Full wwPDB NMR Structure Validation Report (i)

Jun 12, 2024 – 03:05 PM EDT

PDB ID	:	2L2S
BMRB ID	:	17151
Title	:	Solution structure of peptidyl-prolyl cis-trans isomerase from Burkholderia pseudomallei complexed with 1-{[(4-methylphenyl)thio]acetyl}piperidine
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Deposited on	:	2010-08-27

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 (1)) were used in the production of this report:

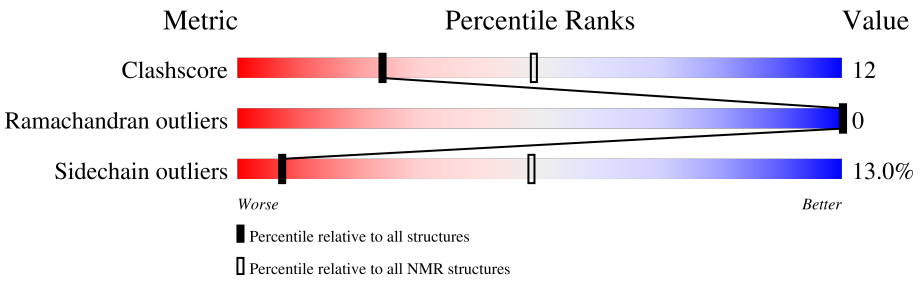
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 is 85%.

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	52% 21% • 26%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 2 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:14-A:61, A:66-A:92, A:106-A:117 (87)	0.35	2

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 3 single-model clusters were found.

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1739 atoms, of which 862 are hydrogens and 0 are deuteriums.

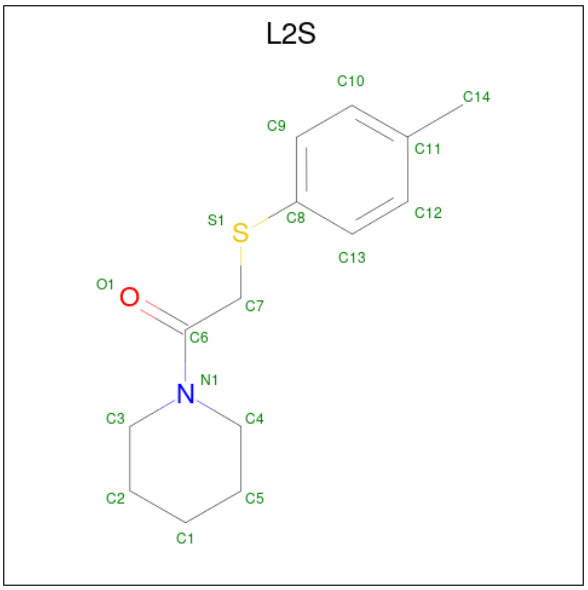
- Molecule 1 is a protein called Peptidyl-prolyl cis-trans isomerase.

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 Q3JK38
A	2	PRO	-	expression tag	UNP Q3JK38
A	3	GLY	-	expression tag	UNP Q3JK38
A	4	SER	-	expression tag	UNP Q3JK38

- Molecule 2 is 1-{[(4-methylphenyl)sulfanyl]acetyl}piperidine (three-letter code: L2S) (formula: $C_{14}H_{19}NOS$).



Mol	Chain	Residues	Atoms					
			Total	C	H	N	O	S
2	A	1	36	14	19	1	1	1

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: 52% 21% • 26%

G1 P2 G3 S4 M5 T6 V7 V8 T9 T10 E11 S12 G13 L14 K15 A27 R28 S34 V35 H36 Y37 T38 L41 T42 D55 P56 L61 G62 G63 G64 M65 G69 W70 V74 V79 V82 L85 T86 I87 Y93 G94 A95 R96 G97 A98 G99 G100 V101 I102

P103 P104 N105 A106 T107 E113 L114 L115 D116 V117

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: Peptidyl-prolyl cis-trans isomerase

