Full wwPDB NMR Structure Validation Report (i)

Feb 14, 2022 – 10:03 AM EST

PDB ID	:	1IYG
Title	:	Solution structure of RSGI RUH-001, a Fis1p-like and CGI-135 homologous domain from a mouse cDNA
Authors	:	Ohashi, W.; Hirota, H.; Yamazaki, T.; Koshiba, S.; Hamada, T.; Yoshida, M.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2002-08-14

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:

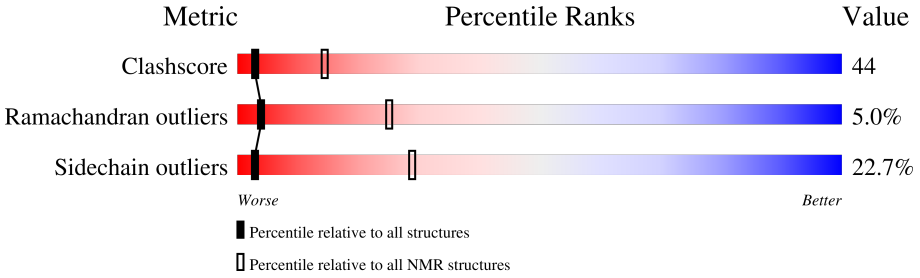
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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	133	21% 63% 7% 9%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 12 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 target function*.

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:7-A:127 (121)	0.36	12

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2125 atoms, of which 1063 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Hypothetical protein (2010003O14).

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	133	2125	666	1063	184	209	3	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	cloning artifact	UNP Q9CQ92
A	2	SER	-	cloning artifact	UNP Q9CQ92
A	3	SER	-	cloning artifact	UNP Q9CQ92
A	4	GLY	-	cloning artifact	UNP Q9CQ92
A	5	SER	-	cloning artifact	UNP Q9CQ92
A	6	SER	-	cloning artifact	UNP Q9CQ92
A	7	GLY	-	cloning artifact	UNP Q9CQ92
A	128	SER	-	cloning artifact	UNP Q9CQ92
A	129	GLY	-	cloning artifact	UNP Q9CQ92
A	130	PRO	-	cloning artifact	UNP Q9CQ92
A	131	SER	-	cloning artifact	UNP Q9CQ92
A	132	SER	-	cloning artifact	UNP Q9CQ92
A	133	GLY	-	cloning artifact	UNP Q9CQ92

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: Hypothetical protein (2010003O14)

Chain A: 21% 63% 7% 9%

G1 S2 S3 G4 S5 S6 G7 M8 L12 N13 E14 L15 V16 E19 D20 L21 K22 N23 F24 E25 R26 K27 F28 Q29 S30 E31 Q32 A33 A34 G35 S36 V37 S38 K39 S40 T41 Q42 F43 E44 Y45 A46 W47 C48 L49 V50 R51 S52 K53 Y54 N55 E56 D57 I58 R59 R60 G61 I62 V63

L64 L65 E66 E67 L68 L69 P70 S73 K74 Q77 R78 D79 Y80 V81 F82 Y83 L84 A85 V86 G87 N88 Y89 R90 L91 K92 E93 Y94 E95 K96 A97 L98 K99 Y100 V101 R102 G103 L104 L105 Q106 T107 E108 P109 Q113 A114 K115 E116 L117 E118 R119 L120 I121 D122 K123 A124 M125 K126 K127

S128 G129 P130 S131 S132 G133

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: Hypothetical protein (2010003O14)

Chain A: 31% 49% 11% • 9%

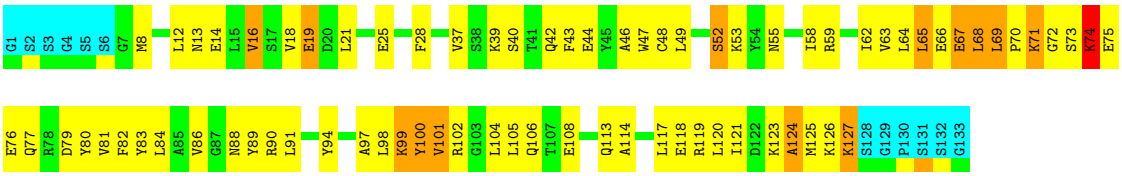
G1 S2 S3 G4 S5 S6 G7 M8 E9 N13 E14 L15 V16 S17 V18 E19 D20 N23 R26 K27 F28 Q29 S30 E31 A34 G35 S36 V37 S38 K39 Q42 F43 E44 Y45 A46 W47 C48 L49 V50 R51 S52 K53 E56 D57 I58 R59 R60 G61 I62 V63 L64 L65 E66 E67

L68 L69 P70 S73 Q77 R78 D79 Y80 V81 F82 Y83 L84 A85 V86 G87 N88 Y89 R90 L91 K92 E93 Y94 E95 K96 A97 L98 K99 Y100 V101 R102 L105 Q106 T107 E108 N112 K115 E116 L117 E118 R119 L120 I121 M125 K126 K127 S128 G129 P130 S131 S132 G133

4.2.2 Score per residue for model 2

• Molecule 1: Hypothetical protein (2010003O14)

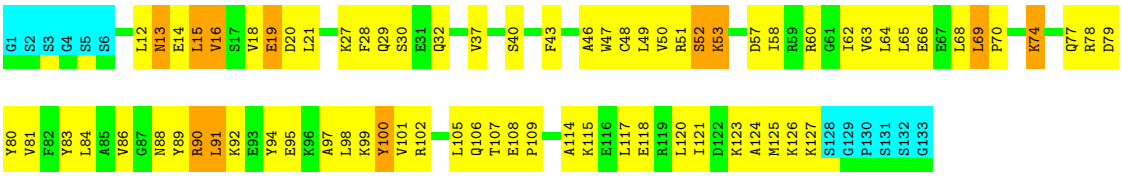
Chain A: 35% 46% 10% • 9%



4.2.3 Score per residue for model 3

- Molecule 1: Hypothetical protein (2010003O14)

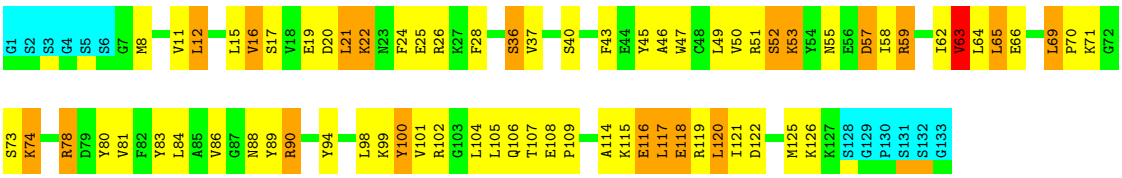
Chain A: 35% 47% 8% 9%



4.2.4 Score per residue for model 4

- Molecule 1: Hypothetical protein (2010003O14)

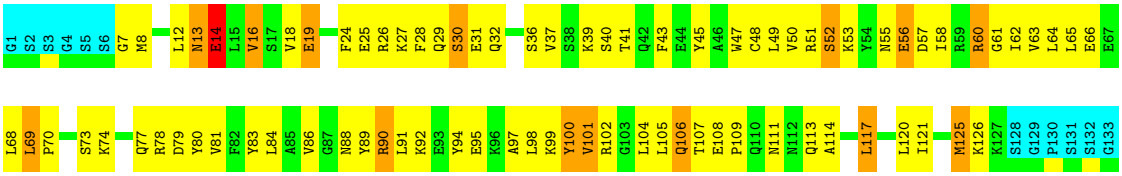
Chain A: 37% 39% 14% • 9%



4.2.5 Score per residue for model 5

- Molecule 1: Hypothetical protein (2010003O14)

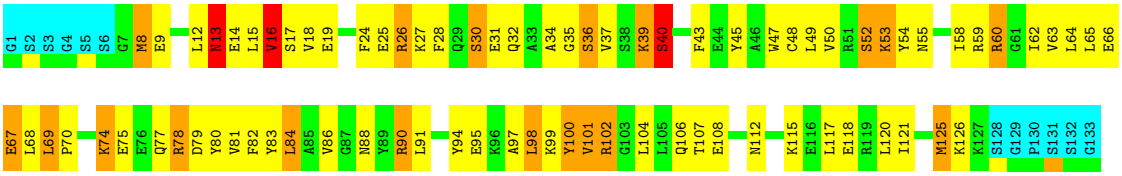
Chain A: 29% 50% 11% • 9%



4.2.6 Score per residue for model 6

- Molecule 1: Hypothetical protein (2010003O14)

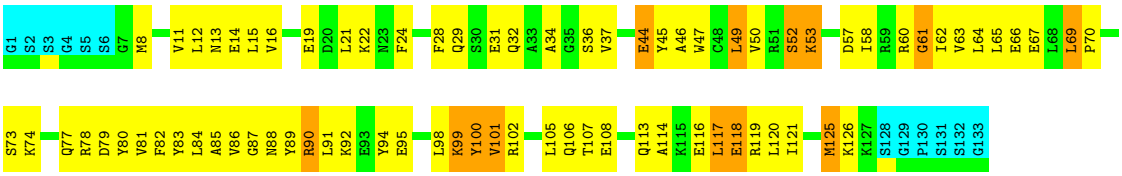
Chain A: 31% 44% 14% • 9%



4.2.7 Score per residue for model 7

- Molecule 1: Hypothetical protein (2010003O14)

