Full wwPDB NMR Structure Validation Report (i)

Apr 26, 2016 – 07:10 PM BST

PDB ID	:	1Y76
Title	:	Solution Structure of Patj/Pals1 L27 Domain Complex
Authors	:	Feng, W.; Long, J.-F.; Zhang, M.
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
http://wwpdb.org/validation/2016/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:

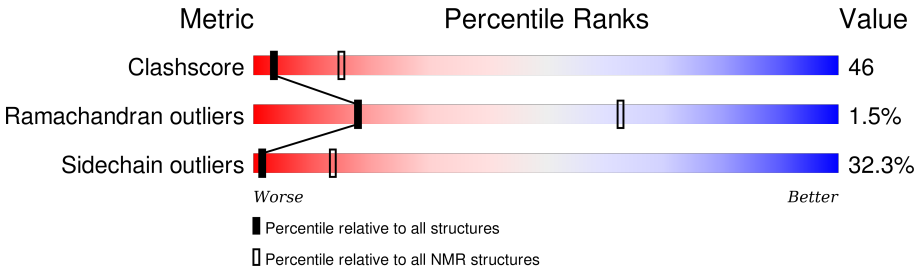
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027457

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	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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	35% 48% 6% 10%
1	C	62	34% 47% 8% 11%
2	B	60	23% 53% 15% 8%
2	D	60	22% 53% 13% 12%

2 Ensemble composition and analysis

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

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
1	A	62	Total	C	H	N	O	S	0
			1017	312	522	87	95	1	
1	C	62	Total	C	H	N	O	S	0
			1017	312	522	87	95	1	

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

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

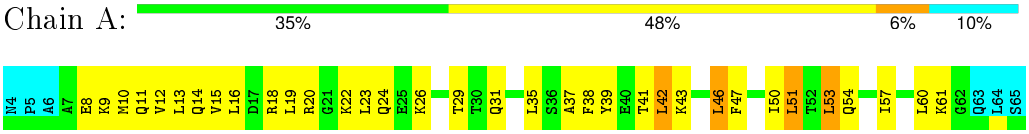
4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA 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.

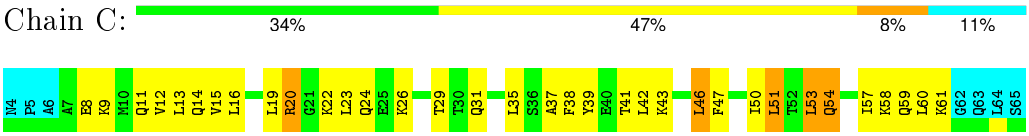
• Molecule 1: protein associated to tight junctions

Chain A:



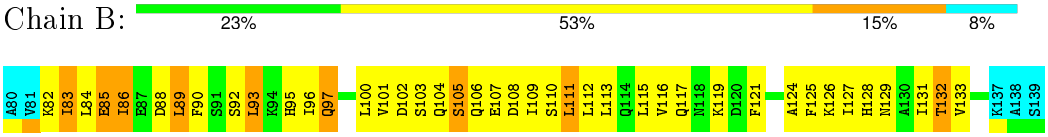
• Molecule 1: protein associated to tight junctions

Chain C:



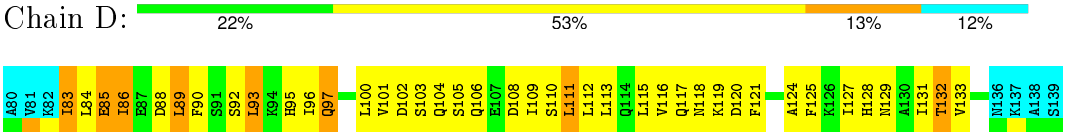
• Molecule 2: MAGUK p55 subfamily member 5

Chain B:



• Molecule 2: MAGUK p55 subfamily member 5

Chain D:



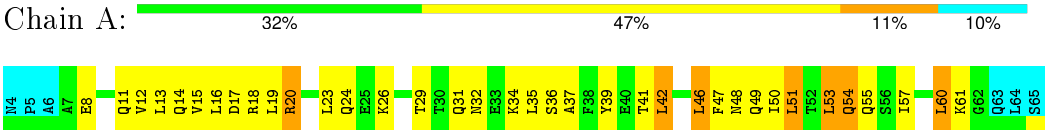
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

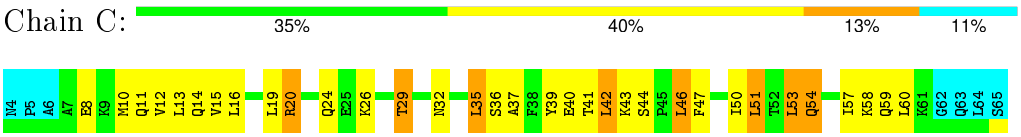
• Molecule 1: protein associated to tight junctions

Chain A:



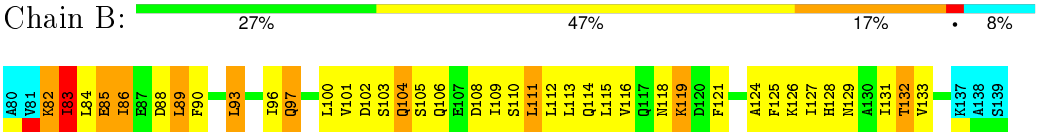
• Molecule 1: protein associated to tight junctions

Chain C:



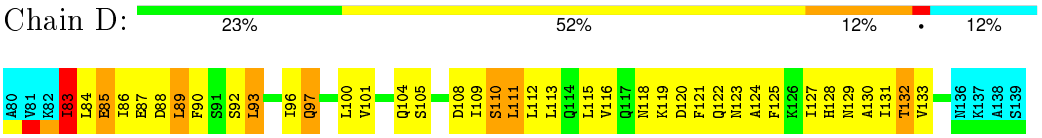
• Molecule 2: MAGUK p55 subfamily member 5

Chain B:



• Molecule 2: MAGUK p55 subfamily member 5

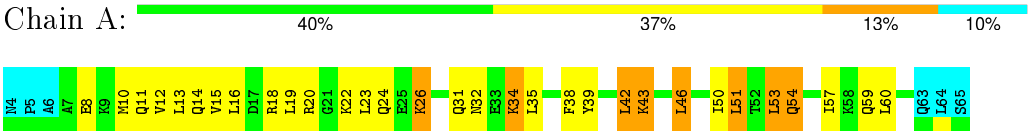
Chain D:



4.2.2 Score per residue for model 2

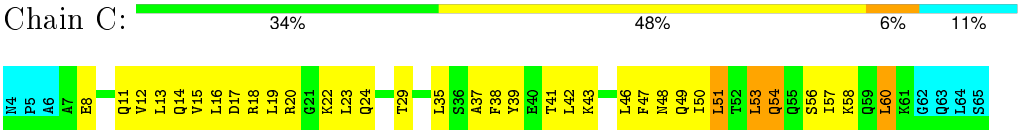
• Molecule 1: protein associated to tight junctions

Chain A:



• Molecule 1: protein associated to tight junctions

Chain C:

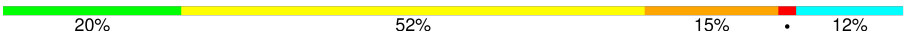


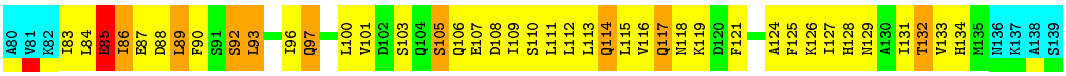
• Molecule 2: MAGUK p55 subfamily member 5

Chain B:

• Molecule 2: MAGUK p55 subfamily member 5

Chain D:

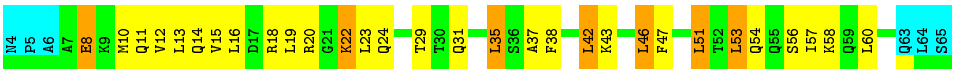




4.2.3 Score per residue for model 3

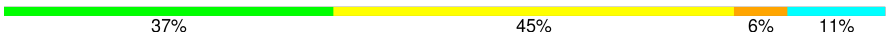
• Molecule 1: protein associated to tight junctions

Chain A:



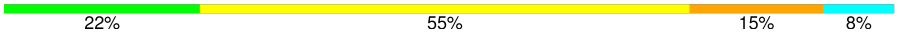
• Molecule 1: protein associated to tight junctions

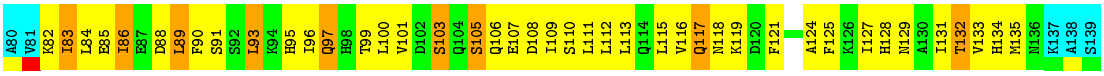
Chain C:



• Molecule 2: MAGUK p55 subfamily member 5

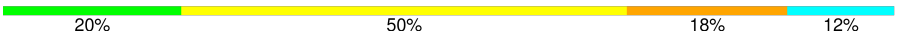
Chain B:





• Molecule 2: MAGUK p55 subfamily member 5

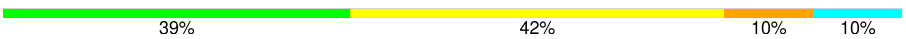
Chain D:

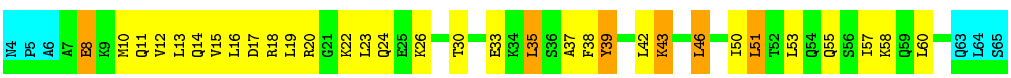


4.2.4 Score per residue for model 4

• Molecule 1: protein associated to tight junctions

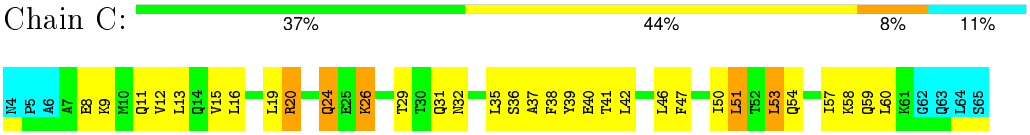
Chain A:





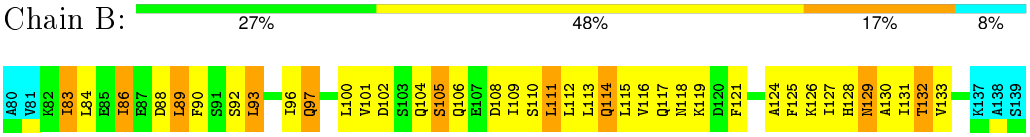
• Molecule 1: protein associated to tight junctions

Chain C:



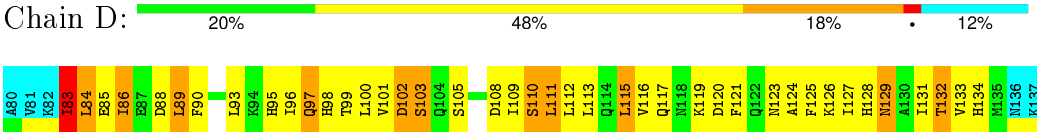
• Molecule 2: MAGUK p55 subfamily member 5

Chain B:



• Molecule 2: MAGUK p55 subfamily member 5

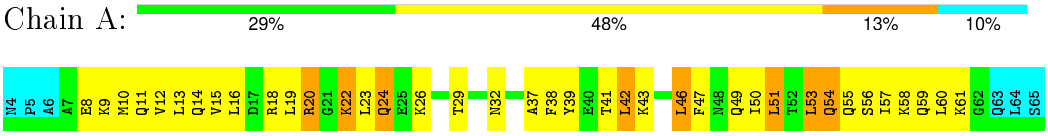
Chain D:



4.2.5 Score per residue for model 5

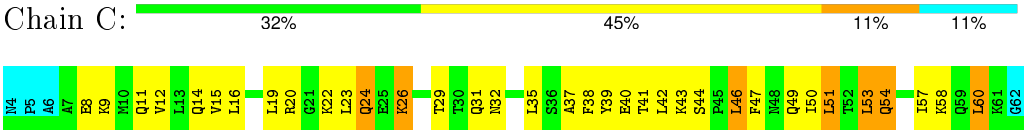
• Molecule 1: protein associated to tight junctions

Chain A:



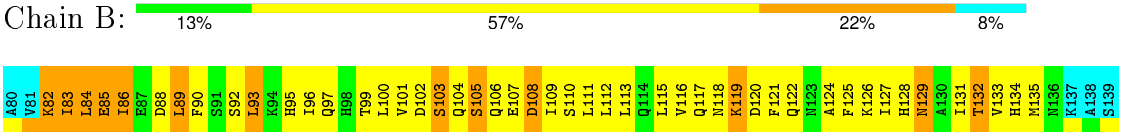
• Molecule 1: protein associated to tight junctions

Chain C:



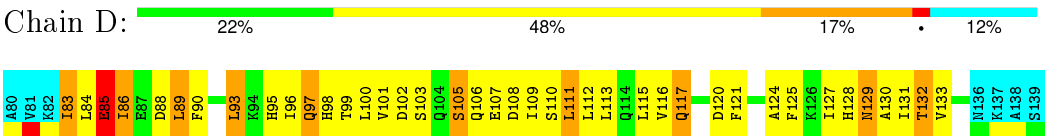
• Molecule 2: MAGUK p55 subfamily member 5

Chain B:



• Molecule 2: MAGUK p55 subfamily member 5

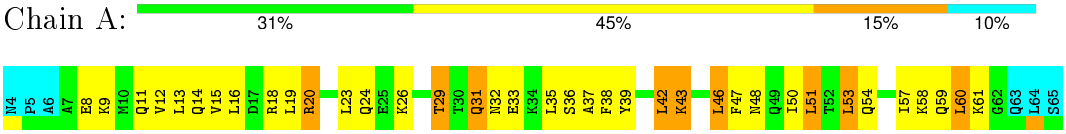
Chain D:



4.2.6 Score per residue for model 6

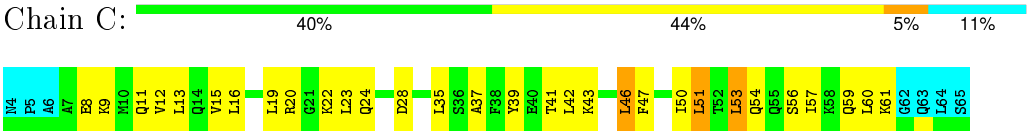
• Molecule 1: protein associated to tight junctions

Chain A:



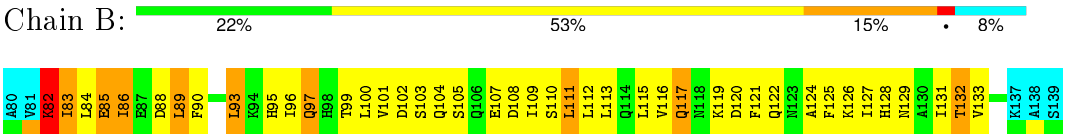
• Molecule 1: protein associated to tight junctions

Chain C:



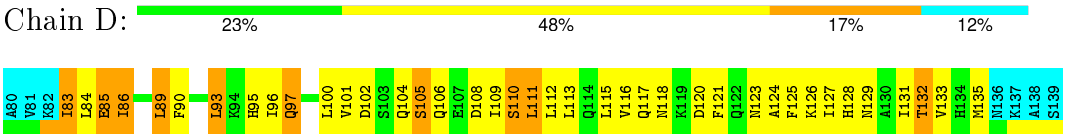
• Molecule 2: MAGUK p55 subfamily member 5

Chain B:



• Molecule 2: MAGUK p55 subfamily member 5

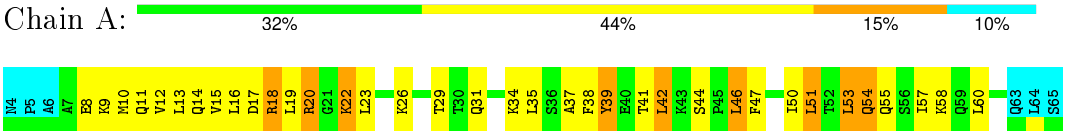
Chain D:



4.2.7 Score per residue for model 7

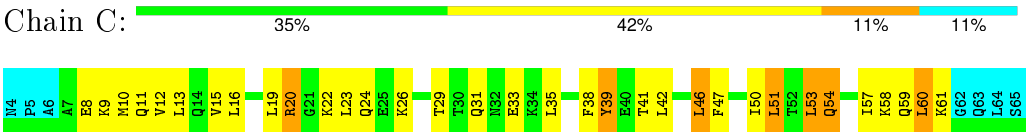
• Molecule 1: protein associated to tight junctions

Chain A:



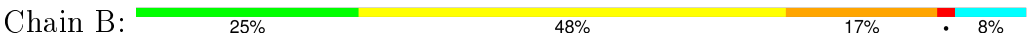
• Molecule 1: protein associated to tight junctions

Chain C:



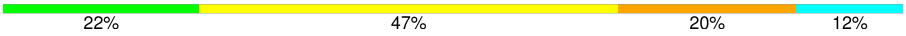
• Molecule 2: MAGUK p55 subfamily member 5

Chain B:



• Molecule 2: MAGUK p55 subfamily member 5

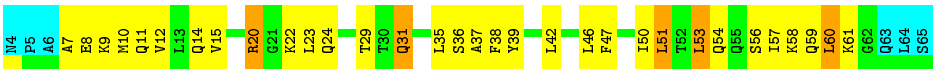
Chain D:



4.2.8 Score per residue for model 8

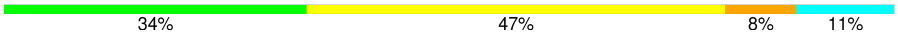
• Molecule 1: protein associated to tight junctions

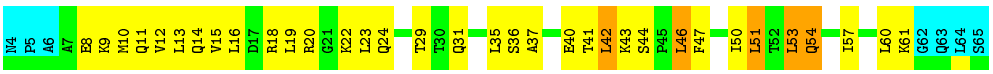
Chain A:



• Molecule 1: protein associated to tight junctions

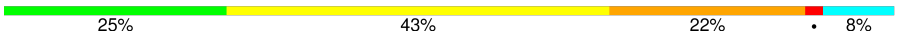
Chain C:





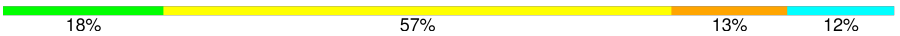
• Molecule 2: MAGUK p55 subfamily member 5

Chain B:



• Molecule 2: MAGUK p55 subfamily member 5

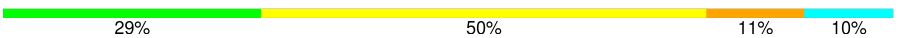
Chain D:



4.2.9 Score per residue for model 9

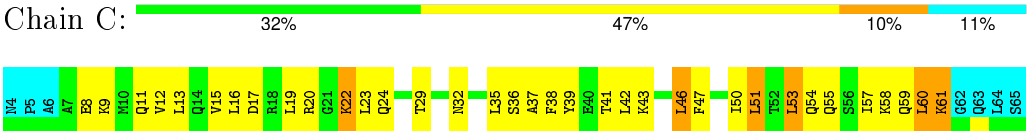
• Molecule 1: protein associated to tight junctions

Chain A:



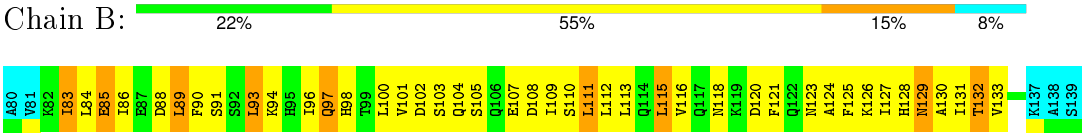
• Molecule 1: protein associated to tight junctions

Chain C:



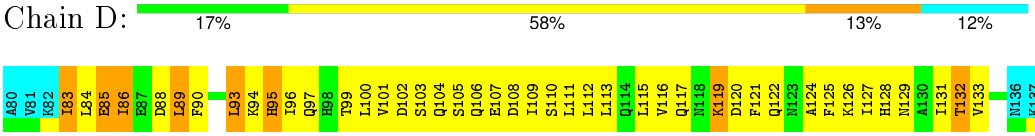
• Molecule 2: MAGUK p55 subfamily member 5

Chain B:



• Molecule 2: MAGUK p55 subfamily member 5

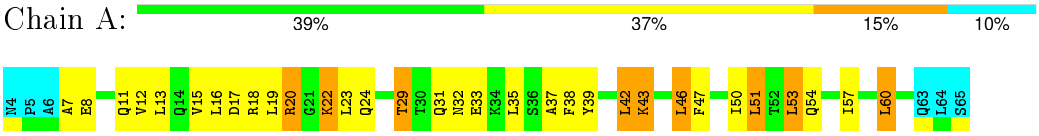
Chain D:



4.2.10 Score per residue for model 10

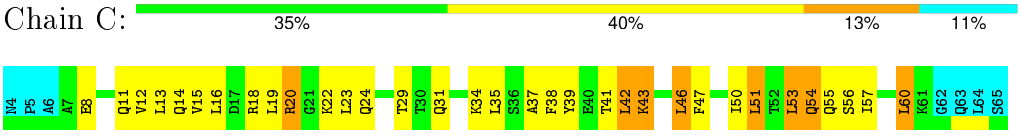
• Molecule 1: protein associated to tight junctions

Chain A:



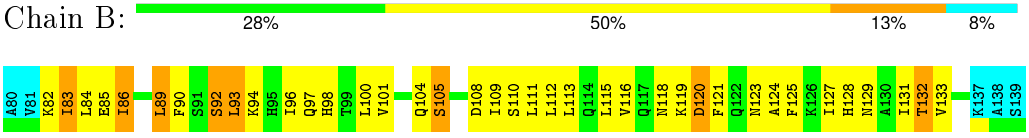
• Molecule 1: protein associated to tight junctions

Chain C:



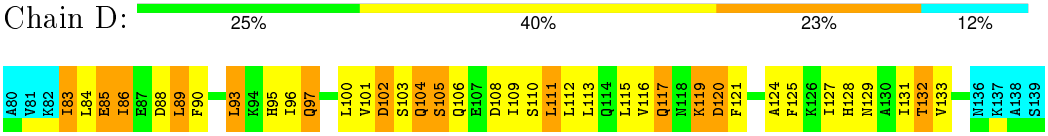
• Molecule 2: MAGUK p55 subfamily member 5

Chain B:



• Molecule 2: MAGUK p55 subfamily member 5

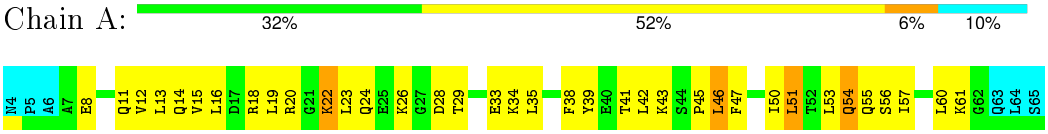
Chain D:



4.2.11 Score per residue for model 11

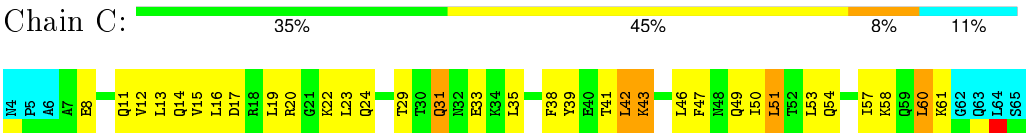
• Molecule 1: protein associated to tight junctions

Chain A:



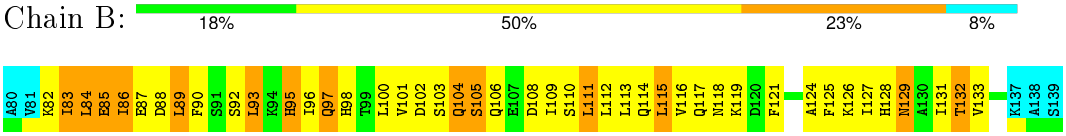
• Molecule 1: protein associated to tight junctions

Chain C:



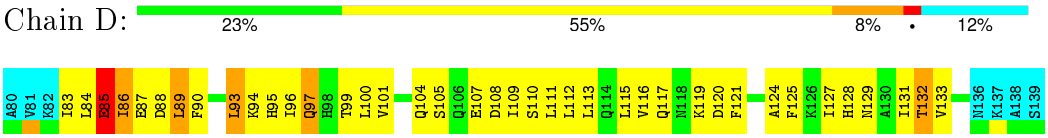
• Molecule 2: MAGUK p55 subfamily member 5

Chain B:



• Molecule 2: MAGUK p55 subfamily member 5

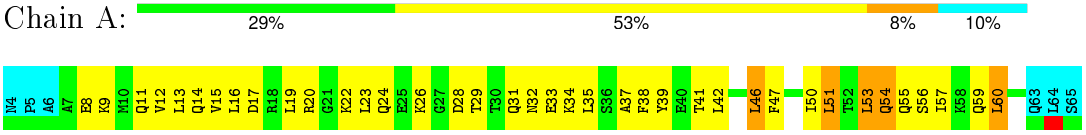
Chain D:



4.2.12 Score per residue for model 12

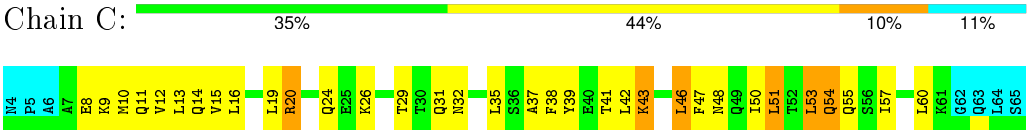
• Molecule 1: protein associated to tight junctions

Chain A:



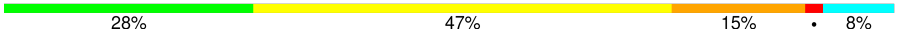
• Molecule 1: protein associated to tight junctions

Chain C:



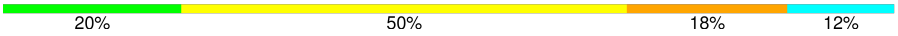
• Molecule 2: MAGUK p55 subfamily member 5

Chain B:



• Molecule 2: MAGUK p55 subfamily member 5

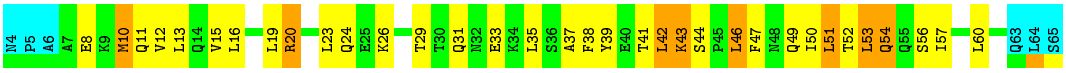
Chain D:



4.2.13 Score per residue for model 13

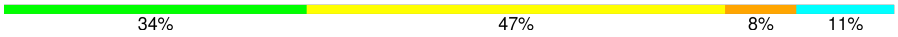
• Molecule 1: protein associated to tight junctions

Chain A:



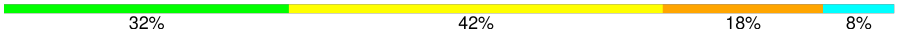
• Molecule 1: protein associated to tight junctions

Chain C:



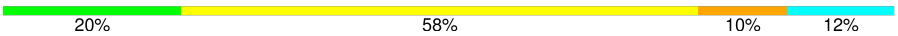
• Molecule 2: MAGUK p55 subfamily member 5

Chain B:



• Molecule 2: MAGUK p55 subfamily member 5

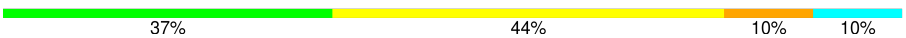
Chain D:

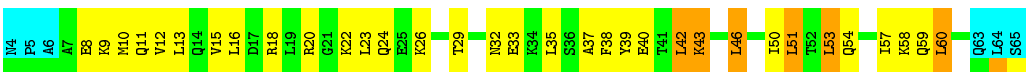


4.2.14 Score per residue for model 14

• Molecule 1: protein associated to tight junctions

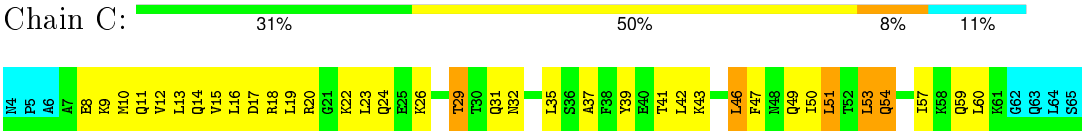
Chain A:





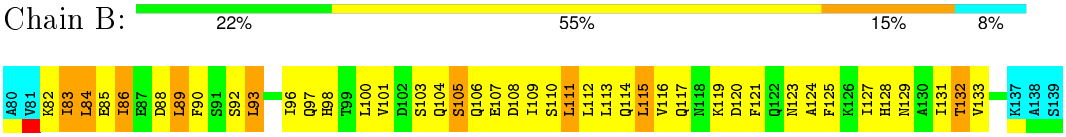
• Molecule 1: protein associated to tight junctions

Chain C:



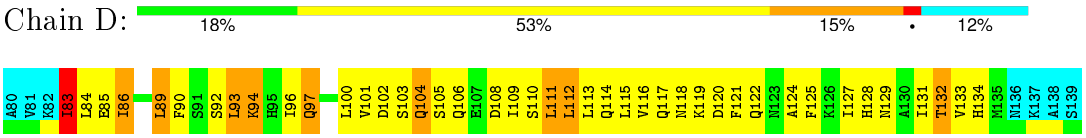
• Molecule 2: MAGUK p55 subfamily member 5

Chain B:



• Molecule 2: MAGUK p55 subfamily member 5

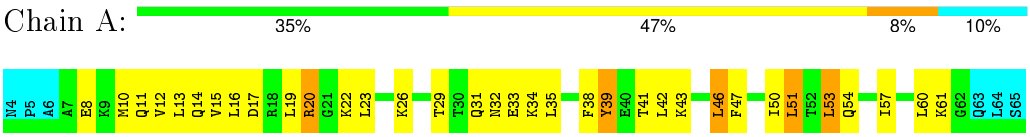
Chain D:



4.2.15 Score per residue for model 15

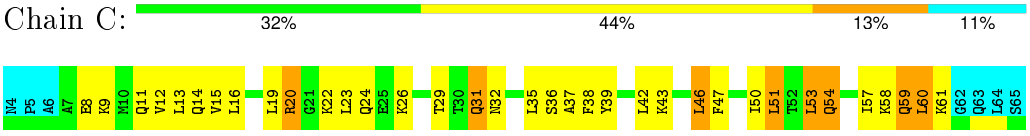
• Molecule 1: protein associated to tight junctions

Chain A:



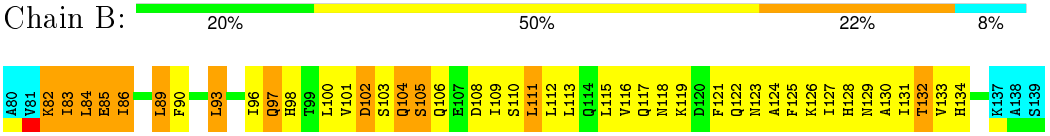
• Molecule 1: protein associated to tight junctions

Chain C:



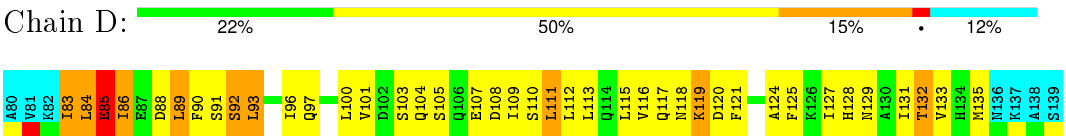
• Molecule 2: MAGUK p55 subfamily member 5

Chain B:



• Molecule 2: MAGUK p55 subfamily member 5

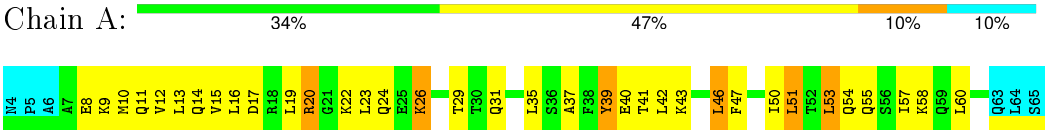
Chain D:



4.2.16 Score per residue for model 16

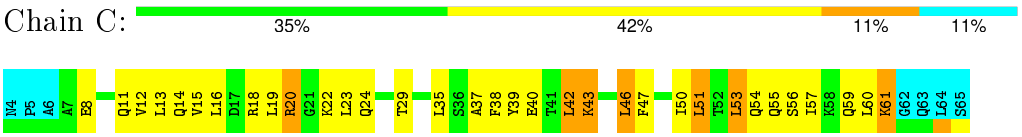
• Molecule 1: protein associated to tight junctions

Chain A:



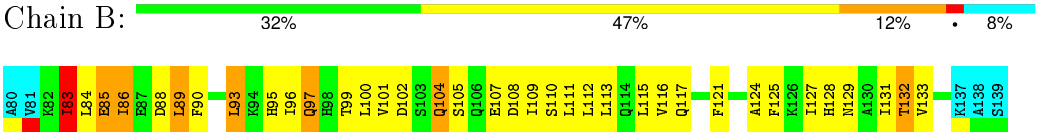
• Molecule 1: protein associated to tight junctions

Chain C:



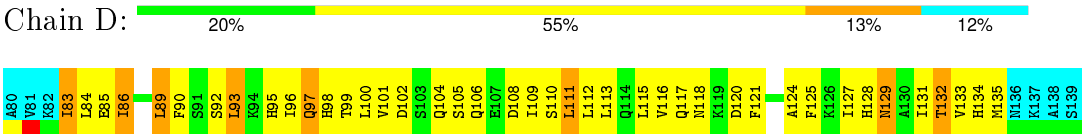
• Molecule 2: MAGUK p55 subfamily member 5

Chain B:



• Molecule 2: MAGUK p55 subfamily member 5

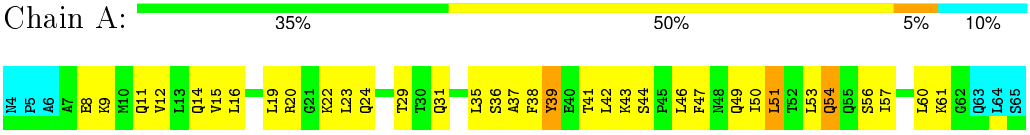
Chain D:



4.2.17 Score per residue for model 17

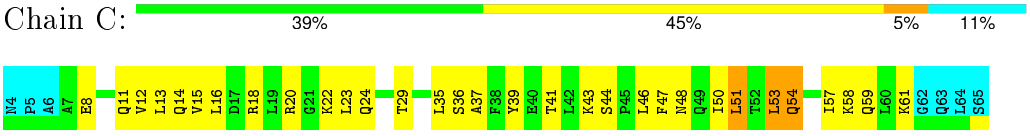
• Molecule 1: protein associated to tight junctions

Chain A:



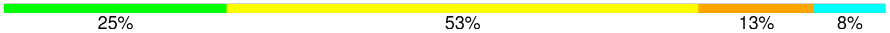
• Molecule 1: protein associated to tight junctions

Chain C:



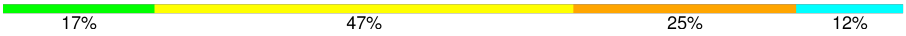
• Molecule 2: MAGUK p55 subfamily member 5

Chain B:



• Molecule 2: MAGUK p55 subfamily member 5

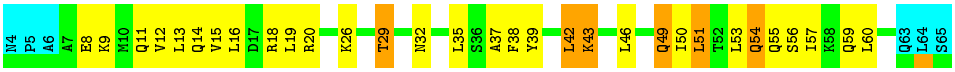
Chain D:



4.2.18 Score per residue for model 18

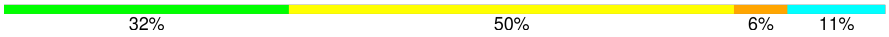
• Molecule 1: protein associated to tight junctions

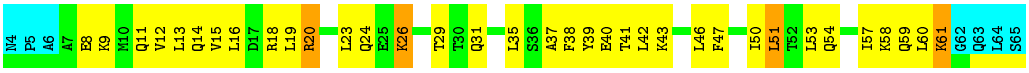
Chain A:



• Molecule 1: protein associated to tight junctions

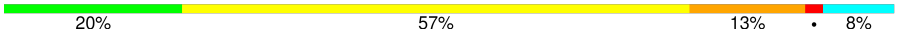
Chain C:

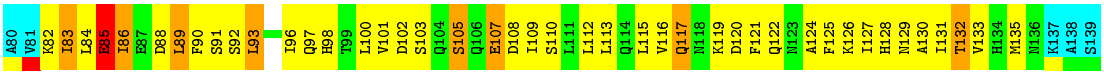




• Molecule 2: MAGUK p55 subfamily member 5

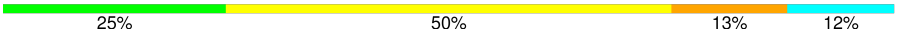
Chain B:

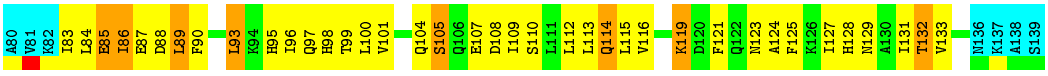




• Molecule 2: MAGUK p55 subfamily member 5

Chain D:

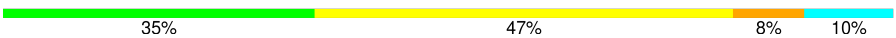




4.2.19 Score per residue for model 19 (medoid)

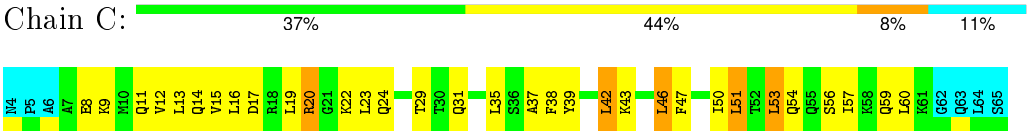
• Molecule 1: protein associated to tight junctions

Chain A:



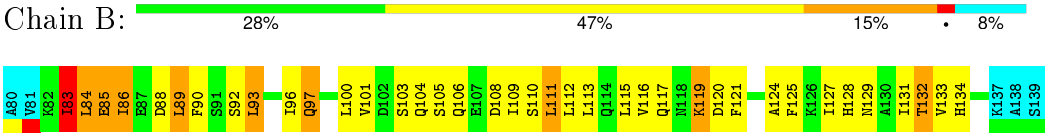
• Molecule 1: protein associated to tight junctions

Chain C:



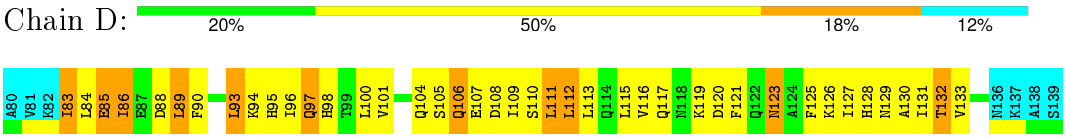
• Molecule 2: MAGUK p55 subfamily member 5

Chain B:



• Molecule 2: MAGUK p55 subfamily member 5

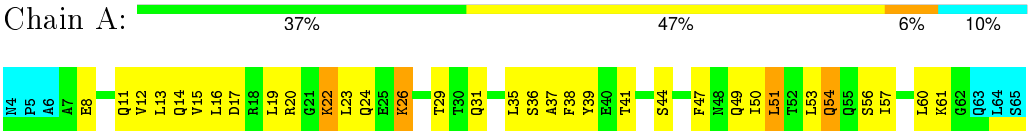
Chain D:



4.2.20 Score per residue for model 20

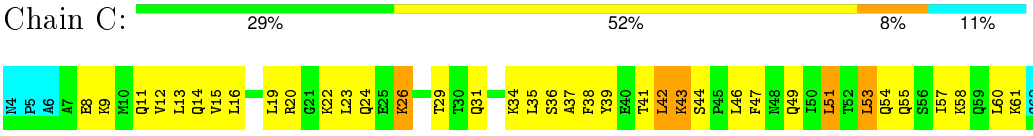
• Molecule 1: protein associated to tight junctions

Chain A:



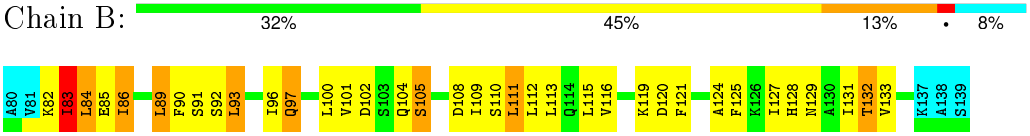
• Molecule 1: protein associated to tight junctions

Chain C:



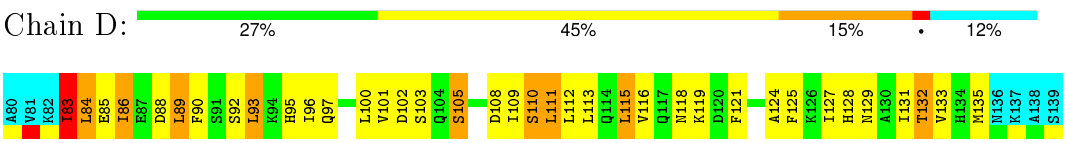
• Molecule 2: MAGUK p55 subfamily member 5

Chain B:



• Molecule 2: MAGUK p55 subfamily member 5

Chain D:



5 Refinement protocol and experimental data overview

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. No validations of the models with respect to experimental NMR restraints is performed at this time.

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	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
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:A:47:PHE:CE1	1:A:51:LEU:HD21	0.84	2.07	12	12
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:D:124:ALA:HA	2:D:127:ILE:HD12	0.74	1.57	12	11
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: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:D:127:ILE:HG22	2:D:131:ILE:HD12	0.72	1.62	6	16
2:B:112:LEU:HD21	1:C:15:VAL:CG1	0.72	2.15	2	19
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
1:A:11:GLN:O	1:A:15:VAL:HG23	0.70	1.86	9	8
2:D:86:ILE:HG13	2:D:89:LEU:HD23	0.70	1.63	17	16
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:C:13:LEU:HA	1:C:16:LEU:HD12	0.70	1.63	6	14
1:A:15:VAL:HG22	2:D:108:ASP:CG	0.70	2.06	17	16
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
1:A:57:ILE:CD1	1:C:46:LEU:HD11	0.69	2.17	13	14
2:B:115:LEU:CD2	1:C:12:VAL:HG21	0.69	2.17	9	16
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:D:84:LEU:HD21	2:D:89:LEU:HD22	0.68	1.63	4	10
2:B:124:ALA:HB2	1:C:54:GLN:NE2	0.68	2.03	2	16
1:C:20:ARG:HB3	1:C:35:LEU:HD12	0.68	1.65	6	8
2:B:111:LEU:HD23	1:C:12:VAL:HG22	0.68	1.64	7	14
1:A:20:ARG:CA	1:A:35:LEU:HD12	0.68	2.18	6	13
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:61:LYS:HE3	2:B:131:ILE:HG23	0.67	1.63	9	1
1:C:20:ARG:N	1:C:35:LEU:HD12	0.67	2.04	1	13
1:A:37:ALA:HB3	2:D:84:LEU:CD2	0.67	2.12	1	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	7
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:57:ILE:HD13	1:C:46:LEU:HD11	0.65	1.69	15	9
1:A:37:ALA:CB	2:D:84:LEU:HD13	0.65	2.21	7	5
1:C:61:LYS:NZ	2:D:131:ILE:HG23	0.65	2.07	20	3
1:C:35:LEU:N	1:C:35:LEU:HD23	0.64	2.07	10	12
2:B:108:ASP:HB3	1:C:15:VAL:HG13	0.64	1.69	8	20
1:C:9:LYS:HE2	1:C:13:LEU:HD11	0.64	1.70	12	3
2:D:100:LEU:HD13	2:D:105:SER:OG	0.64	1.92	10	4
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:61:LYS:HE3	2:D:131:ILE:HG23	0.64	1.70	9	1
1:C:38:PHE:CE1	1:C:42:LEU:HD11	0.64	2.28	18	5
2:D:105:SER:C	2:D:109:ILE:HD12	0.64	2.13	8	19
1:A:35:LEU:HD23	1:A:35:LEU:N	0.64	2.08	12	8
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:C:35:LEU:HD23	1:C:35:LEU:N	0.63	2.08	5	6
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
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
1:A:13:LEU:HD13	1:A:43:LYS:HZ1	0.63	1.52	14	2
2:B:86:ILE:HG23	2:B:116:VAL:CG1	0.63	2.23	13	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:D:86:ILE:HG23	2:D:116:VAL:HG12	0.63	1.69	15	5
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
2:B:89:LEU:HD12	2:B:89:LEU:O	0.62	1.94	1	11
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
2:D:89:LEU:O	2:D:89:LEU:HD12	0.62	1.95	6	7
1:A:57:ILE:HD11	1:C:46:LEU:HD11	0.62	1.72	5	4
1:A:26:LYS:HE2	2:D:100:LEU:HD23	0.62	1.70	2	3
2:D:83:ILE:N	2:D:83:ILE:HD13	0.62	2.08	4	8
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
1:A:35:LEU:N	1:A:35:LEU:HD23	0.62	2.10	3	9
2:B:83:ILE:HD13	2:B:83:ILE:N	0.62	2.10	18	7
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:N	2:D:93:LEU:HD23	0.60	2.11	17	12
1:C:57:ILE:HA	1:C:60:LEU:HD12	0.60	1.72	4	18
1:A:22:LYS:HB3	2:D:100:LEU:HD22	0.60	1.71	16	13
2:D:84:LEU:CD1	2:D:89:LEU:HD22	0.60	2.24	1	1
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
2:D:89:LEU:HD12	2:D:89:LEU:O	0.60	1.95	18	7
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	10
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:38:PHE:CE1	1:A:42:LEU:HD11	0.59	2.32	11	4
2:B:96:ILE:CG2	2:B:100:LEU:HD12	0.59	2.28	10	7
2:D:84:LEU:CD1	2:D:89:LEU:CB	0.59	2.81	1	4
2:B:93:LEU:HD13	2:B:112:LEU:HB2	0.59	1.75	3	20
2:B:86:ILE:HD12	2:B:125:PHE:CD1	0.59	2.33	5	9
1:A:12:VAL:HG22	2:D:111:LEU:HD23	0.59	1.75	7	13
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
2:D:83:ILE:HD13	2:D:83:ILE:N	0.57	2.14	10	5
1:A:60:LEU:CD1	1:C:46:LEU:HD21	0.57	2.28	18	4
1:C:51:LEU:HD23	1:C:51:LEU:N	0.57	2.14	10	10
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:C:20:ARG:CB	1:C:35:LEU:HD12	0.57	2.28	7	17
1:A:51:LEU:HD23	1:A:51:LEU:N	0.57	2.14	6	4
2:D:96:ILE:HG22	2:D:109:ILE:CD1	0.57	2.29	13	2
2:B:100:LEU:HD22	1:C:22:LYS:HB3	0.57	1.75	9	12
2:D:127:ILE:HG22	2:D:131:ILE:CD1	0.57	2.29	6	4
1:A:51:LEU:N	1:A:51:LEU:HD23	0.57	2.14	5	14
2:B:83:ILE:N	2:B:83:ILE:HD13	0.57	2.15	3	5
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:93:LEU:HD23	2:B:93:LEU:N	0.57	2.15	4	6
2:B:119:LYS:CE	2:D:130:ALA:HB1	0.57	2.30	5	2
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:119:LYS:HD2	2:D:130:ALA:HB1	0.56	1.78	19	1
1:C:11:GLN:NE2	1:C:15:VAL:HG21	0.56	2.14	2	1
2:B:93:LEU:N	2:B:93:LEU:HD23	0.56	2.16	14	14
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
2:D:97:GLN:HB2	2:D:109:ILE:HG21	0.55	1.77	16	2
1:A:34:LYS:HA	2:D:84:LEU:HD21	0.55	1.78	1	1
1:A:60:LEU:HD13	1:C:46:LEU:HD21	0.55	1.78	11	4
2:B:111:LEU:CD2	1:C:12:VAL:HG22	0.55	2.31	16	1
2:D:93:LEU:HD23	2:D:93:LEU:N	0.55	2.16	16	8
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:84:LEU:HD23	2:B:89:LEU:HD22	0.54	1.80	10	6
2:B:96:ILE:HD11	1:C:31:GLN:HB3	0.54	1.79	20	8
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
2:D:83:ILE:HG21	2:D:129:ASN:CG	0.54	2.23	10	3
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: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: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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:54:GLN:HE21	2:D:124:ALA:HB2	0.52	1.65	3	5
2:D:84:LEU:HD23	2:D:125:PHE:HZ	0.52	1.65	15	3
1:A:50:ILE:CG1	1:C:53:LEU:HD21	0.52	2.34	2	4
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
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:20:ARG:HA	1:C:23:LEU:HD12	0.51	1.82	15	6
2:B:84:LEU:HD23	2:B:125:PHE:CZ	0.51	2.41	15	6
1:C:23:LEU:HD13	1:C:31:GLN:HB2	0.51	1.82	10	3
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
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:57:ILE:HG21	2:B:131:ILE:HD13	0.51	1.82	3	1
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
2:B:86:ILE:O	2:B:90:PHE:CB	0.50	2.59	2	17
1:A:39:TYR:CZ	1:A:43:LYS:CE	0.50	2.95	2	5
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
2:B:100:LEU:HD12	1:C:19:LEU:HD22	0.50	1.83	3	5
1:A:46:LEU:O	1:A:49:GLN:CG	0.50	2.60	1	1
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:84:LEU:HD23	2:D:89:LEU:HD22	0.49	1.84	3	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:D:83:ILE:HG22	2:D:84:LEU:H	0.49	1.67	1	2
2:D:86:ILE:CG1	2:D:116:VAL:HG13	0.49	2.36	7	6
1:C:29:THR:HG22	1:C:32:ASN:HD21	0.49	1.67	14	2
2:B:130:ALA:HB1	2:D:119:LYS:HE3	0.49	1.83	7	1
2:D:86:ILE:CD1	2:D:125:PHE:CG	0.49	2.96	19	7
1:A:15:VAL:HG22	2:D:108:ASP:OD1	0.49	2.06	17	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
2:B:108:ASP:OD1	1:C:15:VAL:HG22	0.49	2.07	7	8
2:D:89:LEU:HD11	2:D:116:VAL:CG2	0.49	2.38	15	3
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
1:A:38:PHE:CD2	1:A:42:LEU:HD11	0.49	2.43	15	1
2:D:86:ILE:HD11	2:D:125:PHE:CG	0.49	2.42	1	3
1:A:11:GLN:NE2	2:D:111:LEU:HD13	0.49	2.23	19	1
1:C:13:LEU:HD21	1:C:42:LEU:HD22	0.49	1.85	10	1
1:A:16:LEU:CD2	2:D:112:LEU:HD13	0.49	2.38	3	2
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
2:B:86:ILE:HD11	2:B:125:PHE:CG	0.48	2.43	13	5
1:A:38:PHE:CE1	1:A:42:LEU:CD1	0.48	2.96	11	3
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:23:LEU:HD23	2:D:100:LEU:CD2	0.48	2.38	10	1
1:A:47:PHE:CE2	1:A:51:LEU:HD11	0.48	2.43	8	1
1:A:47:PHE:CE2	1:A:51:LEU:HD21	0.48	2.44	8	1
2:B:112:LEU:HD13	1:C:16:LEU:CD2	0.48	2.39	8	3
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:130:ALA:HB1	2:D:119:LYS:CE	0.48	2.38	18	2
2:D:86:ILE:HD11	2:D:125:PHE:CB	0.48	2.39	1	1
1:A:12:VAL:HG21	2:D:115:LEU:HD22	0.48	1.85	19	1
1:C:47:PHE:HD1	1:C:50:ILE:HD12	0.48	1.67	5	1
1:C:54:GLN:NE2	2:D:127:ILE:HD13	0.48	2.23	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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
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
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
2:B:84:LEU:HD23	2:B:125:PHE:CE2	0.47	2.44	5	2
1:A:57:ILE:HG13	1:C:46:LEU:HD12	0.47	1.86	4	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:CD2	1:C:35:LEU:N	0.47	2.77	10	6
2:B:83:ILE:HG22	2:B:84:LEU:H	0.47	1.70	17	2
2:B:114:GLN:HG3	2:B:115:LEU:N	0.47	2.23	4	1
2:D:90:PHE:CE1	2:D:117:GLN:CG	0.47	2.98	9	7
2:B:83:ILE:HG22	2:B:129:ASN:HB2	0.47	1.87	4	1
1:A:38:PHE:CA	2:D:84:LEU:HD22	0.47	2.39	7	1
2:B:124:ALA:HB2	1:C:54:GLN:HE21	0.47	1.68	9	3
1:A:16:LEU:HD21	1:A:38:PHE:HD2	0.47	1.68	7	3
2:B:93:LEU:HD11	2:B:116:VAL:HG21	0.47	1.87	20	3
2:D:86:ILE:HG13	2:D:89:LEU:CD2	0.47	2.37	17	9
2:B:100:LEU:HB2	2:B:109:ILE:HD11	0.46	1.85	10	2
2:B:86:ILE:CG1	2:B:116:VAL:HG13	0.46	2.36	4	3
2:B:83:ILE:CD1	2:B:83:ILE:N	0.46	2.76	18	3
2:B:97:GLN:CG	2:B:109:ILE:HG21	0.46	2.40	19	7
1:A:35:LEU:CD2	1:A:35:LEU:N	0.46	2.78	11	4
2:D:84:LEU:O	2:D:84:LEU:HG	0.46	2.10	17	1
1:C:39:TYR:CZ	1:C:43:LYS:CE	0.46	2.98	12	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:C:30:THR:HG22	1:C:31:GLN:HE21	0.46	1.70	3	1
1:C:38:PHE:CE1	1:C:42:LEU:CD1	0.46	2.98	13	6
2:B:86:ILE:HG23	2:B:116:VAL:HG12	0.46	1.88	4	6
2:B:83:ILE:HD12	2:B:132:THR:HG22	0.46	1.87	18	2
1:A:22:LYS:CB	2:D:100:LEU:HD22	0.46	2.39	2	2
2:B:124:ALA:HB1	1:C:50:ILE:HG22	0.46	1.88	10	1
1:A:39:TYR:CE1	1:A:43:LYS:CD	0.46	2.99	11	2
1:A:41:THR:CG2	1:A:47:PHE:CD2	0.46	2.99	17	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:16:LEU:HD13	1:A:39:TYR:HB2	0.46	1.87	18	3
1:C:39:TYR:CE1	1:C:43:LYS:CD	0.46	2.99	1	2
1:C:16:LEU:HD21	1:C:38:PHE:HD2	0.46	1.70	7	3
1:A:50:ILE:HG12	1:C:53:LEU:HD11	0.46	1.87	2	3
2:B:90:PHE:CE1	2:B:117:GLN:CG	0.46	2.99	16	7
2:B:127:ILE:CD1	2:D:127:ILE:CD1	0.46	2.93	17	3
1:C:38:PHE:O	1:C:42:LEU:HD12	0.46	2.11	11	1
1:C:38:PHE:CE2	1:C:42:LEU:CD1	0.46	2.99	20	2
2:B:96:ILE:HG22	2:B:100:LEU:HD12	0.46	1.88	19	3
1:A:54:GLN:CD	2:D:124:ALA:HB2	0.46	2.31	2	1
1:A:38:PHE:CZ	1:A:42:LEU:CD1	0.46	2.99	14	1
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
1:A:39:TYR:CZ	1:A:43:LYS:NZ	0.45	2.84	10	4
2:D:84:LEU:O	2:D:85:GLU:O	0.45	2.35	2	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:132:THR:CG2	2:D:133:VAL:N	0.45	2.80	15	7
2:D:113:LEU:O	2:D:117:GLN:CG	0.45	2.65	2	5
2:D:97:GLN:CB	2:D:109:ILE:HG21	0.45	2.41	2	2
1:C:41:THR:CG2	1:C:47:PHE:CD1	0.45	2.99	7	1
1:A:31:GLN:NE2	2:D:95:HIS:CD2	0.45	2.84	16	2
2:B:132:THR:HG22	2:B:133:VAL:N	0.45	2.26	7	5
2:B:90:PHE:CE1	2:B:113:LEU:HD23	0.45	2.47	2	2
1:A:53:LEU:HD12	1:C:49:GLN:HB3	0.45	1.89	11	1
1:A:41:THR:CG2	1:A:47:PHE:CE1	0.45	2.99	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:C	2:D:121:PHE:CD1	0.45	2.91	10	4
1:A:46:LEU:CD1	1:C:57:ILE:CD1	0.45	2.94	6	3
1:A:16:LEU:HD11	1:A:42:LEU:HD13	0.45	1.87	6	1
2:D:90:PHE:CE1	2:D:117:GLN:NE2	0.45	2.85	11	2
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: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
2:B:113:LEU:O	2:B:117:GLN:CG	0.44	2.65	18	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:102:ASP:O	2:B:103:SER:CB	0.44	2.65	5	1
1:A:57:ILE:HG12	1:C:46:LEU:CD1	0.44	2.43	4	1
2:D:89:LEU:O	2:D:93:LEU:CD2	0.44	2.66	2	1
1:A:57:ILE:CG2	2:B:131:ILE:CG2	0.44	2.96	16	4
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
1:A:10:MET:HA	1:A:10:MET:HE2	0.44	1.89	14	1
2:D:83:ILE:HG21	2:D:133:VAL:CG2	0.44	2.43	12	1
2:B:89:LEU:CD1	2:B:93:LEU:HD21	0.44	2.41	17	4
2:B:86:ILE:HD12	2:B:125:PHE:CB	0.44	2.42	11	1
2:D:83:ILE:CD1	2:D:83:ILE:N	0.44	2.76	4	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
2:D:84:LEU:CD1	2:D:89:LEU:HB2	0.44	2.43	11	3
1:C:57:ILE:HG22	2:D:131:ILE:HG21	0.44	1.89	5	3
2:B:84:LEU:CD1	2:B:89:LEU:HB2	0.44	2.42	11	1
1:A:41:THR:HG22	1:A:47:PHE:CE2	0.44	2.48	16	2
1:A:22:LYS:O	1:A:26:LYS:CD	0.44	2.66	12	3
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:11:GLN:NE2	1:A:15:VAL:CG2	0.43	2.81	12	10
1:A:57:ILE:CG1	1:C:46:LEU:CD1	0.43	2.96	16	5
2:B:90:PHE:CZ	2:B:117:GLN:HG2	0.43	2.48	17	1
1:A:46:LEU:CD1	1:C:57:ILE:CG1	0.43	2.96	12	6
2:B:121:PHE:CD1	2:B:121:PHE:C	0.43	2.92	11	4
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
2:D:95:HIS:O	2:D:99:THR:N	0.43	2.51	5	6
1:A:13:LEU:O	1:A:39:TYR:CZ	0.43	2.71	4	1
2:D:102:ASP:O	2:D:103:SER:CB	0.43	2.66	4	1
2:B:100:LEU:CD1	1:C:19:LEU:HD22	0.43	2.43	8	3
2:B:130:ALA:HB1	2:D:119:LYS:NZ	0.43	2.28	15	1
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:D:93:LEU:HB2	2:D:113:LEU:HD21	0.43	1.90	4	1
2:D:90:PHE:CE1	2:D:113:LEU:HD23	0.43	2.49	15	1
1:C:57:ILE:CG2	2:D:131:ILE:CG2	0.43	2.96	2	2
1:A:49:GLN:O	1:A:52:THR:HG22	0.43	2.14	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:13:LEU:O	1:C:39:TYR:CE2	0.43	2.71	7	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:D:121:PHE:CD1	2:D:121:PHE:C	0.43	2.92	11	9
2:B:113:LEU:O	2:B:117:GLN:HG3	0.43	2.14	17	2
1:C:13:LEU:HD13	1:C:43:LYS:HZ1	0.43	1.74	11	2
2:B:93:LEU:HB2	2:B:113:LEU:HD21	0.43	1.90	12	3
2:D:84:LEU:O	2:D:85:GLU:C	0.43	2.55	17	1
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:A:35:LEU:N	1:A:35:LEU:CD2	0.43	2.82	9	1
2:B:96:ILE:HG12	1:C:23:LEU:HD11	0.43	1.89	10	1
2:B:95:HIS:CD2	2:B:95:HIS:C	0.43	2.92	11	4
2:D:83:ILE:HG22	2:D:129:ASN:CG	0.43	2.34	13	1
2:D:83:ILE:O	2:D:84:LEU:HB3	0.43	2.14	12	1
2:B:95:HIS:O	2:B:99:THR:N	0.43	2.52	5	5
2:B:120:ASP:OD2	2:D:131:ILE:HD13	0.43	2.13	10	1
1:A:16:LEU:HD13	1:A:39:TYR:CB	0.43	2.43	18	2
2:B:90:PHE:CE1	2:B:117:GLN:HG2	0.43	2.49	17	1
1:C:13:LEU:HD13	1:C:39:TYR:HE1	0.43	1.73	4	1
2:B:83:ILE:CD1	2:B:132:THR:CG2	0.43	2.97	19	3
2:B:104:GLN:O	2:B:107:GLU:HG2	0.43	2.14	16	2
1:A:20:ARG:H	1:A:35:LEU:HD12	0.43	1.72	11	1
1:C:24:GLN:CG	1:C:32:ASN:ND2	0.43	2.81	5	2
2:B:84:LEU:O	2:B:84:LEU:HG	0.43	2.12	14	2
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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
2:D:111:LEU:HD23	2:D:112:LEU:HD23	0.42	1.91	9	1
1:C:11:GLN:NE2	1:C:15:VAL:CG2	0.42	2.82	6	13
2:B:124:ALA:HB1	1:C:50:ILE:CG2	0.42	2.44	10	1
2:B:95:HIS:CD2	1:C:31:GLN:HG3	0.42	2.50	11	2
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
1:A:49:GLN:CD	1:C:53:LEU:HD12	0.42	2.35	18	1
2:B:90:PHE:O	2:B:94:LYS:HG2	0.42	2.15	12	1
2:D:86:ILE:CG2	2:D:116:VAL:HG12	0.42	2.44	15	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:B:100:LEU:CD2	1:C:22:LYS:CB	0.42	2.97	10	1
1:A:46:LEU:HG	1:A:47:PHE:N	0.42	2.29	6	1
1:A:31:GLN:OE1	2:D:95:HIS:CD2	0.42	2.73	20	3
2:D:132:THR:HG22	2:D:133:VAL:N	0.42	2.30	3	2
1:A:19:LEU:CD2	2:D:100:LEU:HD12	0.42	2.41	18	2
1:C:39:TYR:CE1	1:C:43:LYS:HD3	0.42	2.50	9	1
1:A:13:LEU:O	1:A:39:TYR:CE2	0.42	2.73	15	3
2:D:83:ILE:O	2:D:84:LEU:CB	0.42	2.68	4	1
2:B:83:ILE:O	2:B:84:LEU:HB2	0.42	2.14	7	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:96:ILE:HG22	2:B:109:ILE:HD11	0.41	1.90	2	2
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
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
1:A:53:LEU:CD2	1:C:50:ILE:HG23	0.41	2.44	16	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:C:35:LEU:N	1:C:35:LEU:CD2	0.41	2.83	12	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
1:A:23:LEU:HB3	1:A:28:ASP:O	0.41	2.15	12	2
2:D:83:ILE:CD1	2:D:132:THR:HG22	0.41	2.45	7	1
1:A:19:LEU:CD2	2:D:100:LEU:CD1	0.41	2.99	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:121:PHE:C	2:B:121:PHE:CD1	0.41	2.93	1	4
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
2:D:84:LEU:HG	2:D:84:LEU:O	0.41	2.13	8	1
1:C:39:TYR:CE1	1:C:43:LYS:HE3	0.41	2.51	16	1
2:B:109:ILE:HG22	2:B:113:LEU:HD11	0.41	1.93	5	1
1:A:39:TYR:CD1	1:A:43:LYS:HE3	0.41	2.50	4	1
1:C:47:PHE:CE1	1:C:51:LEU:HD11	0.41	2.51	19	1
2:B:83:ILE:CG2	2:B:129:ASN:ND2	0.41	2.84	19	1
1:A:47:PHE:CE1	1:A:51:LEU:HD11	0.41	2.51	10	2
2:B:86:ILE:CD1	2:B:125:PHE:CB	0.41	2.99	8	4
1:A:50:ILE:HG23	1:C:53:LEU:CD2	0.41	2.46	4	1
1:A:16:LEU:HB2	1:A:39:TYR:CD2	0.41	2.51	7	1
1:A:11:GLN:HE22	2:D:111:LEU:HD13	0.41	1.75	19	1
1:A:8:GLU:O	1:A:12:VAL:N	0.41	2.51	19	1
2:D:113:LEU:O	2:D:117:GLN:HG3	0.41	2.16	19	1
1:C:38:PHE:CZ	1:C:42:LEU:CD1	0.41	3.01	10	1
2:D:89:LEU:CD1	2:D:93:LEU:HD21	0.41	2.44	6	1
1:A:31:GLN:NE2	2:D:95:HIS:NE2	0.41	2.68	16	1
2:B:84:LEU:O	2:B:125:PHE:CE1	0.41	2.74	8	1
2:B:124:ALA:N	1:C:54:GLN:NE2	0.41	2.68	19	1
2:B:83:ILE:N	2:B:83:ILE:CD1	0.41	2.83	6	2
1:C:39:TYR:CZ	1:C:43:LYS:HE3	0.41	2.51	11	2
1:A:39:TYR:CE1	1:A:43:LYS:HE3	0.41	2.51	4	1
2:B:84:LEU:CD1	2:B:89:LEU:CB	0.40	2.99	11	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:D:83:ILE:O	2:D:84:LEU:HB2	0.40	2.16	4	1
1:C:22:LYS:O	1:C:26:LYS:N	0.40	2.54	14	1
2:D:97:GLN:NE2	2:D:106:GLN:NE2	0.40	2.69	19	1
2:B:115:LEU:N	2:B:115:LEU:CD1	0.40	2.84	11	1
2:B:103:SER:O	2:B:106:GLN:CG	0.40	2.70	3	1
2:D:84:LEU:O	2:D:125:PHE:CZ	0.40	2.74	8	1
2:B:115:LEU:CD1	2:B:115:LEU:N	0.40	2.84	8	2
2:D:95:HIS:C	2:D:95:HIS:CD2	0.40	2.94	8	1
2:B:125:PHE:CE1	2:B:129:ASN:OD1	0.40	2.74	14	1
2:D:115:LEU:N	2:D:115:LEU:CD1	0.40	2.84	20	1
1:A:54:GLN:NE2	2:D:124:ALA:N	0.40	2.70	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:46:LEU:HG	1:C:47:PHE:N	0.40	2.31	1	1
2:B:84:LEU:HD21	2:B:89:LEU:HB2	0.40	1.93	1	1
2:B:95:HIS:C	2:B:95:HIS:CD2	0.40	2.94	5	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
2:D:127:ILE:CG2	2:D:131:ILE:HD12	0.40	2.45	18	1
1:A:12:VAL:HG22	2:D:111:LEU:CD2	0.40	2.46	19	1
1:A:57:ILE:HG12	1:C:46:LEU:HD11	0.40	1.89	2	1
2:B:84:LEU:CD2	1:C:38:PHE:HB2	0.40	2.45	10	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
1:A:41:THR:CG2	1:A:47:PHE:CE2	0.40	3.05	12	1
2:D:90:PHE:CZ	2:D:117:GLN:OE1	0.40	2.74	15	1
1:A:22:LYS:CB	2:D:100:LEU:CD2	0.40	3.00	15	1
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:125:PHE:CE1	2:D:129:ASN:ND2	0.40	2.90	5	1
1:A:31:GLN:CD	2:D:95:HIS:CD2	0.40	2.95	17	1
1:A:38:PHE:HB2	2:D:84:LEU:HD22	0.40	1.93	4	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
2:D:112:LEU:HD23	2:D:112:LEU:N	0.40	2.31	14	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%)	59	88
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%)	8	37
2	D	53/60 (88%)	48±1 (90±2%)	4±1 (7±2%)	1±1 (2±2%)	11	48
All	All	4380/4880 (90%)	4124 (94%)	191 (4%)	65 (1%)	18	63