Chain A: 52% 21% • 26%

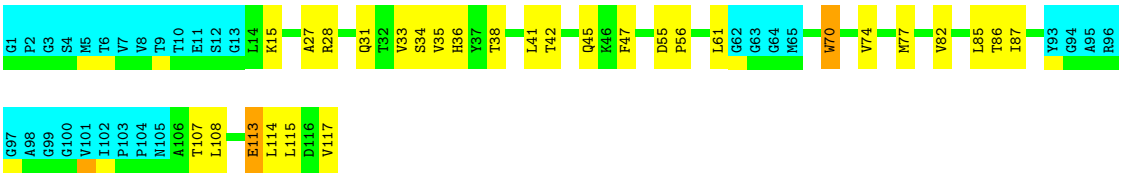
G1 P2 G3 S4 M5 T6 V7 V8 T9 T10 E11 S12 G13 L14 K15 A27 R28 V33 S34 V35 T38 F47 D48 S49 P56 L61 G62 G63 G64 M65 G69 W70 V74 K78 V79 V82 L85 T86 I87 Y93 G94 A95 R96 G97 A98 G99 G100 V101

I102 P103 P104 N105 L108 E113 L114 L115 D116 V117

4.2.2 Score per residue for model 2 (medoid)

• Molecule 1: Peptidyl-prolyl cis-trans isomerase

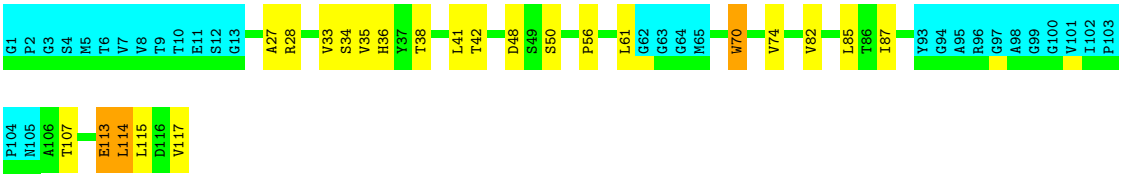
Chain A: 50% 23% • 26%



4.2.3 Score per residue for model 3

- Molecule 1: Peptidyl-prolyl cis-trans isomerase

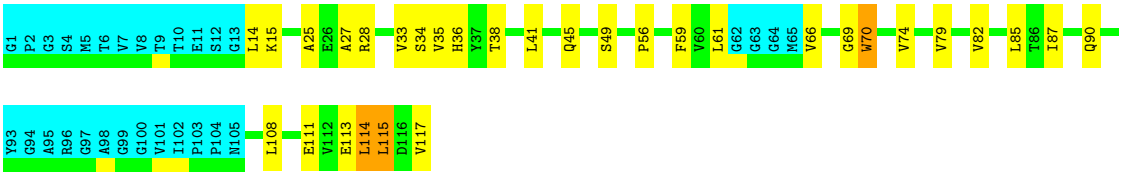
Chain A:



4.2.4 Score per residue for model 4

- Molecule 1: Peptidyl-prolyl cis-trans isomerase

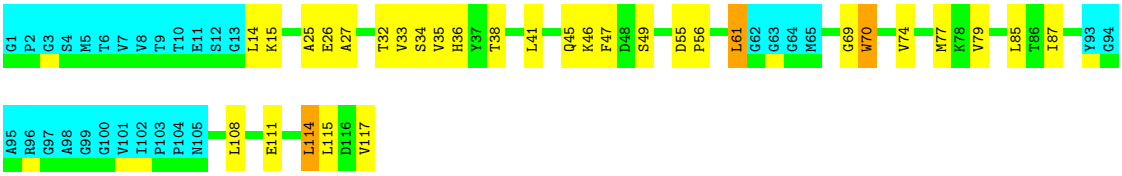
Chain A:



4.2.5 Score per residue for model 5

- Molecule 1: Peptidyl-prolyl cis-trans isomerase

Chain A:



