Full wwPDB NMR Structure Validation Report (i)

Jun 12, 2024 – 06:08 AM EDT

PDB ID	:	1YWY
Title	:	Solution Structure of Pseudomonas aeruginosa Protein PA2021. The Northeast Structural Genomics Consortium Target Pat85.
Authors	:	Lin, Y.C.; Liu, G.; Shen, Y.; Yee, A.; Arrowsmith, C.H.; Szyperski, T.; Northeast Structural Genomics Consortium (NESG)
Deposited on	:	2005-02-18

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

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

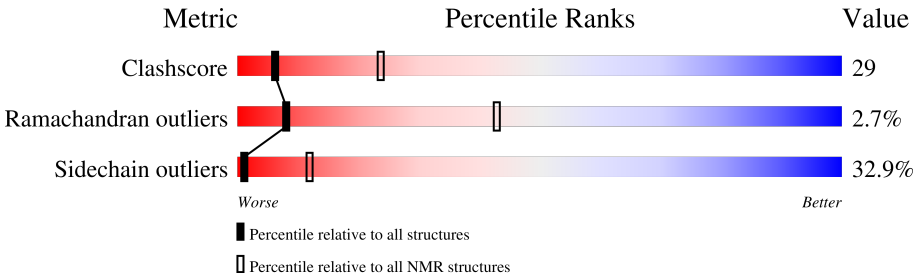
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	74	30% 57% • 9%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 7 is the overall representative, medoid model (most similar to other models). The authors have identified model 20 as representative, based on the following criterion: *fewest violations*.

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:23-A:89 (67)	0.70	7

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 4 clusters and 3 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1132 atoms, of which 559 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called hypothetical protein PA2021.

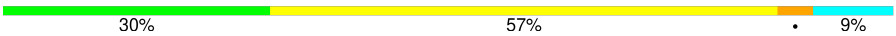
Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	74	1132	344	559	108	118	3	0

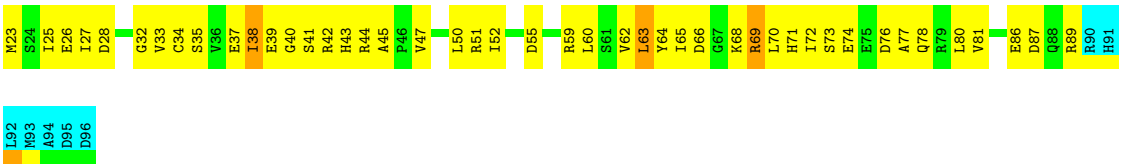
4 Residue-property plots (i)

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 protein PA2021

Chain A: 

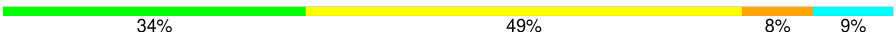


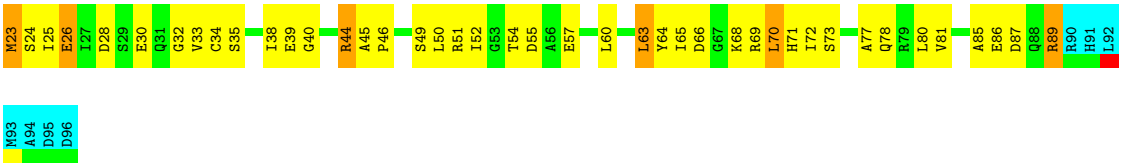
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

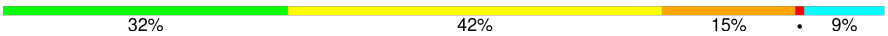
• Molecule 1: hypothetical protein PA2021

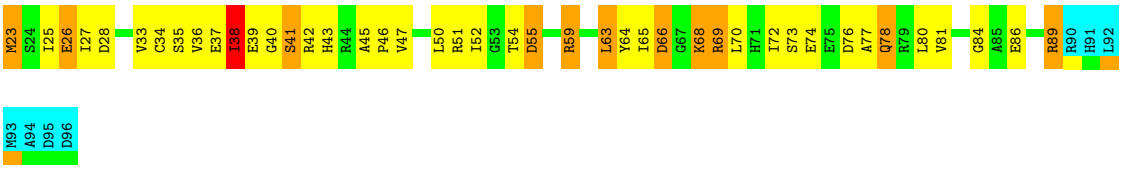
Chain A: 



4.2.2 Score per residue for model 2

• Molecule 1: hypothetical protein PA2021

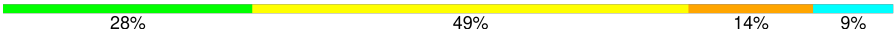
Chain A: 

