:HG22	1:A:62:GLU:CB	0.45	2.42	11	2
1:A:34:GLY:C	1:A:82:ARG:CD	0.45	2.85	13	1
1:A:37:HIS:CD2	1:A:81:LEU:CB	0.44	3.00	2	2
1:A:27:LEU:HD12	1:A:29:TRP:HE3	0.44	1.73	3	1
1:A:87:SER:OG	1:A:88:GLU:N	0.44	2.50	3	3
1:A:27:LEU:HD21	1:A:92:ILE:HG21	0.44	1.89	6	1
1:A:17:LEU:HD22	1:A:27:LEU:CD2	0.44	2.43	5	1
1:A:55:GLU:CD	1:A:55:GLU:O	0.44	2.56	20	1
1:A:17:LEU:HD22	1:A:27:LEU:HD22	0.44	1.87	5	1
1:A:18:ALA:HB2	1:A:28:THR:CG2	0.44	2.43	10	1
1:A:26:HIS:NE2	1:A:62:GLU:OE1	0.44	2.51	2	1
1:A:79:GLN:CD	1:A:87:SER:O	0.44	2.56	7	1
1:A:66:ASP:OD1	1:A:66:ASP:N	0.44	2.51	15	1
1:A:17:LEU:CD2	1:A:19:ALA:C	0.43	2.86	4	1
1:A:88:GLU:OE2	1:A:90:ARG:NH2	0.43	2.51	19	1
1:A:42:CYS:N	1:A:54:ARG:O	0.43	2.52	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:21:THR:HG22	1:A:22:PRO:HD2	0.43	1.91	5	7
1:A:27:LEU:HD21	1:A:92:ILE:CG2	0.43	2.43	15	1
1:A:81:LEU:HD23	1:A:86:GLY:HA3	0.43	1.89	14	1
1:A:12:PRO:O	1:A:15:LEU:CD1	0.42	2.67	7	1
1:A:62:GLU:O	1:A:62:GLU:CG	0.42	2.66	10	2
1:A:27:LEU:HD11	1:A:92:ILE:CG2	0.42	2.41	10	1
1:A:14:ALA:HB3	1:A:30:GLN:HG3	0.42	1.90	19	1
1:A:39:LEU:HB2	1:A:81:LEU:CD2	0.42	2.45	11	2
1:A:32:SER:HB2	1:A:35:ALA:HB3	0.42	1.91	5	1
1:A:73:ASP:OD1	1:A:74:TYR:N	0.42	2.52	13	1
1:A:20:VAL:CG2	1:A:97:PRO:HD3	0.42	2.45	2	1
1:A:20:VAL:O	1:A:20:VAL:CG1	0.42	2.67	5	1
1:A:39:LEU:CB	1:A:81:LEU:HD21	0.42	2.44	5	1
1:A:14:ALA:HB3	1:A:30:GLN:HG2	0.42	1.91	3	1
1:A:28:THR:HG22	1:A:62:GLU:HB3	0.42	1.90	11	1
1:A:14:ALA:HB3	1:A:30:GLN:CG	0.41	2.45	7	1
1:A:17:LEU:HA	1:A:27:LEU:HD12	0.41	1.91	15	1
1:A:37:HIS:CD2	1:A:57:GLN:OE1	0.41	2.72	16	1
1:A:24:THR:HG22	1:A:66:ASP:HA	0.41	1.92	12	1
1:A:37:HIS:NE2	1:A:81:LEU:HB3	0.41	2.31	18	1
1:A:11:PRO:HG2	1:A:90:ARG:CZ	0.41	2.46	14	1
1:A:21:THR:CG2	1:A:22:PRO:HD2	0.41	2.46	17	4
1:A:73:ASP:OD1	1:A:73:ASP:C	0.41	2.58	13	1
1:A:12:PRO:HB3	1:A:29:TRP:CD1	0.41	2.51	14	1
1:A:81:LEU:HD13	1:A:86:GLY:HA3	0.40	1.92	2	1
1:A:78:VAL:CG1	1:A:79:GLN:N	0.40	2.84	16	1
1:A:9:LEU:CD1	1:A:80:SER:HB3	0.40	2.46	18	1
1:A:68:LEU:HD12	1:A:74:TYR:CD2	0.40	2.51	8	1
1:A:79:GLN:OE1	1:A:87:SER:O	0.40	2.40	4	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	83/104 (80%)	76±2 (92±2%)	7±2 (8±2%)	0±1 (0±1%)	44 80

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1660/2080 (80%)	1521 (92%)	134 (8%)	5 (0%)	44 80

All 3 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	83	GLY	3
1	A	34	GLY	1
1	A	99	SER	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	68/83 (82%)	63±2 (93±3%)	5±2 (7±3%)	19 67
All	All	1360/1660 (82%)	1265 (93%)	95 (7%)	19 67

All 24 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	21	THR	13
1	A	36	THR	13
1	A	95	ARG	9
1	A	39	LEU	8
1	A	55	GLU	7
1	A	27	LEU	5
1	A	13	ARG	4
1	A	17	LEU	4
1	A	60	ARG	4
1	A	77	SER	3
1	A	88	GLU	3
1	A	73	ASP	3
1	A	72	ARG	3
1	A	38	TYR	3
1	A	82	ARG	2
1	A	66	ASP	2

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Mol	Chain	Res	Type	Models (Total)
1	A	93	ARG	2
1	A	43	SER	1
1	A	87	SER	1
1	A	62	GLU	1
1	A	85	GLU	1
1	A	68	LEU	1
1	A	23	ARG	1
1	A	9	LEU	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