4.2.6 Score per residue for model 6

- Molecule 1: Peptidyl-prolyl cis-trans isomerase

Chain A: 51% 22% • 26%

G1 P2 G3 S4 M5 T6 V7 V8 T9 T10 E11 S12 G13 L14 K15 A25 E26 A27 R28 V35 H36 Y37 T38 L41 T42 S50 P56 F59 V60 L61 G62 G63 G64 M65 V66 I67 K68 G69 W70 V74 M77 K78 V79 L85 T86 I87 Y93 G94 A95 R96

G97 A98 G99 G100 V101 I102 P103 P104 N105 A106 T107 L114 L115 D116 V117

4.2.7 Score per residue for model 7

- Molecule 1: Peptidyl-prolyl cis-trans isomerase

Chain A: 53% 19% • 26%

G1 P2 G3 S4 M5 T6 V7 V8 T9 T10 E11 S12 G13 L14 L19 A27 R28 V33 S34 V35 H36 Y37 T38 L41 D55 P56 L61 G62 G63 G64 M65 W70 D71 E72 G73 V74 V82 L85 T86 I87 Y93 G94 A95 R96 G97 A98 G99 G100 V101 I102

P103 P104 N105 L108 E113 L114 L115 D116 V117

4.2.8 Score per residue for model 8

- Molecule 1: Peptidyl-prolyl cis-trans isomerase

Chain A: 45% 26% • 26%

G1 P2 G3 S4 M5 T6 V7 V8 T9 T10 E11 S12 G13 L14 K15 Y16 E26 A27 V33 S34 V35 H36 Y37 T38 L41 T42 Q45 K51 P56 L61 G62 G63 G64 M65 K68 G69 W70 D71 E72 G73 V74 M77 K78 V82 R83 R84 L85 T86 I87

L91 G92 Y93 G94 A95 R96 G97 A98 G99 G100 V101 I102 P103 P104 N105 A106 T107 E113 L114 L115 D116 V117

4.2.9 Score per residue for model 9

- Molecule 1: Peptidyl-prolyl cis-trans isomerase

Chain A: 54% 19% • 26%

G1 P2 G3 S4 M5 T6 V7 V8 T9 T10 E11 S12 G13 D18 A27 T32 V33 S34 V35 H36 Y37 T38 L41 T42 S50 D55 P56 L61 G62 G63 G64 M65 W70 V74 M77 V82 L85 T86 I87 Y93 G94 A95 R96 G97 A98 G99 G100

V101 I102 P103 P104 N105 A106 T107 E113 L114 L115 D116 V117

4.2.10 Score per residue for model 10

- Molecule 1: Peptidyl-prolyl cis-trans isomerase

Chain A: 49% 25% • 26%

G1 P2 G3 S4 M5 T6 V7 V8 T9 T10 E11 S12 G13 L14 K15 A27 R28 S34 V35 T38 L41 T42 Q45 D48 S49 S50 D55 P56 F59 V60 L61 G62 G63 G64 M65 V66 I67 K68 G69 W70 V74 V79 L85 T86 I87 L91 G92 Y93

G94 A95 R96 G97 A98 G99 G100 V101 I102 P103 P104 N105 A106 T107 L114 L115 D116 V117

4.2.11 Score per residue for model 11

- Molecule 1: Peptidyl-prolyl cis-trans isomerase

Chain A: 51% 21% • 26%

G1 P2 G3 S4 M5 T6 V7 V8 T9 T10 E11 S12 G13 L14 K15 D18 A27 R28 S34 V35 H36 Y37 T38 L41 T42 S49 P56 F59 V60 L61 G62 G63 G64 M65 V66 W70 D71 E72 G73 V74 V82 L85 T86 I87 Y93 G94 A95 R96 G97

A98 G99 G100 V101 I102 P103 P104 N105 A106 T107 E113 L114 L115 D116 V117

4.2.12 Score per residue for model 12

- Molecule 1: Peptidyl-prolyl cis-trans isomerase

Chain A: 50% 22% • 26%

G1 P2 G3 S4 M5 T6 V7 V8 T9 T10 E11 S12 G13 L14 K15 A25 E26 A27 R28 S34 V35 H36 Y37 T38 L41 T42 D48 S49 S50 P56 L61 G62 G63 G64 M65 G69 W70 D71 V74 V79 V82 L85 T86 I87 Y93 G94 A95 R96

