Full wwPDB NMR Structure Validation Report (i)

Mar 6, 2022 – 12:27 PM EST

PDB ID	:	2KA9
Title	:	Solution structure of PSD-95 PDZ12 complexed with cypin peptide
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Deposited on	:	2008-11-03

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

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

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

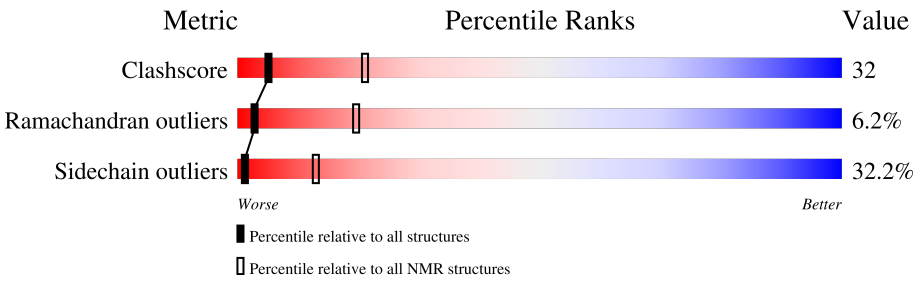
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	189	36% 48% 11% 6%
2	B	9	100%
2	C	9	22% 11% 67%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 14 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:2-A:90 (89)	0.40	1
2	A:97-A:185, C:7-C:9 (92)	0.41	14

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. No single-model clusters were found.

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 3127 atoms, of which 1579 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Disks large homolog 4.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	189	2857	889	1443	248	273	4	0

- Molecule 2 is a protein called cypin peptide.

Mol	Chain	Residues	Atoms					Trace
			Total	C	H	N	O	
2	B	9	135	43	68	10	14	0
2	C	9	135	43	68	10	14	0

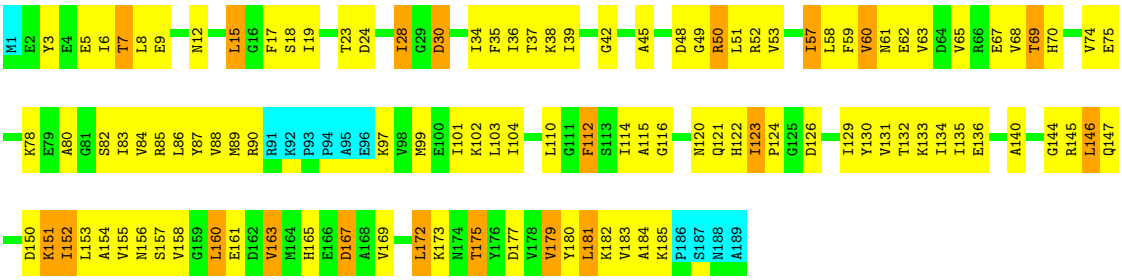
4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• Molecule 1: Disks large homolog 4

Chain A: 36% 48% 11% 6%



• Molecule 2: cypin peptide

Chain B: 100%

• Molecule 2: cypin peptide

Chain C: 22% 11% 67%

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: Disks large homolog 4

Chain A: 36% 41% 17% • 6%

M1 E2 Y3 E4 E5 I6 T7 L8 E9 N12 L15 G16 F17 S18 I19 T23 D24 H27 I28 G29 D30 D31 I34 F35 I36 T37 K38 G42 A45 D48 G49 R50 L51 R52 V53 N54 D55 S56 I57 L58 F59 V60 V65 R66 E67 V68 T69 H70 S71 V74

K78 E79 A80 G81 S82 I83 V84 R85 L86 Y87 V88 R91 K92 P93 P94 A95 E96 K97 V98 M99 K102 L103 I104 K108 G109 L110 G111 F112 S113 I114 A115 G116 N120 Q121 H122 I123 D126 I129 Y130 V131 T132 K133 I134 A140 G144 R145 L146 Q147 I148 G149 D150

K151 I152 L153 A154 V155 N156 S157 V158 G159 L160 E161 D162 V163 M164 H165 E166 D167 A168 V169 L172 K173 N174 T175 Y176 D177 V178 V179 Y180 L181 K182 V183 A184 K185 P186 S187 N188 A189

• Molecule 2: cypin peptide

Chain B: 100%

Q1 V2 V3 P4 F5 S6 S7 S8 V9

• Molecule 2: cypin peptide

Chain C: 22% 11% 67%

Q1 V2 V3 P4 F5 S6 S7 S8 V9

4.2.2 Score per residue for model 2

• Molecule 1: Disks large homolog 4

Chain A: 38% 37% 19% • 6%

M1 E2 Y3 E4 E5 I6 T7 L8 E9 R10 G11 N12 L15 G16 F17 S18 I19 T23 D24 I28 G29 D30 D31 I34 F35 I36 T37 K38 I39 I40 P41 A44 R50 L51 R52 V53 I57 V60 N61 E62 V63 D64 V65 R66 E67 V68 T69 H70 S71 V74 E75

A76 L77 K78 E79 A80 G81 S82 I83 V84 R85 L86 Y87 V88 R91 K92 P93 P94 A95 E96 K97 V98 M99 E100 I101 K102 L103 I104 K105 G106 G109 F112 S113 I114 A115 N120 Q121 H122 I123 P124 G125 D126 I129 Y130 V131 T132 K133 I134 I135 E136 A139 A140 H141 K142 D143

G144 R145 L146 Q147 D150 K151 I152 L153 A154 V155 N156 S157 V158 G159 L160 E161 D162 V163 M164 H165 E166 D167 A168 V169 L172 T175 Y176 D177 V178 V179 Y180 L181 K182 V183 A184 K185 P186 S187 N188 A189

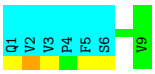
• Molecule 2: cypin peptide

Chain B: 100%

Q1 V2 V3 P4 F5 S6 S7 S8 V9

• Molecule 2: cypin peptide

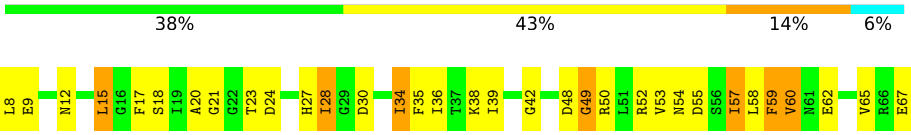
Chain C: 33% 67%

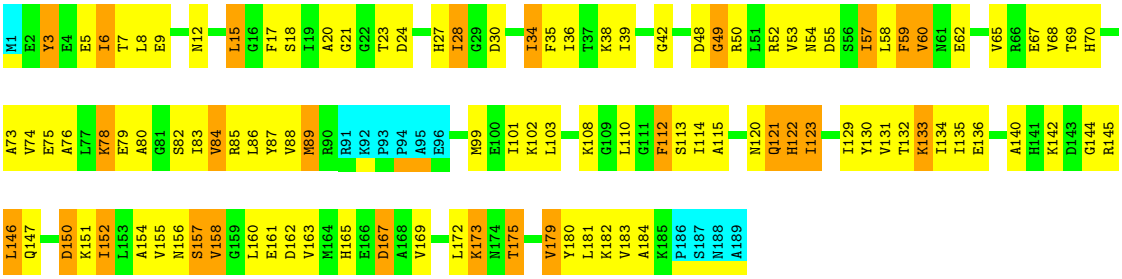


4.2.3 Score per residue for model 3

- Molecule 1: Disks large homolog 4

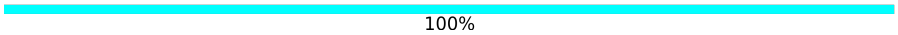
Chain A:





- Molecule 2: cypin peptide

Chain B:



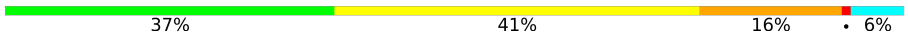
- Molecule 2: cypin peptide

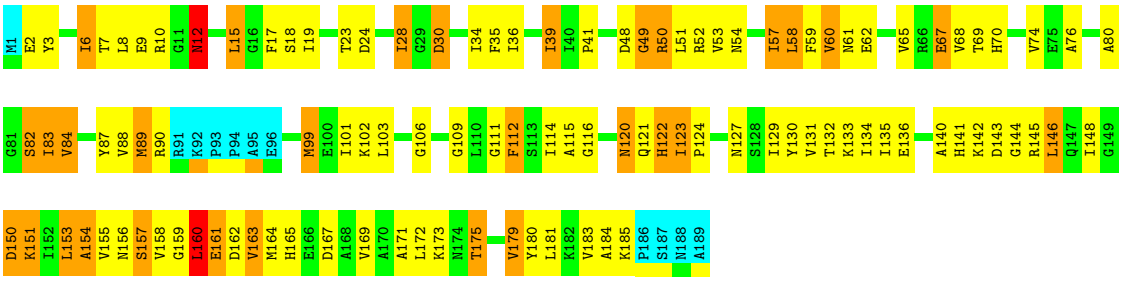
Chain C:

4.2.4 Score per residue for model 4

- Molecule 1: Disks large homolog 4

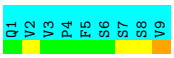
Chain A:





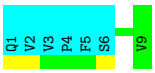
- Molecule 2: cypin peptide

Chain B: 100%



• Molecule 2: cypin peptide

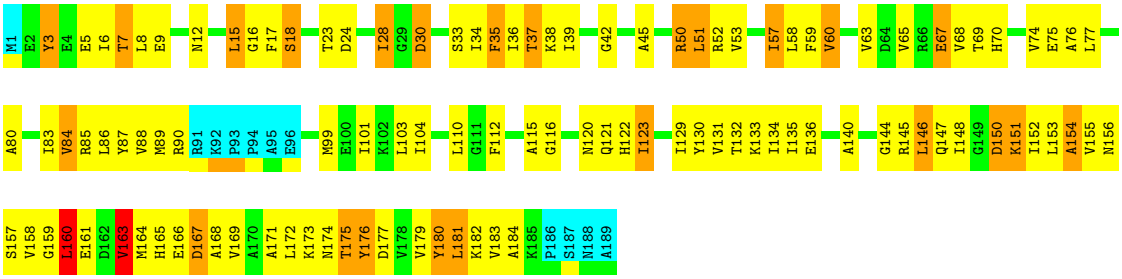
Chain C: 33% 67%



4.2.5 Score per residue for model 5

• Molecule 1: Disks large homolog 4

Chain A: 37% 44% 13% • 6%



• Molecule 2: cypin peptide

Chain B: 100%

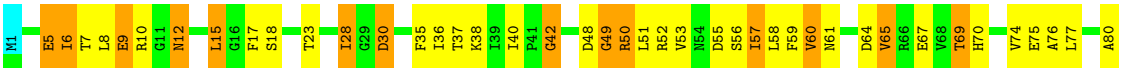
• Molecule 2: cypin peptide

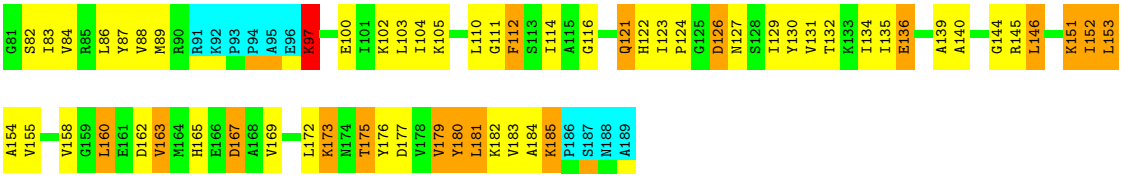
Chain C: 11% 22% 67%

4.2.6 Score per residue for model 6

• Molecule 1: Disks large homolog 4

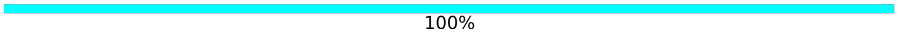
Chain A: 40% 37% 16% • 6%





- Molecule 2: cypin peptide

Chain B:



