Full wwPDB NMR Structure Validation Report (i)

Oct 23, 2021 – 08:48 AM EDT

PDB ID	:	1G3G
Title	:	NMR STRUCTURE OF THE FHA1 DOMAIN OF YEAST RAD53
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Deposited on	:	2000-10-24

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:

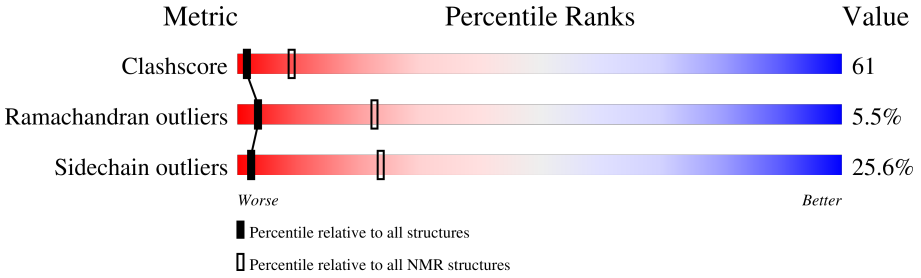
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.23.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	164	20% 35% 10% • 34%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 20 is the overall representative, medoid model (most similar to other models). The authors have identified model 2 as representative, based on the following criterion: *closest to the average*.

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:30-A:52, A:63-A:94, A:99-A:151 (108)	0.28	20

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

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

The models can be grouped into 2 clusters and 2 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2614 atoms, of which 1315 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called PROTEIN KINASE SPK1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	164	2614	808	1315	233	254	4	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	MET	engineered mutation	UNP P22216

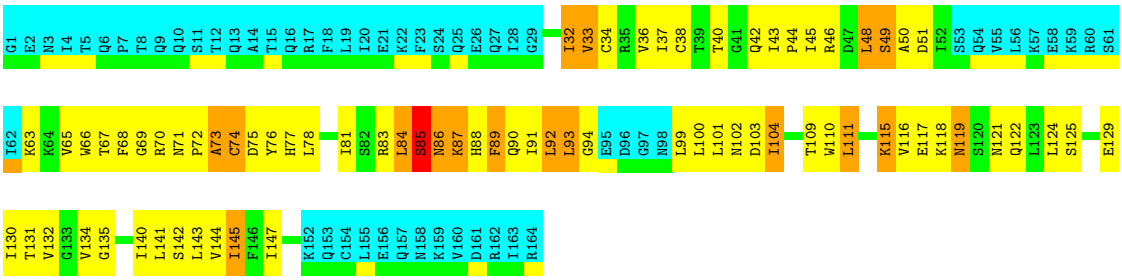
4 Residue-property plots (i)

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 KINASE SPK1

Chain A: 20% 35% 10% • 34%



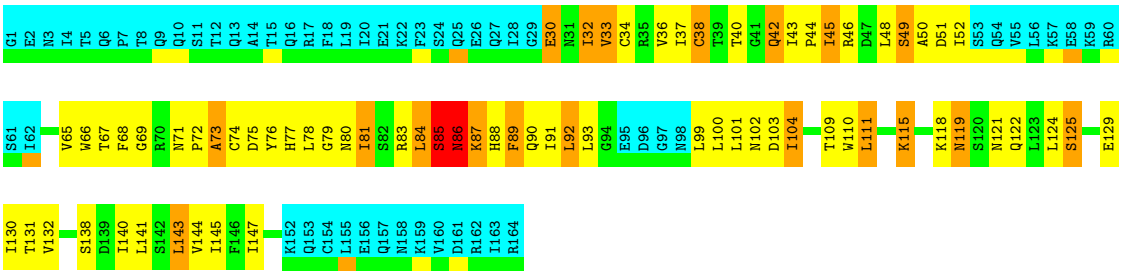
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: PROTEIN KINASE SPK1

