



Full wwPDB NMR Structure Validation Report ⓘ

Mar 29, 2026 – 10:13 PM UTC

PDB ID : 1Y76 / pdb_00001y76
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

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

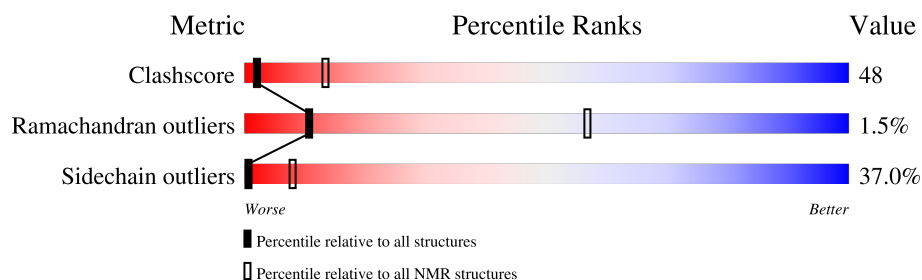
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	62	32% 47% 11% 10%
1	C	62	32% 47% 10% 11%
2	B	60	22% 50% 20% 8%
2	D	60	20% 52% 17% 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)	0.62	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
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.

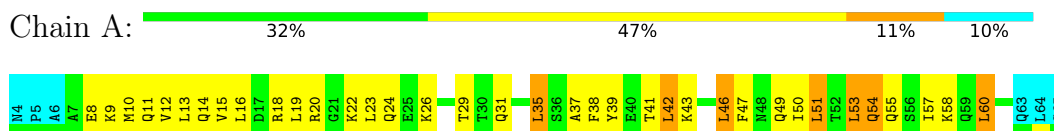
Mol	Chain	Residues	Atoms						Trace
2	B	60	Total	C	H	N	O	S	0
			975	305	493	83	93	1	
2	D	60	Total	C	H	N	O	S	0
			975	305	493	83	93	1	

4 Residue-property plots [i](#)

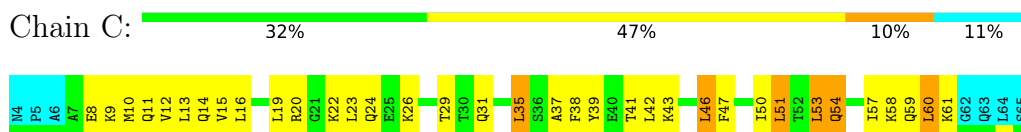
4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, 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.

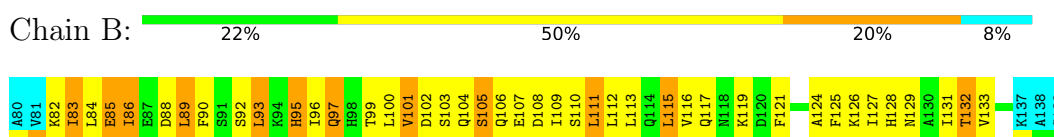
- Molecule 1: protein associated to tight junctions



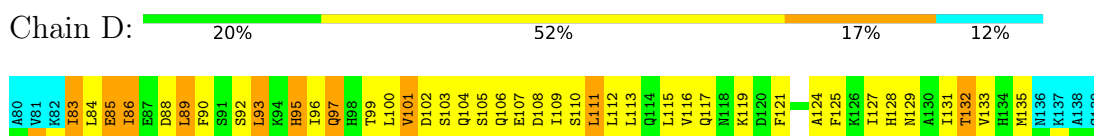
- Molecule 1: protein associated to tight junctions



- Molecule 2: MAGUK p55 subfamily member 5



- Molecule 2: MAGUK p55 subfamily member 5

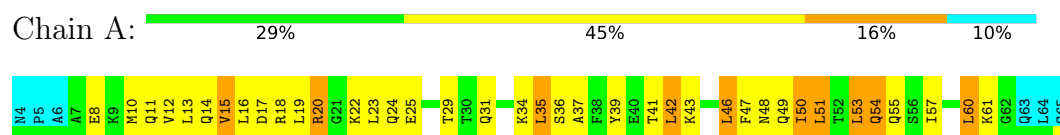


4.2 Scores per residue for each member of the ensemble

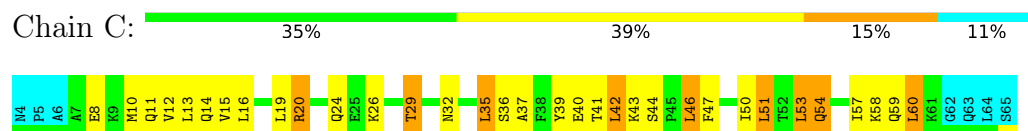
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

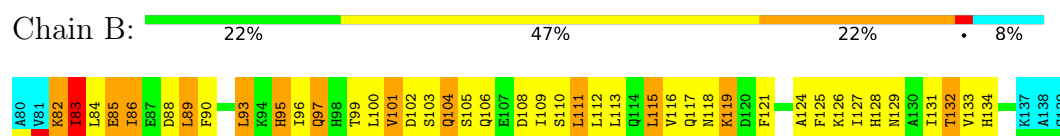
- Molecule 1: protein associated to tight junctions



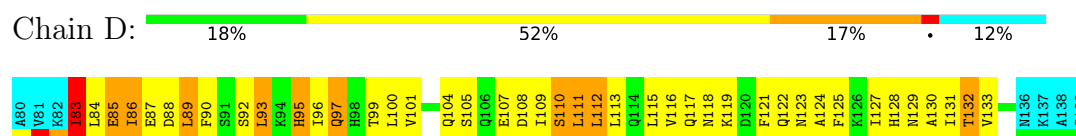
- Molecule 1: protein associated to tight junctions



- Molecule 2: MAGUK p55 subfamily member 5

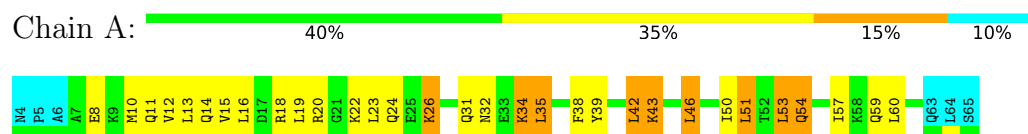


- Molecule 2: MAGUK p55 subfamily member 5

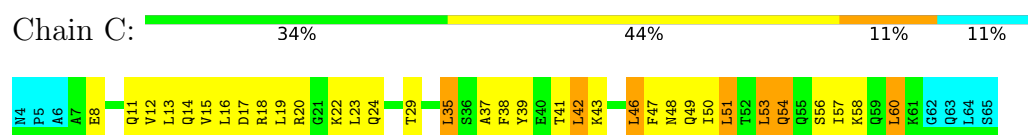


4.2.2 Score per residue for model 2

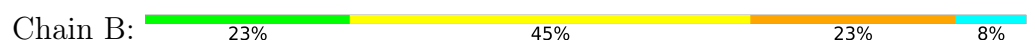
- Molecule 1: protein associated to tight junctions



- Molecule 1: protein associated to tight junctions



- Molecule 2: MAGUK p55 subfamily member 5





- Molecule 2: MAGUK p55 subfamily member 5

Chain D: 13% 55% 18% 12%



4.2.3 Score per residue for model 3

- Molecule 1: protein associated to tight junctions

Chain A: 40% 35% 15% 10%



- Molecule 1: protein associated to tight junctions

Chain C: 37% 40% 11% 11%



- Molecule 2: MAGUK p55 subfamily member 5

Chain B: 20% 52% 20% 8%



- Molecule 2: MAGUK p55 subfamily member 5

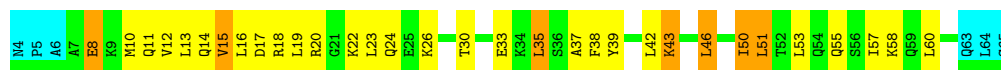
Chain D: 18% 47% 23% 12%



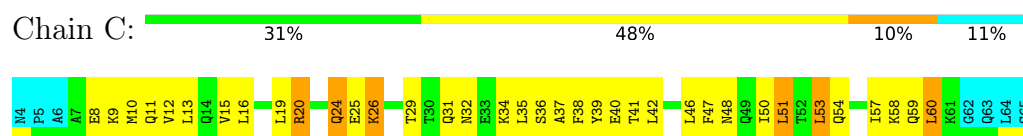
4.2.4 Score per residue for model 4

- Molecule 1: protein associated to tight junctions

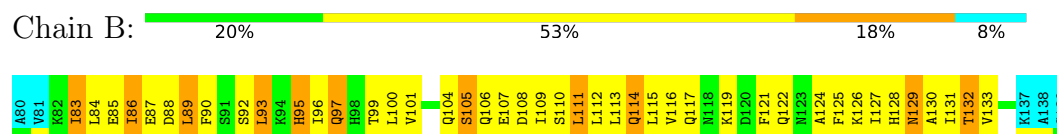
Chain A: 39% 40% 11% 10%



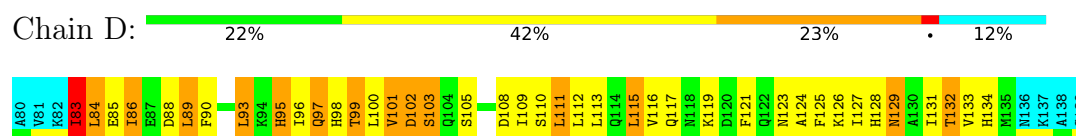
- Molecule 1: protein associated to tight junctions



- Molecule 2: MAGUK p55 subfamily member 5

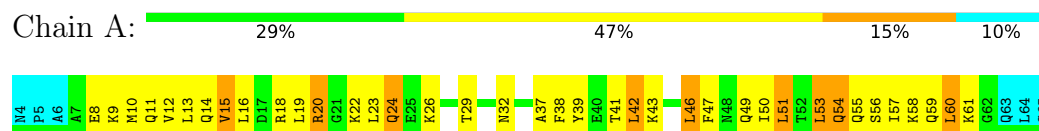


- Molecule 2: MAGUK p55 subfamily member 5

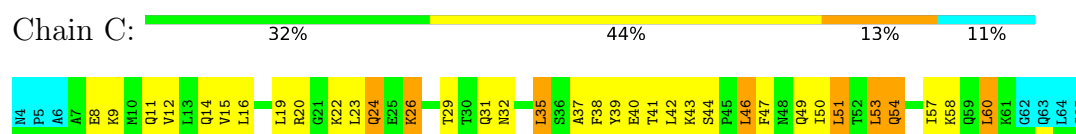


4.2.5 Score per residue for model 5

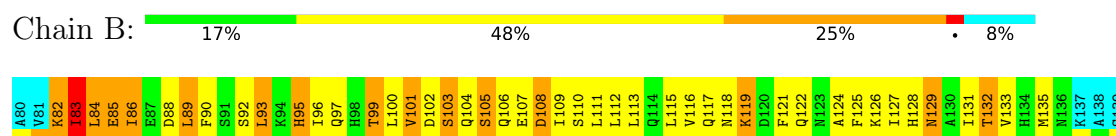
- Molecule 1: protein associated to tight junctions



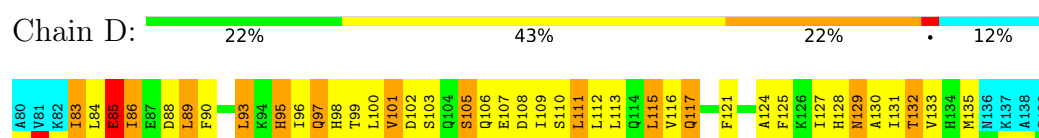
- Molecule 1: protein associated to tight junctions



