Full wwPDB NMR Structure Validation Report (i)

Apr 20, 2024 – 04:17 PM EDT

PDB ID	:	2KE0
Title	:	Solution structure of peptidyl-prolyl cis-trans isomerase from Burkholderia pseudomallei
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Deposited on	:	2009-01-21

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:

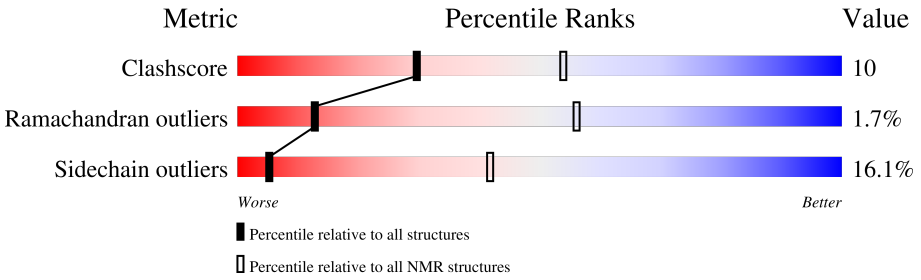
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson 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	117	72% 21% • 7%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:117 (109)	0.53	1

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 1 single-model cluster was found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1703 atoms, of which 843 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Peptidyl-prolyl cis-trans isomerase.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	117	1703	541	843	147	169	3	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP Q63J95
A	2	PRO	-	expression tag	UNP Q63J95
A	3	GLY	-	expression tag	UNP Q63J95
A	4	SER	-	expression tag	UNP Q63J95

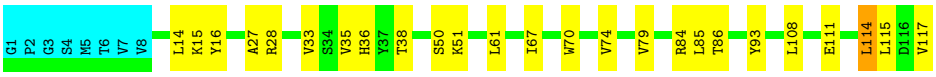
4 Residue-property plots (i)

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: Peptidyl-prolyl cis-trans isomerase

Chain A: 72% 21% • 7%



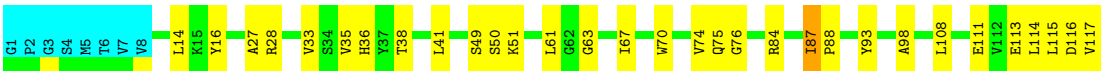
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