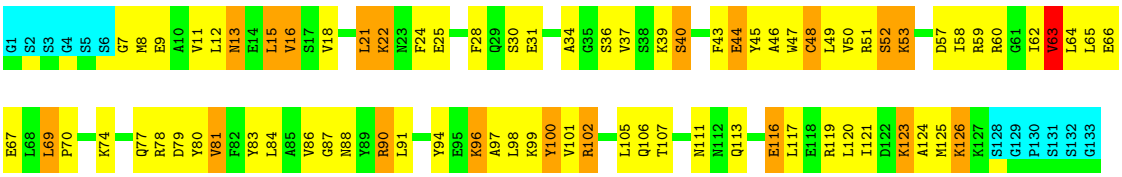
Chain A: 33% 48% 10% 9%



4.2.8 Score per residue for model 8

- Molecule 1: Hypothetical protein (2010003O14)

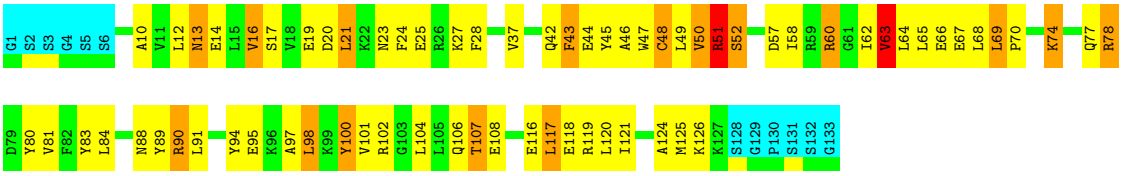
Chain A: 32% 44% 14% • 9%



4.2.9 Score per residue for model 9

- Molecule 1: Hypothetical protein (2010003O14)

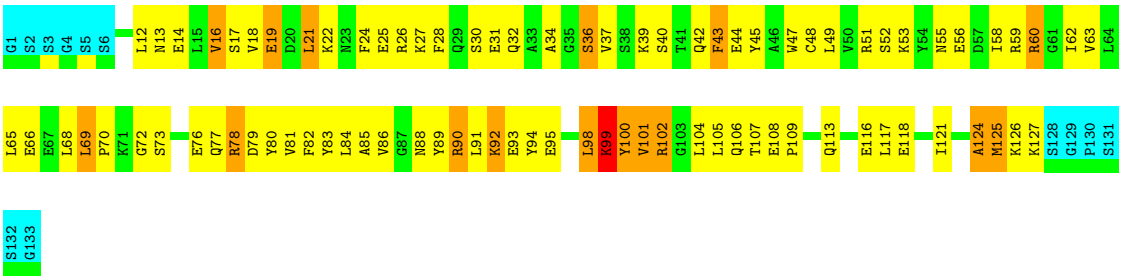
Chain A: 39% 38% 12% • 9%



4.2.10 Score per residue for model 10

- Molecule 1: Hypothetical protein (2010003O14)

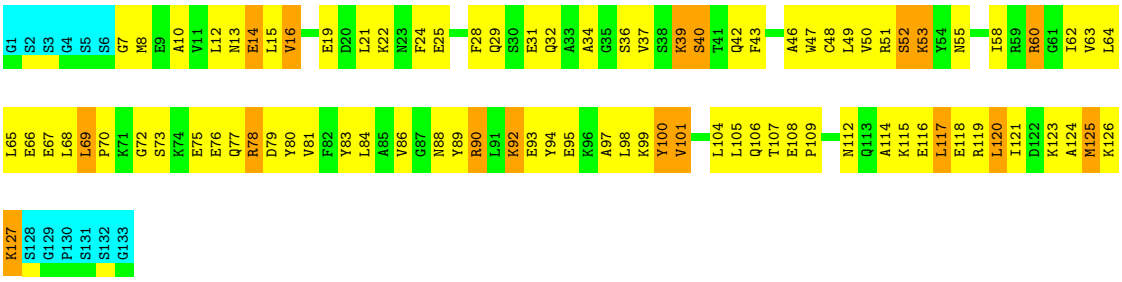
Chain A: 27% 51% 12% • 9%



4.2.11 Score per residue for model 11

- Molecule 1: Hypothetical protein (2010003O14)

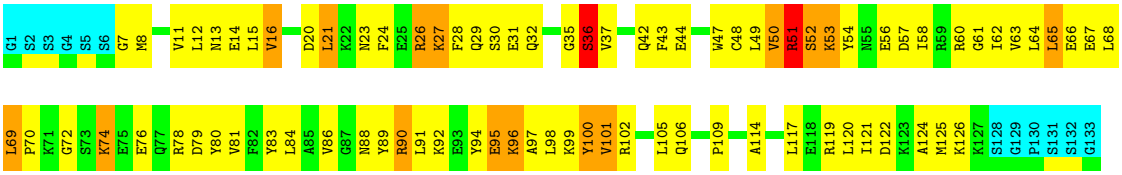
Chain A: 25% 53% 13% 9%



4.2.12 Score per residue for model 12 (medoid)

- Molecule 1: Hypothetical protein (2010003O14)

Chain A: 29% 50% 11% • 9%



4.2.13 Score per residue for model 13

- Molecule 1: Hypothetical protein (2010003O14)

Chain A: 26% 51% 11% • 9%

G1 S2 S3 G4 S5 S6 G7 M8 L12 N13 E14 L15 V16 K22 N23 F24 E25 R26 K27 F28 Q29 S30 E31 Q32 A33 A34 G35 S36 V37 S38 K39 F43 E44 Y45 A46 W47 C48 L49 V50 R51 S52 K53 Y54 N55 I58 R59 R60 G61 I62 V63 L64 L65 E66 E67 L68 L69

P70 K71 G72 S73 K74 Q77 R78 D79 Y80 V81 F82 Y83 L84 A85 V86 G87 N88 Y89 R90 L91 Y94 E95 K96 A97 L98 K99 Y100 V101 R102 G103 L104 L105 Q106 T107 E108 P109 Q113 A114 K115 E116 L117 E118 R119 L120 I121 D122 K123 A124 M125 K126 K127 S128 G129 P130 S131 S132 G133

4.2.14 Score per residue for model 14

- Molecule 1: Hypothetical protein (2010003O14)

Chain A: 35% 40% 15% • 9%

G1 S2 S3 G4 S5 S6 G7 M8 N13 E14 L15 V16 S17 V18 E19 D20 N23 F24 E25 R26 K27 F28 S36 V37 S38 K39 F43 E44 Y45 A46 W47 C48 L49 V50 R51 S52 K53 I58 R59 R60 G61 I62 V63 L64 L65 E66 E67 L68 L69 P70 S73 K74 R78

D79 Y80 V81 F82 Y83 L84 A85 V86 G87 N88 Y89 R90 L91 K92 E93 Y94 E95 K96 A97 L98 K99 Y100 V101 R102 L105 Q106 T107 E108 P109 Q113 A114 K115 E116 L117 E118 R119 L120 I121 D122 K123 A124 M125 K126 K127 S128 G129 P130 S131 S132 G133

4.2.15 Score per residue for model 15

- Molecule 1: Hypothetical protein (2010003O14)

Chain A: 32% 44% 14% • 9%

G1 S2 S3 G4 S5 S6 G7 M8 N13 E14 L15 V16 S17 V18 E19 D20 L21 K22 N23 F24 E25 R26 Q29 S30 E31 Q32 A33 A34 G35 S36 S40 T41 Q42 F43 W47 C48 L49 V50 R51 S52 K53 Y54 D57 I58 R59 R60 G61 I62 V63 L64 L65 E66 E67 L68 L69

P70 S73 K74 E75 E76 Q77 R78 D79 Y80 V81 F82 Y83 L84 G87 N88 Y89 R90 L91 K92 E93 Y94 E95 K96 A97 L98 K99 Y100 V101 R102 G103 L104 L105 Q106 T107 E108 N112 Q113 A114 K115 E116 L117 I121 M125 K126 K127 S128 G129 P130 S131 S132 G133

4.2.16 Score per residue for model 16

- Molecule 1: Hypothetical protein (2010003O14)

Chain A: 37% 41% 13% 9%

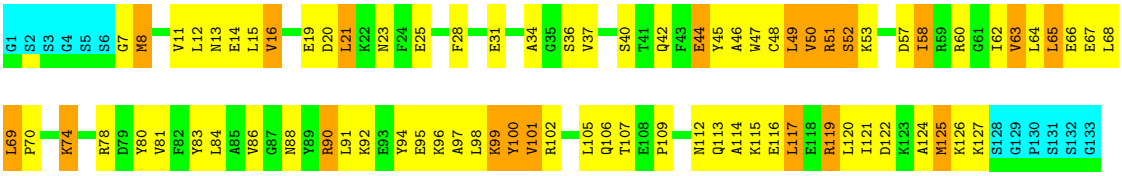
G1 S2 S3 G4 S5 S6 G7 M8 L12 N13 V16 S17 D20 L21 K22 N23 F24 E25 R26 Q29 S30 E31 Q32 A33 A34 K39 S40 F43 E44 Y45 A46 W47 C48 L49 V50 R51 S52 K53 Y54 N55 E56 D57 I58 R59 R60 G61 I62 V63 L64 L65 E66 E67 L68 L69

P70 S73 Y80 V81 F82 Y83 L84 A85 V86 R90 L91 K92 E93 Y94 L98 K99 Y100 V101 R102 L105 Q106 T107 E108 P109 N112 Q113 A114 K115 E116 L117 L120 K123 A124 M125 S128 G129 P130 S131 S132 G133

4.2.17 Score per residue for model 17

• Molecule 1: Hypothetical protein (2010003O14)

