Full wwPDB NMR Structure Validation Report (i)

Feb 28, 2022 – 05:56 PM EST

PDB ID	:	2EH0
Title	:	Solution structure of the FHA domain from human Kinesin-like protein KIF1B
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Deposited on	:	2007-03-02

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:

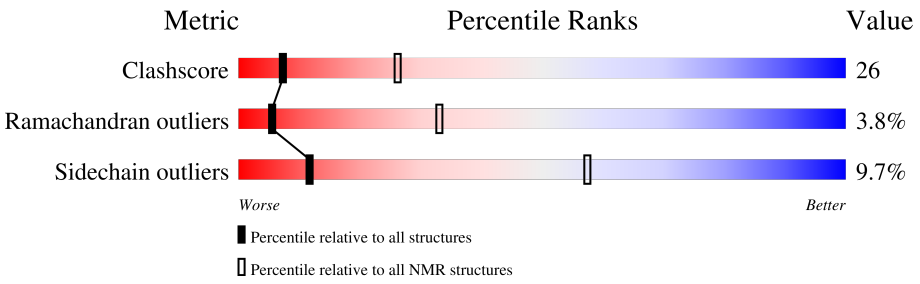
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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	130	41% 32% • 25%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:8-A:16, A:23-A:48, A:52-A:114 (98)	0.36	1

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 2 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2001 atoms, of which 990 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Kinesin-like protein KIF1B.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	130	2001	614	990	193	199	5	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP O60333
A	2	SER	-	expression tag	UNP O60333
A	3	SER	-	expression tag	UNP O60333
A	4	GLY	-	expression tag	UNP O60333
A	5	SER	-	expression tag	UNP O60333
A	6	SER	-	expression tag	UNP O60333
A	7	GLY	-	expression tag	UNP O60333
A	125	SER	-	expression tag	UNP O60333
A	126	GLY	-	expression tag	UNP O60333
A	127	PRO	-	expression tag	UNP O60333
A	128	SER	-	expression tag	UNP O60333
A	129	SER	-	expression tag	UNP O60333
A	130	GLY	-	expression tag	UNP O60333

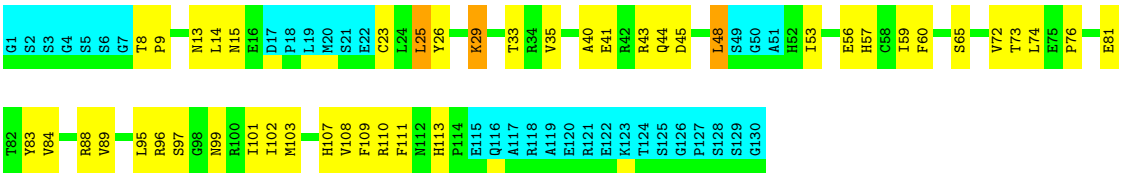
4 Residue-property plots (i)

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: Kinesin-like protein KIF1B

Chain A: 41% 32% • 25%



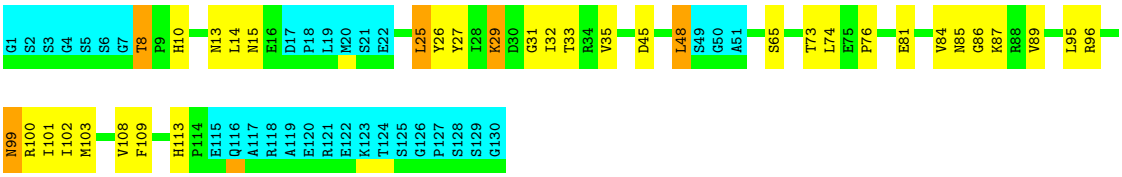
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

• Molecule 1: Kinesin-like protein KIF1B

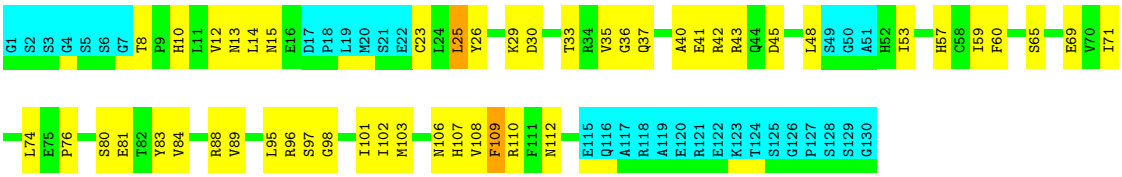
Chain A: 48% 23% • 25%



4.2.2 Score per residue for model 2

• Molecule 1: Kinesin-like protein KIF1B

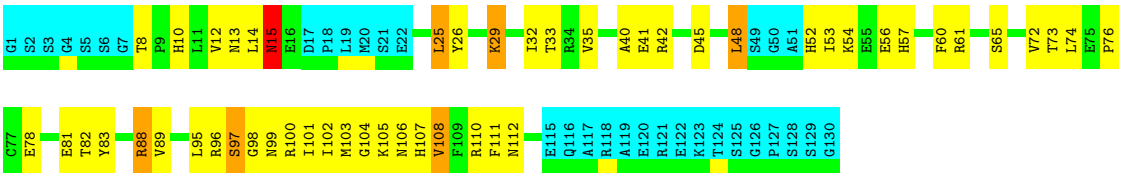
Chain A: 38% 36% • 25%



4.2.3 Score per residue for model 3

- Molecule 1: Kinesin-like protein KIF1B

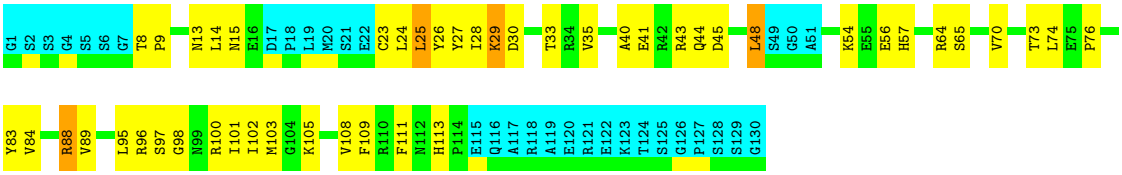
Chain A: 35% 35% 5% • 25%



4.2.4 Score per residue for model 4

- Molecule 1: Kinesin-like protein KIF1B

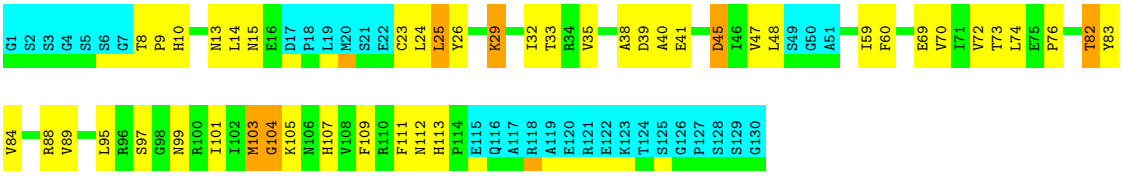
Chain A: 39% 33% • 25%



4.2.5 Score per residue for model 5

- Molecule 1: Kinesin-like protein KIF1B

Chain A: 40% 31% 5% 25%



4.2.6 Score per residue for model 6

- Molecule 1: Kinesin-like protein KIF1B

Chain A: 39% 29% 6% • 25%

G1 S2 S3 G4 S5 S6 G7 T8 P9 L14 N15 E16 D17 P18 L19 M20 S21 E22 C23 L24 L25 Y26 K29 D30 G31 I32 T33 R34 A38 D39 A40 E41 D45 I46 V47 L48 S49 G50 A51 H52 I53 K54 E55 E56 H57 C58 I59 F60 R61 E69 V72 T73 L74 E75