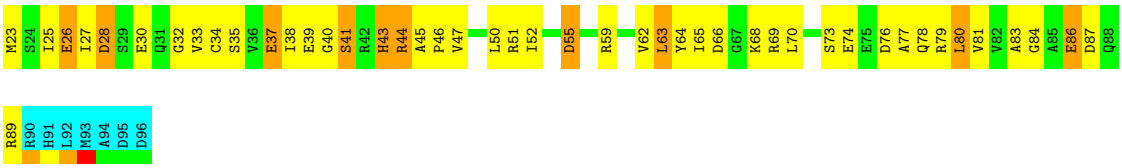


4.2.3 Score per residue for model 3

- Molecule 1: hypothetical protein PA2021

Chain A:

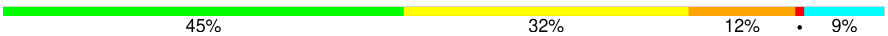


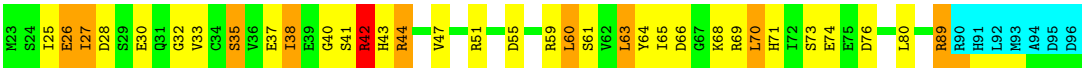


4.2.4 Score per residue for model 4

- Molecule 1: hypothetical protein PA2021

Chain A:

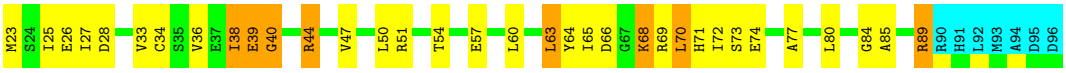




4.2.5 Score per residue for model 5

- Molecule 1: hypothetical protein PA2021

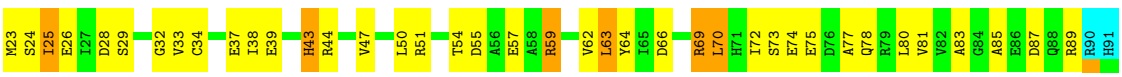
Chain A:



4.2.6 Score per residue for model 6

- Molecule 1: hypothetical protein PA2021

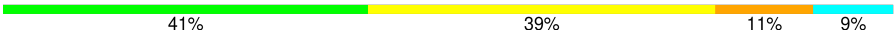
Chain A:



4.2.7 Score per residue for model 7 (medoid)

• Molecule 1: hypothetical protein PA2021

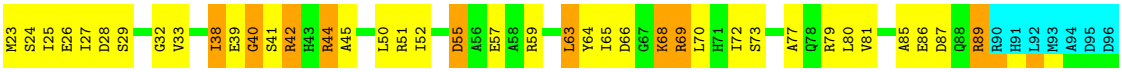
Chain A:



4.2.8 Score per residue for model 8

• Molecule 1: hypothetical protein PA2021

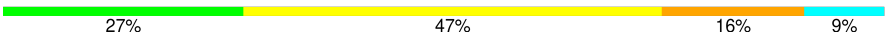
Chain A:

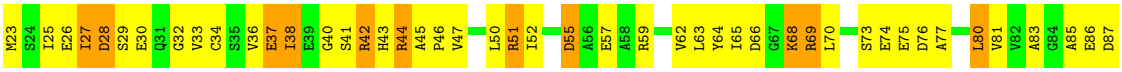


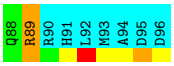
4.2.9 Score per residue for model 9

• Molecule 1: hypothetical protein PA2021

Chain A:



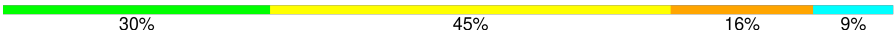


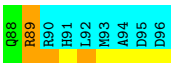


4.2.10 Score per residue for model 10

• Molecule 1: hypothetical protein PA2021

Chain A:





4.2.11 Score per residue for model 11

- Molecule 1: hypothetical protein PA2021

Chain A: 39% 39% 12% 9%

M23 S24 T25 E26 I27 D28 V33 G34 S35 V36 E37 I38 E39 G40 S41 R42 H43 R44 L50 R51 I52 D55 L63 Y64 I65 D66 G67 K68 R69 L70 H71 I72 S73 E74 E75 D76 A77 L80 V81 E86 R89 R90 H91 L92 M93 A94 D95 D96

4.2.12 Score per residue for model 12

- Molecule 1: hypothetical protein PA2021

Chain A: 38% 38% 15% 9%

M23 S24 T25 E26 I27 D28 S29 G32 V33 G34 S35 V36 E37 I38 E39 G40 S41 R42 H43 R44 V47 L50 R51 I52 D55 L60 L63 Y64 I65 K68 R69 L70 H71 I72 S73 E74 R79 L80 V81 E86 R89 R90 H91 L92 M93 A94 D95 D96