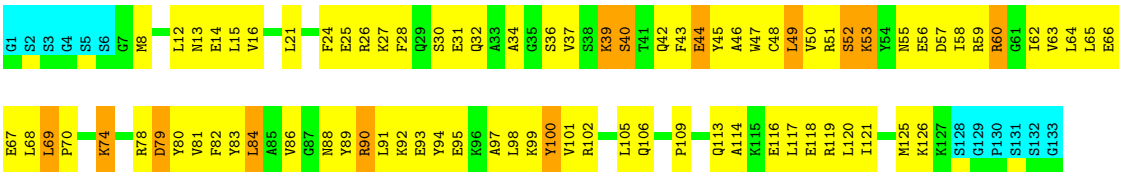
Chain A: 31% 45% 15% 9%



4.2.18 Score per residue for model 18

• Molecule 1: Hypothetical protein (2010003O14)

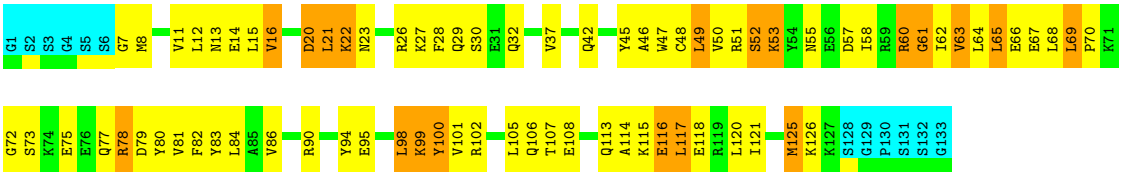
Chain A: 29% 53% 10% 9%



4.2.19 Score per residue for model 19

• Molecule 1: Hypothetical protein (2010003O14)

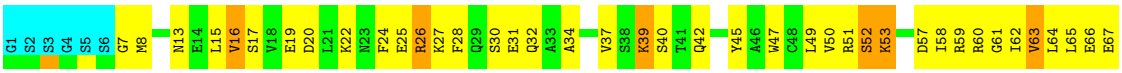
Chain A: 33% 44% 14% 9%

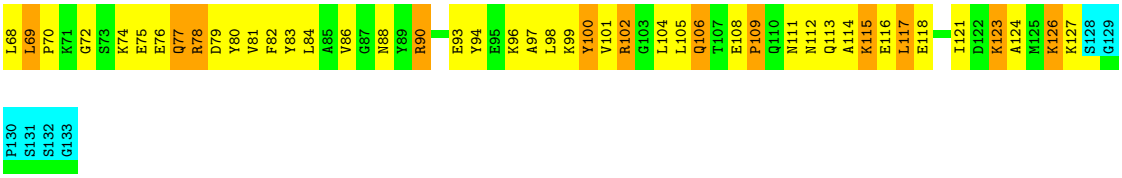


4.2.20 Score per residue for model 20

• Molecule 1: Hypothetical protein (2010003O14)

Chain A: 27% 50% 14% 9%




L68
L69
P70
K71
G72
S73
K74
E75
E76
Q77
R78
D79
Y80
V81
F82
Y83
L84
A85
V86
G87
N88
Y89
R90
E93
Y94
E95
K96
A97
L98
K99
Y100
V101
R102
G103
L104
L105
Q106
T107
E108
P109
Q110
N111
N112
Q113
A114
K115
E116
L117
E118
T121
D122
K123
A124
M125
K126
K127
S128
G129
P130
S131
S132
G133

5 Refinement protocol and experimental data overview (i)

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *The submitted conformer models are those with the lowest number of target function.*

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

Software name	Classification	Version
CYANA	structure solution	1.0.6
CYANA	refinement	1.0.6

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	997	1009	1009	89±9
All	All	19940	20180	20180	1778