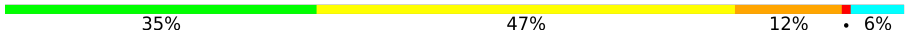
- Molecule 2: cypin peptide

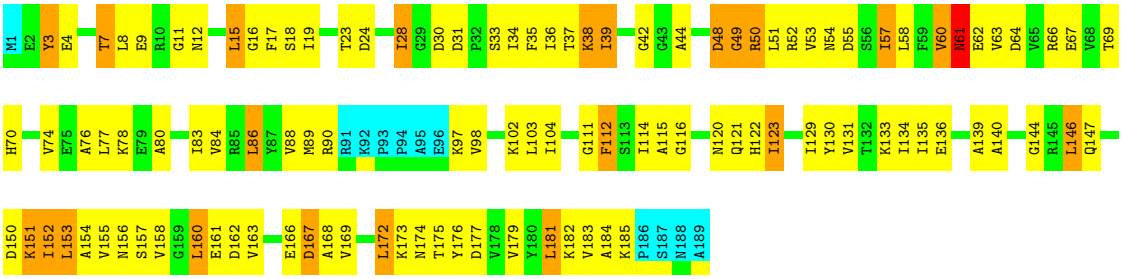
Chain C:

4.2.7 Score per residue for model 7

- Molecule 1: Disks large homolog 4

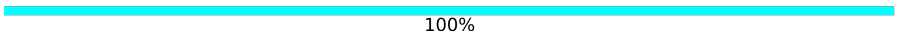
Chain A:





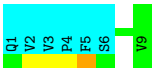
- Molecule 2: cypin peptide

Chain B:



- Molecule 2: cypin peptide

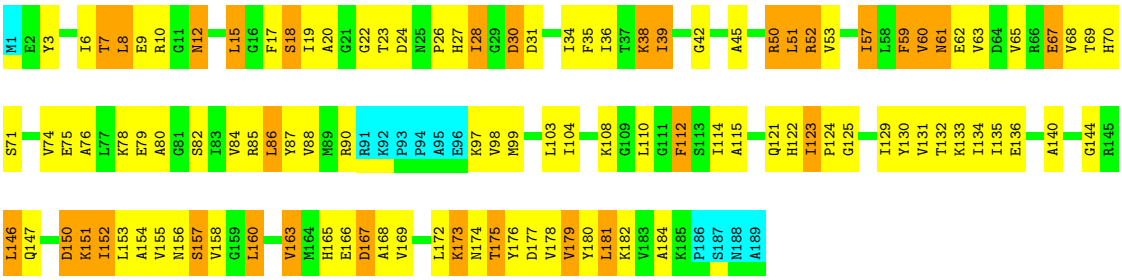
Chain C:



4.2.8 Score per residue for model 8

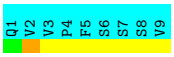
- Molecule 1: Disks large homolog 4

Chain A: 35% 42% 17% 6%



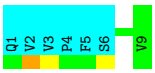
- Molecule 2: cypin peptide

Chain B: 100%



- Molecule 2: cypin peptide

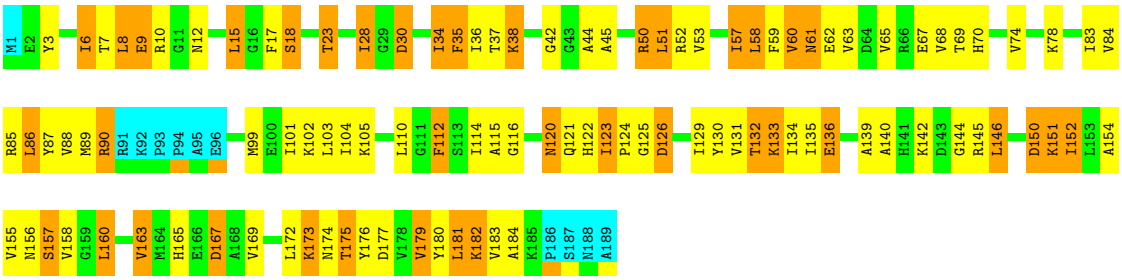
Chain C: 33% 67%



4.2.9 Score per residue for model 9

- Molecule 1: Disks large homolog 4

Chain A: 39% 34% 21% 6%



- Molecule 2: cypin peptide

Chain B: 100%

• Molecule 2: cypin peptide

Chain C: 22% 11% 67%

Q1 V2 V3 P4 F5 S6 S7 S8 V9

4.2.10 Score per residue for model 10

• Molecule 1: Disks large homolog 4

Chain A: 32% 50% 12% • 6%

M1 E2 Y3 E4 E5 I6 T7 L8 E9 N12 L15 G16 F17 S18 I19 A20 G21 G22 T23 D24 N25 P26 H27 I28 G29 D30 D31 I34 F35 I36 T37 K38 I39 G42 A45 D48 G49 R50 L51 R52 V53 N54 D55 S56 I57 L58 F59 V60 V63 D64 V65 R66 E67

V68 T69 H70 V74 E75 A76 L77 K78 E79 A80 G81 S82 I83 V84 R85 L86 Y87 V88 R91 K92 P93 P94 A95 E96 K97 E100 I101 K102 L103 I104 K105 G106 P107 K108 G109 L110 G111 F112 S113 I114 A115 N120 Q121 H122 I123 P124 G125 D126 I129 Y130 V131 T132 K133 I134 I135

E136 A139 A140 H141 K142 D143 G144 R145 L146 K151 I152 L153 A154 V155 N156 S157 V158 G159 L160 E161 D162 V163 M164 H165 E166 D167 A168 V169 A170 A171 L172 K173 N174 V178 V179 Y180 L181 K182 V183 A184 K185 P186 S187 N188 A189

• Molecule 2: cypin peptide

Chain B: 100%

Q1 V2 V3 P4 F5 S6 S7 S8 V9

• Molecule 2: cypin peptide

Chain C: 33% 67%

Q1 V2 V3 P4 F5 S6 V9

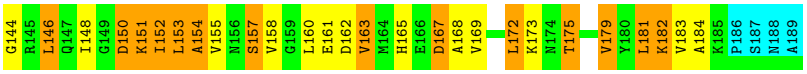
4.2.11 Score per residue for model 11

• Molecule 1: Disks large homolog 4

Chain A: 35% 41% 17% • 6%

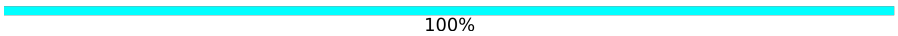
M1 E2 Y3 E4 E5 I6 T7 L8 E9 N12 L15 G16 F17 S18 I19 A20 T23 D24 H27 I28 I34 F35 I36 T37 K38 I39 I40 P41 G42 D48 G49 R50 L51 R52 V53 S56 I57 L58 F59 V60 N61 E62 V63 D64 V65 R66 E67 V68 T69 H70 S71 A72 A73

V74 L77 K78 E79 A80 G81 S82 I83 V84 R85 L86 Y87 V88 N89 R90 R91 K92 P93 P94 A95 E96 K97 I101 K102 L103 G106 G109 L110 G111 F112 S113 I114 A115 G116 N120 Q121 H122 I123 P124 G125 D126 I129 Y130 V131 T132 K133 I134 I135 E136 A140 H141 K142 D143



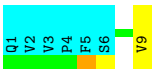
• Molecule 2: cypin peptide

Chain B:



• Molecule 2: cypin peptide

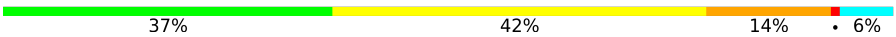
Chain C:

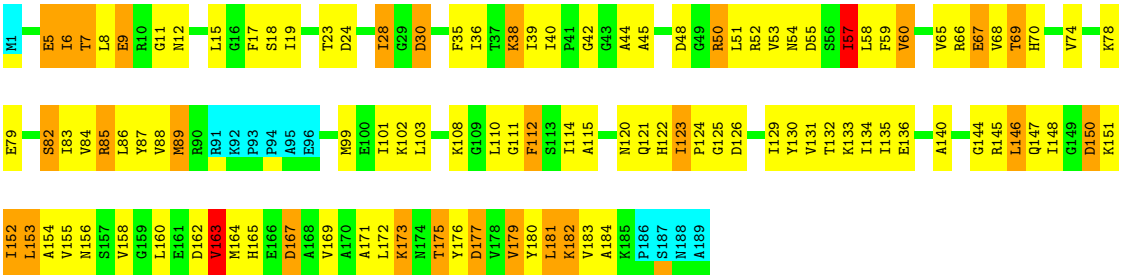


4.2.12 Score per residue for model 12

• Molecule 1: Disks large homolog 4

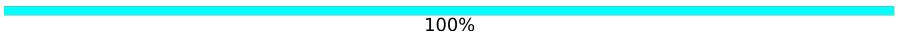
Chain A:

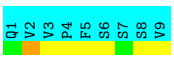




• Molecule 2: cypin peptide

Chain B:





• Molecule 2: cypin peptide

Chain C:

4.2.13 Score per residue for model 13

• Molecule 1: Disks large homolog 4

Chain A: 35% 41% 18% • 6%

M1 E2 Y3 I6 T7 L8 E9 R10 G11 N12 L15 G16 F17 S18 I19 T23 D24 N25 P26 H27 I28 G29 D30 D31 P32 S33 I34 F35 I36 T37 K38 I39 A44 A45 R50 L51 R52 V53 I57 L58 F59 V60 N61 E67 V68 T69 H70 S71 V74 E75 A76 L77

K78 E79 A80 I83 V84 R85 L86 Y87 V88 M89 R90 R91 K92 P93 P94 A95 E96 E100 I101 K102 L103 I104 K108 G109 L110 G111 F112 S113 I114 A115 N120 Q121 H122 I123 P124 G125 D126 I129 Y130 V131 T132 K133 I134 I135 E136 A140 H141 K142 D143 G144 R145 L146 Q147 I148

G149 D150 K151 I152 L153 A154 V155 N156 S157 V158 G159 L160 E161 D162 V163 M164 H165 E166 D167 A168 V169 L172 K173 N174 T175 Y176 D177 V178 V179 Y180 L181 K182 V183 A184 K185 P186 S187 N188 A189

