Full wwPDB NMR Structure Validation Report (i)

Apr 21, 2024 – 03:13 PM EDT

PDB ID	:	2ELL
Title	:	Solution structure of the Leucine Rich Repeat of human Acidic leucine-rich nuclear phosphoprotein 32 family member B
Authors	:	Tochio, N.; Koshiba, S.; Watanabe, S.; Harada, T.; Umehara, T.; Tanaka, A.; Kigawa, T.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2007-03-27

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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

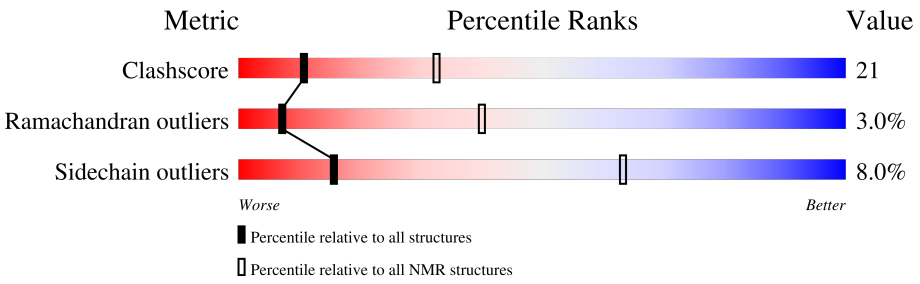
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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	168	

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 20 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:9-A:158 (150)	0.49	20

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 2 clusters and 5 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2668 atoms, of which 1350 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Acidic leucine-rich nuclear phosphoprotein 32 family member B.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	168	2668	827	1350	225	260	6	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP Q92688
A	2	SER	-	expression tag	UNP Q92688
A	3	SER	-	expression tag	UNP Q92688
A	4	GLY	-	expression tag	UNP Q92688
A	5	SER	-	expression tag	UNP Q92688
A	6	SER	-	expression tag	UNP Q92688
A	7	GLY	-	expression tag	UNP Q92688

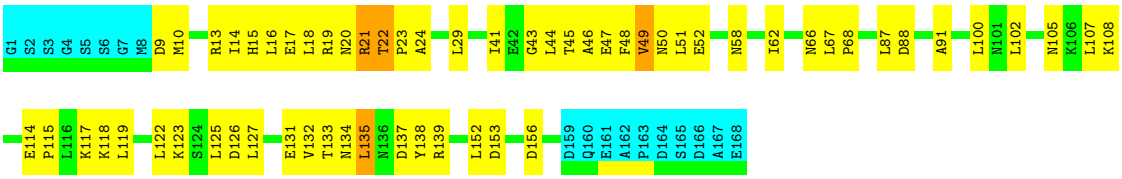
4 Residue-property plots (i)

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: Acidic leucine-rich nuclear phosphoprotein 32 family member B

Chain A: 54% 33% • 11%



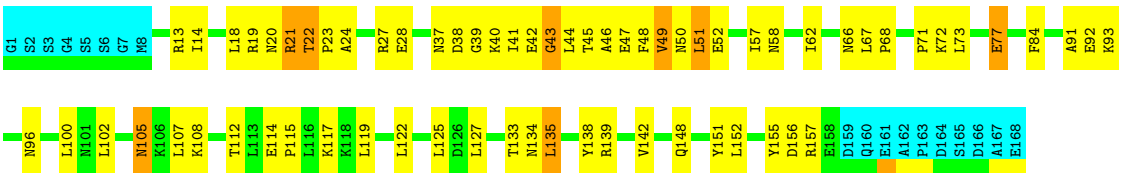
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Acidic leucine-rich nuclear phosphoprotein 32 family member B

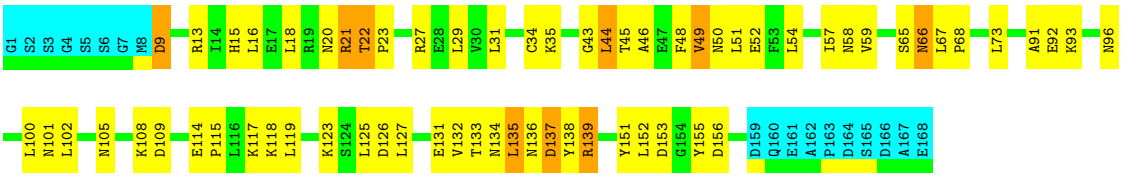
Chain A: 49% 35% 5% 11%



4.2.2 Score per residue for model 2

• Molecule 1: Acidic leucine-rich nuclear phosphoprotein 32 family member B

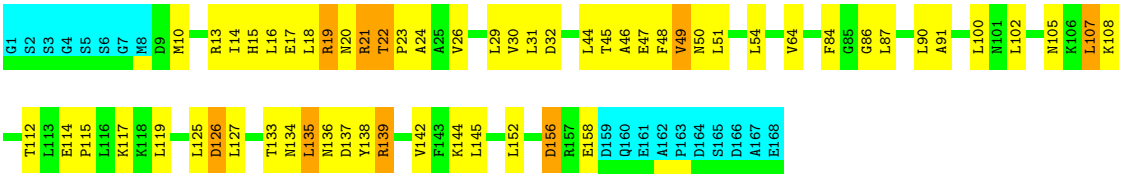
Chain A: 51% 33% 5% 11%



4.2.3 Score per residue for model 3

- Molecule 1: Acidic leucine-rich nuclear phosphoprotein 32 family member B

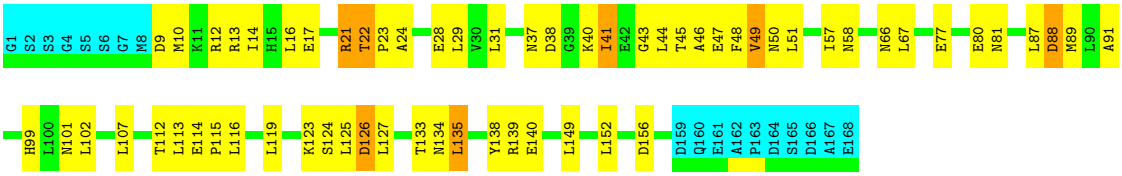
Chain A:



4.2.4 Score per residue for model 4

- Molecule 1: Acidic leucine-rich nuclear phosphoprotein 32 family member B

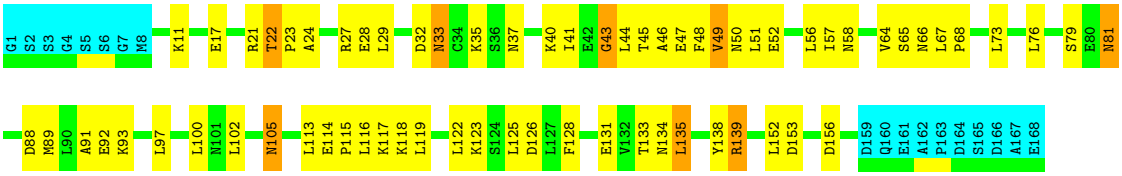
Chain A:



4.2.5 Score per residue for model 5

- Molecule 1: Acidic leucine-rich nuclear phosphoprotein 32 family member B

Chain A:



4.2.6 Score per residue for model 6

- Molecule 1: Acidic leucine-rich nuclear phosphoprotein 32 family member B

Chain A: 51% 35% • 11%

G1 S2 S3 G4 S5 S6 G7 M8 D9 M10 K11 I14 E17 L18 R19 N20 R21 T22 P23 A24 R27 E28 L29 V30 I41 E42 G43 L44 T45 A46 E47 F48 V49 N50 L51 E52 S55 V64 S65 N66 L67 P68 P71 K72 L73 L76 E77 L87 A91

L94 P95 N96 L97 T98 N105 K108 E114 P115 L116 K117 K118 L119 E120 C121 L122 K123 S124 L125 F128 E131 N134 L135 Y138 R139 L146 L149 T150 Y151 L152 D153 D156 D159 Q160 E161 A162 P163 D164 S165 D166 A167 E168

4.2.7 Score per residue for model 7

• Molecule 1: Acidic leucine-rich nuclear phosphoprotein 32 family member B

Chain A: 54% 30% 5% • 11%

G1 S2 S3 G4 S5 S6 G7 M8 K11 E17 R21 T22 P23 A24 R27 E28 L29 G39 K40 I41 E42 G43 L44 T45 A46 E47 F48 V49 N50 L51 E52 S55 L56 I57 N58 V59 I62 S63 V64 S65 N66 L67 P68 K69 L70 L73 K74 K75 L76 E77 L78 S79

E80 N81 R82 A91 N96 L97 T98 H99 L100 N105 K108 D109 I110 E114 P115 K118 L119 L122 L125 C130 T133 D137 Y138 R139 E140 S141 Y155 D159 Q160 E161 A162 P163 D164 S165 D166 A167 E168

4.2.8 Score per residue for model 8

• Molecule 1: Acidic leucine-rich nuclear phosphoprotein 32 family member B

Chain A: 49% 36% • 11%

G1 S2 S3 G4 S5 S6 G7 M8 R12 L16 E17 L18 R19 N20 R21 T22 P23 A24 L29 V30 L31 D38 G43 L44 T45 A46 E47 F48 V49 N50 L51 E52 L56 I62 S65 N66 L67 P68 K69 L70 L73 K74 K75 R82 I83 F84 L87 D88 M89

L90 A91 E92 K93 L94 H99 L102 N105 K106 L107 K108 E114 P115 L116 K117 K118 L119 L125 D126 L127 F128 E131 V132 T133 N134 L135 Y138 R139 L145 L152 D153 G154 Y155 D156 R157 E158 D159 Q160 E161 A162 P163 D164 S165 D166 A167 E168

4.2.9 Score per residue for model 9

• Molecule 1: Acidic leucine-rich nuclear phosphoprotein 32 family member B

Chain A: 53% 29% 7% 11%

G1 S2 S3 G4 S5 S6 G7 M8 D9 M10 R13 I14 E17 R21 T22 P23 A24 L29 N37 D38 I41 E42 G43 L44 T45 A46 E47 F48 V49 N50 L51 I57 N58 V64 L67 P68 L73 L76 E77 L78 S79 E80 N81 L87 D88 M89 L90 A91

E92 K93 L100 N101 N105 K108 E114 P115 L116 K117 K118 L119 L122 L125 E131 N134 L135 N136 D137 Y138 R139 V142 Y151 L152 Y155 D156 R157 E158 D159 Q160 E161 A162 P163 D164 S165 D166 A167 E168

4.2.10 Score per residue for model 10

• Molecule 1: Acidic leucine-rich nuclear phosphoprotein 32 family member B

Chain A: 53% 30% 5% • 11%

G1 S2 S3 G4 S5 S6 G7 M8 D9 M10 R13 I14 H15 L16 E17 L18 R21 T22 P23 R27 E28 L29 V30 N33 N37 D38 G39 K40 G43 L44 T45 A46 E47 F48 V49 N50 L51 S55 L56 I57 N58 I62 P68 K69 L70 E77 D88 M89 L90

A91 L97 L100 N105 K108 L113 E114 P115 L116 K117 K118 L119 L127 E131 V132 T133 N134 L135 N136 D137 Y138 R139 L145 Y151 L152 D153 D156 R157 E158 D159 Q160 E161 A162 P163 D164 S165 D166 A167 E168

4.2.11 Score per residue for model 11

• Molecule 1: Acidic leucine-rich nuclear phosphoprotein 32 family member B

Chain A: 45% 40% • 11%

G1 S2 S3 G4 S5 S6 G7 M8 D9 M10 K11 R12 R13 I14 H15 L16 E17 L18 R19 N20 R21 T22 P23 A24 E28 L29 V30 L31 D32 N33 I41 E42 G43 L44 T45 A46 E47 F48 V49 N50 L51 L54 I62 S65 N66 L67 L76 E77 R82 L87 D88

A91 E92 K93 T98 L102 L107 K108 D109 T112 L113 E114 P115 L116 K117 K118 L119 E120 C121 L122 L125 D126 L127 F128 V132 T133 N134 L135 N136 D137 Y138 R139 V142 L145 Q148 L149 T150 Y151 L152 D153 D156 D159 Q160 E161 A162 P163 D164 S165 D166 A167

E168

4.2.12 Score per residue for model 12

• Molecule 1: Acidic leucine-rich nuclear phosphoprotein 32 family member B

Chain A: 40% 42% 7% 11%

G1 S2 S3 G4 S5 S6 G7 M8 D9 M10 K11 R12 R13 I14 H15 L16 E17 L18 R19 N20 R21 T22 P23 A24 L29 V30 L31 D32 N33 I41 L44 T45 A46 E47 F48 V49 N50 L51 E52 S55 L56 I57 N58 V64 S65 N66 L67 P68 K75 S79 I83 F84

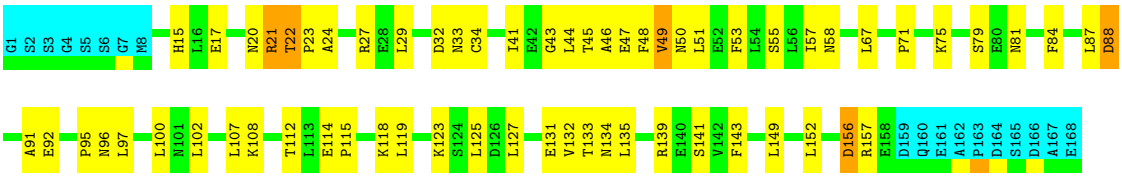
G85 G86 L87 D88 M89 L90 A91 L97 T98 H99 L100 N101 L102 N105 K106 L107 K108 T112 L113 E114 P115 L116 K117 K118 L119 K123 S124 L125 D126 L127 F128 N129 C130 E131 V132 T133 N134 L135 Y138 R139 E140 S141 V142 F143 K144 L145 L146 L149 T150 Y151 L152 D153 G154 Y155