• Molecule 1: Peptidyl-prolyl cis-trans isomerase

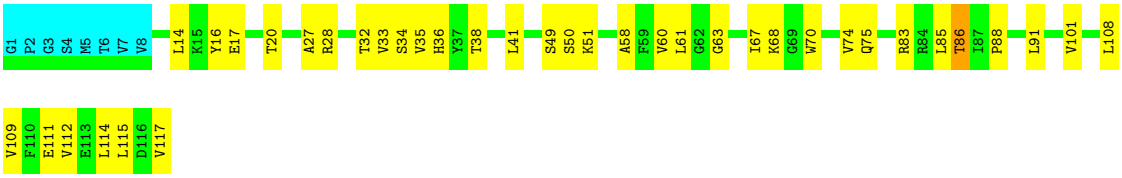
Chain A: 67% 26% • 7%



4.2.2 Score per residue for model 2

• Molecule 1: Peptidyl-prolyl cis-trans isomerase

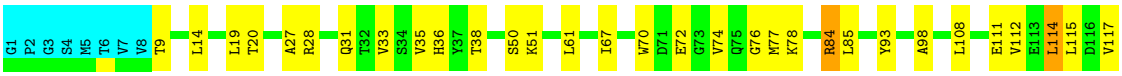
Chain A: 61% 32% • 7%



4.2.3 Score per residue for model 3

- Molecule 1: Peptidyl-prolyl cis-trans isomerase

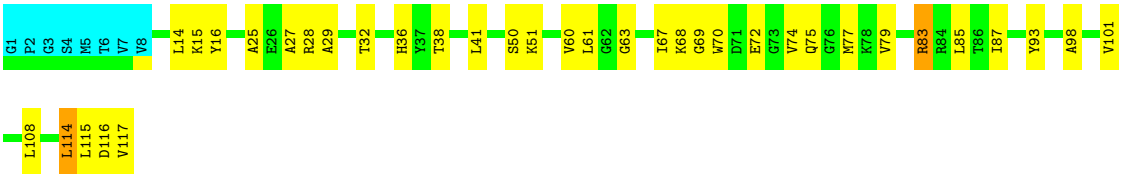
Chain A: 67% 25% • 7%



4.2.4 Score per residue for model 4

- Molecule 1: Peptidyl-prolyl cis-trans isomerase

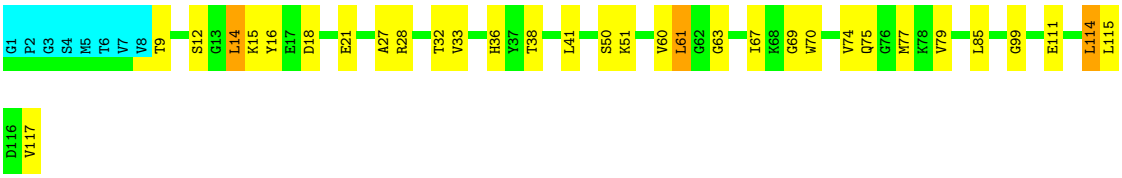
Chain A: 62% 29% • 7%



4.2.5 Score per residue for model 5

- Molecule 1: Peptidyl-prolyl cis-trans isomerase

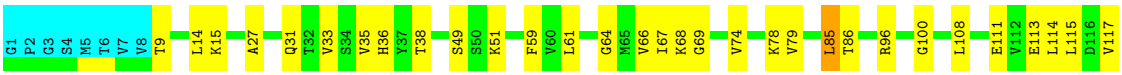
Chain A: 66% 25% • 7%



4.2.6 Score per residue for model 6

- Molecule 1: Peptidyl-prolyl cis-trans isomerase

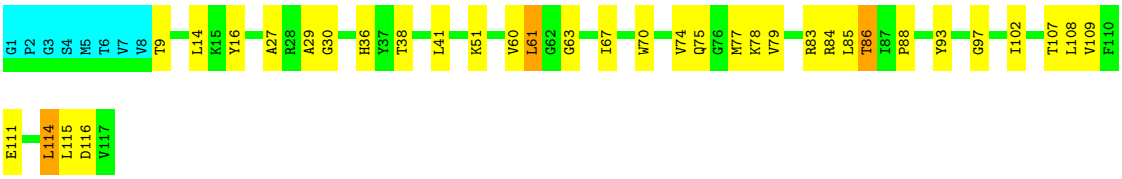
Chain A: 67% 26% • 7%



4.2.7 Score per residue for model 7

- Molecule 1: Peptidyl-prolyl cis-trans isomerase

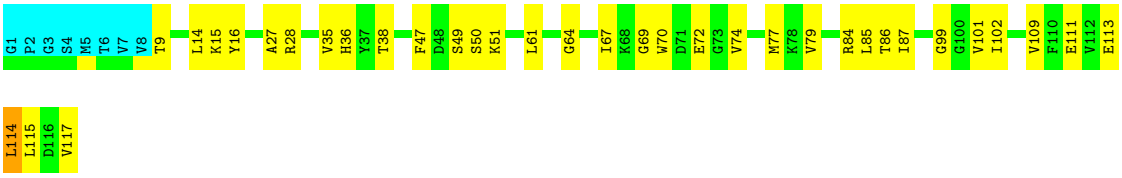
Chain A: 63% 27% • 7%



4.2.8 Score per residue for model 8

- Molecule 1: Peptidyl-prolyl cis-trans isomerase

Chain A: 63% 29% • 7%



4.2.9 Score per residue for model 9

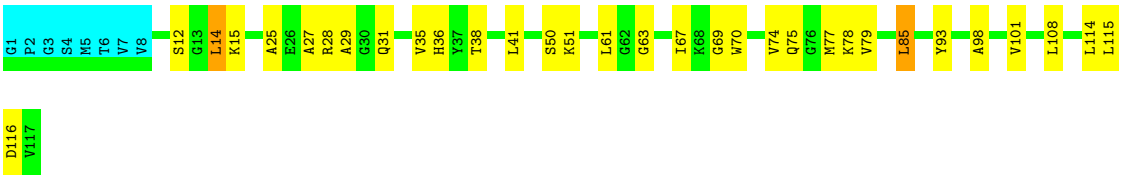
- Molecule 1: Peptidyl-prolyl cis-trans isomerase