• Molecule 2: cypin peptide

Chain B: 100%

Q1 V2 V3 P4 F5 S6 S7 S8 V9

• Molecule 2: cypin peptide

Chain C: 33% 67%

Q1 V2 V3 P4 F5 S6 S7 S8 V9

4.2.14 Score per residue for model 14 (medoid)

• Molecule 1: Disks large homolog 4

Chain A: 38% 41% 15% • 6%

M1 E2 Y3 E4 E5 I6 T7 L8 N12 L15 G16 F17 S18 I19 T23 D24 I28 G29 D30 S33 I34 F35 I36 T37 K38 G42 G43 A44 A45 D48 G49 R50 L51 R52 V53 I57 L58 F59 V60 D64 V65 V68 T69 H70 V74 E75 K78

S82 I83 V84 R85 L86 Y87 V88 M89 R90 R91 K92 P93 P94 A95 E96 K97 V98 M99 E100 I101 K102 L103 I104 K105 G106 G109 F112 S113 I114 N120 Q121 H122 I123 P124 G125 D126 Y130 V131 T132 K133 I134 I135 E136 A139 A140 H141 K142 D143 G144 R145 L146 Q147 I148 G149 D150

K151 I152 L153 A154 V155 N156 S157 V158 G159 L160 E161 D162 V163 M164 H165 E166 D167 A168 V169 L172 K173 N174 T175 V179 Y180 L181 K182 V183 A184 K185 P186 S187 N188 A189

• Molecule 2: cypin peptide

Chain B: 100%

Q1 V2 V3 P4 F5 S6 S7 S8 V9

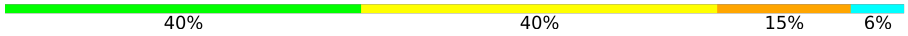
• Molecule 2: cypin peptide

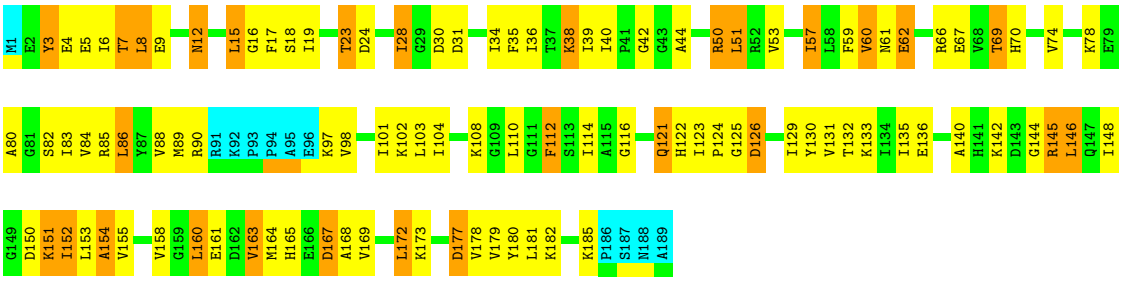
Chain C: 33% 67%

4.2.15 Score per residue for model 15

- Molecule 1: Disks large homolog 4

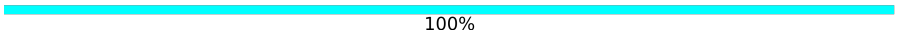
Chain A:





- Molecule 2: cypin peptide

Chain B:



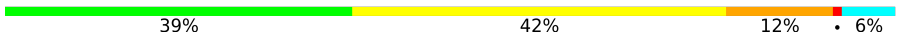
- Molecule 2: cypin peptide

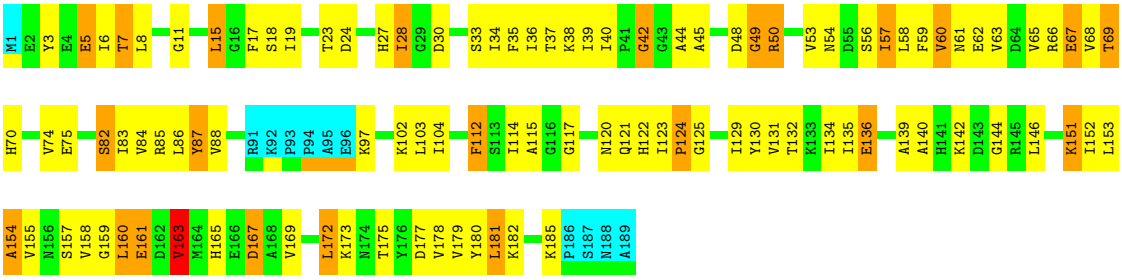
Chain C:

4.2.16 Score per residue for model 16

- Molecule 1: Disks large homolog 4

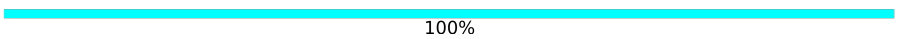
Chain A:





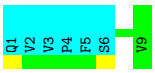
- Molecule 2: cypin peptide

Chain B:



• Molecule 2: cypin peptide

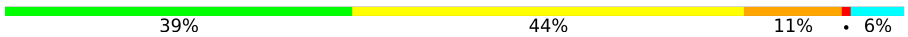
Chain C:

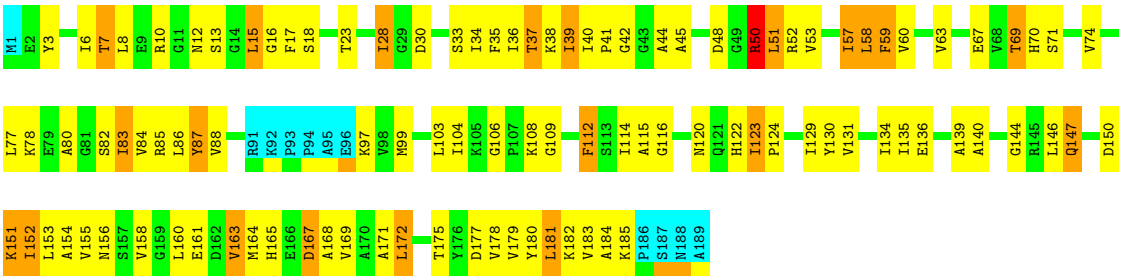


4.2.17 Score per residue for model 17

• Molecule 1: Disks large homolog 4

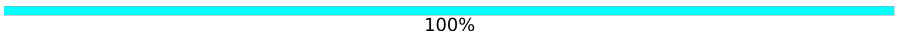
Chain A:





• Molecule 2: cypin peptide

Chain B:



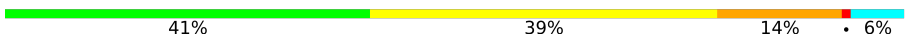
• Molecule 2: cypin peptide

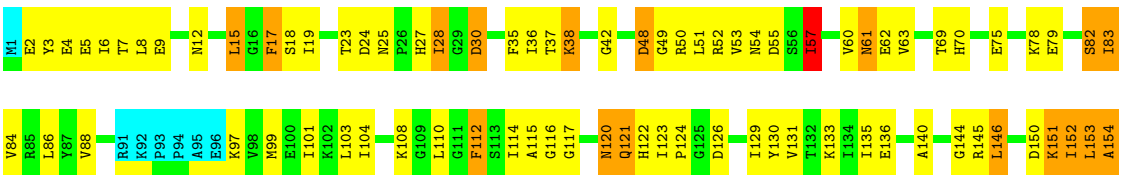
Chain C:

4.2.18 Score per residue for model 18

• Molecule 1: Disks large homolog 4

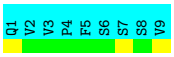
Chain A:





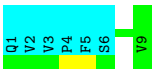
• Molecule 2: cypin peptide

Chain B: 100%



• Molecule 2: cypin peptide

Chain C: 33% 67%



4.2.19 Score per residue for model 19

• Molecule 1: Disks large homolog 4

Chain A: 39% 41% 13% • 6%

• Molecule 2: cypin peptide

Chain B: 100%

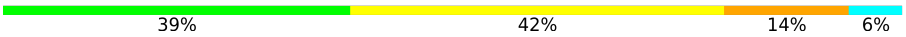
• Molecule 2: cypin peptide

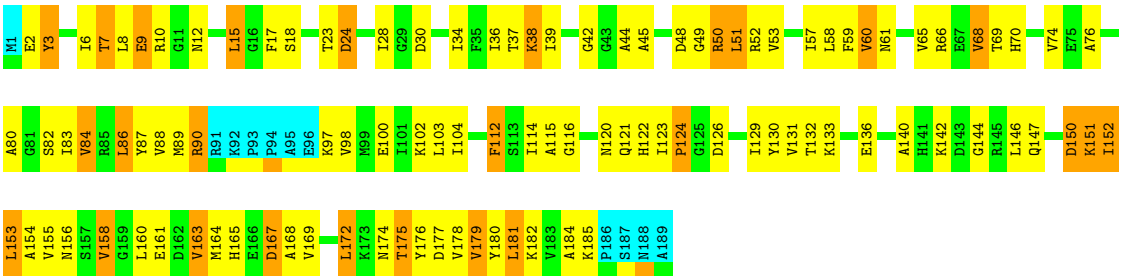
Chain C: 11% 22% 67%

4.2.20 Score per residue for model 20

• Molecule 1: Disks large homolog 4

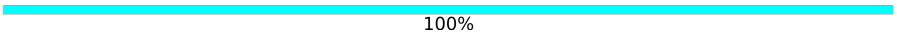
Chain A:

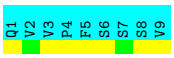




- Molecule 2: cypin peptide

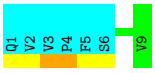
Chain B:





- Molecule 2: cypin peptide

Chain C:



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *simulated annealing*.

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	refinement	

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1331	1358	1353	88±6
2	B	0	0	0	0±0
2	C	20	19	19	1±1
All	All	27020	27540	27440	1761

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 32.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:129:ILE:HD12	1:A:160:LEU:HD22	0.95	1.37	20	4
1:A:155:VAL:HG12	1:A:156:ASN:ND2	0.85	1.87	17	8
1:A:123:ILE:HD11	1:A:130:TYR:CD1	0.84	2.08	6	16
1:A:123:ILE:HD11	1:A:130:TYR:CG	0.84	2.06	17	16
1:A:103:LEU:HD12	1:A:140:ALA:HB2	0.84	1.49	15	2
1:A:172:LEU:HD12	1:A:173:LYS:N	0.83	1.89	6	7
1:A:57:ILE:HD11	1:A:60:VAL:HG13	0.83	1.48	19	1
1:A:80:ALA:HB1	1:A:84:VAL:HG12	0.81	1.51	10	3
1:A:115:ALA:HB3	1:A:122:HIS:CE1	0.81	2.11	3	3
1:A:114:ILE:HG22	1:A:131:VAL:HG22	0.80	1.52	1	9
1:A:15:LEU:HD13	1:A:17:PHE:CZ	0.80	2.11	6	13
1:A:103:LEU:HD12	1:A:181:LEU:HD11	0.80	1.54	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:86:LEU:HD13	1:A:88:VAL:HG13	0.80	1.52	18	5
1:A:57:ILE:HA	1:A:88:VAL:HG12	0.79	1.53	20	14
1:A:57:ILE:HG22	1:A:88:VAL:HG12	0.78	1.56	16	11
1:A:8:LEU:HG	1:A:15:LEU:HD23	0.76	1.57	11	20
1:A:129:ILE:O	1:A:152:ILE:HD12	0.76	1.81	20	1
1:A:114:ILE:HD11	1:A:172:LEU:HD22	0.76	1.57	12	14
1:A:51:LEU:HD13	1:A:90:ARG:CZ	0.75	2.12	20	1
1:A:38:LYS:HA	1:A:53:VAL:HG11	0.75	1.59	7	14
1:A:7:THR:HG23	1:A:85:ARG:HG2	0.75	1.57	10	2
1:A:6:ILE:HG22	1:A:86:LEU:O	0.74	1.82	20	1
1:A:115:ALA:HB3	1:A:122:HIS:HB2	0.74	1.58	7	10
1:A:155:VAL:HG13	1:A:181:LEU:HD23	0.73	1.59	14	4
1:A:80:ALA:HB1	1:A:84:VAL:CG1	0.73	2.12	17	5
1:A:60:VAL:HG12	1:A:63:VAL:HB	0.73	1.59	7	4
1:A:103:LEU:CB	1:A:181:LEU:HD21	0.73	2.12	2	3
1:A:80:ALA:HB1	1:A:84:VAL:HG11	0.73	1.61	17	4
1:A:37:THR:O	1:A:53:VAL:HG21	0.73	1.83	11	10
1:A:57:ILE:O	1:A:65:VAL:HG13	0.72	1.84	16	3
1:A:51:LEU:HD13	1:A:88:VAL:HG21	0.72	1.58	10	1
1:A:131:VAL:HG23	1:A:150:ASP:O	0.72	1.84	17	14
1:A:151:LYS:HD2	1:A:184:ALA:HB3	0.72	1.61	9	5
1:A:86:LEU:CD1	1:A:88:VAL:HG13	0.72	2.15	17	3
1:A:76:ALA:O	1:A:80:ALA:HB2	0.72	1.84	3	10
1:A:8:LEU:HD21	1:A:45:ALA:HB2	0.72	1.60	20	7
1:A:18:SER:O	1:A:36:ILE:HG23	0.71	1.85	19	18
1:A:23:THR:HG22	1:A:69:THR:N	0.71	2.00	8	19
1:A:7:THR:HG23	1:A:85:ARG:CG	0.71	2.15	10	2
1:A:61:ASN:O	1:A:63:VAL:HG23	0.71	1.84	11	1
1:A:57:ILE:HG12	1:A:60:VAL:HG13	0.71	1.63	6	1
1:A:123:ILE:HD12	1:A:126:ASP:HB3	0.71	1.60	11	7
1:A:178:VAL:HG13	1:A:178:VAL:O	0.71	1.85	1	1
1:A:57:ILE:O	1:A:65:VAL:HG23	0.71	1.84	8	2
1:A:86:LEU:HD12	1:A:86:LEU:O	0.70	1.86	18	4
1:A:103:LEU:HG	1:A:140:ALA:HB2	0.70	1.63	19	9
1:A:24:ASP:CB	1:A:69:THR:HG23	0.70	2.16	10	9
1:A:140:ALA:HB1	1:A:146:LEU:HD21	0.70	1.64	10	4
1:A:160:LEU:HD22	1:A:171:ALA:HB1	0.70	1.62	10	1
1:A:60:VAL:HG13	1:A:86:LEU:HG	0.70	1.64	11	1
1:A:60:VAL:HG12	1:A:86:LEU:HG	0.69	1.63	13	1
1:A:111:GLY:O	1:A:134:ILE:HG23	0.69	1.87	7	6
1:A:160:LEU:HD13	1:A:162:ASP:OD2	0.69	1.85	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:173:LYS:HE3	2:C:9:VAL:HG21	0.69	1.65	15	1
1:A:134:ILE:HD11	1:A:146:LEU:O	0.68	1.88	11	11
1:A:6:ILE:HG21	1:A:50:ARG:HB3	0.68	1.65	4	2
1:A:8:LEU:O	1:A:84:VAL:HG22	0.68	1.87	11	4
1:A:116:GLY:HA2	1:A:129:ILE:HG12	0.68	1.64	18	1
1:A:19:ILE:HG22	1:A:36:ILE:HG12	0.68	1.66	10	11
1:A:11:GLY:CA	1:A:44:ALA:HB2	0.68	2.19	16	1
1:A:60:VAL:HG12	1:A:86:LEU:CD2	0.68	2.19	6	1
1:A:51:LEU:HD22	1:A:90:ARG:HG3	0.67	1.65	20	2
1:A:51:LEU:HD12	1:A:55:ASP:OD2	0.67	1.89	1	4
1:A:155:VAL:O	1:A:158:VAL:HG23	0.67	1.89	17	16
1:A:24:ASP:HB2	1:A:69:THR:HG22	0.67	1.66	2	3
1:A:155:VAL:HG13	1:A:181:LEU:HD22	0.67	1.66	13	2
1:A:152:ILE:HG22	1:A:182:LYS:O	0.67	1.89	1	16
1:A:103:LEU:HB2	1:A:181:LEU:HD21	0.66	1.66	2	4
1:A:163:VAL:HG11	1:A:167:ASP:CG	0.66	2.11	9	17
1:A:155:VAL:CG2	1:A:160:LEU:HD21	0.66	2.21	3	3
1:A:9:GLU:HG2	1:A:83:ILE:HG23	0.66	1.66	7	2
1:A:103:LEU:CG	1:A:140:ALA:HB2	0.66	2.21	20	14
1:A:6:ILE:HD13	1:A:6:ILE:N	0.65	2.05	2	9
1:A:60:VAL:HG13	1:A:86:LEU:HB3	0.65	1.66	10	2
1:A:169:VAL:HA	1:A:172:LEU:HD23	0.65	1.68	7	12
1:A:55:ASP:OD2	1:A:88:VAL:HG21	0.65	1.92	19	4
1:A:129:ILE:HD12	1:A:160:LEU:HD13	0.65	1.65	8	2
1:A:129:ILE:CD1	1:A:160:LEU:HD13	0.64	2.21	8	2
1:A:60:VAL:O	1:A:62:GLU:N	0.64	2.30	7	7
1:A:159:GLY:C	1:A:160:LEU:HD12	0.64	2.13	4	2
1:A:173:LYS:HE2	2:C:9:VAL:HG11	0.64	1.69	15	1
1:A:70:HIS:CD2	1:A:74:VAL:HG23	0.64	2.28	5	15
1:A:60:VAL:HG12	1:A:86:LEU:CG	0.64	2.21	13	1
1:A:8:LEU:HD11	1:A:44:ALA:HB3	0.63	1.70	20	5
1:A:155:VAL:HG11	1:A:172:LEU:HB3	0.63	1.70	5	1
1:A:86:LEU:HD23	1:A:86:LEU:O	0.63	1.93	9	1
1:A:7:THR:HG23	1:A:85:ARG:HG3	0.63	1.70	1	1
1:A:103:LEU:HB2	1:A:181:LEU:HD11	0.63	1.71	1	4
1:A:155:VAL:HG11	1:A:172:LEU:CB	0.63	2.23	5	1
1:A:60:VAL:HG22	1:A:65:VAL:HG11	0.63	1.70	3	1
1:A:154:ALA:HB1	1:A:158:VAL:O	0.62	1.93	13	17
1:A:129:ILE:HD12	1:A:160:LEU:HB3	0.62	1.70	16	2
1:A:158:VAL:HG21	1:A:171:ALA:HB1	0.62	1.71	5	1
1:A:104:ILE:HG12	1:A:139:ALA:HB1	0.61	1.70	7	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:86:LEU:HD13	1:A:86:LEU:N	0.61	2.09	8	2
1:A:103:LEU:HD22	1:A:110:LEU:HD23	0.61	1.72	3	2
1:A:155:VAL:HG23	1:A:160:LEU:HD11	0.61	1.71	16	2
1:A:9:GLU:HG3	1:A:83:ILE:HG23	0.61	1.71	20	5
1:A:103:LEU:CD1	1:A:140:ALA:HB2	0.61	2.25	20	7
1:A:114:ILE:CG2	1:A:131:VAL:HG22	0.61	2.23	1	4
1:A:34:ILE:HD13	1:A:73:ALA:HB2	0.61	1.72	3	1
1:A:123:ILE:HG22	1:A:124:PRO:HD2	0.61	1.71	4	8
1:A:60:VAL:HG13	1:A:61:ASN:N	0.61	2.10	7	1
1:A:151:LYS:CE	1:A:184:ALA:HB3	0.61	2.26	8	1
1:A:103:LEU:HD13	1:A:110:LEU:HD23	0.60	1.72	8	4
1:A:80:ALA:HB1	1:A:84:VAL:HG13	0.60	1.73	3	3
1:A:86:LEU:HD21	1:A:88:VAL:CG1	0.60	2.27	12	1
1:A:24:ASP:CB	1:A:69:THR:HG22	0.60	2.26	13	4
1:A:65:VAL:HG23	1:A:68:VAL:CG2	0.60	2.27	16	2
1:A:86:LEU:HD22	1:A:88:VAL:HG13	0.60	1.73	11	1
1:A:158:VAL:CG1	1:A:171:ALA:HB1	0.60	2.27	19	2
1:A:65:VAL:HG13	1:A:68:VAL:CG2	0.60	2.27	19	4
1:A:129:ILE:HD11	1:A:159:GLY:HA3	0.60	1.73	5	1
1:A:153:LEU:O	1:A:154:ALA:HB2	0.59	1.97	4	14
1:A:123:ILE:HD13	1:A:130:TYR:CD1	0.59	2.32	10	2
1:A:155:VAL:HG12	1:A:156:ASN:HD22	0.59	1.58	9	10
1:A:9:GLU:CG	1:A:83:ILE:HG23	0.59	2.27	20	3
1:A:165:HIS:O	1:A:169:VAL:HG23	0.59	1.98	20	19
1:A:6:ILE:HD13	1:A:50:ARG:HG3	0.59	1.72	18	3
1:A:158:VAL:HG11	1:A:171:ALA:HB2	0.59	1.72	5	1
1:A:116:GLY:HA3	1:A:129:ILE:HG12	0.59	1.74	17	9
1:A:103:LEU:HD22	1:A:110:LEU:HD22	0.59	1.73	12	1
1:A:178:VAL:O	1:A:178:VAL:CG1	0.59	2.50	1	1
1:A:24:ASP:HB3	1:A:69:THR:HG23	0.58	1.73	3	7
1:A:129:ILE:HD11	1:A:159:GLY:CA	0.58	2.28	5	1
1:A:50:ARG:NH2	1:A:86:LEU:HD22	0.58	2.14	9	1
1:A:58:LEU:HD11	1:A:89:MET:CG	0.58	2.29	12	1
1:A:36:ILE:HB	1:A:53:VAL:HA	0.58	1.73	12	9
1:A:175:THR:HB	1:A:179:VAL:HG21	0.58	1.76	19	14
1:A:122:HIS:CD2	1:A:123:ILE:HG12	0.58	2.34	18	2
1:A:114:ILE:HD12	1:A:129:ILE:HG21	0.58	1.74	18	1
1:A:154:ALA:CB	1:A:158:VAL:O	0.58	2.52	13	17
1:A:86:LEU:O	1:A:86:LEU:HD22	0.57	1.99	8	2
1:A:8:LEU:CD1	1:A:44:ALA:HB3	0.57	2.30	15	6
1:A:8:LEU:HD22	1:A:50:ARG:NH1	0.57	2.14	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:65:VAL:HG22	1:A:65:VAL:O	0.57	1.99	6	3
1:A:23:THR:HG22	1:A:69:THR:CG2	0.57	2.28	9	2
1:A:103:LEU:HD11	1:A:140:ALA:HB2	0.57	1.74	4	4
1:A:58:LEU:HD21	1:A:87:TYR:CD1	0.57	2.34	10	2
1:A:101:ILE:HD12	1:A:144:GLY:HA2	0.57	1.75	15	1
1:A:38:LYS:CA	1:A:53:VAL:HG11	0.57	2.28	20	8
1:A:112:PHE:CE2	1:A:114:ILE:HD13	0.57	2.35	1	4
1:A:104:ILE:HG22	1:A:178:VAL:HG13	0.57	1.75	17	3
1:A:129:ILE:CD1	1:A:160:LEU:HD22	0.57	2.30	13	1
1:A:40:ILE:O	1:A:46:ALA:HB2	0.57	1.99	19	1
1:A:112:PHE:CE2	1:A:114:ILE:HG21	0.57	2.35	15	16
1:A:35:PHE:CD1	1:A:35:PHE:N	0.56	2.71	9	5
1:A:155:VAL:HG21	1:A:160:LEU:HD21	0.56	1.76	3	2
1:A:65:VAL:HG12	1:A:68:VAL:HG21	0.56	1.78	8	3
1:A:129:ILE:HD12	1:A:160:LEU:CD2	0.56	2.31	13	1
1:A:24:ASP:HB3	1:A:69:THR:HG22	0.56	1.78	13	1
1:A:86:LEU:HD13	1:A:88:VAL:CG1	0.56	2.29	18	1
1:A:51:LEU:HD22	1:A:90:ARG:CG	0.55	2.31	20	1
1:A:146:LEU:HD12	1:A:146:LEU:O	0.55	2.00	20	1
1:A:24:ASP:CG	1:A:69:THR:HG22	0.55	2.21	13	1
1:A:104:ILE:CG1	1:A:139:ALA:HB1	0.55	2.31	6	3
1:A:23:THR:HG22	1:A:69:THR:HG23	0.55	1.78	2	3
1:A:98:VAL:HG13	1:A:153:LEU:HD21	0.55	1.79	7	3
1:A:84:VAL:HG23	1:A:84:VAL:O	0.55	2.02	9	6
1:A:57:ILE:HG22	1:A:88:VAL:CG1	0.55	2.31	17	5
1:A:154:ALA:HB3	1:A:182:LYS:HD2	0.55	1.77	7	1
1:A:65:VAL:O	1:A:65:VAL:HG12	0.55	2.02	19	8
1:A:160:LEU:HD23	1:A:160:LEU:N	0.55	2.17	2	1
1:A:60:VAL:HG12	1:A:86:LEU:HD22	0.55	1.79	6	1
1:A:172:LEU:O	1:A:175:THR:HG23	0.54	2.02	9	7
1:A:24:ASP:HB2	1:A:69:THR:HG23	0.54	1.79	4	9
1:A:129:ILE:HB	1:A:152:ILE:HD12	0.54	1.79	10	12
1:A:114:ILE:CD1	1:A:172:LEU:HD22	0.54	2.32	10	3
1:A:123:ILE:CD1	1:A:130:TYR:CD1	0.54	2.91	10	8
1:A:123:ILE:HD12	1:A:126:ASP:CB	0.54	2.31	11	1
1:A:131:VAL:HG21	1:A:150:ASP:OD1	0.54	2.03	19	1
1:A:60:VAL:HG12	1:A:86:LEU:HD23	0.54	1.78	3	1
1:A:134:ILE:HD12	1:A:147:GLN:HA	0.54	1.80	5	3
1:A:7:THR:HA	1:A:84:VAL:O	0.53	2.03	14	6
1:A:60:VAL:HG23	1:A:65:VAL:HG21	0.53	1.80	10	1
1:A:175:THR:CB	1:A:179:VAL:HG21	0.53	2.33	9	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:155:VAL:CG2	1:A:160:LEU:HD11	0.53	2.34	16	2
1:A:51:LEU:HD23	1:A:51:LEU:N	0.53	2.18	4	3
1:A:172:LEU:HD12	1:A:172:LEU:C	0.53	2.23	3	8
1:A:112:PHE:CE2	1:A:114:ILE:CG2	0.53	2.92	10	19