4.2.13 Score per residue for model 13

- Molecule 1: hypothetical protein PA2021

Chain A: 42% 43% 5% 9%

M23 S24 T25 E26 I27 D28 G32 V33 G34 S35 V36 E37 I38 H43 R44 L50 R51 I52 G53 T54 D55 A56 E57 A58 R59 L60 S61 V62 L63 Y64 I65 D66 G67 K68 R69 L70 H71 I72 S73 D76 A77 L80 V81 D87 R90 H91 L92 M93 A94 D95 D96

4.2.14 Score per residue for model 14

- Molecule 1: hypothetical protein PA2021

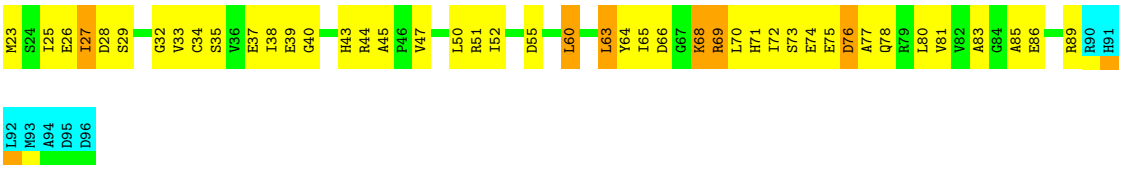
Chain A: 36% 39% 15% 9%

M23 S24 T25 E26 I27 D28 S29 E30 Q31 G32 V33 G34 S35 I38 E39 G40 S41 R42 H43 R44 L50 R51 I52 G53 T54 D55 R59 L60 S61 V62 L63 Y64 I65 D66 G67 K68 R69 L70 H71 I72 S73 E74 E75 D76 A77 L80 V81 G84 A85 E86 D87 Q88 R89 R90 H91 L92 M93 A94 D95 D96

4.2.15 Score per residue for model 15

- Molecule 1: hypothetical protein PA2021

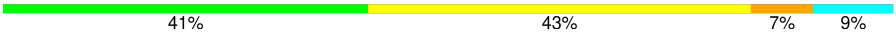
Chain A: 31% 51% 8% 9%

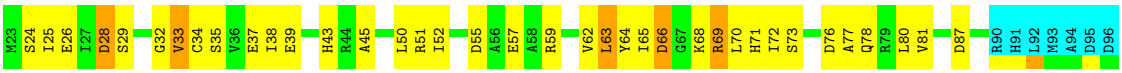


4.2.16 Score per residue for model 16

- Molecule 1: hypothetical protein PA2021

Chain A:

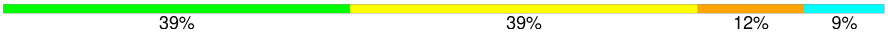


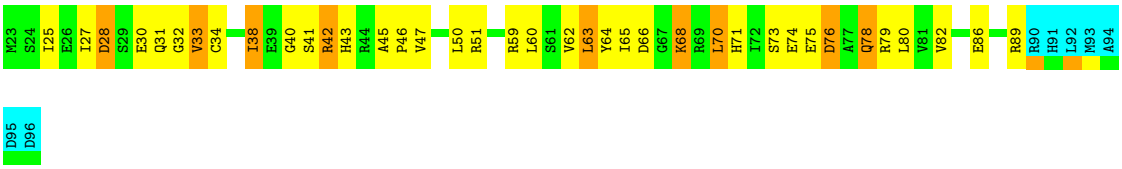


4.2.17 Score per residue for model 17

- Molecule 1: hypothetical protein PA2021

Chain A:

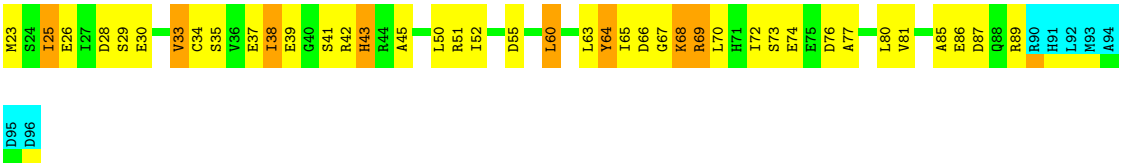




4.2.18 Score per residue for model 18

- Molecule 1: hypothetical protein PA2021

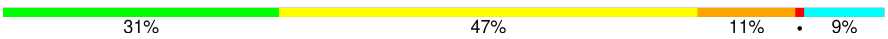
Chain A:



4.2.19 Score per residue for model 19

- Molecule 1: hypothetical protein PA2021

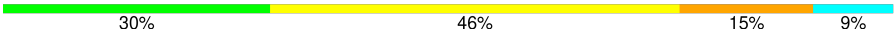
Chain A:

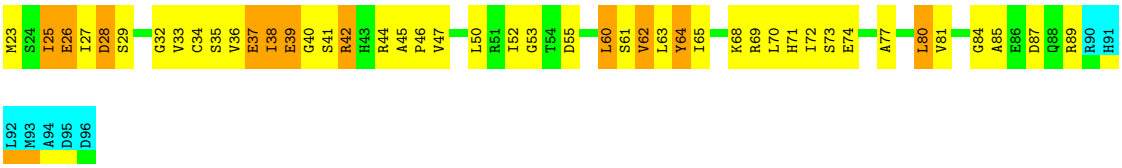


4.2.20 Score per residue for model 20

- Molecule 1: hypothetical protein PA2021

Chain A:





5 Refinement protocol and experimental data overview (i)

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
DYANA	structure solution	1.5
DYANA	refinement	1.5

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	515	506	505	29±4
All	All	10300	10120	10100	589

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 29.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:58:ALA:HB3	1:A:60:LEU:HD12	0.99	1.29	13	1
1:A:33:VAL:HG22	1:A:45:ALA:O	0.92	1.65	17	3
1:A:81:VAL:HG21	1:A:87:ASP:OD2	0.90	1.67	3	3
1:A:63:LEU:HD22	1:A:64:TYR:N	0.89	1.83	12	17
1:A:34:CYS:SG	1:A:47:VAL:HG22	0.88	2.09	15	1
1:A:25:ILE:HD13	1:A:80:LEU:HD11	0.87	1.46	4	5
1:A:81:VAL:HG21	1:A:87:ASP:OD1	0.86	1.70	18	2
1:A:27:ILE:HD13	1:A:28:ASP:N	0.84	1.88	9	2
1:A:50:LEU:HD13	1:A:80:LEU:HD22	0.81	1.53	17	10
1:A:34:CYS:SG	1:A:50:LEU:HD21	0.79	2.17	18	4
1:A:34:CYS:HB3	1:A:47:VAL:HG22	0.79	1.55	19	7
1:A:63:LEU:HD12	1:A:70:LEU:HD21	0.78	1.55	14	3
1:A:45:ALA:HB1	1:A:46:PRO:HD2	0.75	1.57	20	7
1:A:58:ALA:HB3	1:A:60:LEU:CD1	0.72	2.10	13	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:25:ILE:HD13	1:A:80:LEU:HG	0.71	1.62	3	10
1:A:63:LEU:C	1:A:63:LEU:HD13	0.71	2.06	1	16
1:A:63:LEU:CD1	1:A:70:LEU:HD21	0.71	2.15	14	1
1:A:52:ILE:HD12	1:A:81:VAL:HG23	0.70	1.63	13	9
1:A:63:LEU:HD22	1:A:64:TYR:H	0.70	1.45	16	17
1:A:27:ILE:HD12	1:A:27:ILE:O	0.70	1.87	17	3
1:A:55:ASP:HB3	1:A:60:LEU:HD23	0.69	1.63	18	5
1:A:27:ILE:HD11	1:A:47:VAL:HG21	0.69	1.63	4	2
1:A:54:THR:HG23	1:A:60:LEU:O	0.68	1.89	19	2
1:A:45:ALA:HB1	1:A:46:PRO:CD	0.68	2.19	20	4
1:A:68:LYS:HD2	1:A:70:LEU:HD22	0.68	1.65	14	1
1:A:25:ILE:HD13	1:A:80:LEU:CD1	0.68	2.18	4	4
1:A:65:ILE:HG23	1:A:68:LYS:CE	0.68	2.18	11	1
1:A:63:LEU:C	1:A:63:LEU:HD23	0.66	2.11	20	3
1:A:25:ILE:C	1:A:25:ILE:HD12	0.65	2.12	10	9
1:A:32:GLY:O	1:A:47:VAL:HG23	0.65	1.91	15	1
1:A:25:ILE:HG12	1:A:80:LEU:HD12	0.65	1.66	20	1
1:A:72:ILE:HD11	1:A:77:ALA:HB2	0.65	1.67	20	4
1:A:34:CYS:CB	1:A:47:VAL:HG22	0.64	2.21	19	2
1:A:63:LEU:HD23	1:A:64:TYR:N	0.64	2.07	18	3
1:A:62:VAL:HG11	1:A:69:ARG:HE	0.64	1.51	14	1
1:A:60:LEU:HD11	1:A:71:HIS:HB2	0.63	1.70	12	1
1:A:78:GLN:OE1	1:A:82:VAL:HG23	0.63	1.94	17	1
1:A:52:ILE:CD1	1:A:81:VAL:HG23	0.62	2.24	1	10
1:A:60:LEU:C	1:A:60:LEU:HD22	0.62	2.14	13	1
1:A:60:LEU:HD11	1:A:71:HIS:CB	0.61	2.25	12	1
1:A:81:VAL:HG21	1:A:87:ASP:CG	0.61	2.14	10	6
1:A:58:ALA:CB	1:A:60:LEU:HD12	0.61	2.17	13	1
1:A:33:VAL:C	1:A:47:VAL:HG23	0.61	2.16	3	3
1:A:65:ILE:HG23	1:A:68:LYS:NZ	0.61	2.11	11	1
1:A:81:VAL:HG22	1:A:86:GLU:O	0.61	1.96	3	2