- Molecule 2: MAGUK p55 subfamily member 5

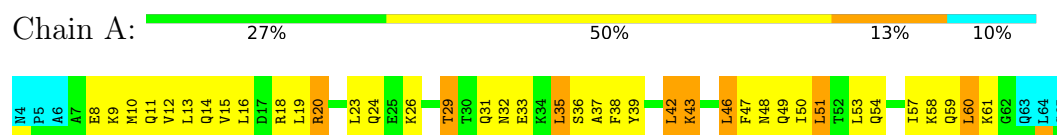


- Molecule 2: MAGUK p55 subfamily member 5

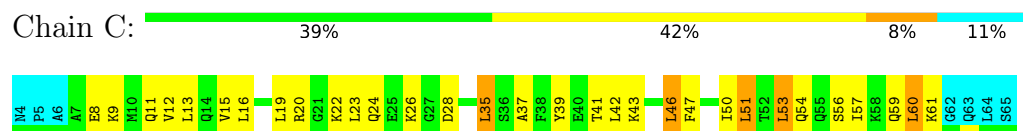


4.2.6 Score per residue for model 6

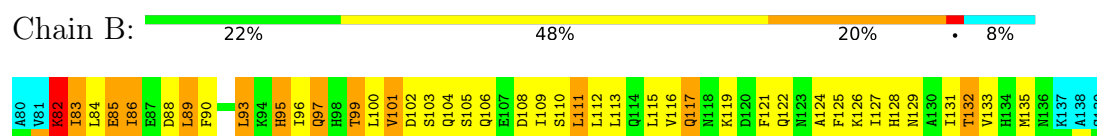
- Molecule 1: protein associated to tight junctions



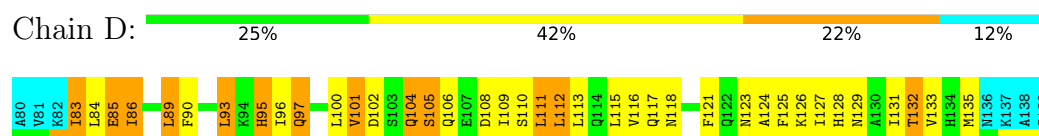
- Molecule 1: protein associated to tight junctions



- Molecule 2: MAGUK p55 subfamily member 5

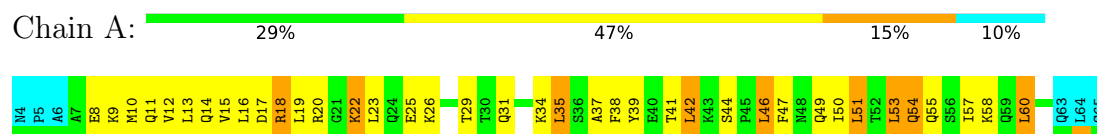


- Molecule 2: MAGUK p55 subfamily member 5

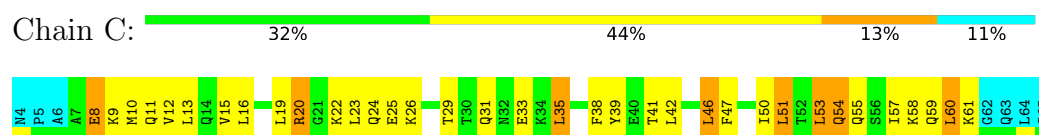


4.2.7 Score per residue for model 7

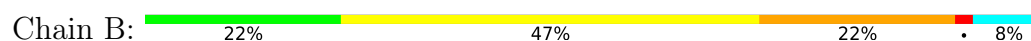
- Molecule 1: protein associated to tight junctions

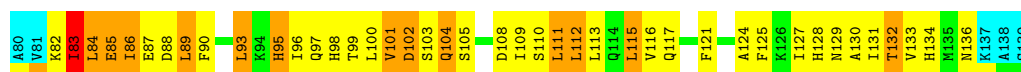


- Molecule 1: protein associated to tight junctions

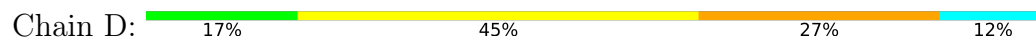


- Molecule 2: MAGUK p55 subfamily member 5



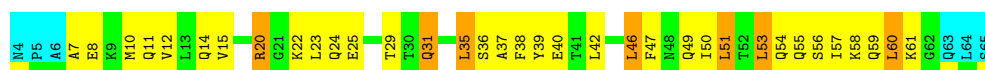


- Molecule 2: MAGUK p55 subfamily member 5



4.2.8 Score per residue for model 8

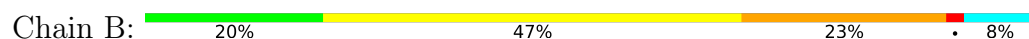
- Molecule 1: protein associated to tight junctions



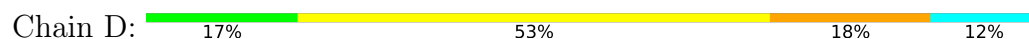
- Molecule 1: protein associated to tight junctions



- Molecule 2: MAGUK p55 subfamily member 5

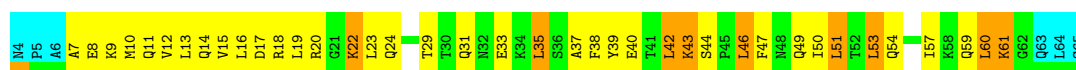


- Molecule 2: MAGUK p55 subfamily member 5

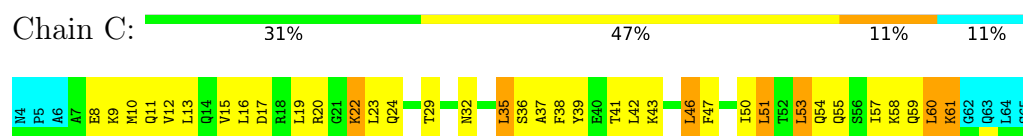


4.2.9 Score per residue for model 9

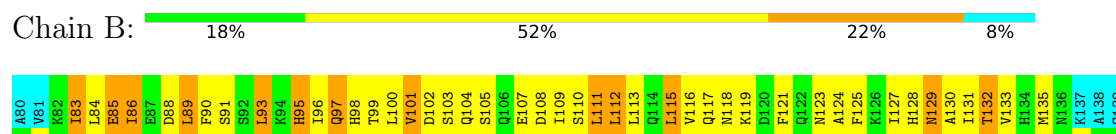
- Molecule 1: protein associated to tight junctions