1:A:86:LEU:C	1:A:86:LEU:HD13	0.53	2.25	12	1
1:A:60:VAL:HG22	1:A:65:VAL:CG1	0.53	2.34	16	2
1:A:23:THR:HG22	1:A:69:THR:CA	0.52	2.33	6	6
1:A:155:VAL:HG11	1:A:175:THR:HG22	0.52	1.81	17	1
1:A:132:THR:O	1:A:148:ILE:HG23	0.52	2.04	4	5
2:C:8:SER:O	2:C:9:VAL:HG13	0.52	2.05	15	5
1:A:101:ILE:HG13	1:A:183:VAL:HG21	0.52	1.81	12	10
1:A:15:LEU:HD13	1:A:17:PHE:CE1	0.52	2.39	14	1
1:A:129:ILE:HD11	1:A:168:ALA:HB1	0.52	1.80	11	5
1:A:181:LEU:N	1:A:181:LEU:HD23	0.52	2.19	2	5
1:A:51:LEU:HD12	1:A:52:ARG:N	0.52	2.20	2	3
1:A:144:GLY:HA3	1:A:146:LEU:HD23	0.52	1.81	15	3
1:A:135:ILE:HG22	1:A:136:GLU:H	0.52	1.63	19	18
1:A:57:ILE:CA	1:A:88:VAL:HG12	0.52	2.34	19	3
1:A:60:VAL:HG12	1:A:63:VAL:CB	0.52	2.33	7	1
1:A:159:GLY:HA2	1:A:168:ALA:HB2	0.52	1.82	5	1
1:A:114:ILE:CG1	1:A:172:LEU:HD22	0.52	2.35	7	2
1:A:19:ILE:HD11	1:A:70:HIS:NE2	0.52	2.20	11	2
1:A:58:LEU:HD12	1:A:59:PHE:HB2	0.51	1.83	3	1
1:A:6:ILE:CG2	1:A:7:THR:N	0.51	2.74	8	4
1:A:121:GLN:O	1:A:122:HIS:HB3	0.51	2.05	18	12
1:A:28:ILE:HG12	1:A:35:PHE:CZ	0.51	2.40	13	16
1:A:50:ARG:O	1:A:51:LEU:HG	0.51	2.05	17	3
1:A:103:LEU:CB	1:A:181:LEU:HD11	0.51	2.36	14	1
1:A:103:LEU:HB3	1:A:181:LEU:HD21	0.51	1.82	2	3
1:A:59:PHE:HA	1:A:65:VAL:HG12	0.51	1.82	16	1
1:A:103:LEU:HD22	1:A:110:LEU:HG	0.51	1.83	1	4
1:A:154:ALA:HB2	1:A:160:LEU:HD23	0.51	1.83	19	1
1:A:8:LEU:CG	1:A:15:LEU:HD23	0.51	2.35	1	1
1:A:158:VAL:HG11	1:A:171:ALA:CB	0.51	2.36	5	1
1:A:104:ILE:O	1:A:139:ALA:HB1	0.51	2.06	14	3
1:A:60:VAL:CG1	1:A:86:LEU:HD12	0.51	2.36	20	1
1:A:110:LEU:O	1:A:139:ALA:HB3	0.50	2.06	10	1
1:A:63:VAL:HG12	1:A:65:VAL:HG13	0.50	1.82	11	1
1:A:103:LEU:HD21	1:A:140:ALA:HB2	0.50	1.84	12	1
1:A:158:VAL:HB	1:A:160:LEU:HD21	0.50	1.83	2	1
1:A:57:ILE:O	1:A:57:ILE:HG13	0.50	2.06	17	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:101:ILE:HD12	1:A:144:GLY:CA	0.50	2.35	15	2
1:A:61:ASN:HD22	1:A:84:VAL:HG12	0.50	1.65	13	1
1:A:158:VAL:CG2	1:A:171:ALA:HB1	0.50	2.36	5	1
1:A:130:TYR:CE1	1:A:151:LYS:CB	0.50	2.94	5	16
1:A:155:VAL:HG21	1:A:160:LEU:HD11	0.50	1.83	2	1
1:A:28:ILE:CD1	1:A:35:PHE:CE1	0.50	2.94	13	1
1:A:11:GLY:HA3	1:A:44:ALA:HB2	0.50	1.84	16	1
1:A:160:LEU:HB3	1:A:168:ALA:HB1	0.50	1.82	17	2
1:A:151:LYS:CD	1:A:184:ALA:HB3	0.50	2.35	11	3
1:A:156:ASN:N	1:A:180:TYR:O	0.50	2.45	5	2
1:A:169:VAL:O	1:A:172:LEU:HG	0.50	2.06	5	4
1:A:154:ALA:HB2	1:A:160:LEU:CD2	0.50	2.37	19	1
1:A:75:GLU:O	1:A:78:LYS:HG3	0.50	2.07	13	2
1:A:60:VAL:O	1:A:61:ASN:C	0.49	2.51	2	3
1:A:86:LEU:HD13	1:A:86:LEU:O	0.49	2.07	12	1
1:A:57:ILE:HB	1:A:86:LEU:HD21	0.49	1.82	11	1
1:A:15:LEU:HB2	1:A:17:PHE:CE2	0.49	2.41	17	16
1:A:98:VAL:HG13	1:A:98:VAL:O	0.49	2.07	8	3
1:A:3:TYR:CD1	1:A:3:TYR:N	0.49	2.81	7	8
1:A:153:LEU:O	1:A:154:ALA:CB	0.49	2.59	4	2
1:A:104:ILE:HB	1:A:177:ASP:O	0.49	2.08	5	5
1:A:11:GLY:N	1:A:44:ALA:HB2	0.49	2.22	2	4
1:A:20:ALA:HB1	1:A:27:HIS:HB2	0.49	1.83	10	3
1:A:131:VAL:HG21	1:A:146:LEU:CD1	0.49	2.37	13	2
1:A:115:ALA:O	1:A:129:ILE:HG23	0.49	2.07	16	2
1:A:113:SER:N	1:A:133:LYS:O	0.49	2.46	3	1
1:A:6:ILE:HG21	1:A:50:ARG:HG3	0.49	1.84	6	1
1:A:60:VAL:HG23	1:A:65:VAL:CG2	0.49	2.37	20	6
1:A:60:VAL:HG22	1:A:61:ASN:H	0.49	1.68	2	3
1:A:7:THR:HG23	1:A:85:ARG:HD2	0.49	1.84	12	1
1:A:57:ILE:CG2	1:A:88:VAL:HG12	0.49	2.34	16	2
1:A:7:THR:HG23	1:A:85:ARG:HA	0.49	1.84	2	1
1:A:160:LEU:HD22	1:A:168:ALA:O	0.49	2.08	11	1
1:A:129:ILE:HD11	1:A:160:LEU:O	0.49	2.08	9	3
1:A:151:LYS:HG3	1:A:184:ALA:HB3	0.49	1.85	3	3
1:A:158:VAL:HG12	1:A:171:ALA:HB1	0.49	1.85	19	2
1:A:103:LEU:HD22	1:A:110:LEU:CD2	0.49	2.37	12	1
2:C:9:VAL:OXT	2:C:9:VAL:HG13	0.49	2.07	11	1
1:A:57:ILE:HD11	1:A:60:VAL:CG1	0.49	2.29	19	1
1:A:8:LEU:HB3	1:A:84:VAL:HG23	0.49	1.83	5	2
1:A:122:HIS:CD2	1:A:123:ILE:CG1	0.49	2.96	18	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:130:TYR:CD1	1:A:151:LYS:CB	0.48	2.96	16	7
1:A:115:ALA:O	1:A:122:HIS:HB3	0.48	2.07	20	2
1:A:57:ILE:CG1	1:A:57:ILE:O	0.48	2.61	10	6
1:A:152:ILE:HG21	1:A:181:LEU:HB3	0.48	1.84	14	3
1:A:57:ILE:HD12	1:A:86:LEU:HB2	0.48	1.84	19	1
1:A:6:ILE:HG22	1:A:50:ARG:NE	0.48	2.23	5	1
1:A:115:ALA:O	1:A:122:HIS:CB	0.48	2.61	7	2
1:A:50:ARG:NH2	1:A:86:LEU:HD21	0.48	2.24	10	2
1:A:110:LEU:HD22	1:A:172:LEU:HD13	0.48	1.83	13	1
1:A:103:LEU:CD1	1:A:181:LEU:HD11	0.48	2.33	2	1
1:A:155:VAL:N	1:A:158:VAL:O	0.48	2.36	5	1
1:A:131:VAL:HG11	1:A:134:ILE:HD11	0.48	1.86	16	2
1:A:176:TYR:CE1	1:A:178:VAL:O	0.48	2.67	20	2
1:A:48:ASP:O	1:A:49:GLY:C	0.48	2.52	16	9
1:A:36:ILE:HB	1:A:53:VAL:CA	0.48	2.39	4	4
1:A:6:ILE:CG2	1:A:50:ARG:NE	0.48	2.77	5	1
1:A:57:ILE:O	1:A:57:ILE:HG23	0.48	2.09	6	1
1:A:160:LEU:HD13	1:A:172:LEU:HB3	0.48	1.85	12	1
1:A:129:ILE:HG13	1:A:160:LEU:O	0.48	2.09	16	2
1:A:6:ILE:HD12	1:A:88:VAL:HG21	0.48	1.85	17	1
1:A:183:VAL:HG12	1:A:184:ALA:N	0.48	2.23	13	15
1:A:51:LEU:HD12	1:A:55:ASP:CG	0.48	2.29	10	1
1:A:102:LYS:CG	1:A:180:TYR:CD2	0.47	2.97	1	1
1:A:153:LEU:CD2	1:A:184:ALA:HB2	0.47	2.39	11	1
1:A:4:GLU:N	1:A:87:TYR:CE1	0.47	2.82	10	3
1:A:104:ILE:HG22	1:A:178:VAL:HG23	0.47	1.84	1	1
1:A:163:VAL:HG11	1:A:167:ASP:OD2	0.47	2.08	3	2
1:A:70:HIS:CD2	1:A:74:VAL:CG2	0.47	2.97	12	11
1:A:10:ARG:O	1:A:12:ASN:N	0.47	2.47	4	2
1:A:59:PHE:O	1:A:86:LEU:HD23	0.47	2.08	11	1
1:A:27:HIS:CD2	1:A:27:HIS:O	0.47	2.67	13	1
1:A:36:ILE:HG22	1:A:53:VAL:HB	0.47	1.87	14	4
1:A:175:THR:HB	1:A:179:VAL:HG11	0.47	1.85	20	1
1:A:58:LEU:HD21	1:A:89:MET:SD	0.47	2.50	7	1
1:A:122:HIS:CE1	1:A:132:THR:HG22	0.47	2.44	5	2
1:A:28:ILE:HG23	1:A:35:PHE:CZ	0.47	2.43	13	1
1:A:155:VAL:O	1:A:157:SER:N	0.47	2.44	4	6
1:A:80:ALA:CB	1:A:84:VAL:HG12	0.47	2.39	8	1
1:A:132:THR:O	1:A:148:ILE:HD13	0.47	2.09	14	1
1:A:53:VAL:HG23	1:A:54:ASN:N	0.47	2.25	16	9
1:A:140:ALA:O	1:A:144:GLY:N	0.47	2.48	11	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:15:LEU:CB	1:A:17:PHE:CE2	0.47	2.98	15	6
1:A:115:ALA:HB3	1:A:122:HIS:CB	0.47	2.40	4	1
1:A:112:PHE:CZ	1:A:114:ILE:HD13	0.47	2.45	6	1
1:A:153:LEU:HD23	1:A:184:ALA:HB2	0.47	1.86	11	1
2:C:9:VAL:OXT	2:C:9:VAL:HG22	0.47	2.09	11	1
1:A:82:SER:O	1:A:83:ILE:HG12	0.47	2.10	3	12
1:A:8:LEU:HB2	1:A:50:ARG:NH2	0.47	2.25	15	1
1:A:51:LEU:HD21	1:A:88:VAL:CG2	0.47	2.39	13	2
1:A:27:HIS:HB3	1:A:35:PHE:CD1	0.47	2.45	11	1
1:A:6:ILE:HD13	1:A:6:ILE:H	0.46	1.70	11	3
1:A:86:LEU:HD12	1:A:86:LEU:C	0.46	2.31	5	2
1:A:103:LEU:C	1:A:103:LEU:HD23	0.46	2.30	20	6
1:A:20:ALA:HB3	1:A:27:HIS:CE1	0.46	2.45	11	1
1:A:51:LEU:HD13	1:A:88:VAL:HG11	0.46	1.87	1	1
1:A:155:VAL:HG23	1:A:160:LEU:CD1	0.46	2.39	16	2
1:A:123:ILE:CD1	1:A:130:TYR:CG	0.46	2.98	3	4
1:A:80:ALA:CB	1:A:84:VAL:HG13	0.46	2.39	4	1
1:A:130:TYR:CD1	1:A:151:LYS:HB3	0.46	2.46	9	9
1:A:134:ILE:HD13	1:A:146:LEU:O	0.46	2.10	5	1
1:A:102:LYS:HE3	1:A:178:VAL:HG12	0.46	1.85	16	1
1:A:15:LEU:HD13	1:A:17:PHE:CE2	0.46	2.46	19	1
1:A:86:LEU:CD2	1:A:88:VAL:HG13	0.46	2.41	12	1
1:A:115:ALA:CB	1:A:122:HIS:CB	0.46	2.93	16	2
1:A:152:ILE:HG21	1:A:181:LEU:HB2	0.46	1.88	9	5
1:A:3:TYR:CD2	1:A:89:MET:CG	0.46	2.99	3	1
1:A:155:VAL:O	1:A:156:ASN:HB2	0.46	2.11	5	1
1:A:65:VAL:HA	1:A:68:VAL:HG23	0.46	1.85	14	2
1:A:58:LEU:HD23	1:A:89:MET:CG	0.46	2.41	6	1
1:A:65:VAL:HG23	1:A:68:VAL:HG22	0.46	1.87	16	1
1:A:122:HIS:CD2	1:A:123:ILE:HD11	0.46	2.46	18	1
1:A:172:LEU:C	1:A:172:LEU:HD12	0.46	2.30	17	10
1:A:175:THR:OG1	1:A:179:VAL:HG22	0.46	2.10	5	1
1:A:155:VAL:HG11	1:A:175:THR:CG2	0.46	2.40	17	1
1:A:121:GLN:NE2	1:A:123:ILE:O	0.46	2.49	3	1
1:A:58:LEU:HD11	1:A:89:MET:HG3	0.46	1.88	12	1
1:A:169:VAL:HG22	2:C:7:SER:CB	0.46	2.41	3	1
1:A:51:LEU:HD13	1:A:86:LEU:HD11	0.46	1.86	12	1
1:A:156:ASN:ND2	1:A:179:VAL:HB	0.46	2.26	19	1
1:A:135:ILE:O	1:A:141:HIS:CE1	0.45	2.69	13	2
1:A:61:ASN:ND2	1:A:84:VAL:HG12	0.45	2.26	13	1
1:A:5:GLU:N	1:A:87:TYR:CE1	0.45	2.84	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:173:LYS:HD3	2:C:9:VAL:HG11	0.45	1.88	19	1
1:A:9:GLU:HA	1:A:82:SER:O	0.45	2.11	6	7
1:A:23:THR:CG2	1:A:69:THR:N	0.45	2.79	12	12
1:A:4:GLU:HG3	1:A:51:LEU:HD22	0.45	1.88	2	1
1:A:123:ILE:CD1	1:A:130:TYR:CD2	0.45	2.99	3	1
1:A:169:VAL:HG22	2:C:7:SER:OG	0.45	2.12	3	1
1:A:156:ASN:OD1	1:A:180:TYR:CZ	0.45	2.69	12	3
1:A:154:ALA:CB	1:A:160:LEU:HG	0.45	2.42	5	1
1:A:17:PHE:CE1	1:A:19:ILE:HG23	0.45	2.46	8	1
1:A:57:ILE:CD1	1:A:60:VAL:HG13	0.45	2.31	19	1
1:A:36:ILE:O	1:A:53:VAL:O	0.45	2.35	12	6
1:A:78:LYS:C	1:A:78:LYS:CD	0.45	2.84	3	2
1:A:6:ILE:O	1:A:85:ARG:HA	0.45	2.12	11	2
1:A:51:LEU:HD21	1:A:88:VAL:HG21	0.45	1.86	15	2
1:A:131:VAL:HG21	1:A:150:ASP:CG	0.45	2.32	19	1
1:A:86:LEU:HD21	1:A:88:VAL:HG13	0.45	1.86	12	1
1:A:112:PHE:CD2	1:A:114:ILE:CG2	0.45	3.00	1	1
1:A:57:ILE:O	1:A:57:ILE:CG1	0.45	2.64	7	1
1:A:106:GLY:N	1:A:109:GLY:O	0.45	2.49	4	6
1:A:110:LEU:N	1:A:110:LEU:HD12	0.45	2.26	15	1
1:A:6:ILE:HG23	1:A:50:ARG:CZ	0.45	2.42	17	1
1:A:57:ILE:CD1	1:A:57:ILE:N	0.45	2.79	14	4
1:A:6:ILE:N	1:A:6:ILE:CD1	0.45	2.79	13	3
1:A:8:LEU:HD11	1:A:45:ALA:N	0.45	2.26	8	4
1:A:11:GLY:H	1:A:44:ALA:HB2	0.44	1.72	7	2
1:A:130:TYR:CE1	1:A:151:LYS:HB3	0.44	2.47	5	6
1:A:159:GLY:O	1:A:161:GLU:N	0.44	2.50	4	1
