Full wwPDB NMR Structure Validation Report

Mar 3, 2022 – 11:15 AM EST

PDB ID	:	2I3E
Title	:	Solution structure of catalytic domain of goldfish RICH protein
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Deposited on	:	2006-08-18

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 ⓘ symbol.

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

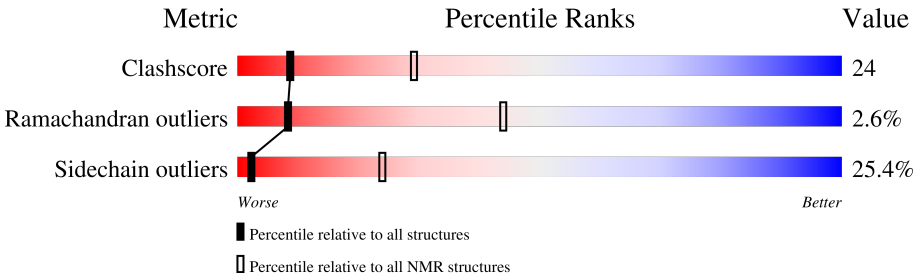
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance

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	222	45% 39% . 13%

2 Ensemble composition and analysis

This entry contains 10 models. Model 9 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:40, A:61-A:219 (193)	0.51	9

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. No single-model clusters were found.

Cluster number	Models
1	1, 4, 5, 6, 7, 8
2	2, 3, 9, 10

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3432 atoms, of which 1701 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called G-RICH.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	222	3432	1105	1701	274	345	7	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	cloning artifact	UNP Q90306
A	2	SER	-	cloning artifact	UNP Q90306
A	3	HIS	-	cloning artifact	UNP Q90306
A	4	MET	-	cloning artifact	UNP Q90306

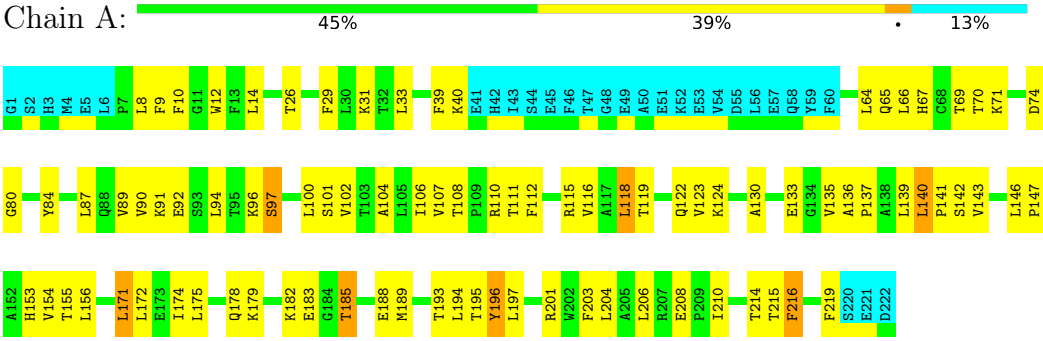
4 Residue-property plots

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: G-RICH

Chain A:



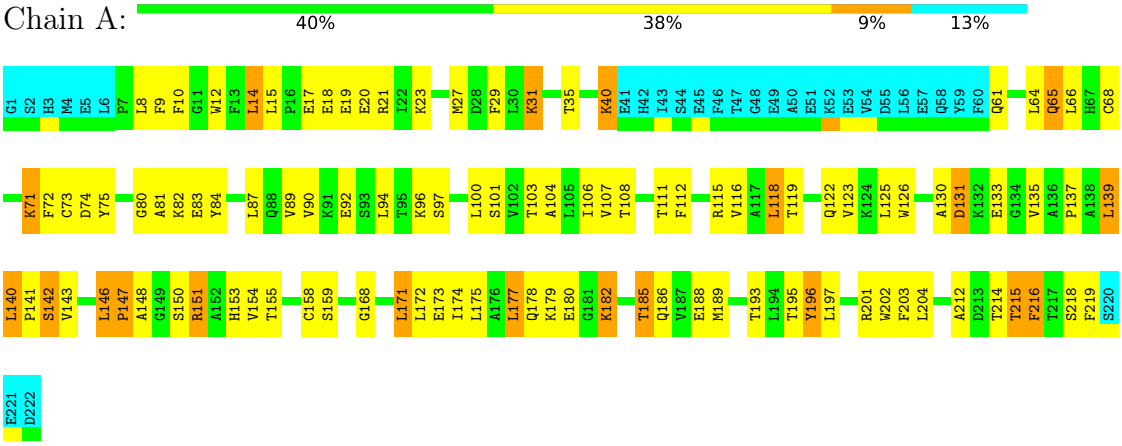
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: G-RICH

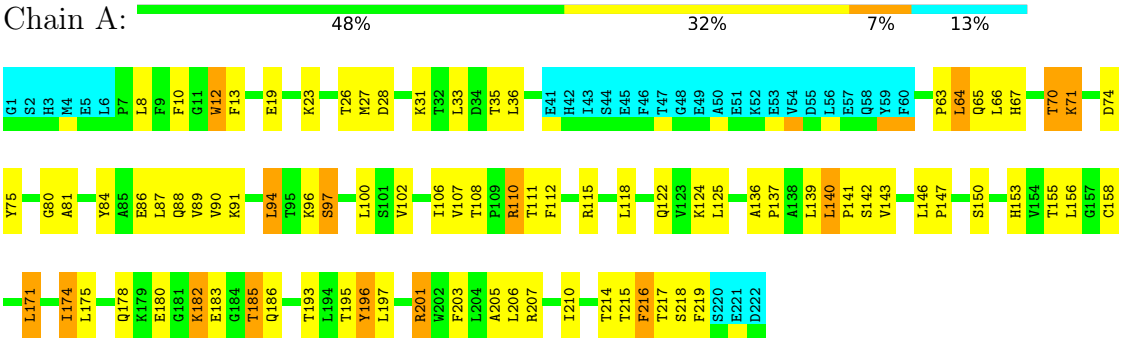
Chain A:



4.2.2 Score per residue for model 2

• Molecule 1: G-RICH

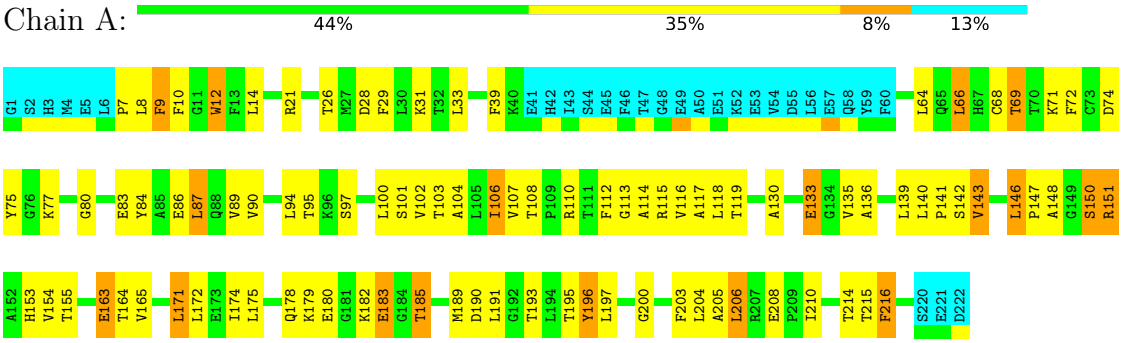
Chain A:



4.2.3 Score per residue for model 3

• Molecule 1: G-RICH

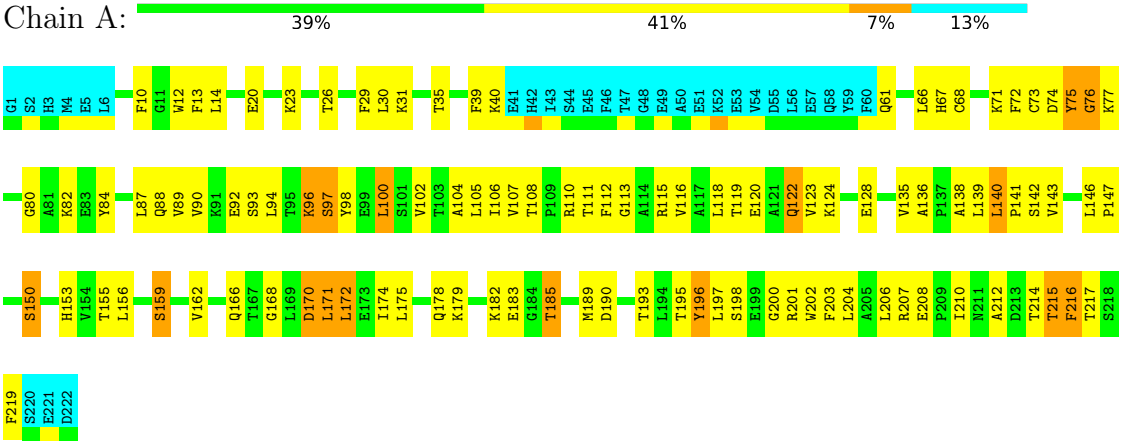
Chain A:



4.2.4 Score per residue for model 4

• Molecule 1: G-RICH

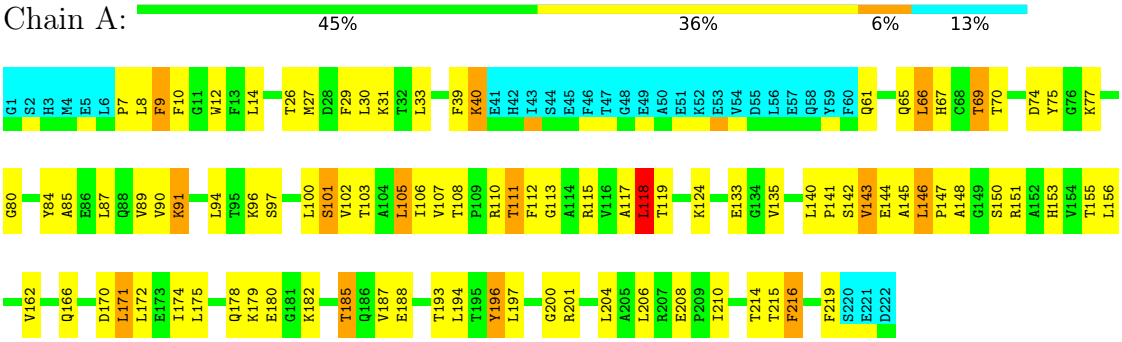
Chain A:



4.2.5 Score per residue for model 5

• Molecule 1: G-RICH

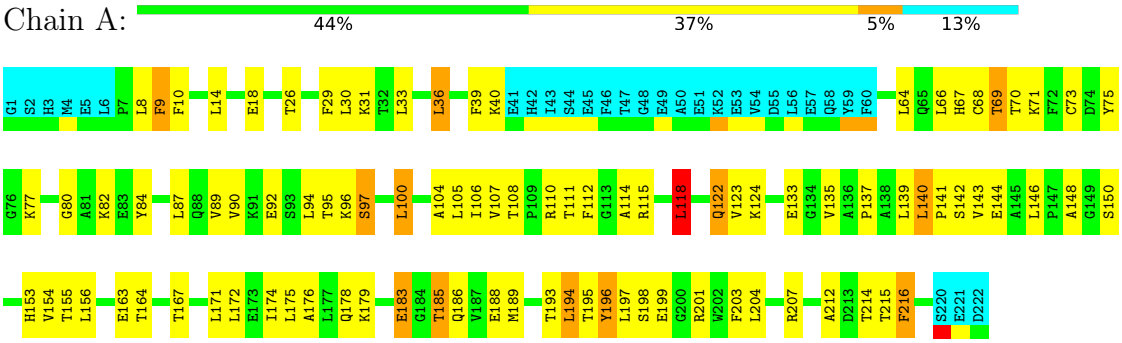
Chain A:



4.2.6 Score per residue for model 6

• Molecule 1: G-RICH

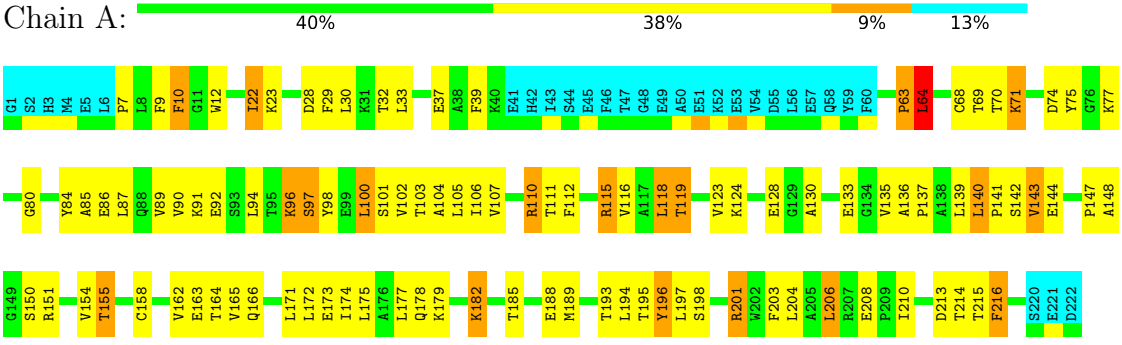
Chain A:



4.2.7 Score per residue for model 7

• Molecule 1: G-RICH

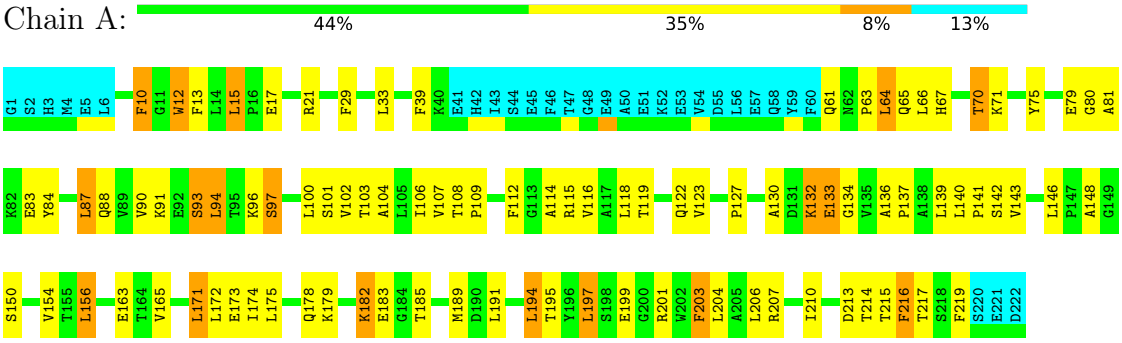
Chain A:



4.2.8 Score per residue for model 8

• Molecule 1: G-RICH

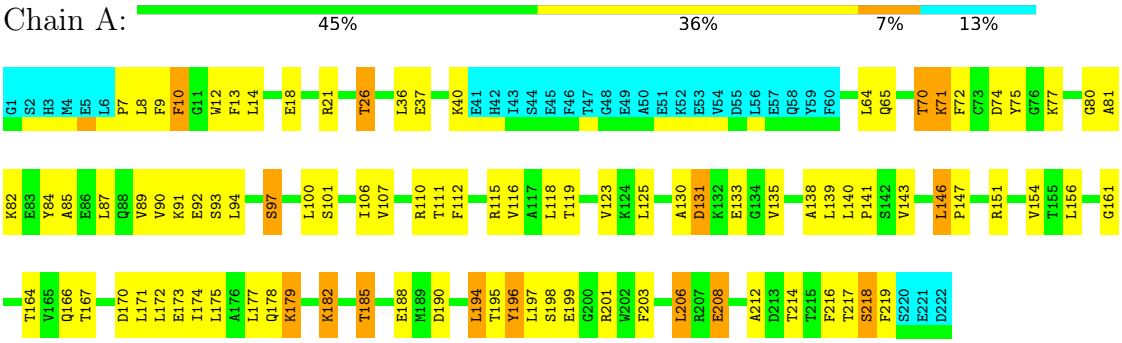
Chain A:



4.2.9 Score per residue for model 9 (medoid)

• Molecule 1: G-RICH

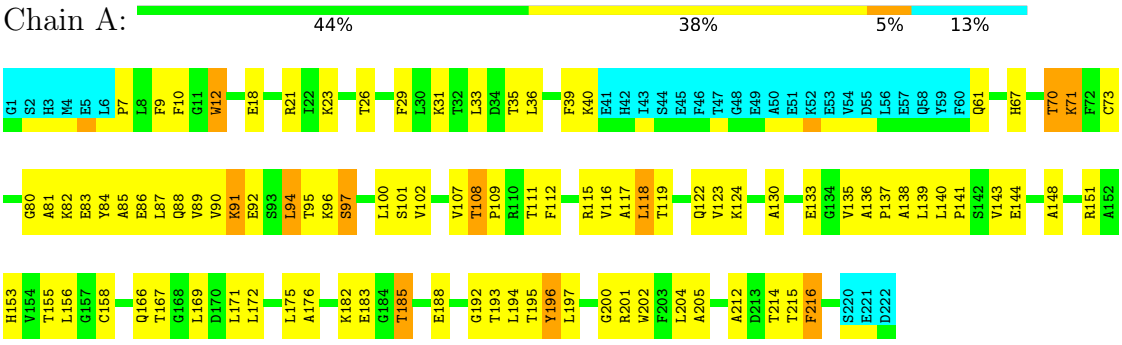
Chain A:



4.2.10 Score per residue for model 10

• Molecule 1: G-RICH

Chain A:



5 Refinement protocol and experimental data overview

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

Of the 150 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy and the least restraint violations*.

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

Software name	Classification	Version
CNS	refinement	1.1

No chemical shift data was provided.

6 Model quality

6.1 Standard geometry

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

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	1493	1497	1497	71±6
All	All	14930	14970	14970	707

