Full wwPDB NMR Structure Validation Report (i)

Apr 26, 2016 – 07:11 PM BST

PDB ID	:	1Y74
Title	:	Solution Structure of mLin-2/mLin-7 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:

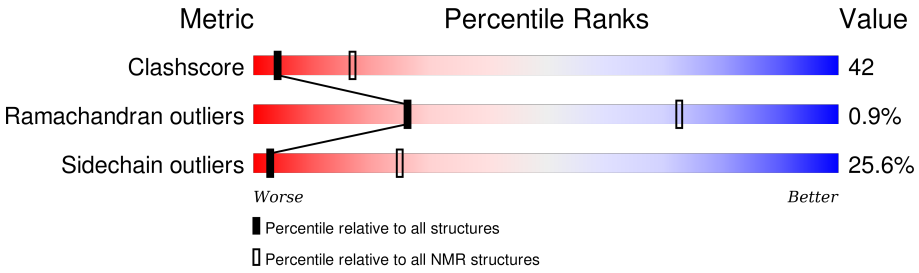
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal 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	57	28% 63% 9%
1	C	57	33% 56% 11%
2	B	50	46% 44% 10%
2	D	50	40% 50% • 6%

2 Ensemble composition and analysis

This entry contains 20 models. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 11 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:17-A:73, B:83-B:132, C:17-C:73, D:83-D:129 (211)	0.32	3

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 5 clusters. No single-model clusters were found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3500 atoms, of which 1758 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called lin 7 homolog b.

Mol	Chain	Residues	Atoms						Trace
1	A	57	Total	C	H	N	O	S	0
			946	291	480	85	89	1	
1	C	57	Total	C	H	N	O	S	0
			946	291	480	85	89	1	

- Molecule 2 is a protein called Peripheral plasma membrane protein CASK.

Mol	Chain	Residues	Atoms						Trace
2	B	50	Total	C	H	N	O	S	0
			804	254	399	70	79	2	
2	D	50	Total	C	H	N	O	S	0
			804	254	399	70	79	2	

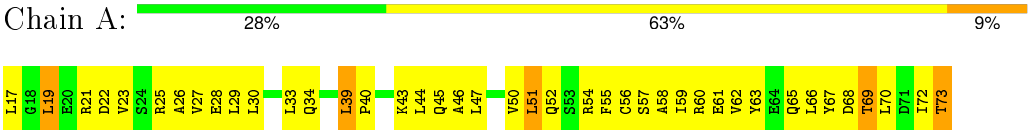
4 Residue-property plots

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.

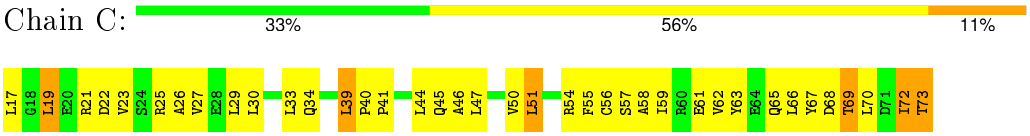
• Molecule 1: lin 7 homolog b

Chain A:



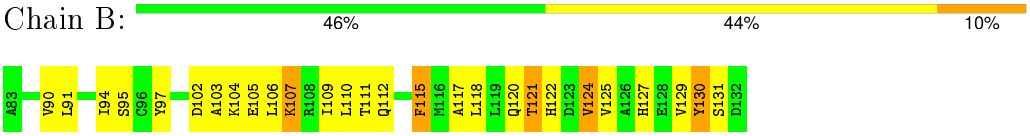
• Molecule 1: lin 7 homolog b

Chain C:



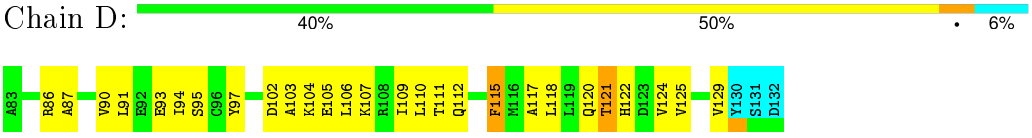
• Molecule 2: Peripheral plasma membrane protein CASK

Chain B:



• Molecule 2: Peripheral plasma membrane protein CASK

Chain D:



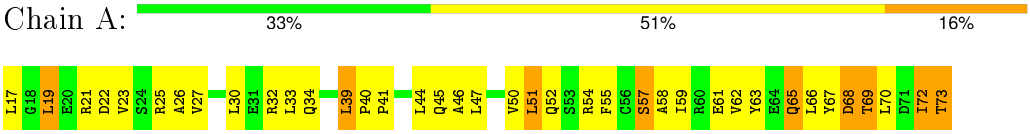
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

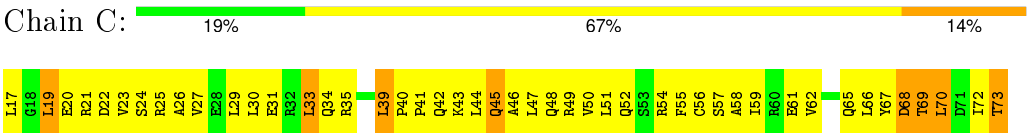
- Molecule 1: lin 7 homolog b

Chain A:



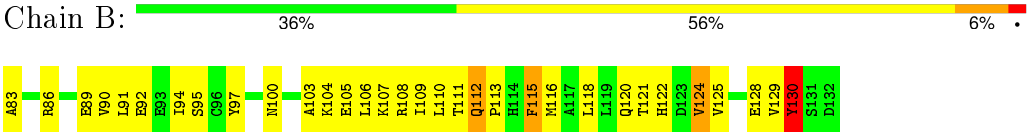
- Molecule 1: lin 7 homolog b

Chain C:



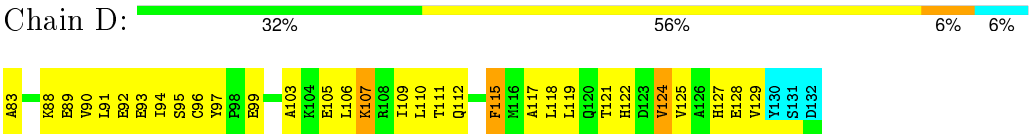
- Molecule 2: Peripheral plasma membrane protein CASK

Chain B:



- Molecule 2: Peripheral plasma membrane protein CASK

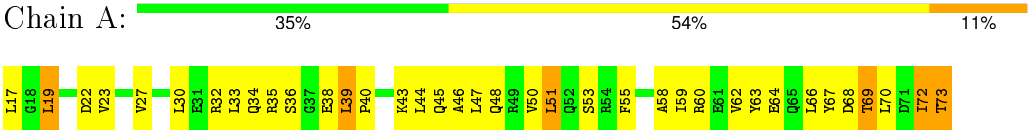
Chain D:



4.2.2 Score per residue for model 2

- Molecule 1: lin 7 homolog b

Chain A:

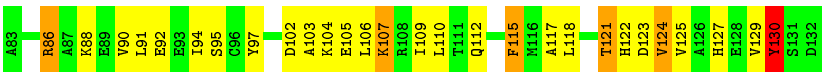


- Molecule 1: lin 7 homolog b

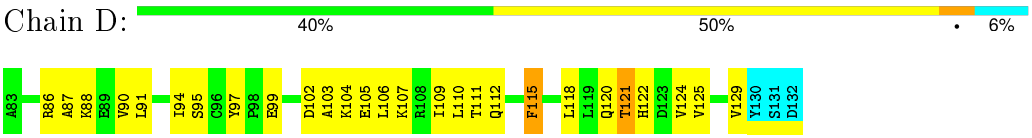
Chain C:

- Molecule 2: Peripheral plasma membrane protein CASK

Chain B:

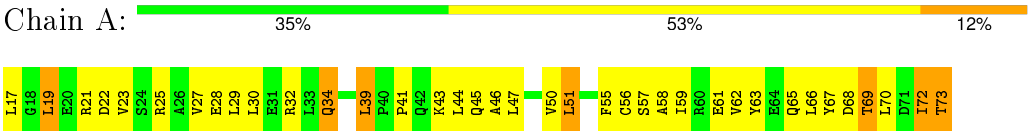


• Molecule 2: Peripheral plasma membrane protein CASK

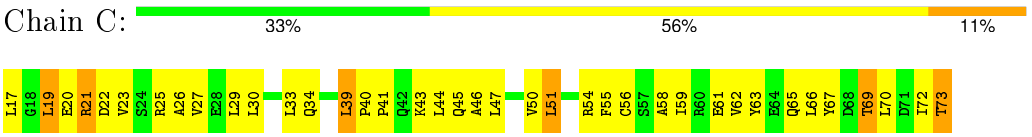


4.2.3 Score per residue for model 3 (medoid)

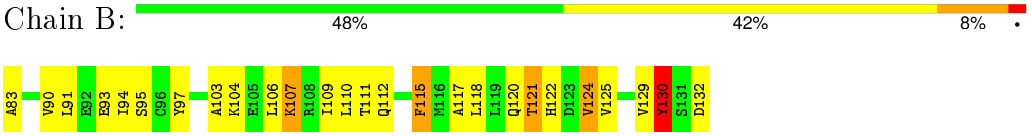
• Molecule 1: lin 7 homolog b



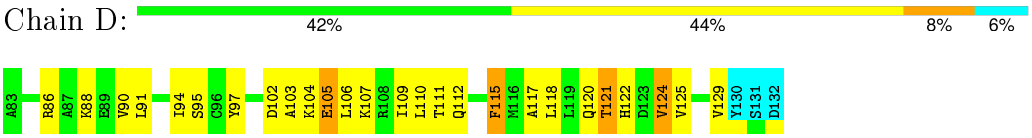
• Molecule 1: lin 7 homolog b



• Molecule 2: Peripheral plasma membrane protein CASK

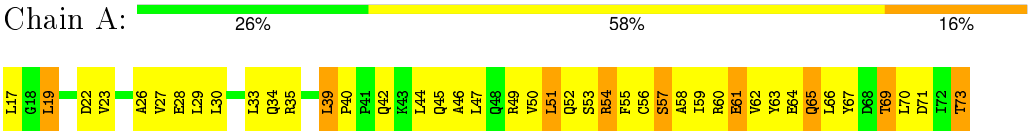


• Molecule 2: Peripheral plasma membrane protein CASK



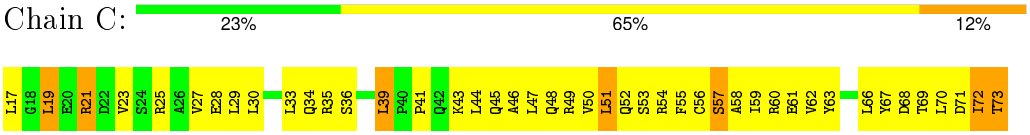
4.2.4 Score per residue for model 4

• Molecule 1: lin 7 homolog b



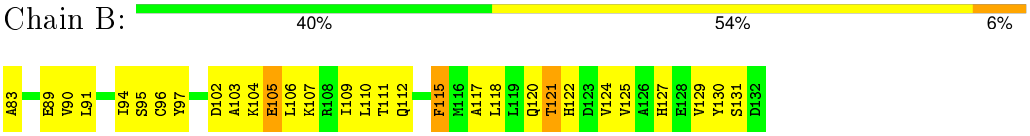
• Molecule 1: lin 7 homolog b

Chain C:



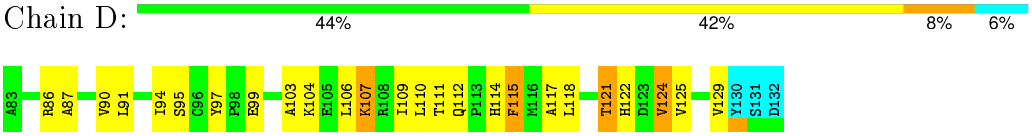
• Molecule 2: Peripheral plasma membrane protein CASK

Chain B:



• Molecule 2: Peripheral plasma membrane protein CASK

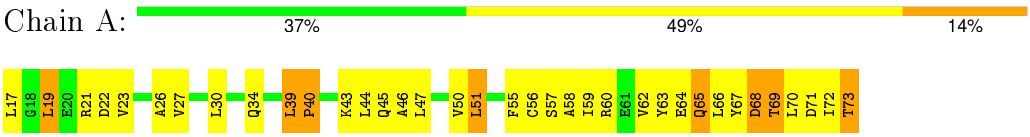
Chain D:



4.2.5 Score per residue for model 5

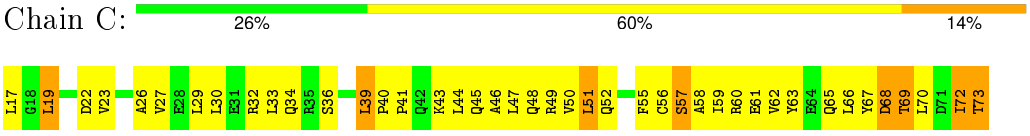
• Molecule 1: lin 7 homolog b

Chain A:



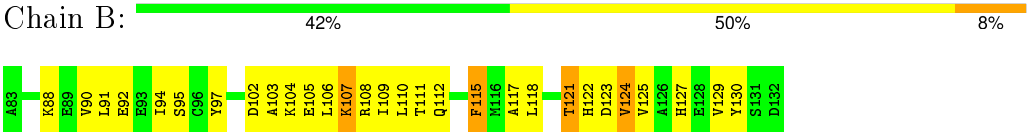
• Molecule 1: lin 7 homolog b

Chain C:



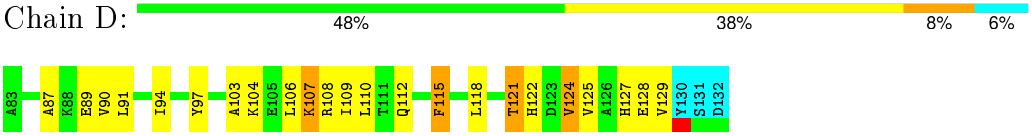
• Molecule 2: Peripheral plasma membrane protein CASK

Chain B:



• Molecule 2: Peripheral plasma membrane protein CASK

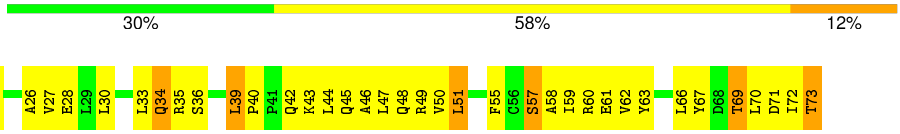
Chain D:



4.2.6 Score per residue for model 6

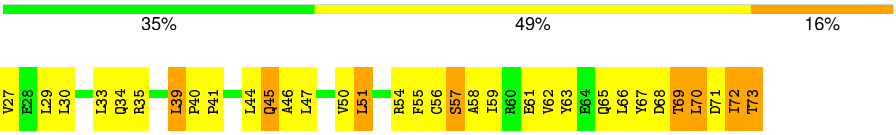
• Molecule 1: lin 7 homolog b

Chain A:



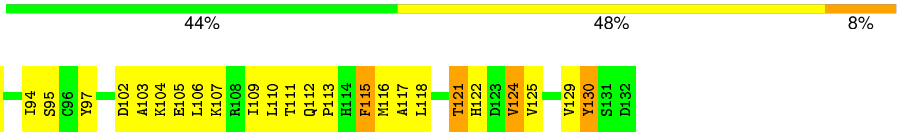
• Molecule 1: lin 7 homolog b

Chain C:



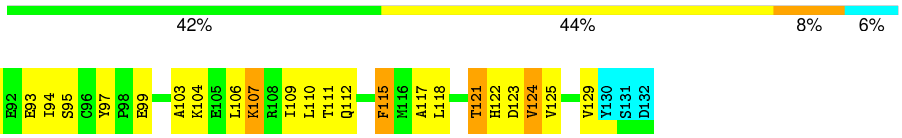
• Molecule 2: Peripheral plasma membrane protein CASK

Chain B:



• Molecule 2: Peripheral plasma membrane protein CASK

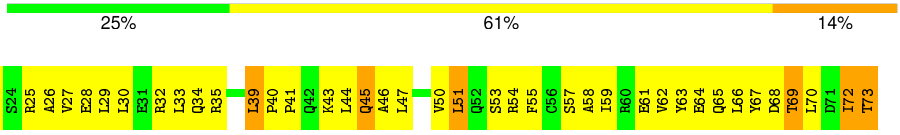
Chain D:



4.2.7 Score per residue for model 7

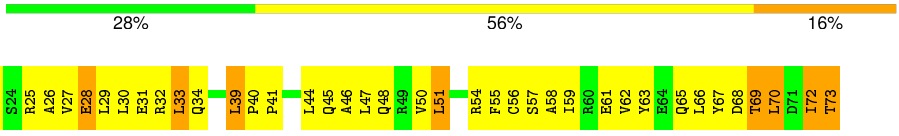
• Molecule 1: lin 7 homolog b

Chain A:



• Molecule 1: lin 7 homolog b

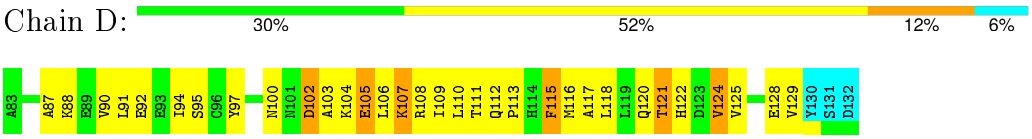
Chain C:



• Molecule 2: Peripheral plasma membrane protein CASK

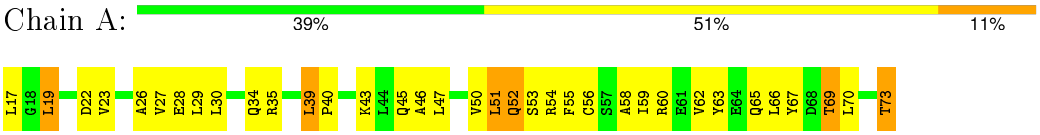
Chain B:

• Molecule 2: Peripheral plasma membrane protein CASK



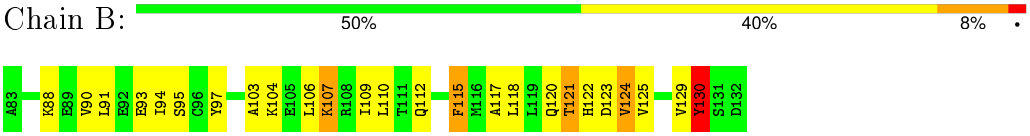
4.2.8 Score per residue for model 8

• Molecule 1: lin 7 homolog b

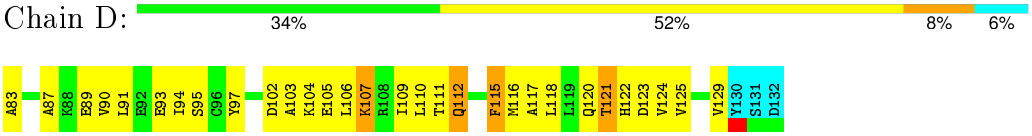


• Molecule 1: lin 7 homolog b

• Molecule 2: Peripheral plasma membrane protein CASK

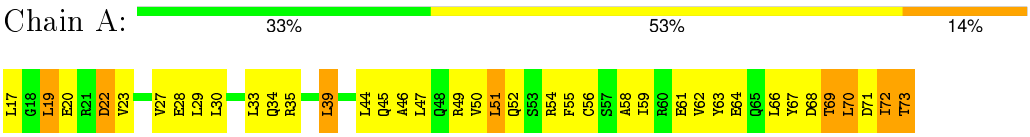


• Molecule 2: Peripheral plasma membrane protein CASK



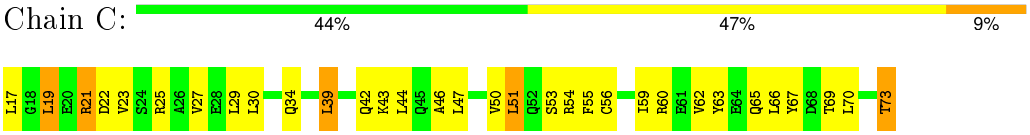
4.2.9 Score per residue for model 9

• Molecule 1: lin 7 homolog b



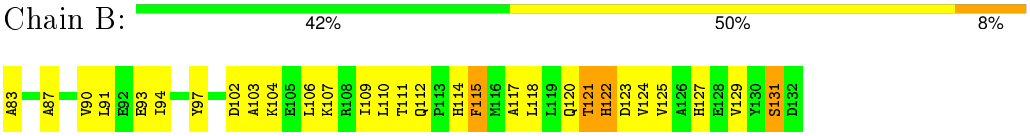
• Molecule 1: lin 7 homolog b

Chain C:



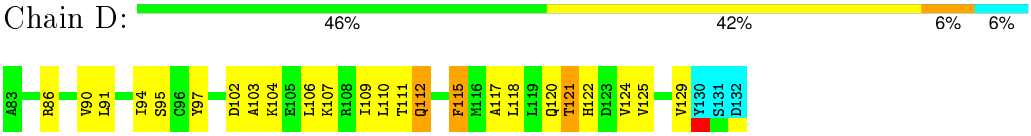
• Molecule 2: Peripheral plasma membrane protein CASK

Chain B:



• Molecule 2: Peripheral plasma membrane protein CASK

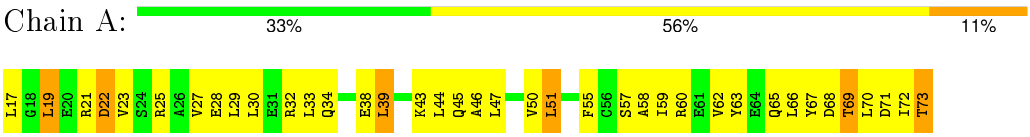
Chain D:



4.2.10 Score per residue for model 10

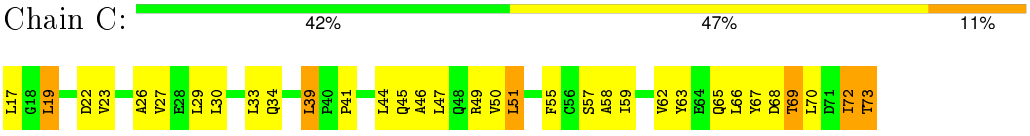
• Molecule 1: lin 7 homolog b

Chain A:



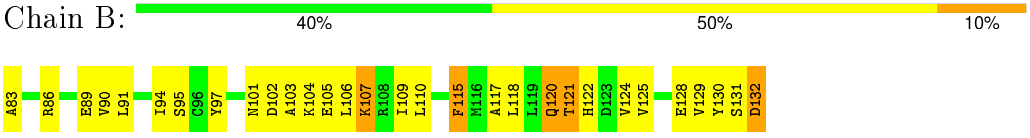
• Molecule 1: lin 7 homolog b

Chain C:



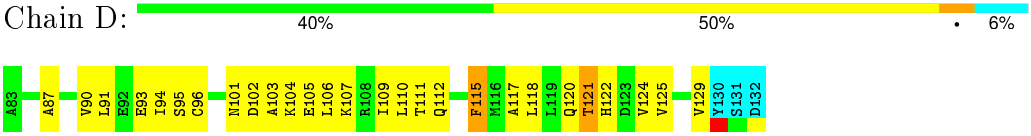
• Molecule 2: Peripheral plasma membrane protein CASK

Chain B:



• Molecule 2: Peripheral plasma membrane protein CASK

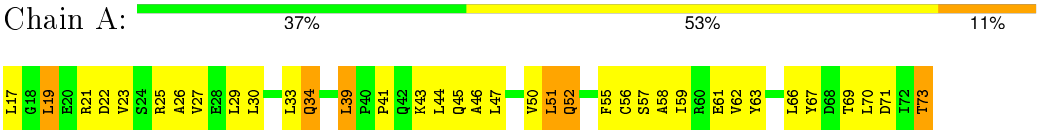
Chain D:



4.2.11 Score per residue for model 11

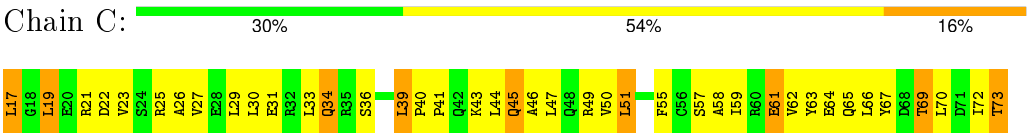
• Molecule 1: lin 7 homolog b

Chain A:



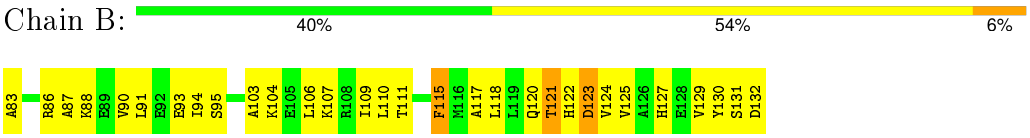
• Molecule 1: lin 7 homolog b

Chain C:



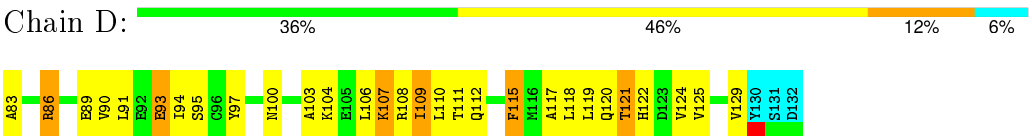
• Molecule 2: Peripheral plasma membrane protein CASK

Chain B:



• Molecule 2: Peripheral plasma membrane protein CASK

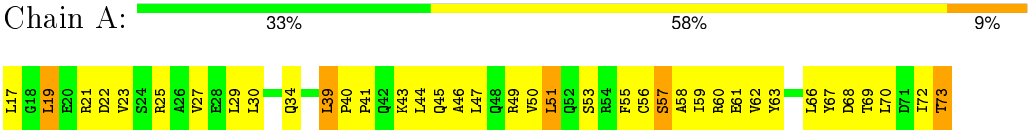
Chain D:



4.2.12 Score per residue for model 12

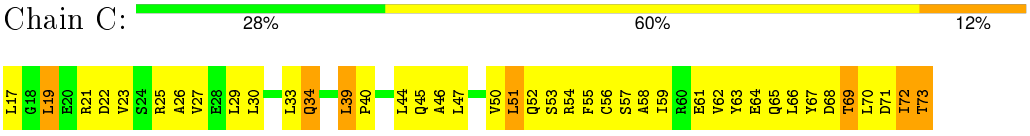
• Molecule 1: lin 7 homolog b

Chain A:



• Molecule 1: lin 7 homolog b

Chain C:

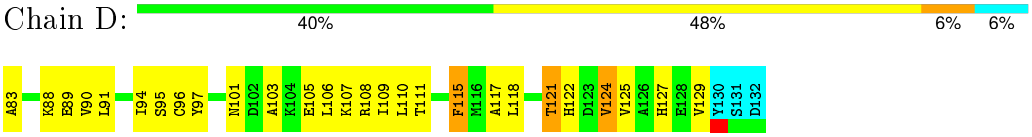


• Molecule 2: Peripheral plasma membrane protein CASK

Chain B:

• Molecule 2: Peripheral plasma membrane protein CASK

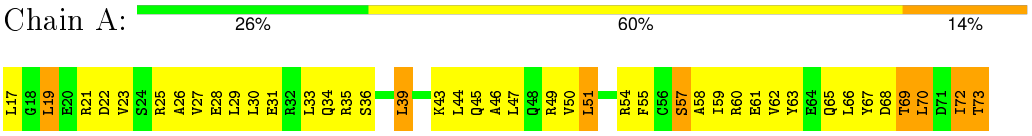
Chain D:



4.2.13 Score per residue for model 13

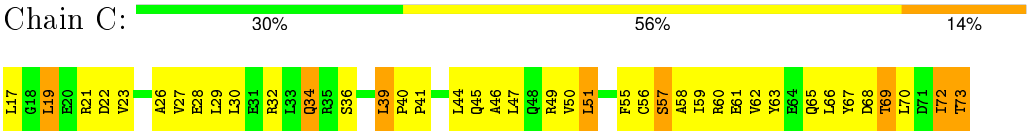
• Molecule 1: lin 7 homolog b

Chain A:



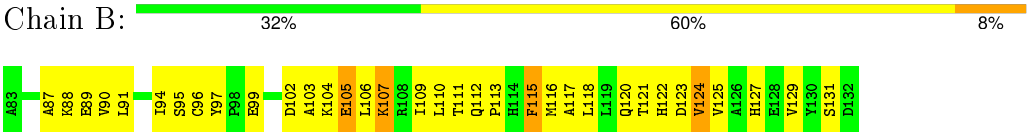
• Molecule 1: lin 7 homolog b

Chain C:



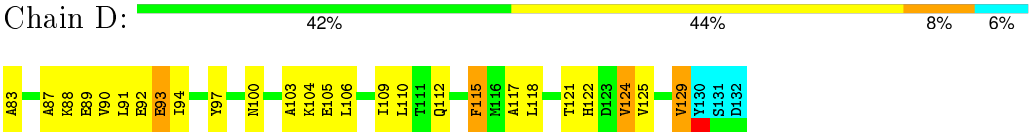
• Molecule 2: Peripheral plasma membrane protein CASK

Chain B:



• Molecule 2: Peripheral plasma membrane protein CASK

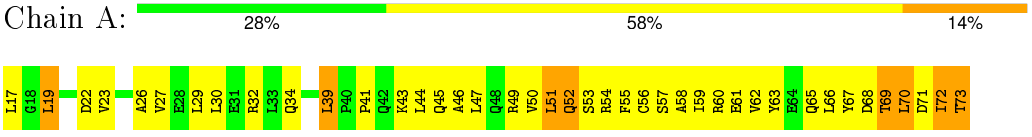
Chain D:



4.2.14 Score per residue for model 14

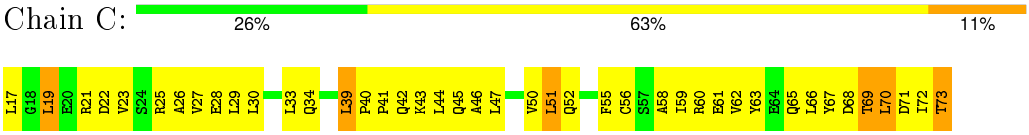
• Molecule 1: lin 7 homolog b

Chain A:



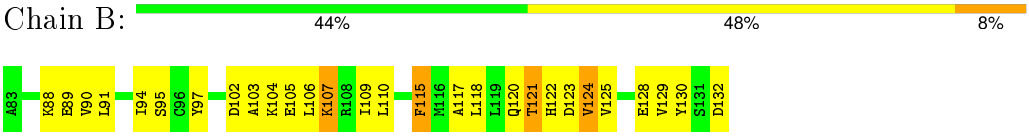
• Molecule 1: lin 7 homolog b

Chain C:



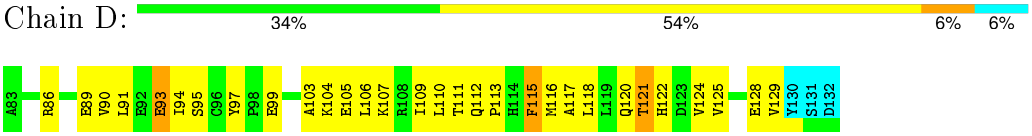
• Molecule 2: Peripheral plasma membrane protein CASK

Chain B:



• Molecule 2: Peripheral plasma membrane protein CASK

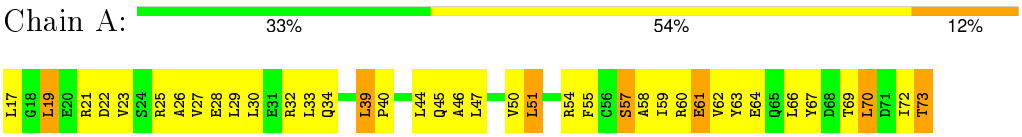
Chain D:



4.2.15 Score per residue for model 15

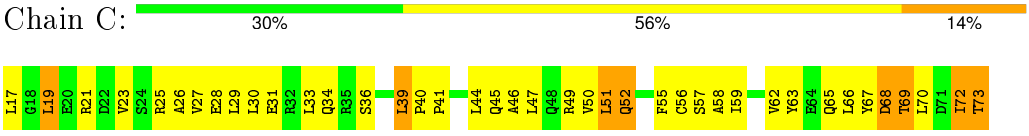
• Molecule 1: lin 7 homolog b

Chain A:



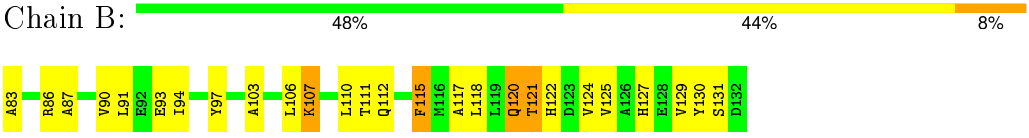
• Molecule 1: lin 7 homolog b

Chain C:



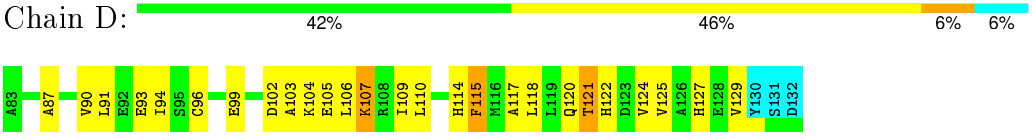
• Molecule 2: Peripheral plasma membrane protein CASK

Chain B:



• Molecule 2: Peripheral plasma membrane protein CASK

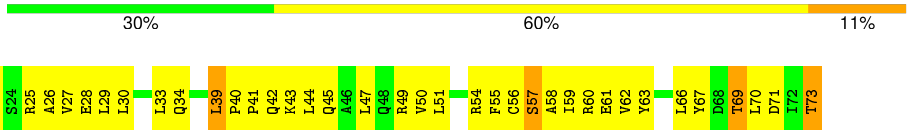
Chain D:



4.2.16 Score per residue for model 16

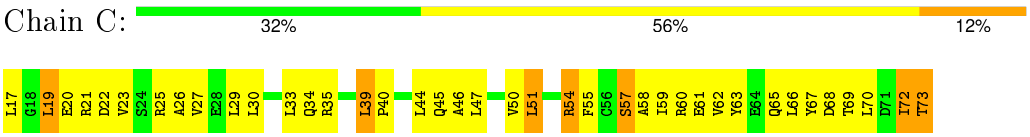
• Molecule 1: lin 7 homolog b

Chain A:



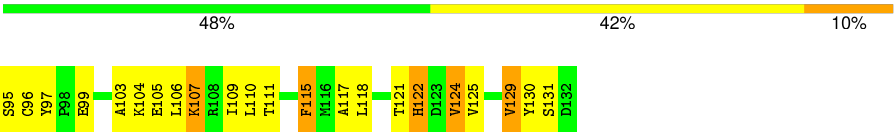
• Molecule 1: lin 7 homolog b

Chain C:



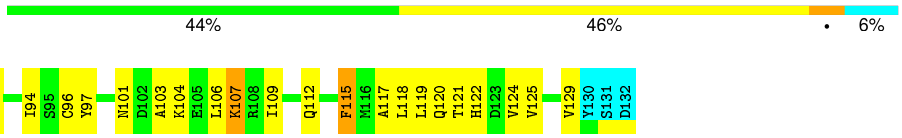
• Molecule 2: Peripheral plasma membrane protein CASK

Chain B:



• Molecule 2: Peripheral plasma membrane protein CASK

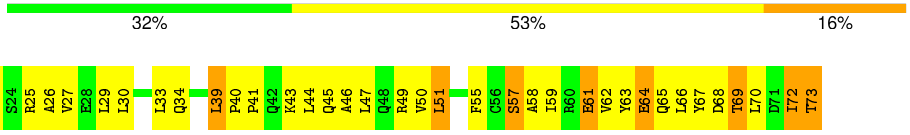
Chain D:



4.2.17 Score per residue for model 17

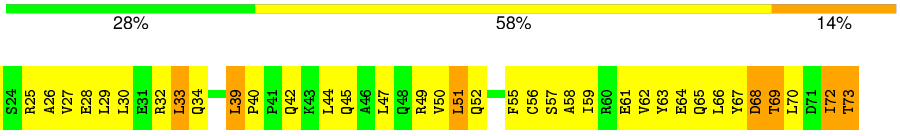
• Molecule 1: lin 7 homolog b

Chain A:



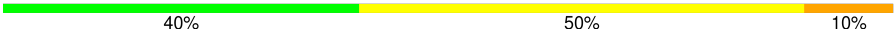
• Molecule 1: lin 7 homolog b

Chain C:



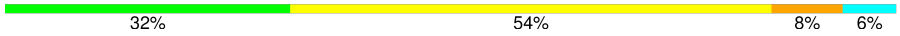
• Molecule 2: Peripheral plasma membrane protein CASK

Chain B:



• Molecule 2: Peripheral plasma membrane protein CASK

Chain D:



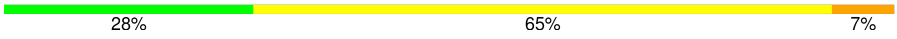
4.2.18 Score per residue for model 18

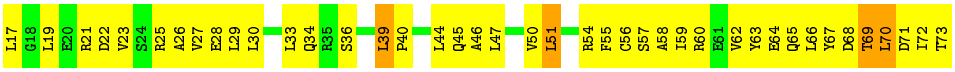
• Molecule 1: lin 7 homolog b

Chain A:

• Molecule 1: lin 7 homolog b

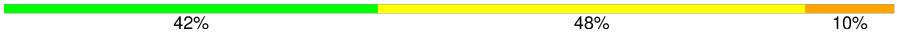
Chain C:





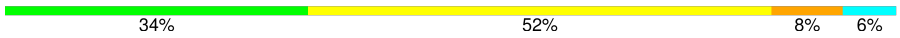
• Molecule 2: Peripheral plasma membrane protein CASK

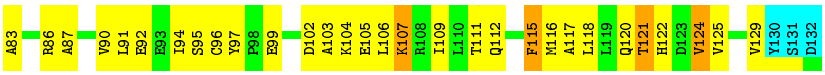
Chain B:



• Molecule 2: Peripheral plasma membrane protein CASK

Chain D:

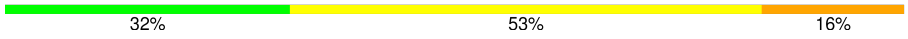


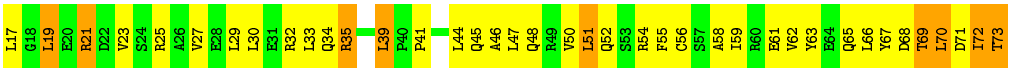


4.2.19 Score per residue for model 19

• Molecule 1: lin 7 homolog b

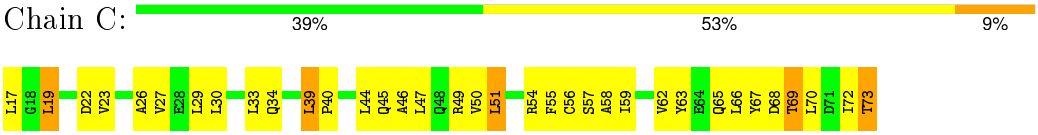
Chain A:





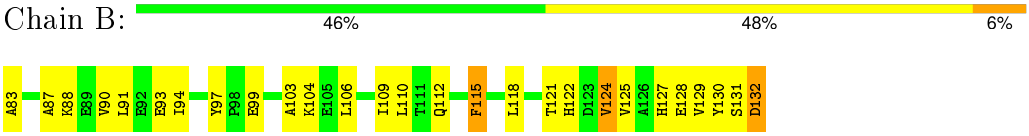
• Molecule 1: lin 7 homolog b

Chain C:



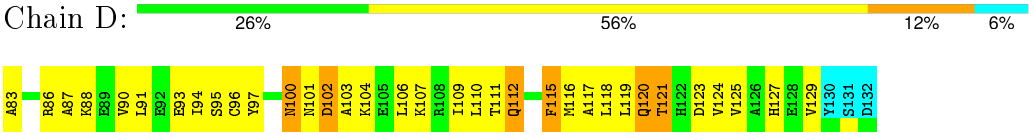
• Molecule 2: Peripheral plasma membrane protein CASK

Chain B:



• Molecule 2: Peripheral plasma membrane protein CASK

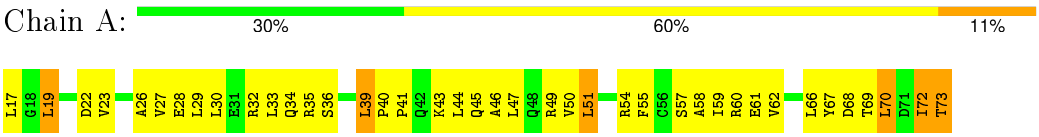
Chain D:



4.2.20 Score per residue for model 20

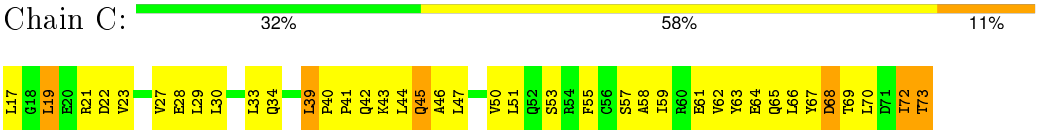
• Molecule 1: lin 7 homolog b

Chain A:



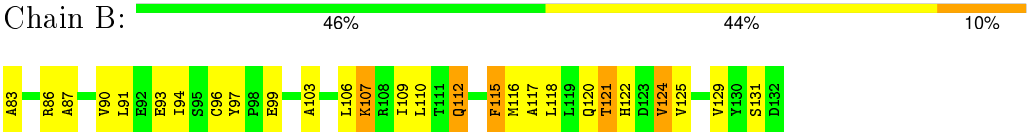
• Molecule 1: lin 7 homolog b

Chain C:



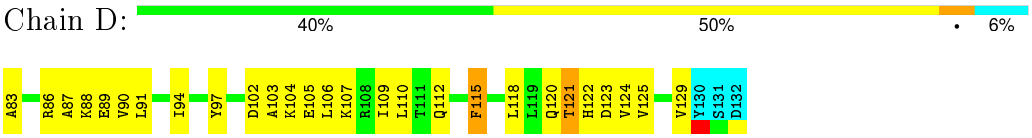
• Molecule 2: Peripheral plasma membrane protein CASK

Chain B:



• Molecule 2: Peripheral plasma membrane protein CASK

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	466	480	479	70±6
1	C	466	480	479	69±5
2	B	405	399	395	43±4
2	D	379	381	377	41±4
All	All	34320	34800	34600	2878

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 42.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:47:LEU:HD22	2:D:90:VAL:HG21	0.93	1.40	16	20
1:A:39:LEU:HD23	2:D:97:TYR:CD2	0.93	1.99	2	6
1:C:70:LEU:CD1	2:D:129:VAL:HG11	0.92	1.93	7	14
2:B:90:VAL:HG21	1:C:47:LEU:HD22	0.92	1.38	5	20
2:B:97:TYR:CD2	1:C:39:LEU:HD23	0.91	2.00	3	1
2:B:125:VAL:O	2:B:129:VAL:HG23	0.90	1.66	8	18
1:C:66:LEU:HD13	2:D:125:VAL:HG11	0.90	1.42	9	20
1:A:70:LEU:CD1	2:B:129:VAL:HG11	0.89	1.97	9	18
1:A:59:ILE:HD11	1:C:66:LEU:HD21	0.89	1.43	6	20
1:A:39:LEU:HD23	2:D:97:TYR:CD1	0.89	2.03	8	10
2:D:125:VAL:O	2:D:129:VAL:HG23	0.88	1.68	4	19