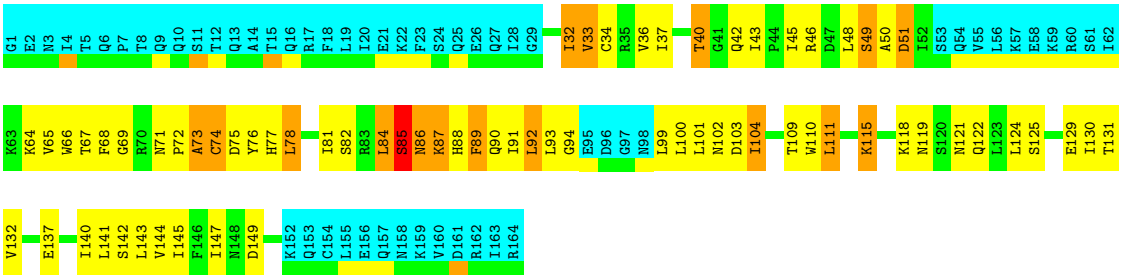
Chain A: 22% 31% 12% • 34%



4.2.2 Score per residue for model 2

• Molecule 1: PROTEIN KINASE SPK1

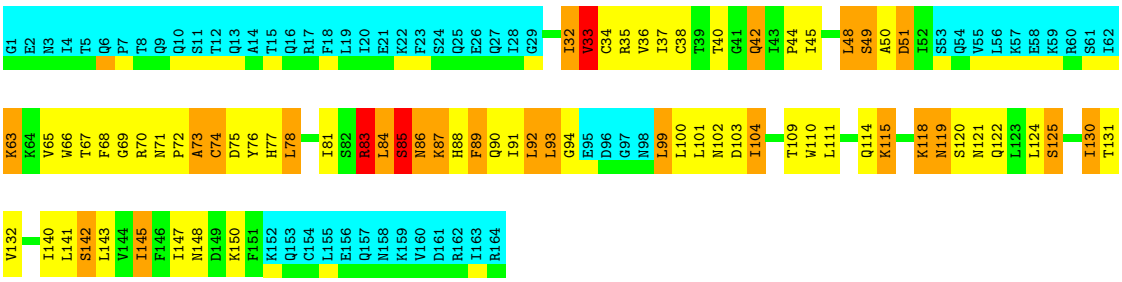
Chain A: 23% 32% 10% • 34%



4.2.3 Score per residue for model 3

• Molecule 1: PROTEIN KINASE SPK1

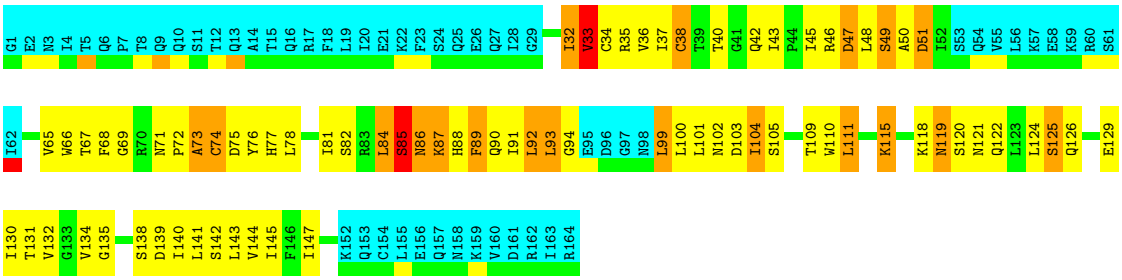
Chain A: 22% 27% 15% • 34%



4.2.4 Score per residue for model 4

• Molecule 1: PROTEIN KINASE SPK1

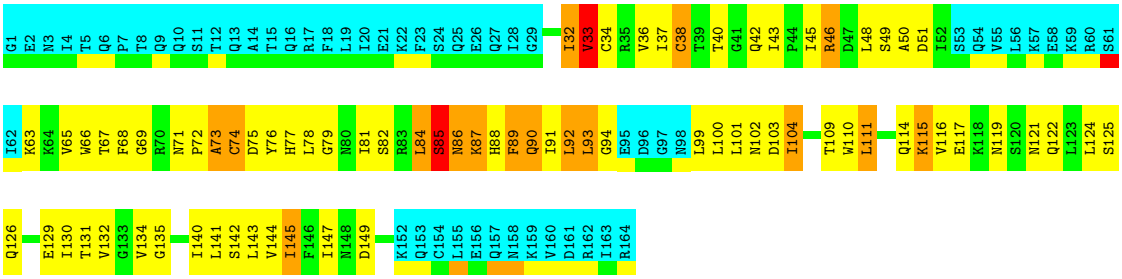
Chain A: 19% 34% 12% • 34%



4.2.5 Score per residue for model 5

• Molecule 1: PROTEIN KINASE SPK1

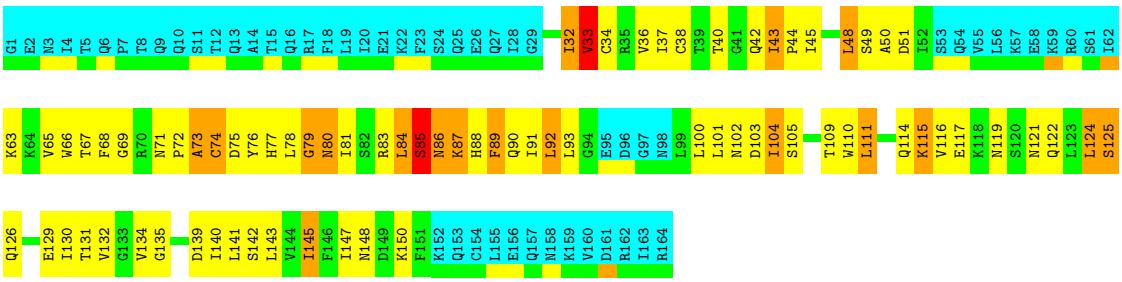
Chain A: 20% 35% 10% • 34%



4.2.6 Score per residue for model 6

• Molecule 1: PROTEIN KINASE SPK1

Chain A: 19% 35% 11% • 34%



4.2.7 Score per residue for model 7

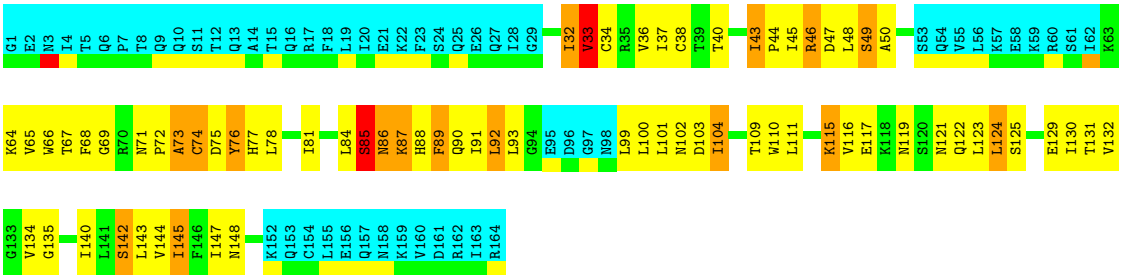
• Molecule 1: PROTEIN KINASE SPK1

Chain A: 21% 34% 10% • 34%

4.2.8 Score per residue for model 8

- Molecule 1: PROTEIN KINASE SPK1