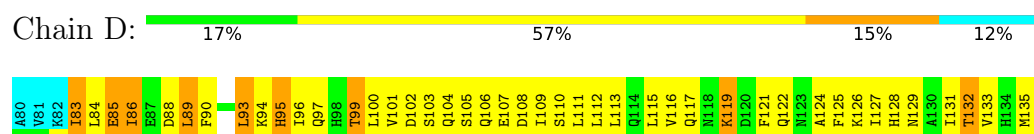
- Molecule 1: protein associated to tight junctions



- Molecule 2: MAGUK p55 subfamily member 5

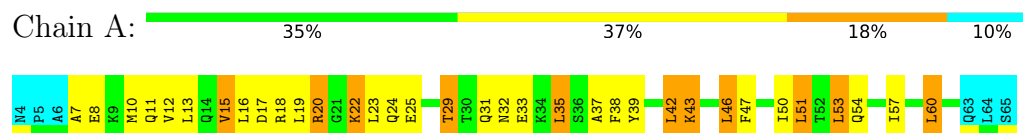


- Molecule 2: MAGUK p55 subfamily member 5

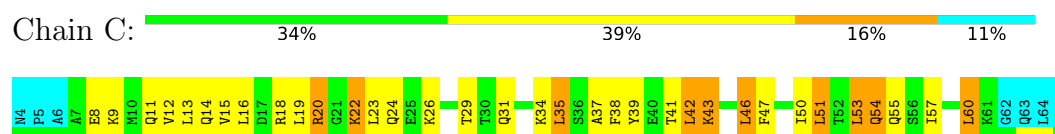


4.2.10 Score per residue for model 10

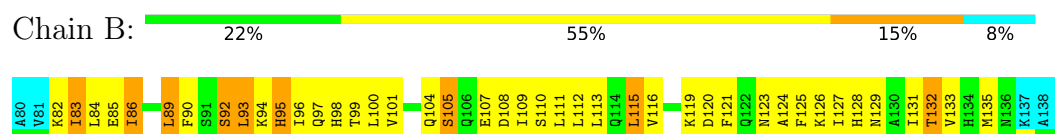
- Molecule 1: protein associated to tight junctions



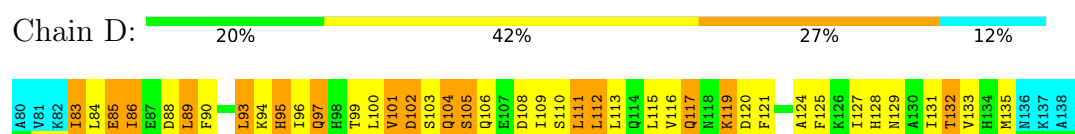
- Molecule 1: protein associated to tight junctions



- Molecule 2: MAGUK p55 subfamily member 5

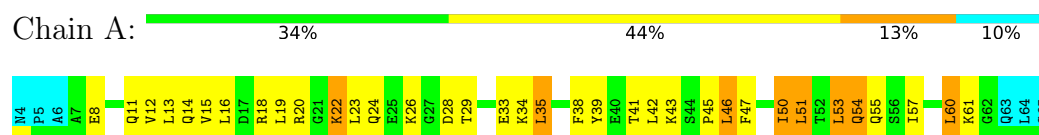


- Molecule 2: MAGUK p55 subfamily member 5

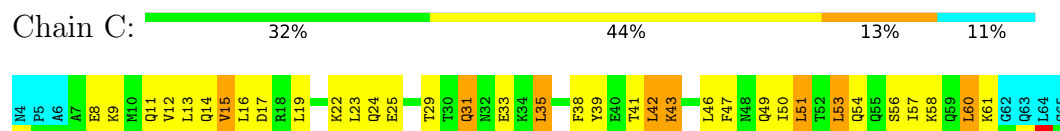


4.2.11 Score per residue for model 11

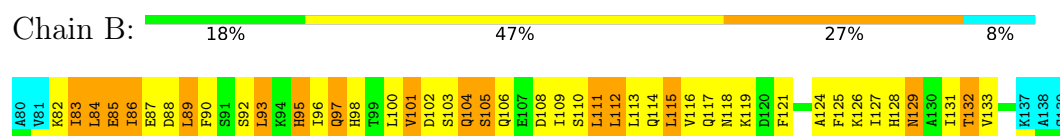
- Molecule 1: protein associated to tight junctions



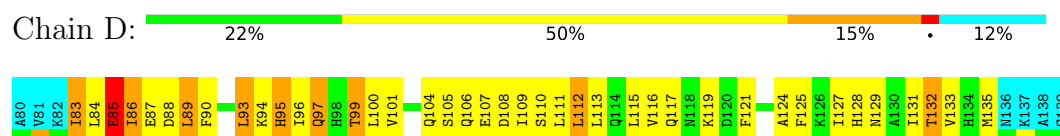
- Molecule 1: protein associated to tight junctions