Chain A: 68% 21% • 7%

4.2.10 Score per residue for model 10

- Molecule 1: Peptidyl-prolyl cis-trans isomerase

Chain A: 66% 26% • 7%



4.2.11 Score per residue for model 11

- Molecule 1: Peptidyl-prolyl cis-trans isomerase

Chain A: 63% 29% • 7%

G1 P2 G3 S4 M5 T6 V7 V8 S12 G13 L14 K15 Y16 E17 D18 A27 R28 Q31 T32 V33 S34 V35 H36 Y37 T38 L41 F47 D48 S49 S50 K51 L61 G64 M65 V66 I67 W70 V74 G75 G76 M77 K78 V79 R83 R84 L85 T86 V101 I102

L108 V109 F110 E111 L114 L115 D116 V117

4.2.12 Score per residue for model 12

- Molecule 1: Peptidyl-prolyl cis-trans isomerase

Chain A: 65% 27% • 7%

G1 P2 G3 S4 M5 T6 V7 V8 S12 G13 L14 K15 T20 A27 R28 Q31 V35 H36 Y37 T38 L41 F47 D48 S49 S50 K51 L61 G64 M65 V66 I67 V74 Q75 V79 T86 I87 L91 G92 Y93 A98 I102 L108 V109 F110

E111 V112 E113 L114 L115 D116 V117

4.2.13 Score per residue for model 13

- Molecule 1: Peptidyl-prolyl cis-trans isomerase

Chain A: 64% 28% • 7%

G1 P2 G3 S4 M5 T6 V7 V8 T9 S12 G13 L14 K15 Y16 A25 E26 A27 V33 S34 V35 T38 F47 S50 K51 F59 V60 L61 G64 M65 V66 I67 K68 G69 V74 V79 R83 R84 L85 T86 Y93 A98 I102 L108 V109 F110

E111 L114 L115 D116 V117

4.2.14 Score per residue for model 14

- Molecule 1: Peptidyl-prolyl cis-trans isomerase

Chain A: 59% 32% • 7%

G1 P2 G3 S4 M5 T6 V7 V8 S12 G13 L14 K15 Y16 T20 E21 G24 A27 R28 A29 G30 V33 H36 Y37 T38 S49 S50 K51 V60 L61 G62 G63 G64 I67 K68 G69 W70 D71 E72 G73 V74 K78 V79 R83 R84 L85 Q90 L91

G100 L108 E111 V112 E113 L114 L115 D116 V117

4.2.15 Score per residue for model 15

- Molecule 1: Peptidyl-prolyl cis-trans isomerase

Chain A: 67% 25% • 7%

G1 P2 G3 S4 M5 T6 V7 V8 L14 A27 R28 A29 G30 Q31 T32 V33 S34 V35 H36 Y37 T38 F47 D48 S49 S50 K51 V60 L61 G62 G63 I67 W70 V74 M77 K78 V79 V82 L85 V101 L108 V109 F110 E111 V112 E113 L114 L115 D116

V117

4.2.16 Score per residue for model 16

- Molecule 1: Peptidyl-prolyl cis-trans isomerase

Chain A: 68% 22% • 7%

G1 P2 G3 S4 M5 T6 V7 V8 T9 S12 G13 L14 K15 Y16 A27 T32 H36 Y37 T38 Q45 S50 K51 V60 L61 G62 G63 V66 I67 W70 V74 Q75 G76 M77 K78 V79 R83 R84 L85 R96 L108 E113 L114 L115 D116 V117

4.2.17 Score per residue for model 17

- Molecule 1: Peptidyl-prolyl cis-trans isomerase

Chain A: 68% 23% • 7%

G1 P2 G3 S4 M5 T6 V7 V8 T9 S12 G13 L14 K15 L19 A27 G30 V35 H36 Y37 T38 K46 S49 S50 K51 D52 R53 F59 V60 L61 G64 I67 K68 G69 W70 V74 V79 L85 T86 I87 Y93 A98 L114 L115 D116

V117

4.2.18 Score per residue for model 18

- Molecule 1: Peptidyl-prolyl cis-trans isomerase

Chain A: 62% 27% • 7%

G1 P2 G3 S4 M5 T6 V7 V8 T9 S12 G13 L14 K15 Y16 L19 V33 S34 V35 H36 Y37 T38 F47 D48 S49 S50 K51 L61 G64 M65 V66 I67 W70 V74 Q75 G76 M77 K78 V79 R84 L85 T86 Q90 Y93 A98 G99 G100 V101 I102

