W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

Full wwPDB NMR Structure Validation Report ⓘ

Mar 1, 2022 – 05:06 PM EST

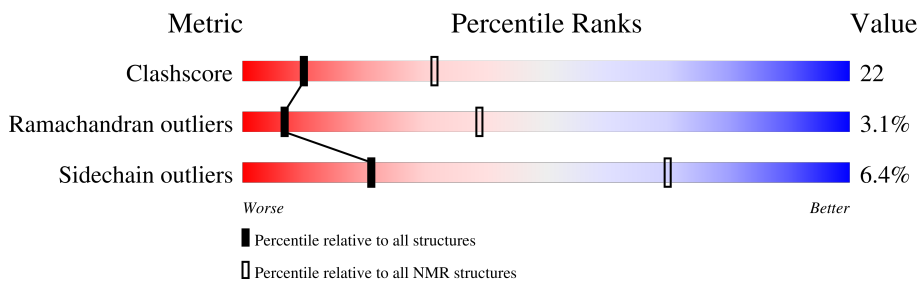|		
PDB ID	:	2FHW
Title	:	Solution structure of human relaxin-3
Authors	:	Rosengren, K.J.; Craik, D.J.
Deposited on	:	2005-12-27

1 Overall quality at a glance ⓘ

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	Percentile Ranks	Value
Clashscore		22
Ramachandran outliers		3.1%
Sidechain outliers		6.4%

Worse   *Better*

▮ Percentile relative to all structures

▯ Percentile relative to all NMR structures

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	B	27	44% 33% • 19%
2	A	24	79% 21%

2   Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 11 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	B:6-B:27, A:1-A:24 (46)	0.22	11

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

3 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 760 atoms, of which 378 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Relaxin 3 (Prorelaxin H3) (Insulin-like peptide INSL7) (Insulin-like peptide 7).

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	B	27	429	136	215	43	33	2	0

- Molecule 2 is a protein called Relaxin 3 (Prorelaxin H3) (Insulin-like peptide INSL7) (Insulin-like peptide 7).

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	A	24	331	101	163	27	36	4	0

W O R L D W I D E
PDB
PROTEIN DATA BANK

4 Residue-property plots ⓘ

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: Relaxin 3 (Prorelaxin H3) (Insulin-like peptide INSL7) (Insulin-like peptide 7)
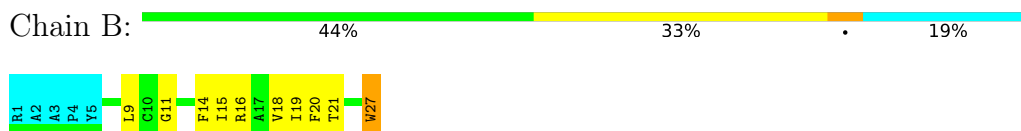
Chain B:

• Molecule 2: Relaxin 3 (Prorelaxin H3) (Insulin-like peptide INSL7) (Insulin-like peptide 7)
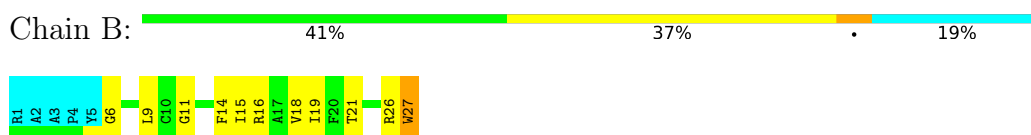
Chain A:
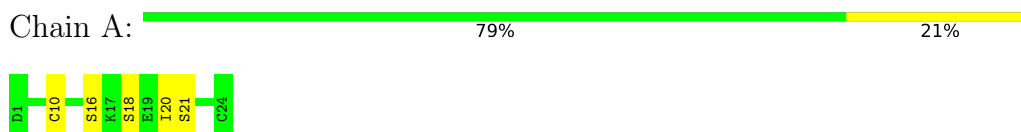
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Relaxin 3 (Prorelaxin H3) (Insulin-like peptide INSL7) (Insulin-like peptide 7)
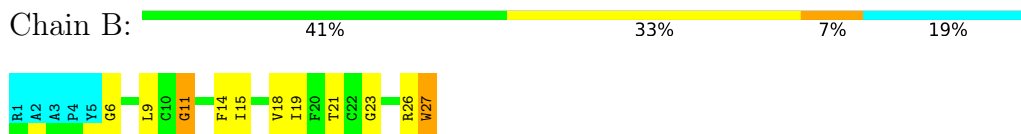
Chain B:

• Molecule 2: Relaxin 3 (Prorelaxin H3) (Insulin-like peptide INSL7) (Insulin-like peptide 7)

Chain A:

4.2.2 Score per residue for model 2

• Molecule 1: Relaxin 3 (Prorelaxin H3) (Insulin-like peptide INSL7) (Insulin-like peptide 7)

Chain B:

• Molecule 2: Relaxin 3 (Prorelaxin H3) (Insulin-like peptide INSL7) (Insulin-like peptide 7)
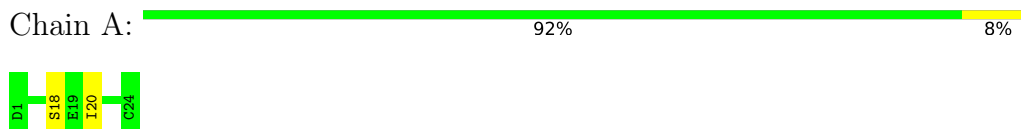
Chain A:

4.2.3 Score per residue for model 3

• Molecule 1: Relaxin 3 (Prorelaxin H3) (Insulin-like peptide INSL7) (Insulin-like peptide 7)

Chain B:
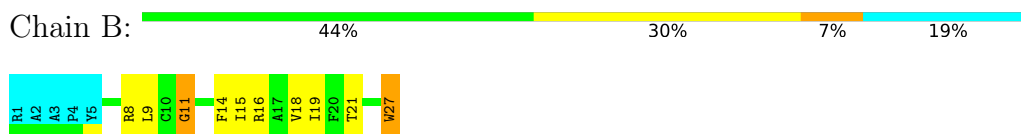

• Molecule 2: Relaxin 3 (Prorelaxin H3) (Insulin-like peptide INSL7) (Insulin-like peptide 7)

Chain A:

4.2.4 Score per residue for model 4

• Molecule 1: Relaxin 3 (Prorelaxin H3) (Insulin-like peptide INSL7) (Insulin-like peptide 7)

Chain B:

• Molecule 2: Relaxin 3 (Prorelaxin H3) (Insulin-like peptide INSL7) (Insulin-like peptide 7)

Chain A:

4.2.5　Score per residue for model 5

• Molecule 1: Relaxin 3 (Prorelaxin H3) (Insulin-like peptide INSL7) (Insulin-like peptide 7)

Chain B:

• Molecule 2: Relaxin 3 (Prorelaxin H3) (Insulin-like peptide INSL7) (Insulin-like peptide 7)
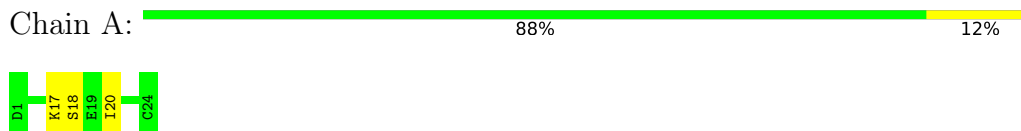
Chain A:

4.2.6　Score per residue for model 6

• Molecule 1: Relaxin 3 (Prorelaxin H3) (Insulin-like peptide INSL7) (Insulin-like peptide 7)

Chain B:

• Molecule 2: Relaxin 3 (Prorelaxin H3) (Insulin-like peptide INSL7) (Insulin-like peptide 7)

