Full wwPDB NMR Structure Validation Report (i)

Feb 16, 2022 – 07:13 AM EST

PDB ID	:	1MKE
Title	:	Structure of the N-WASP EVH1 Domain-WIP complex
Authors	:	Volkman, B.F.; Prehoda, K.E.; Scott, J.A.; Peterson, F.C.; Lim, W.A.
Deposited on	:	2002-08-29

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

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

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

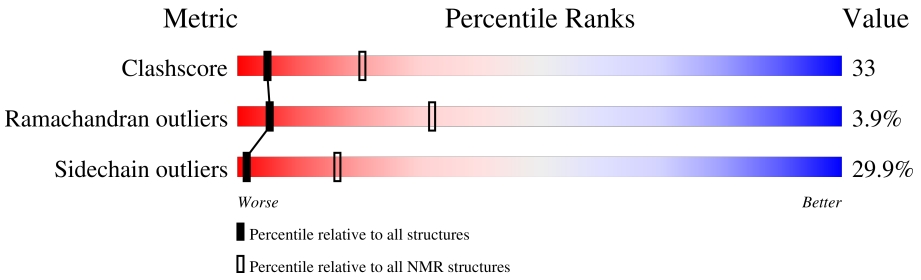
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment was not calculated.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	152	23% 44% 6% 22% 5%

2 Ensemble composition and analysis (i)

This entry contains 21 models. Model 15 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 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:2-A:8, A:14-A:18, A:40-A:72, A:77-A:142 (111)	0.42	15

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 and 2 single-model clusters were found.

Cluster number	Models
1	1, 3, 7, 8, 9, 13, 15
2	4, 14, 18, 21
3	5, 12, 19
4	2, 6, 16
5	10, 20
Single-model clusters	11; 17

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2281 atoms, of which 1132 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Fusion protein consisting of Wiskott-Aldrich syndrome protein interacting protein (WIP), GSGSG linker, and Neural Wiskott-Aldrich syndrome protein (N-WASP).

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	144	2281	729	1132	201	212	7	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	GLY	-	linker	UNP O43516
A	27	SER	-	linker	UNP O43516
A	28	GLY	-	linker	UNP O43516
A	29	SER	-	linker	UNP O43516
A	30	GLY	-	linker	UNP O43516

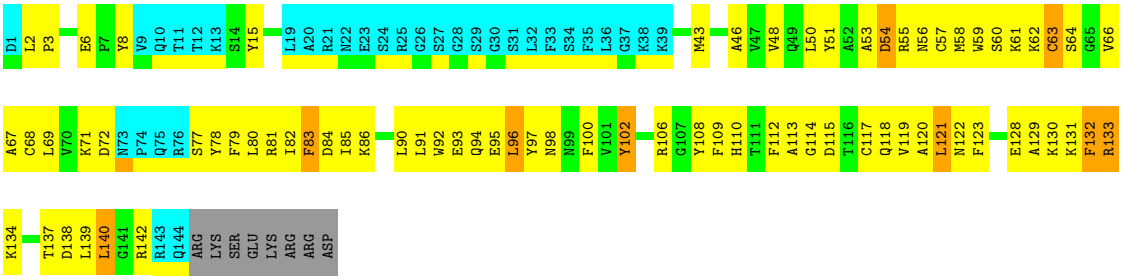
4 Residue-property plots (i)

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: Fusion protein consisting of Wiskott-Aldrich syndrome protein interacting protein (WIP), GSGSG linker, and Neural Wiskott-Aldrich syndrome protein (N-WASP)

Chain A: 23% 44% 6% 22% 5%



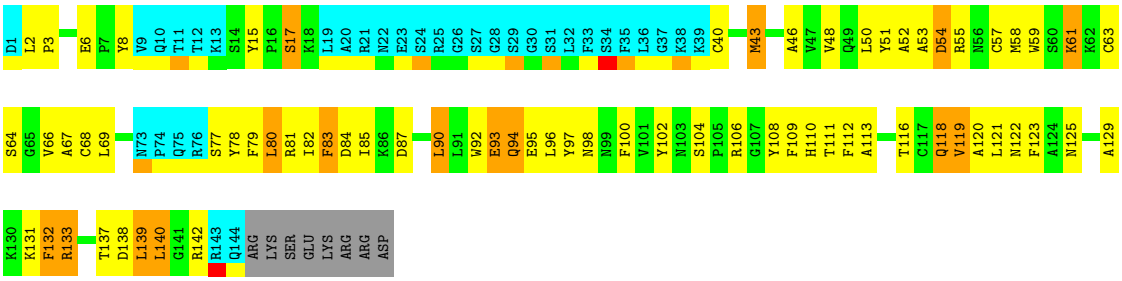
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Fusion protein consisting of Wiskott-Aldrich syndrome protein interacting protein (WIP), GSGSG linker, and Neural Wiskott-Aldrich syndrome protein (N-WASP)

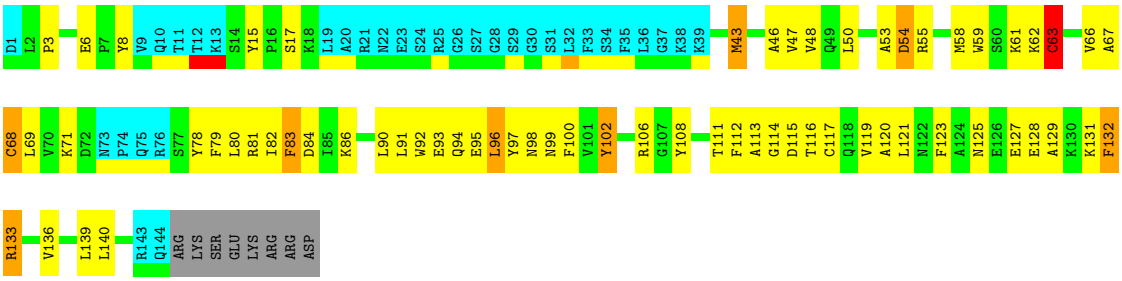
Chain A: 26% 37% 10% 22% 5%



4.2.2 Score per residue for model 2

• Molecule 1: Fusion protein consisting of Wiskott-Aldrich syndrome protein interacting protein (WIP), GSGSG linker, and Neural Wiskott-Aldrich syndrome protein (N-WASP)

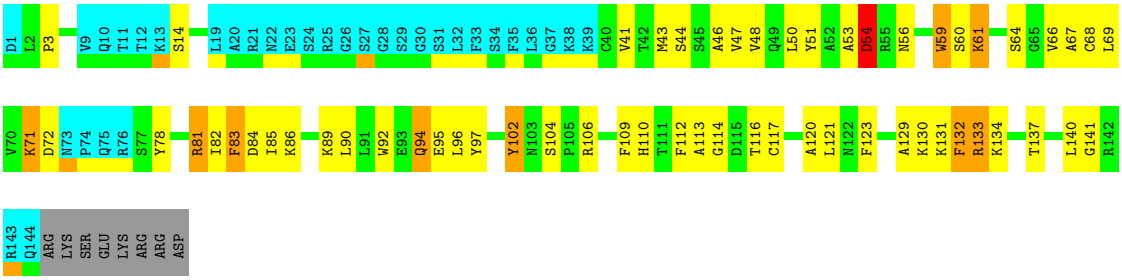
Chain A: 30% 38% 5% • 22% 5%



4.2.3 Score per residue for model 3

• Molecule 1: Fusion protein consisting of Wiskott-Aldrich syndrome protein interacting protein (WIP), GSGSG linker, and Neural Wiskott-Aldrich syndrome protein (N-WASP)

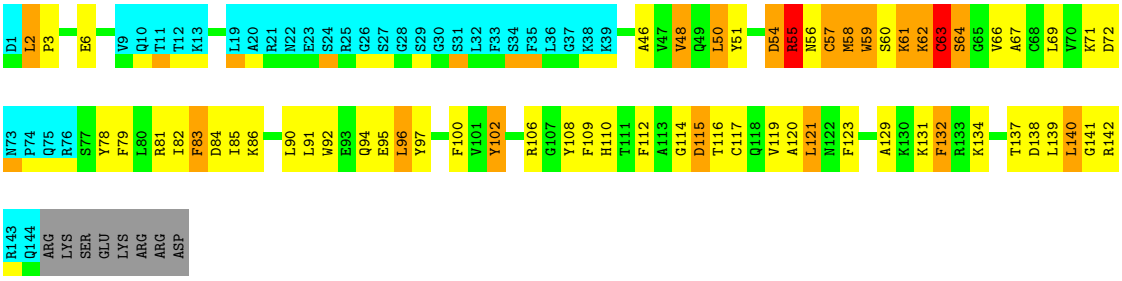
Chain A: 34% 32% 6% • 22% 5%



4.2.4 Score per residue for model 4

• Molecule 1: Fusion protein consisting of Wiskott-Aldrich syndrome protein interacting protein (WIP), GSGSG linker, and Neural Wiskott-Aldrich syndrome protein (N-WASP)