1:A:58:LEU:HD11	1:A:89:MET:SD	0.44	2.52	20	1
1:A:123:ILE:HD11	1:A:130:TYR:CD2	0.44	2.47	3	1
1:A:131:VAL:HG21	1:A:150:ASP:OD2	0.44	2.12	19	1
1:A:176:TYR:CD2	1:A:177:ASP:N	0.44	2.86	8	2
1:A:5:GLU:CG	1:A:87:TYR:CD1	0.44	3.01	12	1
1:A:110:LEU:HD23	1:A:112:PHE:CE1	0.44	2.48	13	1
1:A:70:HIS:CD2	1:A:70:HIS:C	0.44	2.91	13	18
1:A:86:LEU:HD23	1:A:88:VAL:HG13	0.44	1.90	10	1
1:A:37:THR:C	1:A:53:VAL:HG21	0.44	2.32	11	2
1:A:8:LEU:HB3	1:A:84:VAL:CG2	0.44	2.42	8	2
1:A:176:TYR:CG	1:A:177:ASP:N	0.44	2.85	6	4
1:A:7:THR:HG22	1:A:85:ARG:HG2	0.44	1.88	16	2
1:A:160:LEU:CD2	1:A:171:ALA:HB3	0.44	2.43	17	1
1:A:8:LEU:HD21	1:A:45:ALA:HA	0.44	1.88	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:8:LEU:CD2	1:A:50:ARG:NH1	0.44	2.81	8	1
1:A:27:HIS:CB	1:A:35:PHE:CD1	0.44	3.00	11	1
1:A:156:ASN:OD1	1:A:180:TYR:CE2	0.44	2.71	20	4
1:A:160:LEU:HD22	1:A:171:ALA:HB3	0.44	1.90	12	2
1:A:144:GLY:O	1:A:145:ARG:HG3	0.44	2.13	15	1
1:A:176:TYR:CZ	1:A:178:VAL:O	0.44	2.71	20	2
1:A:36:ILE:C	1:A:53:VAL:HB	0.44	2.33	20	2
1:A:60:VAL:HA	1:A:86:LEU:HB3	0.44	1.88	15	2
1:A:115:ALA:HB1	1:A:165:HIS:CE1	0.44	2.48	20	1
1:A:121:GLN:C	1:A:123:ILE:H	0.44	2.15	14	1
1:A:159:GLY:C	1:A:161:GLU:H	0.43	2.16	5	3
1:A:58:LEU:HD12	1:A:89:MET:HB3	0.43	1.88	4	1
1:A:50:ARG:NH1	1:A:51:LEU:CD2	0.43	2.81	6	1
1:A:102:LYS:CG	1:A:180:TYR:CE2	0.43	3.01	6	1
1:A:60:VAL:CG1	1:A:61:ASN:N	0.43	2.79	7	1
1:A:9:GLU:HB3	1:A:83:ILE:HG23	0.43	1.88	9	1
1:A:36:ILE:HB	1:A:53:VAL:O	0.43	2.11	11	3
1:A:17:PHE:CD1	1:A:17:PHE:N	0.43	2.85	14	1
1:A:6:ILE:HD13	1:A:50:ARG:CG	0.43	2.43	16	1
1:A:58:LEU:HD23	1:A:88:VAL:C	0.43	2.33	17	1
1:A:60:VAL:O	1:A:63:VAL:N	0.43	2.48	10	3
1:A:156:ASN:OD1	1:A:180:TYR:CG	0.43	2.71	8	2
1:A:57:ILE:O	1:A:57:ILE:HG12	0.43	2.12	10	4
1:A:45:ALA:O	1:A:49:GLY:N	0.43	2.50	20	2
1:A:65:VAL:HA	1:A:68:VAL:CG2	0.43	2.44	1	1
1:A:103:LEU:HD23	1:A:104:ILE:N	0.43	2.28	5	7
1:A:18:SER:O	1:A:36:ILE:CG2	0.43	2.65	4	1
1:A:8:LEU:HD13	1:A:48:ASP:OD2	0.43	2.13	11	2
1:A:19:ILE:HD11	1:A:74:VAL:CG2	0.43	2.44	12	1
1:A:101:ILE:HG21	1:A:146:LEU:CD2	0.43	2.42	19	1
1:A:158:VAL:HG12	1:A:159:GLY:N	0.43	2.29	16	2
1:A:165:HIS:O	1:A:169:VAL:CG2	0.43	2.66	3	9
1:A:131:VAL:HG21	1:A:146:LEU:HD12	0.43	1.90	13	2
1:A:169:VAL:HG22	2:C:7:SER:HB2	0.43	1.89	6	1
1:A:59:PHE:CA	1:A:65:VAL:HG12	0.43	2.43	16	1
2:C:9:VAL:OXT	2:C:9:VAL:HG23	0.43	2.14	9	1
1:A:180:TYR:CD1	1:A:180:TYR:N	0.43	2.86	13	1
1:A:172:LEU:HD11	2:C:7:SER:OG	0.43	2.13	6	1
1:A:173:LYS:CE	2:C:9:VAL:HG21	0.43	2.42	15	1
1:A:155:VAL:HG21	1:A:160:LEU:CD1	0.43	2.44	2	1
1:A:160:LEU:O	1:A:168:ALA:HB2	0.43	2.14	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:123:ILE:O	1:A:125:GLY:N	0.43	2.52	16	5
1:A:112:PHE:CD1	1:A:112:PHE:O	0.43	2.72	16	3
1:A:23:THR:HG22	1:A:69:THR:OG1	0.43	2.14	11	1
1:A:70:HIS:C	1:A:70:HIS:CD2	0.43	2.92	11	2
1:A:51:LEU:HD23	1:A:90:ARG:HD3	0.43	1.91	14	1
1:A:160:LEU:HD12	1:A:160:LEU:H	0.43	1.73	5	1
1:A:163:VAL:CG1	1:A:167:ASP:CB	0.43	2.97	5	3
1:A:61:ASN:HD21	1:A:84:VAL:HG13	0.43	1.74	20	1
1:A:40:ILE:O	1:A:42:GLY:N	0.43	2.52	11	4
1:A:29:GLY:O	1:A:30:ASP:CB	0.43	2.67	13	1
1:A:58:LEU:O	1:A:59:PHE:CG	0.42	2.72	11	2
1:A:158:VAL:CB	1:A:171:ALA:CB	0.42	2.97	5	1
1:A:8:LEU:O	1:A:84:VAL:HG23	0.42	2.14	16	1
1:A:132:THR:CG2	1:A:133:LYS:N	0.42	2.83	10	3
1:A:123:ILE:HG22	1:A:124:PRO:CD	0.42	2.43	11	2
1:A:8:LEU:HB2	1:A:50:ARG:CZ	0.42	2.44	13	3
1:A:39:ILE:HG13	1:A:53:VAL:HG12	0.42	1.91	8	1
1:A:57:ILE:H	1:A:57:ILE:HD13	0.42	1.74	12	1
1:A:152:ILE:HB	1:A:160:LEU:CD1	0.42	2.45	13	1
1:A:154:ALA:CA	1:A:158:VAL:O	0.42	2.67	20	2
1:A:165:HIS:CD2	2:C:7:SER:OG	0.42	2.72	13	1
1:A:99:MET:SD	1:A:101:ILE:HD11	0.42	2.54	4	1
1:A:130:TYR:CE1	1:A:151:LYS:HB2	0.42	2.49	20	3
1:A:103:LEU:CD2	1:A:140:ALA:HB2	0.42	2.44	12	1
1:A:6:ILE:HG23	1:A:50:ARG:NH2	0.42	2.29	15	1
1:A:172:LEU:O	1:A:175:THR:OG1	0.42	2.37	2	1
1:A:57:ILE:CG1	1:A:60:VAL:HG13	0.42	2.39	6	1
1:A:39:ILE:CG1	1:A:53:VAL:CG1	0.42	2.97	17	2
1:A:2:GLU:O	1:A:90:ARG:N	0.42	2.53	19	1
1:A:15:LEU:HD21	1:A:84:VAL:HG21	0.42	1.91	3	1
1:A:74:VAL:O	1:A:78:LYS:HB3	0.42	2.14	3	2
1:A:156:ASN:OD1	1:A:180:TYR:CD2	0.42	2.73	9	3
1:A:28:ILE:HD11	1:A:35:PHE:CZ	0.42	2.50	5	3
1:A:115:ALA:HB1	1:A:165:HIS:NE2	0.42	2.30	20	1
1:A:163:VAL:HG11	1:A:167:ASP:CB	0.42	2.45	15	6
1:A:61:ASN:HD21	1:A:84:VAL:HG12	0.42	1.74	6	1
1:A:48:ASP:O	1:A:50:ARG:N	0.42	2.53	7	4
1:A:7:THR:O	1:A:50:ARG:NH2	0.42	2.52	14	2
1:A:101:ILE:HG23	1:A:144:GLY:CA	0.42	2.44	5	1
1:A:8:LEU:HB3	1:A:84:VAL:HG22	0.42	1.91	8	2
1:A:156:ASN:ND2	1:A:180:TYR:O	0.42	2.53	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:7:THR:HG23	1:A:85:ARG:HH11	0.42	1.74	19	1
1:A:9:GLU:HA	1:A:83:ILE:HA	0.42	1.92	6	2
1:A:129:ILE:CG2	1:A:152:ILE:CD1	0.42	2.98	9	2
1:A:132:THR:HG23	1:A:133:LYS:N	0.42	2.30	10	1
1:A:80:ALA:HB1	1:A:84:VAL:HG22	0.42	1.92	15	1
1:A:115:ALA:HB2	1:A:122:HIS:CB	0.42	2.45	16	1
1:A:38:LYS:N	1:A:38:LYS:CD	0.42	2.83	20	1
1:A:153:LEU:HD22	1:A:184:ALA:HB2	0.42	1.91	20	1
1:A:146:LEU:HB2	1:A:150:ASP:CG	0.42	2.36	1	1
1:A:50:ARG:HH22	1:A:86:LEU:HD11	0.42	1.75	8	1
1:A:60:VAL:CG2	1:A:65:VAL:HG21	0.42	2.45	9	1
1:A:27:HIS:CD2	1:A:35:PHE:CE2	0.41	3.08	1	4
1:A:156:ASN:OD1	1:A:180:TYR:CD1	0.41	2.73	9	2
1:A:86:LEU:N	1:A:86:LEU:CD1	0.41	2.80	8	1
1:A:16:GLY:HA2	1:A:40:ILE:HD11	0.41	1.91	15	1
1:A:102:LYS:HG2	1:A:180:TYR:CD2	0.41	2.50	1	1
1:A:160:LEU:H	1:A:160:LEU:CD1	0.41	2.28	5	1
1:A:176:TYR:O	1:A:177:ASP:CB	0.41	2.68	5	1
1:A:16:GLY:O	1:A:39:ILE:CG2	0.41	2.69	17	2
1:A:24:ASP:CB	1:A:69:THR:CG2	0.41	2.98	8	2
1:A:34:ILE:HD11	1:A:68:VAL:O	0.41	2.15	9	1
1:A:6:ILE:CG2	1:A:50:ARG:CZ	0.41	2.97	15	1
1:A:79:GLU:CG	1:A:79:GLU:O	0.41	2.68	19	1
1:A:88:VAL:CG2	1:A:90:ARG:NH1	0.41	2.83	20	1
1:A:15:LEU:HD22	1:A:17:PHE:CE2	0.41	2.50	6	1
1:A:23:THR:N	1:A:69:THR:HA	0.41	2.31	18	1
1:A:163:VAL:HB	1:A:167:ASP:CB	0.41	2.45	20	1
1:A:60:VAL:HG13	1:A:86:LEU:CB	0.41	2.45	1	1
1:A:48:ASP:HB3	1:A:50:ARG:CD	0.41	2.46	12	2
1:A:87:TYR:N	1:A:87:TYR:CD1	0.41	2.88	5	1
1:A:101:ILE:O	1:A:180:TYR:CD1	0.41	2.73	5	1
1:A:8:LEU:HD22	1:A:50:ARG:NH2	0.41	2.30	6	1
1:A:57:ILE:HG12	1:A:57:ILE:O	0.41	2.15	12	1
1:A:51:LEU:HD23	1:A:90:ARG:CD	0.41	2.45	14	1
1:A:104:ILE:HA	1:A:177:ASP:O	0.41	2.16	15	1
1:A:59:PHE:O	1:A:87:TYR:N	0.41	2.52	16	1
1:A:59:PHE:CD1	1:A:63:VAL:O	0.41	2.73	9	3
1:A:24:ASP:HB2	1:A:69:THR:CG2	0.41	2.45	1	1
1:A:151:LYS:CG	1:A:184:ALA:HB3	0.41	2.46	3	1
1:A:156:ASN:OD1	1:A:180:TYR:CE1	0.41	2.73	9	2
1:A:53:VAL:HG23	1:A:54:ASN:ND2	0.41	2.31	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:34:ILE:CD1	1:A:73:ALA:HB2	0.41	2.46	11	1
1:A:121:GLN:O	1:A:122:HIS:CB	0.41	2.68	18	1
1:A:8:LEU:HD13	1:A:48:ASP:HB2	0.41	1.93	1	1
1:A:39:ILE:HG13	1:A:53:VAL:CG1	0.41	2.46	4	3
1:A:58:LEU:O	1:A:59:PHE:CD2	0.41	2.73	9	2
1:A:48:ASP:HB3	1:A:50:ARG:HD2	0.41	1.92	11	1
1:A:26:PRO:CG	1:A:30:ASP:HA	0.41	2.46	13	1
1:A:99:MET:N	1:A:183:VAL:O	0.41	2.54	5	1
1:A:17:PHE:HB3	1:A:39:ILE:HG23	0.41	1.91	8	1
1:A:6:ILE:HD12	1:A:88:VAL:CG2	0.41	2.46	17	1
1:A:156:ASN:OD1	1:A:180:TYR:N	0.41	2.54	17	1
1:A:122:HIS:CD2	1:A:123:ILE:CD1	0.41	3.03	18	1
1:A:134:ILE:CD1	1:A:146:LEU:O	0.41	2.67	1	3
1:A:57:ILE:HG21	1:A:86:LEU:CD2	0.41	2.46	2	1
1:A:116:GLY:HA3	1:A:129:ILE:HA	0.41	1.92	4	1
1:A:16:GLY:O	1:A:39:ILE:HG23	0.41	2.16	5	1
1:A:50:ARG:NH1	1:A:50:ARG:CG	0.41	2.84	8	1
1:A:176:TYR:CD1	1:A:179:VAL:HG13	0.41	2.51	8	1
1:A:36:ILE:N	1:A:53:VAL:O	0.41	2.54	14	1
1:A:59:PHE:CD2	1:A:63:VAL:O	0.41	2.74	17	1
1:A:135:ILE:HG22	1:A:136:GLU:N	0.41	2.30	19	1
1:A:155:VAL:HG23	1:A:160:LEU:CG	0.41	2.46	20	1
1:A:113:SER:O	1:A:131:VAL:HG13	0.41	2.16	11	1
1:A:123:ILE:CG2	1:A:126:ASP:CB	0.40	3.00	2	1
1:A:51:LEU:N	1:A:51:LEU:CD2	0.40	2.84	4	1
1:A:5:GLU:HB3	1:A:87:TYR:CD2	0.40	2.51	6	1
1:A:102:LYS:HG3	1:A:180:TYR:CZ	0.40	2.51	6	1
1:A:112:PHE:CZ	1:A:114:ILE:HG21	0.40	2.50	10	1
1:A:59:PHE:CZ	1:A:64:ASP:OD1	0.40	2.74	14	1
1:A:129:ILE:HD12	1:A:160:LEU:HB2	0.40	1.92	18	1
1:A:140:ALA:HB1	1:A:146:LEU:CD2	0.40	2.43	20	1
1:A:74:VAL:HA	1:A:77:LEU:HD21	0.40	1.93	7	1
1:A:58:LEU:O	1:A:59:PHE:CD1	0.40	2.75	11	1
1:A:5:GLU:HG2	1:A:87:TYR:CD1	0.40	2.51	12	1
1:A:60:VAL:HG12	1:A:86:LEU:CD1	0.40	2.46	13	1
1:A:59:PHE:O	1:A:86:LEU:CB	0.40	2.69	15	1
1:A:102:LYS:HE2	1:A:180:TYR:CZ	0.40	2.52	15	1
1:A:8:LEU:HD13	1:A:48:ASP:CB	0.40	2.45	1	1
1:A:116:GLY:O	1:A:165:HIS:HA	0.40	2.17	4	1
1:A:84:VAL:O	1:A:84:VAL:CG2	0.40	2.69	19	1
1:A:141:HIS:O	1:A:145:ARG:HA	0.40	2.16	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:7:THR:HG23	1:A:85:ARG:HD3	0.40	1.93	5	1
1:A:65:VAL:HA	1:A:68:VAL:HG22	0.40	1.93	12	1
1:A:23:THR:HB	1:A:68:VAL:CA	0.40	2.47	14	1
1:A:23:THR:HB	1:A:68:VAL:C	0.40	2.37	20	1
1:A:155:VAL:HB	1:A:158:VAL:HG23	0.40	1.92	20	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	178/189 (94%)	139±3 (78±1%)	28±3 (16±2%)	11±2 (6±1%)	3 19
2	B	0	-	-	-	-
2	C	2/9 (22%)	2±0 (92±18%)	0±0 (8±18%)	0±0 (0±0%)	100 100
All	All	3600/4140 (87%)	2819 (78%)	559 (16%)	222 (6%)	3 19