D156 D159 Q160 E161 A162 P163 D164 S165 D166 A167 E168

4.2.13 Score per residue for model 13

• Molecule 1: Acidic leucine-rich nuclear phosphoprotein 32 family member B

Chain A: 52% 35% • 11%



4.2.14 Score per residue for model 14

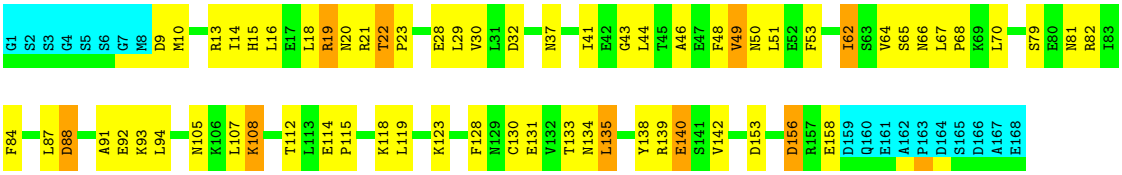
- Molecule 1: Acidic leucine-rich nuclear phosphoprotein 32 family member B

Chain A: 49% 36% 5% 11%

4.2.15 Score per residue for model 15

- Molecule 1: Acidic leucine-rich nuclear phosphoprotein 32 family member B

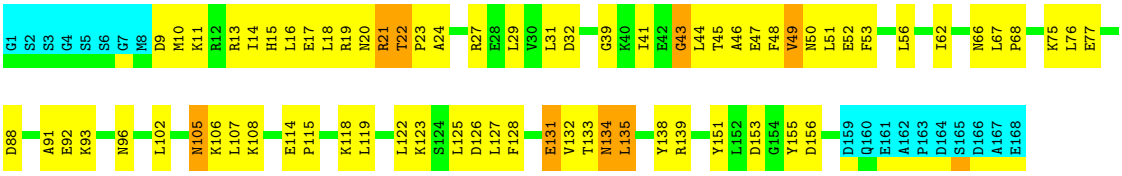
Chain A: 51% 33% 5% 11%



4.2.16 Score per residue for model 16

- Molecule 1: Acidic leucine-rich nuclear phosphoprotein 32 family member B

Chain A: 47% 38% 5% 11%



4.2.17 Score per residue for model 17

- Molecule 1: Acidic leucine-rich nuclear phosphoprotein 32 family member B

Chain A: 49% 34% 6% 11%

G1 S2 S3 G4 S5 S6 G7 M8 D9 M10 I14 E17 L18 R19 N20 R21 T22 P23 A24 E28 L29 V30 L31 K35 S36 N37 D38 G39 K40 I41 E42 G43 L44 T45 A46 E47 F48 V49 N50 L51 L54 L61 S65 N66 L67 P68 L73 L76 E77 L78 S79

E80 N81 R82 L87 L90 A91 L100 N101 L102 K108 E114 P115 L119 E120 C121 L122 K123 S124 L125 D126 C130 E131 V132 T133 N134 L135 Y138 R139 E140 S141 K144 Y151 L152 D156 R157 E158 D159 Q160 E161 A162 P163 D164 S165 D166 A167 E168

4.2.18 Score per residue for model 18

- Molecule 1: Acidic leucine-rich nuclear phosphoprotein 32 family member B

Chain A: 51% 35% • 11%

G1 S2 S3 G4 S5 S6 G7 M8 H15 L16 E17 L18 R19 N20 R21 T22 P23 A24 G39 K40 I41 E42 G43 L44 T45 A46 E47 F48 V49 N50 L51 E52 F53 L54 I62 L67 P68 L76 E77 L78 L87 D88 M89 L90 A91 E92 K93 T98 N101 L102 N105

K108 T112 L113 E114 P115 L116 K117 K118 L119 E120 C121 L122 K123 S124 L125 D126 L127 E131 V132 T133 N134 L135 Y138 R139 F143 L146 P147 Q148 L149 L152 D153 D156 R157 E158 D159 Q160 E161 A162 P163 D164 S165 D166 A167 E168

4.2.19 Score per residue for model 19

- Molecule 1: Acidic leucine-rich nuclear phosphoprotein 32 family member B

Chain A: 46% 36% 7% 11%

G1 S2 S3 G4 S5 S6 G7 M8 D9 M10 K11 I14 H15 L16 E17 L18 R19 N20 R21 T22 P23 A24 L29 D32 K35 S36 N37 D38 G39 K40 I41 E42 G43 L44 T45 A46 E47 F48 V49 N50 L51 E52 I62 S63 V64 S65 N66 L67 P68 L73 F84 D88

M89 L90 A91 L94 L97 T98 L102 L107 K108 T112 L113 E114 P115 L116 K117 K118 L119 E120 C121 L122 K123 S124 L125 C130 E131 V132 T133 N134 L135 N136 D137 Y138 R139 E140 K144 L145 L146 P147 Q148 L149 D159 Q160 E161 A162 P163 D164 S165 D166 A167 E168

4.2.20 Score per residue for model 20 (medoid)

- Molecule 1: Acidic leucine-rich nuclear phosphoprotein 32 family member B

Chain A: 52% 31% 6% • 11%

G1 S2 S3 G4 S5 S6 G7 M8 D9 M10 K11 H15 L16 E17 L18 R19 N20 R21 T22 P23 E28 L29 I41 E42 G43 L44 T45 A46 E47 F48 V49 N50 L51 I62 S65 N66 L67 P68 S79 E80 N81 F84 D88 A91 E92 K93 L97 L100 N101

L102 N105 K108 E114 P115 L116 K117 K118 L119 L122 L125 D126 L127 F128 N129 C130 E131 V132 T133 N134 L135 Y138 R139 V142 P147 Q148 L149 L152 D153 D156 R157 E158 D159 Q160 E161 A162 P163 D164 S165 D166 A167 E168

5 Refinement protocol and experimental data overview (i)

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the least restraint violations, target function*.