1:A:25:ILE:CG2	1:A:72:ILE:HG21	0.60	2.26	6	6
1:A:34:CYS:SG	1:A:47:VAL:HG23	0.60	2.36	12	1
1:A:23:MET:HB3	1:A:38:ILE:HG23	0.60	1.71	2	1
1:A:60:LEU:HD13	1:A:60:LEU:H	0.60	1.56	13	1
1:A:80:LEU:O	1:A:85:ALA:HB3	0.59	1.97	10	6
1:A:45:ALA:HB3	1:A:65:ILE:HD11	0.58	1.75	15	3
1:A:25:ILE:HD13	1:A:80:LEU:HD21	0.58	1.76	6	2
1:A:25:ILE:HD12	1:A:25:ILE:O	0.58	1.98	17	3
1:A:47:VAL:HG11	1:A:83:ALA:HB1	0.57	1.76	15	2
1:A:72:ILE:CD1	1:A:80:LEU:CD1	0.57	2.82	13	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:72:ILE:HD11	1:A:77:ALA:CB	0.57	2.28	20	3
1:A:33:VAL:HG13	1:A:34:CYS:N	0.57	2.14	16	3
1:A:50:LEU:HD13	1:A:80:LEU:HD23	0.57	1.75	13	1
1:A:27:ILE:HD12	1:A:27:ILE:C	0.56	2.21	17	3
1:A:63:LEU:CB	1:A:72:ILE:HG21	0.56	2.29	20	1
1:A:60:LEU:HD22	1:A:60:LEU:O	0.56	2.00	13	1
1:A:50:LEU:HD13	1:A:80:LEU:CD2	0.56	2.30	2	6
1:A:27:ILE:CG2	1:A:80:LEU:HD23	0.56	2.31	5	3
1:A:25:ILE:HG21	1:A:72:ILE:HD13	0.56	1.77	12	2
1:A:72:ILE:CD1	1:A:77:ALA:HB2	0.56	2.30	20	4
1:A:63:LEU:HB2	1:A:72:ILE:HG21	0.55	1.78	20	1
1:A:62:VAL:HG11	1:A:69:ARG:HD3	0.55	1.78	9	1
1:A:25:ILE:HA	1:A:36:VAL:HG23	0.54	1.79	20	1
1:A:25:ILE:HD13	1:A:80:LEU:CD2	0.54	2.31	12	1
1:A:25:ILE:HG21	1:A:72:ILE:HG21	0.54	1.77	6	6
1:A:27:ILE:CD1	1:A:47:VAL:HG21	0.54	2.33	4	1
1:A:25:ILE:HD13	1:A:80:LEU:CG	0.54	2.33	7	7
1:A:64:TYR:CD1	1:A:68:LYS:O	0.53	2.61	8	4
1:A:25:ILE:CG2	1:A:72:ILE:CG2	0.53	2.87	6	3
1:A:23:MET:SD	1:A:71:HIS:CE1	0.53	3.02	1	1
1:A:52:ILE:HD12	1:A:81:VAL:CG2	0.53	2.33	12	3
1:A:25:ILE:HD13	1:A:25:ILE:O	0.52	2.04	14	1
1:A:25:ILE:HG22	1:A:36:VAL:CG2	0.52	2.35	5	1
1:A:62:VAL:HG12	1:A:71:HIS:CD2	0.52	2.40	13	1
1:A:25:ILE:CG2	1:A:63:LEU:HD12	0.52	2.35	20	1
1:A:64:TYR:CD2	1:A:68:LYS:O	0.51	2.63	12	3
1:A:33:VAL:CG1	1:A:34:CYS:N	0.51	2.73	3	13
1:A:62:VAL:HG11	1:A:69:ARG:NE	0.51	2.21	14	1
1:A:65:ILE:O	1:A:66:ASP:CB	0.51	2.58	15	11
1:A:63:LEU:C	1:A:63:LEU:CD2	0.51	2.79	18	3
1:A:52:ILE:CD1	1:A:77:ALA:O	0.51	2.59	20	10
1:A:28:ASP:CB	1:A:33:VAL:O	0.51	2.59	15	5
1:A:47:VAL:HG13	1:A:50:LEU:HD12	0.51	1.82	6	3
1:A:63:LEU:HD13	1:A:63:LEU:O	0.50	2.06	1	3
1:A:52:ILE:HG22	1:A:89:ARG:HB3	0.50	1.83	8	2
1:A:80:LEU:O	1:A:85:ALA:CB	0.50	2.59	18	9
1:A:26:GLU:CB	1:A:35:SER:O	0.50	2.59	14	15
1:A:54:THR:OG1	1:A:89:ARG:CD	0.50	2.60	1	4
1:A:63:LEU:O	1:A:70:LEU:HD23	0.50	2.06	14	1
1:A:54:THR:OG1	1:A:89:ARG:CG	0.50	2.60	7	1
1:A:25:ILE:HD12	1:A:26:GLU:N	0.50	2.21	10	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:25:ILE:CG1	1:A:80:LEU:HD12	0.50	2.37	20	1
1:A:55:ASP:OD2	1:A:69:ARG:CZ	0.50	2.60	2	2
1:A:60:LEU:C	1:A:60:LEU:CD2	0.50	2.79	13	1
1:A:68:LYS:CG	1:A:69:ARG:N	0.50	2.74	18	1
1:A:25:ILE:HG22	1:A:36:VAL:HG22	0.49	1.84	2	1
1:A:63:LEU:C	1:A:63:LEU:CD1	0.49	2.81	8	4