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
1	A	45	PRO	1
2	D	103	SER	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	A	51/56 (91%)	36±2 (70±4%)	15±2 (30±4%)	2 17
1	C	51/56 (91%)	37±2 (72±4%)	14±2 (28±4%)	2 21
2	B	53/56 (95%)	34±3 (65±6%)	19±3 (35±6%)	1 9
2	D	51/56 (91%)	33±2 (64±5%)	19±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)
2	D	101	VAL	20
2	D	132	THR	20
2	B	101	VAL	20
1	C	51	LEU	20
2	B	132	THR	20
2	B	93	LEU	20
2	D	89	LEU	20
1	A	51	LEU	20
2	B	89	LEU	20
1	C	24	GLN	20

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Mol	Chain	Res	Type	Models (Total)
1	C	29	THR	19
2	D	93	LEU	19
2	B	83	ILE	18
2	B	111	LEU	18
1	A	29	THR	18
2	D	86	ILE	18
2	D	85	GLU	17
1	C	53	LEU	17
2	B	88	ASP	17
2	D	111	LEU	17
1	A	24	GLN	17
2	D	97	GLN	17
1	A	14	GLN	17
1	A	53	LEU	17
2	B	86	ILE	17
1	C	14	GLN	16
2	B	104	GLN	16
1	A	46	LEU	16
2	D	83	ILE	15
2	D	119	LYS	15
2	B	97	GLN	15
2	D	88	ASP	15
2	B	119	LYS	14
1	C	54	GLN	14
2	B	85	GLU	14
2	D	120	ASP	14
2	B	82	LYS	13
2	D	104	GLN	13
1	C	46	LEU	13
1	A	42	LEU	13
2	B	105	SER	12
1	A	54	GLN	12
1	A	43	LYS	12
2	D	106	GLN	12
1	C	58	LYS	12
1	A	18	ARG	12
1	C	20	ARG	12
2	D	118	ASN	12
2	B	126	LYS	12
1	C	43	LYS	12
2	B	106	GLN	11
1	C	59	GLN	11

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Mol	Chain	Res	Type	Models (Total)
1	A	10	MET	11
2	B	102	ASP	11
2	B	103	SER	11
1	A	20	ARG	10
2	D	102	ASP	10
1	C	60	LEU	10
1	A	26	LYS	10
1	C	26	LYS	10
2	D	98	HIS	9
1	A	58	LYS	9
2	B	118	ASN	9
1	A	59	GLN	9
2	D	134	HIS	9
2	D	126	LYS	9
2	D	105	SER	9
1	A	55	GLN	9
1	A	9	LYS	9
2	D	103	SER	9
1	C	9	LYS	9
1	A	33	GLU	9
2	D	107	GLU	9
1	A	17	ASP	8
1	C	61	LYS	8
1	C	36	SER	8
2	B	98	HIS	8
2	B	134	HIS	8
1	A	60	LEU	8
2	B	120	ASP	8
1	A	56	SER	8
1	C	42	LEU	7
1	C	18	ARG	7
2	B	107	GLU	7
1	A	22	LYS	7
2	B	115	LEU	7
1	C	40	GLU	6
2	B	91	SER	6
2	B	122	GLN	6
2	B	129	ASN	6
1	C	10	MET	6
1	C	17	ASP	6
2	D	92	SER	6
2	D	135	MET	6

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Mol	Chain	Res	Type	Models (Total)
1	C	55	GLN	6
1	C	44	SER	5
2	D	122	GLN	5
1	A	61	LYS	5
1	A	44	SER	5
1	A	36	SER	5
1	A	39	TYR	5
2	D	95	HIS	5
2	D	87	GLU	5
2	D	94	LYS	5
1	A	49	GLN	5
2	D	117	GLN	5
1	A	32	ASN	5
1	C	56	SER	5
2	D	114	GLN	5
2	B	92	SER	4
1	C	49	GLN	4
2	B	95	HIS	4
2	B	123	ASN	4
1	C	33	GLU	4
1	C	32	ASN	4
2	D	110	SER	4
2	B	114	GLN	4
1	A	34	LYS	4
2	B	117	GLN	3
1	A	48	ASN	3
1	C	48	ASN	3
2	D	123	ASN	3
2	D	115	LEU	3
2	D	91	SER	3
2	D	129	ASN	3
1	C	31	GLN	3
2	B	135	MET	3
1	A	35	LEU	2
1	C	22	LYS	2
1	A	8	GLU	2
1	A	31	GLN	2
2	D	112	LEU	2
1	A	40	GLU	2
2	B	94	LYS	2
2	D	90	PHE	1
2	D	99	THR	1

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Mol	Chain	Res	Type	Models (Total)
2	B	108	ASP	1
2	B	110	SER	1
1	A	30	THR	1
2	B	87	GLU	1
1	C	35	LEU	1
2	B	112	LEU	1
2	B	84	LEU	1
1	C	39	TYR	1
1	C	34	LYS	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 carbohydrates 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