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:55:PHE:CE2	1:C:66:LEU:HD22	0.88	2.04	7	20
1:A:66:LEU:HD21	1:C:59:ILE:HD11	0.88	1.46	5	20
2:B:115:PHE:CE1	1:C:23:VAL:HG22	0.87	2.04	15	20
1:A:66:LEU:HD22	1:C:55:PHE:CE2	0.87	2.04	15	20
1:A:23:VAL:HG22	2:D:115:PHE:CE1	0.87	2.04	13	20
1:A:66:LEU:HD13	2:B:125:VAL:HG11	0.86	1.47	16	20
2:B:97:TYR:CD1	1:C:39:LEU:HD23	0.85	2.05	5	15
1:A:39:LEU:HD23	2:D:97:TYR:CG	0.84	2.07	11	12
1:A:66:LEU:CD1	2:B:125:VAL:HG11	0.84	2.03	14	20
2:B:115:PHE:CZ	1:C:23:VAL:HG22	0.83	2.07	15	19
1:A:55:PHE:CD2	1:C:66:LEU:HD22	0.83	2.09	2	20
1:A:66:LEU:HD22	1:C:55:PHE:CD2	0.82	2.10	4	20
2:B:120:GLN:O	2:B:124:VAL:HG23	0.81	1.76	15	5
1:A:70:LEU:HD13	2:B:130:TYR:CE2	0.81	2.10	19	9
2:B:103:ALA:HB2	1:C:33:LEU:HD21	0.81	1.50	11	3
1:C:46:ALA:O	1:C:50:VAL:HG23	0.80	1.76	14	19
2:D:120:GLN:O	2:D:124:VAL:HG23	0.80	1.75	17	7
1:C:23:VAL:O	1:C:27:VAL:HG23	0.80	1.76	17	20
2:B:122:HIS:CE1	1:C:50:VAL:HG13	0.79	2.12	20	5
2:B:118:LEU:HD12	1:C:59:ILE:HG22	0.79	1.54	20	20
1:A:46:ALA:O	1:A:50:VAL:HG23	0.79	1.78	9	19
1:A:23:VAL:O	1:A:27:VAL:HG23	0.79	1.77	15	20
1:C:27:VAL:HG13	1:C:48:GLN:OE1	0.79	1.78	7	1
1:C:66:LEU:CD1	2:D:125:VAL:HG11	0.78	2.07	2	20
1:A:69:THR:O	1:A:73:THR:HG23	0.78	1.78	6	14
2:B:94:ILE:HD12	2:B:103:ALA:O	0.78	1.79	2	13
1:C:33:LEU:HD22	1:C:39:LEU:HD11	0.77	1.56	12	4
1:C:19:LEU:O	1:C:23:VAL:HG23	0.77	1.80	7	20
1:A:23:VAL:HG22	2:D:115:PHE:CZ	0.77	2.15	9	18
1:A:70:LEU:HD11	2:B:129:VAL:HG11	0.76	1.56	5	12
1:C:69:THR:O	1:C:73:THR:HG23	0.76	1.80	16	13
1:A:59:ILE:HG22	2:D:118:LEU:HD12	0.76	1.55	12	20
1:C:70:LEU:HD11	2:D:129:VAL:HG11	0.75	1.57	6	9
1:A:19:LEU:O	1:A:23:VAL:HG23	0.75	1.81	4	20
2:B:97:TYR:CG	1:C:39:LEU:HD23	0.74	2.16	4	12
1:C:66:LEU:CD1	2:D:125:VAL:HG21	0.74	2.11	19	14
1:C:39:LEU:HD13	1:C:44:LEU:HD11	0.74	1.58	14	9
2:B:90:VAL:HG21	1:C:47:LEU:CD2	0.74	2.12	2	19
1:A:17:LEU:HD11	1:A:67:TYR:CG	0.74	2.17	16	3
1:A:22:ASP:OD2	2:D:109:ILE:HG23	0.74	1.83	9	2
1:A:59:ILE:CD1	1:C:66:LEU:HD21	0.73	2.13	2	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:105:GLU:CD	1:C:29:LEU:HD21	0.73	2.04	7	2
2:B:118:LEU:HD22	1:C:19:LEU:HD22	0.72	1.59	15	13
1:A:47:LEU:CD2	2:D:90:VAL:HG21	0.72	2.14	11	20
1:A:66:LEU:HD21	1:C:59:ILE:CD1	0.72	2.15	16	20
1:A:66:LEU:CD1	2:B:125:VAL:HG21	0.72	2.15	10	17
1:C:17:LEU:HD21	1:C:67:TYR:CE1	0.72	2.20	1	15
1:A:50:VAL:HG13	2:D:122:HIS:CE1	0.72	2.20	18	7
1:A:39:LEU:HB2	1:A:44:LEU:HD11	0.72	1.61	15	4
1:A:33:LEU:HD11	2:D:103:ALA:HA	0.71	1.61	19	3
1:C:70:LEU:HD13	2:D:129:VAL:HG11	0.71	1.60	8	7
1:A:41:PRO:HA	1:A:44:LEU:HD12	0.70	1.64	17	8
1:A:23:VAL:HG11	1:A:60:ARG:NH2	0.70	2.00	12	1
1:A:33:LEU:HD22	1:A:39:LEU:HD11	0.70	1.64	2	6
1:C:41:PRO:HA	1:C:44:LEU:HD12	0.70	1.63	4	11
1:A:39:LEU:HD22	2:D:94:ILE:HG22	0.69	1.62	13	4
2:B:121:THR:HG23	2:D:121:THR:HG23	0.69	1.64	2	2
2:B:87:ALA:HA	1:C:47:LEU:HD21	0.69	1.65	20	4
2:B:91:LEU:HD21	2:B:110:LEU:HB3	0.69	1.64	1	20
1:A:59:ILE:HD11	1:C:66:LEU:CD2	0.68	2.17	13	17
2:D:94:ILE:HB	2:D:103:ALA:HB1	0.68	1.64	7	20
2:B:106:LEU:HD22	1:C:29:LEU:HB3	0.68	1.64	20	6
1:A:22:ASP:O	2:D:109:ILE:HG21	0.68	1.89	20	18
1:A:19:LEU:HD22	2:D:118:LEU:HD22	0.68	1.64	11	18
1:A:66:LEU:CD2	1:C:59:ILE:HD11	0.68	2.19	14	18
1:A:58:ALA:O	1:A:62:VAL:HG23	0.67	1.89	18	20
1:A:30:LEU:HG	2:D:106:LEU:HD21	0.67	1.66	15	20
1:A:27:VAL:HG21	1:A:52:GLN:OE1	0.67	1.90	14	2
1:A:29:LEU:HD21	2:D:105:GLU:CD	0.67	2.10	13	3
1:A:17:LEU:HD21	1:A:67:TYR:CE1	0.67	2.24	16	16
1:A:69:THR:HG21	1:C:55:PHE:CA	0.67	2.20	4	13
1:A:62:VAL:O	1:A:66:LEU:HG	0.66	1.90	16	20
2:B:94:ILE:HB	2:B:103:ALA:HB1	0.66	1.67	2	20
2:B:109:ILE:HG21	1:C:22:ASP:O	0.66	1.91	18	17
1:A:55:PHE:CA	1:C:69:THR:HG21	0.66	2.21	18	8
2:B:106:LEU:HD21	1:C:30:LEU:HG	0.66	1.68	1	18
1:C:70:LEU:HD13	2:D:129:VAL:HG13	0.66	1.67	15	3
2:B:97:TYR:CE1	1:C:39:LEU:HD23	0.66	2.26	14	5
1:C:62:VAL:O	1:C:66:LEU:HG	0.65	1.91	2	20
1:A:39:LEU:CD2	2:D:94:ILE:HG22	0.65	2.21	13	3
2:D:107:LYS:O	2:D:111:THR:HG23	0.65	1.90	18	13
1:C:23:VAL:HG13	1:C:51:LEU:HB3	0.65	1.68	15	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:29:LEU:HD21	2:D:105:GLU:OE2	0.65	1.91	17	4
1:C:27:VAL:HG11	1:C:52:GLN:NE2	0.65	2.05	15	1
1:C:70:LEU:HD11	2:D:129:VAL:CG2	0.65	2.21	13	1
1:A:39:LEU:HD13	1:A:44:LEU:HD11	0.65	1.67	18	5
1:C:70:LEU:HD12	2:D:129:VAL:HG11	0.65	1.68	7	2
1:A:47:LEU:HD22	2:D:90:VAL:CG2	0.64	2.21	6	10
1:A:59:ILE:HG22	2:D:118:LEU:CD1	0.64	2.23	12	11
1:A:17:LEU:HD21	1:A:67:TYR:CD1	0.64	2.28	6	11
2:B:129:VAL:HG12	2:B:130:TYR:CG	0.64	2.27	2	7
1:A:29:LEU:O	1:A:33:LEU:HD12	0.64	1.93	13	3
2:D:91:LEU:HD21	2:D:110:LEU:HB3	0.64	1.68	14	17
1:C:67:TYR:CE1	2:D:129:VAL:HG13	0.63	2.28	18	1
2:B:118:LEU:CD1	1:C:59:ILE:HG22	0.63	2.22	20	11
1:C:70:LEU:CD1	2:D:129:VAL:HG13	0.63	2.23	15	4
1:A:44:LEU:HD23	2:D:90:VAL:HG13	0.63	1.69	6	17
1:A:27:VAL:HG11	1:A:52:GLN:OE1	0.63	1.94	14	2
1:A:33:LEU:HD21	2:D:103:ALA:HB2	0.63	1.70	7	1
1:A:66:LEU:HD22	1:C:55:PHE:CZ	0.63	2.28	6	20
1:A:29:LEU:HD22	2:D:102:ASP:O	0.63	1.93	7	3
1:A:70:LEU:HD13	2:B:129:VAL:HG11	0.62	1.70	17	8
2:B:90:VAL:HG13	1:C:44:LEU:HD23	0.62	1.72	4	17
1:A:27:VAL:HG13	1:A:52:GLN:NE2	0.62	2.10	8	2
1:A:63:TYR:OH	2:D:117:ALA:HB1	0.62	1.94	10	17
1:A:55:PHE:CZ	1:C:66:LEU:HD22	0.61	2.29	6	20
1:A:33:LEU:HD11	2:D:103:ALA:CA	0.61	2.24	7	2
1:A:51:LEU:N	1:A:51:LEU:HD23	0.61	2.10	10	12
2:D:83:ALA:HB1	2:D:119:LEU:HD22	0.61	1.73	19	4
1:C:17:LEU:HD22	1:C:19:LEU:HD12	0.61	1.69	8	1
2:B:117:ALA:HB1	1:C:63:TYR:OH	0.61	1.95	10	18
2:B:105:GLU:OE2	1:C:29:LEU:HD21	0.61	1.96	4	2
1:C:51:LEU:N	1:C:51:LEU:HD23	0.61	2.11	18	5
1:C:62:VAL:HG12	1:C:66:LEU:CD1	0.61	2.25	17	18
1:C:51:LEU:HD23	1:C:51:LEU:N	0.60	2.11	5	11
1:C:17:LEU:HD22	1:C:63:TYR:HB3	0.60	1.73	19	9
2:D:91:LEU:HD13	2:D:111:THR:HG22	0.60	1.72	18	1
1:A:51:LEU:HD23	1:A:51:LEU:N	0.60	2.11	3	6
1:C:70:LEU:HD13	2:D:129:VAL:CG1	0.60	2.27	12	8
2:D:91:LEU:HD13	2:D:111:THR:CG2	0.60	2.26	18	6
1:C:58:ALA:O	1:C:62:VAL:HG23	0.60	1.97	7	19
1:A:59:ILE:HD13	1:C:62:VAL:CG1	0.60	2.27	18	7
2:B:94:ILE:HD11	2:B:107:LYS:CG	0.60	2.27	12	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:129:VAL:HG12	2:B:130:TYR:CD2	0.59	2.32	2	9
1:A:19:LEU:HD21	2:D:115:PHE:HA	0.59	1.74	9	1
1:A:69:THR:HG21	1:C:55:PHE:HA	0.59	1.75	4	14
1:A:69:THR:HG21	1:C:55:PHE:N	0.59	2.13	16	5
2:B:115:PHE:CZ	1:C:51:LEU:HD13	0.59	2.33	4	14
1:C:30:LEU:O	1:C:34:GLN:HG2	0.59	1.98	9	3
1:C:25:ARG:O	1:C:29:LEU:HD12	0.59	1.98	7	1
2:B:109:ILE:HD11	1:C:25:ARG:NH1	0.59	2.13	17	1
2:B:90:VAL:CG2	1:C:47:LEU:HD22	0.58	2.23	5	10
2:B:91:LEU:HD21	2:B:110:LEU:CB	0.58	2.29	1	7
1:C:29:LEU:O	1:C:33:LEU:HD12	0.58	1.98	3	4
2:D:94:ILE:HD12	2:D:103:ALA:O	0.58	1.97	20	9
1:A:62:VAL:HG12	1:A:66:LEU:CD1	0.58	2.29	2	16
2:D:94:ILE:HD11	2:D:107:LYS:CG	0.58	2.28	11	8
1:A:17:LEU:HD11	1:A:67:TYR:CD1	0.58	2.34	13	2
1:C:17:LEU:CD2	1:C:19:LEU:HD12	0.58	2.29	8	1
1:A:55:PHE:N	1:C:69:THR:HG21	0.57	2.12	2	3
2:B:94:ILE:HD11	2:B:107:LYS:HG2	0.57	1.75	8	4
2:B:103:ALA:HA	1:C:33:LEU:HD11	0.57	1.74	14	3
2:B:102:ASP:O	1:C:29:LEU:HD22	0.57	1.99	4	5
2:B:121:THR:CG2	2:D:121:THR:HG23	0.57	2.29	8	2
1:A:51:LEU:HD13	2:D:115:PHE:CZ	0.57	2.35	14	14
1:A:33:LEU:HD21	2:D:103:ALA:N	0.57	2.15	10	8
1:A:70:LEU:CD1	2:B:129:VAL:HG13	0.57	2.30	2	1
1:C:66:LEU:O	1:C:70:LEU:HG	0.57	1.99	4	17
2:B:103:ALA:N	1:C:33:LEU:HD21	0.56	2.15	16	9