G97 A98 G99 G100 V101 I102 P103 P104 N105 A106 T107 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: 50% 20% 5% 26%

G1 P2 G3 S4 M5 T6 V7 V8 T9 T10 E11 S12 G13 L14 K15 A25 E26 A27 R28 S34 V35 H36 Y37 T38 L41 D48 K51 P56 L61 G62 G63 G64 M65 K68 G69 W70 D71 E72 G73 V74 V79 V82 L85 T86 I87 L91 G92 Y93

G94 A95 R96 G97 A98 G99 G100 V101 I102 P103 P104 N105 L108 E111 V112 E113 L114 L115 D116 V117

4.2.14 Score per residue for model 14

- Molecule 1: Peptidyl-prolyl cis-trans isomerase

Chain A: 56% 16% • 26%

G1 P2 G3 S4 M5 T6 V7 V8 T9 T10 E11 S12 G13 L14 K15 A27 R28 S34 V35 T38 L41 S50 D55 P56 L61 G62 G63 G64 M65 G69 W70 V74 M77 L85 T86 I87 Y93 G94 A95 R96 G97 A98 G99 G100 V101 I102 P103 P104

N105 L114 L115 D116 V117

4.2.15 Score per residue for model 15

- Molecule 1: Peptidyl-prolyl cis-trans isomerase

Chain A: 48% 24% • 26%

G1 P2 G3 S4 M5 T6 V7 V8 T9 T10 E11 S12 G13 L14 K15 D18 A25 E26 A27 R28 V33 S34 V35 H36 Y37 T38 T42 K46 F47 D55 P56 L61 G62 G63 G64 M65 K68 G69 W70 V74 K78 V79 V82 L85 T86 I87 Y93

G94 A95 R96 G97 A98 G99 G100 V101 I102 P103 P104 N105 A106 T107 L108 E113 L114 L115 D116 V117

4.2.16 Score per residue for model 16

- Molecule 1: Peptidyl-prolyl cis-trans isomerase

Chain A: 44% 26% • 26%

G1 P2 G3 S4 M5 T6 V7 V8 T9 T10 E11 S12 G13 L14 K15 D18 A27 R28 T32 V33 S34 V35 H36 Y37 T38 T42 D43 D48 D55 P56 F59 V60 L61 G62 G63 G64 M65 V66 G69 W70 V74 N77 K78 V79 V82 L85 T86 I87

Y93 G94 A95 R96 G97 A98 G99 G100 V101 I102 P103 P104 N105 A106 T107 L108 E111 V112 E113 L114 L115 D116 V117

4.2.17 Score per residue for model 17

- Molecule 1: Peptidyl-prolyl cis-trans isomerase

Chain A: 52% 18% • 26%

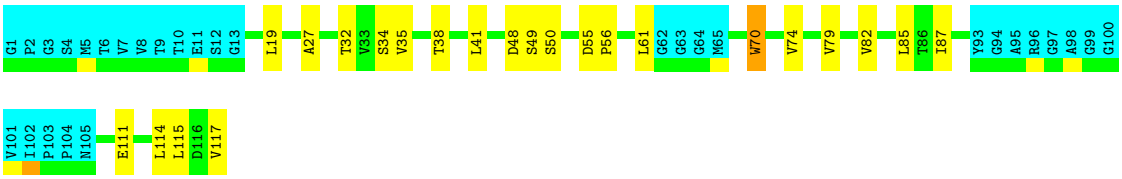
G1 P2 G3 S4 M5 T6 V7 V8 T9 T10 E11 S12 G13 L14 K15 A27 R28 V35 H36 Y37 T38 L41 T42 Q45 D48 S49 S50 V60 L61 G62 G63 G64 M65 G69 W70 D71 E72 G73 V74 V79 L85 T86 I87 Y93 G94 A95 R96 G97 A98 G99