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 24.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:135:VAL:HG23	1:A:175:LEU:HD13	1.07	1.23	10	2
1:A:81:ALA:HB2	1:A:130:ALA:HB2	1.04	1.13	9	1
1:A:135:VAL:HG13	1:A:143:VAL:HG22	0.86	1.45	6	1
1:A:140:LEU:O	1:A:143:VAL:HG22	0.85	1.71	10	1
1:A:139:LEU:O	1:A:143:VAL:HG13	0.85	1.72	10	1
1:A:136:ALA:HB3	1:A:139:LEU:HD13	0.83	1.50	10	6
1:A:107:VAL:HG22	1:A:112:PHE:CE2	0.82	2.09	8	6
1:A:143:VAL:CG1	1:A:148:ALA:HB2	0.82	2.04	6	3
1:A:191:LEU:HD23	1:A:206:LEU:HD22	0.82	1.48	8	1
1:A:81:ALA:HB2	1:A:130:ALA:CB	0.81	2.04	9	1
1:A:150:SER:OG	1:A:175:LEU:HD12	0.80	1.77	3	2
1:A:137:PRO:O	1:A:140:LEU:HD23	0.80	1.77	7	1
1:A:135:VAL:HG22	1:A:146:LEU:HD12	0.80	1.50	1	1
1:A:29:PHE:CZ	1:A:33:LEU:HD13	0.80	2.12	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:118:LEU:HD11	1:A:123:VAL:HG13	0.80	1.53	8	1
1:A:107:VAL:HG22	1:A:112:PHE:CD1	0.80	2.10	2	2
1:A:153:HIS:CG	1:A:171:LEU:HD13	0.80	2.12	3	2
1:A:81:ALA:CB	1:A:130:ALA:HB2	0.79	2.05	9	1
1:A:12:TRP:CH2	1:A:118:LEU:HD21	0.79	2.13	5	4
1:A:29:PHE:CD2	1:A:204:LEU:HD22	0.79	2.11	5	2
1:A:135:VAL:HG22	1:A:146:LEU:CD1	0.79	2.07	1	1
1:A:135:VAL:CG2	1:A:175:LEU:HD13	0.79	2.07	10	2
1:A:135:VAL:CG2	1:A:146:LEU:HD11	0.79	2.07	9	1
1:A:107:VAL:HG22	1:A:112:PHE:CE1	0.78	2.13	9	4
1:A:131:ASP:OD2	1:A:138:ALA:HB3	0.78	1.79	9	1
1:A:119:THR:O	1:A:123:VAL:HG23	0.78	1.79	1	3
1:A:143:VAL:HG21	1:A:148:ALA:HB2	0.78	1.52	7	3
1:A:115:ARG:NH1	1:A:175:LEU:HD21	0.78	1.92	4	2
1:A:174:ILE:HD11	1:A:197:LEU:HD11	0.78	1.53	2	1
1:A:174:ILE:HD11	1:A:203:PHE:CE1	0.77	2.14	6	1
1:A:29:PHE:CD1	1:A:204:LEU:HD22	0.77	2.14	3	1
1:A:14:LEU:HD11	1:A:100:LEU:HD21	0.77	1.57	9	1
1:A:7:PRO:HG2	1:A:85:ALA:HB1	0.77	1.56	9	2
1:A:150:SER:OG	1:A:172:LEU:HD23	0.77	1.79	5	1
1:A:31:LYS:O	1:A:35:THR:HG23	0.76	1.80	1	2
1:A:143:VAL:CG2	1:A:148:ALA:HB2	0.76	2.10	7	3
1:A:112:PHE:CD1	1:A:156:LEU:HD11	0.75	2.16	8	1
1:A:143:VAL:HG11	1:A:148:ALA:HB2	0.75	1.58	6	3
1:A:102:VAL:HG13	1:A:115:ARG:O	0.75	1.82	10	4
1:A:133:GLU:CG	1:A:172:LEU:HD21	0.74	2.12	8	4
1:A:147:PRO:O	1:A:175:LEU:HD13	0.74	1.81	3	5
1:A:140:LEU:O	1:A:143:VAL:HG12	0.74	1.82	7	3
1:A:12:TRP:CE3	1:A:214:THR:HG21	0.74	2.17	8	1
1:A:87:LEU:HD23	1:A:89:VAL:CG1	0.74	2.12	2	9
1:A:150:SER:HB3	1:A:175:LEU:HD12	0.74	1.57	5	2
1:A:84:TYR:CE2	1:A:90:VAL:HG11	0.74	2.17	8	8
1:A:100:LEU:HD11	1:A:214:THR:HG21	0.74	1.60	5	2
1:A:13:PHE:CD1	1:A:217:THR:HG21	0.73	2.18	9	3
1:A:118:LEU:HD21	1:A:137:PRO:CG	0.73	2.13	8	3
1:A:118:LEU:CD1	1:A:123:VAL:HG13	0.73	2.13	8	1
1:A:87:LEU:O	1:A:90:VAL:HG22	0.73	1.83	6	10
1:A:139:LEU:O	1:A:143:VAL:HG23	0.72	1.84	2	3
1:A:12:TRP:CZ3	1:A:70:THR:HG23	0.72	2.19	10	1
1:A:102:VAL:HG23	1:A:115:ARG:O	0.72	1.84	5	3
1:A:175:LEU:HD12	1:A:176:ALA:N	0.72	2.00	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:105:LEU:HD13	1:A:206:LEU:HD11	0.72	1.62	7	2
1:A:171:LEU:HA	1:A:174:ILE:HD12	0.71	1.62	1	2
1:A:150:SER:OG	1:A:175:LEU:HD23	0.71	1.85	6	1
1:A:143:VAL:HG23	1:A:146:LEU:HD11	0.71	1.62	4	1
1:A:106:ILE:HD13	1:A:107:VAL:N	0.71	2.01	3	1
1:A:150:SER:HA	1:A:171:LEU:HD22	0.70	1.62	1	2
1:A:22:ILE:HD13	1:A:22:ILE:O	0.70	1.86	7	1
1:A:133:GLU:OE1	1:A:172:LEU:HD13	0.69	1.86	7	1
1:A:150:SER:CB	1:A:175:LEU:HD12	0.69	2.17	7	1
1:A:111:THR:OG1	1:A:167:THR:HG23	0.69	1.87	9	1
1:A:104:ALA:HB3	1:A:115:ARG:NH1	0.69	2.02	7	1
1:A:177:LEU:HG	1:A:197:LEU:HD13	0.69	1.65	1	1
1:A:174:ILE:HG23	1:A:175:LEU:HD23	0.69	1.65	2	1
1:A:135:VAL:CG1	1:A:143:VAL:HG22	0.69	2.17	6	1
1:A:139:LEU:O	1:A:143:VAL:HG12	0.68	1.88	9	2
1:A:100:LEU:HD12	1:A:100:LEU:O	0.68	1.89	1	2
1:A:150:SER:HB2	1:A:172:LEU:HD23	0.68	1.66	7	1
1:A:153:HIS:HB3	1:A:171:LEU:HD22	0.68	1.65	2	3
1:A:147:PRO:HB2	1:A:175:LEU:HD22	0.67	1.64	9	7
1:A:188:GLU:HA	1:A:193:THR:HG22	0.67	1.67	7	3
1:A:111:THR:HG22	1:A:158:CYS:HA	0.67	1.64	7	3
1:A:135:VAL:HG23	1:A:175:LEU:CD1	0.67	2.12	10	2
1:A:135:VAL:HG13	1:A:143:VAL:CG2	0.67	2.20	4	2
1:A:94:LEU:HD21	1:A:218:SER:HB3	0.66	1.66	1	1
1:A:68:CYS:SG	1:A:116:VAL:HG21	0.66	2.30	3	2
1:A:174:ILE:HD11	1:A:203:PHE:CD1	0.66	2.25	6	1
1:A:142:SER:O	1:A:146:LEU:HD12	0.66	1.90	3	2
1:A:135:VAL:HG13	1:A:143:VAL:HG21	0.66	1.65	9	2
1:A:118:LEU:HD13	1:A:122:GLN:CG	0.66	2.20	4	1
1:A:135:VAL:HG11	1:A:148:ALA:HA	0.65	1.68	1	5
1:A:91:LYS:O	1:A:94:LEU:HD12	0.65	1.92	5	1
1:A:174:ILE:CD1	1:A:197:LEU:HD11	0.65	2.20	2	1
1:A:118:LEU:HD13	1:A:122:GLN:HB3	0.65	1.67	6	1
1:A:106:ILE:HD12	1:A:174:ILE:HG21	0.64	1.68	7	1
1:A:168:GLY:O	1:A:172:LEU:HD22	0.64	1.92	4	1
1:A:7:PRO:CG	1:A:85:ALA:HB1	0.64	2.22	9	2
1:A:150:SER:HB2	1:A:175:LEU:HD12	0.64	1.69	4	1
1:A:118:LEU:HD13	1:A:122:GLN:HB2	0.64	1.67	10	3
1:A:71:LYS:NZ	1:A:85:ALA:HB2	0.64	2.07	7	1
1:A:36:LEU:HD13	1:A:194:LEU:HD22	0.64	1.68	10	1
1:A:173:GLU:O	1:A:177:LEU:HD13	0.63	1.92	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:33:LEU:HD23	1:A:39:PHE:CE1	0.63	2.29	6	1
1:A:182:LYS:HB3	1:A:197:LEU:HD23	0.63	1.69	2	1
1:A:33:LEU:HD11	1:A:39:PHE:CD1	0.63	2.28	3	1
1:A:118:LEU:HD21	1:A:137:PRO:CB	0.63	2.24	8	3
1:A:100:LEU:CD1	1:A:212:ALA:HB3	0.63	2.24	4	1
1:A:169:LEU:HA	1:A:172:LEU:HD12	0.63	1.71	10	1
1:A:135:VAL:CG1	1:A:143:VAL:HG21	0.62	2.24	9	2
1:A:131:ASP:OD2	1:A:139:LEU:HD12	0.62	1.93	1	1
1:A:100:LEU:HD22	1:A:116:VAL:CG1	0.62	2.25	7	1
1:A:18:GLU:HG3	1:A:212:ALA:HB1	0.62	1.72	1	1
1:A:71:LYS:HD3	1:A:81:ALA:HB1	0.62	1.71	10	1
1:A:133:GLU:HB3	1:A:172:LEU:HD22	0.62	1.71	5	2