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 44.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:46:ALA:HB2	1:A:64:LEU:HD12	1.03	1.30	17	8
1:A:84:LEU:HD13	1:A:100:TYR:CE2	1.02	1.88	5	4
1:A:84:LEU:HD13	1:A:100:TYR:CE1	1.01	1.90	13	1
1:A:117:LEU:HD22	1:A:121:ILE:HD11	1.00	1.29	14	11
1:A:84:LEU:HD13	1:A:100:TYR:CZ	0.97	1.94	5	4
1:A:45:TYR:CE2	1:A:49:LEU:HD21	0.96	1.94	18	3
1:A:28:PHE:CD1	1:A:37:VAL:HG11	0.92	1.98	3	12
1:A:62:ILE:HG23	1:A:84:LEU:HD21	0.91	1.43	11	4
1:A:105:LEU:CD2	1:A:114:ALA:HB1	0.87	1.99	5	8
1:A:47:TRP:CE3	1:A:83:TYR:CD2	0.86	2.64	17	18
1:A:81:VAL:HG12	1:A:100:TYR:O	0.84	1.71	13	1
1:A:105:LEU:HD22	1:A:114:ALA:HB1	0.84	1.49	5	9
1:A:12:LEU:HD21	1:A:89:TYR:CE2	0.84	2.08	3	3
1:A:47:TRP:CZ3	1:A:83:TYR:CD1	0.83	2.67	13	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:12:LEU:HD21	1:A:89:TYR:CE1	0.83	2.09	5	2
1:A:66:GLU:HG3	1:A:84:LEU:HD21	0.82	1.51	5	4
1:A:16:VAL:HG12	1:A:52:SER:HA	0.81	1.52	16	15
1:A:45:TYR:O	1:A:49:LEU:HD22	0.81	1.76	19	4
1:A:8:MET:SD	1:A:12:LEU:HD13	0.80	2.16	4	1
1:A:60:ARG:O	1:A:63:VAL:HG22	0.80	1.77	14	4
1:A:62:ILE:HG23	1:A:84:LEU:CD2	0.80	2.05	5	5
1:A:94:TYR:CD1	1:A:121:ILE:HG23	0.79	2.13	1	10
1:A:61:GLY:O	1:A:65:LEU:HD22	0.79	1.78	19	2
1:A:21:LEU:HD12	1:A:48:CYS:HB3	0.78	1.53	19	1
1:A:45:TYR:CZ	1:A:49:LEU:HD21	0.78	2.12	18	1
1:A:47:TRP:CE3	1:A:83:TYR:CG	0.78	2.71	15	20
1:A:47:TRP:CD2	1:A:83:TYR:CE2	0.77	2.72	7	16
1:A:69:LEU:HD23	1:A:77:GLN:HG2	0.77	1.55	11	4
1:A:81:VAL:HG13	1:A:100:TYR:CD1	0.77	2.15	12	19
1:A:45:TYR:CE2	1:A:49:LEU:HD11	0.77	2.15	1	2
1:A:117:LEU:HD22	1:A:121:ILE:CD1	0.76	2.09	9	11
1:A:50:VAL:HG13	1:A:61:GLY:HA3	0.76	1.55	16	1
1:A:55:ASN:HA	1:A:58:ILE:HD12	0.76	1.58	19	6
1:A:47:TRP:CZ3	1:A:83:TYR:CG	0.76	2.74	12	12
1:A:62:ILE:HG22	1:A:66:GLU:CD	0.76	2.00	3	4
1:A:60:ARG:O	1:A:63:VAL:HG12	0.76	1.80	19	1
1:A:45:TYR:CZ	1:A:49:LEU:HD11	0.75	2.16	6	3
1:A:15:LEU:HD22	1:A:53:LYS:CB	0.75	2.12	6	8
1:A:59:ARG:O	1:A:63:VAL:HG23	0.74	1.83	18	1
1:A:107:THR:HG23	1:A:108:GLU:HG2	0.74	1.59	4	8
1:A:59:ARG:O	1:A:63:VAL:HG13	0.74	1.83	16	2
1:A:42:GLN:HG2	1:A:68:LEU:HD11	0.73	1.59	11	7
1:A:83:TYR:HA	1:A:86:VAL:HG12	0.73	1.60	18	5
1:A:78:ARG:NH1	1:A:107:THR:HG21	0.73	1.97	14	3
1:A:94:TYR:CZ	1:A:124:ALA:HB1	0.73	2.18	8	1
1:A:105:LEU:HD21	1:A:114:ALA:HB1	0.73	1.61	3	8
1:A:47:TRP:CG	1:A:83:TYR:CE2	0.72	2.77	20	12
1:A:84:LEU:HD22	1:A:100:TYR:CZ	0.72	2.20	13	10
1:A:47:TRP:CD2	1:A:83:TYR:CZ	0.71	2.78	7	14
1:A:28:PHE:CE1	1:A:42:GLN:CG	0.70	2.74	10	1
1:A:16:VAL:HG21	1:A:48:CYS:O	0.70	1.85	15	1
1:A:47:TRP:CE3	1:A:83:TYR:CD1	0.70	2.80	11	12
1:A:58:ILE:HG22	1:A:91:LEU:HD12	0.70	1.63	3	1
1:A:8:MET:HG2	1:A:120:LEU:HD11	0.69	1.63	12	8
1:A:12:LEU:CD2	1:A:89:TYR:CE2	0.69	2.75	9	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:58:ILE:HG21	1:A:91:LEU:CD1	0.69	2.16	16	3
1:A:12:LEU:HD13	1:A:86:VAL:HG22	0.69	1.63	18	1
1:A:30:SER:O	1:A:34:ALA:HB2	0.69	1.88	18	4
1:A:15:LEU:HD22	1:A:53:LYS:HB3	0.69	1.63	4	8
1:A:84:LEU:HD22	1:A:100:TYR:CE2	0.68	2.23	18	2
1:A:63:VAL:HG23	1:A:64:LEU:HD23	0.68	1.65	16	7
1:A:39:LYS:HB2	1:A:68:LEU:HD22	0.68	1.64	20	1
1:A:69:LEU:HD23	1:A:77:GLN:CG	0.68	2.18	11	4
1:A:28:PHE:CE1	1:A:37:VAL:HG11	0.68	2.24	3	10
1:A:98:LEU:HD22	1:A:102:ARG:HD2	0.68	1.64	20	2
1:A:94:TYR:CE1	1:A:124:ALA:HB1	0.67	2.24	20	3
1:A:62:ILE:HG22	1:A:66:GLU:OE2	0.67	1.90	18	3
1:A:69:LEU:CD1	1:A:84:LEU:HD12	0.67	2.20	11	1
1:A:21:LEU:C	1:A:21:LEU:HD13	0.67	2.10	16	3
1:A:58:ILE:HD13	1:A:90:ARG:HB3	0.66	1.67	14	17
1:A:49:LEU:HD13	1:A:60:ARG:HB3	0.66	1.65	6	5
1:A:61:GLY:O	1:A:65:LEU:HD12	0.66	1.91	7	2
1:A:63:VAL:CG2	1:A:64:LEU:HD23	0.66	2.20	20	3
1:A:8:MET:SD	1:A:12:LEU:HD22	0.66	2.31	4	1
1:A:46:ALA:HB2	1:A:64:LEU:CD1	0.65	2.14	17	1
1:A:117:LEU:HA	1:A:120:LEU:HD12	0.65	1.67	3	8
1:A:21:LEU:HD11	1:A:49:LEU:HD23	0.64	1.69	10	3
1:A:69:LEU:CD1	1:A:84:LEU:HD22	0.64	2.22	15	2
1:A:58:ILE:CG2	1:A:91:LEU:HD12	0.64	2.23	3	1
1:A:105:LEU:HD23	1:A:108:GLU:O	0.64	1.92	2	4
1:A:16:VAL:HG13	1:A:17:SER:N	0.64	2.07	4	3
1:A:15:LEU:HD13	1:A:53:LYS:HB3	0.64	1.68	3	7
1:A:65:LEU:HB3	1:A:84:LEU:HD11	0.64	1.68	16	11
1:A:65:LEU:HD22	1:A:80:TYR:HA	0.63	1.70	6	2
1:A:62:ILE:HG22	1:A:66:GLU:HG3	0.63	1.69	14	2
1:A:42:GLN:HB3	1:A:68:LEU:HD21	0.63	1.69	19	3
1:A:84:LEU:HD23	1:A:100:TYR:CZ	0.63	2.28	20	10
1:A:102:ARG:HA	1:A:105:LEU:HD12	0.63	1.69	13	1
1:A:8:MET:HA	1:A:11:VAL:HG12	0.63	1.70	4	3
1:A:84:LEU:HD13	1:A:100:TYR:HE1	0.63	1.45	13	1
1:A:49:LEU:HD22	1:A:57:ASP:O	0.63	1.93	15	1
1:A:47:TRP:CE3	1:A:83:TYR:CE2	0.62	2.86	17	6
1:A:84:LEU:CD2	1:A:100:TYR:CZ	0.61	2.82	16	16
1:A:12:LEU:CD2	1:A:120:LEU:HD12	0.61	2.24	11	1
1:A:98:LEU:HD12	1:A:102:ARG:CD	0.61	2.25	15	1
1:A:16:VAL:HG21	1:A:48:CYS:SG	0.61	2.35	16	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:28:PHE:CD2	1:A:45:TYR:CD2	0.61	2.87	20	2
1:A:84:LEU:HD22	1:A:100:TYR:HE2	0.61	1.54	18	1
1:A:66:GLU:CG	1:A:84:LEU:HD11	0.61	2.25	11	2
1:A:82:PHE:O	1:A:86:VAL:HG23	0.61	1.96	6	2
1:A:84:LEU:HD23	1:A:100:TYR:CE2	0.61	2.31	16	12
1:A:47:TRP:CH2	1:A:83:TYR:CD1	0.60	2.89	13	6
1:A:43:PHE:HB2	1:A:68:LEU:HD13	0.60	1.71	13	7
1:A:85:ALA:HB2	1:A:100:TYR:HB3	0.60	1.73	13	1
1:A:58:ILE:HG21	1:A:91:LEU:HB2	0.60	1.72	2	1
1:A:66:GLU:HG2	1:A:84:LEU:HD11	0.60	1.74	11	2
1:A:91:LEU:HD12	1:A:91:LEU:O	0.60	1.95	9	2
1:A:16:VAL:HG23	1:A:51:ARG:NH2	0.60	2.11	15	2
1:A:28:PHE:O	1:A:37:VAL:HG22	0.60	1.97	5	7
1:A:62:ILE:HG22	1:A:66:GLU:OE1	0.59	1.97	11	6
1:A:58:ILE:HG21	1:A:87:GLY:O	0.59	1.97	13	4
1:A:85:ALA:CB	1:A:101:VAL:HG23	0.59	2.27	13	2
1:A:49:LEU:HD13	1:A:60:ARG:HG3	0.59	1.73	15	2
1:A:58:ILE:HG21	1:A:91:LEU:CB	0.59	2.27	2	1
1:A:24:PHE:CE2	1:A:48:CYS:SG	0.59	2.95	12	3
1:A:93:GLU:O	1:A:97:ALA:HB2	0.59	1.98	14	2
1:A:45:TYR:CD2	1:A:49:LEU:HD21	0.59	2.32	18	1
1:A:59:ARG:O	1:A:63:VAL:HG12	0.59	1.98	8	3
1:A:65:LEU:CB	1:A:84:LEU:HD11	0.59	2.28	3	7
1:A:47:TRP:CH2	1:A:83:TYR:CE1	0.59	2.91	17	7
1:A:39:LYS:HE2	1:A:68:LEU:HD23	0.59	1.73	18	1
1:A:12:LEU:HD21	1:A:86:VAL:HG22	0.58	1.74	8	1
1:A:62:ILE:O	1:A:66:GLU:N	0.58	2.32	7	14
1:A:21:LEU:HD12	1:A:48:CYS:CB	0.58	2.27	19	1
1:A:12:LEU:HD13	1:A:86:VAL:CG2	0.58	2.27	18	3
1:A:8:MET:CG	1:A:120:LEU:HD11	0.58	2.28	12	1
1:A:46:ALA:CB	1:A:64:LEU:HD12	0.58	2.18	17	6
1:A:66:GLU:CG	1:A:84:LEU:HD21	0.58	2.29	15	5
1:A:12:LEU:HD22	1:A:120:LEU:HD12	0.58	1.74	11	1
1:A:98:LEU:HD12	1:A:102:ARG:HD3	0.58	1.75	15	2
1:A:24:PHE:CD2	1:A:48:CYS:SG	0.58	2.97	15	7
1:A:84:LEU:CD1	1:A:100:TYR:CE1	0.58	2.80	13	1
1:A:104:LEU:HD13	1:A:104:LEU:O	0.57	1.99	6	2
1:A:69:LEU:CD2	1:A:84:LEU:CD1	0.57	2.82	18	2
1:A:16:VAL:HG12	1:A:52:SER:CA	0.57	2.29	16	4
1:A:58:ILE:HG21	1:A:91:LEU:HD13	0.57	1.76	6	2
1:A:81:VAL:HG11	1:A:100:TYR:O	0.57	2.00	20	19