L108 E111 V112 E113 L114 L115 D116 V117

4.2.19 Score per residue for model 19

- Molecule 1: Peptidyl-prolyl cis-trans isomerase

Chain A: 66% 25% • 7%

G1 P2 G3 S4 M5 T6 V7 V8 L14 K15 Y16 L19 A27 R28 T32 V35 T38 L41 F47 S50 K51 L61 I67 W70 D71 E72 G73 V74 Q75 G76 V79 R84 L85 T86 I87 L91 R96 I102 L108 V109 E113

L114 L115 D116 V117

4.2.20 Score per residue for model 20

- Molecule 1: Peptidyl-prolyl cis-trans isomerase

Chain A: 71% 21% • 7%

G1 P2 G3 S4 M5 T6 V7 V8 T9 L14 K15 Y16 A27 V33 H36 Y37 T38 S50 K51 L61 I67 W70 V74 Q75 G76 M77 L85 Y93 A98 L108 V109 F110 E111 V112 E113 L114 L115 D116 V117

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*.

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

Software name	Classification	Version
CYANA	structure solution	2.1
CYANA	refinement	2.1

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	810	791	791	16±4
All	All	16200	15820	15820	323

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 10.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:86:THR:HG23	1:A:109:VAL:HG22	0.87	1.46	7	6
1:A:35:VAL:HG12	1:A:114:LEU:HD13	0.76	1.58	6	9
1:A:61:LEU:HD13	1:A:74:VAL:HG13	0.73	1.59	12	2
1:A:36:HIS:CD2	1:A:115:LEU:HD11	0.67	2.24	10	18
1:A:70:TRP:O	1:A:74:VAL:HG23	0.67	1.90	18	16
1:A:27:ALA:HB3	1:A:74:VAL:O	0.66	1.91	5	19
1:A:25:ALA:HB3	1:A:117:VAL:HG21	0.65	1.67	4	2
1:A:28:ARG:C	1:A:61:LEU:HD23	0.64	2.13	11	11
1:A:108:LEU:N	1:A:108:LEU:HD13	0.63	2.09	19	1
1:A:16:TYR:CB	1:A:85:LEU:HD23	0.63	2.23	19	1
1:A:78:LYS:C	1:A:114:LEU:HD23	0.63	2.13	10	2
1:A:35:VAL:HG12	1:A:114:LEU:HD22	0.63	1.70	15	5
1:A:61:LEU:HD11	1:A:75:GLN:HG2	0.62	1.71	12	4
1:A:77:MET:HB3	1:A:114:LEU:HD13	0.62	1.69	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:16:TYR:HB3	1:A:85:LEU:HD12	0.62	1.71	7	7
1:A:41:LEU:HD21	1:A:101:VAL:O	0.62	1.94	10	4
1:A:25:ALA:O	1:A:79:VAL:HG23	0.62	1.94	10	1
1:A:61:LEU:HD13	1:A:74:VAL:CG1	0.61	2.26	9	13
1:A:14:LEU:C	1:A:14:LEU:HD22	0.61	2.15	16	4
1:A:85:LEU:HD12	1:A:112:VAL:HG21	0.61	1.72	20	4
1:A:14:LEU:HD22	1:A:14:LEU:C	0.59	2.18	10	1
1:A:35:VAL:CG1	1:A:114:LEU:HD22	0.58	2.28	15	4
1:A:69:GLY:HA3	1:A:85:LEU:HD21	0.58	1.74	13	6
1:A:85:LEU:HD12	1:A:112:VAL:CG2	0.58	2.28	20	4
1:A:29:ALA:HB2	1:A:75:GLN:NE2	0.58	2.13	10	1
1:A:79:VAL:HG13	1:A:115:LEU:O	0.57	1.98	14	11
1:A:77:MET:HG3	1:A:114:LEU:HD12	0.57	1.76	7	1
1:A:79:VAL:HG22	1:A:117:VAL:HG13	0.56	1.76	13	4
1:A:77:MET:HG3	1:A:114:LEU:HD23	0.55	1.76	3	2
1:A:16:TYR:HB3	1:A:85:LEU:HD23	0.55	1.78	19	3
1:A:82:VAL:HG22	1:A:113:GLU:HG3	0.55	1.79	15	1
1:A:77:MET:CB	1:A:114:LEU:HD13	0.55	2.31	5	1
1:A:101:VAL:HG23	1:A:102:ILE:HG13	0.55	1.78	18	1
1:A:85:LEU:HD23	1:A:87:ILE:HD11	0.55	1.76	17	2
1:A:108:LEU:HD12	1:A:108:LEU:O	0.55	2.02	15	1
1:A:47:PHE:CD1	1:A:102:ILE:HD11	0.55	2.37	19	2
1:A:78:LYS:C	1:A:114:LEU:HD13	0.54	2.23	7	1
1:A:83:ARG:NH2	1:A:85:LEU:HD13	0.53	2.17	4	3
1:A:79:VAL:CG2	1:A:117:VAL:HG13	0.53	2.33	4	7
1:A:99:GLY:O	1:A:101:VAL:HG23	0.53	2.03	8	1
1:A:61:LEU:HD13	1:A:74:VAL:HB	0.53	1.81	1	10
1:A:12:SER:OG	1:A:91:LEU:HD21	0.53	2.04	12	1