2:D:83:ALA:HB2	2:D:122:HIS:ND1	0.56	2.16	16	8
2:D:125:VAL:HG12	2:D:129:VAL:CG2	0.56	2.31	5	6
2:B:121:THR:HG23	2:D:121:THR:CG2	0.56	2.31	5	5
1:A:62:VAL:CG1	1:C:59:ILE:HD13	0.56	2.31	16	10
2:B:107:LYS:O	2:B:111:THR:HG23	0.55	2.02	16	11
1:A:55:PHE:O	1:A:59:ILE:HG12	0.55	2.02	15	20
1:A:62:VAL:HG21	1:C:62:VAL:HG21	0.55	1.78	12	17
1:A:62:VAL:HG21	1:C:62:VAL:CG2	0.55	2.32	6	7
1:A:17:LEU:HD22	1:A:63:TYR:HB3	0.55	1.76	11	8
2:D:91:LEU:CD1	2:D:111:THR:HG22	0.55	2.31	18	1
2:B:122:HIS:CD2	1:C:55:PHE:CD1	0.55	2.95	16	20
2:B:118:LEU:HD22	1:C:19:LEU:CD2	0.55	2.32	4	1
2:B:109:ILE:HD12	1:C:29:LEU:CD1	0.55	2.32	11	13
1:A:70:LEU:HD13	2:B:129:VAL:HG13	0.55	1.79	2	1
1:A:22:ASP:CG	2:D:109:ILE:HG23	0.54	2.23	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:55:PHE:CD1	2:D:122:HIS:CD2	0.54	2.96	17	19
1:A:70:LEU:HD13	2:B:129:VAL:CG1	0.54	2.32	17	7
2:B:121:THR:HG22	2:D:121:THR:HG23	0.54	1.80	8	1
2:B:121:THR:HG23	2:D:121:THR:HG22	0.54	1.78	9	3
2:D:94:ILE:HD11	2:D:107:LYS:HG3	0.54	1.78	18	1
1:A:32:ARG:O	1:A:35:ARG:HG3	0.54	2.03	19	1
2:B:115:PHE:HZ	1:C:51:LEU:HD13	0.54	1.62	4	15
1:A:22:ASP:HB3	2:D:109:ILE:HG23	0.54	1.80	14	2
1:A:62:VAL:HG12	1:A:66:LEU:HD11	0.53	1.78	2	8
1:C:27:VAL:HG12	1:C:31:GLU:OE2	0.53	2.02	15	2
1:A:30:LEU:O	1:A:34:GLN:HG2	0.53	2.02	14	2
1:A:55:PHE:HA	1:C:69:THR:HG21	0.53	1.79	18	8
1:C:70:LEU:HD11	2:D:129:VAL:HG21	0.53	1.81	13	1
1:C:66:LEU:HD13	2:D:125:VAL:CG1	0.53	2.33	18	17
1:C:27:VAL:HG11	1:C:52:GLN:HE22	0.52	1.60	15	1
2:D:105:GLU:O	2:D:109:ILE:HD12	0.52	2.04	20	12
1:A:51:LEU:HD13	2:D:115:PHE:HZ	0.52	1.64	3	19
2:B:122:HIS:CD2	1:C:55:PHE:CE1	0.52	2.97	11	7
2:B:105:GLU:O	2:B:109:ILE:HD12	0.52	2.05	14	9
2:B:107:LYS:NZ	2:B:111:THR:HG21	0.52	2.19	3	1
1:A:44:LEU:CD2	2:D:90:VAL:HG13	0.52	2.35	7	7
1:A:23:VAL:HG13	1:A:51:LEU:HB3	0.52	1.81	19	9
1:C:69:THR:O	1:C:73:THR:HG22	0.52	2.05	9	6
2:B:102:ASP:HB3	1:C:29:LEU:HD23	0.52	1.79	7	2
1:C:55:PHE:O	1:C:59:ILE:HG12	0.52	2.05	12	20
1:A:39:LEU:HD23	2:D:97:TYR:CE1	0.52	2.39	19	2
1:C:23:VAL:HG13	1:C:51:LEU:CB	0.52	2.35	15	1
2:B:83:ALA:HB2	2:B:122:HIS:ND1	0.52	2.20	10	10
1:A:29:LEU:CD1	2:D:109:ILE:HD12	0.52	2.34	3	8
1:A:55:PHE:CE1	2:D:122:HIS:CD2	0.52	2.98	16	4
2:D:86:ARG:O	2:D:90:VAL:HG23	0.51	2.05	11	4
1:A:23:VAL:HG11	1:A:60:ARG:CZ	0.51	2.35	12	1
1:C:27:VAL:HG11	1:C:52:GLN:CD	0.51	2.26	17	2
1:C:17:LEU:HD21	1:C:67:TYR:CD1	0.51	2.40	12	8
1:A:47:LEU:O	1:A:51:LEU:HG	0.51	2.05	6	19
1:A:70:LEU:HD13	2:B:130:TYR:HE2	0.51	1.63	5	5
2:B:103:ALA:CB	1:C:33:LEU:HD21	0.51	2.31	11	1
1:A:66:LEU:HD13	2:B:125:VAL:CG1	0.51	2.34	1	19
2:B:117:ALA:HB2	2:D:128:GLU:HG3	0.51	1.82	5	1
1:A:66:LEU:O	1:A:70:LEU:HG	0.51	2.06	7	17
1:A:29:LEU:HD13	2:D:106:LEU:HA	0.51	1.81	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:59:ILE:HG21	2:D:121:THR:HB	0.50	1.83	19	6
1:A:62:VAL:CG2	1:C:62:VAL:HG21	0.50	2.36	7	4
1:A:66:LEU:HD12	2:B:125:VAL:HG21	0.50	1.82	20	1
1:C:68:ASP:O	1:C:72:ILE:HG13	0.50	2.05	12	17
1:A:70:LEU:HD13	2:B:130:TYR:CZ	0.50	2.41	6	2
2:B:125:VAL:HG12	2:B:129:VAL:CG2	0.50	2.37	2	3
1:A:23:VAL:HG21	1:A:60:ARG:HD2	0.50	1.81	2	1
1:C:47:LEU:O	1:C:51:LEU:HG	0.50	2.07	15	19
1:A:69:THR:O	1:A:73:THR:HG22	0.50	2.07	8	6
1:C:62:VAL:HG12	1:C:66:LEU:HD11	0.50	1.83	17	10
1:A:29:LEU:HD21	2:D:105:GLU:OE1	0.50	2.06	14	1
1:A:62:VAL:CG2	1:C:62:VAL:CG2	0.50	2.90	15	20
1:A:39:LEU:CD1	1:A:44:LEU:HD11	0.50	2.37	7	3
1:A:27:VAL:HG11	1:A:52:GLN:CG	0.50	2.37	18	1
2:B:90:VAL:HG13	1:C:44:LEU:CD2	0.50	2.36	10	9
1:C:39:LEU:HD12	1:C:39:LEU:H	0.50	1.66	11	1
2:B:109:ILE:HD11	1:C:25:ARG:HH11	0.50	1.66	17	1
1:A:39:LEU:H	1:A:39:LEU:HD12	0.49	1.65	15	1
1:A:66:LEU:HD22	1:C:55:PHE:CG	0.49	2.43	16	1
2:B:124:VAL:CG1	2:B:125:VAL:N	0.49	2.75	16	15
2:D:91:LEU:HD21	2:D:110:LEU:CB	0.49	2.37	14	3
2:B:90:VAL:CG1	1:C:44:LEU:HD23	0.49	2.37	12	2
2:B:106:LEU:HD22	1:C:29:LEU:CB	0.49	2.35	20	2
2:B:86:ARG:O	2:B:90:VAL:HG23	0.49	2.06	2	2
2:D:124:VAL:CG1	2:D:125:VAL:N	0.49	2.75	13	13
1:A:39:LEU:HD12	1:A:39:LEU:H	0.49	1.67	13	3
1:C:27:VAL:HG22	1:C:51:LEU:HB2	0.49	1.85	5	1
1:C:39:LEU:HB2	1:C:44:LEU:HD11	0.49	1.84	11	1
1:A:63:TYR:CE1	2:B:125:VAL:HG22	0.49	2.43	2	1
1:C:30:LEU:HD11	1:C:47:LEU:HB3	0.49	1.85	12	2
1:C:39:LEU:HD12	1:C:39:LEU:N	0.49	2.23	11	1
1:A:17:LEU:CD2	1:A:67:TYR:CE1	0.49	2.95	11	18
1:C:70:LEU:CD1	2:D:129:VAL:CG1	0.49	2.91	17	6
1:A:65:GLN:O	1:A:69:THR:OG1	0.49	2.31	17	12
1:A:68:ASP:O	1:A:72:ILE:HG13	0.48	2.07	2	13
2:B:121:THR:HG22	2:D:121:THR:CG2	0.48	2.38	17	3
1:C:23:VAL:HG21	1:C:60:ARG:HD3	0.48	1.83	18	1
1:A:47:LEU:HD21	2:D:87:ALA:HA	0.48	1.83	7	3
1:C:17:LEU:CD2	1:C:67:TYR:CE1	0.48	2.96	2	16
1:A:70:LEU:CD1	2:B:129:VAL:CG1	0.48	2.90	7	7
1:A:55:PHE:CG	1:C:66:LEU:HD22	0.48	2.43	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:D:125:VAL:O	2:D:129:VAL:N	0.48	2.46	13	2
1:A:66:LEU:HD12	2:B:125:VAL:HG11	0.47	1.85	14	3
1:C:27:VAL:HG11	1:C:52:GLN:OE1	0.47	2.09	17	1
1:A:27:VAL:HG22	1:A:51:LEU:HB2	0.47	1.86	2	2
1:A:59:ILE:HD11	1:C:66:LEU:HD11	0.47	1.86	2	6
1:A:69:THR:HG23	1:C:54:ARG:HB3	0.47	1.86	16	1
1:A:39:LEU:N	1:A:39:LEU:HD12	0.47	2.25	15	1
2:B:121:THR:CG2	2:D:121:THR:HG22	0.47	2.40	11	4
2:B:121:THR:HB	1:C:59:ILE:HG21	0.47	1.87	9	7
2:B:91:LEU:O	2:B:95:SER:CB	0.47	2.63	1	14
2:B:86:ARG:NH1	1:C:46:ALA:HB1	0.47	2.24	7	1
2:D:91:LEU:O	2:D:95:SER:CB	0.47	2.63	3	14
1:A:66:LEU:HD11	1:C:59:ILE:CD1	0.47	2.40	14	8
1:A:67:TYR:CE1	2:B:129:VAL:HG13	0.47	2.45	6	1
1:A:62:VAL:CG2	1:C:62:VAL:HG22	0.47	2.40	9	4
1:A:26:ALA:HA	2:D:106:LEU:HD13	0.47	1.87	17	9
1:A:29:LEU:HD13	2:D:106:LEU:CA	0.47	2.40	17	1
2:B:106:LEU:HD23	1:C:33:LEU:CD1	0.46	2.40	20	1
1:C:69:THR:HG22	1:C:73:THR:CG2	0.46	2.40	12	1
1:A:66:LEU:HD11	1:C:59:ILE:HD11	0.46	1.87	14	7
1:A:67:TYR:HE1	2:B:129:VAL:HG22	0.46	1.69	6	2
2:D:87:ALA:O	2:D:91:LEU:HG	0.46	2.10	17	11
1:A:39:LEU:CD2	2:D:94:ILE:HA	0.46	2.40	13	3
1:A:56:CYS:SG	2:D:118:LEU:HD21	0.46	2.50	19	1
2:D:93:GLU:O	2:D:97:TYR:CD2	0.46	2.69	13	2
1:A:30:LEU:CG	2:D:106:LEU:HD21	0.46	2.39	15	4
1:A:58:ALA:O	1:A:61:GLU:CG	0.46	2.64	18	2
1:C:17:LEU:HD11	1:C:67:TYR:CG	0.46	2.45	18	2
1:C:39:LEU:CD1	1:C:44:LEU:HD11	0.46	2.40	17	2
1:A:29:LEU:HB3	2:D:106:LEU:HD22	0.46	1.87	16	3
1:A:33:LEU:HG	2:D:102:ASP:HB2	0.46	1.88	20	3
1:A:39:LEU:HD12	1:A:39:LEU:N	0.46	2.26	13	2
2:B:103:ALA:CA	1:C:33:LEU:HD11	0.46	2.40	14	1
1:A:67:TYR:CE1	2:B:129:VAL:HG22	0.46	2.46	16	3
2:B:117:ALA:HB2	2:D:128:GLU:OE2	0.46	2.11	17	1
1:A:19:LEU:CD1	1:A:63:TYR:CD2	0.45	2.99	19	2
1:C:67:TYR:HE1	2:D:129:VAL:HG22	0.45	1.71	18	1
1:A:62:VAL:HG22	1:C:62:VAL:HG22	0.45	1.88	17	8
2:B:129:VAL:CG1	2:B:130:TYR:CD2	0.45	2.99	16	2
1:A:23:VAL:HG13	2:D:115:PHE:CZ	0.45	2.46	4	1
1:C:33:LEU:CD2	1:C:39:LEU:HD11	0.45	2.39	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:44:LEU:HD23	2:D:90:VAL:CG1	0.45	2.40	11	3
2:D:94:ILE:HD11	2:D:107:LYS:HA	0.45	1.88	5	1
1:C:65:GLN:O	1:C:69:THR:OG1	0.45	2.35	18	16
1:C:26:ALA:O	1:C:30:LEU:HD12	0.45	2.12	15	1
2:B:97:TYR:CG	1:C:39:LEU:CD2	0.45	2.99	7	4
2:B:115:PHE:HA	1:C:19:LEU:HD21	0.45	1.89	13	1
2:B:125:VAL:O	2:B:129:VAL:N	0.45	2.50	2	1
2:B:129:VAL:O	2:B:130:TYR:CD1	0.45	2.69	14	3
1:C:67:TYR:CZ	2:D:129:VAL:HG13	0.45	2.47	3	2
1:C:21:ARG:O	1:C:25:ARG:CG	0.45	2.65	7	1
2:D:83:ALA:HB1	2:D:119:LEU:CD2	0.45	2.41	19	1
2:B:109:ILE:HG23	1:C:22:ASP:HB3	0.45	1.88	17	1
2:D:94:ILE:HD11	2:D:107:LYS:HG2	0.45	1.89	4	1