G100 V101 I102 P103 P104 N105 A106 T107 L114 L115 D116 V117

4.2.18 Score per residue for model 18

- Molecule 1: Peptidyl-prolyl cis-trans isomerase

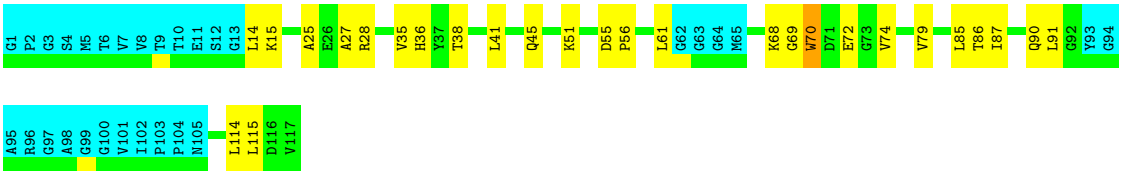
Chain A:



4.2.19 Score per residue for model 19

- Molecule 1: Peptidyl-prolyl cis-trans isomerase

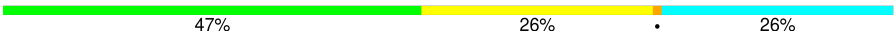
Chain A:

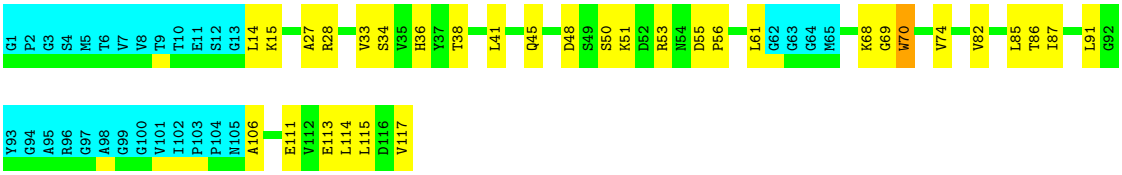


4.2.20 Score per residue for model 20

- Molecule 1: Peptidyl-prolyl cis-trans isomerase

Chain A:





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*.

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

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1250
Number of shifts mapped to atoms	1233
Number of unparsed shifts	0
Number of shifts with mapping errors	17
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	85%

6 Model quality (i)

6.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: L2S

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	671	661	661	16±3
All	All	13760	13600	13600	329