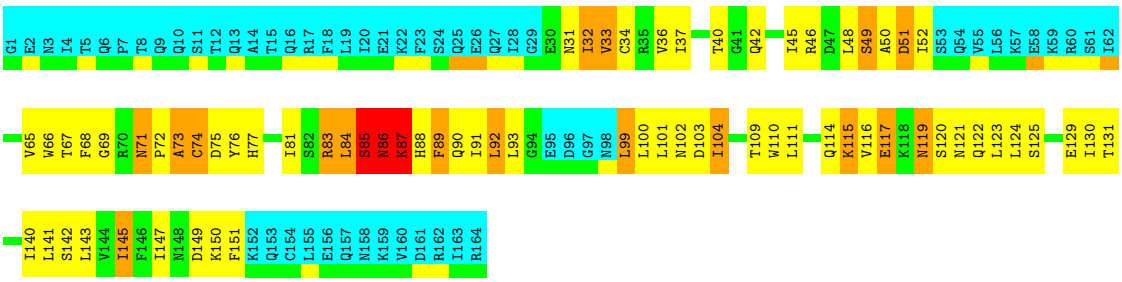
Chain A: 23% 32% 10% • 34%



4.2.9 Score per residue for model 9

- Molecule 1: PROTEIN KINASE SPK1

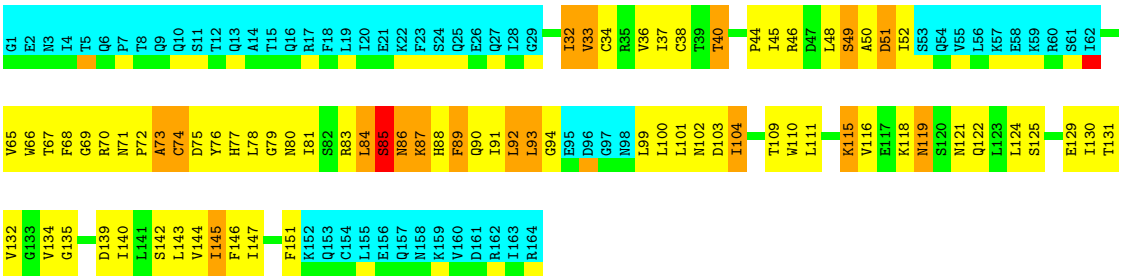
Chain A: 23% 31% 10% • 34%



4.2.10 Score per residue for model 10

- Molecule 1: PROTEIN KINASE SPK1

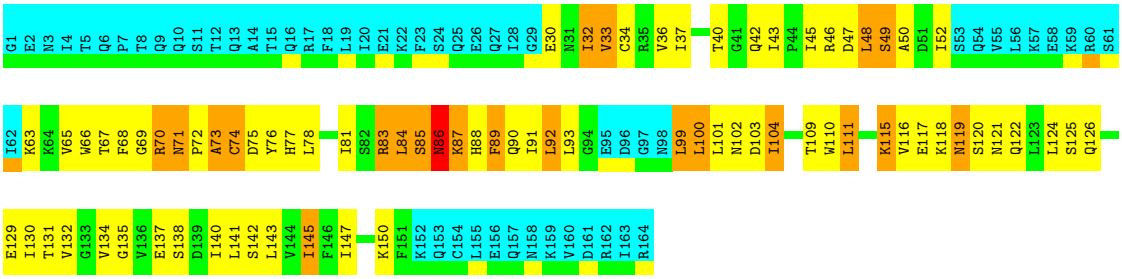
Chain A: 20% 35% 10% • 34%



4.2.11 Score per residue for model 11

- Molecule 1: PROTEIN KINASE SPK1

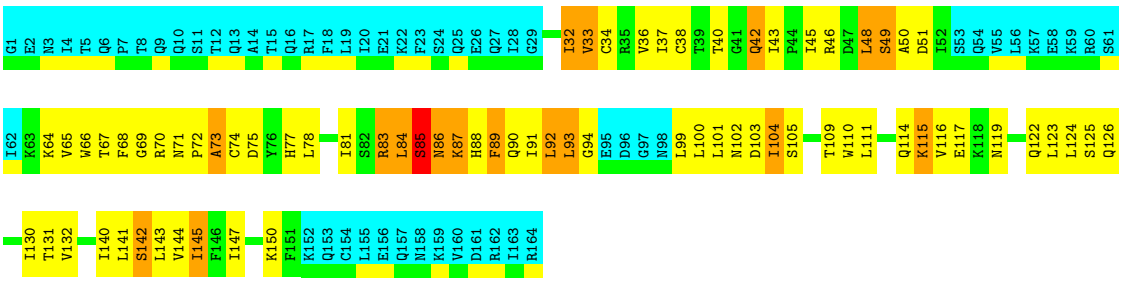
Chain A: 18% 34% 13% • 34%



4.2.12 Score per residue for model 12

- Molecule 1: PROTEIN KINASE SPK1

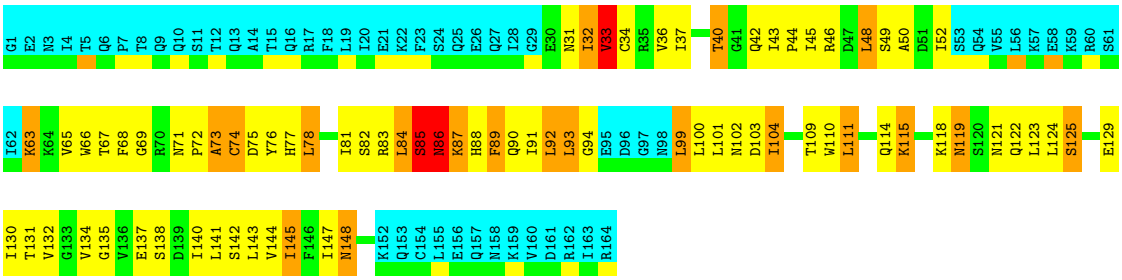
Chain A: 21% 34% 10% • 34%



4.2.13 Score per residue for model 13

- Molecule 1: PROTEIN KINASE SPK1

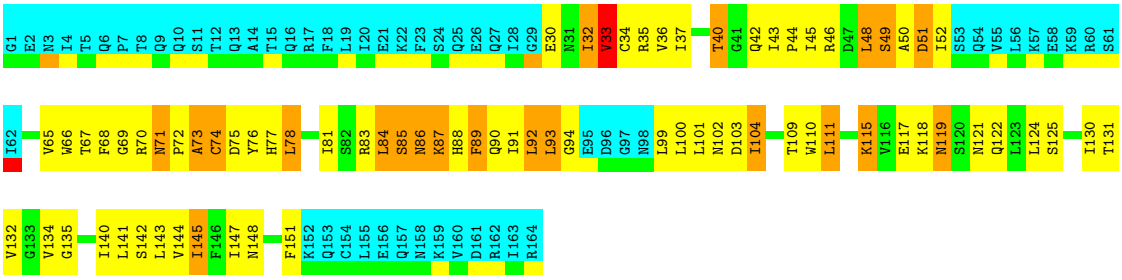
Chain A: 18% 34% 12% • 34%



4.2.14 Score per residue for model 14

- Molecule 1: PROTEIN KINASE SPK1

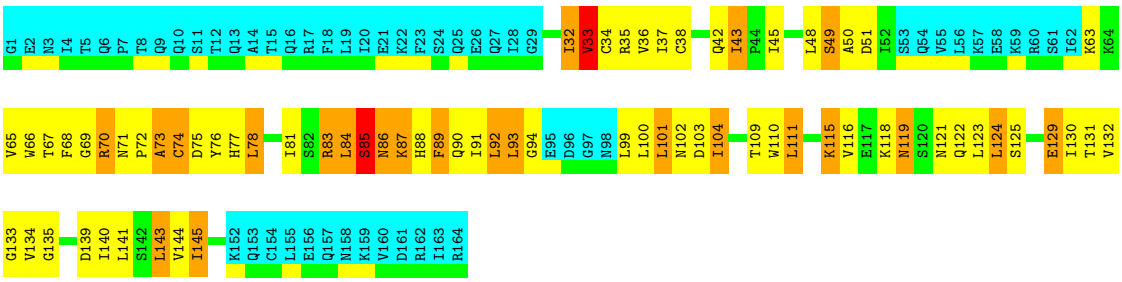
Chain A: 20% 33% 13% • 34%



4.2.15 Score per residue for model 15

- Molecule 1: PROTEIN KINASE SPK1

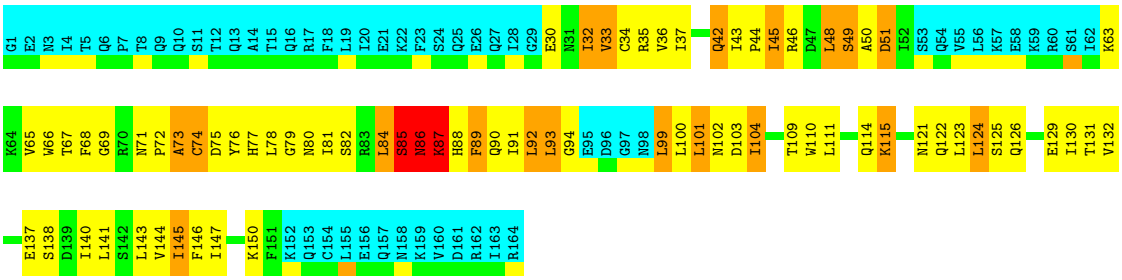
Chain A: 21% 29% 14% • 34%



4.2.16 Score per residue for model 16

- Molecule 1: PROTEIN KINASE SPK1

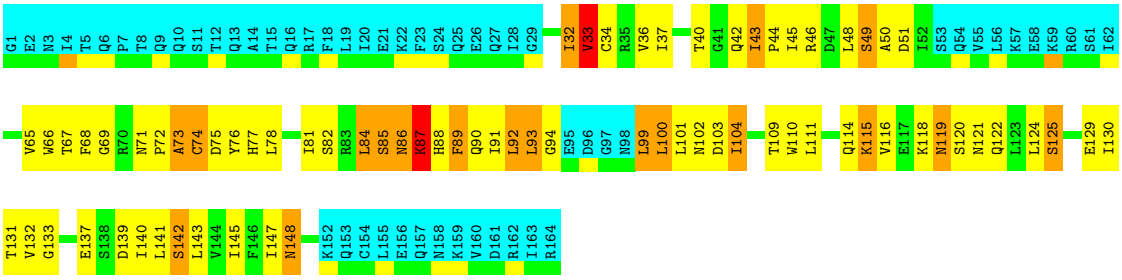
Chain A: 20% 33% 12% • 34%



4.2.17 Score per residue for model 17

- Molecule 1: PROTEIN KINASE SPK1

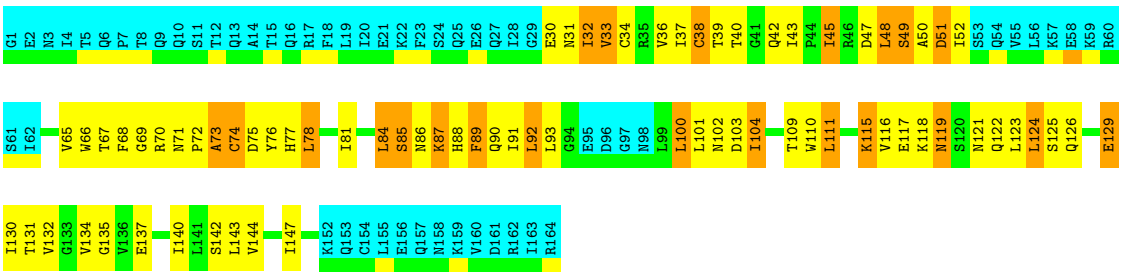
Chain A: 21% 32% 12% • 34%



4.2.18 Score per residue for model 18

- Molecule 1: PROTEIN KINASE SPK1

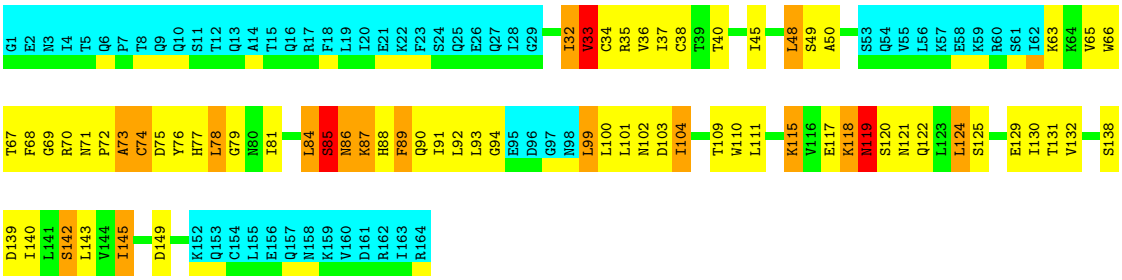
Chain A: 20% 32% 13% 34%



4.2.19 Score per residue for model 19

- Molecule 1: PROTEIN KINASE SPK1

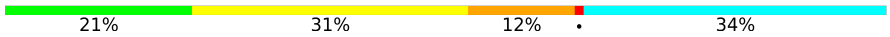
Chain A: 24% 30% 10% • 34%

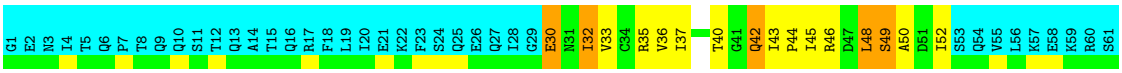


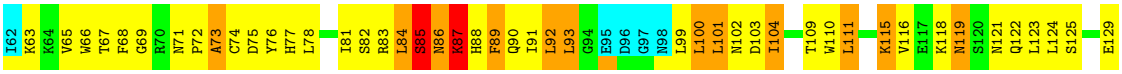
4.2.20 Score per residue for model 20 (medoid)

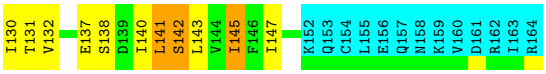
- Molecule 1: PROTEIN KINASE SPK1

Chain A:


21%
31%
12%
34%


G1 E2 N3 I4 T5 Q6 P7 T8 Q9 Q10 S11 T12 Q13 A14 T15 Q16 R17 F18 L19 I20 E21 K22 F23 S24 Q25 E26 Q27 I28 G29 E30 N31 I32 V33 C34 R35 V36 I37 T40 G41 Q42 I43 P44 I45 R46 D47 L48 S49 A50 D51 I52 S53 Q54 V55 L56 K57 E58 K59 R60 S61


I62 K63 K64 V65 W66 T67 F68 G69 R70 N71 P72 A73 C74 D75 Y76 H77 L78 I81 S82 R83 L84 S85 N86 K87 H88 F89 Q90 I91 L92 L93 G94 E95 D96 G97 N98 L99 L100 L101 N102 D103 I104 T109 W110 L111 K115 V116 E117 K118 N119 S120 N121 Q122 L123 L124 S125 E129


I130 T131 V132 E137 S138 D139 I140 L141 S142 L143 V144 I145 F146 I147 K152 Q153 C154 L155 E156 Q157 N158 K159 V160 D161 R162 I163 R164

5 Refinement protocol and experimental data overview (i)

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

Of the 50 calculated structures, 20 were deposited, based on the following criterion: *structures with the least restraint violations,structures with the lowest energy*.

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

Software name	Classification	Version
X-PLOR	structure solution	3.851
X-PLOR	refinement	3.851

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	843	858	856	104±5
All	All	16860	17160	17120	2089

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 61.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:33:VAL:HG23	1:A:50:ALA:HB2	1.08	1.18	9	9
1:A:88:HIS:O	1:A:104:ILE:O	1.07	1.72	18	20
1:A:88:HIS:C	1:A:104:ILE:O	1.04	1.96	8	20
1:A:99:LEU:HD12	1:A:124:LEU:HD22	1.00	1.26	4	2
1:A:36:VAL:HG12	1:A:143:LEU:HD21	1.00	1.29	4	4
1:A:86:ASN:O	1:A:88:HIS:N	0.98	1.97	11	20
1:A:48:LEU:HD21	1:A:91:ILE:HD13	0.96	1.35	10	2
1:A:124:LEU:HD21	1:A:147:ILE:HD13	0.93	1.36	9	3
1:A:33:VAL:CG2	1:A:50:ALA:HB2	0.93	1.92	16	11
1:A:99:LEU:HD22	1:A:124:LEU:HD13	0.93	1.39	10	1
1:A:36:VAL:HG23	1:A:48:LEU:HD21	0.88	1.43	12	5
1:A:101:LEU:HD21	1:A:145:ILE:HD13	0.88	1.44	7	2
1:A:48:LEU:HD22	1:A:66:TRP:CD1	0.87	2.04	5	9
1:A:33:VAL:HG23	1:A:50:ALA:CB	0.84	1.99	16	12