1:A:100:LEU:HD23	1:A:212:ALA:O	0.62	1.93	6	1
1:A:115:ARG:HD3	1:A:175:LEU:HD21	0.62	1.72	2	1
1:A:100:LEU:CD1	1:A:214:THR:HG21	0.61	2.25	5	4
1:A:12:TRP:CZ3	1:A:118:LEU:HD21	0.61	2.28	5	1
1:A:150:SER:HA	1:A:171:LEU:HD12	0.61	1.71	8	1
1:A:197:LEU:HD13	1:A:201:ARG:HB2	0.61	1.73	10	2
1:A:71:LYS:HZ3	1:A:85:ALA:HB2	0.61	1.54	7	1
1:A:155:THR:HG21	1:A:164:THR:HB	0.61	1.70	7	1
1:A:70:THR:HG22	1:A:71:LYS:HE3	0.61	1.72	9	1
1:A:146:LEU:HD12	1:A:147:PRO:O	0.61	1.96	2	2
1:A:96:LYS:O	1:A:215:THR:HG23	0.60	1.96	8	6
1:A:123:VAL:HG12	1:A:137:PRO:HB2	0.60	1.74	8	1
1:A:153:HIS:CE1	1:A:171:LEU:HD13	0.60	2.30	6	1
1:A:143:VAL:HG13	1:A:148:ALA:HB2	0.60	1.71	1	2
1:A:118:LEU:HD11	1:A:123:VAL:CG1	0.60	2.24	8	1
1:A:29:PHE:CZ	1:A:33:LEU:HD22	0.60	2.31	3	2
1:A:101:SER:O	1:A:117:ALA:HB3	0.60	1.97	5	3
1:A:194:LEU:HG	1:A:204:LEU:HD12	0.60	1.72	8	1
1:A:18:GLU:CG	1:A:212:ALA:HB1	0.60	2.25	1	1
1:A:30:LEU:HD21	1:A:112:PHE:CE2	0.60	2.32	4	1
1:A:7:PRO:HG3	1:A:85:ALA:HB1	0.60	1.71	7	1
1:A:12:TRP:CD1	1:A:214:THR:HG21	0.59	2.32	7	1
1:A:133:GLU:HG3	1:A:172:LEU:HD21	0.59	1.74	8	1
1:A:100:LEU:HD13	1:A:116:VAL:CG1	0.59	2.28	1	1
1:A:153:HIS:CD2	1:A:171:LEU:HD13	0.59	2.32	10	2
1:A:70:THR:HG21	1:A:216:PHE:CZ	0.59	2.32	10	1
1:A:115:ARG:HD2	1:A:175:LEU:HD21	0.59	1.75	9	1
1:A:135:VAL:HG13	1:A:143:VAL:HG12	0.59	1.74	10	1
1:A:68:CYS:HA	1:A:154:VAL:HG23	0.59	1.73	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:106:ILE:HG22	1:A:203:PHE:CB	0.59	2.28	2	2
1:A:106:ILE:HG21	1:A:171:LEU:HD11	0.59	1.74	5	1
1:A:135:VAL:CG2	1:A:146:LEU:HD12	0.59	2.27	1	1
1:A:27:MET:HA	1:A:30:LEU:HD12	0.58	1.74	5	1
1:A:106:ILE:HD13	1:A:174:ILE:CD1	0.58	2.28	8	1
1:A:106:ILE:HG22	1:A:203:PHE:HB3	0.58	1.73	2	3
1:A:175:LEU:HD23	1:A:175:LEU:N	0.58	2.14	1	2
1:A:197:LEU:HD22	1:A:201:ARG:HD2	0.58	1.74	7	1
1:A:146:LEU:HD22	1:A:146:LEU:N	0.58	2.14	5	1
1:A:197:LEU:HD13	1:A:201:ARG:CB	0.58	2.28	2	1
1:A:135:VAL:HG21	1:A:146:LEU:HD11	0.58	1.76	9	1
1:A:115:ARG:CZ	1:A:175:LEU:HD21	0.57	2.28	5	3
1:A:153:HIS:CG	1:A:171:LEU:HD22	0.57	2.34	6	1
1:A:105:LEU:CD1	1:A:206:LEU:HD11	0.57	2.29	4	1
1:A:116:VAL:HG23	1:A:153:HIS:HA	0.57	1.76	3	2
1:A:98:TYR:CE2	1:A:100:LEU:HD11	0.57	2.34	7	1
1:A:104:ALA:HB3	1:A:115:ARG:CZ	0.57	2.29	6	3
1:A:206:LEU:HD13	1:A:210:ILE:CD1	0.57	2.30	2	3
1:A:172:LEU:HD13	1:A:172:LEU:N	0.57	2.15	4	1
1:A:185:THR:O	1:A:195:THR:HG23	0.57	1.99	10	1
1:A:29:PHE:CE1	1:A:204:LEU:HD22	0.57	2.35	1	1
1:A:153:HIS:HB3	1:A:171:LEU:HD13	0.57	1.76	1	1
1:A:104:ALA:HB3	1:A:115:ARG:NE	0.56	2.15	6	2
1:A:9:PHE:CE1	1:A:69:THR:HG22	0.56	2.35	6	1
1:A:63:PRO:HB3	1:A:66:LEU:HD11	0.56	1.76	2	1
1:A:118:LEU:HD22	1:A:122:GLN:HB3	0.56	1.76	10	1
1:A:123:VAL:HG22	1:A:137:PRO:HB3	0.56	1.77	1	1
1:A:70:THR:HG21	1:A:216:PHE:CE1	0.56	2.36	10	2
1:A:194:LEU:HD23	1:A:195:THR:N	0.56	2.15	7	1
1:A:187:VAL:O	1:A:193:THR:HG23	0.56	2.01	5	1
1:A:206:LEU:HD21	1:A:210:ILE:CD1	0.56	2.30	3	1
1:A:167:THR:O	1:A:171:LEU:HD12	0.56	2.01	10	2
1:A:197:LEU:HD22	1:A:201:ARG:CD	0.56	2.31	7	1
1:A:94:LEU:HD11	1:A:218:SER:HB2	0.56	1.76	9	1
1:A:145:ALA:C	1:A:146:LEU:HD13	0.56	2.21	5	1
1:A:18:GLU:HB3	1:A:212:ALA:HB1	0.56	1.78	10	2
1:A:15:LEU:HD23	1:A:17:GLU:HB2	0.55	1.77	1	1
1:A:97:SER:HA	1:A:214:THR:O	0.55	2.00	2	10
1:A:84:TYR:CD2	1:A:90:VAL:HG11	0.55	2.37	4	4
1:A:13:PHE:CG	1:A:217:THR:HG21	0.55	2.36	9	1
1:A:96:LYS:O	1:A:215:THR:HG22	0.55	2.01	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:115:ARG:HG2	1:A:171:LEU:HD21	0.55	1.76	1	1
1:A:191:LEU:HD12	1:A:208:GLU:OE2	0.55	2.01	3	1
1:A:107:VAL:HG22	1:A:112:PHE:CZ	0.55	2.37	8	2
1:A:70:THR:HG22	1:A:71:LYS:HE2	0.55	1.77	6	1
1:A:87:LEU:HD23	1:A:89:VAL:HG11	0.55	1.78	3	7
1:A:66:LEU:CD2	1:A:156:LEU:HD23	0.55	2.32	6	1
1:A:118:LEU:HD21	1:A:137:PRO:HB3	0.55	1.79	10	2
1:A:118:LEU:HD13	1:A:122:GLN:CB	0.54	2.33	10	2
1:A:100:LEU:HD23	1:A:118:LEU:HA	0.54	1.79	7	1
1:A:71:LYS:CD	1:A:81:ALA:HB1	0.54	2.32	10	1
1:A:36:LEU:HD13	1:A:194:LEU:CD2	0.54	2.32	10	1
1:A:100:LEU:HD22	1:A:116:VAL:HG12	0.54	1.79	7	1
1:A:14:LEU:HD12	1:A:19:GLU:HB3	0.53	1.79	1	1
1:A:12:TRP:CE3	1:A:70:THR:HG23	0.53	2.38	10	1
1:A:140:LEU:N	1:A:141:PRO:HD2	0.53	2.18	6	10
1:A:196:TYR:CD1	1:A:196:TYR:O	0.53	2.62	6	8
1:A:206:LEU:HD21	1:A:210:ILE:HD11	0.53	1.80	3	1
1:A:106:ILE:HD13	1:A:171:LEU:HG	0.53	1.80	1	1
1:A:66:LEU:HD13	1:A:67:HIS:H	0.53	1.64	5	1
1:A:183:GLU:HB3	1:A:195:THR:HG21	0.53	1.79	3	2
1:A:12:TRP:CZ2	1:A:216:PHE:CZ	0.53	2.97	2	2
1:A:170:ASP:O	1:A:174:ILE:HG22	0.53	2.04	5	1
1:A:162:VAL:HG11	1:A:166:GLN:CD	0.52	2.24	7	1
1:A:63:PRO:CB	1:A:66:LEU:HD11	0.52	2.35	2	1
1:A:174:ILE:CG2	1:A:175:LEU:HD23	0.52	2.33	2	1
1:A:14:LEU:HD12	1:A:14:LEU:O	0.52	2.05	5	1
1:A:100:LEU:HD13	1:A:116:VAL:HG11	0.52	1.81	10	2
1:A:154:VAL:O	1:A:156:LEU:HD12	0.52	2.04	9	1
1:A:84:TYR:CZ	1:A:90:VAL:HG11	0.52	2.39	6	4
1:A:193:THR:O	1:A:205:ALA:HB3	0.52	2.03	3	2
1:A:26:THR:HG21	1:A:156:LEU:CD2	0.51	2.35	2	1
1:A:118:LEU:HD21	1:A:137:PRO:HG2	0.51	1.79	2	2
1:A:68:CYS:HB2	1:A:154:VAL:HG22	0.51	1.80	1	1
1:A:104:ALA:HB1	1:A:204:LEU:O	0.51	2.05	3	2
1:A:84:TYR:O	1:A:90:VAL:HG21	0.51	2.05	7	3
1:A:115:ARG:HD2	1:A:175:LEU:HD11	0.51	1.83	2	1
1:A:94:LEU:HD21	1:A:218:SER:CB	0.51	2.36	1	2
1:A:22:ILE:HD13	1:A:22:ILE:C	0.51	2.27	7	1
1:A:139:LEU:C	1:A:143:VAL:HG13	0.51	2.26	10	1
1:A:182:LYS:CB	1:A:197:LEU:HD23	0.51	2.36	10	2