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 12.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:33:VAL:HG12	1:A:117:VAL:HG23	0.92	1.42	4	5
1:A:85:LEU:HD23	1:A:87:ILE:HD11	0.92	1.40	20	20
1:A:14:LEU:HD11	1:A:85:LEU:HD11	0.76	1.57	11	8
1:A:35:VAL:HG12	1:A:114:LEU:HD13	0.70	1.64	17	10
1:A:36:HIS:CD2	1:A:115:LEU:HD11	0.68	2.23	16	16
1:A:82:VAL:HG22	1:A:113:GLU:HB2	0.67	1.65	20	4
1:A:70:TRP:O	1:A:74:VAL:HG22	0.65	1.91	16	19
1:A:27:ALA:CB	1:A:74:VAL:HG22	0.65	2.22	14	1
1:A:14:LEU:HD11	1:A:85:LEU:CD1	0.64	2.22	6	7
1:A:27:ALA:HB3	1:A:74:VAL:O	0.64	1.91	18	20
1:A:25:ALA:O	1:A:79:VAL:HG23	0.64	1.93	19	7
1:A:27:ALA:HB1	1:A:61:LEU:HD23	0.64	1.70	17	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:79:VAL:HG22	1:A:117:VAL:HG13	0.63	1.70	17	1
1:A:33:VAL:CG1	1:A:117:VAL:HG23	0.63	2.23	1	5
1:A:85:LEU:CD2	1:A:87:ILE:HD11	0.62	2.23	16	12
1:A:56:PRO:HB3	1:A:115:LEU:HD13	0.62	1.71	19	19
1:A:68:LYS:CE	1:A:91:LEU:HD22	0.62	2.25	20	3
1:A:14:LEU:HD22	1:A:69:GLY:HA2	0.61	1.73	5	10
1:A:68:LYS:HE2	1:A:91:LEU:HD22	0.61	1.72	10	3
1:A:33:VAL:HG12	1:A:117:VAL:HG13	0.61	1.73	7	3
1:A:35:VAL:CG1	1:A:114:LEU:HD22	0.60	2.27	4	5
1:A:82:VAL:HG22	1:A:113:GLU:CB	0.59	2.27	20	8
1:A:35:VAL:CG1	1:A:114:LEU:HD13	0.58	2.28	6	10
1:A:78:LYS:C	1:A:114:LEU:HD13	0.57	2.19	15	2
1:A:36:HIS:CG	1:A:115:LEU:HD11	0.57	2.34	13	11
1:A:61:LEU:HD13	1:A:74:VAL:CG1	0.56	2.31	14	1
1:A:47:PHE:CZ	1:A:108:LEU:HD22	0.56	2.35	15	1
1:A:28:ARG:O	1:A:61:LEU:HD23	0.56	2.01	4	13
1:A:41:LEU:HD12	1:A:45:GLN:HB3	0.55	1.78	17	6
1:A:14:LEU:HD13	1:A:85:LEU:HD11	0.53	1.80	1	3
1:A:47:PHE:CZ	1:A:108:LEU:HD12	0.53	2.39	5	3
1:A:33:VAL:HB	1:A:117:VAL:HG23	0.53	1.81	8	1
1:A:14:LEU:HD13	1:A:72:GLU:OE1	0.52	2.04	17	1
1:A:19:LEU:HD23	1:A:82:VAL:CG1	0.52	2.34	18	1
1:A:35:VAL:HA	1:A:115:LEU:HD12	0.52	1.81	10	5
1:A:61:LEU:HD13	1:A:74:VAL:CG2	0.51	2.35	1	7
1:A:82:VAL:HG22	1:A:113:GLU:CD	0.51	2.26	1	1
1:A:68:LYS:NZ	1:A:91:LEU:HD22	0.50	2.21	13	2
1:A:35:VAL:HG11	1:A:114:LEU:HD22	0.50	1.84	4	5
1:A:82:VAL:HG22	1:A:113:GLU:HB3	0.50	1.84	3	7
1:A:82:VAL:HG13	1:A:113:GLU:HB3	0.49	1.84	20	4
1:A:77:MET:CE	1:A:112:VAL:HG12	0.49	2.37	16	1
1:A:79:VAL:CG2	1:A:117:VAL:HG23	0.49	2.37	18	2
1:A:27:ALA:HB1	1:A:61:LEU:CD2	0.49	2.37	16	4
1:A:79:VAL:HA	1:A:114:LEU:HD22	0.49	1.82	15	2
1:A:82:VAL:HG22	1:A:113:GLU:HG3	0.49	1.83	8	2
1:A:79:VAL:N	1:A:114:LEU:HD13	0.49	2.23	1	1
1:A:41:LEU:HD12	1:A:45:GLN:CB	0.49	2.38	10	1
1:A:14:LEU:HD12	1:A:15:LYS:N	0.49	2.22	12	2
1:A:85:LEU:HD23	1:A:87:ILE:CD1	0.49	2.32	14	1
1:A:79:VAL:HG22	1:A:117:VAL:HG23	0.48	1.84	16	1
1:A:14:LEU:HD12	1:A:69:GLY:HA2	0.47	1.87	16	2
1:A:59:PHE:CD2	1:A:66:VAL:HG11	0.47	2.45	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:35:VAL:HG12	1:A:114:LEU:HG	0.47	1.86	13	2
1:A:82:VAL:HG13	1:A:111:GLU:OE2	0.47	2.10	13	1
1:A:82:VAL:HG22	1:A:113:GLU:CG	0.46	2.40	16	2
1:A:59:PHE:CE2	1:A:66:VAL:HG11	0.46	2.45	6	4
1:A:25:ALA:HB3	1:A:117:VAL:HG11	0.45	1.88	5	1
1:A:42:THR:HG22	1:A:107:THR:O	0.45	2.11	8	11
1:A:79:VAL:HG22	1:A:117:VAL:CG1	0.44	2.40	17	1
1:A:78:LYS:C	1:A:114:LEU:HD22	0.44	2.33	8	1
1:A:79:VAL:HG21	1:A:117:VAL:HG12	0.44	1.90	5	1
1:A:27:ALA:HA	1:A:117:VAL:HG21	0.43	1.90	8	1
1:A:70:TRP:O	1:A:74:VAL:HG12	0.43	2.13	14	1
1:A:68:LYS:HD2	1:A:91:LEU:HD22	0.42	1.90	8	1
1:A:77:MET:HB3	1:A:114:LEU:HD13	0.42	1.90	8	1
1:A:69:GLY:C	1:A:85:LEU:HD21	0.41	2.36	4	1
1:A:35:VAL:HG12	1:A:114:LEU:HD22	0.41	1.91	3	1
1:A:61:LEU:HD13	1:A:74:VAL:HG23	0.41	1.92	6	1
1:A:16:TYR:HB3	1:A:85:LEU:HD12	0.41	1.92	8	1
1:A:68:LYS:CD	1:A:91:LEU:HD22	0.41	2.46	8	1
1:A:35:VAL:CA	1:A:115:LEU:HD12	0.41	2.46	18	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	86/117 (74%)	80±2 (93±2%)	6±2 (7±2%)	0±0 (0±0%)	100	100
All	All	1720/2340 (74%)	1592 (93%)	128 (7%)	0 (0%)	100	100