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

Software name	Classification	Version
CYANA	structure solution	2.0.17
CYANA	refinement	2.0.17

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	1200	1258	1256	51±9
All	All	24000	25160	25120	1020

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 21.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:132:VAL:HG23	1:A:135:LEU:HD12	0.94	1.38	19	10
1:A:46:ALA:O	1:A:49:VAL:HG13	0.90	1.67	16	20
1:A:31:LEU:HD12	1:A:54:LEU:HD11	0.88	1.46	2	3
1:A:17:GLU:OE2	1:A:29:LEU:HD21	0.87	1.68	16	1
1:A:44:LEU:HD23	1:A:68:PRO:CD	0.85	2.01	8	16
1:A:10:MET:SD	1:A:41:ILE:HG23	0.84	2.12	9	3
1:A:91:ALA:HA	1:A:119:LEU:HD21	0.83	1.48	19	20
1:A:14:ILE:O	1:A:18:LEU:HD23	0.79	1.77	10	3
1:A:30:VAL:HG12	1:A:55:SER:CB	0.78	2.09	12	3
1:A:44:LEU:HD23	1:A:68:PRO:HD2	0.77	1.55	8	14
1:A:114:GLU:HA	1:A:145:LEU:HD21	0.77	1.54	12	5
1:A:31:LEU:HD11	1:A:56:LEU:HD23	0.77	1.55	8	2
1:A:57:ILE:HG22	1:A:58:ASN:OD1	0.76	1.81	14	3
1:A:70:LEU:HD12	1:A:73:LEU:HD22	0.76	1.56	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:31:LEU:HD11	1:A:56:LEU:CD2	0.76	2.09	8	2
1:A:11:LYS:HA	1:A:14:ILE:HD12	0.75	1.57	19	1
1:A:30:VAL:HG12	1:A:55:SER:HB2	0.74	1.59	12	4
1:A:29:LEU:HD22	1:A:48:PHE:CE1	0.74	2.17	12	6
1:A:70:LEU:CD1	1:A:73:LEU:HD22	0.73	2.13	7	1
1:A:84:PHE:O	1:A:107:LEU:HD23	0.73	1.83	19	6
1:A:98:THR:HG22	1:A:121:CYS:O	0.72	1.84	19	4
1:A:102:LEU:HD12	1:A:125:LEU:HD11	0.72	1.62	2	12
1:A:34:CYS:O	1:A:59:VAL:HG12	0.70	1.86	2	1
1:A:87:LEU:HA	1:A:90:LEU:HD12	0.69	1.62	12	3
1:A:139:ARG:HD2	1:A:152:LEU:HD23	0.69	1.62	1	1
1:A:132:VAL:HG23	1:A:135:LEU:CD1	0.69	2.17	19	1
1:A:73:LEU:HD21	1:A:76:LEU:HD13	0.68	1.66	17	3
1:A:17:GLU:HG3	1:A:29:LEU:HD11	0.67	1.65	12	6
1:A:87:LEU:HD13	1:A:116:LEU:HD11	0.67	1.65	12	3
1:A:132:VAL:CG2	1:A:135:LEU:HD12	0.66	2.19	19	1
1:A:22:THR:HG22	1:A:23:PRO:HD2	0.66	1.65	19	18
1:A:100:LEU:O	1:A:125:LEU:HD12	0.66	1.89	2	4
1:A:57:ILE:O	1:A:59:VAL:HG13	0.65	1.90	7	1
1:A:52:GLU:C	1:A:73:LEU:HD12	0.65	2.12	19	6
1:A:149:LEU:CD2	1:A:152:LEU:HD13	0.64	2.22	12	2
1:A:13:ARG:HD2	1:A:16:LEU:HD12	0.63	1.69	2	2
1:A:142:VAL:HG11	1:A:152:LEU:HD13	0.63	1.70	9	2
1:A:78:LEU:HD12	1:A:100:LEU:HD11	0.63	1.70	9	2
1:A:14:ILE:O	1:A:18:LEU:HD13	0.62	1.94	16	3
1:A:57:ILE:HD11	1:A:77:GLU:OE1	0.62	1.93	1	1
1:A:87:LEU:HD12	1:A:112:THR:O	0.62	1.94	4	6
1:A:138:TYR:CG	1:A:139:ARG:N	0.62	2.68	4	15
1:A:17:GLU:CD	1:A:29:LEU:HD11	0.62	2.15	7	2
1:A:150:THR:HG22	1:A:156:ASP:OD2	0.62	1.93	12	1
1:A:102:LEU:CD1	1:A:125:LEU:HD11	0.61	2.25	5	6
1:A:114:GLU:N	1:A:115:PRO:HD2	0.61	2.11	17	20
1:A:107:LEU:HD22	1:A:112:THR:HB	0.61	1.72	11	6
1:A:122:LEU:HD21	1:A:125:LEU:HD13	0.61	1.71	7	3
1:A:139:ARG:HA	1:A:152:LEU:HD21	0.61	1.73	5	4
1:A:100:LEU:HD23	1:A:125:LEU:HD11	0.60	1.72	17	1
1:A:128:PHE:CZ	1:A:153:ASP:OD1	0.60	2.55	6	2
1:A:54:LEU:HD23	1:A:76:LEU:CD1	0.59	2.28	11	2
1:A:128:PHE:CE1	1:A:153:ASP:OD1	0.59	2.55	5	2
1:A:39:GLY:HA3	1:A:62:ILE:HD12	0.58	1.76	10	7
1:A:56:LEU:HD12	1:A:76:LEU:HD11	0.58	1.76	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:13:ARG:HA	1:A:16:LEU:HD13	0.57	1.76	10	1
1:A:75:LYS:NZ	1:A:99:HIS:CD2	0.57	2.73	7	1
1:A:84:PHE:O	1:A:112:THR:HG21	0.57	1.98	3	2
1:A:128:PHE:CE1	1:A:153:ASP:CG	0.57	2.78	5	2
1:A:78:LEU:HD12	1:A:100:LEU:CD1	0.57	2.30	9	1
1:A:149:LEU:HD21	1:A:152:LEU:HD13	0.56	1.77	12	4
1:A:62:ILE:HG22	1:A:84:PHE:CE2	0.56	2.35	8	1
1:A:125:LEU:HB2	1:A:149:LEU:HD11	0.56	1.77	14	1
1:A:139:ARG:HD3	1:A:152:LEU:HD23	0.56	1.78	20	1
1:A:105:ASN:HD22	1:A:105:ASN:N	0.56	1.97	5	7
1:A:17:GLU:OE1	1:A:29:LEU:HD13	0.56	2.01	6	1
1:A:41:ILE:CD1	1:A:67:LEU:CD2	0.56	2.84	12	7
1:A:41:ILE:CD1	1:A:67:LEU:HD23	0.55	2.32	7	7
1:A:97:LEU:HD21	1:A:100:LEU:HD22	0.55	1.77	5	3
1:A:17:GLU:CB	1:A:29:LEU:HD11	0.54	2.31	20	4
1:A:18:LEU:HD11	1:A:23:PRO:HD3	0.54	1.78	10	3
1:A:49:VAL:HG23	1:A:50:ASN:H	0.54	1.62	3	2
1:A:64:VAL:HB	1:A:67:LEU:HD12	0.54	1.79	9	3
1:A:57:ILE:HG22	1:A:58:ASN:CG	0.54	2.23	14	2
1:A:48:PHE:CD1	1:A:51:LEU:HD22	0.54	2.37	12	6
1:A:117:LYS:HB3	1:A:146:LEU:HD23	0.54	1.79	12	2