P76 E81 T82 Y83 V84 K87 R88 V89 S90 Q91 P92 V93 Q94 L95 R96 N99 R100 I101 I102 M103 R110 F111 N112 H113 P114 E115 Q116 A117 R118 A119 E120 R121 E122 K123 T124 S125 G126 P127 S128 S129 G130

4.2.7 Score per residue for model 7

- Molecule 1: Kinesin-like protein KIF1B

Chain A: 32% 38% 5% 25%

G1 S2 S3 G4 S5 S6 G7 T8 P9 H10 L11 V12 N13 L14 N15 E16 D17 P18 L19 M20 S21 E22 C23 L24 L25 Y26 Y27 I28 K29 D30 G31 I32 T33 R34 V35 D39 A40 E41 R42 R43 Q44 D45 I46 V47 L48 S49 G50 A51 E55 E56 H57 C58 I59 F60 R61 S62 E63

E69 V70 I71 V72 T73 L74 E81 T82 Y83 V84 K87 R88 V89 L95 R96 S97 G98 N99 R100 I101 I102 M103 H107 V108 F109 R110 F111 N112 H113 P114 E115 Q116 A117 R118 A119 E120 R121 E122 K123 T124 S125 G126 P127 S128 S129 G130

4.2.8 Score per residue for model 8

- Molecule 1: Kinesin-like protein KIF1B

Chain A: 30% 39% 6% 25%

G1 S2 S3 G4 S5 S6 G7 T8 P9 H10 L11 V12 N13 L14 N15 E16 D17 P18 L19 M20 S21 E22 C23 L24 L25 Y26 K29 D30 G31 I32 T33 R34 Q37 A38 D39 A40 E41 R42 R43 Q44 D45 I46 V47 L48 S49 G50 A51 H52 I53 K54 E55 E56 H57 C58 I59 F60 E69

V70 I71 V72 T73 L74 E75 P76 Y83 V84 K87 R88 V89 S90 Q91 P92 V93 Q94 L95 R96 S97 G98 N99 R100 I101 I102 M103 H107 V108 F109 R110 F111 N112 H113 P114 E115 Q116 A117 R118 A119 E120 R121 E122 K123 T124 S125 G126 P127 S128 S129 G130

4.2.9 Score per residue for model 9

- Molecule 1: Kinesin-like protein KIF1B

Chain A: 45% 26% 5% 25%

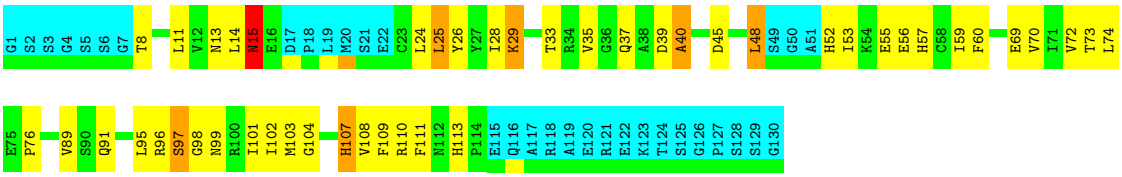
G1 S2 S3 G4 S5 S6 G7 T8 P9 H10 L14 N15 E16 D17 P18 L19 M20 S21 E22 L25 Y26 K29 V35 G36 Q37 A38 D39 A40 E41 Q44 D45 I46 V47 L48 S49 G50 A51 H52 I53 C58 I59 F60 S65 V70 I71 V72 T73 L74 E75 P76 V89

L95 N99 R100 I101 I102 M103 G104 K105 V108 F111 N112 H113 P114 E115 Q116 A117 R118 A119 E120 R121 E122 K123 T124 S125 G126 P127 S128 S129 G130