There are no Ramachandran outliers.

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	71/89 (80%)	62±2 (87±3%)	9±2 (13±3%)	7 48
All	All	1420/1780 (80%)	1236 (87%)	184 (13%)	7 48

All 34 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	38	THR	20
1	A	70	TRP	20
1	A	34	SER	17
1	A	86	THR	15
1	A	55	ASP	11
1	A	114	LEU	10
1	A	50	SER	9
1	A	48	ASP	8
1	A	111	GLU	6
1	A	61	LEU	6
1	A	72	GLU	6
1	A	49	SER	5
1	A	77	MET	5
1	A	113	GLU	5
1	A	115	LEU	4
1	A	32	THR	4
1	A	51	LYS	4
1	A	18	ASP	4
1	A	68	LYS	3
1	A	28	ARG	3
1	A	14	LEU	3
1	A	90	GLN	2
1	A	26	GLU	2
1	A	46	LYS	2
1	A	31	GLN	1
1	A	45	GLN	1
1	A	19	LEU	1
1	A	78	LYS	1
1	A	84	ARG	1
1	A	15	LYS	1
1	A	71	ASP	1
1	A	43	ASP	1
1	A	60	VAL	1

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Mol	Chain	Res	Type	Models (Total)
1	A	53	ARG	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)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	L2S	A	130	-	18,18,18	1.47±0.00	1±0 (5±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	L2S	A	130	-	22,23,23	1.10±0.00	2±0 (9±0%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	L2S	A	130	-	-	0±0,9,17,17	0±0,2,2,2

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	A	130	L2S	C14-C11	3.69	1.40	1.51	3	20

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	A	130	L2S	C4-N1-C3	2.19	117.16	112.68	5	20
2	A	130	L2S	C9-C10-C11	2.14	118.91	121.37	4	20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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)

The completeness of assignment taking into account all chemical shift lists is 85% for the well-defined parts and 83% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping (i)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1250
Number of shifts mapped to atoms	1233
Number of unparsed shifts	0
Number of shifts with mapping errors	17
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. All 17 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	UNMAPPED	1	F191	H9	7.32	0.020	1
1	UNMAPPED	1	F191	H10	7.16	0.020	1
1	UNMAPPED	1	F191	H11	0.98	0.020	2
1	UNMAPPED	1	F191	H12	1.16	0.020	2
1	UNMAPPED	1	F191	H21	3.2	0.020	2
1	UNMAPPED	1	F191	H22	2.94	0.020	2
1	UNMAPPED	1	F191	H31	3.0	0.020	2
1	UNMAPPED	1	F191	H32	2.87	0.020	2
1	UNMAPPED	1	F191	H41	3.0	0.020	2
1	UNMAPPED	1	F191	H42	2.87	0.020	2
1	UNMAPPED	1	F191	H51	3.2	0.020	2
1	UNMAPPED	1	F191	H52	2.94	0.020	2
1	UNMAPPED	1	F191	H71	3.48	0.020	2
1	UNMAPPED	1	F191	H72	3.3	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	UNMAPPED	1	F191	H121	7.16	0.020	1
1	UNMAPPED	1	F191	H131	7.32	0.020	1
1	UNMAPPED	1	F191	H14	2.22	0.020	1