2:B:106:LEU:HD21	1:C:30:LEU:CD2	0.45	2.42	4	1
1:A:59:ILE:CG2	2:D:118:LEU:HD12	0.45	2.38	13	1
2:B:100:ASN:CB	1:C:33:LEU:HD21	0.45	2.41	1	1
1:A:30:LEU:O	1:A:34:GLN:NE2	0.45	2.50	6	3
2:D:124:VAL:HG13	2:D:125:VAL:N	0.45	2.27	2	2
2:B:127:HIS:O	2:B:131:SER:CB	0.44	2.65	15	3
1:C:70:LEU:HD11	2:D:129:VAL:HG22	0.44	1.87	13	1
1:C:19:LEU:CD1	1:C:63:TYR:CD2	0.44	2.99	11	1
2:D:125:VAL:C	2:D:129:VAL:HG23	0.44	2.32	5	1
1:A:39:LEU:CD2	2:D:97:TYR:CG	0.44	2.99	5	2
2:D:112:GLN:OE1	2:D:115:PHE:N	0.44	2.50	9	1
1:A:21:ARG:O	1:A:25:ARG:HB2	0.44	2.12	11	10
2:D:106:LEU:HA	2:D:109:ILE:HG12	0.44	1.90	11	1
1:A:29:LEU:CD1	2:D:109:ILE:CD1	0.44	2.95	17	4
1:C:17:LEU:C	1:C:19:LEU:H	0.44	2.15	8	1
2:B:88:LYS:HA	2:B:91:LEU:HG	0.44	1.90	12	4
1:A:59:ILE:CD1	1:C:66:LEU:HD11	0.44	2.42	2	6
2:B:115:PHE:CZ	1:C:23:VAL:HG13	0.44	2.47	6	2
2:D:112:GLN:O	2:D:116:MET:HG3	0.44	2.13	19	2
1:A:62:VAL:HG22	1:C:62:VAL:CG2	0.44	2.42	20	4
2:B:106:LEU:HD13	1:C:26:ALA:HA	0.44	1.88	19	11
1:A:17:LEU:HD11	1:A:67:TYR:HB2	0.44	1.90	6	1
1:A:70:LEU:N	1:A:70:LEU:HD23	0.44	2.28	6	1
2:B:109:ILE:CD1	1:C:29:LEU:CD1	0.43	2.95	1	7
2:D:125:VAL:HG12	2:D:129:VAL:HG23	0.43	1.88	15	1
2:D:121:THR:O	2:D:124:VAL:HG12	0.43	2.13	2	1
1:A:28:GLU:O	1:A:32:ARG:HB2	0.43	2.12	7	2
1:A:70:LEU:HD12	2:B:129:VAL:HG11	0.43	1.82	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:121:THR:CG2	2:D:121:THR:CG2	0.43	2.96	2	10
2:B:87:ALA:O	2:B:91:LEU:HG	0.43	2.14	9	8
2:D:113:PRO:HA	2:D:116:MET:HG3	0.43	1.90	7	3
1:C:30:LEU:O	1:C:34:GLN:NE2	0.43	2.52	13	2
1:C:21:ARG:O	1:C:25:ARG:HB2	0.43	2.14	18	10
2:D:94:ILE:HD11	2:D:107:LYS:CB	0.43	2.43	16	2
2:D:94:ILE:HD11	2:D:107:LYS:CA	0.43	2.44	17	2
2:B:115:PHE:CE2	1:C:23:VAL:HA	0.43	2.49	17	6
2:B:94:ILE:HD11	2:B:107:LYS:HA	0.43	1.91	20	1
1:A:29:LEU:CD1	2:D:109:ILE:HD11	0.43	2.44	11	1
1:A:17:LEU:HD11	1:A:64:GLU:HA	0.43	1.91	17	1
1:C:70:LEU:N	1:C:70:LEU:HD23	0.43	2.29	18	2
2:B:113:PRO:HA	2:B:116:MET:HG3	0.43	1.90	13	3
2:D:107:LYS:NZ	2:D:111:THR:HG21	0.43	2.29	11	1
1:A:17:LEU:CD2	1:A:67:TYR:CD1	0.43	3.02	12	2
2:B:100:ASN:HB3	1:C:33:LEU:HD21	0.43	1.89	1	1
1:A:26:ALA:HA	2:D:106:LEU:CD1	0.43	2.43	1	4
1:C:31:GLU:CG	1:C:48:GLN:NE2	0.43	2.82	1	2
1:C:51:LEU:N	1:C:51:LEU:CD2	0.43	2.80	9	2
1:C:41:PRO:O	1:C:45:GLN:HG2	0.43	2.13	6	2
2:B:118:LEU:HD12	1:C:59:ILE:CG2	0.43	2.42	9	1
1:A:45:GLN:HA	1:A:45:GLN:NE2	0.43	2.29	11	1
1:A:39:LEU:CD2	2:D:97:TYR:CD2	0.43	3.02	17	1
2:B:106:LEU:HD21	1:C:30:LEU:CG	0.43	2.42	12	7
2:B:121:THR:O	2:B:124:VAL:HG12	0.43	2.13	9	1
2:D:86:ARG:O	2:D:89:GLU:CG	0.43	2.67	17	1
2:B:109:ILE:HG23	1:C:22:ASP:CG	0.43	2.35	5	1
1:A:38:GLU:O	2:D:97:TYR:CZ	0.43	2.72	2	1
1:A:27:VAL:HG13	1:A:52:GLN:CD	0.43	2.34	8	1
1:A:26:ALA:O	1:A:30:LEU:HD12	0.42	2.14	13	2
1:A:29:LEU:HB2	2:D:106:LEU:HD13	0.42	1.90	11	1
1:A:59:ILE:CD1	1:C:62:VAL:CG1	0.42	2.98	2	1
1:C:58:ALA:O	1:C:61:GLU:CG	0.42	2.66	7	1
1:A:27:VAL:HG11	1:A:52:GLN:HG2	0.42	1.91	4	1
1:A:57:SER:O	1:A:61:GLU:CG	0.42	2.67	4	13
2:D:94:ILE:CD1	2:D:103:ALA:O	0.42	2.68	8	5
1:A:55:PHE:CD1	1:A:55:PHE:C	0.42	2.93	2	4
1:C:27:VAL:HG11	1:C:52:GLN:CG	0.42	2.44	5	1
1:A:17:LEU:CD2	1:A:67:TYR:CZ	0.42	3.03	17	1
2:B:130:TYR:N	2:B:130:TYR:CD1	0.42	2.87	8	1
1:A:19:LEU:HD13	1:A:63:TYR:CB	0.42	2.45	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:112:GLN:O	2:B:116:MET:HG3	0.42	2.15	1	2
2:B:106:LEU:CD1	1:C:26:ALA:HA	0.42	2.45	16	6
2:B:123:ASP:OD1	2:B:127:HIS:CE1	0.42	2.73	13	1
2:D:88:LYS:HA	2:D:91:LEU:HG	0.42	1.91	3	3
2:B:97:TYR:CZ	1:C:39:LEU:HB3	0.42	2.50	1	2
2:D:91:LEU:CD2	2:D:110:LEU:HD12	0.42	2.45	11	1
1:A:39:LEU:HD23	2:D:97:TYR:HD1	0.42	1.67	8	1
1:C:20:GLU:O	1:C:24:SER:CB	0.42	2.68	1	1
1:A:51:LEU:CD2	1:A:51:LEU:N	0.42	2.82	5	3
1:A:19:LEU:HD11	1:A:63:TYR:CD2	0.42	2.50	6	1
1:A:54:ARG:HH11	1:C:69:THR:HG23	0.42	1.75	4	1
1:C:17:LEU:HD11	1:C:67:TYR:CD1	0.42	2.49	3	1
1:A:32:ARG:NH1	2:D:105:GLU:OE1	0.42	2.53	20	6
1:C:55:PHE:CD1	1:C:55:PHE:C	0.42	2.93	4	4
2:D:123:ASP:O	2:D:127:HIS:CD2	0.42	2.72	19	1
2:D:91:LEU:HD21	2:D:110:LEU:HB2	0.42	1.91	11	1
1:C:41:PRO:O	1:C:45:GLN:NE2	0.42	2.52	20	1
1:C:57:SER:O	1:C:61:GLU:CG	0.42	2.68	13	10
2:B:94:ILE:CD1	2:B:103:ALA:O	0.42	2.68	1	5
2:D:91:LEU:O	2:D:95:SER:N	0.42	2.52	18	3
1:C:49:ARG:O	1:C:53:SER:CB	0.41	2.68	4	1
1:A:29:LEU:HD12	2:D:109:ILE:CD1	0.41	2.46	14	2
1:A:34:GLN:OE1	1:A:45:GLN:NE2	0.41	2.53	11	1
1:A:55:PHE:CE1	1:A:59:ILE:HD11	0.41	2.50	17	1
2:B:94:ILE:CD1	2:B:107:LYS:CG	0.41	2.98	12	2
1:C:55:PHE:C	1:C:55:PHE:CD1	0.41	2.93	16	2
1:A:33:LEU:HD21	2:D:100:ASN:HB2	0.41	1.91	19	1
1:C:67:TYR:CE1	2:D:129:VAL:HG22	0.41	2.50	18	1
2:B:103:ALA:N	1:C:33:LEU:HD11	0.41	2.29	1	1
1:C:21:ARG:O	1:C:25:ARG:CB	0.41	2.69	15	4
1:C:28:GLU:O	1:C:32:ARG:HB2	0.41	2.16	13	2
2:B:90:VAL:CG2	1:C:47:LEU:CD2	0.41	2.96	12	1
1:A:23:VAL:HA	2:D:115:PHE:CE2	0.41	2.51	19	3
2:B:105:GLU:OE1	1:C:32:ARG:NH1	0.41	2.54	5	2
1:C:39:LEU:CB	1:C:40:PRO:CD	0.41	2.98	2	1
2:D:111:THR:HA	2:D:116:MET:CE	0.41	2.45	18	1
1:A:41:PRO:O	1:A:45:GLN:HG2	0.41	2.15	11	2
2:B:123:ASP:O	2:B:127:HIS:CB	0.41	2.68	11	2
1:A:39:LEU:CB	1:A:40:PRO:CD	0.41	2.98	5	2
1:C:41:PRO:O	1:C:45:GLN:HB2	0.41	2.16	11	1
2:B:121:THR:HB	1:C:59:ILE:CG2	0.41	2.46	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:47:LEU:CD2	2:D:90:VAL:CG2	0.41	2.97	14	1
2:D:109:ILE:O	2:D:112:GLN:HG2	0.41	2.16	14	1
1:A:55:PHE:C	1:A:55:PHE:CD1	0.41	2.94	16	1
2:B:94:ILE:HD11	2:B:107:LYS:HG3	0.41	1.93	1	1
1:A:33:LEU:HD21	2:D:100:ASN:CB	0.41	2.45	7	1
2:B:106:LEU:HA	1:C:29:LEU:HD13	0.41	1.93	7	1
1:A:34:GLN:NE2	1:A:44:LEU:HB2	0.41	2.30	6	1
2:D:93:GLU:O	2:D:97:TYR:CD1	0.41	2.74	11	2
1:A:21:ARG:O	1:A:25:ARG:CB	0.41	2.69	19	1
1:A:51:LEU:N	1:A:51:LEU:CD2	0.41	2.83	4	1
2:B:127:HIS:CE1	2:B:131:SER:OG	0.41	2.74	4	1
2:B:131:SER:O	2:B:131:SER:OG	0.41	2.39	9	1
2:D:108:ARG:HG2	2:D:109:ILE:N	0.41	2.30	11	1
1:C:51:LEU:CD2	1:C:51:LEU:N	0.41	2.81	5	1
2:B:106:LEU:HD13	1:C:29:LEU:CB	0.41	2.46	4	1
1:C:31:GLU:OE1	1:C:48:GLN:NE2	0.41	2.54	2	1
2:B:123:ASP:OD1	2:B:127:HIS:CD2	0.41	2.75	2	1
1:A:62:VAL:CG1	1:C:59:ILE:CD1	0.40	2.98	5	1
2:B:109:ILE:HG23	1:C:22:ASP:CB	0.40	2.47	5	1
2:B:118:LEU:CD1	1:C:59:ILE:CG2	0.40	2.99	20	1
2:B:128:GLU:CD	2:D:117:ALA:HB2	0.40	2.36	10	1
2:B:112:GLN:NE2	1:C:22:ASP:OD1	0.40	2.53	17	1
2:B:125:VAL:HG12	2:B:129:VAL:HG23	0.40	1.92	2	1
2:B:91:LEU:O	2:B:95:SER:N	0.40	2.55	2	1
1:A:27:VAL:HG11	1:A:52:GLN:CD	0.40	2.37	19	1
2:D:102:ASP:O	2:D:106:LEU:HB2	0.40	2.16	19	1
1:A:19:LEU:CD1	1:A:63:TYR:CB	0.40	2.99	13	1
2:B:91:LEU:HD13	2:B:111:THR:CG2	0.40	2.46	13	1
2:B:124:VAL:HG13	2:B:125:VAL:N	0.40	2.30	9	1
2:B:109:ILE:HD12	1:C:29:LEU:HD12	0.40	1.92	11	1
1:A:33:LEU:HD12	2:D:106:LEU:HD23	0.40	1.94	19	1
2:B:127:HIS:CD2	2:B:132:ASP:OD1	0.40	2.74	19	1
2:B:102:ASP:O	2:B:106:LEU:HB2	0.40	2.16	9	1
2:B:130:TYR:O	2:B:132:ASP:N	0.40	2.55	10	1
2:B:94:ILE:HD11	2:B:107:LYS:CB	0.40	2.46	3	1
2:B:118:LEU:HD21	1:C:60:ARG:HG3	0.40	1.92	2	1
2:B:125:VAL:C	2:B:129:VAL:HG23	0.40	2.30	8	1
2:B:123:ASP:O	2:B:127:HIS:N	0.40	2.55	9	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	55/57 (96%)	53±1 (97±2%)	1±1 (2±2%)	1±0 (1±1%)	23	69
1	C	55/57 (96%)	53±1 (97±2%)	1±1 (2±2%)	1±0 (1±1%)	19	64
2	B	48/50 (96%)	45±1 (93±2%)	3±1 (6±2%)	1±1 (1±1%)	24	71
2	D	46/50 (92%)	44±1 (95±2%)	2±1 (5±2%)	0±0 (0±0%)	100	100
All	All	4080/4280 (95%)	3896 (95%)	147 (4%)	37 (1%)	26	73