4.2.10 Score per residue for model 10

- Molecule 1: Kinesin-like protein KIF1B

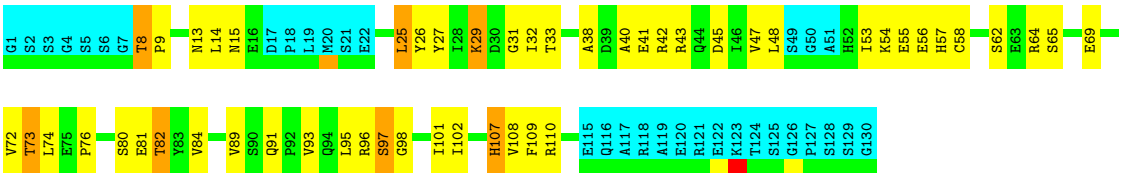
Chain A: 39% 31% 5% • 25%



4.2.11 Score per residue for model 11

- Molecule 1: Kinesin-like protein KIF1B

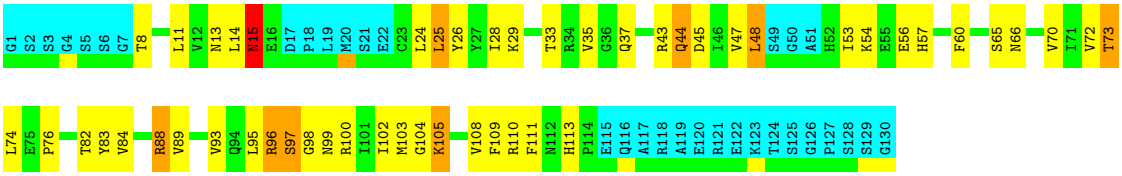
Chain A: 36% 34% 5% 25%



4.2.12 Score per residue for model 12

- Molecule 1: Kinesin-like protein KIF1B

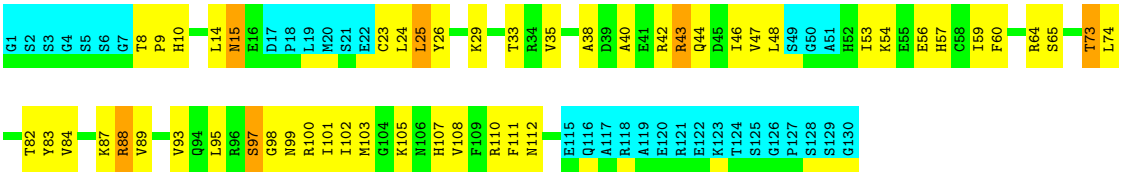
Chain A: 36% 32% 6% • 25%



4.2.13 Score per residue for model 13

- Molecule 1: Kinesin-like protein KIF1B

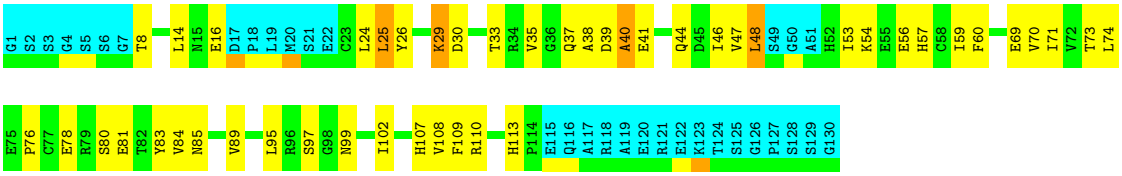
Chain A: 36% 35% 5% 25%



4.2.14 Score per residue for model 14

- Molecule 1: Kinesin-like protein KIF1B

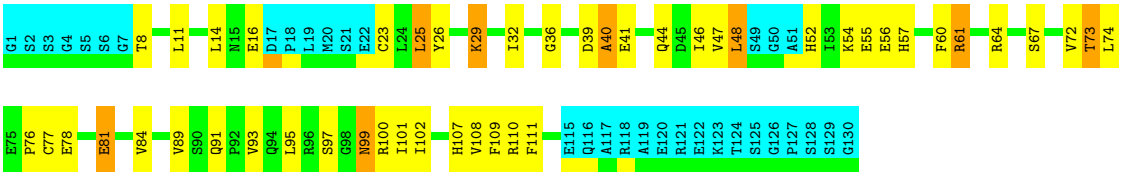
Chain A: 39% 33% • 25%



4.2.15 Score per residue for model 15

- Molecule 1: Kinesin-like protein KIF1B

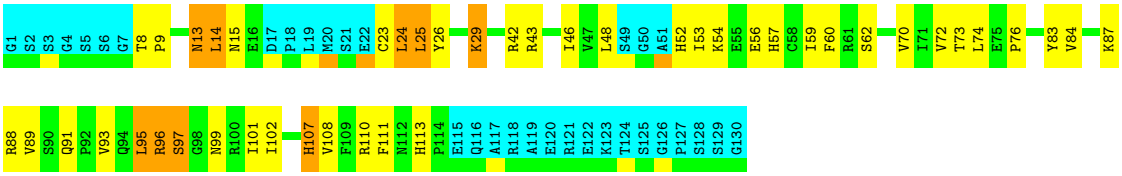
Chain A: 38% 31% 6% 25%



4.2.16 Score per residue for model 16

- Molecule 1: Kinesin-like protein KIF1B

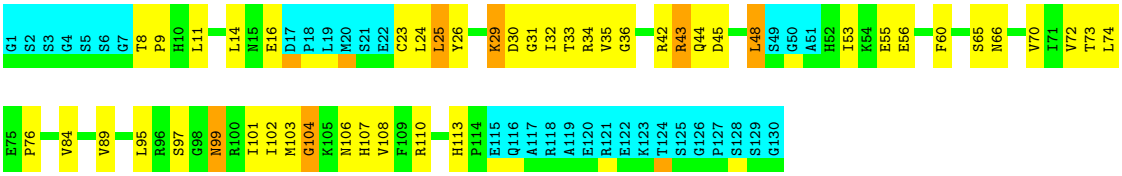
Chain A: 41% 28% 7% 25%



4.2.17 Score per residue for model 17

- Molecule 1: Kinesin-like protein KIF1B

Chain A: 39% 32% 5% 25%



4.2.18 Score per residue for model 18

- Molecule 1: Kinesin-like protein KIF1B

Chain A: 45% 28% • 25%

G1 S2 S3 G4 S5 S6 G7 T8 P9 L14 N15 E16 D17 P18 L19 M20 S21 E22 C23 L24 L25 Y26 K29 D30 G31 I32 V35 E41 R42 R43 Q44 L48 S49 G50 A51 H52 I53 K54 E55 E56 H57 C58 I59 F60 V72 T73 L74 E75 P76 C77 E78 R79 S80

V84 K87 R88 V89 S90 Q91 L95 R100 I101 I102 K105 V108 F109 R110 H113 P114 E115 Q116 A117 R118 A119 E120 R121 E122 K123 T124 S125 G126 P127 S128 S129 G130

4.2.19 Score per residue for model 19

- Molecule 1: Kinesin-like protein KIF1B

Chain A: 42% 28% 6% 25%

G1 S2 S3 G4 S5 S6 G7 T8 P9 H10 L14 N15 E16 D17 P18 L19 M20 S21 E22 L25 Y26 Y27 I28 K29 D30 G31 I32 T33 R34 V35 A40 E41 Q44 D45 L48 S49 G50 A51 E56 H57 C58 I59 F60 S65 I71 V72 T73 L74 E75 P76 E81

V84 V89 V93 Q94 L95 R96 S97 G98 N99 R100 I101 K105 N106 H107 V108 F109 R110 F111 E115 Q116 A117 R118 A119 E120 R121 E122 K123 T124 S125 G126 P127 S128 S129 G130

4.2.20 Score per residue for model 20

- Molecule 1: Kinesin-like protein KIF1B

Chain A: 39% 32% 5% 25%

G1 S2 S3 G4 S5 S6 G7 T8 P9 L14 N15 E16 D17 P18 L19 M20 S21 E22 C23 L24 L25 Y26 Y27 I28 K29 D30 T33 R34 V35 G36 Q37 A38 D39 A40 E41 R42 R43 Q44 D45 L48 S49 G50 A51 H52 I53 K54 E55 E56 H57 C58 I59 F60 S65 I71 V72

T73 L74 E75 P76 E81 T82 Y83 R88 V89 Q94 L95 N99 R100 I101 I102 N106 H107 V108 F109 R110 E115 Q116 A117 R118 A119 E120 R121 E122 K123 T124 S125 G126 P127 S128 S129 G130

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, structures with the lowest energy, target function*.

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

Software name	Classification	Version
CYANA	structure solution	2.1
CYANA	refinement	2.1

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	797	796	795	42±8
All	All	15940	15920	15900	839

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 26.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:25:LEU:HD12	1:A:26:TYR:N	0.91	1.80	11	20
1:A:35:VAL:HG12	1:A:48:LEU:HD21	0.91	1.43	10	11
1:A:74:LEU:HD23	1:A:89:VAL:HG21	0.84	1.46	19	9
1:A:74:LEU:HB2	1:A:95:LEU:HD21	0.83	1.50	14	20
1:A:53:ILE:HD11	1:A:107:HIS:CD2	0.82	2.08	2	5
1:A:14:LEU:HD22	1:A:110:ARG:HB2	0.81	1.50	2	14
1:A:64:ARG:NH1	1:A:70:VAL:HG23	0.80	1.91	4	1
1:A:25:LEU:HD11	1:A:27:TYR:CD1	0.80	2.12	11	2
1:A:46:ILE:CG2	1:A:48:LEU:HD11	0.79	2.08	15	3
1:A:99:ASN:HD21	1:A:101:ILE:HD11	0.77	1.38	3	3
1:A:99:ASN:ND2	1:A:101:ILE:HD11	0.77	1.93	3	2
1:A:48:LEU:HD22	1:A:48:LEU:N	0.77	1.95	9	11
1:A:40:ALA:HB2	1:A:55:GLU:CG	0.77	2.10	10	2
1:A:76:PRO:HG3	1:A:89:VAL:HG22	0.75	1.57	10	18

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:62:SER:OG	1:A:72:VAL:HG22	0.74	1.82	11	1
1:A:74:LEU:HD22	1:A:84:VAL:HG21	0.74	1.59	5	3
1:A:14:LEU:HD22	1:A:110:ARG:CB	0.73	2.11	2	7
1:A:48:LEU:HD23	1:A:53:ILE:HG21	0.73	1.61	18	2
1:A:35:VAL:HG21	1:A:60:PHE:CE2	0.73	2.18	7	3
1:A:102:ILE:HG12	1:A:108:VAL:HG22	0.72	1.60	10	10
1:A:11:LEU:HD11	1:A:60:PHE:CE2	0.71	2.20	10	5
1:A:33:THR:HG23	1:A:45:ASP:HB3	0.70	1.64	10	11
1:A:72:VAL:HG21	1:A:111:PHE:CE1	0.70	2.22	8	2
1:A:60:PHE:CZ	1:A:74:LEU:CD1	0.69	2.75	9	3
1:A:60:PHE:CE1	1:A:74:LEU:CD1	0.69	2.75	9	3
1:A:31:GLY:C	1:A:32:ILE:HD12	0.69	2.07	7	6
1:A:89:VAL:HG13	1:A:89:VAL:O	0.68	1.88	10	19
1:A:72:VAL:HG21	1:A:111:PHE:CZ	0.68	2.24	9	4
1:A:40:ALA:HB2	1:A:55:GLU:HG2	0.68	1.65	10	2
1:A:95:LEU:HD12	1:A:99:ASN:ND2	0.67	2.05	9	2
1:A:61:ARG:O	1:A:72:VAL:HG13	0.66	1.91	6	2
1:A:106:ASN:O	1:A:108:VAL:HG23	0.65	1.91	3	3
1:A:14:LEU:HD23	1:A:14:LEU:N	0.65	2.06	16	4
1:A:35:VAL:CG1	1:A:48:LEU:HD21	0.65	2.22	13	5
1:A:24:LEU:HD22	1:A:24:LEU:N	0.64	2.07	16	2
1:A:84:VAL:HG13	1:A:99:ASN:HD22	0.64	1.52	14	2
1:A:60:PHE:CZ	1:A:101:ILE:HD13	0.64	2.26	6	2
1:A:60:PHE:CZ	1:A:74:LEU:HD13	0.64	2.28	9	3
1:A:33:THR:HG23	1:A:45:ASP:CG	0.63	2.13	7	1
1:A:100:ARG:NE	1:A:102:ILE:HD11	0.63	2.08	15	1
1:A:14:LEU:HD23	1:A:14:LEU:H	0.63	1.53	16	1
1:A:102:ILE:HG13	1:A:108:VAL:HG22	0.63	1.71	17	3
1:A:96:ARG:H	1:A:99:ASN:ND2	0.62	1.93	10	1
1:A:14:LEU:H	1:A:14:LEU:HD23	0.61	1.55	4	16
1:A:59:ILE:O	1:A:74:LEU:HD12	0.61	1.94	6	2
1:A:84:VAL:HG13	1:A:99:ASN:OD1	0.61	1.95	15	4
1:A:46:ILE:HG22	1:A:48:LEU:HD21	0.61	1.72	8	2
1:A:84:VAL:CG2	1:A:101:ILE:HG23	0.61	2.26	5	2
1:A:74:LEU:N	1:A:95:LEU:HD21	0.61	2.10	7	3
1:A:28:ILE:HG23	1:A:33:THR:OG1	0.61	1.96	19	1
1:A:35:VAL:HG21	1:A:60:PHE:HE2	0.60	1.54	7	1
1:A:53:ILE:HD11	1:A:107:HIS:ND1	0.60	2.12	13	1
1:A:74:LEU:CB	1:A:95:LEU:HD21	0.60	2.24	15	15
1:A:35:VAL:HG11	1:A:103:MET:SD	0.60	2.37	13	2
1:A:46:ILE:HG22	1:A:48:LEU:HD11	0.59	1.74	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:38:ALA:HB2	1:A:47:VAL:HG11	0.59	1.74	6	3
1:A:15:ASN:ND2	1:A:108:VAL:N	0.59	2.50	13	1
1:A:14:LEU:HD11	1:A:100:ARG:NE	0.59	2.12	20	1
1:A:103:MET:O	1:A:107:HIS:CD2	0.59	2.55	8	2
1:A:102:ILE:CG1	1:A:108:VAL:HG22	0.59	2.28	13	3
1:A:48:LEU:N	1:A:48:LEU:CD2	0.58	2.66	7	6
1:A:72:VAL:HG12	1:A:95:LEU:HD23	0.58	1.74	9	7
1:A:14:LEU:CD2	1:A:110:ARG:N	0.58	2.67	2	5
1:A:32:ILE:HD12	1:A:32:ILE:N	0.58	2.13	8	5
1:A:70:VAL:O	1:A:113:HIS:CE1	0.58	2.57	14	6
1:A:105:LYS:O	1:A:107:HIS:CE1	0.58	2.57	5	2
1:A:53:ILE:HD11	1:A:107:HIS:CE1	0.58	2.33	13	1
1:A:102:ILE:HG13	1:A:108:VAL:HG13	0.58	1.74	2	10
1:A:102:ILE:CD1	1:A:108:VAL:HG13	0.58	2.28	14	1
1:A:74:LEU:HD22	1:A:84:VAL:CG2	0.58	2.28	5	1
1:A:84:VAL:HG22	1:A:101:ILE:HG23	0.58	1.76	15	4
1:A:23:CYS:SG	1:A:26:TYR:CE1	0.57	2.95	4	1
1:A:37:GLN:HA	1:A:47:VAL:HG13	0.57	1.76	12	1
1:A:10:HIS:CE1	1:A:112:ASN:CB	0.57	2.88	13	4
1:A:102:ILE:CG1	1:A:108:VAL:HG13	0.57	2.29	2	1
1:A:40:ALA:CB	1:A:55:GLU:CG	0.57	2.81	20	2
1:A:74:LEU:HB2	1:A:95:LEU:HD11	0.57	1.77	7	1
1:A:32:ILE:N	1:A:32:ILE:HD12	0.57	2.15	11	1
1:A:95:LEU:H	1:A:95:LEU:HD22	0.56	1.60	8	4
1:A:38:ALA:HB2	1:A:47:VAL:HG21	0.56	1.75	14	2
1:A:24:LEU:N	1:A:24:LEU:CD2	0.56	2.68	16	2
1:A:48:LEU:HD22	1:A:48:LEU:H	0.56	1.59	9	5
1:A:48:LEU:H	1:A:48:LEU:HD22	0.56	1.60	20	5
1:A:32:ILE:HD11	1:A:61:ARG:NH1	0.55	2.15	3	1
1:A:58:CYS:SG	1:A:74:LEU:HD11	0.55	2.41	9	2
1:A:74:LEU:CD2	1:A:89:VAL:HG11	0.55	2.32	13	7
1:A:73:THR:C	1:A:95:LEU:CD2	0.55	2.75	8	2
1:A:33:THR:HG23	1:A:45:ASP:CB	0.55	2.32	20	7
1:A:60:PHE:CE1	1:A:101:ILE:HD13	0.55	2.36	7	1
1:A:59:ILE:HG22	1:A:60:PHE:N	0.55	2.16	7	13
1:A:84:VAL:HG13	1:A:99:ASN:ND2	0.55	2.17	12	2
1:A:54:LYS:N	1:A:54:LYS:CD	0.55	2.70	3	1
1:A:14:LEU:CD2	1:A:109:PHE:C	0.55	2.75	2	2
1:A:107:HIS:N	1:A:107:HIS:ND1	0.55	2.55	11	3
1:A:15:ASN:ND2	1:A:108:VAL:H	0.54	1.99	13	1
1:A:32:ILE:N	1:A:32:ILE:CD1	0.54	2.70	8	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:84:VAL:HG22	1:A:101:ILE:HG12	0.54	1.79	19	4
1:A:45:ASP:CG	1:A:46:ILE:N	0.54	2.60	7	1
1:A:15:ASN:HD21	1:A:108:VAL:N	0.54	2.00	13	1
1:A:74:LEU:N	1:A:95:LEU:CD2	0.54	2.70	7	4
1:A:10:HIS:CE1	1:A:112:ASN:HB2	0.54	2.38	13	1
1:A:48:LEU:HB2	1:A:53:ILE:HG21	0.54	1.80	2	1
1:A:107:HIS:O	1:A:109:PHE:CE1	0.54	2.61	14	3
1:A:10:HIS:NE2	1:A:112:ASN:ND2	0.54	2.56	3	1
1:A:82:THR:C	1:A:83:TYR:CD1	0.53	2.82	5	2
1:A:33:THR:CG2	1:A:45:ASP:CG	0.53	2.76	7	1
1:A:33:THR:HG22	1:A:33:THR:O	0.53	2.04	14	2
1:A:101:ILE:HG22	1:A:103:MET:SD	0.53	2.43	9	2
1:A:84:VAL:HG22	1:A:101:ILE:HG13	0.53	1.81	11	1
1:A:72:VAL:HG21	1:A:111:PHE:HE1	0.53	1.64	8	1
1:A:83:TYR:CE1	1:A:88:ARG:HG3	0.53	2.38	13	3
1:A:57:HIS:CD2	1:A:82:THR:HG1	0.53	2.22	13	1
1:A:14:LEU:HD22	1:A:110:ARG:N	0.52	2.19	8	2
1:A:8:THR:HG23	1:A:9:PRO:HD2	0.52	1.81	20	12
1:A:53:ILE:HG22	1:A:54:LYS:N	0.52	2.19	14	4
1:A:100:ARG:HG2	1:A:108:VAL:HG11	0.52	1.80	3	1
1:A:48:LEU:HD11	1:A:109:PHE:CZ	0.52	2.39	5	1
1:A:15:ASN:HD22	1:A:15:ASN:N	0.52	2.02	10	1
1:A:10:HIS:CD2	1:A:25:LEU:HD13	0.52	2.39	19	3
1:A:84:VAL:HG12	1:A:85:ASN:HD22	0.52	1.64	14	1
1:A:36:GLY:O	1:A:48:LEU:HD22	0.52	2.05	15	2
1:A:23:CYS:HB2	1:A:26:TYR:CE1	0.52	2.40	13	3
1:A:34:ARG:NH1	1:A:44:GLN:NE2	0.52	2.58	19	1
1:A:91:GLN:HG2	1:A:93:VAL:HG13	0.51	1.82	8	3
1:A:29:LYS:NZ	1:A:32:ILE:N	0.51	2.58	5	2
1:A:15:ASN:ND2	1:A:15:ASN:N	0.51	2.57	6	1
1:A:10:HIS:CE1	1:A:112:ASN:HB3	0.51	2.41	3	4
1:A:72:VAL:CG2	1:A:111:PHE:CE1	0.51	2.92	8	1
1:A:46:ILE:HG22	1:A:48:LEU:CD2	0.51	2.35	8	2
1:A:25:LEU:CD1	1:A:26:TYR:N	0.51	2.67	11	2
1:A:99:ASN:ND2	1:A:101:ILE:CD1	0.51	2.73	3	1
1:A:83:TYR:CD1	1:A:88:ARG:HA	0.50	2.41	13	2
1:A:48:LEU:HD23	1:A:53:ILE:CG2	0.50	2.34	2	2
1:A:29:LYS:HZ3	1:A:32:ILE:N	0.50	2.05	5	1
1:A:95:LEU:HB3	1:A:111:PHE:CD2	0.50	2.42	12	1
1:A:83:TYR:CE1	1:A:88:ARG:CG	0.50	2.95	13	1
1:A:48:LEU:HD12	1:A:109:PHE:CZ	0.50	2.41	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:9:PRO:CB	1:A:72:VAL:HG21	0.50	2.37	11	1
1:A:9:PRO:HB3	1:A:72:VAL:HG21	0.50	1.84	11	1
1:A:47:VAL:C	1:A:48:LEU:HD22	0.49	2.28	7	2
1:A:13:ASN:O	1:A:13:ASN:ND2	0.49	2.45	16	3
1:A:96:ARG:O	1:A:98:GLY:N	0.49	2.46	2	6
1:A:10:HIS:NE2	1:A:112:ASN:CB	0.49	2.75	3	1
1:A:15:ASN:ND2	1:A:108:VAL:O	0.49	2.45	3	2
1:A:98:GLY:N	1:A:111:PHE:O	0.49	2.45	4	3
1:A:102:ILE:CG2	1:A:105:LYS:O	0.49	2.61	3	1
1:A:15:ASN:ND2	1:A:15:ASN:H	0.49	2.05	6	1
1:A:37:GLN:NE2	1:A:53:ILE:O	0.49	2.45	9	2
1:A:12:VAL:CG2	1:A:112:ASN:OD1	0.49	2.60	3	1
1:A:72:VAL:HB	1:A:111:PHE:CZ	0.49	2.43	3	5
1:A:100:ARG:NH2	1:A:102:ILE:HD11	0.49	2.23	4	1
1:A:42:ARG:O	1:A:44:GLN:N	0.49	2.45	17	3
1:A:89:VAL:O	1:A:89:VAL:CG1	0.49	2.61	18	14
1:A:13:ASN:CB	1:A:24:LEU:O	0.49	2.61	7	4
1:A:40:ALA:HB2	1:A:55:GLU:HG3	0.49	1.83	20	2
1:A:88:ARG:HE	1:A:89:VAL:N	0.49	2.05	12	1
1:A:57:HIS:CD2	1:A:82:THR:OG1	0.49	2.66	13	1
1:A:46:ILE:CG2	1:A:48:LEU:CD1	0.49	2.86	15	3
1:A:84:VAL:N	1:A:87:LYS:O	0.49	2.46	7	5
1:A:38:ALA:HB2	1:A:47:VAL:CG1	0.49	2.38	6	1
1:A:83:TYR:CD2	1:A:88:ARG:HA	0.49	2.43	5	2
1:A:29:LYS:NZ	1:A:32:ILE:C	0.49	2.66	19	1
1:A:29:LYS:CD	1:A:29:LYS:C	0.49	2.81	14	4
1:A:83:TYR:CE1	1:A:88:ARG:HG2	0.48	2.43	4	2
1:A:95:LEU:HD12	1:A:99:ASN:OD1	0.48	2.07	1	2
1:A:25:LEU:HD12	1:A:25:LEU:C	0.48	2.29	16	2
1:A:108:VAL:O	1:A:109:PHE:CD1	0.48	2.66	1	1
1:A:47:VAL:C	1:A:48:LEU:HD13	0.48	2.29	15	2
1:A:108:VAL:C	1:A:109:PHE:CD1	0.48	2.87	20	1
1:A:73:THR:CG2	1:A:93:VAL:O	0.48	2.62	6	2
1:A:71:ILE:CG2	1:A:72:VAL:N	0.48	2.77	9	1
1:A:99:ASN:OD1	1:A:101:ILE:CG1	0.48	2.62	6	4
1:A:48:LEU:HD12	1:A:107:HIS:CD2	0.48	2.43	7	1
1:A:81:GLU:HG3	1:A:83:TYR:CE2	0.48	2.44	14	2
1:A:48:LEU:HD12	1:A:107:HIS:CG	0.47	2.43	7	1
1:A:40:ALA:HB3	1:A:44:GLN:HG2	0.47	1.85	9	1
1:A:73:THR:HA	1:A:95:LEU:HD22	0.47	1.86	8	1
1:A:25:LEU:HD11	1:A:27:TYR:HD1	0.47	1.63	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:84:VAL:O	1:A:86:GLY:N	0.47	2.47	1	1
1:A:34:ARG:HA	1:A:59:ILE:HG23	0.47	1.87	6	1
1:A:58:CYS:SG	1:A:74:LEU:HD21	0.47	2.49	6	1
1:A:60:PHE:HE1	1:A:101:ILE:HD13	0.47	1.68	7	1
1:A:103:MET:SD	1:A:103:MET:N	0.47	2.87	9	3
1:A:12:VAL:CG2	1:A:112:ASN:ND2	0.47	2.78	2	1
1:A:57:HIS:CD2	1:A:103:MET:HB3	0.47	2.45	4	4
1:A:95:LEU:HD22	1:A:95:LEU:N	0.47	2.25	7	3
1:A:59:ILE:HG22	1:A:60:PHE:H	0.46	1.70	6	2
1:A:60:PHE:CE2	1:A:101:ILE:HD13	0.46	2.46	6	1
1:A:53:ILE:HD11	1:A:107:HIS:HD2	0.46	1.69	16	1
1:A:69:GLU:CG	1:A:69:GLU:O	0.46	2.63	6	2
1:A:46:ILE:O	1:A:46:ILE:HG22	0.46	2.09	13	1
1:A:48:LEU:HD11	1:A:109:PHE:CE2	0.46	2.46	11	1
1:A:73:THR:HG23	1:A:93:VAL:C	0.46	2.31	11	6
1:A:25:LEU:HD12	1:A:26:TYR:CA	0.46	2.40	11	2
1:A:26:TYR:HB2	1:A:46:ILE:HD11	0.46	1.86	16	1
1:A:99:ASN:OD1	1:A:111:PHE:CB	0.46	2.63	5	1
1:A:28:ILE:HG22	1:A:29:LYS:N	0.46	2.26	4	2
1:A:80:SER:O	1:A:82:THR:N	0.46	2.49	11	1
1:A:13:ASN:O	1:A:13:ASN:CG	0.46	2.54	8	2
1:A:44:GLN:NE2	1:A:55:GLU:O	0.46	2.49	7	3
1:A:107:HIS:HB3	1:A:109:PHE:CE2	0.46	2.45	7	1
1:A:71:ILE:CG2	1:A:94:GLN:CD	0.46	2.84	20	1
1:A:15:ASN:OD1	1:A:108:VAL:N	0.45	2.48	19	1
1:A:82:THR:O	1:A:83:TYR:CD1	0.45	2.69	5	1
1:A:99:ASN:ND2	1:A:101:ILE:CG1	0.45	2.79	5	3
1:A:60:PHE:CE1	1:A:74:LEU:HD12	0.45	2.46	9	1
1:A:57:HIS:CE1	1:A:80:SER:HB2	0.45	2.47	18	1
1:A:108:VAL:O	1:A:109:PHE:CG	0.45	2.69	8	3
1:A:96:ARG:O	1:A:99:ASN:N	0.45	2.49	19	1
1:A:40:ALA:O	1:A:41:GLU:C	0.45	2.55	14	11
1:A:35:VAL:CG2	1:A:60:PHE:CD2	0.45	2.99	3	2
1:A:103:MET:O	1:A:105:LYS:N	0.45	2.49	3	2
1:A:39:ASP:O	1:A:40:ALA:C	0.45	2.55	10	9
1:A:40:ALA:O	1:A:42:ARG:N	0.45	2.49	7	1
1:A:102:ILE:C	1:A:103:MET:SD	0.45	2.95	8	1
1:A:56:GLU:O	1:A:57:HIS:C	0.45	2.55	4	13
1:A:102:ILE:HG23	1:A:105:LYS:O	0.45	2.12	3	2
1:A:70:VAL:O	1:A:113:HIS:NE2	0.45	2.50	8	7
1:A:14:LEU:HD13	1:A:110:ARG:HH12	0.45	1.72	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:35:VAL:HG21	1:A:60:PHE:CE1	0.45	2.46	9	1
1:A:23:CYS:HB3	1:A:26:TYR:CE1	0.45	2.47	16	1
1:A:108:VAL:C	1:A:109:PHE:CG	0.45	2.89	20	1
1:A:35:VAL:HG21	1:A:60:PHE:CD1	0.45	2.46	9	1
1:A:44:GLN:CA	1:A:44:GLN:OE1	0.45	2.65	12	1
1:A:10:HIS:ND1	1:A:112:ASN:OD1	0.45	2.50	2	1
1:A:72:VAL:HG21	1:A:111:PHE:HZ	0.45	1.72	15	2