1:A:193:THR:O	1:A:204:LEU:HD12	0.51	2.06	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:12:TRP:CZ3	1:A:216:PHE:CZ	0.50	2.99	3	1
1:A:107:VAL:HG13	1:A:112:PHE:CD2	0.50	2.42	3	2
1:A:196:TYR:CD2	1:A:202:TRP:CE2	0.50	3.00	1	1
1:A:33:LEU:HD21	1:A:39:PHE:CE2	0.50	2.42	5	1
1:A:115:ARG:CD	1:A:175:LEU:HD11	0.50	2.37	2	1
1:A:100:LEU:HD13	1:A:116:VAL:HG13	0.50	1.83	1	1
1:A:115:ARG:CG	1:A:171:LEU:HD21	0.49	2.37	1	1
1:A:106:ILE:HD13	1:A:106:ILE:C	0.49	2.28	3	1
1:A:108:THR:HG22	1:A:109:PRO:HD2	0.49	1.84	10	1
1:A:183:GLU:CB	1:A:195:THR:HG21	0.49	2.37	3	1
1:A:29:PHE:CE2	1:A:204:LEU:HD22	0.49	2.43	4	1
1:A:100:LEU:HD23	1:A:214:THR:HG21	0.49	1.85	1	1
1:A:26:THR:HG21	1:A:156:LEU:HD21	0.49	1.83	2	1
1:A:66:LEU:N	1:A:66:LEU:HD12	0.49	2.23	6	1
1:A:10:PHE:CZ	1:A:216:PHE:CD1	0.49	3.01	1	1
1:A:174:ILE:HA	1:A:197:LEU:HD11	0.49	1.83	1	1
1:A:79:GLU:O	1:A:81:ALA:N	0.49	2.46	8	1
1:A:142:SER:O	1:A:146:LEU:HD23	0.48	2.08	1	1
1:A:114:ALA:HB3	1:A:154:VAL:CG1	0.48	2.38	8	2
1:A:143:VAL:HG21	1:A:148:ALA:CB	0.48	2.38	5	2
1:A:126:TRP:CE3	1:A:151:ARG:NH2	0.48	2.81	1	1
1:A:118:LEU:HD13	1:A:122:GLN:HG2	0.48	1.84	4	1
1:A:66:LEU:HD13	1:A:67:HIS:N	0.48	2.22	5	1
1:A:143:VAL:O	1:A:146:LEU:O	0.48	2.31	2	6
1:A:9:PHE:HE2	1:A:69:THR:HG22	0.48	1.68	7	1
1:A:118:LEU:HD11	1:A:137:PRO:HB3	0.48	1.85	8	2
1:A:18:GLU:CD	1:A:212:ALA:HB1	0.48	2.29	9	1
1:A:123:VAL:HG22	1:A:137:PRO:CB	0.48	2.38	1	1
1:A:135:VAL:CG1	1:A:143:VAL:HG23	0.48	2.39	5	1
1:A:29:PHE:CE1	1:A:107:VAL:HG21	0.48	2.44	10	2
1:A:188:GLU:HG3	1:A:193:THR:HG22	0.48	1.85	1	1
1:A:9:PHE:CE1	1:A:69:THR:HG21	0.48	2.44	3	1
1:A:203:PHE:CD1	1:A:203:PHE:N	0.48	2.81	8	3
1:A:197:LEU:HD12	1:A:197:LEU:N	0.48	2.23	4	2
1:A:155:THR:CG2	1:A:164:THR:HG23	0.48	2.38	6	1
1:A:136:ALA:HB3	1:A:139:LEU:CD1	0.48	2.35	3	2
1:A:14:LEU:CD2	1:A:100:LEU:HD21	0.48	2.39	6	1
1:A:71:LYS:CE	1:A:81:ALA:HB1	0.47	2.38	1	1
1:A:33:LEU:HA	1:A:36:LEU:HD12	0.47	1.86	2	2
1:A:133:GLU:CD	1:A:172:LEU:HD11	0.47	2.29	6	1
1:A:170:ASP:OD1	1:A:174:ILE:HD11	0.47	2.09	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:84:TYR:CE2	1:A:90:VAL:CG1	0.47	2.97	7	8
1:A:115:ARG:CD	1:A:171:LEU:HD21	0.47	2.39	1	1
1:A:135:VAL:HG13	1:A:143:VAL:HG23	0.47	1.85	5	2
1:A:143:VAL:HG23	1:A:146:LEU:CD1	0.47	2.37	4	1
1:A:125:LEU:HD12	1:A:125:LEU:C	0.47	2.30	1	1
1:A:29:PHE:CE1	1:A:204:LEU:HD13	0.47	2.44	3	1
1:A:29:PHE:CE1	1:A:194:LEU:HD21	0.47	2.44	8	1
1:A:206:LEU:HD22	1:A:208:GLU:O	0.47	2.09	9	1
1:A:94:LEU:HA	1:A:216:PHE:HB3	0.47	1.86	4	9
1:A:115:ARG:NH2	1:A:203:PHE:CD2	0.47	2.82	3	1
1:A:146:LEU:HD22	1:A:146:LEU:H	0.47	1.68	5	1
1:A:140:LEU:HG	1:A:141:PRO:CD	0.47	2.39	7	1
1:A:29:PHE:O	1:A:32:THR:HG22	0.47	2.10	7	1
1:A:9:PHE:CE2	1:A:69:THR:HG22	0.46	2.45	7	1
1:A:102:VAL:HG12	1:A:210:ILE:HB	0.46	1.86	5	3
1:A:12:TRP:HE1	1:A:70:THR:HG23	0.46	1.71	8	1
1:A:10:PHE:CE2	1:A:216:PHE:CE1	0.46	3.03	1	1
1:A:100:LEU:HB2	1:A:116:VAL:HG13	0.46	1.87	4	1
1:A:106:ILE:HG23	1:A:115:ARG:HD2	0.46	1.86	6	1
1:A:182:LYS:HB2	1:A:197:LEU:HD23	0.46	1.87	10	1
1:A:115:ARG:HD2	1:A:171:LEU:HD21	0.46	1.88	1	1
1:A:84:TYR:CZ	1:A:90:VAL:CG1	0.46	2.99	9	4
1:A:143:VAL:HB	1:A:148:ALA:HB2	0.46	1.87	10	1
1:A:89:VAL:HG13	1:A:90:VAL:N	0.46	2.26	6	8
1:A:33:LEU:HD11	1:A:39:PHE:CD2	0.46	2.46	7	1
1:A:172:LEU:HA	1:A:175:LEU:HD21	0.46	1.87	6	1
1:A:106:ILE:HD13	1:A:174:ILE:HD13	0.46	1.88	8	1
1:A:118:LEU:HD22	1:A:122:GLN:HG2	0.46	1.87	4	1
1:A:33:LEU:CD2	1:A:39:PHE:CE2	0.46	2.99	10	1
1:A:173:GLU:O	1:A:177:LEU:HD12	0.45	2.11	7	1
1:A:111:THR:HG23	1:A:162:VAL:HG21	0.45	1.88	5	1
1:A:163:GLU:HB3	1:A:165:VAL:HG12	0.45	1.88	3	2
1:A:100:LEU:HD12	1:A:100:LEU:C	0.45	2.30	1	1
1:A:13:PHE:CE1	1:A:217:THR:HG21	0.45	2.47	2	1
1:A:112:PHE:CD1	1:A:113:GLY:N	0.45	2.85	3	2
1:A:133:GLU:HG2	1:A:172:LEU:HD21	0.45	1.88	3	2
1:A:33:LEU:CD2	1:A:39:PHE:CE1	0.45	3.00	6	1
1:A:196:TYR:CD1	1:A:196:TYR:C	0.45	2.90	1	8
1:A:106:ILE:HG21	1:A:171:LEU:CD1	0.45	2.40	5	1
1:A:100:LEU:HD22	1:A:214:THR:CG2	0.45	2.42	6	1
1:A:12:TRP:CE2	1:A:100:LEU:HD13	0.45	2.47	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:112:PHE:CE2	1:A:156:LEU:HD22	0.45	2.47	2	1
1:A:9:PHE:CE1	1:A:69:THR:CG2	0.44	3.00	3	2
1:A:115:ARG:HG3	1:A:171:LEU:HD11	0.44	1.88	8	2
1:A:33:LEU:CD1	1:A:39:PHE:CD1	0.44	3.00	3	1
1:A:98:TYR:O	1:A:214:THR:HG22	0.44	2.13	4	1
1:A:197:LEU:HD22	1:A:201:ARG:HG3	0.44	1.89	5	1
1:A:118:LEU:HD13	1:A:123:VAL:N	0.44	2.27	6	1
1:A:123:VAL:HG13	1:A:138:ALA:HA	0.44	1.89	10	1
1:A:130:ALA:HB1	1:A:151:ARG:HE	0.44	1.72	10	2
1:A:106:ILE:HG22	1:A:113:GLY:O	0.44	2.12	4	1
1:A:14:LEU:HD12	1:A:14:LEU:C	0.44	2.33	5	1
1:A:70:THR:HG22	1:A:71:LYS:CE	0.44	2.43	6	1
1:A:171:LEU:O	1:A:174:ILE:HG22	0.44	2.11	6	1
1:A:10:PHE:HZ	1:A:94:LEU:HD11	0.44	1.73	7	1
1:A:29:PHE:CE2	1:A:105:LEU:CB	0.44	2.99	7	1
1:A:100:LEU:HD12	1:A:214:THR:CG2	0.44	2.42	7	1
1:A:15:LEU:HD22	1:A:213:ASP:HB3	0.44	1.88	8	1
1:A:185:THR:HB	1:A:196:TYR:CD1	0.44	2.47	3	6
1:A:105:LEU:HD22	1:A:114:ALA:CB	0.44	2.43	6	1
1:A:91:LYS:HA	1:A:94:LEU:HD12	0.44	1.87	8	1
1:A:206:LEU:HD13	1:A:210:ILE:HD11	0.44	1.88	2	1
1:A:174:ILE:HG23	1:A:175:LEU:N	0.44	2.28	5	1
1:A:33:LEU:CD2	1:A:39:PHE:CD1	0.44	3.01	6	1
1:A:194:LEU:HD12	1:A:204:LEU:HB2	0.44	1.90	6	1
1:A:12:TRP:CZ2	1:A:100:LEU:HD13	0.44	2.47	8	1
1:A:182:LYS:HG2	1:A:197:LEU:HD21	0.44	1.88	8	1
1:A:33:LEU:CD1	1:A:39:PHE:CD2	0.44	3.00	7	1
1:A:116:VAL:CG2	1:A:154:VAL:HG23	0.44	2.43	9	1
1:A:93:SER:O	1:A:96:LYS:HB2	0.44	2.13	8	1
1:A:13:PHE:CD2	1:A:217:THR:HG21	0.43	2.48	4	1