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:117:LEU:HG	1:A:121:ILE:HD11	0.57	1.76	8	3
1:A:45:TYR:CE1	1:A:49:LEU:HD11	0.57	2.34	18	1
1:A:69:LEU:CD1	1:A:84:LEU:CD2	0.57	2.83	15	3
1:A:101:VAL:HG13	1:A:105:LEU:HD12	0.57	1.75	8	1
1:A:78:ARG:HH11	1:A:107:THR:HG21	0.57	1.60	14	1
1:A:98:LEU:O	1:A:102:ARG:N	0.56	2.36	15	12
1:A:21:LEU:HD13	1:A:21:LEU:O	0.56	1.99	7	7
1:A:91:LEU:CD1	1:A:91:LEU:N	0.56	2.68	15	1
1:A:101:VAL:O	1:A:105:LEU:HD23	0.56	2.00	20	6
1:A:63:VAL:CG2	1:A:64:LEU:N	0.56	2.69	15	4
1:A:43:PHE:CZ	1:A:83:TYR:CE2	0.56	2.94	16	1
1:A:42:GLN:OE1	1:A:68:LEU:HD21	0.56	2.00	20	1
1:A:121:ILE:HA	1:A:124:ALA:HB3	0.56	1.78	2	3
1:A:47:TRP:CE2	1:A:83:TYR:CZ	0.56	2.93	5	11
1:A:12:LEU:HD13	1:A:89:TYR:CE2	0.56	2.35	10	2
1:A:21:LEU:HD11	1:A:49:LEU:HD13	0.56	1.78	19	1
1:A:58:ILE:HG22	1:A:91:LEU:HD11	0.56	1.76	18	5
1:A:117:LEU:CD2	1:A:121:ILE:CD1	0.55	2.84	11	1
1:A:117:LEU:CD2	1:A:121:ILE:HD11	0.55	2.31	11	3
1:A:111:ASN:O	1:A:113:GLN:N	0.55	2.38	20	1
1:A:101:VAL:HG12	1:A:102:ARG:N	0.55	2.16	20	7
1:A:94:TYR:OH	1:A:124:ALA:HB1	0.55	2.01	8	1
1:A:81:VAL:CG1	1:A:100:TYR:O	0.55	2.54	18	19
1:A:62:ILE:O	1:A:63:VAL:C	0.55	2.45	9	10
1:A:77:GLN:O	1:A:81:VAL:HG23	0.55	2.01	5	2
1:A:62:ILE:HG23	1:A:84:LEU:HD23	0.54	1.78	5	2
1:A:21:LEU:C	1:A:21:LEU:CD1	0.54	2.75	16	2
1:A:94:TYR:CD2	1:A:125:MET:HB3	0.54	2.37	10	1
1:A:65:LEU:O	1:A:69:LEU:HD23	0.54	2.02	13	4
1:A:91:LEU:O	1:A:92:LYS:CG	0.54	2.56	15	6
1:A:31:GLU:CB	1:A:37:VAL:HB	0.54	2.32	18	4
1:A:21:LEU:HD21	1:A:49:LEU:CD1	0.54	2.33	17	2
1:A:104:LEU:HD11	1:A:108:GLU:OE1	0.54	2.01	5	1
1:A:21:LEU:HD21	1:A:49:LEU:HD13	0.54	1.79	18	1
1:A:21:LEU:HD11	1:A:49:LEU:CD2	0.54	2.32	4	2
1:A:78:ARG:NH1	1:A:107:THR:CG2	0.54	2.69	14	1
1:A:28:PHE:CE1	1:A:42:GLN:HG2	0.54	2.38	10	1
1:A:60:ARG:O	1:A:62:ILE:N	0.53	2.42	15	7
1:A:21:LEU:HD21	1:A:49:LEU:HD23	0.53	1.79	9	2
1:A:98:LEU:HD12	1:A:125:MET:HE2	0.53	1.80	5	1
1:A:16:VAL:HG23	1:A:51:ARG:CZ	0.53	2.34	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:94:TYR:CD2	1:A:125:MET:HG2	0.53	2.39	12	15
1:A:47:TRP:CZ3	1:A:83:TYR:CE1	0.53	2.96	7	3
1:A:8:MET:CE	1:A:11:VAL:CG1	0.53	2.86	4	1
1:A:69:LEU:HD23	1:A:77:GLN:CD	0.52	2.23	19	4
1:A:80:TYR:O	1:A:83:TYR:N	0.52	2.42	2	13
1:A:69:LEU:CB	1:A:70:PRO:HD3	0.52	2.34	13	20
1:A:78:ARG:O	1:A:104:LEU:HD21	0.52	2.04	20	1
1:A:49:LEU:O	1:A:52:SER:N	0.52	2.43	7	14
1:A:94:TYR:O	1:A:97:ALA:HB3	0.52	2.04	3	1
1:A:76:GLU:O	1:A:80:TYR:CG	0.52	2.63	12	2
1:A:66:GLU:CG	1:A:84:LEU:CD2	0.52	2.88	15	4
1:A:94:TYR:CZ	1:A:124:ALA:CB	0.52	2.91	8	1
1:A:121:ILE:O	1:A:124:ALA:HB3	0.52	2.05	9	1
1:A:60:ARG:O	1:A:63:VAL:CG2	0.52	2.57	10	3
1:A:31:GLU:O	1:A:34:ALA:HB3	0.52	2.05	16	8
1:A:67:GLU:O	1:A:71:LYS:CG	0.52	2.58	2	1
1:A:46:ALA:HB1	1:A:65:LEU:HD13	0.52	1.82	18	1
1:A:79:ASP:O	1:A:83:TYR:CD2	0.52	2.63	18	2
1:A:39:LYS:CE	1:A:68:LEU:CD2	0.52	2.88	18	1
1:A:43:PHE:CE2	1:A:83:TYR:CE2	0.51	2.98	9	1
1:A:64:LEU:N	1:A:64:LEU:HD23	0.51	2.21	8	5
1:A:43:PHE:CE1	1:A:83:TYR:CE2	0.51	2.98	4	3
1:A:26:ARG:O	1:A:30:SER:CB	0.51	2.59	18	3
1:A:49:LEU:O	1:A:52:SER:CB	0.51	2.58	10	7
1:A:65:LEU:O	1:A:69:LEU:HD22	0.51	2.06	6	2
1:A:80:TYR:O	1:A:81:VAL:C	0.51	2.48	8	16
1:A:12:LEU:CD2	1:A:86:VAL:HG13	0.51	2.36	12	2
1:A:78:ARG:O	1:A:104:LEU:CD2	0.51	2.57	20	1
1:A:58:ILE:CG2	1:A:91:LEU:CD1	0.51	2.88	16	2
1:A:7:GLY:O	1:A:11:VAL:CG2	0.51	2.59	8	1
1:A:47:TRP:CE2	1:A:51:ARG:CD	0.51	2.94	18	1
1:A:12:LEU:CD1	1:A:86:VAL:HG13	0.51	2.36	11	1
1:A:12:LEU:CD1	1:A:86:VAL:CG2	0.51	2.89	13	2
1:A:66:GLU:O	1:A:70:PRO:CD	0.51	2.59	11	3
1:A:117:LEU:CA	1:A:120:LEU:HD12	0.51	2.35	3	1
1:A:63:VAL:HG23	1:A:64:LEU:N	0.51	2.21	12	2
1:A:57:ASP:O	1:A:60:ARG:N	0.51	2.44	17	4
1:A:47:TRP:HB2	1:A:83:TYR:CE2	0.50	2.41	11	5
1:A:105:LEU:HG	1:A:114:ALA:HB1	0.50	1.82	2	2
1:A:58:ILE:CG2	1:A:91:LEU:HD11	0.50	2.36	7	4
1:A:84:LEU:CD2	1:A:100:TYR:OH	0.50	2.60	9	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:97:ALA:O	1:A:101:VAL:N	0.50	2.42	8	6
1:A:61:GLY:O	1:A:65:LEU:CD1	0.50	2.59	15	2
1:A:29:GLN:O	1:A:32:GLN:CB	0.50	2.60	12	5
1:A:28:PHE:O	1:A:37:VAL:CG2	0.50	2.60	12	4
1:A:69:LEU:HD21	1:A:84:LEU:HD12	0.50	1.84	13	3
1:A:94:TYR:CE1	1:A:124:ALA:CB	0.50	2.95	20	3
1:A:75:GLU:O	1:A:78:ARG:CD	0.50	2.60	20	1
1:A:65:LEU:HD21	1:A:83:TYR:CB	0.50	2.37	1	4
1:A:116:GLU:O	1:A:119:ARG:N	0.50	2.45	4	4
1:A:91:LEU:O	1:A:91:LEU:CD1	0.49	2.60	9	2
1:A:127:LYS:CG	1:A:127:LYS:O	0.49	2.60	2	1
1:A:47:TRP:CE3	1:A:50:VAL:CG2	0.49	2.95	17	10
1:A:63:VAL:HG13	1:A:64:LEU:HD23	0.49	1.82	19	1
1:A:18:VAL:HG13	1:A:19:GLU:N	0.49	2.22	1	7
1:A:16:VAL:CG1	1:A:17:SER:N	0.49	2.75	4	2
1:A:101:VAL:O	1:A:105:LEU:CD2	0.49	2.60	20	1
1:A:77:GLN:HA	1:A:80:TYR:CD2	0.49	2.42	5	7
1:A:7:GLY:O	1:A:11:VAL:HG23	0.49	2.07	8	1
1:A:12:LEU:HD13	1:A:86:VAL:HG23	0.49	1.84	13	2
1:A:57:ASP:O	1:A:58:ILE:C	0.49	2.49	17	4
1:A:21:LEU:HD22	1:A:48:CYS:HB3	0.49	1.83	9	1
1:A:39:LYS:CD	1:A:40:SER:N	0.49	2.75	11	1
1:A:104:LEU:HD13	1:A:108:GLU:HB2	0.49	1.83	20	1
1:A:94:TYR:O	1:A:98:LEU:HD22	0.49	2.07	9	1
1:A:84:LEU:HB3	1:A:100:TYR:CD2	0.49	2.42	18	2
1:A:47:TRP:NE1	1:A:51:ARG:CD	0.49	2.76	18	1
1:A:47:TRP:HB2	1:A:83:TYR:CD2	0.49	2.41	20	1
1:A:28:PHE:CZ	1:A:42:GLN:HG2	0.49	2.43	10	1
1:A:119:ARG:O	1:A:122:ASP:CB	0.49	2.60	12	3
1:A:98:LEU:O	1:A:100:TYR:N	0.49	2.46	15	16
1:A:53:LYS:HE2	1:A:54:TYR:CD1	0.49	2.43	15	1
1:A:98:LEU:O	1:A:101:VAL:N	0.48	2.46	20	19
1:A:62:ILE:CG2	1:A:66:GLU:OE2	0.48	2.61	6	3
1:A:69:LEU:CD2	1:A:84:LEU:HD12	0.48	2.38	13	4
1:A:39:LYS:CG	1:A:68:LEU:HD22	0.48	2.37	10	1
1:A:18:VAL:CG1	1:A:19:GLU:N	0.48	2.76	2	7
1:A:57:ASP:O	1:A:61:GLY:N	0.48	2.47	1	2
1:A:12:LEU:HG	1:A:89:TYR:CE2	0.48	2.44	4	1
1:A:98:LEU:HD12	1:A:125:MET:CE	0.48	2.38	8	2
1:A:97:ALA:O	1:A:100:TYR:N	0.48	2.45	13	1
1:A:46:ALA:HB3	1:A:65:LEU:HD13	0.48	1.85	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:25:GLU:HG3	1:A:45:TYR:CE1	0.48	2.42	6	7
1:A:47:TRP:CZ2	1:A:51:ARG:HD3	0.48	2.44	19	2
1:A:84:LEU:HD13	1:A:100:TYR:OH	0.48	2.08	11	3
1:A:98:LEU:CD2	1:A:121:ILE:HG21	0.48	2.38	18	2
1:A:84:LEU:O	1:A:88:ASN:ND2	0.48	2.47	13	17
1:A:46:ALA:CB	1:A:65:LEU:HD13	0.48	2.39	16	2
1:A:21:LEU:O	1:A:25:GLU:CB	0.48	2.62	15	2
1:A:61:GLY:C	1:A:65:LEU:HD22	0.48	2.29	19	1
1:A:65:LEU:O	1:A:69:LEU:CD2	0.48	2.62	13	5
1:A:65:LEU:CB	1:A:84:LEU:CD1	0.48	2.92	3	5
1:A:46:ALA:HB2	1:A:64:LEU:HB2	0.47	1.84	9	4
1:A:53:LYS:HD2	1:A:54:TYR:CE1	0.47	2.44	13	3
1:A:47:TRP:O	1:A:50:VAL:HG23	0.47	2.08	7	2
1:A:43:PHE:N	1:A:68:LEU:HD11	0.47	2.25	5	3
1:A:86:VAL:HB	1:A:117:LEU:HD11	0.47	1.84	14	1
1:A:83:TYR:O	1:A:86:VAL:N	0.47	2.47	12	9
1:A:53:LYS:HD2	1:A:54:TYR:CD1	0.47	2.45	6	4
1:A:68:LEU:HB3	1:A:80:TYR:CE2	0.47	2.44	18	1
1:A:105:LEU:O	1:A:109:PRO:N	0.47	2.48	3	11
1:A:86:VAL:HG23	1:A:117:LEU:HD11	0.47	1.86	10	2
1:A:43:PHE:CD2	1:A:44:GLU:N	0.47	2.83	8	1
1:A:21:LEU:O	1:A:21:LEU:HD13	0.47	2.09	15	1
1:A:39:LYS:CE	1:A:68:LEU:HD23	0.47	2.40	18	1
1:A:49:LEU:HD22	1:A:57:ASP:HB3	0.47	1.87	4	2
1:A:62:ILE:O	1:A:65:LEU:N	0.47	2.47	17	4
1:A:84:LEU:CD1	1:A:100:TYR:CZ	0.47	2.86	11	2
1:A:44:GLU:O	1:A:47:TRP:N	0.47	2.47	17	4
1:A:49:LEU:O	1:A:51:ARG:N	0.47	2.45	15	5
1:A:59:ARG:HD3	1:A:91:LEU:HD13	0.47	1.85	13	1
1:A:93:GLU:O	1:A:97:ALA:CB	0.47	2.63	20	2
1:A:58:ILE:HD11	1:A:90:ARG:HD2	0.47	1.86	18	1
1:A:65:LEU:HD21	1:A:83:TYR:HB3	0.47	1.87	1	2
1:A:58:ILE:CG2	1:A:91:LEU:CD2	0.47	2.92	5	1
1:A:98:LEU:HD23	1:A:121:ILE:HG21	0.47	1.86	18	3
1:A:11:VAL:HG13	1:A:12:LEU:N	0.47	2.25	12	4
1:A:47:TRP:CD2	1:A:83:TYR:CD2	0.47	3.01	2	4
1:A:117:LEU:O	1:A:120:LEU:N	0.47	2.48	18	4
1:A:82:PHE:CE1	1:A:113:GLN:HB3	0.47	2.45	15	3
1:A:47:TRP:CE3	1:A:50:VAL:HG23	0.47	2.45	16	3
1:A:94:TYR:CE2	1:A:125:MET:HA	0.47	2.45	10	6
1:A:22:LYS:CD	1:A:22:LYS:C	0.46	2.83	16	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:28:PHE:O	1:A:32:GLN:N	0.46	2.48	18	4
1:A:104:LEU:O	1:A:108:GLU:N	0.46	2.47	15	2
1:A:43:PHE:CB	1:A:68:LEU:HD13	0.46	2.40	13	1
1:A:98:LEU:C	1:A:100:TYR:N	0.46	2.68	15	16
1:A:46:ALA:O	1:A:61:GLY:CA	0.46	2.62	7	2
1:A:92:LYS:HG2	1:A:94:TYR:CZ	0.46	2.45	12	1
1:A:62:ILE:HG23	1:A:66:GLU:HG3	0.46	1.87	19	1
1:A:63:VAL:HG13	1:A:64:LEU:CD2	0.46	2.40	19	1
1:A:69:LEU:O	1:A:77:GLN:NE2	0.46	2.49	6	5
1:A:18:VAL:O	1:A:22:LYS:CG	0.46	2.63	8	1
1:A:25:GLU:HB2	1:A:45:TYR:CE1	0.46	2.45	10	2
1:A:60:ARG:C	1:A:62:ILE:N	0.46	2.68	15	8
1:A:75:GLU:O	1:A:78:ARG:NE	0.46	2.49	11	2
1:A:58:ILE:CG2	1:A:87:GLY:O	0.46	2.63	15	1
1:A:64:LEU:O	1:A:67:GLU:N	0.46	2.48	6	5
1:A:62:ILE:CG2	1:A:66:GLU:OE1	0.46	2.63	11	1
1:A:92:LYS:HA	1:A:94:TYR:CE1	0.46	2.46	12	2
1:A:63:VAL:HG13	1:A:64:LEU:H	0.46	1.71	17	1
1:A:117:LEU:O	1:A:118:GLU:C	0.46	2.54	2	10
1:A:107:THR:HG23	1:A:108:GLU:HG3	0.46	1.88	5	1
1:A:68:LEU:O	1:A:72:GLY:N	0.46	2.49	10	5
1:A:124:ALA:O	1:A:127:LYS:N	0.46	2.49	10	2
1:A:89:TYR:O	1:A:92:LYS:N	0.46	2.47	18	9
1:A:12:LEU:HD21	1:A:86:VAL:HG13	0.46	1.87	6	2
1:A:24:PHE:CE1	1:A:44:GLU:HB3	0.46	2.46	13	2
1:A:16:VAL:HG11	1:A:21:LEU:HD23	0.46	1.86	17	2
1:A:53:LYS:HE2	1:A:54:TYR:CE1	0.46	2.46	15	1
1:A:52:SER:CB	1:A:57:ASP:OD2	0.46	2.63	1	1
1:A:58:ILE:HG22	1:A:91:LEU:CD2	0.46	2.41	5	1
1:A:35:GLY:O	1:A:36:SER:CB	0.46	2.64	12	2
1:A:82:PHE:CZ	1:A:113:GLN:HB3	0.46	2.46	10	4
1:A:39:LYS:O	1:A:43:PHE:N	0.46	2.47	10	1
1:A:78:ARG:HD3	1:A:79:ASP:N	0.46	2.26	11	2
1:A:112:ASN:O	1:A:115:LYS:N	0.45	2.49	16	7
1:A:58:ILE:CG2	1:A:91:LEU:HB2	0.45	2.41	9	2
1:A:106:GLN:CG	1:A:107:THR:N	0.45	2.78	4	1
1:A:117:LEU:O	1:A:121:ILE:HD12	0.45	2.11	4	2
1:A:42:GLN:OE1	1:A:43:PHE:N	0.45	2.49	10	1
1:A:94:TYR:O	1:A:96:LYS:N	0.45	2.49	13	1
1:A:59:ARG:HA	1:A:62:ILE:HD12	0.45	1.88	20	2
1:A:112:ASN:O	1:A:113:GLN:C	0.45	2.54	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:46:ALA:O	1:A:49:LEU:N	0.45	2.49	8	3
1:A:43:PHE:CZ	1:A:79:ASP:HB3	0.45	2.45	18	1
1:A:63:VAL:O	1:A:67:GLU:N	0.45	2.49	17	4
1:A:83:TYR:HA	1:A:86:VAL:CG1	0.45	2.40	3	4
1:A:116:GLU:O	1:A:117:LEU:C	0.45	2.54	4	12
1:A:58:ILE:O	1:A:59:ARG:C	0.45	2.54	15	4
1:A:91:LEU:O	1:A:91:LEU:CG	0.45	2.64	9	2
1:A:15:LEU:CD1	1:A:16:VAL:O	0.45	2.65	4	1
1:A:10:ALA:O	1:A:13:ASN:N	0.45	2.50	9	1
1:A:24:PHE:CD2	1:A:44:GLU:HB3	0.45	2.46	10	1
1:A:76:GLU:O	1:A:80:TYR:CD2	0.45	2.69	11	2
1:A:9:GLU:O	1:A:13:ASN:ND2	0.45	2.50	8	3
1:A:104:LEU:HD13	1:A:104:LEU:C	0.45	2.31	6	2
1:A:81:VAL:HG13	1:A:100:TYR:CG	0.45	2.45	11	2
1:A:12:LEU:HD11	1:A:117:LEU:HD13	0.45	1.89	12	1
1:A:98:LEU:O	1:A:99:LYS:C	0.45	2.55	18	16
1:A:20:ASP:O	1:A:23:ASN:N	0.45	2.50	1	6
1:A:51:ARG:O	1:A:52:SER:C	0.45	2.54	15	4
1:A:55:ASN:O	1:A:58:ILE:N	0.45	2.49	16	2
1:A:98:LEU:CD2	1:A:102:ARG:HD3	0.45	2.42	17	5
1:A:78:ARG:NH1	1:A:107:THR:OG1	0.45	2.49	14	2
1:A:119:ARG:O	1:A:120:LEU:C	0.45	2.55	4	1
1:A:24:PHE:CD1	1:A:44:GLU:HB3	0.45	2.47	9	2
1:A:12:LEU:CD1	1:A:86:VAL:HG22	0.45	2.41	3	4
1:A:8:MET:SD	1:A:12:LEU:CD1	0.45	2.99	4	1
1:A:49:LEU:HD22	1:A:57:ASP:CB	0.45	2.41	8	2
1:A:29:GLN:O	1:A:32:GLN:N	0.45	2.49	12	6
1:A:44:GLU:O	1:A:45:TYR:C	0.45	2.56	8	1
1:A:96:LYS:O	1:A:100:TYR:N	0.45	2.50	13	1
1:A:47:TRP:CE2	1:A:51:ARG:HG3	0.45	2.47	18	1
1:A:66:GLU:CG	1:A:84:LEU:HD23	0.45	2.42	12	1
1:A:48:CYS:O	1:A:49:LEU:C	0.45	2.55	19	3
1:A:94:TYR:O	1:A:95:GLU:C	0.45	2.55	9	8
1:A:44:GLU:O	1:A:48:CYS:N	0.45	2.48	8	1
1:A:74:LYS:O	1:A:76:GLU:N	0.44	2.50	2	1
1:A:101:VAL:CG1	1:A:102:ARG:N	0.44	2.79	20	2
1:A:58:ILE:HD13	1:A:90:ARG:CB	0.44	2.42	20	2
1:A:101:VAL:CG2	1:A:117:LEU:HD13	0.44	2.43	11	1
1:A:116:GLU:O	1:A:120:LEU:N	0.44	2.47	17	2
1:A:49:LEU:HD13	1:A:60:ARG:CG	0.44	2.42	15	1
1:A:8:MET:CE	1:A:11:VAL:HG11	0.44	2.43	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:74:LYS:O	1:A:78:ARG:CD	0.44	2.65	4	1
1:A:114:ALA:O	1:A:115:LYS:C	0.44	2.55	13	3
1:A:47:TRP:HA	1:A:50:VAL:HG22	0.44	1.88	15	2
1:A:39:LYS:O	1:A:40:SER:C	0.44	2.56	6	4
1:A:74:LYS:O	1:A:77:GLN:N	0.44	2.50	2	2
1:A:48:CYS:O	1:A:52:SER:N	0.44	2.51	19	2
1:A:47:TRP:CB	1:A:83:TYR:CE2	0.44	3.00	20	1
1:A:89:TYR:CD1	1:A:121:ILE:HG13	0.44	2.47	11	2
1:A:65:LEU:HD13	1:A:83:TYR:CB	0.44	2.42	5	1
1:A:55:ASN:N	1:A:55:ASN:OD1	0.44	2.50	16	1
1:A:62:ILE:O	1:A:64:LEU:N	0.44	2.50	19	1
1:A:123:LYS:O	1:A:127:LYS:N	0.44	2.50	20	1
1:A:24:PHE:CE2	1:A:44:GLU:HB3	0.44	2.47	8	3
1:A:47:TRP:O	1:A:50:VAL:CG2	0.44	2.66	17	6
1:A:88:ASN:O	1:A:91:LEU:N	0.44	2.50	15	1
1:A:87:GLY:O	1:A:91:LEU:CD1	0.44	2.66	7	1
1:A:94:TYR:C	1:A:98:LEU:HD22	0.44	2.33	9	1
1:A:55:ASN:OD1	1:A:90:ARG:NH1	0.44	2.51	11	1
1:A:66:GLU:HG3	1:A:84:LEU:CD2	0.43	2.43	15	1
1:A:45:TYR:O	1:A:48:CYS:N	0.43	2.51	18	1
1:A:60:ARG:O	1:A:61:GLY:C	0.43	2.57	15	1
1:A:63:VAL:HG22	1:A:64:LEU:HD23	0.43	1.89	1	2
1:A:60:ARG:O	1:A:63:VAL:N	0.43	2.51	3	1
1:A:74:LYS:O	1:A:78:ARG:NH1	0.43	2.51	6	1