1:A:15:HIS:CD2	1:A:15:HIS:C	0.53	2.81	19	10
1:A:24:ALA:HB1	1:A:50:ASN:HD22	0.53	1.63	8	2
1:A:17:GLU:CG	1:A:29:LEU:HD11	0.53	2.33	9	5
1:A:44:LEU:HD12	1:A:48:PHE:CE2	0.53	2.39	15	7
1:A:45:THR:HG23	1:A:47:GLU:HB2	0.53	1.81	17	13
1:A:125:LEU:CD2	1:A:142:VAL:HG11	0.53	2.34	14	1
1:A:133:THR:O	1:A:138:TYR:CD2	0.53	2.62	1	2
1:A:148:GLN:OE1	1:A:149:LEU:N	0.53	2.42	18	4
1:A:48:PHE:O	1:A:51:LEU:N	0.52	2.42	12	20
1:A:108:LYS:CG	1:A:108:LYS:O	0.52	2.55	11	5
1:A:57:ILE:HG22	1:A:58:ASN:N	0.52	2.20	2	3
1:A:128:PHE:CZ	1:A:153:ASP:O	0.52	2.62	12	1
1:A:44:LEU:HD12	1:A:48:PHE:HE2	0.52	1.64	3	1
1:A:130:CYS:O	1:A:133:THR:HG23	0.52	2.05	15	5
1:A:24:ALA:HB1	1:A:50:ASN:ND2	0.52	2.20	18	3
1:A:91:ALA:O	1:A:119:LEU:HD21	0.52	2.05	6	6
1:A:70:LEU:O	1:A:94:LEU:HD23	0.52	2.05	8	2
1:A:149:LEU:HD21	1:A:152:LEU:CD1	0.52	2.34	12	1
1:A:62:ILE:HG23	1:A:82:ARG:O	0.52	2.05	8	3
1:A:29:LEU:HB3	1:A:51:LEU:HD21	0.51	1.82	2	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:57:ILE:HG23	1:A:79:SER:HB3	0.51	1.81	12	2
1:A:31:LEU:CD1	1:A:56:LEU:HD23	0.51	2.30	8	1
1:A:30:VAL:HG12	1:A:55:SER:HB3	0.51	1.81	12	1
1:A:108:LYS:CD	1:A:108:LYS:O	0.51	2.59	19	1
1:A:107:LEU:HD12	1:A:127:LEU:CD2	0.51	2.34	14	2
1:A:148:GLN:OE1	1:A:148:GLN:C	0.51	2.49	19	4
1:A:48:PHE:O	1:A:49:VAL:C	0.51	2.49	12	20
1:A:11:LYS:CE	1:A:11:LYS:O	0.51	2.59	7	1
1:A:29:LEU:HD22	1:A:48:PHE:CZ	0.51	2.41	12	1
1:A:143:PHE:CE1	1:A:157:ARG:HG2	0.51	2.41	13	1
1:A:91:ALA:CA	1:A:119:LEU:HD21	0.51	2.34	7	4
1:A:48:PHE:O	1:A:50:ASN:N	0.50	2.44	20	11
1:A:127:LEU:O	1:A:133:THR:CG2	0.50	2.60	1	12
1:A:18:LEU:O	1:A:20:ASN:N	0.50	2.45	19	13
1:A:114:GLU:N	1:A:115:PRO:CD	0.50	2.74	17	20
1:A:114:GLU:O	1:A:117:LYS:CD	0.50	2.60	14	7
1:A:13:ARG:O	1:A:16:LEU:N	0.50	2.45	10	8
1:A:57:ILE:O	1:A:58:ASN:ND2	0.50	2.45	12	2
1:A:57:ILE:HD11	1:A:77:GLU:C	0.50	2.27	4	1
1:A:17:GLU:OE2	1:A:29:LEU:HD12	0.50	2.06	8	1
1:A:18:LEU:HD11	1:A:23:PRO:CD	0.50	2.37	10	3
1:A:71:PRO:O	1:A:96:ASN:ND2	0.50	2.45	1	3
1:A:29:LEU:CD2	1:A:48:PHE:CZ	0.50	2.94	12	2
1:A:29:LEU:HD23	1:A:31:LEU:HD11	0.50	1.83	11	1
1:A:24:ALA:O	1:A:50:ASN:ND2	0.50	2.45	12	6
1:A:131:GLU:O	1:A:134:ASN:ND2	0.50	2.45	5	7
1:A:57:ILE:HG23	1:A:79:SER:HB2	0.49	1.83	5	1
1:A:88:ASP:CG	1:A:89:MET:N	0.49	2.66	10	2
1:A:79:SER:O	1:A:81:ASN:ND2	0.49	2.45	15	3
1:A:117:LYS:HA	1:A:146:LEU:HD22	0.49	1.84	19	1
1:A:44:LEU:HD23	1:A:68:PRO:CG	0.49	2.37	8	2
1:A:79:SER:N	1:A:81:ASN:OD1	0.49	2.45	5	5
1:A:31:LEU:HD23	1:A:31:LEU:H	0.49	1.67	8	1
1:A:10:MET:HG2	1:A:14:ILE:HD11	0.49	1.84	3	5
1:A:74:LYS:NZ	1:A:98:THR:HG21	0.49	2.22	7	1
1:A:142:VAL:HG11	1:A:152:LEU:CD1	0.49	2.36	9	1
1:A:134:ASN:OD1	1:A:135:LEU:N	0.49	2.45	12	2
1:A:64:VAL:HG23	1:A:89:MET:SD	0.49	2.48	5	1
1:A:125:LEU:CB	1:A:149:LEU:HD11	0.49	2.38	14	2
1:A:88:ASP:OD1	1:A:89:MET:N	0.49	2.46	8	2
1:A:117:LYS:CG	1:A:146:LEU:HD23	0.49	2.37	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:117:LYS:CA	1:A:146:LEU:CD2	0.48	2.91	19	1
1:A:132:VAL:O	1:A:135:LEU:N	0.48	2.45	19	1
1:A:138:TYR:CD2	1:A:139:ARG:HD3	0.48	2.43	5	1
1:A:139:ARG:HG2	1:A:152:LEU:HD23	0.48	1.85	17	1
1:A:132:VAL:O	1:A:138:TYR:CB	0.48	2.62	20	1
1:A:64:VAL:HG21	1:A:86:GLY:O	0.48	2.09	3	1
1:A:110:ILE:HD11	1:A:141:SER:OG	0.48	2.08	7	1
1:A:37:ASN:O	1:A:40:LYS:N	0.48	2.46	4	4
1:A:41:ILE:HD13	1:A:67:LEU:HD23	0.48	1.84	18	3
1:A:83:ILE:HD12	1:A:105:ASN:OD1	0.48	2.08	14	1
1:A:139:ARG:CD	1:A:153:ASP:OD2	0.48	2.61	18	1
1:A:65:SER:O	1:A:67:LEU:N	0.48	2.46	7	4
1:A:138:TYR:CE1	1:A:139:ARG:HD2	0.48	2.44	9	1
1:A:40:LYS:O	1:A:41:ILE:C	0.48	2.53	17	1
1:A:140:GLU:N	1:A:140:GLU:CD	0.47	2.67	15	1
1:A:84:PHE:O	1:A:112:THR:CG2	0.47	2.62	3	1
1:A:74:LYS:HZ2	1:A:98:THR:HG21	0.47	1.68	7	1
1:A:88:ASP:O	1:A:91:ALA:HB3	0.47	2.09	11	1
1:A:87:LEU:HB3	1:A:116:LEU:HD21	0.47	1.85	11	1
1:A:50:ASN:O	1:A:51:LEU:C	0.47	2.52	12	20
1:A:57:ILE:CG2	1:A:58:ASN:N	0.47	2.78	2	2
1:A:156:ASP:OD1	1:A:158:GLU:N	0.47	2.47	9	6
1:A:94:LEU:HD13	1:A:97:LEU:HD13	0.47	1.85	19	2
1:A:128:PHE:CZ	1:A:153:ASP:HB2	0.47	2.45	11	1
1:A:123:LYS:HG3	1:A:124:SER:N	0.47	2.24	6	3
1:A:151:TYR:CE1	1:A:156:ASP:HB3	0.46	2.45	1	6