Chain A:

4.2.7　Score per residue for model 7

• Molecule 1: Relaxin 3 (Prorelaxin H3) (Insulin-like peptide INSL7) (Insulin-like peptide 7)

Chain B:

• Molecule 2: Relaxin 3 (Prorelaxin H3) (Insulin-like peptide INSL7) (Insulin-like peptide 7)

Chain A:

4.2.8　Score per residue for model 8

• Molecule 1: Relaxin 3 (Prorelaxin H3) (Insulin-like peptide INSL7) (Insulin-like peptide 7)

Chain B:

• Molecule 2: Relaxin 3 (Prorelaxin H3) (Insulin-like peptide INSL7) (Insulin-like peptide 7)

Chain A:

4.2.9　Score per residue for model 9

• Molecule 1: Relaxin 3 (Prorelaxin H3) (Insulin-like peptide INSL7) (Insulin-like peptide 7)

Chain B:
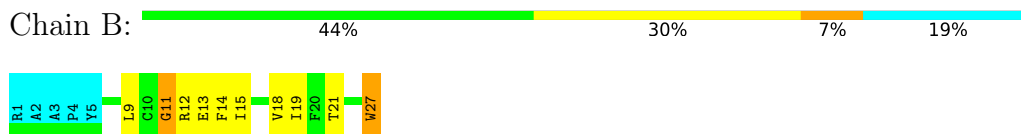

• Molecule 2: Relaxin 3 (Prorelaxin H3) (Insulin-like peptide INSL7) (Insulin-like peptide 7)

Chain A:

4.2.10　Score per residue for model 10

• Molecule 1: Relaxin 3 (Prorelaxin H3) (Insulin-like peptide INSL7) (Insulin-like peptide 7)

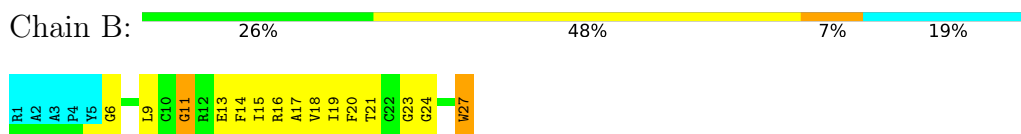Chain B:

• Molecule 2: Relaxin 3 (Prorelaxin H3) (Insulin-like peptide INSL7) (Insulin-like peptide 7)

Chain A:

4.2.11 Score per residue for model 11 (medoid)

• Molecule 1: Relaxin 3 (Prorelaxin H3) (Insulin-like peptide INSL7) (Insulin-like peptide 7)

Chain B:

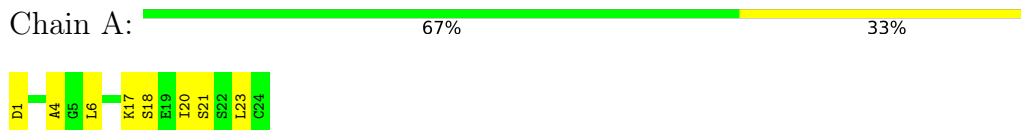• Molecule 2: Relaxin 3 (Prorelaxin H3) (Insulin-like peptide INSL7) (Insulin-like peptide 7)

Chain A:

4.2.12 Score per residue for model 12

• Molecule 1: Relaxin 3 (Prorelaxin H3) (Insulin-like peptide INSL7) (Insulin-like peptide 7)

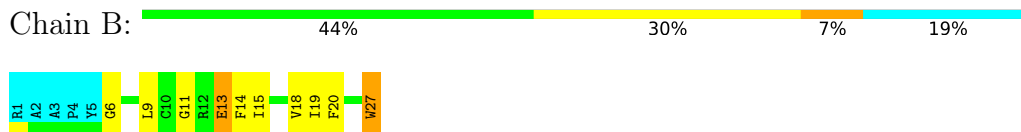Chain B:

• Molecule 2: Relaxin 3 (Prorelaxin H3) (Insulin-like peptide INSL7) (Insulin-like peptide 7)

Chain A:

4.2.13 Score per residue for model 13

• Molecule 1: Relaxin 3 (Prorelaxin H3) (Insulin-like peptide INSL7) (Insulin-like peptide 7)

Chain B:

• Molecule 2: Relaxin 3 (Prorelaxin H3) (Insulin-like peptide INSL7) (Insulin-like peptide 7)

Chain A:

4.2.14 Score per residue for model 14

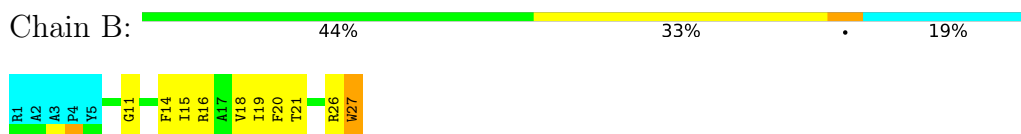• Molecule 1: Relaxin 3 (Prorelaxin H3) (Insulin-like peptide INSL7) (Insulin-like peptide 7)

Chain B:

• Molecule 2: Relaxin 3 (Prorelaxin H3) (Insulin-like peptide INSL7) (Insulin-like peptide 7)

Chain A:

4.2.15 Score per residue for model 15

• Molecule 1: Relaxin 3 (Prorelaxin H3) (Insulin-like peptide INSL7) (Insulin-like peptide 7)

Chain B:

• Molecule 2: Relaxin 3 (Prorelaxin H3) (Insulin-like peptide INSL7) (Insulin-like peptide 7)

Chain A:
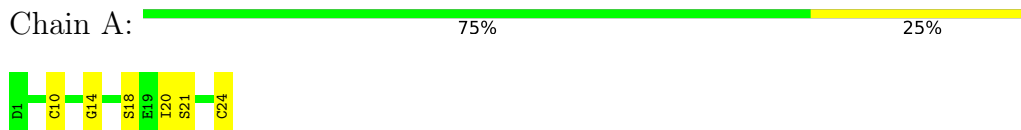
4.2.16 Score per residue for model 16

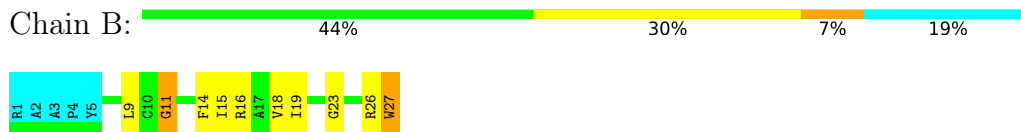• Molecule 1: Relaxin 3 (Prorelaxin H3) (Insulin-like peptide INSL7) (Insulin-like peptide 7)
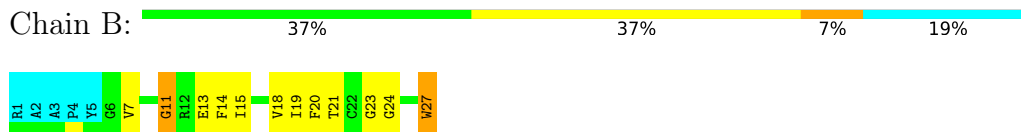
Chain B:

• Molecule 2: Relaxin 3 (Prorelaxin H3) (Insulin-like peptide INSL7) (Insulin-like peptide 7)

Chain A:
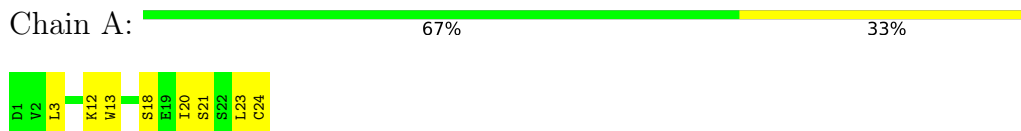
4.2.17 Score per residue for model 17

• Molecule 1: Relaxin 3 (Prorelaxin H3) (Insulin-like peptide INSL7) (Insulin-like peptide 7)

Chain B:

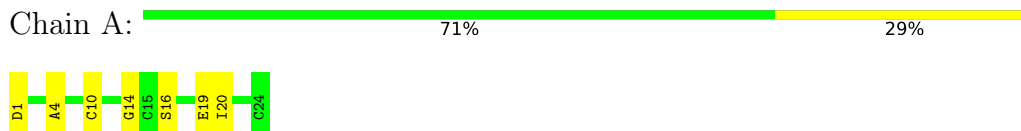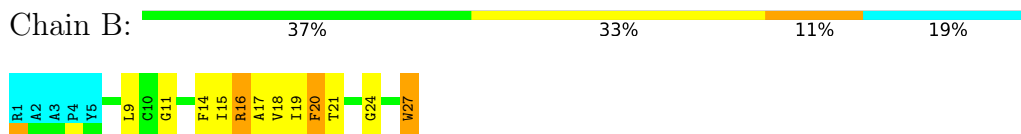• Molecule 2: Relaxin 3 (Prorelaxin H3) (Insulin-like peptide INSL7) (Insulin-like peptide 7)

Chain A:
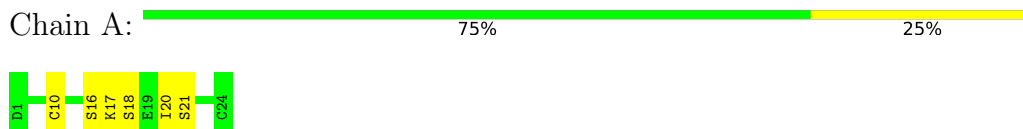
4.2.18 Score per residue for model 18

• Molecule 1: Relaxin 3 (Prorelaxin H3) (Insulin-like peptide INSL7) (Insulin-like peptide 7)
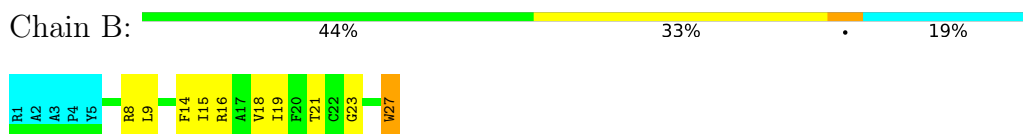
Chain B:

• Molecule 2: Relaxin 3 (Prorelaxin H3) (Insulin-like peptide INSL7) (Insulin-like peptide 7)

Chain A:
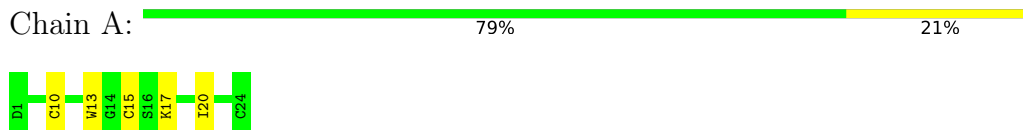
4.2.19 Score per residue for model 19

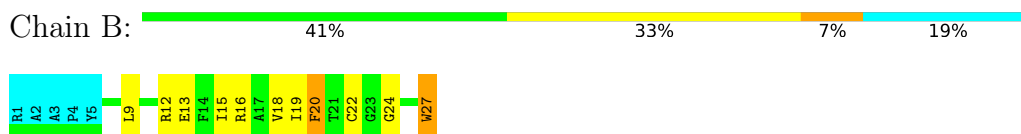• Molecule 1: Relaxin 3 (Prorelaxin H3) (Insulin-like peptide INSL7) (Insulin-like peptide 7)

Chain B:

• Molecule 2: Relaxin 3 (Prorelaxin H3) (Insulin-like peptide INSL7) (Insulin-like peptide 7)
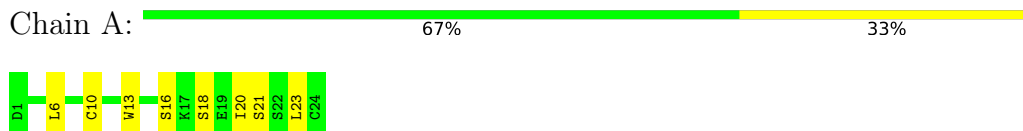
Chain A:

4.2.20 Score per residue for model 20

• Molecule 1: Relaxin 3 (Prorelaxin H3) (Insulin-like peptide INSL7) (Insulin-like peptide 7)

Chain B:

• Molecule 2: Relaxin 3 (Prorelaxin H3) (Insulin-like peptide INSL7) (Insulin-like peptide 7)

Chain A:

5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: *Structures were calculated using torsion angle dynamics and further refined using Cartesian dynamics in explicit solvent.*.

Of the 50 calculated structures, 20 were deposited, based on the following criterion: *structures with the least restraint violations,structures with the lowest energy.*

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

Software name	Classification	Version
CYANA	structure solution	1.0
CNS	structure solution	1.1
CNS	refinement	1.1

No chemical shift data was provided.

6 Model quality ⓘ

6.1 Standard geometry ⓘ

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 ⓘ

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	B	174	174	174	12±2
2	A	168	163	163	6±2
All	All	6840	6740	6740	294

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 22.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:B:9:LEU:HB2	2:A:10:CYS:HB3	0.76	1.57	17	7
1:B:19:ILE:HD12	1:B:27:TRP:CD1	0.76	2.15	2	20
1:B:21:THR:HG21	2:A:20:ILE:HB	0.71	1.61	9	7
1:B:18:VAL:HA	2:A:20:ILE:HG22	0.65	1.65	12	18
1:B:19:ILE:HG23	1:B:27:TRP:HD1	0.63	1.54	7	19
1:B:7:VAL:HG22	1:B:8:ARG:H	0.62	1.54	20	1
1:B:12:ARG:HB2	1:B:12:ARG:NH1	0.60	2.11	11	1
2:A:6:LEU:HD23	2:A:23:LEU:HD11	0.59	1.74	1	3
1:B:21:THR:HG22	2:A:17:LYS:HG2	0.59	1.74	9	3
2:A:6:LEU:HD12	2:A:23:LEU:HD11	0.59	1.74	8	2
1:B:19:ILE:HG23	1:B:27:TRP:CD1	0.57	2.33	16	16
1:B:14:PHE:O	1:B:18:VAL:HG23	0.57	1.99	17	19
1:B:16:ARG:CZ	1:B:19:ILE:HG13	0.57	2.29	5	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
2:A:2:VAL:O	2:A:6:LEU:HG	0.55	2.00	10	3
1:B:15:ILE:O	1:B:19:ILE:HG12	0.54	2.03	18	20
1:B:27:TRP:CD1	1:B:27:TRP:N	0.52	2.78	18	20
2:A:10:CYS:O	2:A:14:GLY:HA2	0.51	2.06	14	8
1:B:16:ARG:NH2	1:B:19:ILE:HG13	0.51	2.21	14	3
2:A:16:SER:HB2	2:A:19:GLU:OE1	0.51	2.06	13	8
2:A:21:SER:HA	2:A:24:CYS:SG	0.51	2.45	15	3
1:B:9:LEU:HB3	1:B:14:PHE:HA	0.50	1.83	10	10
1:B:21:THR:HG22	2:A:17:LYS:HG3	0.50	1.84	18	2
1:B:18:VAL:HA	2:A:20:ILE:CG2	0.49	2.37	6	15
1:B:20:PHE:HA	1:B:24:GLY:HA2	0.49	1.84	5	5
1:B:21:THR:HB	2:A:21:SER:OG	0.47	2.10	12	8
2:A:3:LEU:HD23	2:A:23:LEU:HD13	0.46	1.86	16	1
1:B:9:LEU:HD12	1:B:13:GLU:HG3	0.46	1.86	8	1
2:A:16:SER:HB3	2:A:19:GLU:OE1	0.45	2.10	10	1
1:B:26:ARG:HA	1:B:26:ARG:NE	0.45	2.26	13	1
1:B:16:ARG:NH1	1:B:19:ILE:HG21	0.45	2.27	15	1
1:B:11:GLY:O	1:B:14:PHE:HB3	0.44	2.12	11	12
2:A:1:ASP:OD1	2:A:4:ALA:HB3	0.44	2.13	6	9
1:B:26:ARG:NH1	2:A:24:CYS:HB3	0.44	2.28	12	2
2:A:12:LYS:HD2	2:A:13:TRP:CE2	0.44	2.48	7	3
2:A:6:LEU:HG	2:A:10:CYS:SG	0.44	2.52	19	1
2:A:16:SER:O	2:A:20:ILE:HG13	0.44	2.13	1	10
1:B:12:ARG:O	1:B:12:ARG:HD2	0.43	2.14	8	1
2:A:17:LYS:HD3	2:A:21:SER:OG	0.43	2.14	9	2
1:B:9:LEU:HD23	2:A:15:CYS:SG	0.43	2.52	18	1
1:B:8:ARG:HG2	2:A:13:TRP:O	0.43	2.13	18	4
1:B:9:LEU:HD23	1:B:14:PHE:HA	0.43	1.90	17	1
1:B:9:LEU:HD12	1:B:13:GLU:HB3	0.42	1.90	9	2
1:B:17:ALA:HB1	2:A:20:ILE:HD13	0.42	1.91	9	1
1:B:20:PHE:HA	1:B:24:GLY:CA	0.42	2.45	9	1
1:B:16:ARG:HA	1:B:16:ARG:HD2	0.42	1.59	6	1
1:B:12:ARG:HB2	1:B:12:ARG:CZ	0.42	2.44	11	1
1:B:6:GLY:H	2:A:16:SER:HA	0.41	1.75	10	1
2:A:12:LYS:HG2	2:A:13:TRP:CD1	0.41	2.51	3	1
1:B:12:ARG:HG3	1:B:13:GLU:N	0.40	2.31	15	1
1:B:18:VAL:O	1:B:22:CYS:SG	0.40	2.80	15	1
1:B:16:ARG:NH1	1:B:19:ILE:HG13	0.40	2.31	6	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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	B	21/27 (78%)	17±1 (79±4%)	3±1 (14±5%)	1±1 (6±5%)	3	19
2	A	22/24 (92%)	22±1 (98±3%)	0±1 (2±3%)	0±0 (0±0%)	100	100
All	All	860/1020 (84%)	763 (89%)	70 (8%)	27 (3%)	7	39

All 5 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	B	11	GLY	13
1	B	23	GLY	7
1	B	6	GLY	5
1	B	26	ARG	1
1	B	7	VAL	1

6.3.2 Protein sidechains ⓘ

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	B	17/20 (85%)	16±1 (91±4%)	2±1 (9±4%)	13	60
2	A	21/21 (100%)	20±0 (95±2%)	1±0 (5±2%)	31	80
All	All	760/820 (93%)	711 (94%)	49 (6%)	21	70

All 6 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	B	27	TRP	20
2	A	18	SER	18

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Mol	Chain	Res	Type	Models (Total)
1	B	20	PHE	7
1	B	13	GLU	2
2	A	1	ASP	1
1	B	16	ARG	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.6 Ligand geometry ⓘ

There are no ligands in this entry.

6.7 Other polymers ⓘ

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation ⓘ

No chemical shift data were provided