1:A:21:LEU:O	1:A:25:GLU:N	0.43	2.48	10	2
1:A:81:VAL:O	1:A:82:PHE:C	0.43	2.57	2	3
1:A:69:LEU:CB	1:A:70:PRO:CD	0.43	2.97	13	9
1:A:94:TYR:O	1:A:98:LEU:N	0.43	2.47	5	1
1:A:123:LYS:O	1:A:126:LYS:N	0.43	2.52	14	3
1:A:47:TRP:NE1	1:A:51:ARG:NH1	0.43	2.67	17	1
1:A:15:LEU:HD12	1:A:16:VAL:O	0.43	2.13	6	1
1:A:61:GLY:O	1:A:65:LEU:CG	0.43	2.67	7	1
1:A:101:VAL:CG2	1:A:117:LEU:HD23	0.43	2.44	13	2
1:A:84:LEU:HB3	1:A:100:TYR:CD1	0.43	2.49	13	1
1:A:42:GLN:CB	1:A:68:LEU:HD21	0.43	2.43	19	1
1:A:25:GLU:HG3	1:A:45:TYR:CZ	0.43	2.49	20	1
1:A:17:SER:O	1:A:20:ASP:N	0.43	2.51	1	2
1:A:119:ARG:O	1:A:122:ASP:N	0.43	2.52	4	1
1:A:111:ASN:OD1	1:A:113:GLN:N	0.43	2.52	5	1
1:A:96:LYS:O	1:A:97:ALA:C	0.43	2.57	1	7
1:A:66:GLU:HG2	1:A:84:LEU:CD2	0.43	2.43	15	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:47:TRP:O	1:A:51:ARG:CG	0.43	2.67	14	3
1:A:10:ALA:O	1:A:14:GLU:N	0.43	2.50	11	1
1:A:78:ARG:HB2	1:A:104:LEU:CD2	0.43	2.44	11	1
1:A:16:VAL:HG21	1:A:48:CYS:CA	0.43	2.44	15	1
1:A:16:VAL:CG2	1:A:48:CYS:SG	0.43	3.05	16	1
1:A:65:LEU:HB3	1:A:84:LEU:CD1	0.43	2.43	7	8
1:A:74:LYS:C	1:A:76:GLU:N	0.43	2.71	2	1
1:A:24:PHE:C	1:A:26:ARG:N	0.43	2.72	12	3
1:A:65:LEU:HD21	1:A:83:TYR:HD2	0.43	1.73	12	1
1:A:64:LEU:HD23	1:A:64:LEU:N	0.42	2.29	1	1
1:A:104:LEU:C	1:A:104:LEU:HD13	0.42	2.34	5	2
1:A:28:PHE:CZ	1:A:42:GLN:CG	0.42	3.01	10	1
1:A:81:VAL:HG11	1:A:104:LEU:HB2	0.42	1.90	9	1
1:A:8:MET:SD	1:A:8:MET:O	0.42	2.77	4	1
1:A:65:LEU:CD2	1:A:83:TYR:HB2	0.42	2.44	18	1
1:A:62:ILE:C	1:A:64:LEU:N	0.42	2.72	19	1
1:A:64:LEU:O	1:A:68:LEU:N	0.42	2.49	6	1
1:A:25:GLU:O	1:A:29:GLN:NE2	0.42	2.52	16	1
1:A:51:ARG:O	1:A:52:SER:O	0.42	2.38	5	9
1:A:69:LEU:HD21	1:A:84:LEU:CD1	0.42	2.45	1	1
1:A:55:ASN:OD1	1:A:90:ARG:CD	0.42	2.67	6	1
1:A:94:TYR:C	1:A:96:LYS:N	0.42	2.71	13	1
1:A:86:VAL:CG2	1:A:117:LEU:HD11	0.42	2.45	10	1
1:A:79:ASP:O	1:A:83:TYR:CG	0.42	2.72	13	1
1:A:81:VAL:HG12	1:A:100:TYR:C	0.42	2.35	13	1
1:A:83:TYR:O	1:A:84:LEU:C	0.42	2.58	2	5
1:A:68:LEU:HB3	1:A:80:TYR:CZ	0.42	2.49	5	1
1:A:47:TRP:CE3	1:A:83:TYR:CZ	0.42	3.07	7	1
1:A:78:ARG:HG3	1:A:107:THR:CG2	0.42	2.44	9	2
1:A:89:TYR:CD1	1:A:90:ARG:N	0.42	2.88	14	1
1:A:46:ALA:HA	1:A:49:LEU:HD22	0.42	1.90	17	1
1:A:105:LEU:O	1:A:108:GLU:C	0.42	2.58	14	2
1:A:93:GLU:O	1:A:94:TYR:C	0.42	2.58	10	1
1:A:43:PHE:CE1	1:A:79:ASP:HB3	0.42	2.50	18	1
1:A:43:PHE:HA	1:A:65:LEU:CD1	0.42	2.45	12	3
1:A:8:MET:HE2	1:A:11:VAL:HG11	0.42	1.90	4	1
1:A:24:PHE:O	1:A:26:ARG:N	0.42	2.53	12	2
1:A:58:ILE:HG21	1:A:91:LEU:HD11	0.42	1.86	7	1
1:A:18:VAL:O	1:A:22:LYS:CB	0.42	2.67	8	1
1:A:78:ARG:HA	1:A:104:LEU:HD23	0.42	1.91	13	2
1:A:47:TRP:CE3	1:A:83:TYR:CE1	0.42	3.08	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:49:LEU:HD13	1:A:60:ARG:CB	0.42	2.42	13	1
1:A:108:GLU:N	1:A:109:PRO:HD3	0.42	2.30	20	1
1:A:18:VAL:O	1:A:19:GLU:C	0.41	2.58	14	2
1:A:102:ARG:O	1:A:106:GLN:OE1	0.41	2.38	5	1
1:A:42:GLN:CD	1:A:68:LEU:HD21	0.41	2.34	20	1
1:A:8:MET:SD	1:A:113:GLN:O	0.41	2.79	17	10
1:A:24:PHE:O	1:A:25:GLU:C	0.41	2.58	4	2
1:A:81:VAL:O	1:A:84:LEU:N	0.41	2.53	14	2
1:A:22:LYS:O	1:A:25:GLU:N	0.41	2.53	11	2
1:A:47:TRP:CD2	1:A:83:TYR:CE1	0.41	3.08	11	1
1:A:69:LEU:HD11	1:A:84:LEU:HD12	0.41	1.88	11	1
1:A:65:LEU:HB2	1:A:84:LEU:HD11	0.41	1.92	15	1
1:A:40:SER:C	1:A:44:GLU:OE1	0.41	2.58	8	1
1:A:26:ARG:O	1:A:30:SER:N	0.41	2.49	18	1
1:A:61:GLY:O	1:A:65:LEU:CD2	0.41	2.61	19	1
1:A:94:TYR:CB	1:A:125:MET:SD	0.41	3.09	2	1
1:A:31:GLU:OE1	1:A:41:THR:HG21	0.41	2.15	5	1
1:A:16:VAL:CG2	1:A:48:CYS:O	0.41	2.66	15	1
1:A:47:TRP:HA	1:A:50:VAL:CG2	0.41	2.46	4	4
1:A:94:TYR:HB3	1:A:125:MET:CE	0.41	2.46	12	5
1:A:8:MET:HG3	1:A:120:LEU:CD1	0.41	2.46	7	1
1:A:69:LEU:HD13	1:A:77:GLN:HG2	0.41	1.92	8	1
1:A:94:TYR:HB3	1:A:121:ILE:CG2	0.41	2.46	12	2
1:A:84:LEU:HD22	1:A:100:TYR:OH	0.41	2.15	17	2
1:A:98:LEU:HB3	1:A:102:ARG:CD	0.41	2.45	20	1
1:A:123:LYS:O	1:A:124:ALA:C	0.41	2.58	14	2
1:A:60:ARG:HA	1:A:63:VAL:HG22	0.41	1.91	7	1
1:A:43:PHE:O	1:A:44:GLU:C	0.41	2.58	8	1
1:A:101:VAL:O	1:A:105:LEU:N	0.41	2.52	8	1
1:A:22:LYS:C	1:A:24:PHE:N	0.41	2.74	13	1
1:A:12:LEU:HD21	1:A:89:TYR:CD2	0.41	2.51	3	2
1:A:20:ASP:O	1:A:21:LEU:C	0.41	2.58	3	2
1:A:49:LEU:C	1:A:51:ARG:N	0.41	2.74	3	1
1:A:58:ILE:CD1	1:A:90:ARG:HB3	0.41	2.45	7	1
1:A:69:LEU:HD21	1:A:84:LEU:HD13	0.41	1.93	9	1
1:A:94:TYR:CD1	1:A:94:TYR:N	0.41	2.89	9	3
1:A:27:LYS:O	1:A:31:GLU:CG	0.41	2.68	12	1
1:A:14:GLU:OE1	1:A:15:LEU:O	0.41	2.39	15	1
1:A:108:GLU:HB3	1:A:111:ASN:CB	0.41	2.46	20	1
1:A:13:ASN:O	1:A:14:GLU:C	0.41	2.59	9	2
1:A:121:ILE:O	1:A:124:ALA:N	0.41	2.54	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:65:LEU:HD12	1:A:68:LEU:HD12	0.41	1.92	16	1
1:A:104:LEU:HD22	1:A:104:LEU:O	0.41	2.16	20	1
1:A:46:ALA:O	1:A:50:VAL:HG22	0.41	2.16	1	1
1:A:55:ASN:OD1	1:A:56:GLU:N	0.41	2.54	5	1
1:A:78:ARG:HA	1:A:104:LEU:CD2	0.41	2.46	10	1
1:A:39:LYS:HA	1:A:68:LEU:CD2	0.41	2.46	11	1
1:A:22:LYS:O	1:A:23:ASN:C	0.41	2.58	13	1
1:A:26:ARG:O	1:A:27:LYS:C	0.41	2.59	13	1
1:A:86:VAL:CB	1:A:117:LEU:HD11	0.41	2.45	14	1
1:A:84:LEU:HD23	1:A:100:TYR:OH	0.41	2.16	15	1
1:A:87:GLY:O	1:A:91:LEU:HD13	0.41	2.16	7	1
1:A:42:GLN:OE1	1:A:42:GLN:C	0.41	2.59	10	1
1:A:48:CYS:O	1:A:51:ARG:N	0.41	2.53	19	1
1:A:28:PHE:CD2	1:A:45:TYR:CE2	0.41	3.09	20	1
1:A:76:GLU:O	1:A:80:TYR:CD1	0.41	2.74	20	1
1:A:45:TYR:O	1:A:49:LEU:N	0.40	2.50	1	1
1:A:27:LYS:O	1:A:31:GLU:CD	0.40	2.60	5	1
1:A:58:ILE:CD1	1:A:90:ARG:HD2	0.40	2.45	5	1
1:A:98:LEU:CD1	1:A:102:ARG:HD3	0.40	2.46	14	1
1:A:107:THR:O	1:A:108:GLU:OE2	0.40	2.40	15	1
1:A:124:ALA:O	1:A:125:MET:CB	0.40	2.69	2	1
1:A:116:GLU:O	1:A:120:LEU:HD23	0.40	2.17	4	1
1:A:111:ASN:OD1	1:A:111:ASN:C	0.40	2.60	5	1
1:A:85:ALA:O	1:A:86:VAL:C	0.40	2.60	7	2
1:A:91:LEU:C	1:A:93:GLU:N	0.40	2.73	15	1
1:A:98:LEU:HD23	1:A:121:ILE:CG2	0.40	2.47	6	1
1:A:46:ALA:CB	1:A:64:LEU:HB2	0.40	2.46	7	1
1:A:60:ARG:HA	1:A:63:VAL:CG2	0.40	2.47	7	1
1:A:28:PHE:CE1	1:A:42:GLN:HG3	0.40	2.49	10	1
1:A:47:TRP:CE2	1:A:51:ARG:CG	0.40	3.04	19	1
1:A:31:GLU:HB2	1:A:37:VAL:CG2	0.40	2.46	20	1
1:A:43:PHE:CD1	1:A:80:TYR:CE1	0.40	3.10	1	1
1:A:98:LEU:HD11	1:A:118:GLU:HG2	0.40	1.94	4	1
1:A:55:ASN:OD1	1:A:56:GLU:OE1	0.40	2.40	5	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	121/133 (91%)	87±4 (72±4%)	28±4 (23±3%)	6±2 (5±1%)	4 25
All	All	2420/2660 (91%)	1738 (72%)	560 (23%)	122 (5%)	4 25