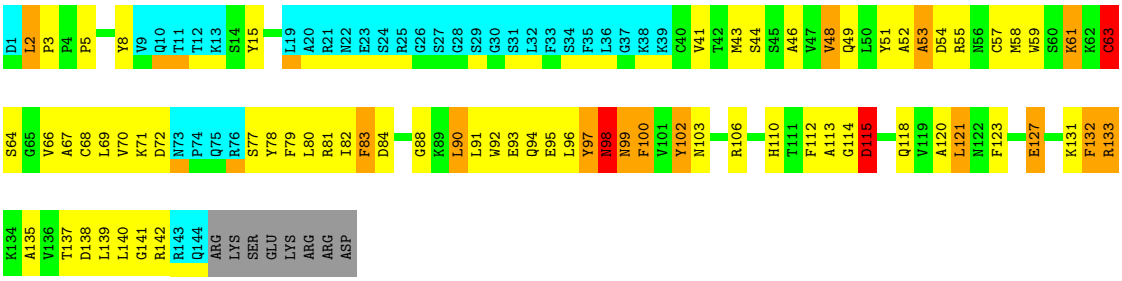
Chain A: 32% 29% 11% • 22% 5%



4.2.5 Score per residue for model 5

• Molecule 1: Fusion protein consisting of Wiskott-Aldrich syndrome protein interacting protein (WIP), GSGSG linker, and Neural Wiskott-Aldrich syndrome protein (N-WASP)

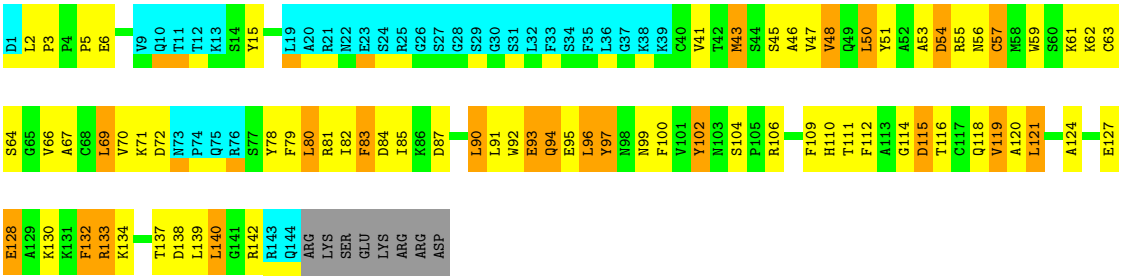
Chain A: 26% 36% 9% • 22% 5%



4.2.6 Score per residue for model 6

• Molecule 1: Fusion protein consisting of Wiskott-Aldrich syndrome protein interacting protein (WIP), GSGSG linker, and Neural Wiskott-Aldrich syndrome protein (N-WASP)

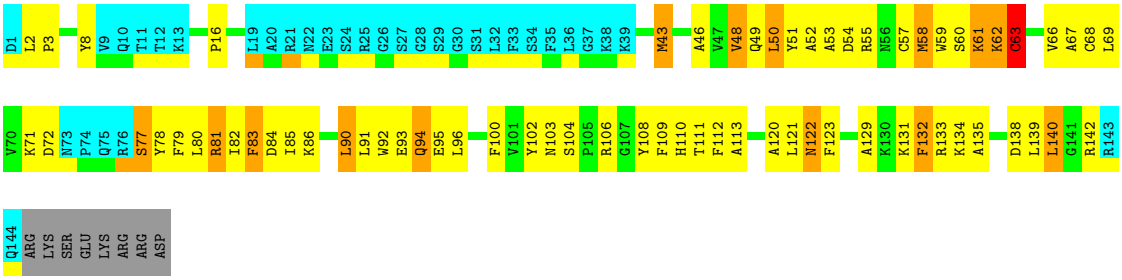
Chain A: 24% 35% 14% 22% 5%



4.2.7 Score per residue for model 7

• Molecule 1: Fusion protein consisting of Wiskott-Aldrich syndrome protein interacting protein (WIP), GSGSG linker, and Neural Wiskott-Aldrich syndrome protein (N-WASP)

Chain A: 28% 36% 9% • 22% 5%



4.2.8 Score per residue for model 8

• Molecule 1: Fusion protein consisting of Wiskott-Aldrich syndrome protein interacting protein (WIP), GSGSG linker, and Neural Wiskott-Aldrich syndrome protein (N-WASP)

Chain A: 34% 34% 5% • 22% 5%

D1 L2 P3 E6 V9 Q10 T11 T12 K13 S14 Y15 K18 L19 A20 R21 N22 E23 S24 R25 G26 S27 G28 S29 G30 S31 L32 F33 S34 F35 L36 G37 K38 K39 M43 S44 S45 A46 V47 V48 Q49 L50 A53 D54 M58 W59 S60 K61 K62 C63 S64 G65 V66 A67 C68

L69 V70 K71 D72 N73 P74 Q75 R76 S77 Y78 F79 L80 R81 I82 F83 D84 I85 K86 D87 W92 E93 Q94 E95 L96 Y97 F100 V101 Y102 R106 G107 Y108 F109 H110 D115 A120 L121 N122 F123 A124 N125 E126 E127 E128 A129 K130 K131 F132 R133 K134 A135 V136 T137 D138 L139 L140

G141 R142 R143 Q144 ARG LYS SER GLU LYS ARG ARG ASP

4.2.9 Score per residue for model 9

• Molecule 1: Fusion protein consisting of Wiskott-Aldrich syndrome protein interacting protein (WIP), GSGSG linker, and Neural Wiskott-Aldrich syndrome protein (N-WASP)

Chain A: 28% 36% 9% • 22% 5%

D1 L2 P3 V9 Q10 T11 T12 K13 P16 S17 K18 L19 A20 R21 N22 E23 S24 R25 G26 S27 G28 S29 G30 S31 L32 F33 S34 F35 L36 G37 K38 K39 C40 V41 T42 M43 A46 V47 V48 Q49 L50 Y51 D54 R55 N56 C57 M58 W59 S60 K61 K62 C63 S64 G65 V66 A67

C68 K71 D72 N73 P74 Q75 R76 S77 Y78 I82 F83 K86 K89 L90 L91 W92 E93 Q94 E95 L96 Y97 N98 N99 F100 V101 Y102 N103 S104 P105 R106 G107 Y108 F109 H110 T111 F112 A113 G114 D115 Q118 V119 A120 L121 N122 F123 A124 N125 A129 K130 K131 F132 R133 K134

T137 D138 L139 L140 G141 R142 R143 Q144 ARG LYS SER GLU LYS ARG ARG ASP

4.2.10 Score per residue for model 10

• Molecule 1: Fusion protein consisting of Wiskott-Aldrich syndrome protein interacting protein (WIP), GSGSG linker, and Neural Wiskott-Aldrich syndrome protein (N-WASP)

Chain A: 30% 35% 7% • 22% 5%

D1 L2 P3 V9 Q10 T11 T12 K13 S14 L19 A20 R21 N22 E23 S24 R25 G26 S27 G28 S29 G30 S31 L32 F33 S34 F35 L36 G37 K38 K39 M43 S44 S45 A46 V47 V48 Q49 L50 Y51 A52 A53 D54 R55 N56 W59 S60 K61 K62 C63 V66 A67 C68 L69 V70 K71

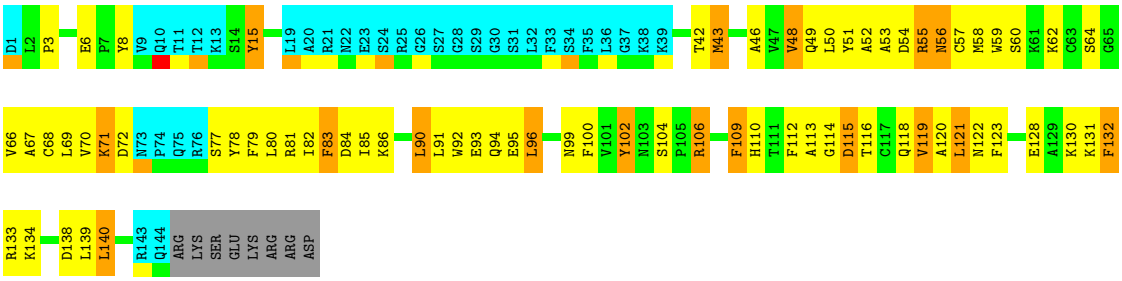
D72 N73 P74 Q75 R76 S77 Y78 F79 L80 R81 I82 F83 D84 I85 K86 L90 L91 W92 E93 Q94 E95 L96 Y97 N98 N99 F100 V101 Y102 R106 G107 Y108 F109 H110 T111 F112 A113 G114 D115 T116 C117 Q118 V119 A120 L121 N122 F123 E128 A129 K130 K131 F132 R133 K134 T137 D138 L139

L140 R143 Q144 ARG LYS SER GLU LYS ARG ARG ASP

4.2.11 Score per residue for model 11

• Molecule 1: Fusion protein consisting of Wiskott-Aldrich syndrome protein interacting protein (WIP), GSGSG linker, and Neural Wiskott-Aldrich syndrome protein (N-WASP)

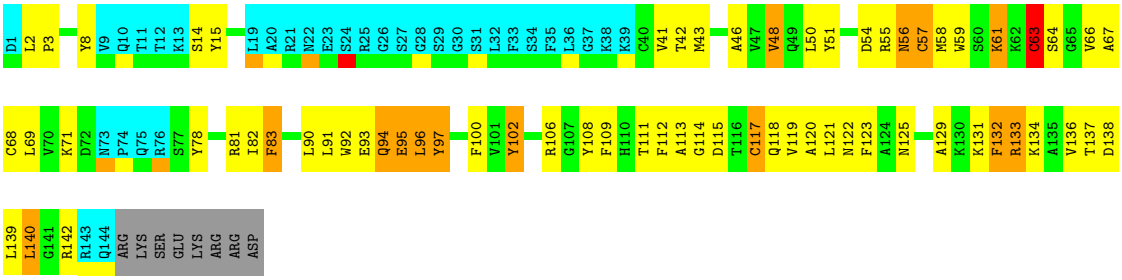
Chain A: 25% 37% 11% 22% 5%



4.2.12 Score per residue for model 12

• Molecule 1: Fusion protein consisting of Wiskott-Aldrich syndrome protein interacting protein (WIP), GSGSG linker, and Neural Wiskott-Aldrich syndrome protein (N-WASP)

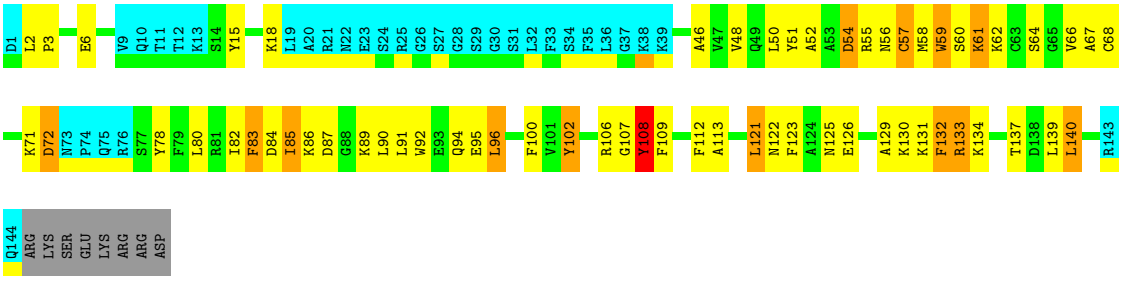
Chain A: 29% 34% 9% • 22% 5%



4.2.13 Score per residue for model 13

• Molecule 1: Fusion protein consisting of Wiskott-Aldrich syndrome protein interacting protein (WIP), GSGSG linker, and Neural Wiskott-Aldrich syndrome protein (N-WASP)

Chain A: 32% 32% 9% • 22% 5%



4.2.14 Score per residue for model 14

• Molecule 1: Fusion protein consisting of Wiskott-Aldrich syndrome protein interacting protein (WIP), GSGSG linker, and Neural Wiskott-Aldrich syndrome protein (N-WASP)

Chain A: 24% 39% 9% • 22% 5%

D1 L2 P3 P4 P5 Y8 V9 Q10 T11 T12 K13 S14 Y15 P16 L19 A20 R21 N22 E23 S24 R25 G26 S27 G28 S29 G30 S31 L32 F33 S34 F35 L36 G37 K38 K39 M43 A46 V47 V48 Q49 L50 Y51 A52 A53 D54 R55 W59 S60 K61 K62 C63 V66 A67 C68

L69 D72 N73 P74 Q75 R76 S77 Y78 F79 L80 R81 I82 F83 D84 I85 K86 D87 G88 K89 L90 L91 W92 E93 Q94 E95 L96 Y97 N98 N99 F100 V101 Y102 R106 G107 Y108 F109 H110 T111 F112 A113 G114 D115 T116 C117 Q118 V119 A120 L121 N122 F123 E127 E128 A129 K130 K131 F132 R133

K134 T137 D138 L139 L140 G141 R142 R143 Q144 ARG LYS SER GLU LYS ARG ARG ASP

4.2.15 Score per residue for model 15 (medoid)

• Molecule 1: Fusion protein consisting of Wiskott-Aldrich syndrome protein interacting protein (WIP), GSGSG linker, and Neural Wiskott-Aldrich syndrome protein (N-WASP)

Chain A: 28% 38% 7% 22% 5%

D1 L2 P3 P4 P5 E6 P7 Y8 V9 Q10 T11 T12 K13 L19 A20 R21 N22 E23 S24 R25 G26 S27 G28 S29 G30 S31 L32 F33 S34 F35 L36 G37 K38 K39 T42 M43 A46 V47 V48 Q49 L50 Y51 A52 A53 D54 R55 N56 C57 M58 W59 S60 K61 K62 C63 S64 G65 V66

A67 C68 L69 V70 K71 D72 N73 P74 Q75 R76 S77 Y78 F79 L80 R81 I82 F83 D84 I85 K86 K89 L90 L91 W92 E93 Q94 E95 L96 F100 V101 Y102 N103 R106 G107 Y108 F109 H110 T111 F112 A113 C117 A120 L121 N122 F123 A124 N125 E128 A129 K130 K131 F132 R133 K134

A135 V136 T137 D138 L139 L140 G141 R142 R143 Q144 ARG LYS SER GLU LYS ARG ARG ASP

4.2.16 Score per residue for model 16

• Molecule 1: Fusion protein consisting of Wiskott-Aldrich syndrome protein interacting protein (WIP), GSGSG linker, and Neural Wiskott-Aldrich syndrome protein (N-WASP)

Chain A: 22% 41% 10% • 22% 5%

D1 L2 P3 E6 P7 Y8 V9 Q10 T11 T12 K13 S14 Y15 P16 L19 A20 R21 N22 E23 S24 R25 G26 S27 G28 S29 G30 S31 L32 F33 S34 F35 L36 G37 K38 K39 C40 V41 T42 M43 S44 V48 Q49 L50 Y51 A52 A53 D54 R55 N56 C57 M58 W59 S60 K61 K62 C63

V66 A67 C68 L69 V70 K71 D72 N73 P74 Q75 R76 S77 Y78 F79 L80 R81 I82 F83 D84 I85 K86 D87 L90 L91 W92 E93 Q94 E95 L96 Y97 N98 N99 F100 V101 Y102 N103 S104 P105 R106 G107 Y108 F109 H110 T111 F112 A113 G114 D115 T116 C117 Q118 V119 A120 L121 N122 F123 A124 N125 E126

E127 E128 A129 K130 K131 F132 R133 K134 T137 D138 L139 R142 R143 Q144 ARG LYS SER GLU LYS ARG ARG ASP

4.2.17 Score per residue for model 17

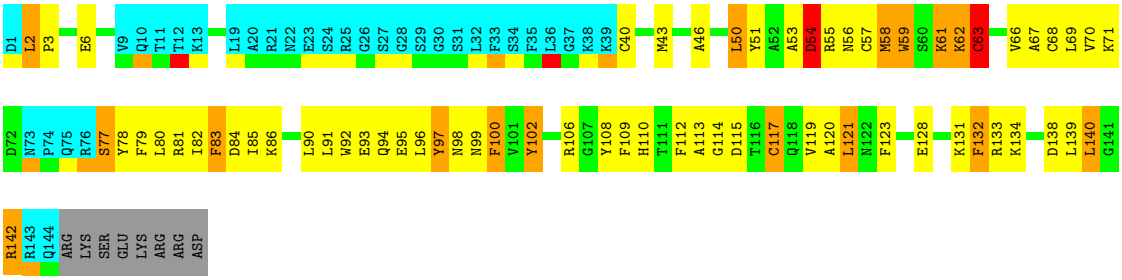
• Molecule 1: Fusion protein consisting of Wiskott-Aldrich syndrome protein interacting protein (WIP), GSGSG linker, and Neural Wiskott-Aldrich syndrome protein (N-WASP)

Chain A: 28% 34% 11% • 22% 5%

4.2.18 Score per residue for model 18

• Molecule 1: Fusion protein consisting of Wiskott-Aldrich syndrome protein interacting protein (WIP), GSGSG linker, and Neural Wiskott-Aldrich syndrome protein (N-WASP)

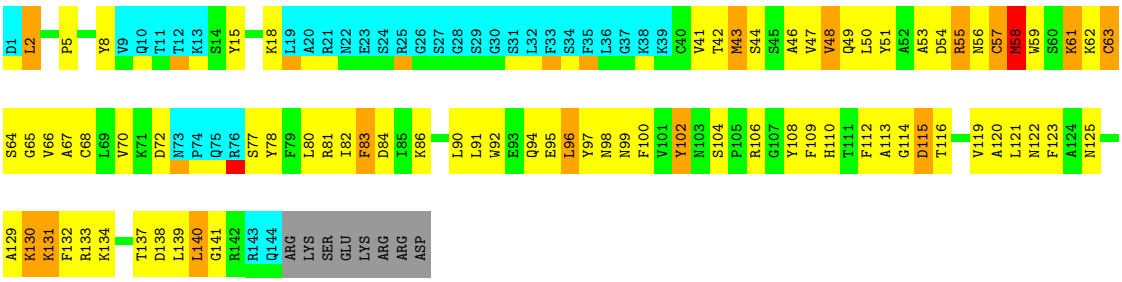
Chain A: 28% 33% 11% • 22% 5%



4.2.19 Score per residue for model 19

• Molecule 1: Fusion protein consisting of Wiskott-Aldrich syndrome protein interacting protein (WIP), GSGSG linker, and Neural Wiskott-Aldrich syndrome protein (N-WASP)

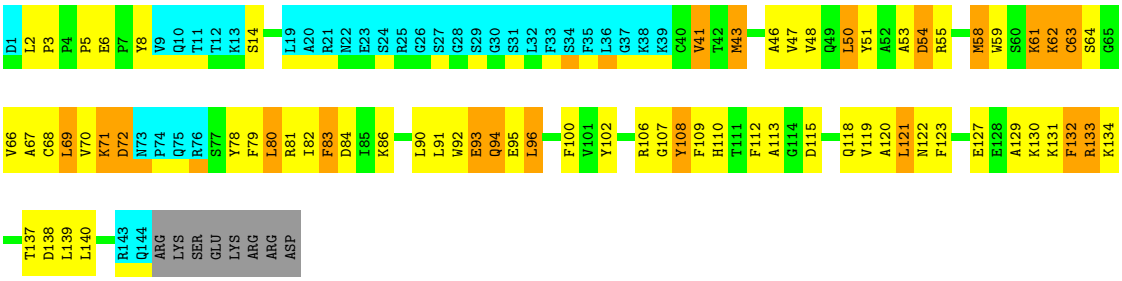
Chain A: 22% 41% 9% • 22% 5%



4.2.20 Score per residue for model 20

• Molecule 1: Fusion protein consisting of Wiskott-Aldrich syndrome protein interacting protein (WIP), GSGSG linker, and Neural Wiskott-Aldrich syndrome protein (N-WASP)

Chain A: 26% 34% 13% 22% 5%



4.2.21 Score per residue for model 21

• Molecule 1: Fusion protein consisting of Wiskott-Aldrich syndrome protein interacting protein (WIP), GSGSG linker, and Neural Wiskott-Aldrich syndrome protein (N-WASP)

Chain A: 31% 31% 10% • 22% 5%

5 Refinement protocol and experimental data overview (i)

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

Of the 50 calculated structures, 21 were deposited, based on the following criterion: *LOWEST TARGET FUNCTION*.

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

Software name	Classification	Version
DYANA	structure solution	1.5
DYANA	refinement	1.5

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	893	872	872	58±6
All	All	18753	18312	18312	1220

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 33.

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:VAL:HG13	1:A:124:ALA:HB3	1.01	1.32	6	3
1:A:82:ILE:HD12	1:A:92:TRP:CE3	0.97	1.93	14	21
1:A:84:ASP:N	1:A:91:LEU:HD21	0.93	1.78	14	2
1:A:100:PHE:O	1:A:140:LEU:HD21	0.92	1.64	13	17
1:A:69:LEU:HD12	1:A:80:LEU:HD21	0.90	1.40	17	1
1:A:80:LEU:HD12	1:A:96:LEU:HD21	0.88	1.46	20	1
1:A:78:TYR:CE1	1:A:139:LEU:HD11	0.86	2.05	14	1
1:A:47:VAL:HG13	1:A:65:GLY:O	0.86	1.70	15	3
1:A:112:PHE:CE1	1:A:121:LEU:HD23	0.83	2.08	4	1
1:A:139:LEU:O	1:A:139:LEU:HD12	0.82	1.74	10	1
1:A:78:TYR:CE2	1:A:139:LEU:HD21	0.81	2.11	13	3
1:A:43:MET:SD	1:A:139:LEU:HD12	0.80	2.16	14	4
1:A:112:PHE:CZ	1:A:119:VAL:HG23	0.79	2.13	21	10
1:A:90:LEU:HD13	1:A:93:GLU:OE1	0.78	1.78	10	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:81:ARG:HB3	1:A:90:LEU:HD21	0.78	1.56	19	4
1:A:47:VAL:CG1	1:A:124:ALA:HB3	0.78	2.08	6	3
1:A:133:ARG:O	1:A:137:THR:HG23	0.77	1.77	10	14
1:A:121:LEU:HD22	1:A:121:LEU:O	0.77	1.78	9	1
1:A:67:ALA:HB2	1:A:82:ILE:HG12	0.77	1.54	15	18
1:A:46:ALA:HB3	1:A:132:PHE:CE2	0.77	2.14	8	7
1:A:82:ILE:O	1:A:90:LEU:HD23	0.76	1.80	19	3
1:A:90:LEU:HD11	1:A:93:GLU:HB3	0.75	1.55	12	2
1:A:46:ALA:HB3	1:A:132:PHE:CE1	0.75	2.17	12	13
1:A:78:TYR:CZ	1:A:139:LEU:HD21	0.74	2.17	11	5
1:A:8:TYR:CZ	1:A:113:ALA:HB1	0.74	2.18	16	4
1:A:78:TYR:HB2	1:A:96:LEU:HD12	0.74	1.58	1	10
1:A:139:LEU:HD12	1:A:139:LEU:C	0.73	2.03	10	1
1:A:112:PHE:CE1	1:A:119:VAL:HG23	0.73	2.19	6	9
1:A:102:TYR:CE2	1:A:136:VAL:HG21	0.73	2.17	15	3
1:A:83:PHE:CD1	1:A:83:PHE:N	0.73	2.56	11	21
1:A:43:MET:CE	1:A:135:ALA:HB1	0.72	2.14	7	3
1:A:123:PHE:CD2	1:A:129:ALA:CB	0.71	2.73	9	14
1:A:90:LEU:HD11	1:A:93:GLU:HB2	0.71	1.61	16	2
1:A:66:VAL:HG13	1:A:83:PHE:CD2	0.70	2.22	12	4
1:A:47:VAL:HG13	1:A:124:ALA:CB	0.70	2.13	6	2
1:A:2:LEU:HD12	1:A:59:TRP:CD1	0.70	2.21	18	2
1:A:2:LEU:CD2	1:A:109:PHE:CE1	0.70	2.74	17	1
1:A:41:VAL:O	1:A:70:VAL:HG13	0.70	1.87	19	5
1:A:8:TYR:CE1	1:A:113:ALA:HB1	0.69	2.23	1	4
1:A:123:PHE:CD2	1:A:129:ALA:HB2	0.69	2.23	1	11
1:A:112:PHE:CE2	1:A:121:LEU:HD22	0.69	2.22	6	1
1:A:123:PHE:CD1	1:A:129:ALA:CB	0.68	2.77	19	2
1:A:3:PRO:CG	1:A:109:PHE:CD1	0.68	2.76	1	8
1:A:82:ILE:HD12	1:A:92:TRP:HE3	0.68	1.49	11	15
1:A:132:PHE:O	1:A:136:VAL:HG23	0.68	1.89	15	2
1:A:8:TYR:CE2	1:A:113:ALA:HB1	0.67	2.25	11	2
1:A:2:LEU:CD1	1:A:109:PHE:CE2	0.67	2.78	9	2
1:A:69:LEU:CD1	1:A:80:LEU:HD21	0.67	2.20	17	1
1:A:82:ILE:O	1:A:90:LEU:HD13	0.66	1.91	7	1
1:A:63:CYS:HB3	1:A:91:LEU:HD13	0.66	1.67	4	3
1:A:102:TYR:OH	1:A:121:LEU:HD11	0.66	1.90	21	3
1:A:42:THR:OG1	1:A:70:VAL:HG22	0.65	1.92	11	1
1:A:78:TYR:HB3	1:A:96:LEU:HD12	0.65	1.66	10	6
1:A:46:ALA:O	1:A:48:VAL:HG13	0.65	1.91	17	7
1:A:78:TYR:CB	1:A:96:LEU:HD12	0.65	2.21	4	18

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:46:ALA:HB2	1:A:128:GLU:OE1	0.65	1.91	2	1
1:A:112:PHE:CZ	1:A:119:VAL:CG2	0.65	2.79	19	9
1:A:59:TRP:CZ3	1:A:120:ALA:HB2	0.65	2.27	8	15
1:A:102:TYR:CE2	1:A:110:HIS:ND1	0.65	2.64	9	9
1:A:69:LEU:HD12	1:A:80:LEU:HD11	0.65	1.67	1	1
1:A:2:LEU:HD22	1:A:59:TRP:CD1	0.65	2.27	7	1
1:A:46:ALA:HB3	1:A:132:PHE:HE2	0.64	1.52	8	7
1:A:43:MET:SD	1:A:139:LEU:HD11	0.64	2.32	9	2
1:A:110:HIS:HB2	1:A:121:LEU:HD21	0.64	1.70	9	1
1:A:59:TRP:CZ3	1:A:120:ALA:CB	0.64	2.81	6	13
1:A:78:TYR:CE1	1:A:139:LEU:HD13	0.64	2.28	8	1
1:A:46:ALA:HB3	1:A:132:PHE:HE1	0.63	1.54	7	9
1:A:15:TYR:CE1	1:A:96:LEU:O	0.63	2.52	11	2
1:A:43:MET:HE3	1:A:135:ALA:HB1	0.63	1.71	15	2
1:A:50:LEU:HD12	1:A:62:LYS:HB2	0.63	1.71	4	1
1:A:102:TYR:CD2	1:A:136:VAL:HG21	0.62	2.30	8	3
1:A:97:TYR:N	1:A:97:TYR:CD1	0.62	2.67	14	2
1:A:112:PHE:CE2	1:A:113:ALA:O	0.62	2.53	3	3
1:A:41:VAL:HG23	1:A:71:LYS:CG	0.62	2.25	17	1
1:A:8:TYR:CE1	1:A:113:ALA:HB2	0.62	2.30	2	2
1:A:123:PHE:CD1	1:A:129:ALA:HB2	0.62	2.29	19	1
1:A:2:LEU:HD22	1:A:109:PHE:CE2	0.61	2.30	1	1
1:A:123:PHE:CE1	1:A:132:PHE:CD2	0.61	2.89	9	4
1:A:84:ASP:OD2	1:A:91:LEU:HD11	0.61	1.95	6	4
1:A:53:ALA:HB2	1:A:59:TRP:CZ3	0.61	2.31	10	3
1:A:41:VAL:HG23	1:A:71:LYS:HG2	0.61	1.72	17	1
1:A:50:LEU:HD21	1:A:112:PHE:CZ	0.61	2.30	19	1
1:A:121:LEU:N	1:A:121:LEU:HD13	0.61	2.11	9	1
1:A:15:TYR:CE1	1:A:95:GLU:O	0.61	2.54	1	6
1:A:82:ILE:CD1	1:A:92:TRP:CE3	0.61	2.84	4	11
1:A:139:LEU:C	1:A:139:LEU:HD23	0.60	2.16	14	4
1:A:96:LEU:HD22	1:A:100:PHE:CZ	0.60	2.31	13	5
1:A:112:PHE:CE1	1:A:113:ALA:O	0.60	2.55	13	2
1:A:110:HIS:CE1	1:A:123:PHE:CE2	0.60	2.89	4	7
1:A:78:TYR:O	1:A:79:PHE:CD1	0.60	2.54	5	3
1:A:112:PHE:CD1	1:A:113:ALA:N	0.60	2.69	13	2
1:A:66:VAL:HG12	1:A:83:PHE:O	0.60	1.96	15	2
1:A:111:THR:HG22	1:A:120:ALA:CB	0.60	2.27	1	6
1:A:108:TYR:CE1	1:A:122:ASN:OD1	0.60	2.54	20	1
1:A:96:LEU:CD2	1:A:100:PHE:CE2	0.60	2.85	9	2
1:A:66:VAL:O	1:A:83:PHE:CE2	0.60	2.55	13	4

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:50:LEU:HD13	1:A:51:TYR:N	0.59	2.12	6	7
1:A:92:TRP:CZ2	1:A:112:PHE:CZ	0.59	2.91	6	3
1:A:112:PHE:HE2	1:A:121:LEU:HD22	0.59	1.58	6	1
1:A:109:PHE:CE1	1:A:120:ALA:HB1	0.59	2.31	3	9
1:A:66:VAL:O	1:A:83:PHE:CD2	0.59	2.55	13	8
1:A:78:TYR:CE1	1:A:139:LEU:HD23	0.59	2.33	4	3
1:A:71:LYS:CD	1:A:139:LEU:HD11	0.59	2.28	6	2
1:A:43:MET:HE2	1:A:69:LEU:HD11	0.59	1.73	20	1
1:A:94:GLN:NE2	1:A:97:TYR:CE2	0.58	2.71	18	1
1:A:50:LEU:HD12	1:A:62:LYS:CB	0.58	2.27	4	1
1:A:123:PHE:CE1	1:A:132:PHE:CG	0.58	2.92	10	10
1:A:77:SER:OG	1:A:79:PHE:CE2	0.58	2.57	1	1
1:A:43:MET:CE	1:A:139:LEU:HD12	0.58	2.28	2	1
1:A:121:LEU:CD1	1:A:123:PHE:CZ	0.58	2.86	18	2
1:A:91:LEU:N	1:A:91:LEU:HD22	0.58	2.13	21	2
1:A:78:TYR:C	1:A:79:PHE:CD1	0.57	2.77	18	8
1:A:90:LEU:C	1:A:91:LEU:HD13	0.57	2.20	14	2
1:A:112:PHE:CD2	1:A:113:ALA:O	0.57	2.57	1	4
1:A:42:THR:HG23	1:A:68:CYS:SG	0.57	2.39	17	4
1:A:121:LEU:HD12	1:A:123:PHE:CE2	0.57	2.35	18	1
1:A:112:PHE:CG	1:A:113:ALA:N	0.57	2.72	9	7
1:A:67:ALA:HB2	1:A:82:ILE:CG1	0.57	2.28	12	7
1:A:97:TYR:CZ	1:A:100:PHE:CD2	0.57	2.93	19	1
1:A:115:ASP:OD2	1:A:116:THR:HG22	0.57	1.98	19	1
1:A:43:MET:CE	1:A:139:LEU:HD21	0.56	2.29	9	1
1:A:112:PHE:CE1	1:A:121:LEU:CD2	0.56	2.87	4	2
1:A:5:PRO:CB	1:A:53:ALA:HB1	0.56	2.31	20	8
1:A:47:VAL:HG22	1:A:66:VAL:HG22	0.56	1.78	20	3
1:A:67:ALA:HB2	1:A:82:ILE:HG13	0.56	1.78	12	1
1:A:84:ASP:HB2	1:A:91:LEU:HD11	0.56	1.78	14	3
1:A:108:TYR:CD2	1:A:122:ASN:OD1	0.55	2.59	1	2
1:A:92:TRP:CZ2	1:A:94:GLN:HB2	0.55	2.37	20	17
1:A:50:LEU:HD21	1:A:112:PHE:HZ	0.55	1.61	19	1
1:A:2:LEU:CB	1:A:3:PRO:CD	0.55	2.85	18	3
1:A:46:ALA:HB2	1:A:128:GLU:OE2	0.55	2.01	6	1
1:A:2:LEU:HD13	1:A:109:PHE:CE2	0.55	2.37	13	2
1:A:3:PRO:HG3	1:A:109:PHE:CD1	0.55	2.38	3	3
1:A:78:TYR:CE2	1:A:139:LEU:CD2	0.55	2.89	11	1
1:A:80:LEU:HD23	1:A:96:LEU:HD11	0.55	1.79	16	1
1:A:41:VAL:CG2	1:A:71:LYS:CG	0.55	2.85	17	1
1:A:3:PRO:HG2	1:A:109:PHE:CD1	0.54	2.37	1	4

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:66:VAL:O	1:A:83:PHE:CD1	0.54	2.61	9	6
1:A:123:PHE:CD2	1:A:129:ALA:HB1	0.54	2.38	17	5
1:A:2:LEU:HD23	1:A:2:LEU:N	0.54	2.17	19	2
1:A:2:LEU:HD12	1:A:109:PHE:CE2	0.54	2.37	6	2
1:A:108:TYR:CZ	1:A:122:ASN:OD1	0.54	2.61	20	2
1:A:136:VAL:HG12	1:A:140:LEU:CD1	0.54	2.33	15	1
1:A:108:TYR:CD1	1:A:108:TYR:N	0.54	2.75	14	6
1:A:72:ASP:OD1	1:A:79:PHE:CE1	0.54	2.61	7	1
1:A:97:TYR:CE1	1:A:100:PHE:CD2	0.53	2.96	19	1
1:A:114:GLY:O	1:A:116:THR:N	0.53	2.40	3	6
1:A:96:LEU:HD23	1:A:100:PHE:CE2	0.53	2.38	9	1
1:A:96:LEU:CD2	1:A:100:PHE:CZ	0.53	2.91	6	3
1:A:3:PRO:CG	1:A:109:PHE:CD2	0.53	2.91	4	2
1:A:63:CYS:O	1:A:64:SER:CB	0.53	2.57	4	1
1:A:2:LEU:HD23	1:A:109:PHE:CE1	0.53	2.37	17	1
1:A:102:TYR:HE2	1:A:136:VAL:HG21	0.53	1.59	15	1
1:A:104:SER:HB2	1:A:110:HIS:CD2	0.53	2.39	7	6
1:A:79:PHE:CD2	1:A:81:ARG:NH2	0.53	2.77	4	1
1:A:96:LEU:HD22	1:A:100:PHE:CE1	0.53	2.39	11	4
1:A:3:PRO:HG3	1:A:109:PHE:CD2	0.53	2.39	11	1
1:A:91:LEU:HD22	1:A:91:LEU:H	0.53	1.64	14	2
1:A:8:TYR:CZ	1:A:113:ALA:CB	0.53	2.91	2	2
1:A:115:ASP:CG	1:A:116:THR:HG23	0.53	2.24	4	2
1:A:84:ASP:CG	1:A:91:LEU:HD11	0.52	2.25	20	3
1:A:110:HIS:CE1	1:A:123:PHE:CE1	0.52	2.98	19	1
1:A:84:ASP:CB	1:A:91:LEU:HD11	0.52	2.33	18	4
1:A:123:PHE:CE2	1:A:132:PHE:CG	0.52	2.98	13	2
1:A:112:PHE:CE2	1:A:119:VAL:HG23	0.52	2.39	20	1
1:A:66:VAL:HB	1:A:83:PHE:CE2	0.52	2.39	8	12
1:A:5:PRO:HB3	1:A:53:ALA:HB1	0.52	1.81	20	3
1:A:83:PHE:C	1:A:91:LEU:HD21	0.52	2.24	14	2
1:A:84:ASP:N	1:A:84:ASP:OD1	0.52	2.42	17	1
1:A:95:GLU:O	1:A:96:LEU:C	0.52	2.48	4	18
1:A:92:TRP:CH2	1:A:94:GLN:HB2	0.52	2.40	12	11
1:A:3:PRO:HG2	1:A:109:PHE:CD2	0.52	2.40	4	1
1:A:107:GLY:O	1:A:108:TYR:CB	0.52	2.58	13	2
1:A:47:VAL:CG1	1:A:124:ALA:CB	0.52	2.86	8	2
1:A:122:ASN:HD22	1:A:122:ASN:N	0.52	2.01	7	1
1:A:121:LEU:HD11	1:A:123:PHE:CZ	0.51	2.40	2	1
1:A:104:SER:HB3	1:A:110:HIS:CD2	0.51	2.40	19	2
1:A:72:ASP:N	1:A:72:ASP:OD1	0.51	2.42	16	4

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:50:LEU:C	1:A:50:LEU:HD13	0.51	2.26	11	1
1:A:41:VAL:HG12	1:A:71:LYS:O	0.51	2.05	3	2
1:A:72:ASP:OD1	1:A:79:PHE:CD1	0.51	2.63	7	1
1:A:112:PHE:CZ	1:A:113:ALA:O	0.51	2.64	9	1
1:A:85:ILE:HG23	1:A:86:LYS:HD2	0.51	1.82	11	1
1:A:96:LEU:HD22	1:A:100:PHE:CE2	0.51	2.41	2	5
1:A:48:VAL:HG12	1:A:123:PHE:CD1	0.51	2.40	10	1
1:A:108:TYR:O	1:A:108:TYR:CG	0.51	2.64	20	1
1:A:3:PRO:HG2	1:A:109:PHE:CE1	0.50	2.42	14	6
1:A:81:ARG:HB3	1:A:90:LEU:HD11	0.50	1.83	7	1
1:A:66:VAL:O	1:A:83:PHE:CZ	0.50	2.65	14	4
1:A:108:TYR:CD1	1:A:108:TYR:C	0.50	2.84	8	1
1:A:57:CYS:O	1:A:58:MET:CG	0.50	2.59	19	1
1:A:112:PHE:CE2	1:A:119:VAL:CG2	0.50	2.94	19	2
1:A:3:PRO:O	1:A:59:TRP:NE1	0.50	2.44	7	19
1:A:123:PHE:CZ	1:A:132:PHE:CD2	0.50	2.99	13	3
1:A:63:CYS:SG	1:A:91:LEU:HD22	0.50	2.47	4	2
1:A:78:TYR:N	1:A:78:TYR:CD1	0.50	2.79	18	3
1:A:111:THR:HG22	1:A:120:ALA:HB1	0.50	1.83	12	3
1:A:50:LEU:HD23	1:A:62:LYS:HB2	0.50	1.82	20	1
1:A:51:TYR:CE1	1:A:61:LYS:CB	0.50	2.94	3	1
1:A:110:HIS:O	1:A:121:LEU:CD2	0.50	2.60	5	2
1:A:109:PHE:CE2	1:A:122:ASN:OD1	0.50	2.65	7	2
1:A:61:LYS:CD	1:A:61:LYS:C	0.49	2.80	1	1
1:A:46:ALA:CB	1:A:128:GLU:OE2	0.49	2.60	6	1
1:A:63:CYS:HB2	1:A:91:LEU:HD13	0.49	1.83	6	1
1:A:109:PHE:CD2	1:A:122:ASN:OD1	0.49	2.65	7	2
1:A:80:LEU:O	1:A:94:GLN:N	0.49	2.45	11	1
1:A:15:TYR:CE2	1:A:95:GLU:O	0.49	2.65	16	1
1:A:48:VAL:CG1	1:A:123:PHE:CD2	0.49	2.95	11	2
1:A:108:TYR:CG	1:A:108:TYR:O	0.49	2.66	8	1
1:A:109:PHE:CZ	1:A:122:ASN:HB3	0.49	2.43	11	1
1:A:104:SER:CB	1:A:110:HIS:CD2	0.49	2.96	19	5
1:A:94:GLN:HG3	1:A:112:PHE:CZ	0.49	2.42	3	2
1:A:110:HIS:O	1:A:121:LEU:HD23	0.49	2.07	8	2
1:A:66:VAL:CG1	1:A:83:PHE:CE2	0.49	2.95	8	1
1:A:56:ASN:O	1:A:57:CYS:CB	0.49	2.59	6	5
1:A:62:LYS:O	1:A:63:CYS:CB	0.49	2.61	7	4
1:A:15:TYR:CD1	1:A:95:GLU:O	0.49	2.66	13	2
1:A:81:ARG:HD2	1:A:90:LEU:HD12	0.49	1.85	16	1
1:A:57:CYS:O	1:A:58:MET:CB	0.49	2.60	19	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:54:ASP:CB	1:A:58:MET:O	0.49	2.60	5	2
1:A:43:MET:CE	1:A:139:LEU:HD11	0.49	2.38	8	1
1:A:66:VAL:HB	1:A:83:PHE:CD2	0.49	2.43	4	14
1:A:123:PHE:CG	1:A:129:ALA:HB2	0.49	2.43	19	4
1:A:110:HIS:CE1	1:A:123:PHE:CZ	0.48	3.01	4	1
1:A:111:THR:HG22	1:A:120:ALA:HB2	0.48	1.84	6	2
1:A:66:VAL:O	1:A:83:PHE:CG	0.48	2.66	9	8
1:A:78:TYR:CE2	1:A:139:LEU:HD23	0.48	2.43	5	2
1:A:15:TYR:CZ	1:A:95:GLU:O	0.48	2.67	1	1
1:A:121:LEU:HD13	1:A:121:LEU:H	0.48	1.68	9	1
1:A:90:LEU:HD22	1:A:93:GLU:OE1	0.48	2.08	10	1
1:A:99:ASN:O	1:A:100:PHE:O	0.48	2.32	5	1
1:A:77:SER:OG	1:A:78:TYR:N	0.48	2.46	7	2
1:A:90:LEU:CD1	1:A:93:GLU:OE1	0.48	2.59	10	1
1:A:122:ASN:N	1:A:122:ASN:ND2	0.48	2.62	7	1
1:A:3:PRO:CD	1:A:109:PHE:CD1	0.48	2.96	8	2
1:A:2:LEU:HD12	1:A:59:TRP:HD1	0.48	1.64	18	1
1:A:137:THR:O	1:A:141:GLY:N	0.48	2.46	19	7
1:A:104:SER:OG	1:A:110:HIS:CD2	0.48	2.67	6	1
1:A:94:GLN:HG3	1:A:112:PHE:CE1	0.48	2.44	16	1
1:A:94:GLN:NE2	1:A:95:GLU:N	0.48	2.61	16	1
1:A:90:LEU:HD23	1:A:93:GLU:HB2	0.48	1.84	5	1
1:A:92:TRP:CZ3	1:A:94:GLN:HB2	0.48	2.44	11	2
1:A:72:ASP:OD2	1:A:77:SER:N	0.48	2.47	16	1
1:A:97:TYR:CZ	1:A:100:PHE:CE2	0.48	3.02	19	1
1:A:6:GLU:O	1:A:118:GLN:NE2	0.47	2.47	11	2
1:A:42:THR:CG2	1:A:68:CYS:SG	0.47	3.02	19	2
1:A:78:TYR:HE2	1:A:139:LEU:HD23	0.47	1.68	5	1
1:A:2:LEU:HD22	1:A:2:LEU:N	0.47	2.24	12	1
1:A:40:CYS:HB3	1:A:70:VAL:HG11	0.47	1.86	16	1
1:A:2:LEU:HD23	1:A:3:PRO:HD2	0.47	1.86	21	1
1:A:68:CYS:SG	1:A:83:PHE:CZ	0.47	3.07	1	8
1:A:133:ARG:O	1:A:137:THR:CG2	0.47	2.60	5	5
1:A:121:LEU:CD1	1:A:123:PHE:CE2	0.47	2.97	18	1
1:A:51:TYR:CE1	1:A:61:LYS:HB2	0.47	2.45	9	3
1:A:59:TRP:CZ3	1:A:120:ALA:HB3	0.47	2.44	6	2
1:A:66:VAL:HG12	1:A:83:PHE:CE2	0.47	2.43	7	2
1:A:49:GLN:HB2	1:A:51:TYR:CE2	0.47	2.43	16	1
1:A:109:PHE:CE2	1:A:122:ASN:HB2	0.47	2.44	16	5
1:A:8:TYR:CZ	1:A:113:ALA:HB2	0.47	2.44	20	2
1:A:68:CYS:SG	1:A:70:VAL:HG23	0.47	2.49	15	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:81:ARG:O	1:A:83:PHE:CE1	0.47	2.67	19	1
1:A:78:TYR:CD1	1:A:78:TYR:N	0.47	2.82	20	3
1:A:3:PRO:HG2	1:A:109:PHE:CE2	0.47	2.45	4	2
1:A:72:ASP:OD2	1:A:79:PHE:CD1	0.47	2.68	4	1
1:A:43:MET:CE	1:A:69:LEU:CD2	0.47	2.92	11	1
1:A:109:PHE:CE2	1:A:122:ASN:HB3	0.47	2.45	11	1
1:A:123:PHE:CE2	1:A:132:PHE:CD2	0.47	3.02	13	1
1:A:54:ASP:O	1:A:55:ARG:CB	0.47	2.63	4	1
1:A:47:VAL:HG11	1:A:124:ALA:HB3	0.47	1.87	9	1
1:A:43:MET:HE3	1:A:139:LEU:HD21	0.47	1.86	9	1
1:A:84:ASP:OD1	1:A:85:ILE:N	0.47	2.47	7	11
1:A:52:ALA:O	1:A:60:SER:N	0.47	2.48	11	5
1:A:68:CYS:O	1:A:80:LEU:HD12	0.47	2.10	11	1
1:A:49:GLN:HG2	1:A:51:TYR:CE2	0.47	2.45	15	1
1:A:78:TYR:HE2	1:A:139:LEU:HD22	0.47	1.69	19	1
1:A:79:PHE:CE2	1:A:95:GLU:HG2	0.46	2.44	4	1
1:A:99:ASN:O	1:A:100:PHE:C	0.46	2.53	18	2
1:A:123:PHE:CD1	1:A:129:ALA:HB1	0.46	2.45	19	1
1:A:115:ASP:OD1	1:A:116:THR:HG23	0.46	2.10	4	1
1:A:108:TYR:O	1:A:108:TYR:CD2	0.46	2.68	4	3
1:A:52:ALA:O	1:A:54:ASP:N	0.46	2.49	5	3
1:A:58:MET:O	1:A:59:TRP:C	0.46	2.53	18	9
1:A:2:LEU:CB	1:A:3:PRO:HD2	0.46	2.41	18	2
1:A:43:MET:HG3	1:A:139:LEU:HD21	0.46	1.85	7	1
1:A:84:ASP:OD1	1:A:89:LYS:O	0.46	2.34	17	1
1:A:71:LYS:HB2	1:A:78:TYR:CD1	0.46	2.46	11	2
1:A:115:ASP:CG	1:A:116:THR:HG22	0.46	2.29	19	1
1:A:55:ARG:O	1:A:57:CYS:N	0.46	2.49	9	4
1:A:112:PHE:CE1	1:A:119:VAL:CG2	0.46	2.97	1	1
1:A:114:GLY:CA	1:A:117:CYS:O	0.46	2.64	18	6
1:A:72:ASP:N	1:A:77:SER:O	0.46	2.47	14	2
1:A:72:ASP:CB	1:A:77:SER:O	0.46	2.64	15	1
1:A:68:CYS:SG	1:A:83:PHE:CE1	0.45	3.06	1	5
1:A:114:GLY:N	1:A:117:CYS:O	0.45	2.49	12	2
1:A:112:PHE:CZ	1:A:119:VAL:HG21	0.45	2.45	19	1
1:A:78:TYR:CE2	1:A:139:LEU:HB3	0.45	2.46	17	1
1:A:71:LYS:HG3	1:A:78:TYR:CE2	0.45	2.46	9	1
1:A:49:GLN:N	1:A:122:ASN:O	0.45	2.48	7	1
1:A:51:TYR:CD2	1:A:61:LYS:N	0.45	2.84	1	1
1:A:79:PHE:CD1	1:A:79:PHE:N	0.45	2.85	2	2
1:A:136:VAL:HG12	1:A:140:LEU:HD13	0.45	1.88	12	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:79:PHE:CB	1:A:81:ARG:NH1	0.45	2.80	1	1
1:A:82:ILE:C	1:A:83:PHE:CD1	0.45	2.90	12	3
1:A:109:PHE:CD2	1:A:122:ASN:HB3	0.45	2.46	15	1
1:A:51:TYR:CE1	1:A:61:LYS:HB3	0.45	2.46	3	1
1:A:115:ASP:CG	1:A:116:THR:N	0.45	2.70	19	4
1:A:96:LEU:HD22	1:A:100:PHE:CD1	0.45	2.47	11	2
1:A:106:ARG:O	1:A:108:TYR:N	0.45	2.50	10	1
1:A:64:SER:O	1:A:91:LEU:HD13	0.45	2.12	17	1
1:A:97:TYR:CD1	1:A:97:TYR:N	0.45	2.85	6	2