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:101:LEU:HD22	1:A:145:ILE:HD13	0.82	1.50	15	1
1:A:36:VAL:HG23	1:A:48:LEU:CD2	0.82	2.03	12	5
1:A:37:ILE:HG23	1:A:45:ILE:HG12	0.81	1.51	14	20
1:A:103:ASP:OD1	1:A:130:ILE:HD13	0.81	1.75	14	4
1:A:93:LEU:HD22	1:A:94:GLY:N	0.80	1.91	15	12
1:A:36:VAL:HG13	1:A:48:LEU:HD11	0.80	1.51	13	1
1:A:99:LEU:HD13	1:A:124:LEU:HD22	0.79	1.55	20	1
1:A:92:LEU:HD13	1:A:121:ASN:OD1	0.78	1.79	4	1
1:A:48:LEU:HD12	1:A:66:TRP:CD1	0.78	2.14	16	5
1:A:42:GLN:OE1	1:A:141:LEU:HD21	0.77	1.78	2	1
1:A:67:THR:HG23	1:A:90:GLN:HG3	0.77	1.55	16	9
1:A:33:VAL:HG12	1:A:99:LEU:CD2	0.77	2.08	20	1
1:A:48:LEU:HD11	1:A:91:ILE:HD13	0.77	1.56	15	7
1:A:67:THR:HG23	1:A:90:GLN:CG	0.77	2.10	11	16
1:A:36:VAL:HG13	1:A:143:LEU:HD11	0.76	1.56	16	2
1:A:103:ASP:HB3	1:A:109:THR:HG21	0.76	1.56	13	20
1:A:36:VAL:CG2	1:A:48:LEU:HD11	0.76	2.10	14	6
1:A:92:LEU:HD12	1:A:93:LEU:N	0.76	1.96	20	3
1:A:124:LEU:HD21	1:A:147:ILE:CD1	0.75	2.11	9	3
1:A:36:VAL:CG1	1:A:143:LEU:HD21	0.75	2.11	7	4
1:A:143:LEU:HD22	1:A:144:VAL:N	0.75	1.95	15	5
1:A:33:VAL:HG13	1:A:99:LEU:HD21	0.75	1.57	2	3
1:A:33:VAL:CG2	1:A:93:LEU:HD13	0.75	2.11	18	4
1:A:43:ILE:HG22	1:A:44:PRO:HD2	0.75	1.58	6	3
1:A:78:LEU:HD11	1:A:85:SER:O	0.74	1.82	20	9
1:A:52:ILE:HD11	1:A:151:PHE:CE2	0.74	2.17	14	3
1:A:100:LEU:HD13	1:A:122:GLN:O	0.74	1.82	14	3
1:A:78:LEU:HD12	1:A:79:GLY:O	0.74	1.83	10	5
1:A:33:VAL:HG23	1:A:50:ALA:HB3	0.73	1.60	6	8
1:A:40:THR:HG21	1:A:142:SER:CB	0.73	2.13	8	5
1:A:34:CYS:SG	1:A:48:LEU:HD12	0.73	2.24	13	5
1:A:87:LYS:HB2	1:A:104:ILE:HD11	0.72	1.61	15	10
1:A:43:ILE:HG21	1:A:76:TYR:CE2	0.72	2.19	17	1
1:A:129:GLU:HG2	1:A:144:VAL:HG22	0.72	1.60	8	2
1:A:124:LEU:HD21	1:A:147:ILE:HG12	0.72	1.60	11	9
1:A:81:ILE:HD12	1:A:85:SER:CB	0.72	2.14	10	2
1:A:32:ILE:HD13	1:A:48:LEU:O	0.71	1.84	4	8
1:A:33:VAL:HG21	1:A:93:LEU:HD13	0.71	1.59	18	4
1:A:40:THR:HG21	1:A:142:SER:HB2	0.71	1.62	7	7
1:A:100:LEU:HD23	1:A:121:ASN:HB3	0.71	1.61	2	5
1:A:142:SER:C	1:A:143:LEU:HD12	0.71	2.06	14	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:38:CYS:SG	1:A:143:LEU:HD12	0.70	2.26	12	2
1:A:93:LEU:HD23	1:A:99:LEU:HD22	0.70	1.64	12	1
1:A:87:LYS:HB3	1:A:104:ILE:HD11	0.70	1.61	3	6
1:A:100:LEU:HD22	1:A:121:ASN:HB3	0.69	1.62	18	4
1:A:81:ILE:HD12	1:A:85:SER:OG	0.69	1.87	2	5
1:A:103:ASP:OD2	1:A:116:VAL:HG11	0.69	1.87	7	5
1:A:36:VAL:CG1	1:A:48:LEU:HD11	0.69	2.18	13	1
1:A:92:LEU:HD13	1:A:121:ASN:ND2	0.69	2.03	14	13
1:A:48:LEU:CD1	1:A:91:ILE:HD13	0.68	2.18	15	7
1:A:81:ILE:HD13	1:A:85:SER:HB3	0.68	1.63	12	3
1:A:103:ASP:OD2	1:A:116:VAL:HG21	0.68	1.88	10	5
1:A:124:LEU:HD11	1:A:147:ILE:HG12	0.68	1.65	9	9
1:A:36:VAL:HG22	1:A:145:ILE:HG13	0.68	1.62	12	7
1:A:93:LEU:CD1	1:A:99:LEU:HD22	0.67	2.19	9	1
1:A:37:ILE:HG23	1:A:45:ILE:CG1	0.67	2.20	17	8
1:A:124:LEU:HD11	1:A:147:ILE:CD1	0.67	2.18	14	1
1:A:43:ILE:HG21	1:A:76:TYR:CD2	0.67	2.25	17	1
1:A:124:LEU:HD12	1:A:147:ILE:HG12	0.67	1.65	3	1
1:A:99:LEU:C	1:A:100:LEU:HD22	0.67	2.10	8	3
1:A:110:TRP:CE2	1:A:115:LYS:HB2	0.67	2.25	17	20
1:A:125:SER:O	1:A:147:ILE:HD11	0.67	1.90	4	4
1:A:36:VAL:CG1	1:A:143:LEU:HD11	0.67	2.20	16	3
1:A:129:GLU:CG	1:A:144:VAL:HG22	0.66	2.20	16	2
1:A:93:LEU:HD13	1:A:93:LEU:O	0.66	1.91	17	9
1:A:38:CYS:SG	1:A:143:LEU:HD23	0.66	2.31	18	6
1:A:99:LEU:HB2	1:A:124:LEU:HD13	0.66	1.67	3	4
1:A:142:SER:C	1:A:143:LEU:HD22	0.65	2.11	2	1
1:A:124:LEU:HD21	1:A:147:ILE:CG1	0.65	2.20	11	6
1:A:90:GLN:OE1	1:A:104:ILE:HD13	0.65	1.91	6	8
1:A:103:ASP:CB	1:A:109:THR:HG21	0.65	2.22	19	20
1:A:142:SER:O	1:A:143:LEU:HD13	0.65	1.92	6	2
1:A:36:VAL:HG23	1:A:48:LEU:HD11	0.64	1.68	19	4
1:A:93:LEU:HD23	1:A:99:LEU:CD2	0.64	2.23	12	1
1:A:84:LEU:HD22	1:A:84:LEU:H	0.64	1.51	14	8
1:A:33:VAL:HG12	1:A:99:LEU:HD21	0.64	1.69	20	1
1:A:84:LEU:HD13	1:A:84:LEU:N	0.64	2.07	9	8
1:A:65:VAL:HG23	1:A:91:ILE:O	0.64	1.93	8	1
1:A:43:ILE:CG1	1:A:78:LEU:HD13	0.64	2.22	18	1
1:A:33:VAL:HG11	1:A:93:LEU:HD13	0.64	1.69	7	1
1:A:36:VAL:HG12	1:A:145:ILE:HG13	0.63	1.69	13	2
1:A:99:LEU:O	1:A:100:LEU:HD22	0.63	1.93	16	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:78:LEU:HD11	1:A:85:SER:HA	0.63	1.68	18	2
1:A:33:VAL:CG1	1:A:34:CYS:N	0.63	2.61	4	18
1:A:36:VAL:HG22	1:A:145:ILE:CG1	0.63	2.24	19	4
1:A:34:CYS:SG	1:A:147:ILE:HG23	0.63	2.33	3	1
1:A:43:ILE:HG12	1:A:78:LEU:HD13	0.63	1.69	18	1
1:A:42:GLN:C	1:A:43:ILE:HD13	0.63	2.13	17	1
1:A:78:LEU:N	1:A:78:LEU:HD13	0.62	2.08	15	1
1:A:36:VAL:HG21	1:A:91:ILE:HD11	0.62	1.71	12	5
1:A:147:ILE:HD12	1:A:147:ILE:N	0.62	2.09	11	1
1:A:42:GLN:HG2	1:A:141:LEU:HD12	0.62	1.72	3	1
1:A:36:VAL:CG2	1:A:48:LEU:HD21	0.62	2.24	12	6
1:A:32:ILE:CG2	1:A:32:ILE:O	0.62	2.48	13	15
1:A:130:ILE:O	1:A:143:LEU:HD12	0.61	1.96	3	2
1:A:36:VAL:HG23	1:A:48:LEU:HD13	0.61	1.72	10	2
1:A:49:SER:OG	1:A:50:ALA:N	0.61	2.32	13	2
1:A:99:LEU:O	1:A:100:LEU:HD12	0.61	1.96	15	4
1:A:93:LEU:HD13	1:A:99:LEU:HA	0.61	1.72	8	1
1:A:123:LEU:HD13	1:A:124:LEU:O	0.61	1.96	12	3
1:A:99:LEU:CB	1:A:124:LEU:HD13	0.61	2.26	2	3
1:A:73:ALA:HB2	1:A:77:HIS:HB2	0.60	1.72	16	19
1:A:100:LEU:HA	1:A:122:GLN:O	0.60	1.96	13	20
1:A:88:HIS:O	1:A:88:HIS:CD2	0.60	2.54	19	20
1:A:124:LEU:HD13	1:A:125:SER:N	0.60	2.12	13	1
1:A:143:LEU:HD13	1:A:144:VAL:N	0.60	2.11	13	2
1:A:33:VAL:HG12	1:A:34:CYS:N	0.60	2.12	16	18
1:A:65:VAL:HG13	1:A:91:ILE:O	0.60	1.96	20	19
1:A:81:ILE:N	1:A:81:ILE:HD12	0.60	2.12	6	5
1:A:83:ARG:HB3	1:A:84:LEU:HD13	0.60	1.73	6	1
1:A:99:LEU:HD22	1:A:99:LEU:N	0.60	2.11	11	1
1:A:67:THR:HG23	1:A:90:GLN:HG2	0.60	1.73	18	10
1:A:36:VAL:HG23	1:A:48:LEU:CD1	0.60	2.26	2	4
1:A:67:THR:N	1:A:75:ASP:HB2	0.60	2.12	15	16
1:A:65:VAL:HG22	1:A:92:LEU:HD23	0.59	1.73	17	1
1:A:69:GLY:HA2	1:A:85:SER:O	0.59	1.96	18	19
1:A:68:PHE:CD2	1:A:76:TYR:CE2	0.59	2.90	17	1
1:A:71:ASN:O	1:A:77:HIS:CD2	0.59	2.56	17	20
1:A:48:LEU:HD23	1:A:48:LEU:N	0.59	2.13	14	5
1:A:33:VAL:CG1	1:A:93:LEU:HD13	0.59	2.28	7	1
1:A:100:LEU:HD13	1:A:122:GLN:C	0.59	2.18	14	3
1:A:93:LEU:HD11	1:A:99:LEU:HD22	0.59	1.72	9	1
1:A:103:ASP:OD1	1:A:130:ILE:HG21	0.59	1.98	19	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:78:LEU:HD11	1:A:85:SER:C	0.58	2.18	2	4
1:A:99:LEU:HD12	1:A:99:LEU:N	0.58	2.13	20	2
1:A:48:LEU:HD22	1:A:66:TRP:CG	0.58	2.34	19	1
1:A:43:ILE:HG23	1:A:78:LEU:HD21	0.58	1.75	5	1
1:A:92:LEU:HD22	1:A:121:ASN:ND2	0.58	2.14	6	3
1:A:42:GLN:OE1	1:A:141:LEU:HD13	0.58	1.99	12	1
1:A:40:THR:HG21	1:A:142:SER:H	0.58	1.57	19	8
1:A:92:LEU:HD11	1:A:102:ASN:CG	0.58	2.19	19	1
1:A:67:THR:O	1:A:75:ASP:N	0.58	2.35	6	20
1:A:49:SER:O	1:A:66:TRP:CZ2	0.58	2.57	5	11
1:A:33:VAL:CG2	1:A:50:ALA:HB3	0.57	2.29	6	6
1:A:129:GLU:CD	1:A:144:VAL:HG22	0.57	2.18	16	1
1:A:36:VAL:HG21	1:A:68:PHE:CZ	0.57	2.34	5	4
1:A:42:GLN:HB3	1:A:43:ILE:HD12	0.57	1.76	1	3
1:A:81:ILE:HB	1:A:85:SER:HB2	0.57	1.76	20	18
1:A:81:ILE:N	1:A:86:ASN:OD1	0.57	2.38	17	10
1:A:68:PHE:CE1	1:A:75:ASP:CG	0.57	2.78	15	11
1:A:48:LEU:N	1:A:48:LEU:HD13	0.57	2.15	7	4
1:A:123:LEU:HD13	1:A:124:LEU:N	0.57	2.14	13	2
1:A:69:GLY:CA	1:A:78:LEU:HD21	0.57	2.30	12	5
1:A:129:GLU:HG3	1:A:144:VAL:HG22	0.57	1.75	10	4
1:A:87:LYS:CB	1:A:104:ILE:HD11	0.57	2.30	17	1
1:A:99:LEU:HD22	1:A:124:LEU:CD1	0.57	2.22	10	1
1:A:72:PRO:O	1:A:73:ALA:CB	0.56	2.53	19	20
1:A:33:VAL:HG22	1:A:99:LEU:HD11	0.56	1.78	17	1
1:A:66:TRP:CZ3	1:A:93:LEU:HD23	0.56	2.35	8	1
1:A:129:GLU:HG3	1:A:144:VAL:HG13	0.56	1.77	16	2
1:A:42:GLN:HG2	1:A:141:LEU:HD22	0.56	1.75	15	2
1:A:93:LEU:HD22	1:A:94:GLY:H	0.56	1.59	19	4
1:A:143:LEU:HD22	1:A:144:VAL:H	0.56	1.59	5	5
1:A:92:LEU:C	1:A:93:LEU:HD22	0.56	2.22	8	1
1:A:103:ASP:HB3	1:A:109:THR:CG2	0.56	2.31	13	20
1:A:48:LEU:HD12	1:A:48:LEU:N	0.55	2.15	10	1
1:A:42:GLN:NE2	1:A:141:LEU:HD23	0.55	2.15	16	2
1:A:69:GLY:HA3	1:A:87:LYS:N	0.55	2.17	11	1