1:A:108:LEU:O	1:A:108:LEU:HD12	0.52	2.04	20	3
1:A:90:GLN:HG3	1:A:91:LEU:HD12	0.52	1.81	14	1
1:A:69:GLY:O	1:A:85:LEU:HD11	0.52	2.05	10	1
1:A:35:VAL:CG1	1:A:114:LEU:HD13	0.51	2.34	6	4
1:A:33:VAL:CG1	1:A:117:VAL:HG12	0.51	2.36	2	1
1:A:32:THR:OG1	1:A:60:VAL:HG12	0.51	2.06	16	4
1:A:69:GLY:HA3	1:A:85:LEU:HD11	0.51	1.82	5	1
1:A:108:LEU:HD13	1:A:110:PHE:CE2	0.51	2.41	15	2
1:A:85:LEU:CD2	1:A:87:ILE:HD11	0.51	2.35	17	1
1:A:61:LEU:HD11	1:A:75:GLN:CA	0.50	2.37	5	1
1:A:9:THR:HG22	1:A:15:LYS:CD	0.50	2.37	6	1
1:A:16:TYR:CB	1:A:85:LEU:HD12	0.50	2.36	8	4
1:A:33:VAL:HG12	1:A:117:VAL:HA	0.50	1.82	15	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:47:PHE:CE1	1:A:102:ILE:HD11	0.49	2.41	19	6
1:A:77:MET:CG	1:A:114:LEU:HD23	0.49	2.36	15	1
1:A:25:ALA:CB	1:A:117:VAL:HG21	0.49	2.36	4	1
1:A:59:PHE:CZ	1:A:66:VAL:HG11	0.49	2.42	6	2
1:A:93:TYR:CE2	1:A:98:ALA:HB2	0.49	2.42	13	6
1:A:88:PRO:HA	1:A:107:THR:HG23	0.49	1.82	7	1
1:A:69:GLY:C	1:A:85:LEU:HD11	0.49	2.28	10	1
1:A:83:ARG:CZ	1:A:85:LEU:HD13	0.49	2.38	11	2
1:A:88:PRO:CG	1:A:91:LEU:HD12	0.48	2.37	2	1
1:A:19:LEU:HD21	1:A:84:ARG:HD2	0.48	1.84	9	2
1:A:77:MET:HG2	1:A:114:LEU:HD23	0.48	1.84	15	1
1:A:29:ALA:N	1:A:61:LEU:HD23	0.48	2.24	10	3
1:A:77:MET:HB3	1:A:114:LEU:HD23	0.48	1.86	16	2
1:A:70:TRP:O	1:A:74:VAL:HG12	0.48	2.08	11	1
1:A:79:VAL:HG23	1:A:117:VAL:HG13	0.48	1.84	14	1
1:A:61:LEU:HG	1:A:74:VAL:HG12	0.48	1.84	18	1
1:A:69:GLY:CA	1:A:85:LEU:HD11	0.48	2.39	5	1
1:A:14:LEU:HD22	1:A:15:LYS:N	0.48	2.24	13	5
1:A:61:LEU:CD1	1:A:74:VAL:HG13	0.47	2.39	11	1
1:A:36:HIS:CD2	1:A:115:LEU:HD21	0.47	2.45	15	1
1:A:33:VAL:HG12	1:A:117:VAL:C	0.47	2.30	14	1
1:A:14:LEU:HD12	1:A:15:LYS:N	0.47	2.25	5	2
1:A:61:LEU:HD13	1:A:74:VAL:HG12	0.46	1.86	3	5
1:A:19:LEU:HD11	1:A:84:ARG:HD3	0.45	1.87	3	2
1:A:30:GLY:C	1:A:60:VAL:HG23	0.45	2.32	14	2
1:A:61:LEU:HD13	1:A:74:VAL:CB	0.44	2.41	3	9
1:A:87:ILE:HG22	1:A:88:PRO:HD2	0.44	1.90	1	1
1:A:108:LEU:HD13	1:A:110:PHE:CD2	0.44	2.47	15	1
1:A:86:THR:OG1	1:A:109:VAL:HG22	0.44	2.12	19	1
1:A:25:ALA:HB3	1:A:117:VAL:CG2	0.44	2.41	4	1
1:A:34:SER:OG	1:A:58:ALA:HB2	0.43	2.13	2	1
1:A:35:VAL:HG12	1:A:114:LEU:CD1	0.43	2.43	10	1
1:A:61:LEU:HD11	1:A:75:GLN:CG	0.43	2.42	12	1
1:A:91:LEU:HD23	1:A:91:LEU:O	0.43	2.14	19	1
1:A:108:LEU:HD22	1:A:108:LEU:O	0.43	2.14	19	1
1:A:93:TYR:CE2	1:A:102:ILE:HD12	0.43	2.49	7	1
1:A:14:LEU:N	1:A:14:LEU:CD1	0.42	2.82	13	3
1:A:93:TYR:HE2	1:A:98:ALA:HB2	0.42	1.74	17	4
1:A:14:LEU:CD1	1:A:14:LEU:N	0.42	2.83	10	1
1:A:30:GLY:C	1:A:60:VAL:HG13	0.42	2.35	15	2
1:A:32:THR:OG1	1:A:60:VAL:HG22	0.42	2.15	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:61:LEU:HD21	1:A:75:GLN:HG2	0.42	1.92	4	2
1:A:61:LEU:HD11	1:A:75:GLN:HA	0.41	1.93	16	1
1:A:108:LEU:N	1:A:108:LEU:CD1	0.41	2.80	19	1
1:A:9:THR:HG22	1:A:15:LYS:CG	0.41	2.46	6	1
1:A:61:LEU:HD22	1:A:74:VAL:HG12	0.41	1.93	10	1
1:A:47:PHE:HB2	1:A:101:VAL:HG11	0.40	1.92	15	1
1:A:59:PHE:HZ	1:A:74:VAL:HG21	0.40	1.77	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	108/117 (92%)	95±2 (88±2%)	11±2 (10±2%)	2±1 (2±1%)	13	56
All	All	2160/2340 (92%)	1907 (88%)	216 (10%)	37 (2%)	13	56