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	112	-0.16 ± 0.22	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	94	-0.01 ± 0.21	None needed (< 0.5 ppm)
$^{13}C'$	0	—	None (insufficient data)
^{15}N	109	-0.26 ± 0.41	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 85%, i.e. 985 atoms were assigned a chemical shift out of a possible 1158. 0 out of 19 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	352/440 (80%)	182/182 (100%)	86/174 (49%)	84/84 (100%)
Sidechain	556/629 (88%)	379/409 (93%)	172/198 (87%)	5/22 (23%)
Aromatic	77/89 (87%)	40/44 (91%)	36/42 (86%)	1/3 (33%)
Overall	985/1158 (85%)	601/635 (95%)	294/414 (71%)	90/109 (83%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 83%, i.e. 1233 atoms were assigned a chemical shift out of a possible 1478. 0 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

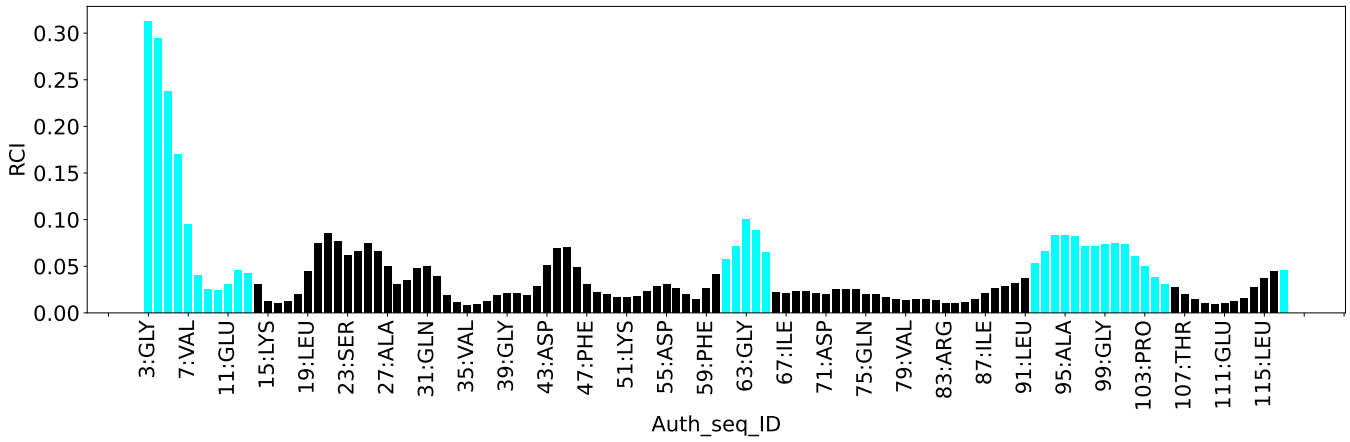
	Total	^{1}H	^{13}C	^{15}N
Backbone	465/594 (78%)	244/249 (98%)	112/234 (48%)	109/111 (98%)
Sidechain	683/786 (87%)	466/514 (91%)	211/246 (86%)	6/26 (23%)
Aromatic	85/98 (87%)	44/48 (92%)	40/47 (85%)	1/3 (33%)
Overall	1233/1478 (83%)	754/811 (93%)	363/527 (69%)	116/140 (83%)

7.1.4 Statistically unusual chemical shifts (i)

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	39	GLY	HA3	2.01	2.08 – 5.71	-5.2

7.1.5 Random Coil Index (RCI) plots (i)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A: