Full wwPDB NMR Structure Validation Report (i)

Jun 12, 2024 – 01:46 AM EDT

PDB ID	:	2KCU
BMRB ID	:	16097
Title	:	NMR solution structure of an uncharacterized protein from Chlorobium tepidum. Northeast Structural Genomics target CtR107
Authors	:	Mills, J.L.; Zhang, Q.; Sukumaran, D.K.; Wang, D.; Jiang, M.; Foote, E.L.; Xiao, R.; Nair, R.; Everett, J.K.; Swapna, G.V.T.; Acton, T.B.; Rost, B.; Montelione, G.T.; Szyperski, T.; Northeast Structural Genomics Consortium (NESG)
Deposited on	:	2008-12-29

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

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

The 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:

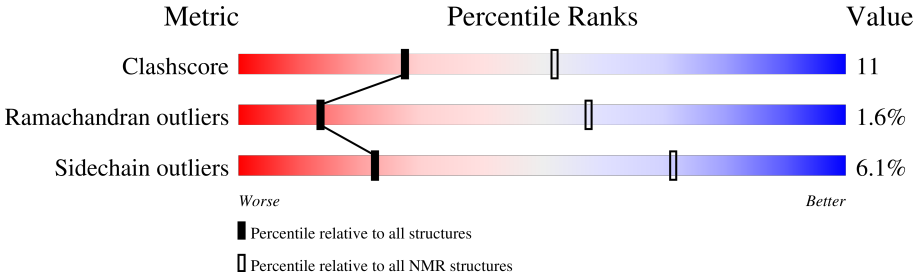
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson 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 is 78%.

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	166	76% 13% 11%

2 Ensemble composition and analysis (i)

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

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

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:7-A:154 (148)	2.19	14

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 4 clusters and 4 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2495 atoms, of which 1218 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called protein CtR107.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	166	2495	813	1218	209	248	7	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	ALA	THR	SEE REMARK 999	UNP Q8KFZ1
A	159	LEU	-	expression tag	UNP Q8KFZ1
A	160	GLU	-	expression tag	UNP Q8KFZ1
A	161	HIS	-	expression tag	UNP Q8KFZ1
A	162	HIS	-	expression tag	UNP Q8KFZ1
A	163	HIS	-	expression tag	UNP Q8KFZ1
A	164	HIS	-	expression tag	UNP Q8KFZ1
A	165	HIS	-	expression tag	UNP Q8KFZ1
A	166	HIS	-	expression tag	UNP Q8KFZ1

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: protein CtR107

Chain A: 76% 13% 11%

M1 D2 F3 E4 C5 Q6 L11 L20 L21 I42 R60 Y61 F62 E70 V71 E72 F73 G74 A98 L101 Y102 I103 L116 V120 E130 I134 Y135 L136 T142 R150 L153 M154 L155 H156 E157 S158 L159 E160 H161 H162 H163 H164 H165 H166

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: protein CtR107

Chain A: 60% 27% • 11%

M1 D2 F3 E4 C5 Q6 P16 L20 L21 I22 R23 T26 E30 L34 G38 L43 Q44 L45 P56 Y61 E70 V71 E72 F73 G74 E78 G83 R86 V87 V88 T89 T92 A98 L101 Y102 I103 G104 I109 E110 A111 V112 Y113

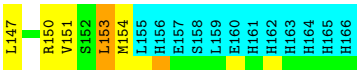
L116 W119 V120 N123 G124 F125 D126 L127 E130 L136 D137 N138 P139 A143 P144 D145 Q146 L147 R150 V151 S152 L153 M154 L155 H156 E157 S158 L159 E160 H161 H162 H163 H164 H165 H166

4.2.2 Score per residue for model 2

• Molecule 1: protein CtR107

Chain A: 69% 19% • 11%

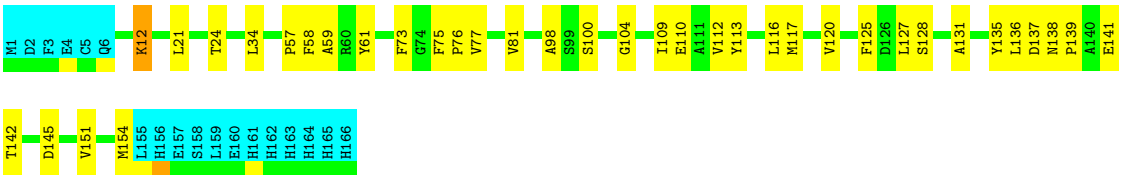
M1 D2 F3 E4 C5 Q6 E13 R23 I42 F58 Y61 S65 E70 V71 E72 F73 G74 E78 V81 G95 I103 G104 E108 I109 V112 Y113 D114 M117 F125 D126 L127 S128 G129 E130 E133 I134 N138 T142 A143 P144 D145 Q146



4.2.3 Score per residue for model 3

- Molecule 1: protein CtR107

Chain A:



4.2.4 Score per residue for model 4

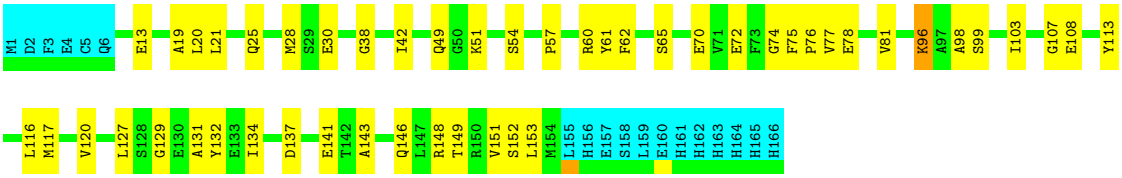
- Molecule 1: protein CtR107

Chain A:

4.2.5 Score per residue for model 5

- Molecule 1: protein CtR107

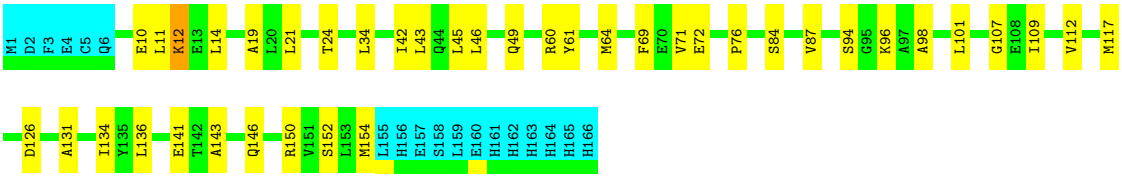
Chain A:



4.2.6 Score per residue for model 6

- Molecule 1: protein CtR107

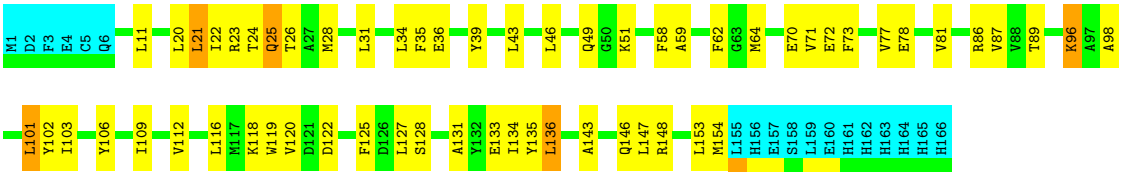
Chain A:



4.2.7 Score per residue for model 7

- Molecule 1: protein CtR107

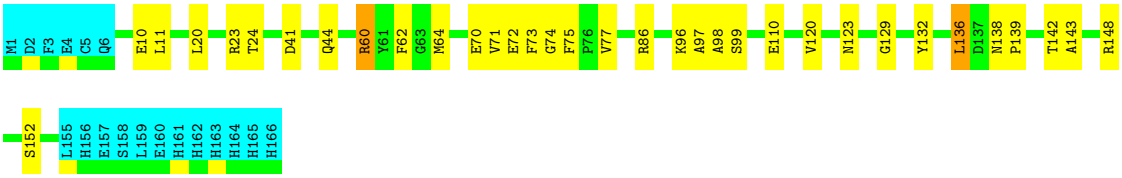
Chain A:



4.2.8 Score per residue for model 8

- Molecule 1: protein CtR107

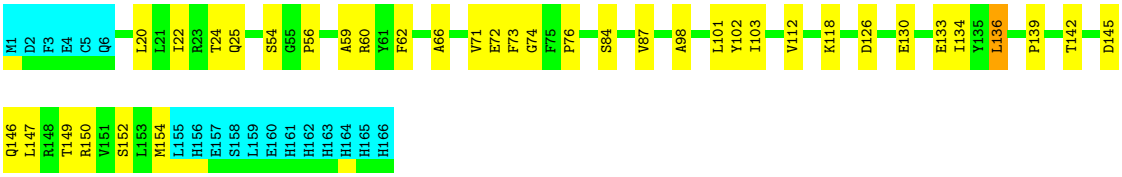
Chain A:



4.2.9 Score per residue for model 9

- Molecule 1: protein CtR107

Chain A:



4.2.10 Score per residue for model 10

- Molecule 1: protein CtR107

Chain A: 63% 24% • 11%

M1 D2 F3 E4 C5 Q6 F7 V8 C9 E10 L11 K12 E13 L20 L21 M28 G38 I42 Q49 P56 P57 F62 E70 V71 E72 F73 G74 E78 V81 E82 V87 V88 T89 K96 A97 A98 S99 S100 L101 Y106 Y113 L116 W119 V120

D126 L127 E130 E133 I134 Y135 L136 D137 T142 A143 V151 S152 L153 M154 L155 H156 E157 S158 L159 E160 H161 H162 H163 H164 H165 H166

4.2.11 Score per residue for model 11

- Molecule 1: protein CtR107

Chain A: 69% 18% • 11%

M1 D2 F3 E4 C5 Q6 F7 L14 A19 L20 L21 L45 A59 R60 Y61 F62 E70 V71 E72 F73 G74 F75 P76 G83 S84 V88 L101 Y102 I103 G104 P105 V112 Y113 D114 A115 L116 E130 D145 Q146 L147 R148 T149 R150 L153 M154 L155 H156 E157

S158 L159 E160 H161 H162 H163 H164 H165 H166

4.2.12 Score per residue for model 12

- Molecule 1: protein CtR107

Chain A: 70% 18% • 11%

M1 D2 F3 E4 C5 Q6 L11 K12 E13 L14 V17 P18 R23 D41 I42 A47 K51 A59 T68 G74 G90 L91 S94 G95 K96 L101 Y102 I103 G104 P105 K118 W119 D126 L127 Y132 E133 L136 D137 N138 P139 R148 T149 R150

V151 L155 H156 E157 S158 L159 E160 H161 H162 H163 H164 H165 H166

4.2.13 Score per residue for model 13

- Molecule 1: protein CtR107

Chain A: 64% 24% • 11%

M1 D2 F3 E4 C5 Q6 K12 E13 L14 A15 P16 A19 L20 L21 I42 L45 L46 A47 K51 P57 R60 Y61 F62 F69 E70 V71 E72 F73 G74 F75 P76 V77 E78 V81 E82 G83 V87 T92 P93 S94 A98 G104 E108 L116

V120 L127 E130 L136 D137 T142 D145 R148 L153 M154 L155 H156 E157 S158 L159 E160 H161 H162 H163 H164 H165 H166

4.2.14 Score per residue for model 14 (medoid)

- Molecule 1: protein CtR107

Chain A: 65% 22% • 11%

M1 D2 F3 E4 C5 Q6 C9 E10 L11 L21 I22 R23 T24 Q25 T26 A27 L45 P57 F58 A59 R60 Y61 F62 G63 M64 G67 T68 F69 E70 V71 E72 G83 S84 V87 L101 E110 Y113 L116 M117 K118 W119 N123 G124 F125 E130 A131 Y132

E133 I134 Y135 R150 V151 S152 L153 M154 L155 H156 E157 S158 L159 E160 H161 H162 H163 H164 H165 H166

4.2.15 Score per residue for model 15

- Molecule 1: protein CtR107

Chain A: 62% 24% • 11%

M1 D2 F3 E4 C5 Q6 F7 V8 L11 L14 L20 L21 I22 Q25 M28 S29 E30 L31 L34 I42 L45 F58 A59 R60 Y61 F62 E70 V71 E72 F73 G74 F75 P76 V77 E78 S84 V87 V88 T89 S99 S100 L101 Y102 D114 S128

G129 E130 A131 Y132 E133 I134 D145 R148 T149 R150 V151 S152 L153 M154 L155 H156 E157 S158 L159 E160 H161 H162 H163 H164 H165 H166

4.2.16 Score per residue for model 16

- Molecule 1: protein CtR107

Chain A: 62% 25% • 11%

M1 D2 F3 E4 C5 Q6 C9 E10 L11 K12 E13 L14 A15 P16 L20 L21 I22 Q25 T26 E30 S33 Y39 I42 K51 P56 A59 G63 M64 F69 E72 F73 G74 G79 P93 S94 T103 G107 L116 W119 V120

N123 G124 F125 D126 L127 A131 Y132 E133 I134 Y135 L136 P139 A140 E141 T142 L147 R148 L153 M154 L155 H156 E157 S158 L159 E160 H161 H162 H163 H164 H165 H166

4.2.17 Score per residue for model 17

- Molecule 1: protein CtR107

Chain A: 58% 28% • 11%

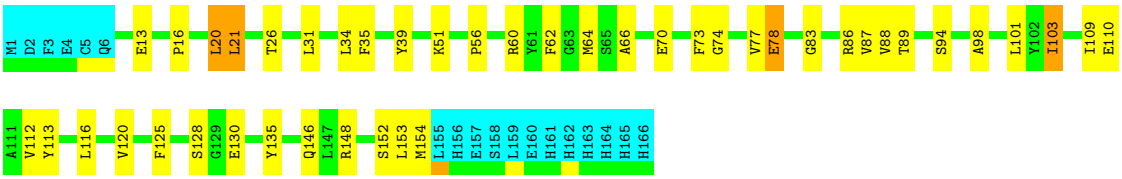
M1 D2 F3 E4 C5 Q6 L11 K12 E13 L14 L21 I22 Q25 L31 L34 F35 E36 D41 I42 Q49 P53 R60 Y61 F62 A66 G67 E70 V71 E72 F73 G74 F75 P76 T89 G90 L91 S94 G95 K96 A97 A98 L101 Y102 L116

F125 D126 E130 A131 Y132 E133 I134 D137 N138 P139 A140 E141 P144 D145 Q146 L147 R148 T149 R150 L153 M154 L155 H156 E157 S158 L159 E160 H161 H162 H163 H164 H165 H166

4.2.18 Score per residue for model 18

- Molecule 1: protein CtR107

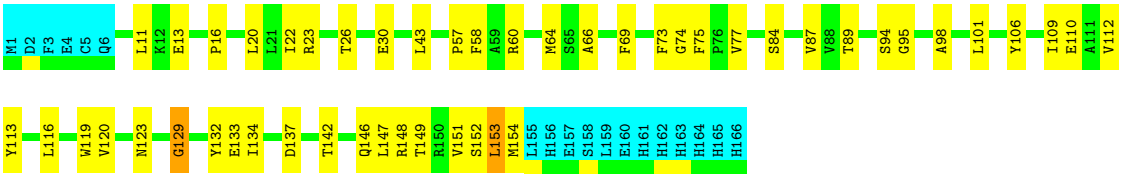
Chain A: 63% 24% • 11%



4.2.19 Score per residue for model 19

- Molecule 1: protein CtR107

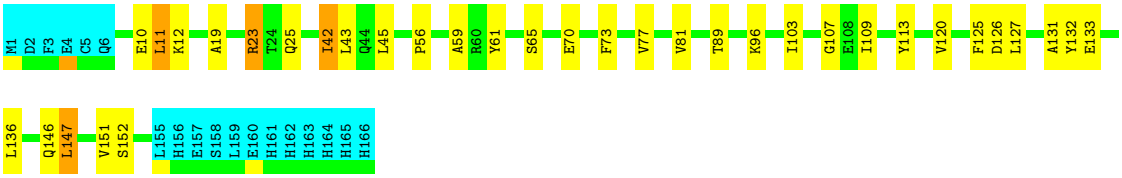
Chain A: 60% 28% • 11%



4.2.20 Score per residue for model 20

- Molecule 1: protein CtR107

Chain A: 68% 19% • 11%



5 Refinement protocol and experimental data overview (i)

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

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

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

Software name	Classification	Version
CSI	structure solution	
TALOS	structure solution	
CYANA	structure solution	
CNS	geometry optimization	
PSVS	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1677
Number of shifts mapped to atoms	1677
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	78%

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	1115	1080	1079	24±6
All	All	22300	21600	21580	476