All 4 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	C	40	PRO	15
1	A	40	PRO	12
2	B	130	TYR	6
2	B	131	SER	4

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	52/52 (100%)	37±3 (71±6%)	15±3 (29±6%)	2	19
1	C	52/52 (100%)	38±2 (72±4%)	14±2 (28±4%)	2	21
2	B	45/45 (100%)	35±2 (78±4%)	10±2 (22±4%)	4	31
2	D	42/45 (93%)	33±2 (78±4%)	9±2 (22±4%)	4	31
All	All	3820/3880 (98%)	2843 (74%)	977 (26%)	3	25

All 122 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	39	LEU	20
2	B	115	PHE	20
1	A	73	THR	20
2	D	121	THR	20
1	C	73	THR	20
1	A	19	LEU	20
2	B	121	THR	20
1	C	39	LEU	20
2	D	115	PHE	20
1	A	51	LEU	19
1	C	19	LEU	19
1	A	45	GLN	19
1	C	45	GLN	19
2	B	104	LYS	18
1	C	51	LEU	18
1	C	34	GLN	18
1	A	34	GLN	18
2	D	104	LYS	17
1	A	69	THR	16
2	B	112	GLN	16
1	C	56	CYS	16
2	D	112	GLN	16
1	C	69	THR	15
1	A	43	LYS	15
1	A	72	ILE	14
1	C	72	ILE	14
2	B	124	VAL	13
2	B	107	LYS	13
1	C	57	SER	13
1	A	54	ARG	12
1	C	54	ARG	11
1	A	57	SER	11
2	D	107	LYS	11
1	A	60	ARG	10
1	A	56	CYS	10
2	B	120	GLN	10
1	A	28	GLU	10
1	C	49	ARG	9
2	D	124	VAL	9
2	D	120	GLN	9
1	A	71	ASP	9
1	A	49	ARG	9
1	C	43	LYS	9

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Mol	Chain	Res	Type	Models (Total)
1	A	35	ARG	9
2	B	93	GLU	9
2	D	89	GLU	9
2	D	93	GLU	8
2	B	130	TYR	8
1	A	70	LEU	7
2	D	99	GLU	7
2	D	86	ARG	7
2	D	96	CYS	7
1	A	64	GLU	7
1	A	53	SER	7
2	B	132	ASP	7
1	C	64	GLU	7
1	C	28	GLU	7
1	C	60	ARG	7
1	C	71	ASP	7
2	D	88	LYS	7
2	B	102	ASP	6
1	C	70	LEU	6
1	C	21	ARG	6
1	C	36	SER	6
2	D	102	ASP	6
2	B	89	GLU	6
2	B	86	ARG	6
1	C	42	GLN	6
2	B	88	LYS	6
2	B	99	GLU	6
2	B	92	GLU	5
2	D	92	GLU	5
1	A	52	GLN	5
1	C	68	ASP	5
1	C	61	GLU	5
1	A	36	SER	5
1	C	52	GLN	5
1	A	61	GLU	4
2	D	101	ASN	4
2	B	105	GLU	4
1	C	53	SER	4
1	C	35	ARG	4
1	A	48	GLN	4
2	D	127	HIS	4
2	B	96	CYS	4

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Mol	Chain	Res	Type	Models (Total)
1	A	65	GLN	3
1	A	68	ASP	3
2	B	123	ASP	3
1	A	20	GLU	3
2	D	100	ASN	3
1	A	21	ARG	3
2	D	105	GLU	3
2	B	131	SER	3
2	B	108	ARG	3
1	C	33	LEU	3
2	B	114	HIS	3
2	B	128	GLU	3
2	D	123	ASP	3
2	D	108	ARG	3
1	A	42	GLN	3
1	C	48	GLN	3
2	D	128	GLU	3
2	B	127	HIS	2
1	C	65	GLN	2
1	C	20	GLU	2
2	B	101	ASN	2
2	B	122	HIS	2
1	A	22	ASP	2
2	D	114	HIS	2
1	C	40	PRO	1
1	A	33	LEU	1
1	C	50	VAL	1
2	D	129	VAL	1
1	A	50	VAL	1
2	D	111	THR	1
1	C	17	LEU	1
1	A	31	GLU	1
1	A	38	GLU	1
2	D	109	ILE	1
2	B	111	THR	1
2	B	129	VAL	1
1	A	17	LEU	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