- Molecule 2: MAGUK p55 subfamily member 5

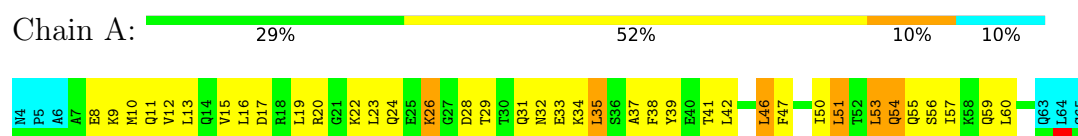


- Molecule 2: MAGUK p55 subfamily member 5

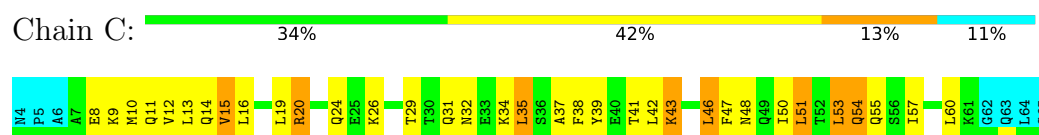


4.2.12 Score per residue for model 12

- Molecule 1: protein associated to tight junctions



- Molecule 1: protein associated to tight junctions

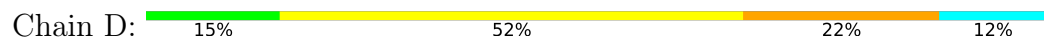


- Molecule 2: MAGUK p55 subfamily member 5





- Molecule 2: MAGUK p55 subfamily member 5

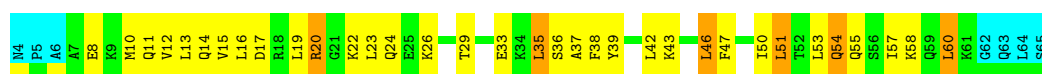


4.2.13 Score per residue for model 13

- Molecule 1: protein associated to tight junctions



- Molecule 1: protein associated to tight junctions



- Molecule 2: MAGUK p55 subfamily member 5

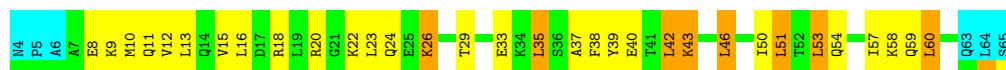
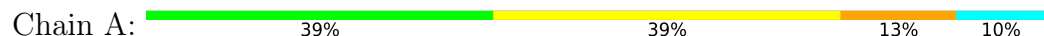


- Molecule 2: MAGUK p55 subfamily member 5

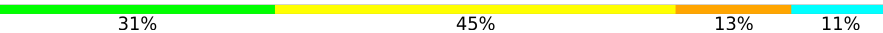


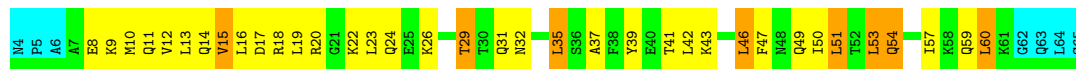
4.2.14 Score per residue for model 14

- Molecule 1: protein associated to tight junctions



- Molecule 1: protein associated to tight junctions

Chain C: 



- Molecule 2: MAGUK p55 subfamily member 5

Chain B: 



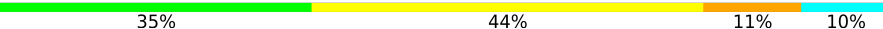
- Molecule 2: MAGUK p55 subfamily member 5

Chain D: 



4.2.15 Score per residue for model 15

- Molecule 1: protein associated to tight junctions

Chain A: 

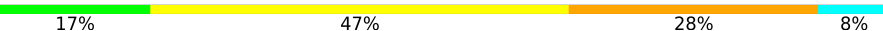


- Molecule 1: protein associated to tight junctions

Chain C: 

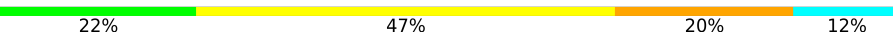


- Molecule 2: MAGUK p55 subfamily member 5

Chain B: 



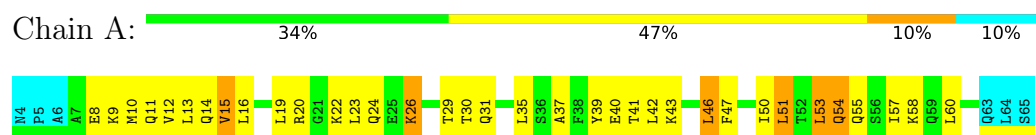
- Molecule 2: MAGUK p55 subfamily member 5

Chain D: 

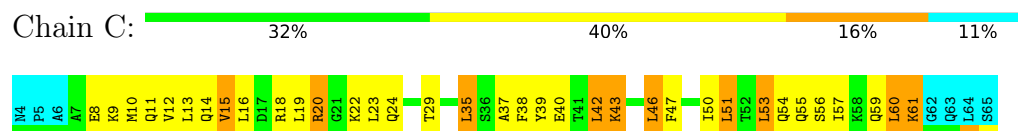


4.2.16 Score per residue for model 16

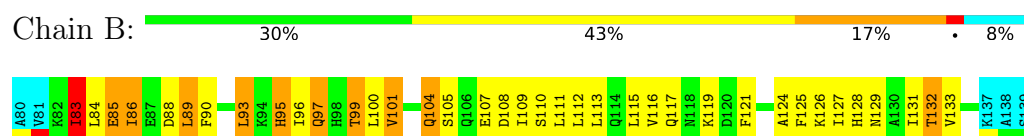
- Molecule 1: protein associated to tight junctions



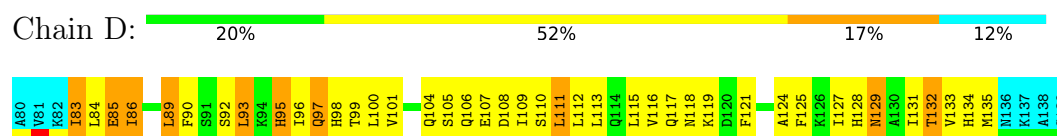
- Molecule 1: protein associated to tight junctions



