Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	1Y76
Title	:	Solution Structure of Patj/Pals1 L27 Domain Complex
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Deposited on	:	2004-12-08

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

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

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

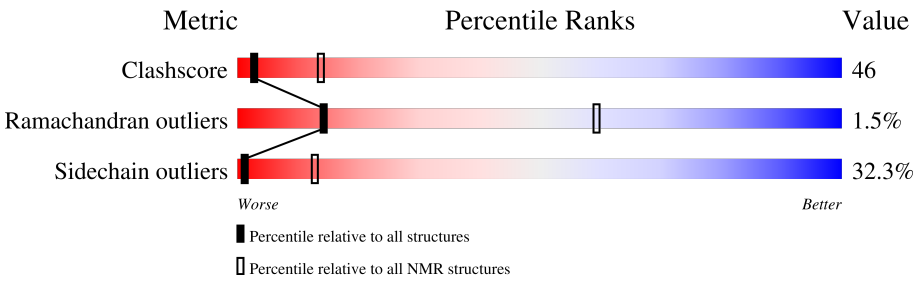
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

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	62	37% 47% 6% 10%
1	C	62	34% 47% 8% 11%
2	B	60	25% 52% 15% 8%
2	D	60	22% 53% 13% 12%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 19 is the overall representative, medoid model (most similar to other models). The authors have identified model 10 as representative, based on the following criterion: *minimized average structure*.

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:7-A:62, B:82-B:136, C:7-C:61, D:83-D:135 (219)	0.36	19

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 2 single-model clusters were found.

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 3984 atoms, of which 2030 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called protein associated to tight junctions.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	62	1017	312	522	87	95	1	0
1	C	62	1017	312	522	87	95	1	0

- Molecule 2 is a protein called MAGUK p55 subfamily member 5.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	B	60	975	305	493	83	93	1	0
2	D	60	975	305	493	83	93	1	0

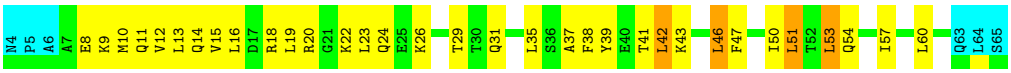
4 Residue-property plots (i)

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.

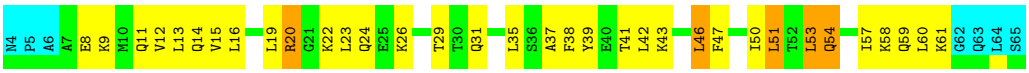
• Molecule 1: protein associated to tight junctions

Chain A: 37% 47% 6% 10%



• Molecule 1: protein associated to tight junctions

Chain C: 34% 47% 8% 11%



• Molecule 2: MAGUK p55 subfamily member 5

Chain B: 25% 52% 15% 8%

• Molecule 2: MAGUK p55 subfamily member 5

Chain D: 22% 53% 13% 12%

4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

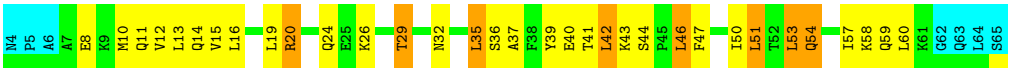
4.2.1 Score per residue for model 1

- Molecule 1: protein associated to tight junctions

Chain A: 32% 47% 11% 10%

- Molecule 1: protein associated to tight junctions

Chain C: 35% 40% 13% 11%



- Molecule 2: MAGUK p55 subfamily member 5

Chain B: 27% 47% 17% • 8%

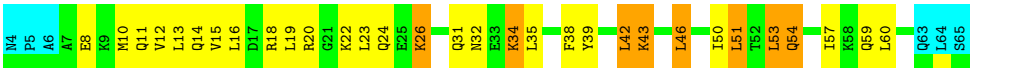
- Molecule 2: MAGUK p55 subfamily member 5

Chain D: 23% 52% 12% • 12%

4.2.2 Score per residue for model 2

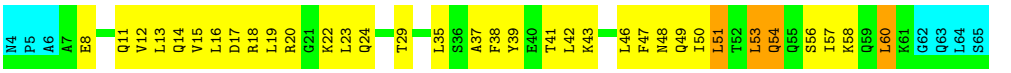
- Molecule 1: protein associated to tight junctions

Chain A: 40% 37% 13% 10%



- Molecule 1: protein associated to tight junctions

Chain C: 34% 48% 6% 11%

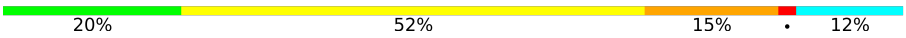


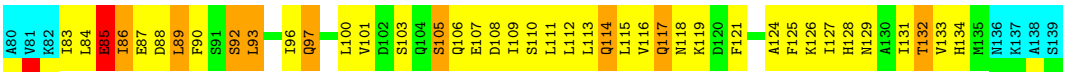
- Molecule 2: MAGUK p55 subfamily member 5

Chain B: 23% 50% 18% 8%

• Molecule 2: MAGUK p55 subfamily member 5

Chain D:

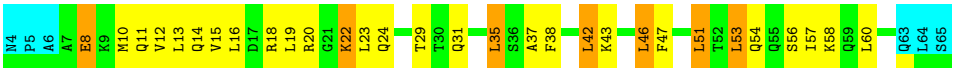




4.2.3 Score per residue for model 3

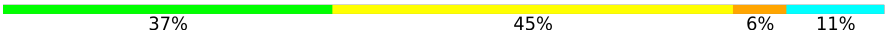
• Molecule 1: protein associated to tight junctions

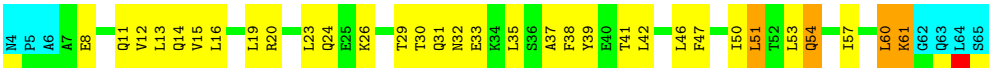
Chain A:



• Molecule 1: protein associated to tight junctions

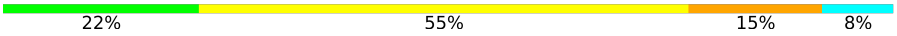
Chain C:

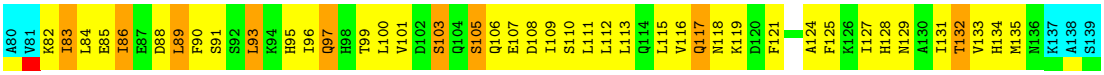




• Molecule 2: MAGUK p55 subfamily member 5

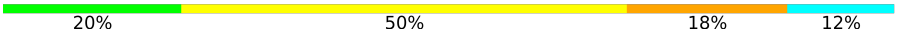
Chain B:





• Molecule 2: MAGUK p55 subfamily member 5

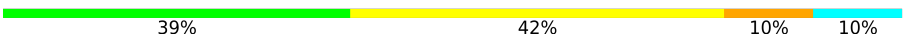
Chain D:

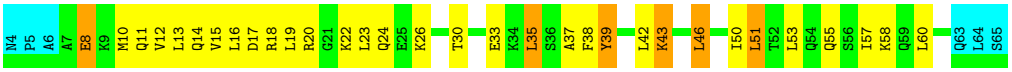


4.2.4 Score per residue for model 4

• Molecule 1: protein associated to tight junctions

Chain A:





- Molecule 1: protein associated to tight junctions

Chain C: 37% 44% 8% 11%

N4 P5 A6 A7 E8 K9 M10 Q11 V12 L13 Q14 V15 L16 L19 R20 Q24 E25 K26 T29 T30 Q31 N32 L35 S36 A37 F38 Y39 E40 T41 L42 L46 F47 I50 L51 T52 L53 Q54 I57 K58 Q59 L60 K61 G62 Q63 L64 S65

- Molecule 2: MAGUK p55 subfamily member 5

Chain B: 27% 48% 17% 8%

A80 V81 K82 I83 L84 E85 I86 E87 D88 L89 F90 S91 S92 L93 I96 Q97 L100 V101 D102 S103 Q104 S105 Q106 E107 D108 I109 S110 L111 L112 L113 Q114 L115 V116 Q117 N118 K119 D120 F121 A124 F125 K126 I127 H128 N129 A130 I131 T132 V133 K137 A138 S139

- Molecule 2: MAGUK p55 subfamily member 5

Chain D: 20% 48% 18% • 12%

A80 V81 K82 I83 L84 E85 I86 E87 D88 L89 F90 L93 K94 H95 I96 Q97 H98 T99 L100 V101 D102 S103 Q104 S105 D108 I109 S110 L111 L112 L113 Q114 L115 V116 Q117 N118 K119 D120 F121 Q122 N123 A124 F125 K126 I127 H128 N129 A130 I131 T132 V133 H134 M135 N136 K137 A138 S139

4.2.5 Score per residue for model 5

- Molecule 1: protein associated to tight junctions

Chain A: 29% 48% 13% 10%

N4 P5 A6 A7 E8 K9 M10 Q11 V12 L13 Q14 V15 L16 D17 R18 L19 R20 G21 K22 L23 Q24 E25 K26 T29 N32 A37 F38 Y39 E40 T41 L42 K43 L46 F47 N48 Q49 I50 L51 T52 L53 Q54 Q55 S56 I57 K58 Q59 L60 K61 G62 Q63 L64 S65

- Molecule 1: protein associated to tight junctions

Chain C: 32% 45% 11% 11%

N4 P5 A6 A7 E8 K9 M10 Q11 V12 L13 Q14 V15 L16 L19 R20 G21 K22 L23 Q24 E25 K26 T29 T30 Q31 N32 L35 S36 A37 F38 Y39 E40 T41 L42 K43 S44 P45 L46 F47 N48 Q49 I50 L51 T52 L53 Q54 I57 K58 Q59 L60 K61 G62 Q63 L64 S65

- Molecule 2: MAGUK p55 subfamily member 5

Chain B: 13% 57% 22% 8%

A80 V81 K82 I83 L84 E85 I86 E87 D88 L89 F90 S91 S92 L93 K94 H95 I96 Q97 H98 T99 L100 V101 D102 S103 Q104 S105 Q106 E107 D108 I109 S110 L111 L112 L113 Q114 L115 V116 Q117 N118 K119 D120 F121 Q122 N123 A124 F125 K126 I127 H128 N129 A130 I131 T132 V133 H134 M135 N136 K137 A138 S139

- Molecule 2: MAGUK p55 subfamily member 5

Chain D: 22% 48% 17% • 12%

A80 V81 K82 I83 L84 E85 I86 E87 D88 L89 F90 L93 K94 H95 I96 Q97 H98 T99 L100 V101 D102 S103 Q104 S105 Q106 E107 D108 I109 S110 L111 L112 L113 Q114 L115 V116 Q117 D120 F121 A124 F125 K126 I127 H128 N129 A130 I131 T132 V133 N136 K137 A138 S139

4.2.6 Score per residue for model 6

- Molecule 1: protein associated to tight junctions

Chain A: 31% 45% 15% 10%

- Molecule 1: protein associated to tight junctions

Chain C: 40% 44% 5% 11%

- Molecule 2: MAGUK p55 subfamily member 5

Chain B: 22% 53% 15% • 8%

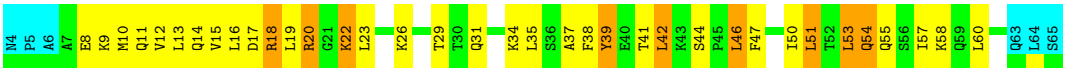
- Molecule 2: MAGUK p55 subfamily member 5

Chain D: 23% 48% 17% 12%

4.2.7 Score per residue for model 7

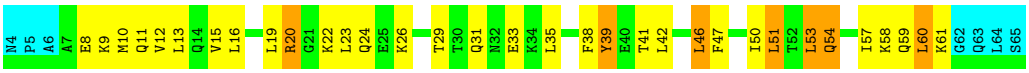
- Molecule 1: protein associated to tight junctions

Chain A: 32% 44% 15% 10%



- Molecule 1: protein associated to tight junctions

Chain C: 35% 42% 11% 11%

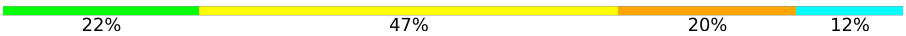


- Molecule 2: MAGUK p55 subfamily member 5

Chain B: 25% 48% 17% • 8%

• Molecule 2: MAGUK p55 subfamily member 5

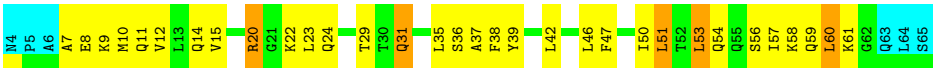
Chain D:



4.2.8 Score per residue for model 8

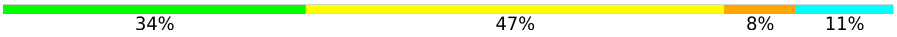
• Molecule 1: protein associated to tight junctions

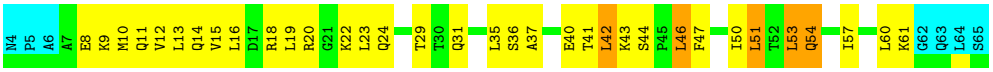
Chain A:



• Molecule 1: protein associated to tight junctions

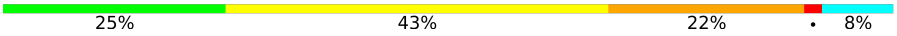
Chain C:

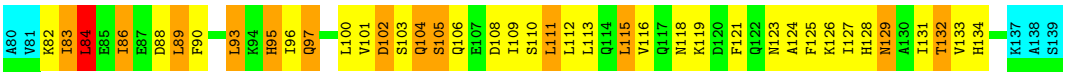




• Molecule 2: MAGUK p55 subfamily member 5

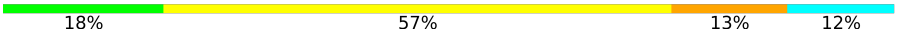
Chain B:





• Molecule 2: MAGUK p55 subfamily member 5

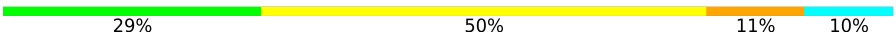
Chain D:

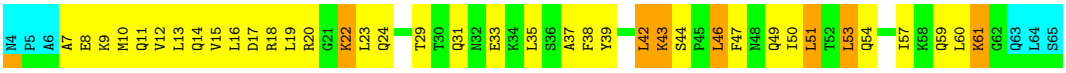


4.2.9 Score per residue for model 9

• Molecule 1: protein associated to tight junctions

Chain A:





• Molecule 1: protein associated to tight junctions

Chain C: 32% 47% 10% 11%

N4 P5 A6 A7 E8 K9 M10 Q11 V12 L13 Q14 V15 L16 D17 R18 L19 R20 G21 K22 L23 Q24 T29 N32 L35 S36 A37 F38 Y39 E40 T41 L42 K43 L46 F47 I50 L51 T52 L53 Q54 Q55 S56 I57 K58 Q59 L60 K61 G62 Q63 L64 S65

• Molecule 2: MAGUK p55 subfamily member 5

Chain B: 22% 55% 15% 8%

A80 V81 K82 I83 L84 E85 I86 E87 D88 L89 F90 S91 S92 L93 K94 H95 I96 Q97 H98 T99 L100 V101 D102 S103 Q104 S105 Q106 E107 D108 I109 S110 L111 L112 L113 Q114 L115 V116 Q117 N118 K119 D120 F121 Q122 N123 A124 F125 K126 I127 H128 N129 A130 I131 T132 V133 K137 A138 S139

• Molecule 2: MAGUK p55 subfamily member 5

Chain D: 17% 58% 13% 12%

A80 V81 K82 I83 L84 E85 I86 E87 D88 L89 F90 L93 K94 H95 I96 Q97 H98 T99 L100 V101 D102 S103 Q104 S105 Q106 E107 D108 I109 S110 L111 L112 L113 Q114 L115 V116 Q117 N118 K119 D120 F121 Q122 N123 A124 F125 K126 I127 H128 N129 A130 I131 T132 V133 N136 K137 A138 S139

4.2.10 Score per residue for model 10

• Molecule 1: protein associated to tight junctions

Chain A: 39% 37% 15% 10%

N4 P5 A6 A7 E8 Q11 V12 L13 Q14 V15 L16 D17 R18 L19 R20 G21 K22 L23 Q24 T29 T30 Q31 N32 E33 K34 L35 S36 A37 F38 Y39 L42 K43 L46 F47 I50 L51 T52 L53 Q54 I57 L60 Q63 L64 S65

• Molecule 1: protein associated to tight junctions

Chain C: 35% 40% 13% 11%

N4 P5 A6 A7 E8 Q11 V12 L13 Q14 V15 L16 D17 R18 L19 R20 G21 K22 L23 Q24 T29 T30 Q31 K34 L35 S36 A37 F38 Y39 E40 T41 L42 K43 L46 F47 I50 L51 T52 L53 Q54 Q55 S56 I57 L60 K61 G62 Q63 L64 S65

• Molecule 2: MAGUK p55 subfamily member 5

Chain B: 28% 50% 13% 8%

A80 V81 K82 I83 L84 E85 I86 L89 F90 S91 S92 L93 K94 H95 I96 Q97 H98 T99 L100 V101 Q104 S105 D108 I109 S110 L111 L112 L113 Q114 L115 V116 Q117 N118 K119 D120 F121 Q122 N123 A124 F125 K126 I127 H128 N129 A130 I131 T132 V133 K137 A138 S139

• Molecule 2: MAGUK p55 subfamily member 5

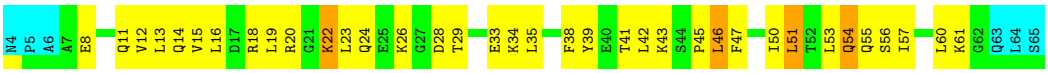
Chain D: 25% 40% 23% 12%

A80 V81 K82 I83 L84 E85 I86 E87 D88 L89 F90 L93 K94 H95 I96 Q97 L100 V101 D102 S103 Q104 S105 Q106 E107 D108 I109 S110 L111 L112 L113 Q114 L115 V116 Q117 N118 K119 D120 F121 A124 F125 K126 I127 H128 N129 A130 I131 T132 V133 N136 K137 A138 S139

4.2.11 Score per residue for model 11

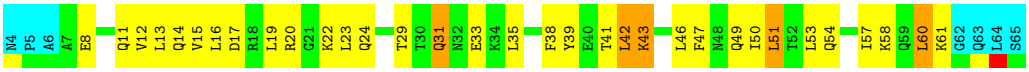
- Molecule 1: protein associated to tight junctions

Chain A: 32% 52% 6% 10%



- Molecule 1: protein associated to tight junctions

Chain C: 35% 45% 8% 11%

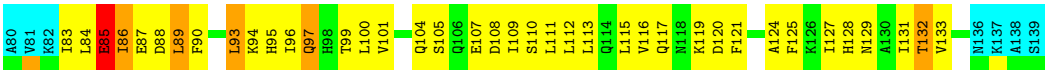


- Molecule 2: MAGUK p55 subfamily member 5

Chain B: 18% 50% 23% 8%

- Molecule 2: MAGUK p55 subfamily member 5

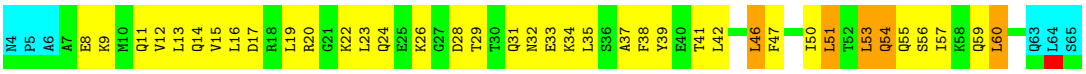
Chain D: 23% 55% 8% • 12%



4.2.12 Score per residue for model 12

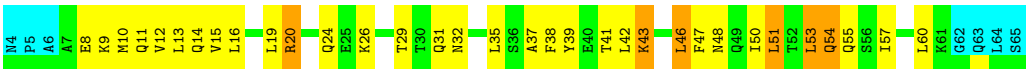
- Molecule 1: protein associated to tight junctions

Chain A: 29% 53% 8% 10%



- Molecule 1: protein associated to tight junctions

Chain C: 35% 44% 10% 11%



- Molecule 2: MAGUK p55 subfamily member 5

Chain B: 28% 47% 15% • 8%

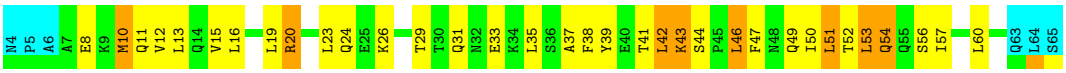
• Molecule 2: MAGUK p55 subfamily member 5

Chain D: 20% 50% 18% 12%

4.2.13 Score per residue for model 13

• Molecule 1: protein associated to tight junctions

Chain A: 35% 42% 13% 10%



• Molecule 1: protein associated to tight junctions

Chain C: 34% 47% 8% 11%

• Molecule 2: MAGUK p55 subfamily member 5

Chain B: 32% 42% 18% 8%

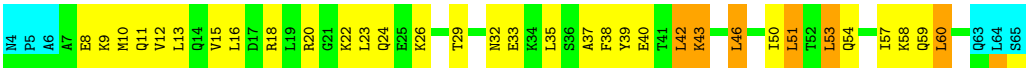
• Molecule 2: MAGUK p55 subfamily member 5

Chain D: 20% 58% 10% 12%

4.2.14 Score per residue for model 14

• Molecule 1: protein associated to tight junctions

Chain A: 37% 44% 10% 10%



• Molecule 1: protein associated to tight junctions

Chain C: 31% 50% 8% 11%

N4 P5 A6 A7 E8 K9 M10 Q11 V12 L13 Q14 V15 L16 D17 R18 L19 R20 G21 K22 L23 Q24 E25 K26 T29 T30 Q31 N32 L35 S36 A37 F38 Y39 E40 T41 L42 K43 L46 F47 N48 Q49 I50 L51 T52 L53 Q54 I57 K58 Q59 L60 K61 G62 Q63 L64 S65

• Molecule 2: MAGUK p55 subfamily member 5

Chain B: 22% 55% 15% 8%

A80 V81 K82 I83 L84 E85 I86 E87 D88 L89 F90 S91 S92 L93 I96 Q97 H98 T99 L100 V101 D102 S103 Q104 S105 Q106 E107 D108 I109 S110 L111 L112 L113 Q114 L115 V116 Q117 N118 K119 D120 F121 Q122 N123 A124 F125 K126 I127 H128 N129 A130 I131 T132 V133 K137 A138 S139

• Molecule 2: MAGUK p55 subfamily member 5

Chain D: 18% 53% 15% • 12%

A80 V81 K82 I83 L84 E85 I86 L89 F90 S91 S92 L93 K94 H95 I96 Q97 L100 V101 D102 S103 Q104 S105 Q106 E107 D108 I109 S110 L111 L112 L113 Q114 L115 V116 Q117 N118 K119 D120 F121 Q122 N123 A124 F125 K126 I127 H128 N129 A130 I131 T132 V133 H134 M135 N136 K137 A138 S139

4.2.15 Score per residue for model 15

• Molecule 1: protein associated to tight junctions

Chain A: 35% 47% 8% 10%

N4 P5 A6 A7 E8 K9 M10 Q11 V12 L13 Q14 V15 L16 D17 R18 L19 R20 G21 K22 L23 K26 T29 T30 Q31 N32 E33 K34 L35 F38 Y39 E40 T41 L42 K43 L46 F47 I50 L51 T52 L53 Q54 I57 L60 K61 G62 Q63 L64 S65

• Molecule 1: protein associated to tight junctions

Chain C: 32% 44% 13% 11%

N4 P5 A6 A7 E8 K9 M10 Q11 V12 L13 Q14 V15 L16 L19 R20 G21 K22 L23 Q24 E25 K26 T29 T30 Q31 N32 L35 S36 A37 F38 Y39 L42 K43 L46 F47 I50 L51 T52 L53 Q54 I57 K58 Q59 L60 K61 G62 Q63 L64 S65

• Molecule 2: MAGUK p55 subfamily member 5

Chain B: 20% 50% 22% 8%

A80 V81 K82 I83 L84 E85 I86 L89 F90 L93 I96 Q97 H98 T99 L100 V101 D102 S103 Q104 S105 Q106 E107 D108 I109 S110 L111 L112 L113 Q114 L115 V116 Q117 N118 K119 D120 F121 Q122 N123 A124 F125 K126 I127 H128 N129 A130 I131 T132 V133 H134 K137 A138 S139

• Molecule 2: MAGUK p55 subfamily member 5

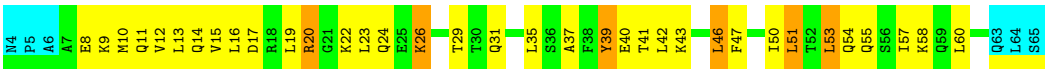
Chain D: 22% 50% 15% • 12%

A80 V81 K82 I83 L84 E85 I86 E87 D88 L89 F90 S91 S92 L93 I96 Q97 L100 V101 D102 S103 Q104 S105 Q106 E107 D108 I109 S110 L111 L112 L113 Q114 L115 V116 Q117 N118 K119 D120 F121 A124 F125 K126 I127 H128 N129 A130 I131 T132 V133 H134 M135 N136 K137 A138 S139

4.2.16 Score per residue for model 16

- Molecule 1: protein associated to tight junctions

Chain A: 34% 47% 10% 10%



- Molecule 1: protein associated to tight junctions

Chain C: 35% 42% 11% 11%

- Molecule 2: MAGUK p55 subfamily member 5

Chain B: 32% 47% 12% • 8%

- Molecule 2: MAGUK p55 subfamily member 5

Chain D: 20% 55% 13% 12%

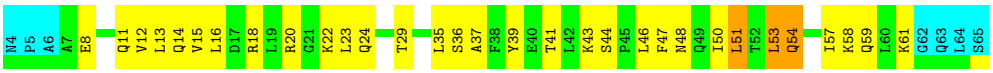
4.2.17 Score per residue for model 17

- Molecule 1: protein associated to tight junctions

Chain A: 35% 50% 5% 10%

- Molecule 1: protein associated to tight junctions

Chain C: 39% 45% 5% 11%

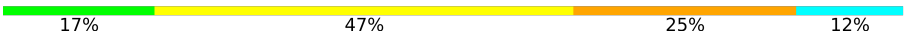


- Molecule 2: MAGUK p55 subfamily member 5

Chain B: 25% 53% 13% 8%

• Molecule 2: MAGUK p55 subfamily member 5

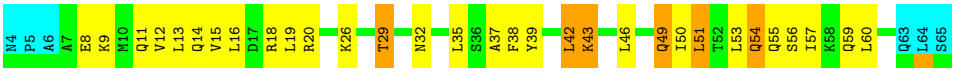
Chain D:



4.2.18 Score per residue for model 18

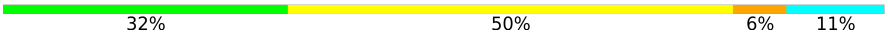
• Molecule 1: protein associated to tight junctions

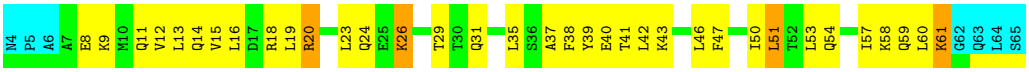
Chain A:



• Molecule 1: protein associated to tight junctions

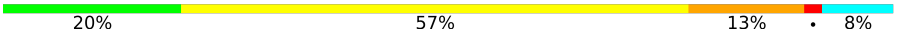
Chain C:

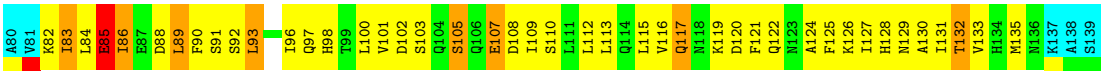




• Molecule 2: MAGUK p55 subfamily member 5

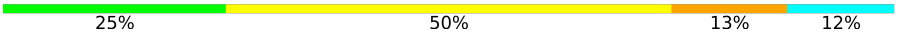
Chain B:

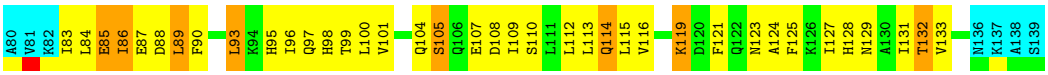




• Molecule 2: MAGUK p55 subfamily member 5

Chain D:

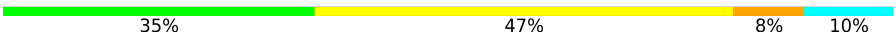


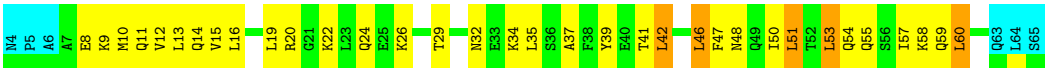


4.2.19 Score per residue for model 19 (medoid)

• Molecule 1: protein associated to tight junctions

Chain A:





• Molecule 1: protein associated to tight junctions

Chain C: 37% 44% 8% 11%

N4 P5 A6 A7 E8 K9 M10 Q11 V12 L13 Q14 V15 L16 D17 R18 L19 R20 G21 K22 L23 Q24 T29 T30 Q31 L35 S36 A37 F38 Y39 L42 K43 L46 F47 I50 L51 T52 L53 Q54 Q55 S56 I57 K58 Q59 L60 K61 G62 Q63 L64 S65

• Molecule 2: MAGUK p55 subfamily member 5

Chain B: 28% 47% 15% • 8%

A80 V81 K82 I83 L84 E85 I86 E87 D88 L89 F90 S91 S92 L93 I96 Q97 L100 V101 D102 S103 Q104 S105 Q106 E107 D108 I109 S110 L111 L112 L113 Q114 L115 V116 Q117 N118 K119 D120 F121 A124 F125 K126 I127 H128 N129 A130 I131 T132 V133 H134 K137 A138 S139

• Molecule 2: MAGUK p55 subfamily member 5

Chain D: 20% 50% 18% 12%

A80 V81 K82 I83 L84 E85 I86 E87 D88 L89 F90 L93 K94 H95 I96 Q97 H98 T99 L100 V101 Q104 S105 Q106 E107 D108 I109 S110 L111 L112 L113 Q114 L115 V116 Q117 N118 K119 D120 F121 Q122 N123 A124 F125 K126 I127 H128 N129 A130 I131 T132 V133 N136 K137 A138 S139

4.2.20 Score per residue for model 20

• Molecule 1: protein associated to tight junctions

Chain A: 37% 47% 6% 10%

N4 P5 A6 A7 E8 Q11 V12 L13 Q14 V15 L16 D17 R18 L19 R20 G21 K22 L23 Q24 E25 K26 T29 T30 Q31 L35 S36 A37 F38 Y39 E40 T41 S44 F47 N48 Q49 I50 L51 T52 L53 Q54 Q55 S56 I57 L60 K61 G62 Q63 L64 S65

• Molecule 1: protein associated to tight junctions

Chain C: 29% 52% 8% 11%

N4 P5 A6 A7 E8 K9 M10 Q11 V12 L13 Q14 V15 L16 L19 R20 G21 K22 L23 Q24 E25 K26 T29 T30 Q31 K34 L35 S36 A37 F38 Y39 E40 T41 L42 K43 S44 P45 L46 F47 N48 Q49 I50 L51 T52 L53 Q54 Q55 S56 I57 K58 Q59 L60 K61 G62 Q63 L64 S65

• Molecule 2: MAGUK p55 subfamily member 5

Chain B: 32% 45% 13% • 8%

A80 V81 K82 I83 L84 E85 I86 L89 F90 S91 S92 L93 I96 Q97 L100 V101 D102 S103 Q104 S105 D108 I109 S110 L111 L112 L113 Q114 L115 V116 K119 D120 F121 A124 F125 K126 I127 H128 N129 A130 I131 T132 V133 K137 A138 S139

• Molecule 2: MAGUK p55 subfamily member 5

Chain D: 27% 45% 15% • 12%

A80 V81 K82 I83 L84 E85 I86 E87 D88 L89 F90 S91 S92 L93 K94 H95 I96 Q97 L100 V101 D102 S103 Q104 S105 D108 I109 S110 L111 L112 L113 Q114 L115 V116 Q117 N118 K119 D120 F121 A124 F125 K126 I127 H128 N129 A130 I131 T132 V133 H134 M135 N136 K137 A138 S139

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *torsion angle dynamics*.

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CNS	structure solution	1.1
CNS	refinement	1.1

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	452	480	480	44±5
1	C	448	477	477	44±4
2	B	449	456	452	61±4
2	D	432	437	433	62±3
All	All	35620	37000	36840	3313

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 46.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:127:ILE:HD11	2:D:127:ILE:HD11	1.08	1.25	15	20
2:B:84:LEU:HD13	1:C:37:ALA:HB3	1.07	1.26	10	18
1:A:37:ALA:HB3	2:D:84:LEU:HD23	1.04	1.21	1	1
2:D:86:ILE:HA	2:D:89:LEU:HD23	0.96	1.33	1	20
2:D:100:LEU:HD12	2:D:109:ILE:HD11	0.93	1.41	17	18
2:B:127:ILE:CD1	2:D:127:ILE:HD11	0.93	1.92	18	20
2:B:100:LEU:HD12	2:B:109:ILE:HD11	0.92	1.39	7	18
1:A:37:ALA:HB3	2:D:84:LEU:HD13	0.91	1.42	18	16
1:A:57:ILE:HG21	2:B:131:ILE:HG21	0.91	1.43	5	18
1:C:57:ILE:HG21	2:D:131:ILE:HG21	0.88	1.42	18	20
1:A:41:THR:HG22	1:A:47:PHE:CD2	0.86	2.04	5	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:129:ASN:O	2:B:133:VAL:HG23	0.85	1.71	6	20
1:A:47:PHE:CE1	1:A:51:LEU:HD21	0.84	2.07	12	12
2:B:127:ILE:HD11	2:D:127:ILE:CD1	0.84	2.03	7	20
2:B:100:LEU:HD21	1:C:23:LEU:HD23	0.84	1.48	17	10
1:C:41:THR:HG22	1:C:47:PHE:CD2	0.84	2.06	6	11
2:D:129:ASN:O	2:D:133:VAL:HG23	0.84	1.73	6	19
1:A:38:PHE:CZ	1:A:42:LEU:HD11	0.83	2.07	11	8
1:A:37:ALA:CB	2:D:84:LEU:HD23	0.82	2.02	1	1
1:C:47:PHE:CE1	1:C:51:LEU:HD21	0.82	2.10	13	16
1:C:11:GLN:O	1:C:15:VAL:HG23	0.81	1.75	8	9
1:A:13:LEU:HD13	1:A:43:LYS:NZ	0.81	1.91	14	2
2:B:83:ILE:HD12	2:B:132:THR:CG2	0.80	2.07	6	8
1:C:38:PHE:CZ	1:C:42:LEU:HD11	0.79	2.13	5	8
2:D:83:ILE:HD11	2:D:133:VAL:HG22	0.79	1.53	1	6
2:D:112:LEU:O	2:D:116:VAL:HG23	0.79	1.77	10	20
2:B:112:LEU:O	2:B:116:VAL:HG23	0.79	1.78	5	20
2:D:84:LEU:HD12	2:D:89:LEU:HD22	0.78	1.55	1	1
2:B:86:ILE:HG12	2:B:116:VAL:HG13	0.77	1.54	1	20
2:B:105:SER:O	2:B:109:ILE:HD12	0.77	1.79	7	20
2:D:86:ILE:HG12	2:D:116:VAL:HG13	0.77	1.56	12	17
2:D:86:ILE:HG23	2:D:116:VAL:CG1	0.77	2.10	2	20
2:B:83:ILE:CD1	2:B:133:VAL:HG22	0.76	2.10	5	6
2:D:105:SER:O	2:D:109:ILE:HD12	0.76	1.81	8	20
2:B:112:LEU:HD21	1:C:15:VAL:HG11	0.76	1.58	2	18
1:C:8:GLU:O	1:C:12:VAL:HG23	0.76	1.80	15	20
2:B:84:LEU:HD13	1:C:37:ALA:CB	0.76	2.09	10	4
1:A:57:ILE:CG2	2:B:131:ILE:HG21	0.75	2.12	13	16
1:A:8:GLU:O	1:A:12:VAL:HG23	0.75	1.81	3	20
2:B:83:ILE:HG22	2:B:129:ASN:ND2	0.75	1.97	2	2
2:B:124:ALA:HA	2:B:127:ILE:HD12	0.74	1.59	5	14
1:C:29:THR:HG22	1:C:32:ASN:ND2	0.74	1.98	14	2
2:D:124:ALA:HA	2:D:127:ILE:HD12	0.74	1.57	12	11
2:B:92:SER:O	2:B:96:ILE:HD12	0.74	1.82	4	7
2:B:84:LEU:CD2	2:B:89:LEU:HD22	0.74	2.12	7	16
1:A:46:LEU:HD13	1:C:57:ILE:HG12	0.74	1.59	11	3
1:A:54:GLN:NE2	2:D:124:ALA:HB2	0.74	1.98	20	15
2:B:119:LYS:NZ	2:D:130:ALA:HB1	0.73	1.98	5	1
2:B:86:ILE:HA	2:B:89:LEU:HD23	0.73	1.60	3	20
1:C:57:ILE:CG2	2:D:131:ILE:HG21	0.73	2.13	10	18
2:D:83:ILE:CD1	2:D:133:VAL:HG22	0.73	2.13	1	6
2:D:84:LEU:CD2	2:D:89:LEU:HD22	0.73	2.14	4	12

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:D:83:ILE:HD12	2:D:132:THR:CG2	0.73	2.14	6	10
2:D:128:HIS:O	2:D:132:THR:HB	0.72	1.84	6	20
1:A:15:VAL:CG1	2:D:112:LEU:HD21	0.72	2.14	3	20
1:A:20:ARG:CB	1:A:35:LEU:HD12	0.72	2.14	10	13
2:B:97:GLN:HA	2:B:109:ILE:HD13	0.72	1.61	16	17
2:B:112:LEU:HD21	1:C:15:VAL:CG1	0.72	2.15	2	19
2:D:127:ILE:HG22	2:D:131:ILE:HD12	0.72	1.62	6	16
2:B:83:ILE:HD11	2:B:133:VAL:HG22	0.72	1.62	5	6
2:B:92:SER:C	2:B:96:ILE:HD12	0.71	2.05	10	7
2:B:83:ILE:HG21	2:B:129:ASN:HA	0.71	1.61	11	2
2:D:92:SER:C	2:D:96:ILE:HD12	0.71	2.05	2	9
1:A:13:LEU:HD13	1:A:43:LYS:HE2	0.71	1.60	18	3
2:B:84:LEU:HD21	2:B:89:LEU:HD22	0.71	1.62	2	13
1:A:15:VAL:HG11	2:D:112:LEU:HD21	0.71	1.62	18	20
1:A:23:LEU:HD23	2:D:100:LEU:HD21	0.71	1.61	17	6
2:D:83:ILE:HG22	2:D:129:ASN:ND2	0.71	2.00	13	1
2:D:86:ILE:HG13	2:D:89:LEU:HD23	0.70	1.63	17	16
1:A:11:GLN:O	1:A:15:VAL:HG23	0.70	1.86	9	8
2:D:86:ILE:HD12	2:D:125:PHE:CD1	0.70	2.21	12	6
1:C:47:PHE:CD1	1:C:51:LEU:HD21	0.70	2.20	18	11
1:A:15:VAL:HG22	2:D:108:ASP:CG	0.70	2.06	17	16
1:C:13:LEU:HA	1:C:16:LEU:HD12	0.70	1.63	6	14
2:D:83:ILE:HG21	2:D:129:ASN:HA	0.70	1.62	4	4
1:A:50:ILE:HG12	1:C:53:LEU:HD21	0.70	1.64	5	19
2:D:92:SER:O	2:D:96:ILE:HD12	0.70	1.86	13	8
2:B:112:LEU:HD22	1:C:12:VAL:HG13	0.70	1.63	7	6
1:C:13:LEU:HD13	1:C:43:LYS:HZ3	0.69	1.46	16	1
2:B:115:LEU:CD2	1:C:12:VAL:HG21	0.69	2.17	9	16
1:A:57:ILE:CD1	1:C:46:LEU:HD11	0.69	2.17	13	14
2:D:97:GLN:HA	2:D:109:ILE:HD13	0.69	1.62	6	15
2:B:128:HIS:O	2:B:132:THR:HB	0.69	1.86	14	20
2:B:83:ILE:HG23	2:B:132:THR:HG21	0.69	1.64	7	1
1:A:13:LEU:HA	1:A:16:LEU:HD12	0.69	1.64	1	15
2:B:108:ASP:CG	1:C:15:VAL:HG22	0.69	2.08	4	16
2:B:97:GLN:HB3	2:B:109:ILE:HG21	0.69	1.64	7	4
2:B:124:ALA:HB2	1:C:54:GLN:NE2	0.68	2.03	2	16
2:D:84:LEU:HD21	2:D:89:LEU:HD22	0.68	1.63	4	10
1:C:20:ARG:HB3	1:C:35:LEU:HD12	0.68	1.65	6	8
1:A:20:ARG:CA	1:A:35:LEU:HD12	0.68	2.18	6	13
2:B:111:LEU:HD23	1:C:12:VAL:HG22	0.68	1.64	7	14
1:A:46:LEU:HD11	1:C:57:ILE:CG1	0.68	2.18	2	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:100:LEU:HD13	2:B:105:SER:OG	0.68	1.88	13	6
1:C:38:PHE:CE2	1:C:42:LEU:HD11	0.67	2.24	5	7
1:A:53:LEU:HD21	1:C:50:ILE:HG12	0.67	1.67	16	18
1:A:37:ALA:HB3	2:D:84:LEU:CD2	0.67	2.12	1	1
1:C:20:ARG:N	1:C:35:LEU:HD12	0.67	2.04	1	13
1:A:61:LYS:HE3	2:B:131:ILE:HG23	0.67	1.63	9	1
2:B:83:ILE:HD13	2:B:83:ILE:H	0.66	1.50	11	1
1:A:12:VAL:HG21	2:D:115:LEU:CD2	0.66	2.21	12	18
1:A:57:ILE:CG1	1:C:46:LEU:HD11	0.66	2.20	2	4
2:D:97:GLN:HB3	2:D:109:ILE:HG21	0.66	1.66	17	2
2:B:89:LEU:O	2:B:89:LEU:HD12	0.65	1.91	17	5
2:B:130:ALA:HB1	2:D:119:LYS:CD	0.65	2.20	9	1
1:A:57:ILE:HG12	1:C:46:LEU:HD13	0.65	1.68	1	4
1:A:37:ALA:CB	2:D:84:LEU:HD13	0.65	2.21	7	5
1:A:57:ILE:HD13	1:C:46:LEU:HD11	0.65	1.69	15	9
1:C:61:LYS:NZ	2:D:131:ILE:HG23	0.65	2.07	20	3
1:C:35:LEU:HD23	1:C:35:LEU:N	0.64	2.07	10	18
2:B:108:ASP:HB3	1:C:15:VAL:HG13	0.64	1.69	8	20
2:D:100:LEU:HD13	2:D:105:SER:OG	0.64	1.92	10	4
1:C:9:LYS:HE2	1:C:13:LEU:HD11	0.64	1.70	12	3
1:A:19:LEU:HD12	2:D:112:LEU:HD11	0.64	1.70	13	16
1:A:20:ARG:N	1:A:35:LEU:HD12	0.64	2.08	13	8
1:A:46:LEU:HD11	1:C:57:ILE:CD1	0.64	2.23	5	16
1:C:38:PHE:CE1	1:C:42:LEU:HD11	0.64	2.28	18	5
1:C:61:LYS:HE3	2:D:131:ILE:HG23	0.64	1.70	9	1
1:A:35:LEU:N	1:A:35:LEU:HD23	0.64	2.08	12	17
2:D:105:SER:C	2:D:109:ILE:HD12	0.64	2.13	8	19
2:D:84:LEU:HD11	2:D:89:LEU:HB2	0.64	1.69	1	4
1:A:38:PHE:CE2	1:A:42:LEU:HD11	0.64	2.27	17	5
2:B:105:SER:C	2:B:109:ILE:HD12	0.63	2.13	16	20
1:C:16:LEU:HD13	1:C:39:TYR:HA	0.63	1.68	6	15
1:A:9:LYS:HD2	1:A:42:LEU:HD22	0.63	1.70	17	2
2:B:108:ASP:CB	1:C:15:VAL:HG13	0.63	2.22	5	2
2:B:93:LEU:HA	2:B:96:ILE:HD12	0.63	1.70	11	9
1:A:13:LEU:HD13	1:A:43:LYS:HZ1	0.63	1.52	14	2
2:D:93:LEU:HA	2:D:96:ILE:HD12	0.63	1.71	9	9
1:C:16:LEU:HD21	1:C:38:PHE:CD2	0.63	2.28	16	6
1:C:13:LEU:HD13	1:C:43:LYS:HE2	0.63	1.71	12	4
1:A:10:MET:CE	1:A:13:LEU:HD12	0.63	2.24	13	1
2:B:86:ILE:HG23	2:B:116:VAL:CG1	0.63	2.23	13	20
2:D:86:ILE:HG23	2:D:116:VAL:HG12	0.63	1.69	15	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:ARG:HB2	1:A:35:LEU:HD12	0.62	1.70	9	10
1:A:15:VAL:HG13	2:D:108:ASP:HB3	0.62	1.71	9	20
2:D:83:ILE:HG22	2:D:129:ASN:OD1	0.62	1.94	17	1
1:A:20:ARG:HA	1:A:23:LEU:HD12	0.62	1.69	11	6
1:A:57:ILE:HA	1:A:60:LEU:HD12	0.62	1.72	5	13
1:A:20:ARG:HB3	1:A:35:LEU:HD12	0.62	1.71	10	4
1:A:26:LYS:HE2	2:D:100:LEU:HD23	0.62	1.70	2	3
1:A:57:ILE:HD11	1:C:46:LEU:HD11	0.62	1.72	5	4
2:D:89:LEU:HD12	2:D:89:LEU:O	0.62	1.95	6	14
2:D:83:ILE:N	2:D:83:ILE:HD13	0.62	2.08	4	13
2:B:86:ILE:HG13	2:B:89:LEU:HD23	0.62	1.71	1	16
1:A:57:ILE:CG1	1:C:46:LEU:HD12	0.62	2.24	4	1
2:B:83:ILE:HD13	2:B:83:ILE:N	0.62	2.10	18	12
1:A:57:ILE:HG21	2:B:131:ILE:CG2	0.61	2.23	5	4
2:B:100:LEU:HD21	1:C:23:LEU:CD2	0.61	2.23	17	3
2:B:112:LEU:HD11	1:C:19:LEU:HD12	0.61	1.73	4	16
1:C:20:ARG:CA	1:C:35:LEU:HD12	0.61	2.26	17	17
2:B:86:ILE:HD12	2:B:125:PHE:CG	0.61	2.30	17	11
1:A:11:GLN:NE2	1:A:15:VAL:HG21	0.61	2.11	12	2
2:B:127:ILE:HG22	2:B:131:ILE:HD12	0.61	1.73	16	18
2:D:93:LEU:HD23	2:D:93:LEU:N	0.60	2.11	17	20
1:C:57:ILE:HA	1:C:60:LEU:HD12	0.60	1.72	4	18
2:D:84:LEU:CD1	2:D:89:LEU:HD22	0.60	2.24	1	1
1:A:22:LYS:HB3	2:D:100:LEU:HD22	0.60	1.71	16	13
1:A:16:LEU:HD13	1:A:39:TYR:HA	0.60	1.73	13	17
2:D:86:ILE:HD12	2:D:125:PHE:CG	0.60	2.30	19	4
2:B:112:LEU:HD13	1:C:16:LEU:HD23	0.60	1.72	8	3
1:A:19:LEU:HD22	2:D:100:LEU:HD12	0.60	1.73	18	6
1:A:46:LEU:HD11	1:C:57:ILE:HD13	0.60	1.72	1	9
2:D:86:ILE:HG23	2:D:116:VAL:HG13	0.60	1.73	2	2
1:A:46:LEU:HD11	1:C:57:ILE:HD11	0.60	1.73	17	7
1:C:47:PHE:CE2	1:C:51:LEU:HD21	0.60	2.32	7	1
2:D:96:ILE:CG2	2:D:100:LEU:HD12	0.59	2.27	1	3
1:C:51:LEU:N	1:C:51:LEU:HD23	0.59	2.13	11	20
1:C:13:LEU:HD13	1:C:43:LYS:HG3	0.59	1.75	14	3
1:A:31:GLN:HB3	2:D:96:ILE:HD11	0.59	1.74	2	10
2:D:83:ILE:HD12	2:D:132:THR:HG22	0.59	1.74	5	3
1:A:38:PHE:CE1	1:A:42:LEU:HD11	0.59	2.32	11	4
2:D:84:LEU:CD1	2:D:89:LEU:CB	0.59	2.81	1	4
2:B:96:ILE:CG2	2:B:100:LEU:HD12	0.59	2.28	10	7
1:A:12:VAL:HG22	2:D:111:LEU:HD23	0.59	1.75	7	13

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:86:ILE:HD12	2:B:125:PHE:CD1	0.59	2.33	5	9
2:B:93:LEU:HD13	2:B:112:LEU:HB2	0.59	1.75	3	20
2:D:109:ILE:HG22	2:D:113:LEU:CD1	0.59	2.28	8	20
2:B:108:ASP:CG	1:C:15:VAL:HG13	0.59	2.18	5	1
2:B:89:LEU:HD12	2:B:93:LEU:HD21	0.59	1.75	17	20
2:D:84:LEU:HD11	2:D:89:LEU:CB	0.59	2.28	1	1
1:A:57:ILE:HG22	2:B:131:ILE:HG21	0.58	1.73	13	1
1:A:47:PHE:CD1	1:A:51:LEU:HD21	0.58	2.33	19	5
1:A:23:LEU:HD21	2:D:96:ILE:HG23	0.58	1.75	1	12
2:B:83:ILE:HG21	2:B:129:ASN:OD1	0.58	1.98	6	1
1:C:16:LEU:HD13	1:C:39:TYR:CA	0.58	2.29	15	15
1:C:20:ARG:HB2	1:C:35:LEU:HD12	0.58	1.76	7	9
1:A:60:LEU:CD1	1:C:46:LEU:HD21	0.57	2.28	18	4
2:B:115:LEU:HD21	1:C:12:VAL:HG21	0.57	1.76	14	7
2:D:89:LEU:HD12	2:D:93:LEU:HD21	0.57	1.76	6	17
2:B:96:ILE:HG23	1:C:23:LEU:HD21	0.57	1.77	6	12
1:A:51:LEU:HD23	1:A:51:LEU:N	0.57	2.14	6	18
1:C:20:ARG:CB	1:C:35:LEU:HD12	0.57	2.28	7	17
2:D:96:ILE:HG22	2:D:109:ILE:CD1	0.57	2.29	13	2
2:D:127:ILE:HG22	2:D:131:ILE:CD1	0.57	2.29	6	4
2:B:100:LEU:HD22	1:C:22:LYS:HB3	0.57	1.75	9	12
2:B:93:LEU:HD23	2:B:93:LEU:N	0.57	2.15	4	20
2:B:119:LYS:CE	2:D:130:ALA:HB1	0.57	2.30	5	2
2:B:89:LEU:HD11	2:B:116:VAL:HG21	0.57	1.76	10	8
2:D:89:LEU:HD11	2:D:116:VAL:HG21	0.57	1.77	8	9
2:B:83:ILE:HG22	2:B:129:ASN:OD1	0.57	2.00	18	1
2:D:93:LEU:HD13	2:D:112:LEU:HB2	0.56	1.76	6	20
2:B:109:ILE:HG22	2:B:113:LEU:CD1	0.56	2.30	5	20
1:C:13:LEU:HD21	1:C:42:LEU:HB3	0.56	1.77	12	9
1:C:13:LEU:HD13	1:C:43:LYS:CE	0.56	2.29	12	4
1:C:13:LEU:HD13	1:C:43:LYS:NZ	0.56	2.13	16	4
2:B:84:LEU:O	2:B:85:GLU:O	0.56	2.24	11	2
1:A:16:LEU:HD13	1:A:39:TYR:CA	0.56	2.31	10	14
1:C:11:GLN:NE2	1:C:15:VAL:HG21	0.56	2.14	2	1
2:B:119:LYS:HD2	2:D:130:ALA:HB1	0.56	1.78	19	1
2:B:110:SER:HA	2:B:113:LEU:HD12	0.55	1.77	2	20
1:A:13:LEU:HD13	1:A:43:LYS:CE	0.55	2.30	18	4
1:A:16:LEU:HD21	1:A:38:PHE:CD2	0.55	2.36	6	9
1:A:34:LYS:HA	2:D:84:LEU:HD21	0.55	1.78	1	1
2:D:97:GLN:HB2	2:D:109:ILE:HG21	0.55	1.77	16	2
1:A:60:LEU:HD13	1:C:46:LEU:HD21	0.55	1.78	11	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:111:LEU:CD2	1:C:12:VAL:HG22	0.55	2.31	16	1
2:B:84:LEU:CD1	1:C:37:ALA:HB3	0.55	2.19	10	1
2:D:84:LEU:HD23	2:D:125:PHE:CZ	0.55	2.36	6	10
2:B:100:LEU:HD23	1:C:26:LYS:HE2	0.55	1.78	14	4
1:A:54:GLN:NE2	2:B:127:ILE:HD13	0.55	2.16	20	1
2:D:86:ILE:HD12	2:D:125:PHE:CB	0.54	2.32	3	2
1:A:16:LEU:HD11	1:A:42:LEU:HD12	0.54	1.79	4	2
2:B:130:ALA:HB1	2:D:119:LYS:HE2	0.54	1.79	18	1
2:D:110:SER:HA	2:D:113:LEU:HD12	0.54	1.78	4	20
2:B:96:ILE:HD11	1:C:31:GLN:HB3	0.54	1.79	20	8
2:B:84:LEU:HD23	2:B:89:LEU:HD22	0.54	1.80	10	6
1:A:13:LEU:HD21	1:A:42:LEU:HB3	0.54	1.78	2	7
1:A:16:LEU:HD11	1:A:42:LEU:CD1	0.54	2.32	4	8
2:D:97:GLN:CG	2:D:109:ILE:HG21	0.54	2.33	6	8
1:A:12:VAL:HG21	2:D:115:LEU:HD21	0.54	1.77	5	9
1:A:38:PHE:N	2:D:84:LEU:HD22	0.54	2.17	7	1
2:D:83:ILE:HG21	2:D:129:ASN:CG	0.54	2.23	10	3
2:D:86:ILE:HD12	2:D:125:PHE:HB3	0.54	1.79	3	2
2:B:100:LEU:CD2	1:C:23:LEU:HD23	0.54	2.27	17	1
2:B:84:LEU:HD11	2:B:89:LEU:HB2	0.53	1.80	11	2
1:A:29:THR:HG22	1:A:32:ASN:ND2	0.53	2.18	6	3
1:A:53:LEU:HD21	1:C:50:ILE:CG1	0.53	2.33	16	1
2:D:86:ILE:HA	2:D:89:LEU:CD2	0.53	2.33	11	3
2:B:86:ILE:CD1	2:B:125:PHE:CG	0.53	2.92	18	18
2:D:86:ILE:O	2:D:90:PHE:CB	0.53	2.57	8	16
2:B:86:ILE:O	2:B:90:PHE:HB2	0.53	2.04	1	20
1:A:61:LYS:NZ	2:B:131:ILE:HG23	0.53	2.19	17	4
2:D:86:ILE:O	2:D:90:PHE:HB2	0.53	2.03	19	20
1:A:13:LEU:HD21	1:A:42:LEU:HD22	0.53	1.78	6	1
2:B:89:LEU:HD12	2:B:89:LEU:O	0.53	2.04	9	13
2:D:96:ILE:HG22	2:D:109:ILE:HD11	0.52	1.81	13	1
2:B:83:ILE:HG22	2:B:129:ASN:CG	0.52	2.25	2	2
1:C:11:GLN:NE2	1:C:15:VAL:HG23	0.52	2.20	14	9
1:A:35:LEU:O	1:A:39:TYR:HB2	0.52	2.04	4	7
2:D:109:ILE:HG22	2:D:113:LEU:HD12	0.52	1.81	8	14
1:A:50:ILE:CG1	1:C:53:LEU:HD21	0.52	2.34	2	4
2:D:84:LEU:HD23	2:D:125:PHE:HZ	0.52	1.65	15	3
1:A:54:GLN:HE21	2:D:124:ALA:HB2	0.52	1.65	3	5
2:B:124:ALA:CB	1:C:50:ILE:HG22	0.52	2.35	10	1
2:B:111:LEU:HD21	1:C:12:VAL:HG22	0.52	1.81	16	1
1:A:11:GLN:NE2	1:A:15:VAL:HG23	0.52	2.20	16	12

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:13:LEU:HD13	1:A:43:LYS:CD	0.51	2.36	2	1
1:A:23:LEU:CD2	2:D:100:LEU:HD21	0.51	2.33	17	6
2:D:123:ASN:O	2:D:127:ILE:HG13	0.51	2.05	6	5
1:C:23:LEU:HD13	1:C:31:GLN:HB2	0.51	1.82	10	3
2:B:84:LEU:HD23	2:B:125:PHE:CZ	0.51	2.41	15	6
1:C:20:ARG:HA	1:C:23:LEU:HD12	0.51	1.82	15	6
1:A:19:LEU:CD1	2:D:112:LEU:HD11	0.51	2.35	13	2
1:A:34:LYS:HG3	2:D:84:LEU:HD12	0.51	1.83	2	1
1:A:57:ILE:HG21	2:B:131:ILE:HD13	0.51	1.82	3	1
2:B:123:ASN:O	2:B:127:ILE:HG13	0.51	2.06	9	2
2:B:100:LEU:HD22	1:C:22:LYS:CB	0.51	2.36	17	2
1:A:50:ILE:CG2	2:D:127:ILE:HD12	0.51	2.36	6	2
2:B:83:ILE:CD1	2:B:133:VAL:CG2	0.51	2.89	8	6
2:D:89:LEU:O	2:D:93:LEU:HG	0.51	2.06	11	12
2:D:83:ILE:HG21	2:D:129:ASN:OD1	0.51	2.06	10	2
2:D:83:ILE:CD1	2:D:133:VAL:CG2	0.50	2.88	3	6
1:A:39:TYR:CZ	1:A:43:LYS:CE	0.50	2.95	2	5
2:B:86:ILE:O	2:B:90:PHE:CB	0.50	2.59	2	17
1:A:9:LYS:NZ	1:A:51:LEU:HD12	0.50	2.22	16	2
2:B:109:ILE:HG22	2:B:113:LEU:HD12	0.50	1.84	9	18
2:D:83:ILE:HG23	2:D:132:THR:HG21	0.50	1.83	15	2
2:D:86:ILE:HD11	2:D:125:PHE:HB3	0.50	1.82	11	3
1:A:53:LEU:HD11	1:C:50:ILE:HG12	0.50	1.81	2	3
2:D:114:GLN:HG3	2:D:115:LEU:N	0.50	2.21	2	3
1:A:46:LEU:O	1:A:49:GLN:CG	0.50	2.60	1	1
2:B:100:LEU:HD12	1:C:19:LEU:HD22	0.50	1.83	3	5
1:A:29:THR:HG22	1:A:32:ASN:HD21	0.50	1.66	6	1
1:C:35:LEU:O	1:C:39:TYR:HB2	0.50	2.07	16	2
2:B:86:ILE:O	2:B:90:PHE:N	0.50	2.45	16	20
2:D:86:ILE:O	2:D:90:PHE:N	0.50	2.45	3	20
2:D:93:LEU:HD11	2:D:116:VAL:HG21	0.50	1.84	13	2
2:D:83:ILE:HG22	2:D:84:LEU:H	0.49	1.67	1	2
2:D:84:LEU:HD23	2:D:89:LEU:HD22	0.49	1.84	3	7
1:C:29:THR:HG22	1:C:32:ASN:HD21	0.49	1.67	14	2
2:D:86:ILE:CG1	2:D:116:VAL:HG13	0.49	2.36	7	6
2:B:130:ALA:HB1	2:D:119:LYS:HE3	0.49	1.83	7	1
1:A:15:VAL:HG22	2:D:108:ASP:OD1	0.49	2.06	17	7
2:D:86:ILE:CD1	2:D:125:PHE:CG	0.49	2.96	19	7
1:C:57:ILE:HG21	2:D:131:ILE:CG2	0.49	2.29	18	3
1:A:10:MET:HE1	1:A:13:LEU:HD12	0.49	1.83	13	1
2:B:115:LEU:O	2:B:121:PHE:CD1	0.49	2.66	11	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:108:ASP:OD1	1:C:15:VAL:HG22	0.49	2.07	7	8
1:A:46:LEU:HD13	1:C:57:ILE:CG1	0.49	2.37	6	2
1:C:23:LEU:HB3	1:C:28:ASP:O	0.49	2.06	6	1
2:B:83:ILE:O	2:B:84:LEU:CB	0.49	2.60	7	1
2:D:89:LEU:HD11	2:D:116:VAL:CG2	0.49	2.38	15	3
2:D:86:ILE:HD11	2:D:125:PHE:CG	0.49	2.42	1	3
1:A:38:PHE:CD2	1:A:42:LEU:HD11	0.49	2.43	15	1
1:A:16:LEU:CD2	2:D:112:LEU:HD13	0.49	2.38	3	2
1:C:13:LEU:HD21	1:C:42:LEU:HD22	0.49	1.85	10	1
1:A:11:GLN:NE2	2:D:111:LEU:HD13	0.49	2.23	19	1
2:D:84:LEU:HD12	2:D:89:LEU:CD2	0.49	2.34	1	1
2:D:115:LEU:O	2:D:121:PHE:CG	0.48	2.65	17	14
2:B:89:LEU:O	2:B:93:LEU:HG	0.48	2.08	11	14
1:A:57:ILE:HG12	1:C:46:LEU:HD12	0.48	1.84	4	1
1:A:38:PHE:CE1	1:A:42:LEU:CD1	0.48	2.96	11	3
2:B:86:ILE:HD11	2:B:125:PHE:CG	0.48	2.43	13	5
1:A:19:LEU:HD22	2:D:100:LEU:CD1	0.48	2.38	5	3
2:D:115:LEU:O	2:D:121:PHE:CD1	0.48	2.67	10	20
2:B:86:ILE:HD12	2:B:125:PHE:HB3	0.48	1.85	11	1
2:B:115:LEU:O	2:B:121:PHE:CG	0.48	2.66	6	13
1:A:47:PHE:CE2	1:A:51:LEU:HD21	0.48	2.44	8	1
1:A:47:PHE:CE2	1:A:51:LEU:HD11	0.48	2.43	8	1
1:A:23:LEU:HD23	2:D:100:LEU:CD2	0.48	2.38	10	1
2:D:96:ILE:HG22	2:D:100:LEU:HD12	0.48	1.85	1	1
1:A:23:LEU:HD12	1:A:32:ASN:OD1	0.48	2.08	5	1
2:B:83:ILE:HG23	2:B:132:THR:CG2	0.48	2.38	7	1
2:B:112:LEU:HD13	1:C:16:LEU:CD2	0.48	2.39	8	3
2:D:86:ILE:HD11	2:D:125:PHE:CB	0.48	2.39	1	1
2:B:130:ALA:HB1	2:D:119:LYS:CE	0.48	2.38	18	2
1:C:47:PHE:HD1	1:C:50:ILE:HD12	0.48	1.67	5	1
1:A:12:VAL:HG21	2:D:115:LEU:HD22	0.48	1.85	19	1
1:A:16:LEU:HD23	2:D:112:LEU:HD13	0.48	1.85	5	4
1:A:49:GLN:HG3	1:C:53:LEU:HD11	0.48	1.85	1	1
1:C:54:GLN:NE2	2:D:127:ILE:HD13	0.48	2.23	2	1
2:B:86:ILE:HG13	2:B:89:LEU:CD2	0.48	2.39	5	11
1:A:57:ILE:HD11	1:C:50:ILE:HD11	0.48	1.85	2	1
1:A:46:LEU:O	1:A:50:ILE:HG13	0.48	2.09	1	1
2:D:86:ILE:HG21	2:D:122:GLN:NE2	0.48	2.24	17	1
1:C:41:THR:CG2	1:C:47:PHE:CD2	0.47	2.97	4	5
1:A:57:ILE:HG13	1:C:46:LEU:HD12	0.47	1.86	4	1
2:B:84:LEU:HD23	2:B:125:PHE:CE2	0.47	2.44	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:D:83:ILE:HD12	2:D:132:THR:HG21	0.47	1.86	10	1
1:A:41:THR:HG22	1:A:47:PHE:CZ	0.47	2.44	11	1
1:C:39:TYR:CZ	1:C:43:LYS:NZ	0.47	2.82	10	4
1:A:34:LYS:O	2:D:84:LEU:HD13	0.47	2.09	15	3
2:B:97:GLN:CA	2:B:109:ILE:HD13	0.47	2.39	5	1
1:C:35:LEU:N	1:C:35:LEU:CD2	0.47	2.77	10	7
2:B:114:GLN:HG3	2:B:115:LEU:N	0.47	2.23	4	1
2:B:83:ILE:HG22	2:B:84:LEU:H	0.47	1.70	17	2
2:B:83:ILE:HG22	2:B:129:ASN:HB2	0.47	1.87	4	1
2:D:90:PHE:CE1	2:D:117:GLN:CG	0.47	2.98	9	7
1:A:38:PHE:CA	2:D:84:LEU:HD22	0.47	2.39	7	1
1:A:16:LEU:HD21	1:A:38:PHE:HD2	0.47	1.68	7	3
2:B:124:ALA:HB2	1:C:54:GLN:HE21	0.47	1.68	9	3
2:D:86:ILE:HG13	2:D:89:LEU:CD2	0.47	2.37	17	9
2:B:93:LEU:HD11	2:B:116:VAL:HG21	0.47	1.87	20	3
2:B:86:ILE:CG1	2:B:116:VAL:HG13	0.46	2.36	4	3
2:B:83:ILE:N	2:B:83:ILE:CD1	0.46	2.76	18	5
2:B:100:LEU:HB2	2:B:109:ILE:HD11	0.46	1.85	10	2
2:B:97:GLN:CG	2:B:109:ILE:HG21	0.46	2.40	19	7
1:A:35:LEU:N	1:A:35:LEU:CD2	0.46	2.78	11	5
2:D:84:LEU:O	2:D:84:LEU:HG	0.46	2.10	17	2
1:C:39:TYR:CZ	1:C:43:LYS:CE	0.46	2.98	12	1
1:C:30:THR:HG22	1:C:31:GLN:HE21	0.46	1.70	3	1
1:A:39:TYR:CZ	1:A:43:LYS:HE3	0.46	2.45	18	3
2:B:83:ILE:HD12	2:B:132:THR:HG23	0.46	1.87	13	1
1:A:22:LYS:CB	2:D:100:LEU:HD22	0.46	2.39	2	2
2:B:86:ILE:HG23	2:B:116:VAL:HG12	0.46	1.88	4	6
1:A:39:TYR:CE1	1:A:43:LYS:CD	0.46	2.99	11	2
1:C:38:PHE:CE1	1:C:42:LEU:CD1	0.46	2.98	13	6
2:B:124:ALA:HB1	1:C:50:ILE:HG22	0.46	1.88	10	1
2:B:83:ILE:HD12	2:B:132:THR:HG22	0.46	1.87	18	2
1:A:16:LEU:HD13	1:A:39:TYR:HB2	0.46	1.87	18	3
1:A:41:THR:CG2	1:A:47:PHE:CD2	0.46	2.99	17	3
1:C:39:TYR:CE1	1:C:43:LYS:CD	0.46	2.99	1	2
1:A:50:ILE:HG12	1:C:53:LEU:HD11	0.46	1.87	2	3
1:C:16:LEU:HD21	1:C:38:PHE:HD2	0.46	1.70	7	3
2:B:127:ILE:CD1	2:D:127:ILE:CD1	0.46	2.93	17	3
2:B:90:PHE:CE1	2:B:117:GLN:CG	0.46	2.99	16	7
1:C:38:PHE:O	1:C:42:LEU:HD12	0.46	2.11	11	1
1:A:54:GLN:CD	2:D:124:ALA:HB2	0.46	2.31	2	1
2:B:96:ILE:HG22	2:B:100:LEU:HD12	0.46	1.88	19	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:38:PHE:CZ	1:A:42:LEU:CD1	0.46	2.99	14	1
1:C:38:PHE:CE2	1:C:42:LEU:CD1	0.46	2.99	20	2
2:D:83:ILE:HG23	2:D:129:ASN:HA	0.46	1.87	1	1
1:A:20:ARG:HA	1:A:35:LEU:HD12	0.46	1.88	6	1
1:C:47:PHE:CZ	1:C:51:LEU:HD21	0.46	2.45	2	1
1:A:15:VAL:HG12	2:D:112:LEU:HD21	0.45	1.84	1	5
1:C:47:PHE:CD2	1:C:51:LEU:HD21	0.45	2.47	7	1
2:D:84:LEU:O	2:D:85:GLU:O	0.45	2.35	2	4
1:A:39:TYR:CZ	1:A:43:LYS:NZ	0.45	2.84	10	4
2:D:84:LEU:CD1	2:D:89:LEU:HB3	0.45	2.40	1	1
2:B:86:ILE:HD11	2:B:125:PHE:CB	0.45	2.42	3	2
2:D:83:ILE:CD1	2:D:132:THR:CG2	0.45	2.95	7	5
2:D:97:GLN:CB	2:D:109:ILE:HG21	0.45	2.41	2	2
2:D:113:LEU:O	2:D:117:GLN:CG	0.45	2.65	2	5
1:C:41:THR:CG2	1:C:47:PHE:CD1	0.45	2.99	7	1
2:D:132:THR:CG2	2:D:133:VAL:N	0.45	2.80	15	7
2:B:90:PHE:CE1	2:B:113:LEU:HD23	0.45	2.47	2	2
2:B:132:THR:HG22	2:B:133:VAL:N	0.45	2.26	7	5
1:A:31:GLN:NE2	2:D:95:HIS:CD2	0.45	2.84	16	2
1:A:41:THR:CG2	1:A:47:PHE:CE1	0.45	2.99	11	1
1:A:53:LEU:HD12	1:C:49:GLN:HB3	0.45	1.89	11	1
2:B:112:LEU:HD21	1:C:15:VAL:HG12	0.45	1.89	14	3
1:A:38:PHE:CE2	1:A:42:LEU:CD1	0.45	2.99	5	1
2:D:121:PHE:CD1	2:D:121:PHE:C	0.45	2.91	10	13
2:D:90:PHE:CE1	2:D:117:GLN:NE2	0.45	2.85	11	2
1:A:16:LEU:HD11	1:A:42:LEU:HD13	0.45	1.87	6	1
1:A:46:LEU:CD1	1:C:57:ILE:CD1	0.45	2.94	6	3
1:C:16:LEU:HD11	1:C:42:LEU:CD1	0.45	2.42	10	3
2:D:113:LEU:O	2:D:117:GLN:HG2	0.45	2.12	2	2
2:B:113:LEU:O	2:B:117:GLN:CG	0.44	2.65	18	3
1:A:57:ILE:HG12	1:C:46:LEU:CD1	0.44	2.43	4	1
2:B:102:ASP:O	2:B:103:SER:CB	0.44	2.65	5	1
2:D:111:LEU:CD2	2:D:112:LEU:HD23	0.44	2.41	9	1
1:A:22:LYS:O	1:A:26:LYS:N	0.44	2.50	19	2
1:A:57:ILE:CG2	2:B:131:ILE:CG2	0.44	2.96	16	4
2:D:89:LEU:O	2:D:93:LEU:CD2	0.44	2.66	2	1
2:B:111:LEU:HD21	1:C:12:VAL:CG2	0.44	2.43	16	1
2:B:112:LEU:CD2	1:C:12:VAL:HG13	0.44	2.40	7	1
1:C:41:THR:CG2	1:C:47:PHE:CE1	0.44	3.01	7	1
2:D:83:ILE:HG21	2:D:133:VAL:CG2	0.44	2.43	12	1
1:A:10:MET:HA	1:A:10:MET:HE2	0.44	1.89	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:89:LEU:CD1	2:B:93:LEU:HD21	0.44	2.41	17	4
2:D:83:ILE:N	2:D:83:ILE:CD1	0.44	2.76	4	1
2:B:86:ILE:HD12	2:B:125:PHE:CB	0.44	2.42	11	1
1:C:53:LEU:HD23	1:C:54:GLN:OE1	0.44	2.12	5	1
2:D:120:ASP:N	2:D:120:ASP:OD1	0.44	2.51	7	1
2:B:84:LEU:HD12	1:C:34:LYS:NZ	0.44	2.28	20	1
1:C:57:ILE:HG22	2:D:131:ILE:HG21	0.44	1.89	5	3
2:D:84:LEU:CD1	2:D:89:LEU:HB2	0.44	2.43	11	3
1:A:22:LYS:O	1:A:26:LYS:CD	0.44	2.66	12	3
1:A:41:THR:HG22	1:A:47:PHE:CE2	0.44	2.48	16	2
2:B:84:LEU:CD1	2:B:89:LEU:HB2	0.44	2.42	11	1
2:B:115:LEU:HD22	1:C:12:VAL:HG21	0.44	1.90	2	1
2:B:124:ALA:HA	1:C:50:ILE:HG21	0.44	1.88	18	1
1:A:57:ILE:CG1	1:C:46:LEU:CD1	0.43	2.96	16	5
1:A:11:GLN:NE2	1:A:15:VAL:CG2	0.43	2.81	12	10
1:A:46:LEU:CD1	1:C:57:ILE:CG1	0.43	2.96	12	6
2:B:90:PHE:CZ	2:B:117:GLN:HG2	0.43	2.48	17	1
2:B:121:PHE:CD1	2:B:121:PHE:C	0.43	2.92	11	8
1:A:13:LEU:HB3	1:A:39:TYR:CE1	0.43	2.48	13	1
2:B:107:GLU:HG3	2:B:108:ASP:N	0.43	2.28	18	1
1:A:13:LEU:O	1:A:39:TYR:CZ	0.43	2.71	4	1
2:D:95:HIS:O	2:D:99:THR:N	0.43	2.51	5	6
2:D:102:ASP:O	2:D:103:SER:CB	0.43	2.66	4	1
2:D:93:LEU:HB2	2:D:113:LEU:HD21	0.43	1.90	4	1
2:B:100:LEU:CD1	1:C:19:LEU:HD22	0.43	2.43	8	3
2:B:86:ILE:HA	2:B:89:LEU:CD2	0.43	2.41	11	1
1:A:23:LEU:HD13	1:A:31:GLN:HB2	0.43	1.89	13	1
1:A:39:TYR:CE1	1:A:43:LYS:NZ	0.43	2.85	13	1
2:B:130:ALA:HB1	2:D:119:LYS:NZ	0.43	2.28	15	1
1:C:57:ILE:CG2	2:D:131:ILE:CG2	0.43	2.96	2	2
1:C:13:LEU:O	1:C:39:TYR:CE2	0.43	2.71	7	1
1:A:49:GLN:O	1:A:52:THR:HG22	0.43	2.14	13	1
2:D:90:PHE:CE1	2:D:113:LEU:HD23	0.43	2.49	15	1
1:A:20:ARG:O	1:A:24:GLN:NE2	0.43	2.51	5	1
1:A:17:ASP:OD1	1:A:18:ARG:N	0.43	2.52	7	1
1:A:31:GLN:HG3	2:D:95:HIS:CD2	0.43	2.48	8	1
2:B:113:LEU:O	2:B:117:GLN:HG3	0.43	2.14	17	2
2:B:93:LEU:HB2	2:B:113:LEU:HD21	0.43	1.90	12	3
1:A:19:LEU:O	1:A:23:LEU:HG	0.43	2.13	12	2
1:A:38:PHE:CZ	2:D:116:VAL:HG22	0.43	2.49	8	1
1:C:13:LEU:HD13	1:C:43:LYS:HZ1	0.43	1.74	11	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:D:84:LEU:O	2:D:85:GLU:C	0.43	2.55	17	1
2:B:95:HIS:CD2	2:B:95:HIS:C	0.43	2.92	11	5
2:B:96:ILE:HG12	1:C:23:LEU:HD11	0.43	1.89	10	1
2:D:83:ILE:O	2:D:84:LEU:HB3	0.43	2.14	12	1
2:D:83:ILE:HG22	2:D:129:ASN:CG	0.43	2.34	13	1
2:B:95:HIS:O	2:B:99:THR:N	0.43	2.52	5	5
1:C:13:LEU:HD13	1:C:39:TYR:HE1	0.43	1.73	4	1
1:A:16:LEU:HD13	1:A:39:TYR:CB	0.43	2.43	18	2
2:B:120:ASP:OD2	2:D:131:ILE:HD13	0.43	2.13	10	1
2:B:90:PHE:CE1	2:B:117:GLN:HG2	0.43	2.49	17	1
2:B:104:GLN:O	2:B:107:GLU:HG2	0.43	2.14	16	2
1:C:24:GLN:CG	1:C:32:ASN:ND2	0.43	2.81	5	2
1:A:20:ARG:H	1:A:35:LEU:HD12	0.43	1.72	11	1
2:B:84:LEU:HG	2:B:84:LEU:O	0.43	2.12	14	1
2:B:83:ILE:CD1	2:B:132:THR:CG2	0.43	2.97	19	3
2:B:102:ASP:O	2:B:104:GLN:N	0.42	2.52	7	6
1:A:56:SER:O	1:A:60:LEU:HD23	0.42	2.14	12	1
2:B:86:ILE:CG2	2:B:116:VAL:CG1	0.42	2.97	6	2
2:B:128:HIS:HB2	1:C:50:ILE:HD12	0.42	1.91	11	1
1:A:57:ILE:CD1	1:C:46:LEU:CD1	0.42	2.98	1	2
2:B:132:THR:CG2	2:B:133:VAL:N	0.42	2.83	14	5
2:D:86:ILE:CD1	2:D:125:PHE:HB3	0.42	2.44	7	2
2:D:125:PHE:CE1	2:D:129:ASN:OD1	0.42	2.72	12	2
2:B:84:LEU:HD22	1:C:38:PHE:HB2	0.42	1.91	12	1
2:B:96:ILE:HG23	2:B:100:LEU:CD1	0.42	2.45	20	1
2:B:90:PHE:CE1	2:B:117:GLN:NE2	0.42	2.88	7	2
2:D:119:LYS:HG2	2:D:120:ASP:N	0.42	2.29	10	1
2:D:100:LEU:HB2	2:D:109:ILE:HD11	0.42	1.90	16	1
2:B:125:PHE:HA	1:C:47:PHE:CE1	0.42	2.48	17	1
1:A:57:ILE:CG1	1:C:46:LEU:HD13	0.42	2.43	1	1
1:C:41:THR:CG2	1:C:47:PHE:CE2	0.42	3.03	1	1
1:A:41:THR:HG22	1:A:47:PHE:CE1	0.42	2.49	11	1
2:D:94:LYS:HE2	2:D:113:LEU:HD22	0.42	1.91	14	1
2:B:127:ILE:CG2	2:B:131:ILE:HD12	0.42	2.43	20	1
1:C:11:GLN:NE2	1:C:15:VAL:CG2	0.42	2.82	6	13
1:C:30:THR:HG22	1:C:31:GLN:NE2	0.42	2.29	3	1
2:B:129:ASN:CG	2:B:130:ALA:N	0.42	2.73	4	1
2:B:95:HIS:CD2	1:C:31:GLN:HG3	0.42	2.50	11	2
2:D:111:LEU:HD23	2:D:112:LEU:HD23	0.42	1.91	9	1
2:B:124:ALA:HB1	1:C:50:ILE:CG2	0.42	2.44	10	1
2:B:90:PHE:O	2:B:94:LYS:HG2	0.42	2.15	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:49:GLN:CD	1:C:53:LEU:HD12	0.42	2.35	18	1
1:A:20:ARG:CD	1:A:32:ASN:ND2	0.42	2.83	2	1
1:C:8:GLU:O	1:C:12:VAL:N	0.42	2.53	2	1
2:D:132:THR:HG22	2:D:133:VAL:N	0.42	2.30	3	2
1:A:31:GLN:OE1	2:D:95:HIS:CD2	0.42	2.73	20	3
1:A:46:LEU:HG	1:A:47:PHE:N	0.42	2.29	6	1
2:B:100:LEU:CD2	1:C:22:LYS:CB	0.42	2.97	10	1
1:A:19:LEU:CD2	2:D:100:LEU:HD12	0.42	2.41	18	2
2:D:86:ILE:CG2	2:D:116:VAL:HG12	0.42	2.44	15	1
2:D:83:ILE:O	2:D:84:LEU:CB	0.42	2.68	4	1
1:A:13:LEU:O	1:A:39:TYR:CE2	0.42	2.73	15	3
2:B:83:ILE:O	2:B:84:LEU:HB2	0.42	2.14	7	1
1:C:39:TYR:CE1	1:C:43:LYS:HD3	0.42	2.50	9	1
2:B:96:ILE:HG22	2:B:109:ILE:HD11	0.41	1.90	2	2
2:D:97:GLN:HG2	2:D:109:ILE:HG21	0.41	1.92	3	1
2:D:86:ILE:CD1	2:D:125:PHE:CB	0.41	2.98	7	3
2:D:86:ILE:CG2	2:D:116:VAL:CG1	0.41	2.97	17	3
2:B:89:LEU:O	2:B:93:LEU:CD2	0.41	2.68	13	1
2:D:104:GLN:O	2:D:107:GLU:HG2	0.41	2.15	13	1
1:A:11:GLN:OE1	2:D:111:LEU:HD22	0.41	2.14	19	1
1:A:12:VAL:CG2	2:D:111:LEU:CD2	0.41	2.98	19	1
2:B:84:LEU:O	2:B:85:GLU:C	0.41	2.59	14	2
2:B:84:LEU:O	2:B:125:PHE:CZ	0.41	2.73	8	1
1:A:53:LEU:CD2	1:C:50:ILE:HG23	0.41	2.44	16	1
2:D:96:ILE:CG2	2:D:100:LEU:CD1	0.41	2.98	1	1
1:C:41:THR:HG22	1:C:47:PHE:CE2	0.41	2.49	6	1
2:D:83:ILE:CD1	2:D:132:THR:HG22	0.41	2.45	7	1
1:A:23:LEU:HB3	1:A:28:ASP:O	0.41	2.15	12	2
1:A:19:LEU:CD2	2:D:100:LEU:CD1	0.41	2.99	18	1
2:D:102:ASP:O	2:D:104:GLN:N	0.41	2.53	7	8
1:A:39:TYR:CE1	1:A:43:LYS:HD3	0.41	2.49	5	1
2:B:128:HIS:CE1	1:C:41:THR:HG23	0.41	2.50	18	1
1:A:46:LEU:O	1:A:49:GLN:HG2	0.41	2.15	1	1
2:B:105:SER:O	2:B:109:ILE:CD1	0.41	2.66	13	1
1:A:39:TYR:CD1	1:A:43:LYS:HE3	0.41	2.50	4	1
2:B:109:ILE:HG22	2:B:113:LEU:HD11	0.41	1.93	5	1
1:C:39:TYR:CE1	1:C:43:LYS:HE3	0.41	2.51	16	1
1:A:47:PHE:CE1	1:A:51:LEU:HD11	0.41	2.51	10	2
2:B:83:ILE:CG2	2:B:129:ASN:ND2	0.41	2.84	19	1
1:C:47:PHE:CE1	1:C:51:LEU:HD11	0.41	2.51	19	1
1:A:50:ILE:HG23	1:C:53:LEU:CD2	0.41	2.46	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:86:ILE:CD1	2:B:125:PHE:CB	0.41	2.99	8	4
1:A:16:LEU:HB2	1:A:39:TYR:CD2	0.41	2.51	7	1
2:B:84:LEU:O	2:B:84:LEU:HG	0.41	2.15	8	1
2:D:89:LEU:CD1	2:D:93:LEU:HD21	0.41	2.44	6	1
2:B:84:LEU:O	2:B:125:PHE:CE1	0.41	2.74	8	1
1:C:38:PHE:CZ	1:C:42:LEU:CD1	0.41	3.01	10	1
1:A:31:GLN:NE2	2:D:95:HIS:NE2	0.41	2.68	16	1
1:A:8:GLU:O	1:A:12:VAL:N	0.41	2.51	19	1
1:A:11:GLN:HE22	2:D:111:LEU:HD13	0.41	1.75	19	1
2:D:113:LEU:O	2:D:117:GLN:HG3	0.41	2.16	19	1
1:A:39:TYR:CE1	1:A:43:LYS:HE3	0.41	2.51	4	1
1:C:39:TYR:CZ	1:C:43:LYS:HE3	0.41	2.51	11	2
2:B:124:ALA:N	1:C:54:GLN:NE2	0.41	2.68	19	1
2:D:83:ILE:O	2:D:84:LEU:HB2	0.40	2.16	4	1
2:B:95:HIS:CE1	2:B:99:THR:HG1	0.40	2.33	5	1
2:B:119:LYS:HE2	2:D:130:ALA:HB1	0.40	1.92	5	1
2:B:84:LEU:CD1	2:B:89:LEU:CB	0.40	2.99	11	1
1:C:22:LYS:O	1:C:26:LYS:N	0.40	2.54	14	1
2:B:103:SER:O	2:B:106:GLN:CG	0.40	2.70	3	1
2:B:115:LEU:N	2:B:115:LEU:CD1	0.40	2.84	8	3
2:D:84:LEU:O	2:D:125:PHE:CZ	0.40	2.74	8	1
2:D:95:HIS:CD2	2:D:95:HIS:C	0.40	2.94	8	1
2:B:125:PHE:CE1	2:B:129:ASN:OD1	0.40	2.74	14	1
2:D:97:GLN:NE2	2:D:106:GLN:NE2	0.40	2.69	19	1
2:D:115:LEU:N	2:D:115:LEU:CD1	0.40	2.84	20	1
2:B:84:LEU:HD21	2:B:89:LEU:HB2	0.40	1.93	1	1
1:C:46:LEU:HG	1:C:47:PHE:N	0.40	2.31	1	1
1:C:13:LEU:HD22	1:C:39:TYR:CD1	0.40	2.52	4	1
1:A:38:PHE:CA	2:D:84:LEU:CD2	0.40	2.99	7	1
1:A:54:GLN:NE2	2:D:124:ALA:N	0.40	2.70	8	2
2:D:127:ILE:CG2	2:D:131:ILE:HD12	0.40	2.45	18	1
1:A:57:ILE:HG12	1:C:46:LEU:HD11	0.40	1.89	2	1
1:A:51:LEU:O	1:A:54:GLN:CG	0.40	2.69	6	1
2:B:113:LEU:O	2:B:117:GLN:HG2	0.40	2.17	6	1
2:B:84:LEU:CD2	1:C:38:PHE:HB2	0.40	2.45	10	1
1:A:41:THR:CG2	1:A:47:PHE:CE2	0.40	3.05	12	1
1:A:12:VAL:HG22	2:D:111:LEU:CD2	0.40	2.46	19	1
1:A:38:PHE:HB2	2:D:84:LEU:HD22	0.40	1.93	4	1
2:D:125:PHE:CE1	2:D:129:ASN:ND2	0.40	2.90	5	1
1:A:22:LYS:NZ	2:D:102:ASP:CB	0.40	2.84	7	1
2:B:112:LEU:CD1	1:C:16:LEU:HD23	0.40	2.46	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:23:LEU:HD13	1:C:31:GLN:CB	0.40	2.47	10	1
1:A:39:TYR:CE1	1:A:43:LYS:CE	0.40	3.05	13	1
2:D:112:LEU:HD23	2:D:112:LEU:N	0.40	2.31	14	1
1:A:22:LYS:CB	2:D:100:LEU:CD2	0.40	3.00	15	1
2:D:90:PHE:CZ	2:D:117:GLN:OE1	0.40	2.74	15	1
1:A:31:GLN:CD	2:D:95:HIS:CD2	0.40	2.95	17	1
2:B:100:LEU:HD23	1:C:26:LYS:CE	0.40	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	56/62 (90%)	55±1 (98±1%)	1±1 (2±1%)	0±0 (0±0%)	54	85
1	C	55/62 (89%)	54±1 (98±1%)	1±1 (2±1%)	0±0 (0±0%)	100	100
2	B	55/60 (92%)	50±1 (90±2%)	3±1 (6±2%)	2±1 (3±2%)	6	35
2	D	53/60 (88%)	48±1 (90±2%)	4±1 (7±2%)	1±1 (2±2%)	9	45
All	All	4380/4880 (90%)	4124 (94%)	191 (4%)	65 (1%)	14	59

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)
2	D	85	GLU	17
2	B	85	GLU	15
2	B	84	LEU	8
2	B	83	ILE	7
2	B	82	LYS	6
2	D	83	ILE	4
2	D	84	LEU	4
2	B	103	SER	2
2	D	103	SER	1
1	A	45	PRO	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	51/56 (91%)	36±2 (70±4%)	15±2 (30±4%)	1 16
1	C	51/56 (91%)	37±2 (72±4%)	14±2 (28±4%)	2 20
2	B	53/56 (95%)	34±3 (65±6%)	19±3 (35±6%)	1 9
2	D	51/56 (91%)	32±2 (64±5%)	18±2 (36±5%)	1 8
All	All	4120/4480 (92%)	2788 (68%)	1332 (32%)	1 13

All 145 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	51	LEU	20
2	B	89	LEU	20
2	B	93	LEU	20
2	B	101	VAL	20
2	B	132	THR	20
1	C	24	GLN	20
1	C	51	LEU	20
2	D	89	LEU	20
2	D	101	VAL	20
2	D	132	THR	20
1	C	29	THR	19
2	D	93	LEU	19
1	A	29	THR	18
2	B	83	ILE	18
2	B	111	LEU	18
2	D	86	ILE	18
1	A	14	GLN	17
1	A	24	GLN	17
1	A	53	LEU	17
2	B	86	ILE	17
2	B	88	ASP	17
1	C	53	LEU	17
2	D	85	GLU	17
2	D	97	GLN	17
2	D	111	LEU	17

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Mol	Chain	Res	Type	Models (Total)
1	A	46	LEU	16
2	B	104	GLN	16
1	C	14	GLN	16
2	B	97	GLN	15
2	D	83	ILE	15
2	D	88	ASP	15
2	D	119	LYS	15
2	B	85	GLU	14
2	B	119	LYS	14
1	C	54	GLN	14
2	D	120	ASP	14
1	A	42	LEU	13
2	B	82	LYS	13
1	C	46	LEU	13
2	D	104	GLN	13
1	A	18	ARG	12
1	A	54	GLN	12
2	B	126	LYS	12
1	C	20	ARG	12
1	C	58	LYS	12
2	D	118	ASN	12
1	A	43	LYS	12
2	B	105	SER	12
1	C	43	LYS	12
2	D	106	GLN	12
2	B	103	SER	11
2	B	106	GLN	11
1	C	59	GLN	11
1	A	10	MET	11
2	B	102	ASP	11
1	A	20	ARG	10
1	A	26	LYS	10
1	C	26	LYS	10
1	C	60	LEU	10
2	D	102	ASP	10
1	A	55	GLN	9
2	B	118	ASN	9
1	A	59	GLN	9
2	D	103	SER	9
2	D	105	SER	9
2	D	107	GLU	9
2	D	126	LYS	9

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Mol	Chain	Res	Type	Models (Total)
2	D	134	HIS	9
1	A	58	LYS	9
2	D	98	HIS	9
1	A	33	GLU	9
1	C	9	LYS	9
1	A	9	LYS	9
1	A	17	ASP	8
1	A	60	LEU	8
1	C	36	SER	8
2	B	134	HIS	8
1	A	56	SER	8
1	C	61	LYS	8
2	B	120	ASP	8
2	B	98	HIS	8
1	C	42	LEU	7
2	B	115	LEU	7
1	C	18	ARG	7
1	A	22	LYS	7
2	B	107	GLU	7
1	C	10	MET	6
1	C	40	GLU	6
2	B	91	SER	6
1	C	17	ASP	6
2	D	92	SER	6
2	D	135	MET	6
2	B	129	ASN	6
2	B	122	GLN	6
1	C	55	GLN	6
1	A	32	ASN	5
1	A	36	SER	5
1	A	61	LYS	5
1	C	44	SER	5
2	D	87	GLU	5
2	D	122	GLN	5
1	C	56	SER	5
2	D	114	GLN	5
2	D	117	GLN	5
1	A	39	TYR	5
1	A	49	GLN	5
1	A	44	SER	5
2	D	94	LYS	5
2	D	95	HIS	5

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Mol	Chain	Res	Type	Models (Total)
2	B	114	GLN	4
2	D	110	SER	4
1	A	34	LYS	4
1	C	49	GLN	4
1	C	32	ASN	4
1	C	33	GLU	4
2	B	92	SER	4
2	B	95	HIS	4
2	B	123	ASN	4
1	A	48	ASN	3
1	C	48	ASN	3
2	B	117	GLN	3
2	B	135	MET	3
2	D	115	LEU	3
2	D	129	ASN	3
1	C	31	GLN	3
2	D	91	SER	3
2	D	123	ASN	3
1	A	8	GLU	2
1	A	35	LEU	2
1	A	31	GLN	2
2	B	94	LYS	2
1	C	22	LYS	2
1	A	40	GLU	2
2	D	112	LEU	2
1	C	35	LEU	1
2	B	110	SER	1
2	B	112	LEU	1
1	A	30	THR	1
2	B	108	ASP	1
1	C	39	TYR	1
2	B	84	LEU	1
1	C	34	LYS	1
2	B	87	GLU	1
2	D	99	THR	1
2	D	90	PHE	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