1:A:13:ASN:N	1:A:13:ASN:HD22	0.45	2.09	8	1
1:A:42:ARG:O	1:A:44:GLN:CD	0.45	2.56	8	1
1:A:54:LYS:O	1:A:55:GLU:C	0.45	2.55	11	2
1:A:42:ARG:O	1:A:43:ARG:C	0.45	2.56	20	7
1:A:73:THR:C	1:A:95:LEU:HD21	0.45	2.32	8	1
1:A:101:ILE:HG22	1:A:103:MET:CE	0.44	2.42	1	1
1:A:36:GLY:O	1:A:48:LEU:CD2	0.44	2.65	15	1
1:A:73:THR:CA	1:A:95:LEU:CD2	0.44	2.95	8	1
1:A:46:ILE:O	1:A:48:LEU:CD2	0.44	2.65	7	1
1:A:63:GLU:OE1	1:A:63:GLU:C	0.44	2.55	7	1
1:A:14:LEU:N	1:A:14:LEU:CD2	0.44	2.77	16	1
1:A:14:LEU:HD21	1:A:109:PHE:C	0.44	2.31	2	2
1:A:23:CYS:C	1:A:24:LEU:HD22	0.44	2.33	16	1
1:A:53:ILE:CG2	1:A:54:LYS:N	0.44	2.80	3	5
1:A:57:HIS:NE2	1:A:81:GLU:O	0.44	2.50	3	1
1:A:106:ASN:O	1:A:108:VAL:N	0.44	2.50	3	1
1:A:56:GLU:O	1:A:58:CYS:N	0.44	2.50	6	1
1:A:44:GLN:OE1	1:A:44:GLN:N	0.44	2.50	12	1
1:A:98:GLY:O	1:A:110:ARG:NH1	0.44	2.51	2	1
1:A:44:GLN:O	1:A:45:ASP:C	0.44	2.56	17	1
1:A:69:GLU:O	1:A:69:GLU:CG	0.44	2.66	14	3
1:A:91:GLN:CG	1:A:93:VAL:HG13	0.44	2.43	6	2
1:A:48:LEU:N	1:A:48:LEU:HD13	0.44	2.28	18	1
1:A:100:ARG:CB	1:A:100:ARG:CZ	0.43	2.96	4	1
1:A:23:CYS:O	1:A:24:LEU:C	0.43	2.56	17	1
1:A:84:VAL:O	1:A:87:LYS:N	0.43	2.51	18	1
1:A:52:HIS:ND1	1:A:105:LYS:NZ	0.43	2.65	3	1
1:A:12:VAL:HG23	1:A:112:ASN:ND2	0.43	2.28	2	1
1:A:102:ILE:HG22	1:A:103:MET:N	0.43	2.29	7	1
1:A:110:ARG:CZ	1:A:110:ARG:HB3	0.43	2.44	10	1
1:A:64:ARG:CZ	1:A:64:ARG:CB	0.43	2.96	11	3
1:A:46:ILE:HG22	1:A:48:LEU:CD1	0.43	2.44	15	1
1:A:28:ILE:HD11	1:A:60:PHE:CD2	0.43	2.48	10	1
1:A:103:MET:O	1:A:104:GLY:C	0.43	2.56	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:95:LEU:HB3	1:A:111:PHE:CG	0.43	2.49	10	1
1:A:36:GLY:O	1:A:37:GLN:NE2	0.43	2.52	2	1
1:A:29:LYS:O	1:A:31:GLY:N	0.43	2.52	6	1
1:A:37:GLN:O	1:A:44:GLN:CG	0.43	2.66	9	2
1:A:26:TYR:CB	1:A:46:ILE:HD11	0.43	2.43	16	1
1:A:29:LYS:NZ	1:A:45:ASP:OD2	0.43	2.52	20	1
1:A:110:ARG:CZ	1:A:110:ARG:CB	0.42	2.96	10	1
1:A:15:ASN:OD1	1:A:15:ASN:N	0.42	2.52	12	1
1:A:64:ARG:CZ	1:A:70:VAL:HG23	0.42	2.43	4	1
1:A:103:MET:SD	1:A:109:PHE:CE1	0.42	3.12	4	1
1:A:25:LEU:HD12	1:A:26:TYR:C	0.42	2.35	11	1
1:A:23:CYS:HB2	1:A:26:TYR:CZ	0.42	2.49	8	2
1:A:60:PHE:HZ	1:A:101:ILE:HD13	0.42	1.69	6	1
1:A:81:GLU:C	1:A:81:GLU:OE1	0.42	2.57	19	1
1:A:69:GLU:HG3	1:A:71:ILE:HD11	0.42	1.92	2	1
1:A:96:ARG:O	1:A:97:SER:C	0.42	2.57	3	3
1:A:28:ILE:CD1	1:A:60:PHE:CD2	0.42	3.03	10	1
1:A:13:ASN:OD1	1:A:15:ASN:CG	0.42	2.58	12	1
1:A:57:HIS:CE1	1:A:81:GLU:H	0.42	2.32	20	3
1:A:99:ASN:ND2	1:A:101:ILE:HG12	0.42	2.29	5	1
1:A:100:ARG:CG	1:A:108:VAL:CG1	0.41	2.98	1	1
1:A:48:LEU:CD2	1:A:53:ILE:HG21	0.41	2.42	2	1
1:A:98:GLY:HA2	1:A:110:ARG:NE	0.41	2.30	2	1
1:A:11:LEU:HD11	1:A:28:ILE:HD11	0.41	1.92	7	1
1:A:88:ARG:NE	1:A:89:VAL:N	0.41	2.68	12	1
1:A:100:ARG:HG2	1:A:102:ILE:HD11	0.41	1.91	12	1
1:A:101:ILE:O	1:A:108:VAL:HG13	0.41	2.15	19	1
1:A:83:TYR:CE1	1:A:88:ARG:HD3	0.41	2.50	3	1
1:A:58:CYS:SG	1:A:74:LEU:CG	0.41	3.08	6	2
1:A:59:ILE:CG2	1:A:60:PHE:N	0.41	2.83	7	1
1:A:102:ILE:O	1:A:102:ILE:HG22	0.41	2.15	13	1
1:A:84:VAL:C	1:A:86:GLY:N	0.41	2.72	1	1
1:A:101:ILE:CG2	1:A:103:MET:CE	0.41	2.98	2	2
1:A:34:ARG:CB	1:A:44:GLN:OE1	0.41	2.68	8	1
1:A:44:GLN:NE2	1:A:56:GLU:OE1	0.41	2.53	15	1
1:A:29:LYS:NZ	1:A:32:ILE:O	0.41	2.52	19	1
1:A:10:HIS:CG	1:A:112:ASN:OD1	0.41	2.74	2	1
1:A:100:ARG:HG2	1:A:108:VAL:CG1	0.41	2.45	3	1
1:A:58:CYS:SG	1:A:82:THR:HG21	0.41	2.56	11	2
1:A:59:ILE:C	1:A:60:PHE:CD1	0.41	2.93	9	1
1:A:101:ILE:O	1:A:109:PHE:N	0.41	2.53	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:10:HIS:CD2	1:A:112:ASN:HB2	0.41	2.50	3	1
1:A:37:GLN:CG	1:A:53:ILE:O	0.41	2.68	10	1
1:A:35:VAL:C	1:A:44:GLN:OE1	0.41	2.59	4	1
1:A:25:LEU:HD11	1:A:27:TYR:CE2	0.41	2.50	20	1
1:A:25:LEU:HD11	1:A:27:TYR:CE1	0.41	2.50	1	1
1:A:25:LEU:HD11	1:A:27:TYR:CD2	0.41	2.51	4	1
1:A:54:LYS:N	1:A:54:LYS:HD3	0.41	2.30	3	1
1:A:48:LEU:HD12	1:A:109:PHE:HZ	0.41	1.74	19	1
1:A:83:TYR:CE1	1:A:88:ARG:HD2	0.41	2.51	2	1
1:A:10:HIS:NE2	1:A:112:ASN:CG	0.41	2.75	3	1
1:A:29:LYS:C	1:A:29:LYS:CD	0.41	2.89	20	2
1:A:82:THR:CG2	1:A:89:VAL:CG1	0.41	2.99	3	1
1:A:102:ILE:CG2	1:A:103:MET:N	0.41	2.83	7	1
1:A:32:ILE:CD1	1:A:61:ARG:HG2	0.41	2.46	15	1
1:A:29:LYS:N	1:A:29:LYS:HD3	0.40	2.31	1	1
1:A:74:LEU:HD21	1:A:82:THR:HG21	0.40	1.93	3	1
1:A:53:ILE:CD1	1:A:104:GLY:HA3	0.40	2.46	10	1
1:A:43:ARG:C	1:A:44:GLN:OE1	0.40	2.60	12	1
1:A:32:ILE:HG21	1:A:34:ARG:NH1	0.40	2.31	17	1
1:A:104:GLY:HA3	1:A:107:HIS:CD2	0.40	2.51	17	1
1:A:69:GLU:HG3	1:A:71:ILE:CD1	0.40	2.47	7	1
1:A:53:ILE:O	1:A:54:LYS:C	0.40	2.60	13	1
1:A:108:VAL:HG12	1:A:109:PHE:N	0.40	2.31	1	1
1:A:10:HIS:CD2	1:A:112:ASN:HD21	0.40	2.34	2	1
1:A:61:ARG:O	1:A:72:VAL:CG1	0.40	2.65	6	1
1:A:100:ARG:CG	1:A:108:VAL:HG11	0.40	2.47	3	1
1:A:58:CYS:C	1:A:59:ILE:CG1	0.40	2.90	6	1
1:A:37:GLN:NE2	1:A:37:GLN:CA	0.40	2.85	8	1
1:A:53:ILE:O	1:A:53:ILE:HG22	0.40	2.15	13	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	98/130 (75%)	83±3 (84±3%)	12±2 (12±3%)	4±1 (4±1%)	5 33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1960/2600 (75%)	1654 (84%)	231 (12%)	75 (4%)	5 33