All 34 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	30	ASP	19
1	A	12	ASN	18
1	A	57	ILE	17
1	A	42	GLY	16
1	A	67	GLU	16
1	A	163	VAL	15
1	A	175	THR	15
1	A	120	ASN	15
1	A	124	PRO	11
1	A	49	GLY	9
1	A	61	ASN	8
1	A	154	ALA	7
1	A	51	LEU	6
1	A	160	LEU	5
1	A	157	SER	5

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Mol	Chain	Res	Type	Models (Total)
1	A	161	GLU	5
1	A	10	ARG	4
1	A	83	ILE	4
1	A	41	PRO	3
1	A	69	THR	3
1	A	148	ILE	2
1	A	97	LYS	2
1	A	22	GLY	2
1	A	26	PRO	2
1	A	125	GLY	2
1	A	82	SER	2
1	A	117	GLY	2
1	A	21	GLY	1
1	A	162	ASP	1
1	A	164	MET	1
1	A	176	TYR	1
1	A	65	VAL	1
1	A	32	PRO	1
1	A	50	ARG	1

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	140/149 (94%)	95±5 (68±4%)	45±5 (32±4%)	1 12
2	B	0	-	-	-
2	C	3/9 (33%)	2±1 (78±24%)	1±1 (22±24%)	3 30
All	All	2860/3340 (86%)	1939 (68%)	921 (32%)	1 13