All 10 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	63	GLY	10
1	A	64	GLY	8
1	A	76	GLY	7
1	A	61	LEU	3
1	A	99	GLY	2
1	A	100	GLY	2
1	A	65	MET	2
1	A	97	GLY	1
1	A	24	GLY	1
1	A	66	VAL	1

6.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR

entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	83/89 (93%)	70±2 (84±2%)	13±2 (16±2%)	5 42
All	All	1660/1780 (93%)	1393 (84%)	267 (16%)	5 42

All 44 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	14	LEU	20
1	A	38	THR	20
1	A	51	LYS	20
1	A	67	ILE	20
1	A	50	SER	14
1	A	111	GLU	14
1	A	108	LEU	12
1	A	114	LEU	10
1	A	49	SER	9
1	A	9	THR	9
1	A	113	GLU	8
1	A	12	SER	8
1	A	84	ARG	7
1	A	41	LEU	6
1	A	61	LEU	6
1	A	68	LYS	6
1	A	85	LEU	6
1	A	116	ASP	5
1	A	83	ARG	5
1	A	86	THR	5
1	A	31	GLN	5
1	A	72	GLU	5
1	A	15	LYS	5
1	A	87	ILE	4
1	A	20	THR	4
1	A	78	LYS	4
1	A	65	MET	4
1	A	75	GLN	3
1	A	96	ARG	3
1	A	19	LEU	3
1	A	28	ARG	2
1	A	18	ASP	2
1	A	21	GLU	2

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Mol	Chain	Res	Type	Models (Total)
1	A	17	GLU	1
1	A	23	SER	1
1	A	77	MET	1
1	A	115	LEU	1
1	A	48	ASP	1
1	A	45	GLN	1
1	A	46	LYS	1
1	A	53	ARG	1
1	A	90	GLN	1
1	A	32	THR	1
1	A	91	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