- Molecule 2: MAGUK p55 subfamily member 5

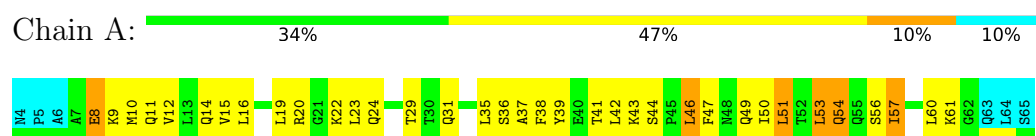


- Molecule 2: MAGUK p55 subfamily member 5

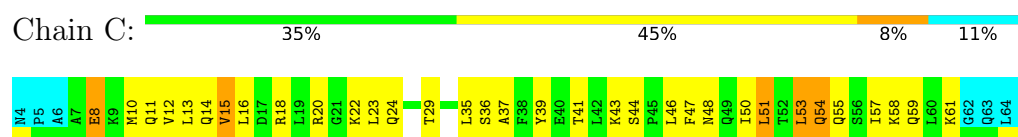


4.2.17 Score per residue for model 17

- Molecule 1: protein associated to tight junctions

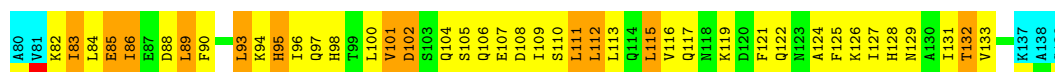


- Molecule 1: protein associated to tight junctions

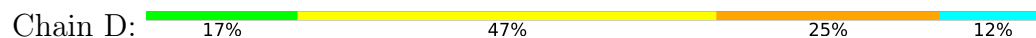


- Molecule 2: MAGUK p55 subfamily member 5



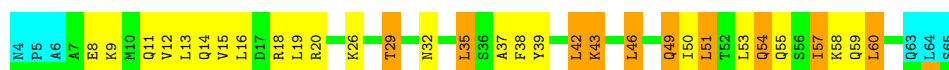


- Molecule 2: MAGUK p55 subfamily member 5



4.2.18 Score per residue for model 18

- Molecule 1: protein associated to tight junctions



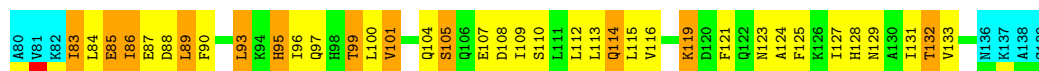
- Molecule 1: protein associated to tight junctions



- Molecule 2: MAGUK p55 subfamily member 5

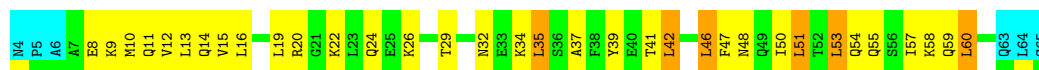


- Molecule 2: MAGUK p55 subfamily member 5

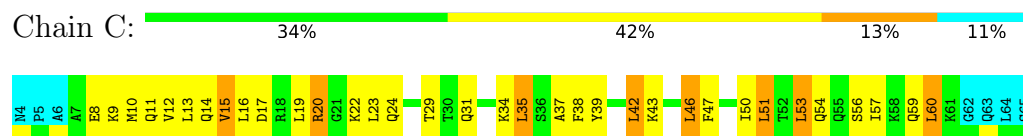


4.2.19 Score per residue for model 19 (medoid)

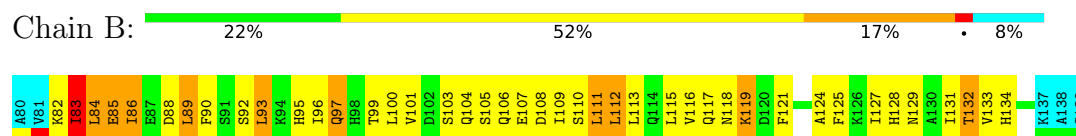
- Molecule 1: protein associated to tight junctions



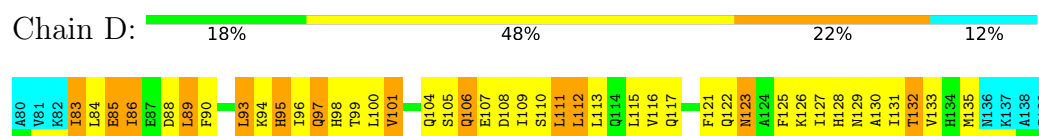
- Molecule 1: protein associated to tight junctions



- Molecule 2: MAGUK p55 subfamily member 5

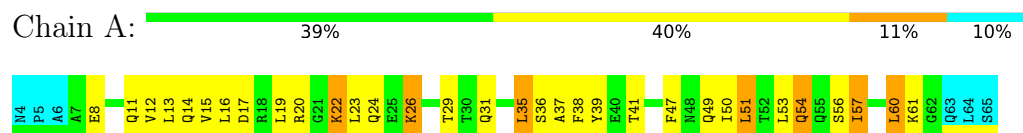


- Molecule 2: MAGUK p55 subfamily member 5

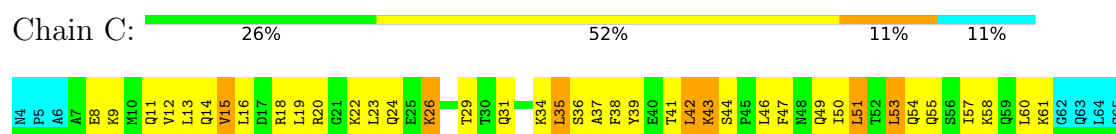


4.2.20 Score per residue for model 20

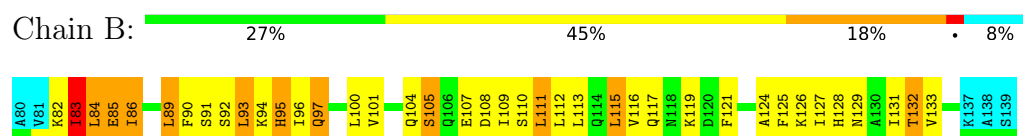
- Molecule 1: protein associated to tight junctions



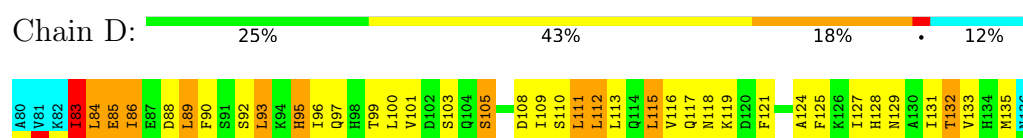
- Molecule 1: protein associated to tight junctions



- Molecule 2: MAGUK p55 subfamily member 5



- Molecule 2: MAGUK p55 subfamily member 5



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.

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	45±5
1	C	448	477	477	44±4
2	B	449	456	452	65±4
2	D	432	437	433	65±4
All	All	35620	37000	36840	3463

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 48.

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:92:SER:C	2:D:96:ILE:HD12	0.76	2.05	2	9
2:B:92:SER:C	2:B:96:ILE:HD12	0.76	2.05	10	7
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
1:A:15:VAL:HG22	2:D:108:ASP:CG	0.74	2.06	17	17
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:108:ASP:CG	1:C:15:VAL:HG22	0.73	2.08	4	16
2:B:119:LYS:NZ	2:D:130:ALA:HB1	0.73	1.98	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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
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:83:ILE:HG21	2:B:129:ASN:HA	0.71	1.61	11	2
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: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
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: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:105:SER:C	2:D:109:ILE:HD12	0.68	2.13	8	19
2:D:84:LEU:HD21	2:D:89:LEU:HD22	0.68	1.63	4	10
2:B:105:SER:C	2:B:109:ILE:HD12	0.68	2.13	16	20
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:46:LEU:HD11	1:C:57:ILE:CG1	0.68	2.18	2	7
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
2:B:108:ASP:CG	1:C:15:VAL:HG13	0.64	2.18	5	1
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: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
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: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:C:13:LEU:HD13	1:C:43:LYS:NZ	0.59	2.13	16	4
2:B:132:THR:HA	2:B:135:MET:HE3	0.58	1.74	13	6
2:D:132:THR:HA	2:D:135:MET:HE3	0.58	1.73	10	7
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
2:D:83:ILE:HG21	2:D:129:ASN:CG	0.58	2.23	10	3
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:83:ILE:HG22	2:B:129:ASN:CG	0.57	2.25	2	3
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
2:B:84:LEU:O	2:B:85:GLU:O	0.56	2.24	11	2
1:A:10:MET:HA	1:A:10:MET:HE3	0.56	1.77	1	1
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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
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: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
1:C:10:MET:HE3	1:C:10:MET:HA	0.53	1.79	17	2
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
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:124:ALA:CB	1:C:50:ILE:HG22	0.52	2.35	10	1
1:C:10:MET:HA	1:C:10:MET:HE2	0.52	1.82	19	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: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:C:61:LYS:HZ1	2:D:131:ILE:HG23	0.51	1.64	20	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
1:A:54:GLN:CD	2:D:124:ALA:HB2	0.51	2.31	2	1
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:10:MET:HA	1:A:10:MET:HE2	0.50	1.83	10	4
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:D:121:PHE:C	2:D:121:PHE:CD1	0.49	2.91	10	8
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
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
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:B:121:PHE:CD1	2:B:121:PHE:C	0.48	2.92	11	17
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:B:95:HIS:CD2	2:B:95:HIS:C	0.48	2.92	11	20
2:D:83:ILE:HG22	2:D:129:ASN:CG	0.48	2.34	13	2
2:D:84:LEU:O	2:D:85:GLU:C	0.48	2.55	17	2
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
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:61:LYS:HZ1	2:B:131:ILE:HG23	0.47	1.69	15	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:129:ASN:CG	2:B:130:ALA:N	0.47	2.73	4	1
2:B:93:LEU:HD11	2:B:116:VAL:HG21	0.47	1.87	20	3
1:A:49:GLN:CD	1:C:53:LEU:HD12	0.47	2.35	18	1
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:D:121:PHE:CD1	2:D:121:PHE:C	0.46	2.92	20	11
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:84:LEU:O	2:B:85:GLU:C	0.46	2.59	14	4
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
2:B:121:PHE:C	2:B:121:PHE:CD1	0.46	2.93	19	3
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
2:B:96:ILE:HG22	2:B:100:LEU:HD12	0.46	1.88	19	3
1:A:10:MET:HE2	1:A:13:LEU:HD12	0.46	1.87	13	1
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	6
2:D:95:HIS:CD2	2:D:95:HIS:C	0.45	2.94	8	19
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	4
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:A:31:GLN:CD	2:D:95:HIS:CD2	0.45	2.95	17	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:B:83:ILE:HG21	2:B:129:ASN:CG	0.45	2.37	6	1
2:B:125:PHE:CD1	2:B:125:PHE:C	0.44	2.95	5	4
2:B:100:LEU:C	2:B:101:VAL:CG2	0.44	2.90	7	12
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
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
2:D:90:PHE:CZ	2:D:117:GLN:CD	0.44	2.96	19	9
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
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:B:90:PHE:CZ	2:B:117:GLN:CD	0.43	2.96	9	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:D:100:LEU:C	2:D:101:VAL:CG2	0.43	2.92	4	12
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:10:MET:HE3	1:A:13:LEU:HD12	0.43	1.90	12	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:C:13:LEU:HD13	1:C:43:LYS:HZ1	0.43	1.73	10	2
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:61:LYS:HZ2	2:D:131:ILE:HG23	0.43	1.72	16	1
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: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
2:B:84:LEU:O	2:B:84:LEU:HG	0.43	2.12	14	2
1:A:20:ARG:H	1:A:35:LEU:HD12	0.43	1.72	11	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
2:B:89:LEU:HD12	2:B:89:LEU:C	0.42	2.38	12	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:13:LEU:HD13	1:A:43:LYS:HZ3	0.42	1.74	6	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
2:D:89:LEU:HD12	2:D:89:LEU:C	0.42	2.39	6	2
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: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
1:A:20:ARG:CD	1:A:32:ASN:ND2	0.42	2.83	2	1
2:B:90:PHE:CE1	2:B:117:GLN:CD	0.42	2.98	11	7
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:B:119:LYS:HZ1	2:D:130:ALA:HB1	0.41	1.71	5	1
2:D:86:ILE:CG2	2:D:116:VAL:CG1	0.41	2.97	17	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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: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:39:TYR:CD1	1:A:39:TYR:C	0.41	2.98	11	1
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:C:39:TYR:C	1:C:39:TYR:CD1	0.41	2.98	4	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
2:B:86:ILE:CD1	2:B:125:PHE:CB	0.41	2.99	8	4
2:D:90:PHE:CE1	2:D:117:GLN:CD	0.41	2.99	16	5
1:A:16:LEU:HB2	1:A:39:TYR:CD2	0.41	2.51	7	1
2:D:125:PHE:C	2:D:125:PHE:CD1	0.41	2.99	19	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:10:MET:HE3	1:C:13:LEU:HD12	0.41	1.92	9	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
2:B:82:LYS:C	2:B:83:ILE:HD13	0.41	2.41	18	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:D:83:ILE:O	2:D:84:LEU:HB2	0.40	2.16	4	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: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
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
2:B:100:LEU:HD23	1:C:26:LYS:CE	0.40	2.46	18	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	56/62 (90%)	55±1 (98±1%)	1±1 (2±1%)	0±0 (0±0%)	49	83
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%)	4	33
2	D	53/60 (88%)	48±1 (90±2%)	4±1 (7±2%)	1±1 (2±2%)	6	43
All	All	4380/4880 (90%)	4124 (94%)	191 (4%)	65 (1%)	11	57