All 28 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	52	SER	19
1	A	36	SER	14
1	A	7	GLY	9
1	A	95	GLU	8
1	A	63	VAL	7
1	A	44	GLU	7
1	A	74	LYS	7
1	A	61	GLY	6
1	A	50	VAL	6
1	A	51	ARG	6
1	A	13	ASN	5
1	A	14	GLU	3
1	A	73	SER	3
1	A	40	SER	3
1	A	99	LYS	3
1	A	124	ALA	2
1	A	97	ALA	2
1	A	81	VAL	2
1	A	72	GLY	1
1	A	75	GLU	1
1	A	115	LYS	1
1	A	30	SER	1
1	A	16	VAL	1
1	A	111	ASN	1
1	A	127	LYS	1
1	A	58	ILE	1
1	A	106	GLN	1
1	A	109	PRO	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	107/115 (93%)	83±2 (77±2%)	24±2 (23±2%)	3 29
All	All	2140/2300 (93%)	1654 (77%)	486 (23%)	3 29

All 67 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	69	LEU	20
1	A	13	ASN	19
1	A	16	VAL	19
1	A	100	TYR	19
1	A	106	GLN	19
1	A	126	LYS	19
1	A	53	LYS	18
1	A	90	ARG	18
1	A	78	ARG	17
1	A	14	GLU	14
1	A	79	ASP	14
1	A	60	ARG	13
1	A	101	VAL	12
1	A	19	GLU	12
1	A	74	LYS	12
1	A	117	LEU	11
1	A	26	ARG	10
1	A	39	LYS	10
1	A	99	LYS	10
1	A	73	SER	9
1	A	27	LYS	9
1	A	40	SER	9
1	A	30	SER	8
1	A	65	LEU	8
1	A	67	GLU	8
1	A	125	MET	8
1	A	22	LYS	8
1	A	107	THR	7
1	A	119	ARG	7
1	A	123	LYS	7
1	A	21	LEU	7
1	A	63	VAL	6
1	A	116	GLU	6

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Mol	Chain	Res	Type	Models (Total)
1	A	102	ARG	6
1	A	56	GLU	5
1	A	98	LEU	5
1	A	48	CYS	5
1	A	36	SER	5
1	A	49	LEU	5
1	A	8	MET	4
1	A	43	PHE	4
1	A	51	ARG	4
1	A	57	ASP	3
1	A	71	LYS	3
1	A	127	LYS	3
1	A	20	ASP	3
1	A	118	GLU	3
1	A	75	GLU	3
1	A	84	LEU	3
1	A	96	LYS	3
1	A	17	SER	3
1	A	92	LYS	3
1	A	68	LEU	2
1	A	15	LEU	2
1	A	91	LEU	2
1	A	59	ARG	2
1	A	120	LEU	2
1	A	12	LEU	1
1	A	76	GLU	1
1	A	93	GLU	1
1	A	52	SER	1
1	A	89	TYR	1
1	A	104	LEU	1
1	A	55	ASN	1
1	A	23	ASN	1
1	A	77	GLN	1
1	A	115	LYS	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