1:A:54:ASP:N	1:A:58:MET:O	0.45	2.50	16	2
1:A:112:PHE:CD1	1:A:121:LEU:CD2	0.44	3.00	20	2
1:A:71:LYS:HD2	1:A:78:TYR:CE1	0.44	2.47	12	1
1:A:109:PHE:CD2	1:A:122:ASN:HB2	0.44	2.47	1	1
1:A:68:CYS:HB3	1:A:83:PHE:CE1	0.44	2.47	8	2
1:A:68:CYS:HB3	1:A:83:PHE:CZ	0.44	2.48	8	2
1:A:84:ASP:O	1:A:88:GLY:HA2	0.44	2.11	5	2
1:A:78:TYR:CE2	1:A:139:LEU:HD11	0.44	2.47	10	1
1:A:112:PHE:CE2	1:A:119:VAL:HG21	0.44	2.46	19	1
1:A:51:TYR:CZ	1:A:61:LYS:HB3	0.44	2.47	7	4
1:A:2:LEU:HD12	1:A:109:PHE:CZ	0.44	2.47	6	1
1:A:78:TYR:CB	1:A:96:LEU:CD1	0.44	2.95	6	2
1:A:123:PHE:CE1	1:A:132:PHE:CD1	0.44	3.06	10	2
1:A:139:LEU:C	1:A:139:LEU:CD1	0.44	2.77	10	1
1:A:43:MET:SD	1:A:139:LEU:HD22	0.44	2.53	12	1
1:A:102:TYR:O	1:A:133:ARG:NH1	0.44	2.50	6	2
1:A:114:GLY:O	1:A:115:ASP:C	0.44	2.56	16	6
1:A:51:TYR:CE1	1:A:61:LYS:HG2	0.44	2.48	12	1
1:A:98:ASN:O	1:A:100:PHE:N	0.44	2.51	14	1
1:A:98:ASN:O	1:A:99:ASN:CB	0.44	2.66	19	1
1:A:82:ILE:HG22	1:A:91:LEU:HD23	0.44	1.88	14	1
1:A:48:VAL:HG11	1:A:123:PHE:CD2	0.44	2.47	11	2
1:A:69:LEU:CD1	1:A:80:LEU:CD2	0.44	2.94	17	1
1:A:51:TYR:CZ	1:A:61:LYS:HB2	0.44	2.48	1	4
1:A:2:LEU:HB3	1:A:3:PRO:CD	0.44	2.43	18	2
1:A:48:VAL:CG1	1:A:123:PHE:CD1	0.44	3.01	10	2
1:A:121:LEU:N	1:A:121:LEU:CD1	0.44	2.81	9	1
1:A:97:TYR:CZ	1:A:100:PHE:CD1	0.44	3.06	16	1
1:A:78:TYR:HB2	1:A:96:LEU:CD1	0.43	2.43	20	4
1:A:56:ASN:O	1:A:57:CYS:C	0.43	2.56	13	2
1:A:96:LEU:HD13	1:A:100:PHE:CD2	0.43	2.48	8	1
1:A:68:CYS:HB2	1:A:83:PHE:CE1	0.43	2.49	16	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:8:TYR:CE2	1:A:113:ALA:HB2	0.43	2.49	19	1
1:A:63:CYS:HB3	1:A:91:LEU:HD22	0.43	1.90	9	1
1:A:66:VAL:O	1:A:83:PHE:CE1	0.43	2.72	14	2
1:A:15:TYR:CZ	1:A:96:LEU:O	0.43	2.71	11	1
1:A:112:PHE:CD1	1:A:119:VAL:O	0.43	2.72	11	1
1:A:69:LEU:HD12	1:A:80:LEU:CD1	0.43	2.44	6	1
1:A:82:ILE:N	1:A:92:TRP:O	0.43	2.48	17	1
1:A:108:TYR:CE2	1:A:122:ASN:OD1	0.43	2.72	1	1
1:A:78:TYR:CZ	1:A:139:LEU:HD23	0.43	2.48	1	1
1:A:109:PHE:CZ	1:A:122:ASN:HB2	0.43	2.49	10	1
1:A:78:TYR:CZ	1:A:139:LEU:HB3	0.43	2.49	17	1
1:A:40:CYS:HB2	1:A:70:VAL:HG12	0.43	1.90	18	1
1:A:95:GLU:O	1:A:97:TYR:CD2	0.43	2.71	18	1
1:A:109:PHE:CD2	1:A:122:ASN:ND2	0.43	2.87	16	1
1:A:3:PRO:HG3	1:A:109:PHE:CG	0.43	2.48	7	1
1:A:43:MET:CE	1:A:135:ALA:CB	0.43	2.95	7	1
1:A:107:GLY:O	1:A:110:HIS:NE2	0.43	2.52	20	1
1:A:97:TYR:CE1	1:A:100:PHE:CD1	0.43	3.07	2	2
1:A:78:TYR:HB3	1:A:96:LEU:CD1	0.42	2.44	6	3
1:A:41:VAL:CG2	1:A:71:LYS:HG2	0.42	2.44	17	1
1:A:43:MET:HE3	1:A:69:LEU:HD21	0.42	1.91	20	1
1:A:54:ASP:O	1:A:58:MET:O	0.42	2.37	4	1
1:A:79:PHE:CE2	1:A:95:GLU:HG3	0.42	2.48	21	1
1:A:78:TYR:HE2	1:A:139:LEU:HD11	0.42	1.74	10	1
1:A:2:LEU:N	1:A:2:LEU:CD2	0.42	2.82	12	1
1:A:91:LEU:HD13	1:A:91:LEU:N	0.42	2.28	14	1
1:A:64:SER:O	1:A:91:LEU:CD1	0.42	2.67	17	2
1:A:97:TYR:CZ	1:A:100:PHE:CE1	0.42	3.07	2	1
1:A:127:GLU:O	1:A:131:LYS:CG	0.42	2.67	5	1
1:A:56:ASN:C	1:A:57:CYS:SG	0.42	2.97	6	2
1:A:112:PHE:CD1	1:A:112:PHE:C	0.42	2.92	6	1
1:A:84:ASP:CA	1:A:91:LEU:HD21	0.42	2.44	21	1
1:A:102:TYR:OH	1:A:121:LEU:CD1	0.42	2.64	21	1
1:A:68:CYS:HB2	1:A:83:PHE:CZ	0.42	2.49	16	2
1:A:81:ARG:HD3	1:A:90:LEU:HD11	0.42	1.91	3	1
1:A:48:VAL:HG11	1:A:123:PHE:CD1	0.42	2.50	4	1
1:A:56:ASN:O	1:A:57:CYS:SG	0.42	2.77	13	2
1:A:100:PHE:O	1:A:140:LEU:CD2	0.42	2.59	5	1
1:A:96:LEU:HD22	1:A:100:PHE:CG	0.42	2.49	10	1
1:A:122:ASN:ND2	1:A:123:PHE:O	0.42	2.53	12	1
1:A:109:PHE:CZ	1:A:120:ALA:HB1	0.42	2.49	18	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:43:MET:SD	1:A:139:LEU:CD1	0.42	3.08	1	2
1:A:78:TYR:CZ	1:A:139:LEU:CD2	0.42	3.02	1	1
1:A:97:TYR:O	1:A:98:ASN:O	0.42	2.38	5	2
1:A:113:ALA:O	1:A:114:GLY:O	0.42	2.37	16	1
1:A:80:LEU:C	1:A:81:ARG:CG	0.42	2.88	5	1
1:A:125:ASN:ND2	1:A:128:GLU:OE2	0.42	2.52	16	1
1:A:121:LEU:HD12	1:A:123:PHE:CZ	0.42	2.48	18	1
1:A:102:TYR:HB2	1:A:136:VAL:HG11	0.42	1.92	21	1
1:A:90:LEU:CD2	1:A:93:GLU:HB3	0.42	2.45	1	1
1:A:2:LEU:HB3	1:A:3:PRO:HD2	0.42	1.92	4	1
1:A:112:PHE:CD1	1:A:121:LEU:HD23	0.42	2.49	20	2
1:A:46:ALA:O	1:A:48:VAL:CG1	0.42	2.67	12	1
1:A:67:ALA:CB	1:A:82:ILE:HG13	0.42	2.43	12	2
1:A:40:CYS:HB2	1:A:70:VAL:CG1	0.42	2.45	17	1
1:A:8:TYR:CE1	1:A:113:ALA:CB	0.42	3.01	1	1
1:A:54:ASP:OD1	1:A:55:ARG:N	0.42	2.53	19	2
1:A:55:ARG:O	1:A:56:ASN:C	0.42	2.56	11	1
1:A:53:ALA:O	1:A:54:ASP:O	0.41	2.38	18	6
1:A:69:LEU:HD23	1:A:69:LEU:C	0.41	2.36	2	1
1:A:50:LEU:HD13	1:A:50:LEU:C	0.41	2.36	6	2
1:A:55:ARG:C	1:A:57:CYS:N	0.41	2.71	15	2
1:A:56:ASN:O	1:A:57:CYS:O	0.41	2.38	4	1
1:A:53:ALA:O	1:A:54:ASP:C	0.41	2.58	7	5
1:A:2:LEU:HD23	1:A:109:PHE:CZ	0.41	2.50	14	1
1:A:49:GLN:NE2	1:A:64:SER:OG	0.41	2.53	15	1
1:A:92:TRP:CZ2	1:A:94:GLN:CB	0.41	3.03	13	1
1:A:78:TYR:CD2	1:A:139:LEU:HD11	0.41	2.51	18	1
1:A:43:MET:HE2	1:A:139:LEU:HD22	0.41	1.92	5	1
1:A:47:VAL:C	1:A:48:VAL:CG1	0.41	2.89	6	1
1:A:114:GLY:O	1:A:117:CYS:O	0.41	2.38	4	1
1:A:109:PHE:CD1	1:A:122:ASN:HB3	0.41	2.50	19	1
1:A:81:ARG:HB2	1:A:90:LEU:HD11	0.41	1.92	3	1
1:A:8:TYR:CE2	1:A:114:GLY:O	0.41	2.74	5	1
1:A:72:ASP:CB	1:A:79:PHE:CE2	0.41	3.04	5	1
1:A:84:ASP:HB2	1:A:91:LEU:CD1	0.41	2.46	11	2
1:A:84:ASP:N	1:A:89:LYS:O	0.41	2.48	13	1
1:A:110:HIS:CD2	1:A:110:HIS:N	0.41	2.89	14	1
1:A:48:VAL:HG12	1:A:123:PHE:CD2	0.41	2.51	16	1
1:A:54:ASP:O	1:A:56:ASN:N	0.41	2.50	16	1
1:A:62:LYS:O	1:A:63:CYS:SG	0.41	2.79	10	1
1:A:49:GLN:O	1:A:122:ASN:OD1	0.41	2.39	11	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:109:PHE:CD1	1:A:121:LEU:O	0.41	2.74	11	1
1:A:95:GLU:O	1:A:96:LEU:O	0.40	2.39	16	2
1:A:96:LEU:CD2	1:A:100:PHE:CE1	0.40	3.04	11	1
1:A:6:GLU:O	1:A:118:GLN:OE1	0.40	2.39	20	1
1:A:81:ARG:CZ	1:A:93:GLU:HG3	0.40	2.46	20	1
1:A:133:ARG:CZ	1:A:137:THR:HG21	0.40	2.45	21	1
1:A:122:ASN:OD1	1:A:122:ASN:O	0.40	2.40	13	1
1:A:94:GLN:HG2	1:A:112:PHE:CZ	0.40	2.50	13	1
1:A:130:LYS:HG3	1:A:131:LYS:N	0.40	2.32	19	1
1:A:72:ASP:OD2	1:A:79:PHE:CE1	0.40	2.75	4	1
1:A:53:ALA:HB3	1:A:118:GLN:CB	0.40	2.47	11	1
1:A:112:PHE:O	1:A:119:VAL:O	0.40	2.39	12	1
1:A:112:PHE:CD1	1:A:112:PHE:N	0.40	2.89	20	1
1:A:41:VAL:CG1	1:A:71:LYS:HG3	0.40	2.46	3	1
1:A:127:GLU:O	1:A:131:LYS:N	0.40	2.50	5	1
1:A:109:PHE:HE1	1:A:120:ALA:HB1	0.40	1.76	16	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	111/152 (73%)	97±2 (87±2%)	10±2 (9±2%)	4±2 (4±2%)	5	32
All	All	2331/3192 (73%)	2030 (87%)	210 (9%)	91 (4%)	5	32