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 11.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:21:LEU:HB3	1:A:74:GLY:HA3	0.90	1.42	5	3
1:A:19:ALA:HA	1:A:76:PRO:HA	0.89	1.42	11	4
1:A:120:VAL:HA	1:A:123:ASN:HD22	0.83	1.34	19	3
1:A:62:PHE:HB2	1:A:70:GLU:HB3	0.81	1.49	18	2
1:A:102:TYR:HB3	1:A:149:THR:HB	0.77	1.54	17	2
1:A:120:VAL:HA	1:A:123:ASN:ND2	0.77	1.93	8	3
1:A:62:PHE:HB3	1:A:70:GLU:HB3	0.77	1.55	13	3
1:A:61:TYR:HB2	1:A:131:ALA:HB3	0.76	1.54	5	4
1:A:22:ILE:HB	1:A:87:VAL:HG22	0.75	1.57	1	2
1:A:100:SER:HB2	1:A:112:VAL:HG23	0.74	1.60	3	1
1:A:54:SER:HB3	1:A:76:PRO:HB2	0.73	1.59	9	2
1:A:60:ARG:HB3	1:A:132:TYR:HD1	0.73	1.42	15	1
1:A:57:PRO:HA	1:A:75:PHE:HB3	0.72	1.60	5	2
1:A:62:PHE:HB3	1:A:70:GLU:HB2	0.72	1.60	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:137:ASP:HB3	1:A:142:THR:HG21	0.71	1.62	19	4
1:A:116:LEU:HG	1:A:153:LEU:HD21	0.71	1.61	17	1
1:A:132:TYR:HB3	1:A:152:SER:HB2	0.71	1.61	20	1
1:A:139:PRO:HA	1:A:147:LEU:HD21	0.71	1.61	1	1
1:A:21:LEU:HG	1:A:72:GLU:HB3	0.71	1.61	11	2
1:A:110:GLU:HA	1:A:113:TYR:HD2	0.69	1.46	18	3
1:A:25:GLN:HA	1:A:70:GLU:HA	0.69	1.61	20	4
1:A:23:ARG:HA	1:A:72:GLU:HG2	0.67	1.66	2	2
1:A:46:LEU:HG	1:A:51:LYS:HG3	0.66	1.68	13	1
1:A:110:GLU:HA	1:A:113:TYR:HB3	0.66	1.67	14	1
1:A:131:ALA:HB2	1:A:154:MET:HG3	0.66	1.68	7	2
1:A:21:LEU:HB2	1:A:72:GLU:HG2	0.65	1.68	10	1
1:A:12:LYS:HE3	1:A:12:LYS:HA	0.65	1.67	3	2
1:A:59:ALA:HA	1:A:73:PHE:HA	0.65	1.67	3	6
1:A:101:LEU:HD13	1:A:148:ARG:HD3	0.65	1.67	17	1
1:A:20:LEU:HD13	1:A:77:VAL:HG21	0.65	1.68	19	1
1:A:23:ARG:HB3	1:A:72:GLU:HG2	0.65	1.69	7	1
1:A:120:VAL:HG23	1:A:125:PHE:HB2	0.64	1.69	7	2
1:A:101:LEU:HB3	1:A:150:ARG:HG2	0.64	1.69	11	1
1:A:102:TYR:O	1:A:148:ARG:HA	0.64	1.92	15	1
1:A:11:LEU:HD11	1:A:96:LYS:HD3	0.64	1.69	20	1
1:A:84:SER:HB3	1:A:87:VAL:HB	0.64	1.70	6	1
1:A:31:LEU:HD13	1:A:31:LEU:H	0.64	1.51	15	1
1:A:45:LEU:HD21	1:A:83:GLY:HA2	0.63	1.70	13	1
1:A:83:GLY:HA3	1:A:88:VAL:HA	0.63	1.71	11	3
1:A:133:GLU:HB3	1:A:151:VAL:HA	0.63	1.69	15	1
1:A:116:LEU:HG	1:A:153:LEU:HD23	0.63	1.70	14	1
1:A:23:ARG:H	1:A:23:ARG:HD3	0.63	1.53	20	1
1:A:112:VAL:HG21	1:A:151:VAL:HG13	0.63	1.71	3	1
1:A:153:LEU:HD13	1:A:153:LEU:H	0.63	1.52	19	1
1:A:113:TYR:CD2	1:A:153:LEU:HD13	0.63	2.29	5	1
1:A:103:ILE:HD12	1:A:148:ARG:HG2	0.63	1.69	16	1
1:A:134:ILE:HB	1:A:150:ARG:HB2	0.62	1.69	17	2
1:A:96:LYS:HD2	1:A:127:LEU:HD22	0.62	1.71	20	1
1:A:61:TYR:HB3	1:A:71:VAL:HG12	0.62	1.72	14	3
1:A:22:ILE:O	1:A:72:GLU:HA	0.62	1.95	16	2
1:A:84:SER:H	1:A:87:VAL:HG13	0.62	1.54	9	2
1:A:116:LEU:HD21	1:A:153:LEU:HD12	0.62	1.70	5	1
1:A:56:PRO:HG2	1:A:134:ILE:HD11	0.61	1.71	16	1
1:A:57:PRO:HG2	1:A:135:TYR:HB2	0.61	1.71	3	1
1:A:136:LEU:H	1:A:136:LEU:HD23	0.61	1.54	20	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:116:LEU:HB3	1:A:153:LEU:HD21	0.61	1.71	4	1
1:A:60:ARG:HB3	1:A:132:TYR:HB3	0.61	1.72	19	2
1:A:136:LEU:H	1:A:136:LEU:HD13	0.61	1.55	9	4
1:A:116:LEU:HD11	1:A:153:LEU:HD22	0.61	1.71	13	1
1:A:11:LEU:HD23	1:A:11:LEU:H	0.61	1.55	19	1
1:A:104:GLY:HA2	1:A:144:PRO:HB2	0.61	1.72	2	1
1:A:11:LEU:HD21	1:A:96:LYS:HB3	0.60	1.73	20	1
1:A:102:TYR:HE2	1:A:106:TYR:HA	0.60	1.56	7	1
1:A:11:LEU:HB2	1:A:119:TRP:HH2	0.60	1.57	10	2
1:A:129:GLY:HA2	1:A:154:MET:SD	0.59	2.38	2	1
1:A:116:LEU:HD13	1:A:153:LEU:HD21	0.59	1.73	11	1
1:A:11:LEU:HB2	1:A:119:TRP:CH2	0.59	2.31	10	4
1:A:127:LEU:HD12	1:A:127:LEU:H	0.59	1.57	16	3
1:A:10:GLU:HB2	1:A:12:LYS:HE2	0.59	1.75	20	1
1:A:133:GLU:HB2	1:A:135:TYR:CE2	0.58	2.34	7	1
1:A:109:ILE:O	1:A:112:VAL:HG12	0.58	1.96	18	6
1:A:104:GLY:HA2	1:A:145:ASP:HA	0.58	1.76	1	2
1:A:132:TYR:HB3	1:A:152:SER:HB3	0.58	1.73	14	2
1:A:16:PRO:HG3	1:A:94:SER:HB3	0.57	1.75	13	2
1:A:60:ARG:HG3	1:A:72:GLU:HB2	0.57	1.73	9	1
1:A:139:PRO:HB3	1:A:147:LEU:HD11	0.57	1.75	9	1
1:A:137:ASP:HB3	1:A:142:THR:HB	0.57	1.75	10	1
1:A:103:ILE:HA	1:A:147:LEU:O	0.57	2.00	20	3
1:A:138:ASN:OD1	1:A:139:PRO:HD2	0.57	1.98	3	4
1:A:22:ILE:HG13	1:A:87:VAL:HB	0.57	1.75	15	1
1:A:25:GLN:HG2	1:A:70:GLU:HG2	0.57	1.77	15	1
1:A:11:LEU:HG	1:A:96:LYS:HB3	0.57	1.77	8	1
1:A:16:PRO:HD3	1:A:94:SER:HB3	0.57	1.76	19	1
1:A:21:LEU:HD22	1:A:72:GLU:HB3	0.56	1.77	13	2
1:A:20:LEU:HD13	1:A:87:VAL:HG21	0.56	1.77	15	1
1:A:58:PHE:CZ	1:A:76:PRO:HG3	0.56	2.35	15	1
1:A:116:LEU:HA	1:A:119:TRP:CD1	0.56	2.35	1	1
1:A:99:SER:HB3	1:A:152:SER:HB2	0.56	1.76	8	1
1:A:120:VAL:CG2	1:A:125:PHE:HA	0.56	2.31	20	1
1:A:20:LEU:HA	1:A:89:THR:HA	0.56	1.76	15	2
1:A:23:ARG:HD2	1:A:23:ARG:H	0.56	1.61	2	1
1:A:24:THR:HG21	1:A:34:LEU:HD21	0.56	1.77	6	2
1:A:102:TYR:CG	1:A:149:THR:HG22	0.56	2.36	15	1
1:A:101:LEU:HA	1:A:150:ARG:HA	0.56	1.76	14	2
1:A:60:ARG:HB3	1:A:132:TYR:CD1	0.56	2.31	15	1
1:A:43:LEU:H	1:A:43:LEU:HD23	0.56	1.60	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:98:ALA:O	1:A:152:SER:HA	0.55	2.02	19	5
1:A:96:LYS:O	1:A:96:LYS:HD2	0.55	2.01	7	1
1:A:13:GLU:HB3	1:A:96:LYS:HD3	0.55	1.79	17	1
1:A:45:LEU:HD23	1:A:84:SER:HB3	0.54	1.79	14	1
1:A:24:THR:HB	1:A:34:LEU:HD21	0.54	1.79	4	1
1:A:8:VAL:O	1:A:100:SER:HA	0.54	2.02	15	1
1:A:20:LEU:HD13	1:A:77:VAL:HG11	0.54	1.78	8	1
1:A:103:ILE:HB	1:A:145:ASP:O	0.54	2.02	11	1
1:A:98:ALA:HB2	1:A:119:TRP:HZ2	0.54	1.62	19	1
1:A:62:PHE:HD1	1:A:130:GLU:HG2	0.54	1.63	15	1
1:A:39:TYR:HA	1:A:42:ILE:HG22	0.54	1.80	16	1
1:A:26:THR:HG21	1:A:31:LEU:HD22	0.54	1.78	18	1
1:A:77:VAL:HG21	1:A:81:VAL:HB	0.53	1.80	13	1
1:A:61:TYR:HB3	1:A:69:PHE:CE2	0.53	2.38	13	1
1:A:137:ASP:O	1:A:139:PRO:HD3	0.53	2.03	17	1
1:A:59:ALA:HB3	1:A:133:GLU:HB2	0.53	1.79	20	1
1:A:62:PHE:HB2	1:A:70:GLU:HB2	0.53	1.79	11	1
1:A:110:GLU:HA	1:A:113:TYR:CB	0.53	2.33	14	1
1:A:22:ILE:HD13	1:A:73:PHE:HB3	0.53	1.79	16	1
1:A:98:ALA:HB1	1:A:116:LEU:HD12	0.53	1.79	17	2
1:A:60:ARG:HG3	1:A:72:GLU:O	0.53	2.03	15	1
1:A:34:LEU:HG	1:A:73:PHE:HZ	0.53	1.63	1	1
1:A:42:ILE:HG22	1:A:43:LEU:H	0.53	1.64	20	1
1:A:62:PHE:HD1	1:A:130:GLU:HB3	0.52	1.63	9	2
1:A:102:TYR:CD1	1:A:149:THR:HG22	0.52	2.39	15	1
1:A:43:LEU:HD22	1:A:45:LEU:HD23	0.52	1.81	1	1
1:A:26:THR:HG21	1:A:34:LEU:HD22	0.52	1.82	1	1
1:A:21:LEU:HD23	1:A:74:GLY:HA3	0.52	1.82	15	1
1:A:110:GLU:HA	1:A:113:TYR:CD2	0.52	2.40	19	2
1:A:51:LYS:O	1:A:51:LYS:HE2	0.52	2.03	13	1
1:A:26:THR:O	1:A:69:PHE:HB3	0.52	2.05	19	1
1:A:133:GLU:HB3	1:A:151:VAL:HG23	0.51	1.81	2	1
1:A:98:ALA:HB3	1:A:153:LEU:HD21	0.51	1.82	13	1
1:A:31:LEU:O	1:A:35:PHE:HB2	0.51	2.05	7	1
1:A:139:PRO:HB3	1:A:147:LEU:HD13	0.51	1.83	16	1
1:A:38:GLY:HA3	1:A:73:PHE:CE2	0.51	2.40	1	1
1:A:101:LEU:HD13	1:A:103:ILE:HD11	0.51	1.83	7	1
1:A:61:TYR:O	1:A:130:GLU:HA	0.51	2.05	11	1
1:A:24:THR:O	1:A:71:VAL:HG22	0.51	2.06	7	4
1:A:41:ASP:O	1:A:44:GLN:HG2	0.51	2.06	8	1
1:A:153:LEU:HD23	1:A:153:LEU:H	0.51	1.66	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:41:ASP:O	1:A:42:ILE:HG12	0.51	2.06	12	2
1:A:36:GLU:HA	1:A:39:TYR:CE2	0.51	2.41	7	1
1:A:20:LEU:HD23	1:A:77:VAL:HG21	0.51	1.82	18	1
1:A:134:ILE:HG12	1:A:150:ARG:HB2	0.51	1.83	6	1
1:A:136:LEU:HB2	1:A:148:ARG:HG3	0.51	1.83	12	1
1:A:60:ARG:HD3	1:A:72:GLU:OE1	0.50	2.06	11	4
1:A:56:PRO:HB3	1:A:136:LEU:HA	0.50	1.82	20	2
1:A:116:LEU:O	1:A:120:VAL:HG12	0.50	2.07	3	2
1:A:11:LEU:O	1:A:11:LEU:HD12	0.50	2.06	17	2
1:A:31:LEU:H	1:A:31:LEU:CD1	0.50	2.20	15	1
1:A:132:TYR:CE2	1:A:152:SER:HB3	0.50	2.42	8	1
1:A:109:ILE:HD11	1:A:151:VAL:HG21	0.50	1.82	20	1
1:A:59:ALA:O	1:A:132:TYR:HA	0.50	2.07	4	3
1:A:61:TYR:HD1	1:A:71:VAL:HG12	0.50	1.65	11	1
1:A:64:MET:HG2	1:A:129:GLY:O	0.49	2.07	19	1
1:A:56:PRO:CB	1:A:136:LEU:HA	0.49	2.37	4	3
1:A:20:LEU:HD12	1:A:87:VAL:HG22	0.49	1.83	9	1
1:A:114:ASP:O	1:A:117:MET:HG2	0.49	2.08	2	1
1:A:20:LEU:HB3	1:A:89:THR:HG22	0.49	1.84	7	1
1:A:109:ILE:O	1:A:112:VAL:HG22	0.49	2.07	2	1
1:A:101:LEU:HG	1:A:150:ARG:HG2	0.49	1.84	12	1
1:A:120:VAL:HG22	1:A:125:PHE:HA	0.49	1.83	20	1
1:A:25:GLN:NE2	1:A:25:GLN:H	0.49	2.04	16	1
1:A:14:LEU:HB2	1:A:94:SER:HB3	0.49	1.84	16	1
1:A:20:LEU:HD11	1:A:45:LEU:HD23	0.49	1.84	11	1
1:A:24:THR:HG22	1:A:26:THR:HG23	0.49	1.84	7	1
1:A:24:THR:HG23	1:A:71:VAL:HG23	0.49	1.85	9	1
1:A:58:PHE:CD1	1:A:134:ILE:HD12	0.49	2.43	15	1
1:A:143:ALA:HB1	1:A:146:GLN:HB2	0.48	1.85	7	3
1:A:42:ILE:HG13	1:A:87:VAL:HG13	0.48	1.84	13	1
1:A:133:GLU:HA	1:A:151:VAL:HA	0.48	1.85	19	1
1:A:120:VAL:HG21	1:A:153:LEU:HD11	0.48	1.84	13	1
1:A:49:GLN:HB3	1:A:51:LYS:HE3	0.48	1.83	5	1
1:A:54:SER:CB	1:A:78:GLU:HG3	0.48	2.39	5	1
1:A:24:THR:HG21	1:A:34:LEU:HD22	0.48	1.85	7	1
1:A:46:LEU:O	1:A:51:LYS:HB3	0.48	2.08	13	1
1:A:103:ILE:CG2	1:A:145:ASP:HA	0.48	2.38	2	1
1:A:14:LEU:O	1:A:94:SER:HA	0.48	2.08	12	3
1:A:30:GLU:HG3	1:A:33:SER:HB2	0.48	1.84	16	1
1:A:56:PRO:HB2	1:A:135:TYR:O	0.48	2.08	18	1
1:A:78:GLU:OE2	1:A:81:VAL:HG23	0.48	2.08	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:64:MET:HA	1:A:64:MET:CE	0.48	2.39	7	1
1:A:99:SER:HB3	1:A:152:SER:CB	0.48	2.38	8	1
1:A:134:ILE:HD11	1:A:150:ARG:HB3	0.48	1.85	9	1
1:A:45:LEU:HD23	1:A:87:VAL:HB	0.48	1.85	13	1
1:A:64:MET:HG3	1:A:129:GLY:C	0.47	2.29	8	1
1:A:9:CYS:HA	1:A:100:SER:OG	0.47	2.10	10	1
1:A:60:ARG:HG3	1:A:132:TYR:CE2	0.47	2.43	17	1
1:A:120:VAL:HA	1:A:125:PHE:CE1	0.47	2.44	18	1
1:A:45:LEU:H	1:A:45:LEU:HD23	0.47	1.69	20	1
1:A:13:GLU:HA	1:A:95:GLY:O	0.47	2.09	19	3
1:A:43:LEU:HD21	1:A:87:VAL:HB	0.47	1.86	1	1
1:A:56:PRO:HG2	1:A:136:LEU:HG	0.47	1.85	1	1
1:A:20:LEU:HD12	1:A:87:VAL:HG12	0.47	1.84	18	2
1:A:102:TYR:CD1	1:A:112:VAL:HG11	0.47	2.45	9	1
1:A:11:LEU:HD13	1:A:123:ASN:HD21	0.47	1.70	14	1
1:A:64:MET:SD	1:A:64:MET:N	0.47	2.87	14	1
1:A:51:LYS:HE2	1:A:79:GLY:O	0.47	2.09	16	1
1:A:60:ARG:HD2	1:A:72:GLU:OE1	0.47	2.10	8	2
1:A:101:LEU:HA	1:A:149:THR:O	0.47	2.10	9	1
1:A:46:LEU:HG	1:A:51:LYS:CG	0.47	2.37	13	1
1:A:31:LEU:HB3	1:A:71:VAL:HG11	0.47	1.85	15	1
1:A:61:TYR:HB3	1:A:69:PHE:CZ	0.47	2.44	6	1
1:A:27:ALA:HB2	1:A:68:THR:HA	0.47	1.85	14	1
1:A:83:GLY:HA3	1:A:87:VAL:O	0.47	2.10	14	1
1:A:116:LEU:HA	1:A:119:TRP:HD1	0.47	1.68	1	2
1:A:130:GLU:HG3	1:A:154:MET:HG3	0.47	1.87	9	1
1:A:77:VAL:HB	1:A:81:VAL:HG21	0.47	1.87	20	3
1:A:113:TYR:HA	1:A:153:LEU:HD11	0.47	1.88	10	1
1:A:21:LEU:HB3	1:A:74:GLY:CA	0.47	2.37	11	1
1:A:20:LEU:HD11	1:A:89:THR:HG22	0.46	1.86	19	1
1:A:58:PHE:HB3	1:A:134:ILE:HG12	0.46	1.85	19	1
1:A:58:PHE:CE1	1:A:76:PRO:HG3	0.46	2.46	3	1
1:A:18:PRO:HA	1:A:90:GLY:O	0.46	2.11	12	1
1:A:21:LEU:HB3	1:A:74:GLY:H	0.46	1.70	1	1
1:A:63:GLY:HA3	1:A:69:PHE:CE2	0.46	2.44	16	1
1:A:116:LEU:HB3	1:A:153:LEU:HB2	0.46	1.88	14	1
1:A:142:THR:HG23	1:A:147:LEU:HD23	0.46	1.86	2	1
1:A:63:GLY:HA3	1:A:69:PHE:CD2	0.46	2.45	4	1
1:A:43:LEU:HG	1:A:46:LEU:HB3	0.46	1.87	6	1
1:A:61:TYR:CE2	1:A:131:ALA:HB3	0.46	2.46	17	1
1:A:103:ILE:HG13	1:A:148:ARG:HG2	0.46	1.85	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:150:ARG:O	1:A:150:ARG:HG3	0.46	2.11	14	1
1:A:120:VAL:HG22	1:A:125:PHE:CZ	0.46	2.46	18	1
1:A:23:ARG:HB3	1:A:72:GLU:CG	0.46	2.40	7	1
1:A:22:ILE:HB	1:A:73:PHE:HD2	0.46	1.70	19	1
1:A:98:ALA:HB1	1:A:116:LEU:HD22	0.46	1.88	3	1
1:A:110:GLU:HA	1:A:113:TYR:CD1	0.46	2.46	3	1
1:A:38:GLY:O	1:A:42:ILE:HG12	0.46	2.11	10	2
1:A:101:LEU:HD12	1:A:101:LEU:O	0.46	2.11	10	2
1:A:21:LEU:HB3	1:A:74:GLY:HA2	0.46	1.88	4	2
1:A:45:LEU:O	1:A:49:GLN:HB2	0.46	2.11	6	1
1:A:104:GLY:HA2	1:A:145:ASP:H	0.46	1.71	11	1
1:A:31:LEU:HD21	1:A:71:VAL:HG11	0.46	1.87	17	1
1:A:42:ILE:HB	1:A:87:VAL:HG21	0.45	1.86	6	1
1:A:14:LEU:HD22	1:A:150:ARG:HH22	0.45	1.72	15	1
1:A:20:LEU:HD11	1:A:75:PHE:CZ	0.45	2.46	15	1
1:A:116:LEU:CB	1:A:153:LEU:HD21	0.45	2.41	4	1
1:A:142:THR:HG23	1:A:143:ALA:H	0.45	1.72	8	1
1:A:120:VAL:HG13	1:A:125:PHE:O	0.45	2.12	18	1
1:A:99:SER:HA	1:A:151:VAL:O	0.45	2.12	15	2
1:A:42:ILE:HG22	1:A:43:LEU:N	0.45	2.27	20	1
1:A:22:ILE:HD13	1:A:87:VAL:HB	0.45	1.88	9	1
1:A:51:LYS:HD3	1:A:51:LYS:H	0.45	1.71	13	1
1:A:102:TYR:CE1	1:A:149:THR:HB	0.45	2.47	11	1
1:A:23:ARG:HD3	1:A:70:GLU:OE1	0.45	2.12	1	1
1:A:22:ILE:HG13	1:A:86:ARG:HD2	0.45	1.88	7	1
1:A:153:LEU:HG	1:A:154:MET:H	0.45	1.71	7	1
1:A:103:ILE:H	1:A:103:ILE:HD13	0.45	1.72	11	1
1:A:136:LEU:H	1:A:136:LEU:CD1	0.45	2.24	8	1
1:A:127:LEU:HD12	1:A:130:GLU:HB3	0.45	1.88	13	1
1:A:61:TYR:HA	1:A:70:GLU:O	0.44	2.11	11	2
1:A:113:TYR:HD2	1:A:153:LEU:HD13	0.44	1.69	5	1
1:A:142:THR:O	1:A:146:GLN:HB3	0.44	2.12	9	1
1:A:16:PRO:HB3	1:A:93:PRO:HA	0.44	1.88	16	1
1:A:58:PHE:HB3	1:A:134:ILE:HG13	0.44	1.88	4	1
1:A:39:TYR:HB3	1:A:73:PHE:CE2	0.44	2.47	18	1
1:A:153:LEU:HD13	1:A:154:MET:H	0.44	1.72	2	1
1:A:62:PHE:HB2	1:A:130:GLU:HG3	0.44	1.89	4	1
1:A:153:LEU:HG	1:A:154:MET:N	0.44	2.27	7	1
1:A:56:PRO:HG2	1:A:136:LEU:HA	0.44	1.89	9	1
1:A:133:GLU:HG2	1:A:151:VAL:HG23	0.44	1.89	12	3
1:A:60:ARG:HG2	1:A:72:GLU:HB2	0.44	1.89	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:127:LEU:HG	1:A:129:GLY:H	0.44	1.71	5	1
1:A:101:LEU:HB3	1:A:150:ARG:HB3	0.44	1.87	14	1
1:A:134:ILE:HD11	1:A:150:ARG:HG2	0.44	1.88	14	1
1:A:139:PRO:C	1:A:141:GLU:H	0.44	2.15	17	1
1:A:20:LEU:HB3	1:A:89:THR:HB	0.44	1.89	15	1
1:A:123:ASN:HB3	1:A:125:PHE:HD2	0.44	1.72	1	1
1:A:46:LEU:HG	1:A:51:LYS:CB	0.44	2.43	13	1
1:A:139:PRO:HG3	1:A:147:LEU:HD21	0.44	1.88	17	1
1:A:57:PRO:HB3	1:A:75:PHE:CE2	0.44	2.47	3	2
1:A:136:LEU:HD13	1:A:136:LEU:N	0.44	2.27	16	3
1:A:57:PRO:HD2	1:A:135:TYR:O	0.44	2.13	14	2
1:A:62:PHE:CD1	1:A:130:GLU:HG3	0.44	2.48	17	1
1:A:154:MET:CE	1:A:154:MET:HA	0.43	2.43	15	1
1:A:61:TYR:HB3	1:A:69:PHE:HE2	0.43	1.71	13	1
1:A:34:LEU:HG	1:A:73:PHE:CZ	0.43	2.48	1	1
1:A:12:LYS:HA	1:A:12:LYS:CE	0.43	2.43	3	1
1:A:127:LEU:HD21	1:A:130:GLU:HB2	0.43	1.91	2	1
1:A:147:LEU:HD12	1:A:147:LEU:O	0.43	2.13	2	1
1:A:28:MET:HG2	1:A:28:MET:O	0.43	2.14	7	1
1:A:17:VAL:O	1:A:91:LEU:HA	0.43	2.13	12	1
1:A:49:GLN:HE22	1:A:81:VAL:HG13	0.43	1.74	10	1
1:A:128:SER:OG	1:A:153:LEU:HG	0.43	2.14	15	1
1:A:23:ARG:H	1:A:23:ARG:CD	0.43	2.25	20	1
1:A:60:ARG:O	1:A:71:VAL:HA	0.43	2.14	13	1
1:A:128:SER:CB	1:A:154:MET:HB3	0.43	2.44	18	1
1:A:60:ARG:HA	1:A:132:TYR:HA	0.43	1.90	19	1
1:A:20:LEU:HD12	1:A:89:THR:HB	0.42	1.91	4	1
1:A:64:MET:H	1:A:69:PHE:HE1	0.42	1.57	6	1
1:A:123:ASN:HB3	1:A:125:PHE:CD2	0.42	2.49	1	1
1:A:142:THR:HG23	1:A:143:ALA:N	0.42	2.27	8	1
1:A:9:CYS:HB2	1:A:119:TRP:CD1	0.42	2.49	14	1
1:A:21:LEU:HD13	1:A:21:LEU:N	0.42	2.30	14	3
1:A:19:ALA:HA	1:A:77:VAL:HG22	0.42	1.92	20	1
1:A:26:THR:HB	1:A:34:LEU:HD22	0.42	1.90	4	1
1:A:47:ALA:HA	1:A:51:LYS:O	0.42	2.14	12	1
1:A:30:GLU:O	1:A:34:LEU:HG	0.42	2.14	15	1
1:A:101:LEU:HD11	1:A:148:ARG:CG	0.42	2.44	19	1
1:A:64:MET:SD	1:A:130:GLU:HB2	0.42	2.54	18	1
1:A:103:ILE:N	1:A:103:ILE:HD13	0.42	2.29	18	1
1:A:60:ARG:HG2	1:A:72:GLU:HG2	0.42	1.91	14	1
1:A:58:PHE:HD1	1:A:134:ILE:HG12	0.42	1.74	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:51:LYS:HG3	1:A:81:VAL:HG22	0.42	1.91	7	1
1:A:112:VAL:O	1:A:116:LEU:HG	0.42	2.15	11	1
1:A:47:ALA:HA	1:A:51:LYS:CD	0.42	2.44	13	1
1:A:12:LYS:CB	1:A:99:SER:HB3	0.42	2.44	10	1
1:A:63:GLY:HA3	1:A:69:PHE:HD2	0.42	1.74	4	1
1:A:20:LEU:HD23	1:A:77:VAL:HG12	0.42	1.91	7	1
1:A:25:GLN:H	1:A:25:GLN:CD	0.42	2.19	7	1
1:A:20:LEU:O	1:A:74:GLY:HA2	0.42	2.15	16	1
1:A:11:LEU:HG	1:A:11:LEU:O	0.42	2.14	19	1
1:A:134:ILE:O	1:A:149:THR:HG23	0.42	2.15	5	1
1:A:64:MET:HG3	1:A:154:MET:SD	0.42	2.55	6	1
1:A:98:ALA:HB2	1:A:119:TRP:CZ2	0.41	2.48	19	1
1:A:143:ALA:O	1:A:147:LEU:HG	0.41	2.15	7	1
1:A:154:MET:SD	1:A:154:MET:N	0.41	2.93	14	1
1:A:110:GLU:HA	1:A:113:TYR:HD1	0.41	1.76	3	1
1:A:9:CYS:SG	1:A:116:LEU:HG	0.41	2.55	16	1
1:A:77:VAL:HG12	1:A:78:GLU:H	0.41	1.75	18	1
1:A:137:ASP:CB	1:A:142:THR:HG21	0.41	2.44	3	1
1:A:13:GLU:HA	1:A:96:LYS:HA	0.41	1.91	5	1
1:A:54:SER:HB2	1:A:78:GLU:HG3	0.41	1.91	5	1
1:A:45:LEU:HD21	1:A:84:SER:HB3	0.41	1.93	15	1
1:A:113:TYR:HA	1:A:116:LEU:HD12	0.41	1.92	18	1
1:A:106:TYR:OH	1:A:149:THR:HG21	0.41	2.14	19	1
1:A:23:ARG:O	1:A:86:ARG:HD3	0.41	2.16	1	1
1:A:60:ARG:HG2	1:A:72:GLU:CG	0.41	2.45	14	1
1:A:119:TRP:O	1:A:119:TRP:HE3	0.41	1.98	14	1
1:A:26:THR:HG22	1:A:69:PHE:HB3	0.41	1.92	16	1
1:A:21:LEU:HG	1:A:60:ARG:NH2	0.41	2.29	18	1
1:A:20:LEU:HB3	1:A:89:THR:HG23	0.41	1.93	1	1
1:A:136:LEU:O	1:A:137:ASP:HB2	0.41	2.16	3	1
1:A:62:PHE:CZ	1:A:65:SER:HB2	0.41	2.50	5	1
1:A:116:LEU:HD22	1:A:153:LEU:HB3	0.41	1.91	16	1
1:A:53:PRO:HA	1:A:76:PRO:O	0.41	2.16	17	1
1:A:58:PHE:CB	1:A:134:ILE:HG12	0.41	2.46	19	1
1:A:129:GLY:HA2	1:A:154:MET:HG3	0.41	1.93	2	1
1:A:73:PHE:HB3	1:A:75:PHE:HE1	0.41	1.76	8	1
1:A:123:ASN:OD1	1:A:125:PHE:HB2	0.41	2.16	14	1
1:A:104:GLY:HA2	1:A:145:ASP:O	0.41	2.16	3	1
1:A:51:LYS:HD2	1:A:78:GLU:HB3	0.41	1.91	7	1
1:A:62:PHE:CD1	1:A:130:GLU:HG2	0.41	2.50	15	1
1:A:101:LEU:HD11	1:A:148:ARG:HG2	0.41	1.93	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:LEU:HD11	1:A:96:LYS:HB3	0.40	1.92	6	1
1:A:20:LEU:HD21	1:A:46:LEU:HD21	0.40	1.93	7	1
1:A:61:TYR:CD1	1:A:71:VAL:HG12	0.40	2.50	11	1
1:A:35:PHE:HB2	1:A:73:PHE:CD1	0.40	2.50	18	1
1:A:77:VAL:HB	1:A:81:VAL:CG2	0.40	2.46	5	1
1:A:49:GLN:OE1	1:A:81:VAL:HA	0.40	2.17	7	1
1:A:103:ILE:HD13	1:A:103:ILE:N	0.40	2.31	11	1
1:A:136:LEU:HB2	1:A:148:ARG:HB3	0.40	1.92	13	1
1:A:7:PHE:HA	1:A:101:LEU:O	0.40	2.17	11	1
1:A:16:PRO:HA	1:A:92:THR:O	0.40	2.16	1	1
1:A:129:GLY:HA2	1:A:154:MET:CG	0.40	2.46	2	1
1:A:110:GLU:H	1:A:110:GLU:CD	0.40	2.20	4	1
1:A:144:PRO:O	1:A:145:ASP:HB3	0.40	2.17	17	1
1:A:150:ARG:HG3	1:A:150:ARG:O	0.40	2.16	1	1
1:A:138:ASN:O	1:A:142:THR:HG22	0.40	2.16	2	1
1:A:20:LEU:HD11	1:A:83:GLY:HA2	0.40	1.93	18	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	148/166 (89%)	132±2 (90±2%)	13±3 (9±2%)	2±1 (2±1%)	13	57
All	All	2960/3320 (89%)	2650 (90%)	264 (9%)	46 (2%)	13	57

All 20 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	74	GLY	11
1	A	42	ILE	5
1	A	107	GLY	5
1	A	66	ALA	4
1	A	28	MET	3
1	A	43	LEU	2

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Mol	Chain	Res	Type	Models (Total)
1	A	143	ALA	2
1	A	67	GLY	2
1	A	30	GLU	1
1	A	65	SER	1
1	A	50	GLY	1
1	A	137	ASP	1
1	A	105	PRO	1
1	A	108	GLU	1
1	A	63	GLY	1
1	A	7	PHE	1
1	A	142	THR	1
1	A	49	GLN	1
1	A	140	ALA	1
1	A	129	GLY	1

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	116/134 (87%)	109±2 (94±2%)	7±2 (6±2%)	22 71
All	All	2320/2680 (87%)	2179 (94%)	141 (6%)	22 71

All 57 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	LEU	9
1	A	78	GLU	6
1	A	89	THR	5
1	A	153	LEU	5
1	A	136	LEU	5
1	A	101	LEU	4
1	A	23	ARG	4
1	A	12	LYS	4
1	A	117	MET	4
1	A	141	GLU	4
1	A	25	GLN	4

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Mol	Chain	Res	Type	Models (Total)
1	A	96	LYS	4
1	A	130	GLU	3
1	A	154	MET	3
1	A	14	LEU	3
1	A	142	THR	3
1	A	20	LEU	3
1	A	126	ASP	3
1	A	118	LYS	3
1	A	148	ARG	3
1	A	103	ILE	3
1	A	11	LEU	3
1	A	13	GLU	3
1	A	150	ARG	2
1	A	36	GLU	2
1	A	110	GLU	2
1	A	30	GLU	2
1	A	10	GLU	2
1	A	60	ARG	2
1	A	86	ARG	2
1	A	133	GLU	2
1	A	114	ASP	2
1	A	91	LEU	2
1	A	51	LYS	2
1	A	64	MET	2
1	A	31	LEU	2
1	A	34	LEU	2
1	A	146	GLN	2
1	A	147	LEU	2
1	A	24	THR	1
1	A	33	SER	1
1	A	44	GLN	1
1	A	108	GLU	1
1	A	116	LEU	1
1	A	122	ASP	1
1	A	82	GLU	1
1	A	106	TYR	1
1	A	84	SER	1
1	A	68	THR	1
1	A	92	THR	1
1	A	22	ILE	1
1	A	58	PHE	1
1	A	119	TRP	1

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Mol	Chain	Res	Type	Models (Total)
1	A	149	THR	1
1	A	123	ASN	1
1	A	138	ASN	1
1	A	113	TYR	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)

The completeness of assignment taking into account all chemical shift lists is 78% for the well-defined parts and 78% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping (i)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1677
Number of shifts mapped to atoms	1677
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	156	0.12 ± 0.14	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	138	-0.05 ± 0.13	None needed (< 0.5 ppm)
$^{13}C'$	0	—	None (insufficient data)
^{15}N	149	-0.10 ± 0.22	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 78%, i.e. 1488 atoms were assigned a chemical shift out of a possible 1904. 0 out of 26 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	563/738 (76%)	291/304 (96%)	139/296 (47%)	133/138 (96%)
Sidechain	821/1003 (82%)	565/660 (86%)	252/318 (79%)	4/25 (16%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	104/163 (64%)	67/78 (86%)	36/82 (44%)	1/3 (33%)
Overall	1488/1904 (78%)	923/1042 (89%)	427/696 (61%)	138/166 (83%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 78%, i.e. 1677 atoms were assigned a chemical shift out of a possible 2161. 0 out of 28 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	629/828 (76%)	324/340 (95%)	156/332 (47%)	149/156 (96%)
Sidechain	908/1104 (82%)	624/725 (86%)	279/353 (79%)	5/26 (19%)
Aromatic	140/229 (61%)	86/111 (77%)	53/101 (52%)	1/17 (6%)
Overall	1677/2161 (78%)	1034/1176 (88%)	488/786 (62%)	155/199 (78%)

7.1.4 Statistically unusual chemical shifts (i)

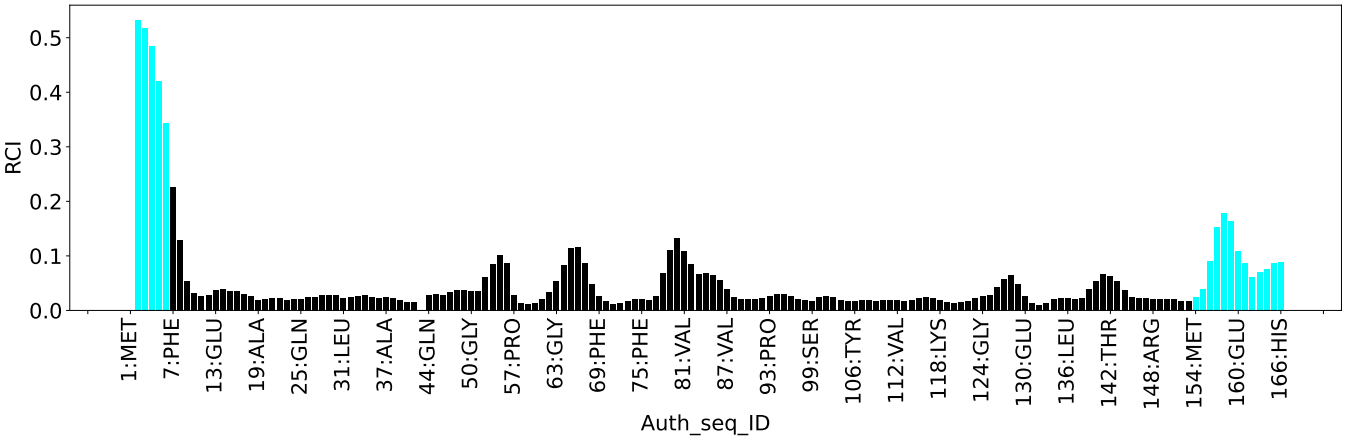
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	22	ILE	HB	0.24	0.35 – 3.22	-5.4

7.1.5 Random Coil Index (RCI) plots (i)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:


RCI
0.0
0.1
0.2
0.3
0.4
0.5
1:MET
7:PHE
13:GLU
19:ALA
25:GLN
31:LEU
37:ALA
44:GLN
50:GLY
57:PRO
63:GLY
69:PHE
75:PHE
81:VAL
87:VAL
93:PRO
99:SER
106:TYR
112:VAL
118:LYS
124:GLY
130:GLU
136:LEU
142:THR
148:ARG
154:MET
160:GLU
166:HIS
Auth_seq_ID