1:A:12:ARG:O	1:A:16:LEU:HD13	0.46	2.10	8	1
1:A:77:GLU:N	1:A:77:GLU:OE1	0.46	2.48	11	2
1:A:138:TYR:CE1	1:A:139:ARG:HG3	0.46	2.45	18	2
1:A:39:GLY:HA2	1:A:61:LEU:HD12	0.46	1.86	17	1
1:A:136:ASN:C	1:A:137:ASP:CG	0.46	2.73	9	2
1:A:128:PHE:CE1	1:A:153:ASP:HA	0.46	2.44	15	2
1:A:78:LEU:CD1	1:A:100:LEU:HD11	0.46	2.37	9	1
1:A:88:ASP:OD1	1:A:88:ASP:N	0.46	2.49	20	2
1:A:134:ASN:O	1:A:135:LEU:C	0.46	2.54	17	18
1:A:57:ILE:O	1:A:58:ASN:CG	0.46	2.54	9	5
1:A:64:VAL:O	1:A:65:SER:C	0.46	2.53	15	1
1:A:21:ARG:O	1:A:22:THR:C	0.46	2.54	10	16
1:A:41:ILE:HD11	1:A:67:LEU:CD2	0.46	2.41	4	1
1:A:134:ASN:OD1	1:A:134:ASN:C	0.46	2.54	16	7
1:A:79:SER:O	1:A:81:ASN:CG	0.46	2.53	17	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:32:ASP:C	1:A:33:ASN:CG	0.46	2.74	5	1
1:A:150:THR:HG22	1:A:156:ASP:OD1	0.46	2.10	11	1
1:A:24:ALA:O	1:A:50:ASN:CG	0.46	2.55	5	10
1:A:65:SER:O	1:A:66:ASN:C	0.46	2.55	8	9
1:A:138:TYR:O	1:A:142:VAL:HG23	0.45	2.10	15	3
1:A:138:TYR:O	1:A:139:ARG:C	0.45	2.54	19	2
1:A:87:LEU:HD22	1:A:90:LEU:HD12	0.45	1.88	17	1
1:A:136:ASN:O	1:A:137:ASP:C	0.45	2.55	10	5
1:A:136:ASN:O	1:A:137:ASP:CG	0.45	2.55	9	2
1:A:17:GLU:CB	1:A:29:LEU:CD1	0.45	2.95	14	1
1:A:108:LYS:CB	1:A:131:GLU:HB3	0.45	2.42	15	3
1:A:32:ASP:OD1	1:A:57:ILE:N	0.45	2.49	13	1
1:A:29:LEU:CD2	1:A:31:LEU:HD11	0.45	2.42	4	1
1:A:17:GLU:O	1:A:20:ASN:CG	0.45	2.55	13	1
1:A:108:LYS:CB	1:A:131:GLU:HB2	0.45	2.42	6	5
1:A:43:GLY:O	1:A:44:LEU:C	0.45	2.55	13	14
1:A:156:ASP:OD1	1:A:156:ASP:C	0.45	2.55	14	9
1:A:121:CYS:O	1:A:122:LEU:C	0.45	2.55	17	1
1:A:101:ASN:CG	1:A:126:ASP:OD1	0.45	2.55	2	1
1:A:12:ARG:O	1:A:16:LEU:CD1	0.45	2.65	4	1
1:A:58:ASN:OD1	1:A:80:GLU:CD	0.45	2.55	4	1
1:A:72:LYS:O	1:A:73:LEU:C	0.45	2.56	6	2
1:A:101:ASN:CG	1:A:126:ASP:OD2	0.45	2.55	4	1
1:A:49:VAL:HA	1:A:70:LEU:HD23	0.45	1.88	10	1
1:A:100:LEU:HD23	1:A:125:LEU:CD1	0.45	2.41	17	1
1:A:152:LEU:O	1:A:153:ASP:CG	0.45	2.55	18	3
1:A:117:LYS:CB	1:A:146:LEU:HD23	0.45	2.41	19	1
1:A:66:ASN:O	1:A:67:LEU:C	0.44	2.56	16	9
1:A:118:LYS:N	1:A:118:LYS:CD	0.44	2.79	20	1
1:A:97:LEU:HD21	1:A:100:LEU:HD13	0.44	1.88	12	1
1:A:18:LEU:C	1:A:20:ASN:N	0.44	2.71	18	9
1:A:30:VAL:CG1	1:A:32:ASP:OD1	0.44	2.65	3	1
1:A:87:LEU:CD1	1:A:116:LEU:HD11	0.44	2.42	6	1
1:A:73:LEU:CD2	1:A:76:LEU:HD13	0.44	2.41	17	1
1:A:88:ASP:OD1	1:A:88:ASP:C	0.44	2.55	8	2
1:A:140:GLU:O	1:A:142:VAL:N	0.44	2.51	12	1
1:A:132:VAL:O	1:A:134:ASN:N	0.44	2.51	19	1
1:A:108:LYS:O	1:A:109:ASP:CG	0.44	2.55	2	3
1:A:32:ASP:OD2	1:A:33:ASN:ND2	0.44	2.50	14	2
1:A:64:VAL:CG2	1:A:89:MET:SD	0.44	3.06	5	1
1:A:41:ILE:HD12	1:A:67:LEU:CD2	0.44	2.42	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:126:ASP:C	1:A:126:ASP:OD1	0.44	2.55	17	1
1:A:64:VAL:HG23	1:A:89:MET:CG	0.44	2.42	5	2
1:A:139:ARG:CD	1:A:152:LEU:HD23	0.44	2.43	13	1
1:A:77:GLU:C	1:A:77:GLU:OE1	0.44	2.55	14	1
1:A:32:ASP:C	1:A:32:ASP:OD1	0.44	2.56	16	2
1:A:138:TYR:CD1	1:A:139:ARG:HD2	0.44	2.46	9	1
1:A:102:LEU:O	1:A:127:LEU:HD23	0.44	2.13	14	1
1:A:15:HIS:O	1:A:17:GLU:N	0.44	2.51	18	1
1:A:150:THR:O	1:A:156:ASP:CG	0.44	2.56	12	1
1:A:102:LEU:C	1:A:126:ASP:O	0.44	2.56	16	1
1:A:147:PRO:O	1:A:149:LEU:N	0.44	2.51	20	2
1:A:102:LEU:N	1:A:126:ASP:O	0.43	2.51	17	5
1:A:57:ILE:O	1:A:58:ASN:C	0.43	2.57	7	1
1:A:32:ASP:OD1	1:A:55:SER:C	0.43	2.56	13	1
1:A:62:ILE:HG22	1:A:84:PHE:CD2	0.43	2.48	8	1
1:A:143:PHE:CD1	1:A:149:LEU:HD23	0.43	2.48	18	1
1:A:57:ILE:HD11	1:A:77:GLU:CD	0.43	2.33	1	1
1:A:17:GLU:OE2	1:A:29:LEU:CD2	0.43	2.66	6	1
1:A:9:ASP:O	1:A:10:MET:C	0.43	2.56	10	6
1:A:49:VAL:HG23	1:A:50:ASN:N	0.43	2.28	3	2
1:A:117:LYS:HB3	1:A:146:LEU:CD2	0.43	2.42	6	3
1:A:62:ILE:CG2	1:A:84:PHE:CZ	0.43	3.01	20	1
1:A:102:LEU:CA	1:A:105:ASN:OD1	0.43	2.66	1	2
1:A:48:PHE:O	1:A:51:LEU:CB	0.43	2.67	12	1
1:A:102:LEU:HD22	1:A:107:LEU:HD11	0.43	1.91	12	1
1:A:14:ILE:O	1:A:18:LEU:CD2	0.43	2.63	14	1
1:A:96:ASN:O	1:A:96:ASN:CG	0.43	2.57	14	1
1:A:14:ILE:O	1:A:17:GLU:CG	0.43	2.67	6	1
1:A:91:ALA:HA	1:A:119:LEU:HD11	0.43	1.90	13	2
1:A:125:LEU:HB3	1:A:149:LEU:HD11	0.43	1.91	6	1
1:A:140:GLU:C	1:A:142:VAL:N	0.43	2.72	12	1
1:A:11:LYS:CA	1:A:14:ILE:HD12	0.43	2.37	19	1