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 ⓘ

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%)	33±2 (65±5%)	18±2 (35±5%)	1	10
1	C	51/56 (91%)	34±2 (67±4%)	17±2 (33±4%)	1	12
2	B	53/56 (95%)	32±3 (60±5%)	21±3 (40±5%)	0	5
2	D	51/56 (91%)	31±2 (60±5%)	20±2 (40±5%)	0	5
All	All	4120/4480 (92%)	2597 (63%)	1523 (37%)	1	8

All 150 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	83	ILE	20
2	B	86	ILE	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	83	ILE	20
2	D	86	ILE	20
2	D	89	LEU	20
2	D	93	LEU	20
2	D	95	HIS	20
2	D	101	VAL	20
2	D	132	THR	20
1	A	46	LEU	19
2	B	95	HIS	19
1	C	29	THR	19
1	C	53	LEU	19
1	A	29	THR	18
1	A	53	LEU	18
2	B	111	LEU	18
1	C	35	LEU	18
1	C	60	LEU	18
2	D	85	GLU	18
2	D	99	THR	18
1	A	24	GLN	17
1	A	35	LEU	17
2	B	88	ASP	17
2	B	119	LYS	17
2	D	111	LEU	17
1	A	14	GLN	16
1	A	60	LEU	16
2	B	82	LYS	16
2	B	104	GLN	16
1	C	14	GLN	16
2	D	97	GLN	16
2	B	85	GLU	15
2	B	97	GLN	15
2	B	99	THR	15
2	B	126	LYS	15
1	C	46	LEU	15

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Mol	Chain	Res	Type	Models (Total)
2	D	88	ASP	15
2	D	119	LYS	15
1	A	18	ARG	14
1	C	54	GLN	14
1	A	42	LEU	13
1	A	43	LYS	13
1	A	54	GLN	13
2	D	104	GLN	13
2	D	106	GLN	13
2	B	106	GLN	12
2	B	115	LEU	12
1	C	58	LYS	12
1	A	26	LYS	12
2	B	105	SER	12
1	C	43	LYS	12
1	C	9	LYS	12
1	A	55	GLN	11
2	B	103	SER	11
1	C	20	ARG	11
1	C	26	LYS	11
1	C	59	GLN	11
2	D	107	GLU	11
1	A	10	MET	11
1	A	58	LYS	11
2	D	134	HIS	10
2	B	107	GLU	10
2	D	112	LEU	9
2	D	118	ASN	9
1	A	59	GLN	9
2	D	102	ASP	9
2	D	103	SER	9
2	D	126	LYS	9
1	A	9	LYS	9
1	A	33	GLU	9
1	C	55	GLN	9
1	A	20	ARG	8
2	B	118	ASN	8
2	B	134	HIS	8
1	C	10	MET	8
1	C	36	SER	8
1	C	42	LEU	8
2	B	112	LEU	8

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Mol	Chain	Res	Type	Models (Total)
1	C	18	ARG	8
2	D	105	SER	8
2	B	122	GLN	8
1	C	15	VAL	8
1	C	61	LYS	8
2	D	98	HIS	8
1	A	49	GLN	8
2	B	98	HIS	8
1	A	17	ASP	7
1	A	22	LYS	7
2	D	122	GLN	7
2	B	102	ASP	7
2	D	115	LEU	7
1	A	15	VAL	6
1	C	40	GLU	6
2	D	87	GLU	6
2	B	91	SER	6
1	C	17	ASP	6
2	D	92	SER	6
2	D	135	MET	6
2	D	94	LYS	6
1	A	36	SER	5
1	A	61	LYS	5
1	C	44	SER	5
1	C	56	SER	5
2	D	114	GLN	5
2	D	117	GLN	5
1	A	40	GLU	5
1	A	56	SER	5
1	C	33	GLU	5
2	B	129	ASN	5
2	B	123	ASN	5
1	A	25	GLU	4
1	A	48	ASN	4
1	A	34	LYS	4
1	C	48	ASN	4
1	C	49	GLN	4
1	C	34	LYS	4
2	B	92	SER	4
1	A	44	SER	4
1	C	22	LYS	4
1	A	57	ILE	4

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Mol	Chain	Res	Type	Models (Total)
1	A	50	ILE	3
1	A	8	GLU	3
2	B	117	GLN	3
2	B	135	MET	3
1	C	32	ASN	3
2	B	87	GLU	3
2	B	114	GLN	3
1	C	25	GLU	3
2	D	129	ASN	3
1	C	31	GLN	3
2	B	94	LYS	3
2	D	123	ASN	3
1	A	30	THR	2
1	C	8	GLU	2
2	D	91	SER	2
1	A	32	ASN	2
2	D	110	SER	1
2	B	110	SER	1
2	B	108	ASP	1
2	D	120	ASP	1
1	A	31	GLN	1
2	B	84	LEU	1
1	C	50	ILE	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 oligosaccharides in this entry.

6.6 Ligand geometry ⓘ

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

No chemical shift data were provided