1:A:39:GLU:CG	1:A:39:GLU:O	0.49	2.61	20	1
1:A:38:ILE:HD11	1:A:43:HIS:ND1	0.49	2.22	3	1
1:A:50:LEU:CD1	1:A:80:LEU:HD22	0.49	2.33	5	3
1:A:47:VAL:HG12	1:A:84:GLY:C	0.49	2.27	5	1
1:A:63:LEU:HD11	1:A:65:ILE:HG22	0.49	1.84	5	1
1:A:64:TYR:CE1	1:A:69:ARG:NH1	0.49	2.81	16	1
1:A:38:ILE:O	1:A:40:GLY:N	0.49	2.44	14	6
1:A:55:ASP:OD1	1:A:69:ARG:CZ	0.49	2.61	12	1
1:A:34:CYS:SG	1:A:50:LEU:HD11	0.49	2.48	11	1
1:A:55:ASP:CB	1:A:60:LEU:HD23	0.49	2.37	10	1
1:A:23:MET:CE	1:A:71:HIS:CE1	0.48	2.96	11	1
1:A:41:SER:O	1:A:42:ARG:CG	0.48	2.61	4	2
1:A:65:ILE:HG23	1:A:65:ILE:O	0.48	2.09	12	2
1:A:62:VAL:CB	1:A:70:LEU:O	0.48	2.62	6	2
1:A:33:VAL:HG22	1:A:45:ALA:C	0.48	2.27	17	2
1:A:53:GLY:C	1:A:62:VAL:CG2	0.48	2.82	20	1
1:A:38:ILE:O	1:A:39:GLU:C	0.48	2.51	19	5
1:A:38:ILE:O	1:A:39:GLU:CG	0.47	2.62	8	3
1:A:60:LEU:HD13	1:A:60:LEU:N	0.47	2.24	13	1
1:A:34:CYS:HB3	1:A:50:LEU:HD11	0.47	1.87	20	1
1:A:80:LEU:C	1:A:85:ALA:HB3	0.47	2.28	15	5
1:A:25:ILE:HD11	1:A:76:ASP:HB3	0.47	1.85	15	2
1:A:37:GLU:C	1:A:38:ILE:CG1	0.47	2.83	19	11
1:A:25:ILE:HD12	1:A:76:ASP:CB	0.47	2.40	14	1
1:A:63:LEU:HG	1:A:80:LEU:HD11	0.47	1.87	10	2
1:A:71:HIS:O	1:A:71:HIS:CG	0.47	2.67	14	2
1:A:69:ARG:CD	1:A:69:ARG:C	0.47	2.83	10	1
1:A:74:GLU:CG	1:A:75:GLU:N	0.46	2.77	9	5
1:A:78:GLN:OE1	1:A:82:VAL:CG2	0.46	2.63	17	1
1:A:80:LEU:O	1:A:83:ALA:HB3	0.46	2.09	9	2
1:A:25:ILE:HG22	1:A:72:ILE:HG21	0.46	1.87	18	1
1:A:28:ASP:O	1:A:32:GLY:N	0.46	2.49	12	15
1:A:55:ASP:O	1:A:59:ARG:N	0.46	2.49	19	10
1:A:27:ILE:HD13	1:A:28:ASP:H	0.46	1.66	9	2
1:A:25:ILE:HG22	1:A:36:VAL:HG23	0.46	1.88	9	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:52:ILE:HD11	1:A:77:ALA:O	0.45	2.10	9	6
1:A:28:ASP:N	1:A:33:VAL:O	0.45	2.49	8	6
1:A:33:VAL:C	1:A:47:VAL:CG2	0.45	2.84	19	1
1:A:34:CYS:CB	1:A:50:LEU:HD11	0.45	2.41	20	1
1:A:45:ALA:CB	1:A:46:PRO:CD	0.45	2.89	20	1
1:A:51:ARG:NH1	1:A:52:ILE:O	0.45	2.50	9	1
1:A:40:GLY:O	1:A:41:SER:C	0.45	2.55	3	9
1:A:73:SER:O	1:A:77:ALA:N	0.45	2.50	10	2
1:A:71:HIS:CD2	1:A:71:HIS:C	0.45	2.90	20	1
1:A:34:CYS:SG	1:A:50:LEU:CD2	0.45	3.00	18	1
1:A:81:VAL:O	1:A:84:GLY:N	0.45	2.49	20	6
1:A:65:ILE:O	1:A:67:GLY:N	0.45	2.50	18	3
1:A:63:LEU:HD12	1:A:70:LEU:CD2	0.44	2.42	6	1
1:A:65:ILE:O	1:A:65:ILE:HG23	0.44	2.12	1	1
1:A:55:ASP:OD1	1:A:69:ARG:NH1	0.44	2.50	6	2
1:A:23:MET:CB	1:A:37:GLU:O	0.44	2.65	3	1
1:A:54:THR:OG1	1:A:89:ARG:NE	0.44	2.50	2	1
1:A:68:LYS:CD	1:A:68:LYS:C	0.44	2.84	11	1
1:A:72:ILE:HD11	1:A:77:ALA:HA	0.44	1.89	13	3
1:A:33:VAL:HG12	1:A:34:CYS:N	0.44	2.27	12	1
1:A:23:MET:HG3	1:A:38:ILE:HG23	0.44	1.90	19	1
1:A:63:LEU:CD2	1:A:65:ILE:HG22	0.44	2.43	20	1
1:A:43:HIS:CE1	1:A:68:LYS:HE3	0.44	2.47	11	1
1:A:25:ILE:N	1:A:76:ASP:OD2	0.44	2.50	10	1