All 18 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	15	ASN	16
1	A	97	SER	12
1	A	65	SER	11
1	A	40	ALA	7
1	A	104	GLY	5
1	A	43	ARG	5
1	A	29	LYS	4
1	A	8	THR	2
1	A	81	GLU	2
1	A	95	LEU	2
1	A	23	CYS	2
1	A	85	ASN	1
1	A	107	HIS	1
1	A	30	ASP	1
1	A	57	HIS	1
1	A	41	GLU	1
1	A	37	GLN	1
1	A	52	HIS	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	90/113 (80%)	81±2 (90±2%)	9±2 (10±2%)	12 57
All	All	1800/2260 (80%)	1625 (90%)	175 (10%)	12 57

All 46 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	25	LEU	20

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Mol	Chain	Res	Type	Models (Total)
1	A	29	LYS	19
1	A	73	THR	16
1	A	48	LEU	15
1	A	8	THR	8
1	A	30	ASP	7
1	A	97	SER	7
1	A	81	GLU	4
1	A	15	ASN	4
1	A	78	GLU	4
1	A	88	ARG	4
1	A	103	MET	4
1	A	41	GLU	4
1	A	105	LYS	4
1	A	107	HIS	4
1	A	96	ARG	3
1	A	99	ASN	3
1	A	82	THR	3
1	A	52	HIS	3
1	A	91	GLN	3
1	A	80	SER	2
1	A	54	LYS	2
1	A	45	ASP	2
1	A	13	ASN	2
1	A	56	GLU	2
1	A	75	GLU	2
1	A	44	GLN	2
1	A	66	ASN	2
1	A	100	ARG	2
1	A	71	ILE	2
1	A	106	ASN	1
1	A	109	PHE	1
1	A	42	ARG	1
1	A	108	VAL	1
1	A	55	GLU	1
1	A	69	GLU	1
1	A	87	LYS	1
1	A	61	ARG	1
1	A	67	SER	1
1	A	77	CYS	1
1	A	14	LEU	1
1	A	24	LEU	1
1	A	62	SER	1

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Mol	Chain	Res	Type	Models (Total)
1	A	16	GLU	1
1	A	39	ASP	1
1	A	94	GLN	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