1:A:32:ASP:O	1:A:33:ASN:CG	0.43	2.57	5	2
1:A:143:PHE:CE1	1:A:157:ARG:CG	0.43	3.02	13	1
1:A:102:LEU:HB3	1:A:127:LEU:HD23	0.43	1.91	3	1
1:A:75:LYS:HD3	1:A:99:HIS:CB	0.43	2.44	8	2
1:A:138:TYR:OH	1:A:153:ASP:CB	0.43	2.67	12	1
1:A:144:LYS:HG3	1:A:145:LEU:N	0.42	2.29	3	1
1:A:113:LEU:HA	1:A:116:LEU:HD12	0.42	1.91	10	1
1:A:117:LYS:HA	1:A:146:LEU:CD2	0.42	2.44	19	1
1:A:130:CYS:O	1:A:131:GLU:C	0.42	2.57	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:88:ASP:O	1:A:91:ALA:N	0.42	2.51	5	1
1:A:113:LEU:HB3	1:A:116:LEU:HD12	0.42	1.90	5	1
1:A:17:GLU:CD	1:A:29:LEU:CD1	0.42	2.85	7	1
1:A:22:THR:CG2	1:A:23:PRO:HD2	0.42	2.42	6	9
1:A:95:PRO:HA	1:A:119:LEU:CD2	0.42	2.44	6	2
1:A:92:GLU:HG3	1:A:93:LYS:N	0.42	2.30	15	8
1:A:101:ASN:CB	1:A:126:ASP:OD1	0.42	2.67	4	1
1:A:142:VAL:O	1:A:145:LEU:N	0.42	2.51	12	1
1:A:138:TYR:CZ	1:A:139:ARG:HG3	0.42	2.48	15	1
1:A:107:LEU:HD13	1:A:127:LEU:CD2	0.42	2.44	16	1
1:A:27:ARG:HD2	1:A:27:ARG:N	0.42	2.29	14	2
1:A:83:ILE:HG21	1:A:87:LEU:HD21	0.42	1.90	8	1
1:A:83:ILE:O	1:A:106:LYS:N	0.42	2.50	12	1
1:A:147:PRO:C	1:A:149:LEU:N	0.42	2.72	20	2
1:A:102:LEU:C	1:A:105:ASN:OD1	0.42	2.57	8	1
1:A:122:LEU:O	1:A:148:GLN:OE1	0.42	2.38	11	4
1:A:30:VAL:CG1	1:A:55:SER:HB3	0.42	2.44	12	1
1:A:119:LEU:O	1:A:148:GLN:NE2	0.42	2.52	1	1
1:A:26:VAL:O	1:A:51:LEU:HD12	0.42	2.14	3	1
1:A:37:ASN:O	1:A:38:ASP:C	0.42	2.58	9	1
1:A:14:ILE:CD1	1:A:44:LEU:N	0.42	2.82	10	2
1:A:107:LEU:CD1	1:A:127:LEU:CD2	0.42	2.97	16	1
1:A:13:ARG:O	1:A:14:ILE:C	0.42	2.58	10	6
1:A:74:LYS:O	1:A:97:LEU:HD12	0.42	2.14	7	1
1:A:10:MET:O	1:A:11:LYS:C	0.42	2.57	6	1
1:A:30:VAL:CG1	1:A:55:SER:CB	0.42	2.92	12	1
1:A:42:GLU:O	1:A:42:GLU:CD	0.41	2.58	1	1
1:A:24:ALA:O	1:A:50:ASN:CB	0.41	2.68	18	2
1:A:24:ALA:C	1:A:50:ASN:ND2	0.41	2.74	12	1
1:A:53:PHE:CD1	1:A:75:LYS:HE3	0.41	2.50	13	2
1:A:15:HIS:O	1:A:18:LEU:N	0.41	2.53	14	1
1:A:49:VAL:HG23	1:A:50:ASN:HD22	0.41	1.75	19	1
1:A:17:GLU:CD	1:A:29:LEU:HD13	0.41	2.35	6	1
1:A:74:LYS:HZ2	1:A:98:THR:CG2	0.41	2.26	7	1
1:A:144:LYS:HG2	1:A:145:LEU:N	0.41	2.30	12	1
1:A:97:LEU:HD21	1:A:100:LEU:HB2	0.41	1.92	13	1
1:A:64:VAL:O	1:A:64:VAL:HG23	0.41	2.15	7	1
1:A:75:LYS:CE	1:A:77:GLU:OE2	0.41	2.68	7	1
1:A:38:ASP:O	1:A:38:ASP:CG	0.41	2.58	4	1
1:A:15:HIS:C	1:A:17:GLU:N	0.41	2.73	18	1
1:A:102:LEU:HD12	1:A:125:LEU:HD21	0.41	1.93	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:125:LEU:HD23	1:A:152:LEU:CD1	0.41	2.46	14	1
1:A:92:GLU:CG	1:A:93:LYS:N	0.41	2.83	2	3
1:A:17:GLU:HG2	1:A:29:LEU:HD11	0.41	1.92	10	1
1:A:138:TYR:CZ	1:A:139:ARG:HG2	0.41	2.51	14	1
1:A:151:TYR:CE1	1:A:156:ASP:HB2	0.41	2.51	2	1
1:A:75:LYS:HZ3	1:A:99:HIS:CD2	0.41	2.34	7	1
1:A:136:ASN:O	1:A:138:TYR:N	0.41	2.54	10	1
1:A:88:ASP:C	1:A:90:LEU:N	0.41	2.74	12	1
1:A:141:SER:HA	1:A:144:LYS:CD	0.41	2.46	12	1
1:A:105:ASN:N	1:A:105:ASN:ND2	0.41	2.67	5	1
1:A:125:LEU:HG	1:A:126:ASP:N	0.41	2.31	2	1
1:A:31:LEU:CD1	1:A:44:LEU:CD1	0.41	2.99	3	1
1:A:48:PHE:C	1:A:50:ASN:N	0.41	2.74	8	2
1:A:123:LYS:CD	1:A:123:LYS:C	0.41	2.89	12	1
1:A:108:LYS:O	1:A:108:LYS:CG	0.41	2.68	13	1
1:A:138:TYR:CE2	1:A:139:ARG:HD3	0.41	2.51	5	1
1:A:57:ILE:HG22	1:A:58:ASN:H	0.40	1.76	7	1
1:A:50:ASN:O	1:A:52:GLU:OE1	0.40	2.39	8	1
1:A:30:VAL:CG1	1:A:53:PHE:CE2	0.40	3.04	15	1
1:A:37:ASN:OD1	1:A:40:LYS:O	0.40	2.40	17	1
1:A:123:LYS:O	1:A:150:THR:N	0.40	2.53	6	1
1:A:132:VAL:C	1:A:134:ASN:N	0.40	2.73	19	1
1:A:78:LEU:O	1:A:101:ASN:O	0.40	2.39	9	2
1:A:13:ARG:O	1:A:15:HIS:N	0.40	2.54	10	1
1:A:27:ARG:N	1:A:27:ARG:HD3	0.40	2.32	7	1
1:A:118:LYS:N	1:A:118:LYS:HD2	0.40	2.30	7	1
1:A:88:ASP:CG	1:A:92:GLU:OE2	0.40	2.60	13	1
1:A:18:LEU:O	1:A:19:ARG:C	0.40	2.59	15	1
1:A:89:MET:O	1:A:93:LYS:CG	0.40	2.69	18	1
1:A:58:ASN:O	1:A:58:ASN:OD1	0.40	2.40	5	1
1:A:128:PHE:CE1	1:A:153:ASP:OD2	0.40	2.75	5	1
1:A:142:VAL:HG11	1:A:152:LEU:HD11	0.40	1.92	11	1
1:A:88:ASP:OD1	1:A:92:GLU:OE2	0.40	2.40	13	1
1:A:27:ARG:N	1:A:27:ARG:CD	0.40	2.85	14	1
1:A:84:PHE:CD1	1:A:84:PHE:N	0.40	2.90	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	150/168 (89%)	123±3 (82±2%)	22±3 (15±2%)	4±2 (3±1%)	7 40
All	All	3000/3360 (89%)	2461 (82%)	449 (15%)	90 (3%)	7 40