All 16 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	57	CYS	13
1	A	63	CYS	13
1	A	96	LEU	11
1	A	115	ASP	10
1	A	54	ASP	9
1	A	56	ASN	6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	55	ARG	4
1	A	98	ASN	4
1	A	59	TRP	4
1	A	77	SER	4
1	A	58	MET	4
1	A	53	ALA	3
1	A	100	PHE	2
1	A	108	TYR	2
1	A	45	SER	1
1	A	114	GLY	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	97/133 (73%)	68±3 (70±3%)	29±3 (30±3%)	1 16
All	All	2037/2793 (73%)	1427 (70%)	610 (30%)	1 16

All 72 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	83	PHE	21
1	A	102	TYR	21
1	A	106	ARG	20
1	A	121	LEU	20
1	A	61	LYS	19
1	A	48	VAL	18
1	A	131	LYS	18
1	A	133	ARG	18
1	A	50	LEU	17
1	A	132	PHE	17
1	A	140	LEU	17
1	A	71	LYS	16
1	A	134	LYS	16
1	A	63	CYS	15
1	A	62	LYS	15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	86	LYS	15
1	A	80	LEU	14
1	A	138	ASP	14
1	A	54	ASP	13
1	A	64	SER	13
1	A	90	LEU	12
1	A	69	LEU	12
1	A	94	GLN	11
1	A	55	ARG	11
1	A	72	ASP	11
1	A	43	MET	10
1	A	142	ARG	10
1	A	130	LYS	10
1	A	93	GLU	9
1	A	125	ASN	9
1	A	81	ARG	9
1	A	118	GLN	8
1	A	6	GLU	8
1	A	128	GLU	8
1	A	87	ASP	7
1	A	97	TYR	7
1	A	127	GLU	7
1	A	115	ASP	7
1	A	58	MET	6
1	A	99	ASN	6
1	A	60	SER	6
1	A	89	LYS	6
1	A	2	LEU	6
1	A	108	TYR	6
1	A	18	LYS	6
1	A	68	CYS	5
1	A	14	SER	5
1	A	44	SER	5
1	A	119	VAL	4
1	A	77	SER	4
1	A	117	CYS	4
1	A	98	ASN	3
1	A	103	ASN	3
1	A	56	ASN	3
1	A	109	PHE	3
1	A	17	SER	2
1	A	139	LEU	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	49	GLN	2
1	A	45	SER	2
1	A	126	GLU	2
1	A	41	VAL	2
1	A	95	GLU	2
1	A	91	LEU	2
1	A	8	TYR	2
1	A	40	CYS	1
1	A	116	THR	1
1	A	111	THR	1
1	A	122	ASN	1
1	A	70	VAL	1
1	A	15	TYR	1
1	A	85	ILE	1
1	A	84	ASP	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