1:A:64:TYR:OH	1:A:69:ARG:NH1	0.44	2.51	14	1
1:A:25:ILE:CD1	1:A:80:LEU:HD11	0.44	2.31	4	1
1:A:47:VAL:CG2	1:A:50:LEU:HD12	0.43	2.44	12	1
1:A:25:ILE:HG12	1:A:72:ILE:HG21	0.43	1.91	5	1
1:A:47:VAL:HG12	1:A:84:GLY:O	0.43	2.13	5	1
1:A:72:ILE:CD1	1:A:80:LEU:HD12	0.43	2.43	8	2
1:A:52:ILE:HD11	1:A:81:VAL:HG23	0.43	1.88	1	2
1:A:63:LEU:HD13	1:A:64:TYR:N	0.43	2.28	2	1
1:A:41:SER:O	1:A:42:ARG:CB	0.43	2.66	4	1
1:A:47:VAL:HG11	1:A:83:ALA:CB	0.43	2.42	15	1
1:A:38:ILE:C	1:A:40:GLY:N	0.43	2.71	5	7
1:A:34:CYS:SG	1:A:47:VAL:CG2	0.43	3.06	12	1
1:A:27:ILE:HG23	1:A:47:VAL:HG21	0.43	1.90	20	1
1:A:55:ASP:OD2	1:A:69:ARG:NE	0.43	2.50	8	1
1:A:25:ILE:HG22	1:A:72:ILE:CG2	0.42	2.44	18	1
1:A:36:VAL:HG21	1:A:63:LEU:HD13	0.42	1.91	20	1
1:A:70:LEU:HD12	1:A:71:HIS:N	0.42	2.29	4	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:27:ILE:HG21	1:A:83:ALA:HB1	0.42	1.91	10	1
1:A:55:ASP:N	1:A:60:LEU:O	0.42	2.51	19	1
1:A:81:VAL:HA	1:A:85:ALA:HB3	0.42	1.90	9	1
1:A:61:SER:OG	1:A:89:ARG:CD	0.42	2.67	10	1
1:A:65:ILE:CG2	1:A:68:LYS:CE	0.42	2.96	11	1
1:A:43:HIS:CE1	1:A:68:LYS:CE	0.42	3.03	11	1
1:A:65:ILE:CG2	1:A:68:LYS:HE2	0.42	2.44	11	1
1:A:34:CYS:SG	1:A:47:VAL:CB	0.42	3.08	12	1
1:A:27:ILE:C	1:A:27:ILE:CD1	0.42	2.87	17	1
1:A:63:LEU:HD11	1:A:65:ILE:CG2	0.42	2.44	5	1
1:A:52:ILE:O	1:A:89:ARG:NH1	0.42	2.53	9	1
1:A:72:ILE:HD11	1:A:77:ALA:CA	0.42	2.44	1	1
1:A:43:HIS:O	1:A:44:ARG:CB	0.42	2.67	11	1
1:A:26:GLU:N	1:A:35:SER:O	0.41	2.52	2	1
1:A:25:ILE:CD1	1:A:76:ASP:CG	0.41	2.89	14	1
1:A:33:VAL:HG13	1:A:45:ALA:O	0.41	2.15	7	1
1:A:25:ILE:CD1	1:A:80:LEU:HG	0.41	2.46	15	1
1:A:73:SER:O	1:A:77:ALA:HB2	0.41	2.15	16	1
1:A:62:VAL:CA	1:A:70:LEU:O	0.41	2.68	6	1
1:A:62:VAL:HG12	1:A:70:LEU:O	0.41	2.16	6	2
1:A:72:ILE:HD13	1:A:80:LEU:CD1	0.41	2.45	13	1
1:A:41:SER:O	1:A:42:ARG:C	0.41	2.59	18	1
1:A:54:THR:CG2	1:A:60:LEU:O	0.41	2.67	19	1
1:A:33:VAL:HG11	1:A:44:ARG:CG	0.41	2.46	12	1
1:A:61:SER:OG	1:A:89:ARG:NE	0.41	2.54	4	1
1:A:55:ASP:OD1	1:A:69:ARG:NH2	0.41	2.49	11	2
1:A:38:ILE:HD11	1:A:70:LEU:HD22	0.41	1.91	1	1
1:A:55:ASP:OD2	1:A:69:ARG:NH2	0.41	2.54	6	1
1:A:81:VAL:HG11	1:A:87:ASP:OD2	0.41	2.16	6	1
1:A:50:LEU:CD2	1:A:65:ILE:CD1	0.41	2.99	1	1
1:A:40:GLY:O	1:A:41:SER:O	0.41	2.39	3	1
1:A:38:ILE:O	1:A:39:GLU:CB	0.41	2.69	6	1
1:A:34:CYS:SG	1:A:45:ALA:O	0.40	2.78	3	1
1:A:25:ILE:CD1	1:A:76:ASP:OD2	0.40	2.69	14	1
1:A:27:ILE:CD1	1:A:34:CYS:SG	0.40	3.09	15	1
1:A:25:ILE:O	1:A:76:ASP:CG	0.40	2.60	17	1
1:A:68:LYS:HD2	1:A:70:LEU:HD23	0.40	1.93	5	1
1:A:34:CYS:SG	1:A:46:PRO:O	0.40	2.80	17	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	66/74 (89%)	58±1 (88±2%)	6±1 (9±2%)	2±1 (3±1%)	8 43
All	All	1320/1480 (89%)	1163 (88%)	121 (9%)	36 (3%)	8 43