1:A:123:VAL:HG21	1:A:138:ALA:HA	0.43	1.89	4	1
1:A:12:TRP:CD1	1:A:12:TRP:O	0.43	2.71	7	1
1:A:153:HIS:CE1	1:A:167:THR:CG2	0.43	3.00	10	1
1:A:12:TRP:NE1	1:A:100:LEU:HD11	0.43	2.28	3	1
1:A:170:ASP:O	1:A:174:ILE:HD12	0.43	2.12	4	1
1:A:142:SER:O	1:A:146:LEU:HD22	0.43	2.13	5	1
1:A:12:TRP:CH2	1:A:118:LEU:HD22	0.43	2.48	3	1
1:A:74:ASP:O	1:A:76:GLY:N	0.43	2.51	4	1
1:A:140:LEU:CA	1:A:143:VAL:HG12	0.43	2.43	9	2
1:A:63:PRO:O	1:A:64:LEU:CB	0.43	2.66	8	1
1:A:13:PHE:CD1	1:A:217:THR:CG2	0.43	2.98	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:LEU:HD13	1:A:194:LEU:CD1	0.43	2.43	9	1
1:A:146:LEU:HB3	1:A:179:LYS:HB2	0.43	1.88	9	1
1:A:118:LEU:HD22	1:A:122:GLN:NE2	0.43	2.28	1	1
1:A:71:LYS:HD2	1:A:81:ALA:HB1	0.43	1.89	2	1
1:A:193:THR:C	1:A:204:LEU:HD12	0.43	2.34	6	1
1:A:12:TRP:CZ3	1:A:70:THR:CG2	0.43	2.99	10	1
1:A:66:LEU:HD12	1:A:154:VAL:HG21	0.43	1.90	3	1
1:A:63:PRO:O	1:A:64:LEU:HD23	0.43	2.14	7	1
1:A:123:VAL:HG12	1:A:137:PRO:CB	0.43	2.41	8	1
1:A:12:TRP:CE3	1:A:216:PHE:CZ	0.43	3.06	3	1
1:A:140:LEU:C	1:A:140:LEU:HD13	0.43	2.34	8	1
1:A:126:TRP:CE3	1:A:151:ARG:CZ	0.43	3.01	1	1
1:A:12:TRP:CE2	1:A:216:PHE:CZ	0.43	3.07	2	1
1:A:197:LEU:HD12	1:A:201:ARG:O	0.43	2.14	2	1
1:A:130:ALA:HB1	1:A:151:ARG:NE	0.42	2.29	7	1
1:A:135:VAL:CG1	1:A:143:VAL:CG2	0.42	2.94	9	1
1:A:195:THR:O	1:A:203:PHE:CD1	0.42	2.72	9	1
1:A:9:PHE:CE1	1:A:72:PHE:CZ	0.42	3.07	1	1
1:A:140:LEU:HA	1:A:143:VAL:CG1	0.42	2.44	9	2
1:A:29:PHE:HE2	1:A:204:LEU:HD13	0.42	1.74	5	1
1:A:163:GLU:OE1	1:A:165:VAL:HG23	0.42	2.14	7	1
1:A:130:ALA:HB1	1:A:151:ARG:HH21	0.42	1.74	9	1
1:A:70:THR:HG21	1:A:216:PHE:HE1	0.42	1.73	2	1
1:A:174:ILE:CG2	1:A:175:LEU:N	0.42	2.81	2	1
1:A:170:ASP:C	1:A:174:ILE:HD12	0.42	2.35	4	1
1:A:133:GLU:CD	1:A:172:LEU:HD21	0.42	2.34	9	1
1:A:182:LYS:O	1:A:197:LEU:HD22	0.42	2.15	9	1
1:A:12:TRP:CE3	1:A:70:THR:OG1	0.42	2.72	7	2
1:A:29:PHE:CE1	1:A:107:VAL:CG2	0.42	3.03	7	1
1:A:150:SER:CA	1:A:171:LEU:HD22	0.42	2.40	1	1
1:A:154:VAL:O	1:A:154:VAL:HG13	0.42	2.14	7	1
1:A:177:LEU:CG	1:A:197:LEU:HD13	0.42	2.39	1	1
1:A:33:LEU:HD21	1:A:39:PHE:CE1	0.42	2.50	3	1
1:A:26:THR:HG22	1:A:105:LEU:HD21	0.42	1.90	5	1
1:A:29:PHE:CE2	1:A:204:LEU:HD13	0.42	2.50	5	1
1:A:150:SER:HA	1:A:171:LEU:HD23	0.42	1.91	6	1
1:A:106:ILE:HD11	1:A:171:LEU:CD2	0.42	2.45	9	1
1:A:91:LYS:HG3	1:A:92:GLU:N	0.42	2.30	10	1
1:A:200:GLY:O	1:A:202:TRP:CD1	0.42	2.73	10	1
1:A:153:HIS:CB	1:A:171:LEU:HD13	0.42	2.45	1	1
1:A:159:SER:HB2	1:A:162:VAL:HG21	0.42	1.90	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:98:TYR:HE2	1:A:100:LEU:HD11	0.42	1.74	7	1
1:A:107:VAL:CG2	1:A:112:PHE:CE2	0.42	2.99	7	1
1:A:10:PHE:CE2	1:A:216:PHE:CD1	0.42	3.08	1	1
1:A:153:HIS:CE1	1:A:168:GLY:CA	0.42	3.03	1	1
1:A:185:THR:OG1	1:A:196:TYR:HB2	0.41	2.14	4	1
1:A:10:PHE:CE1	1:A:94:LEU:HD21	0.41	2.50	8	1
1:A:79:GLU:O	1:A:130:ALA:N	0.41	2.53	8	1
1:A:174:ILE:HD12	1:A:197:LEU:HD21	0.41	1.92	3	1
1:A:36:LEU:CD1	1:A:194:LEU:HD22	0.41	2.40	10	1
1:A:72:PHE:CD2	1:A:72:PHE:O	0.41	2.73	3	1
1:A:104:ALA:CB	1:A:115:ARG:NH1	0.41	2.84	8	1
1:A:12:TRP:CH2	1:A:118:LEU:HD11	0.41	2.49	9	1
1:A:12:TRP:NE1	1:A:100:LEU:CD1	0.41	2.83	5	2
1:A:146:LEU:HD12	1:A:179:LYS:HB3	0.41	1.90	5	1
1:A:64:LEU:C	1:A:64:LEU:HD12	0.41	2.35	8	1
1:A:133:GLU:O	1:A:134:GLY:C	0.41	2.58	8	1
1:A:133:GLU:CG	1:A:172:LEU:CD2	0.41	2.99	3	1
1:A:26:THR:HG21	1:A:156:LEU:HD22	0.41	1.90	9	1
1:A:91:LYS:O	1:A:94:LEU:HD13	0.41	2.15	10	2
1:A:7:PRO:O	1:A:8:LEU:HD23	0.41	2.16	3	1
1:A:94:LEU:HA	1:A:216:PHE:O	0.41	2.16	4	1
1:A:197:LEU:N	1:A:197:LEU:CD1	0.41	2.84	5	2
1:A:177:LEU:HD22	1:A:182:LYS:HE3	0.41	1.92	7	1
1:A:115:ARG:NH1	1:A:175:LEU:HD22	0.41	2.30	1	1
1:A:126:TRP:CZ2	1:A:130:ALA:CB	0.41	3.04	1	1
1:A:185:THR:CG2	1:A:196:TYR:CD1	0.41	3.04	3	2
1:A:30:LEU:HD21	1:A:112:PHE:HE2	0.41	1.72	4	1
1:A:74:ASP:O	1:A:75:TYR:CD2	0.41	2.73	4	1
1:A:150:SER:O	1:A:153:HIS:CE1	0.41	2.74	3	1
1:A:72:PHE:O	1:A:72:PHE:CD1	0.41	2.75	4	1
1:A:113:GLY:CA	1:A:156:LEU:HD12	0.41	2.46	5	1
1:A:123:VAL:HG23	1:A:137:PRO:HB2	0.41	1.93	6	1
1:A:153:HIS:CG	1:A:171:LEU:CD2	0.41	3.03	6	1
1:A:112:PHE:CD1	1:A:156:LEU:CD1	0.41	2.99	8	1
1:A:114:ALA:HB3	1:A:154:VAL:HG12	0.41	1.92	8	1
1:A:195:THR:O	1:A:203:PHE:CE1	0.40	2.74	9	2
1:A:12:TRP:CD1	1:A:100:LEU:HD11	0.40	2.52	3	1
1:A:146:LEU:N	1:A:146:LEU:CD2	0.40	2.83	5	1
1:A:146:LEU:N	1:A:146:LEU:HD13	0.40	2.31	5	1
1:A:12:TRP:CE3	1:A:98:TYR:OH	0.40	2.74	7	1
1:A:29:PHE:CD1	1:A:29:PHE:C	0.40	2.94	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:192:GLY:HA3	1:A:205:ALA:O	0.40	2.16	10	1
1:A:174:ILE:HD12	1:A:197:LEU:CD2	0.40	2.46	3	1
1:A:182:LYS:O	1:A:197:LEU:HG	0.40	2.17	3	1
1:A:120:GLU:O	1:A:123:VAL:HG12	0.40	2.16	4	1
1:A:147:PRO:CB	1:A:175:LEU:HD22	0.40	2.46	4	1
1:A:178:GLN:OE1	1:A:203:PHE:CG	0.40	2.74	4	1
1:A:9:PHE:CE1	1:A:10:PHE:O	0.40	2.74	9	1
1:A:74:ASP:OD1	1:A:75:TYR:CE2	0.40	2.75	4	1
1:A:12:TRP:O	1:A:12:TRP:CD1	0.40	2.74	1	1
1:A:84:TYR:CD1	1:A:84:TYR:C	0.40	2.95	3	2
1:A:146:LEU:HB3	1:A:179:LYS:CB	0.40	2.47	4	1
1:A:72:PHE:CD1	1:A:72:PHE:O	0.40	2.74	9	1
1:A:140:LEU:HA	1:A:143:VAL:HG12	0.40	1.92	4	1
1:A:170:ASP:OD2	1:A:174:ILE:HD11	0.40	2.16	4	1
1:A:70:THR:CG2	1:A:71:LYS:NZ	0.40	2.84	6	1
1:A:81:ALA:N	1:A:127:PRO:CB	0.40	2.85	8	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	193/222 (87%)	175±4 (91±2%)	13±3 (7±2%)	5±2 (3±1%)	8	44
All	All	1930/2220 (87%)	1749 (91%)	130 (7%)	51 (3%)	8	44