All 106 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	7	THR	20
1	A	28	ILE	20
1	A	112	PHE	20
1	A	167	ASP	20

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Mol	Chain	Res	Type	Models (Total)
1	A	15	LEU	19
1	A	50	ARG	19
1	A	146	LEU	19
1	A	179	VAL	19
1	A	181	LEU	19
1	A	52	ARG	18
1	A	151	LYS	18
1	A	152	ILE	18
1	A	3	TYR	16
1	A	34	ILE	16
1	A	60	VAL	16
1	A	38	LYS	15
1	A	78	LYS	15
1	A	133	LYS	15
1	A	121	GLN	13
1	A	172	LEU	13
1	A	173	LYS	13
1	A	5	GLU	12
1	A	39	ILE	12
1	A	150	ASP	12
1	A	6	ILE	11
1	A	30	ASP	11
1	A	97	LYS	11
1	A	126	ASP	11
1	A	85	ARG	11
1	A	123	ILE	11
1	A	145	ARG	11
1	A	153	LEU	11
1	A	90	ARG	11
1	A	9	GLU	10
1	A	59	PHE	10
1	A	99	MET	10
1	A	108	LYS	10
1	A	161	GLU	10
1	A	163	VAL	10
1	A	185	LYS	10
1	A	160	LEU	10
1	A	87	TYR	10
1	A	86	LEU	9
1	A	182	LYS	9
1	A	102	LYS	9
1	A	142	LYS	9

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Mol	Chain	Res	Type	Models (Total)
1	A	147	GLN	9
1	A	75	GLU	9
1	A	174	ASN	9
1	A	67	GLU	8
1	A	69	THR	8
1	A	157	SER	8
1	A	89	MET	8
2	C	7	SER	8
1	A	164	MET	8
1	A	12	ASN	7
1	A	31	ASP	7
1	A	48	ASP	7
1	A	71	SER	7
1	A	166	GLU	7
1	A	62	GLU	7
1	A	177	ASP	7
1	A	58	LEU	7
1	A	33	SER	7
1	A	57	ILE	7
1	A	4	GLU	6
1	A	37	THR	6
1	A	79	GLU	6
1	A	120	ASN	6
1	A	132	THR	6
1	A	18	SER	6
1	A	84	VAL	6
1	A	162	ASP	6
1	A	136	GLU	6
2	C	8	SER	5
1	A	8	LEU	5
1	A	100	GLU	5
1	A	61	ASN	5
1	A	82	SER	5
1	A	51	LEU	5
1	A	180	TYR	5
1	A	66	ARG	5
1	A	122	HIS	4
1	A	158	VAL	4
1	A	2	GLU	4
1	A	143	ASP	4
1	A	10	ARG	4
1	A	56	SER	4

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Mol	Chain	Res	Type	Models (Total)
1	A	68	VAL	3
1	A	175	THR	3
1	A	35	PHE	3
1	A	105	LYS	3
1	A	17	PHE	3
1	A	74	VAL	2
1	A	83	ILE	2
1	A	127	ASN	2
1	A	64	ASP	2
1	A	23	THR	2
1	A	141	HIS	2
1	A	165	HIS	2
1	A	24	ASP	2
1	A	113	SER	1
1	A	54	ASN	1
1	A	19	ILE	1
1	A	13	SER	1
1	A	25	ASN	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

No chemical shift data were provided