All 25 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	49	VAL	19
1	A	135	LEU	13
1	A	43	GLY	11
1	A	19	ARG	10
1	A	41	ILE	9
1	A	66	ASN	4
1	A	122	LEU	3
1	A	51	LEU	2
1	A	137	ASP	2
1	A	37	ASN	2
1	A	105	ASN	1
1	A	9	ASP	1
1	A	44	LEU	1
1	A	107	LEU	1
1	A	58	ASN	1
1	A	38	ASP	1
1	A	136	ASN	1
1	A	14	ILE	1
1	A	22	THR	1
1	A	85	GLY	1
1	A	141	SER	1
1	A	73	LEU	1
1	A	16	LEU	1
1	A	133	THR	1
1	A	148	GLN	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	139/152 (91%)	128±2 (92±2%)	11±2 (8±2%)	16	63
All	All	2780/3040 (91%)	2558 (92%)	222 (8%)	16	63

All 51 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	21	ARG	20
1	A	22	THR	20
1	A	88	ASP	13
1	A	118	LYS	12
1	A	108	LYS	10
1	A	105	ASN	9
1	A	28	GLU	8
1	A	123	LYS	8
1	A	27	ARG	7
1	A	156	ASP	7
1	A	11	LYS	7
1	A	52	GLU	6
1	A	96	ASN	5
1	A	9	ASP	5
1	A	134	ASN	5
1	A	38	ASP	4
1	A	77	GLU	4
1	A	157	ARG	4
1	A	35	LYS	4
1	A	139	ARG	4
1	A	137	ASP	4
1	A	148	GLN	4
1	A	131	GLU	3
1	A	117	LYS	3
1	A	126	ASP	3
1	A	81	ASN	3
1	A	140	GLU	3
1	A	33	ASN	3
1	A	32	ASP	3

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Mol	Chain	Res	Type	Models (Total)
1	A	144	LYS	3
1	A	19	ARG	2
1	A	113	LEU	2
1	A	82	ARG	2
1	A	75	LYS	2
1	A	89	MET	2
1	A	141	SER	2
1	A	106	LYS	2
1	A	45	THR	1
1	A	99	HIS	1
1	A	42	GLU	1
1	A	55	SER	1
1	A	58	ASN	1
1	A	69	LYS	1
1	A	74	LYS	1
1	A	17	GLU	1
1	A	153	ASP	1
1	A	120	GLU	1
1	A	34	CYS	1
1	A	62	ILE	1
1	A	36	SER	1
1	A	84	PHE	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