All 16 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	80	GLY	10
1	A	75	TYR	8
1	A	74	ASP	6
1	A	201	ARG	5
1	A	118	LEU	4
1	A	64	LEU	3

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Mol	Chain	Res	Type	Models (Total)
1	A	110	ARG	3
1	A	200	GLY	3
1	A	65	GLN	2
1	A	147	PRO	1
1	A	182	LYS	1
1	A	76	GLY	1
1	A	63	PRO	1
1	A	206	LEU	1
1	A	132	LYS	1
1	A	161	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	160/186 (86%)	119±4 (75±3%)	41±4 (25±3%)	2 24
All	All	1600/1860 (86%)	1194 (75%)	406 (25%)	2 24

All 111 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	185	THR	10
1	A	216	PHE	10
1	A	196	TYR	9
1	A	10	PHE	9
1	A	71	LYS	8
1	A	108	THR	8
1	A	178	GLN	8
1	A	155	THR	7
1	A	182	LYS	7
1	A	97	SER	7
1	A	31	LYS	6
1	A	171	LEU	6
1	A	179	LYS	6
1	A	189	MET	6
1	A	219	PHE	6

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Mol	Chain	Res	Type	Models (Total)
1	A	64	LEU	6
1	A	110	ARG	6
1	A	124	LYS	6
1	A	183	GLU	6
1	A	77	LYS	6
1	A	119	THR	6
1	A	21	ARG	5
1	A	23	LYS	5
1	A	40	LYS	5
1	A	61	GLN	5
1	A	66	LEU	5
1	A	82	LYS	5
1	A	92	GLU	5
1	A	101	SER	5
1	A	103	THR	5
1	A	140	LEU	5
1	A	142	SER	5
1	A	67	HIS	5
1	A	26	THR	5
1	A	8	LEU	4
1	A	65	GLN	4
1	A	73	CYS	4
1	A	83	GLU	4
1	A	111	THR	4
1	A	146	LEU	4
1	A	180	GLU	4
1	A	215	THR	4
1	A	12	TRP	4
1	A	70	THR	4
1	A	86	GLU	4
1	A	88	GLN	4
1	A	91	LYS	4
1	A	207	ARG	4
1	A	9	PHE	4
1	A	166	GLN	4
1	A	198	SER	4
1	A	208	GLU	4
1	A	144	GLU	4
1	A	194	LEU	4
1	A	14	LEU	3
1	A	151	ARG	3
1	A	186	GLN	3

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Mol	Chain	Res	Type	Models (Total)
1	A	28	ASP	3
1	A	94	LEU	3
1	A	150	SER	3
1	A	195	THR	3
1	A	69	THR	3
1	A	95	THR	3
1	A	143	VAL	3
1	A	190	ASP	3
1	A	206	LEU	3
1	A	93	SER	3
1	A	96	LYS	3
1	A	100	LEU	3
1	A	156	LEU	3
1	A	118	LEU	3
1	A	188	GLU	3
1	A	199	GLU	3
1	A	20	GLU	2
1	A	27	MET	2
1	A	131	ASP	2
1	A	159	SER	2
1	A	173	GLU	2
1	A	35	THR	2
1	A	125	LEU	2
1	A	87	LEU	2
1	A	133	GLU	2
1	A	163	GLU	2
1	A	164	THR	2
1	A	122	GLN	2
1	A	128	GLU	2
1	A	201	ARG	2
1	A	30	LEU	2
1	A	197	LEU	2
1	A	37	GLU	2
1	A	139	LEU	1
1	A	158	CYS	1
1	A	177	LEU	1
1	A	19	GLU	1
1	A	174	ILE	1
1	A	106	ILE	1
1	A	75	TYR	1
1	A	170	ASP	1
1	A	172	LEU	1

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Mol	Chain	Res	Type	Models (Total)
1	A	193	THR	1
1	A	105	LEU	1
1	A	36	LEU	1
1	A	22	ILE	1
1	A	115	ARG	1
1	A	204	LEU	1
1	A	213	ASP	1
1	A	15	LEU	1
1	A	17	GLU	1
1	A	132	LYS	1
1	A	203	PHE	1
1	A	218	SER	1

6.3.3 RNA

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates

There are no monosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation (i)

No chemical shift data were provided