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	44	ARG	10
1	A	42	ARG	9
1	A	40	GLY	4
1	A	38	ILE	4
1	A	41	SER	2
1	A	39	GLU	2
1	A	43	HIS	2
1	A	66	ASP	2
1	A	67	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	56/62 (90%)	38±3 (67±5%)	18±3 (33±5%)	1 12
All	All	1120/1240 (90%)	751 (67%)	369 (33%)	1 12

All 41 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	69	ARG	19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	70	LEU	19
1	A	73	SER	19
1	A	68	LYS	18
1	A	51	ARG	17
1	A	63	LEU	16
1	A	89	ARG	15
1	A	23	MET	14
1	A	26	GLU	13
1	A	44	ARG	13
1	A	43	HIS	13
1	A	55	ASP	12
1	A	86	GLU	12
1	A	38	ILE	12
1	A	76	ASP	12
1	A	60	LEU	11
1	A	28	ASP	10
1	A	29	SER	10
1	A	57	GLU	8
1	A	42	ARG	8
1	A	74	GLU	8
1	A	30	GLU	7
1	A	27	ILE	7
1	A	66	ASP	7
1	A	37	GLU	7
1	A	79	ARG	7
1	A	71	HIS	7
1	A	78	GLN	6
1	A	80	LEU	6
1	A	24	SER	5
1	A	62	VAL	5
1	A	25	ILE	5
1	A	59	ARG	4
1	A	39	GLU	3
1	A	35	SER	3
1	A	64	TYR	3
1	A	33	VAL	3
1	A	61	SER	2
1	A	49	SER	1
1	A	47	VAL	1
1	A	31	GLN	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