1:A:48:LEU:HD13	1:A:66:TRP:CG	0.55	2.37	15	1
1:A:89:PHE:CZ	1:A:91:ILE:HD11	0.55	2.36	17	3
1:A:93:LEU:C	1:A:93:LEU:HD13	0.55	2.22	19	9
1:A:131:THR:HG23	1:A:140:ILE:CG2	0.55	2.31	20	12
1:A:70:ARG:HD2	1:A:86:ASN:ND2	0.55	2.16	14	1
1:A:145:ILE:CG2	1:A:147:ILE:HD11	0.55	2.31	3	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:40:THR:HG21	1:A:142:SER:N	0.55	2.16	19	4
1:A:91:ILE:HG12	1:A:145:ILE:HD11	0.55	1.79	19	2
1:A:131:THR:CG2	1:A:140:ILE:CG2	0.54	2.85	5	20
1:A:124:LEU:HD11	1:A:147:ILE:HD11	0.54	1.77	14	1
1:A:69:GLY:HA2	1:A:78:LEU:HD21	0.54	1.79	20	6
1:A:32:ILE:O	1:A:32:ILE:HG22	0.54	2.03	15	19
1:A:33:VAL:HG23	1:A:50:ALA:N	0.54	2.18	20	2
1:A:92:LEU:HD23	1:A:121:ASN:ND2	0.54	2.18	20	1
1:A:33:VAL:HG23	1:A:49:SER:HA	0.54	1.80	20	2
1:A:123:LEU:HD23	1:A:124:LEU:O	0.54	2.01	20	1
1:A:42:GLN:CB	1:A:43:ILE:HD12	0.54	2.32	4	2
1:A:104:ILE:O	1:A:104:ILE:CG1	0.53	2.56	4	20
1:A:111:LEU:HD12	1:A:116:VAL:HG11	0.53	1.80	9	1
1:A:89:PHE:C	1:A:89:PHE:CD1	0.53	2.81	15	3
1:A:101:LEU:HD21	1:A:145:ILE:CD1	0.53	2.28	7	1
1:A:78:LEU:HD21	1:A:85:SER:O	0.53	2.03	10	2
1:A:93:LEU:HD13	1:A:93:LEU:C	0.53	2.24	13	3
1:A:69:GLY:C	1:A:78:LEU:HD11	0.53	2.24	7	1
1:A:36:VAL:HG11	1:A:68:PHE:CE2	0.53	2.39	8	2
1:A:42:GLN:HB3	1:A:141:LEU:HD22	0.53	1.79	14	1
1:A:33:VAL:HB	1:A:49:SER:C	0.52	2.25	13	2
1:A:37:ILE:HG22	1:A:39:THR:CG2	0.52	2.34	18	1
1:A:33:VAL:HG11	1:A:93:LEU:CG	0.52	2.34	20	1
1:A:48:LEU:HB3	1:A:66:TRP:CE2	0.52	2.39	20	14
1:A:68:PHE:CD2	1:A:89:PHE:CD2	0.52	2.98	3	6
1:A:52:ILE:HD11	1:A:151:PHE:CD2	0.52	2.40	10	1
1:A:43:ILE:HG12	1:A:78:LEU:HD11	0.52	1.81	5	1
1:A:142:SER:O	1:A:143:LEU:HD12	0.52	2.05	9	1
1:A:92:LEU:HD11	1:A:102:ASN:HB2	0.52	1.80	9	5
1:A:101:LEU:HD23	1:A:130:ILE:HD11	0.52	1.82	14	1
1:A:69:GLY:CA	1:A:86:ASN:C	0.52	2.78	4	11
1:A:86:ASN:O	1:A:87:LYS:C	0.52	2.48	11	1
1:A:78:LEU:HD11	1:A:85:SER:CA	0.52	2.35	14	1
1:A:90:GLN:O	1:A:102:ASN:O	0.52	2.29	2	20
1:A:92:LEU:HD12	1:A:102:ASN:HB2	0.52	1.81	4	1
1:A:99:LEU:N	1:A:99:LEU:HD23	0.52	2.20	4	2
1:A:37:ILE:HG12	1:A:45:ILE:HG23	0.52	1.82	13	1
1:A:100:LEU:HD23	1:A:122:GLN:C	0.51	2.25	18	2
1:A:42:GLN:HG3	1:A:141:LEU:HD12	0.51	1.83	13	3
1:A:68:PHE:CE1	1:A:89:PHE:CE2	0.51	2.98	9	3
1:A:124:LEU:C	1:A:124:LEU:HD22	0.51	2.26	8	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:89:PHE:CD1	1:A:90:GLN:N	0.51	2.79	19	19
1:A:129:GLU:OE2	1:A:144:VAL:HG22	0.51	2.05	16	1
1:A:36:VAL:HG21	1:A:91:ILE:CD1	0.51	2.35	12	5
1:A:69:GLY:HA3	1:A:86:ASN:C	0.51	2.26	12	15
1:A:99:LEU:HD23	1:A:100:LEU:N	0.51	2.21	10	1
1:A:42:GLN:NE2	1:A:143:LEU:HD11	0.51	2.20	14	1
1:A:124:LEU:HD21	1:A:147:ILE:HG13	0.51	1.81	14	1
1:A:48:LEU:CD1	1:A:48:LEU:N	0.51	2.74	2	2
1:A:33:VAL:HG11	1:A:93:LEU:HG	0.51	1.82	20	1
1:A:81:ILE:N	1:A:86:ASN:ND2	0.51	2.59	14	1
1:A:68:PHE:CE2	1:A:89:PHE:CE2	0.50	2.99	6	6
1:A:69:GLY:C	1:A:78:LEU:HD21	0.50	2.26	19	1
1:A:143:LEU:HD12	1:A:143:LEU:N	0.50	2.21	17	5
1:A:42:GLN:NE2	1:A:141:LEU:HD11	0.50	2.20	2	1
1:A:36:VAL:HG22	1:A:145:ILE:HG12	0.50	1.83	19	1
1:A:43:ILE:HD12	1:A:43:ILE:N	0.50	2.22	13	2
1:A:43:ILE:HG22	1:A:76:TYR:CD2	0.50	2.41	6	1
1:A:93:LEU:HD12	1:A:99:LEU:CD1	0.50	2.37	11	1
1:A:81:ILE:O	1:A:86:ASN:ND2	0.50	2.45	11	6
1:A:89:PHE:CE1	1:A:91:ILE:HG13	0.50	2.42	15	3
1:A:92:LEU:HD11	1:A:102:ASN:OD1	0.50	2.07	19	1
1:A:84:LEU:O	1:A:85:SER:CB	0.50	2.60	6	17
1:A:103:ASP:CG	1:A:109:THR:HG21	0.50	2.26	10	16
1:A:68:PHE:CD1	1:A:89:PHE:CD2	0.50	3.00	9	2
1:A:30:GLU:O	1:A:52:ILE:HD11	0.50	2.07	1	2
1:A:140:ILE:C	1:A:141:LEU:HD22	0.50	2.28	1	1
1:A:33:VAL:CG2	1:A:50:ALA:N	0.50	2.75	7	2
1:A:36:VAL:HG11	1:A:68:PHE:CZ	0.49	2.42	8	6
1:A:110:TRP:CD1	1:A:115:LYS:N	0.49	2.81	19	20
1:A:33:VAL:HG12	1:A:34:CYS:H	0.49	1.66	18	10
1:A:43:ILE:CG2	1:A:76:TYR:CD2	0.49	2.95	6	2
1:A:124:LEU:HD13	1:A:124:LEU:C	0.49	2.27	13	1
1:A:32:ILE:O	1:A:32:ILE:CG2	0.49	2.61	20	5
1:A:110:TRP:O	1:A:130:ILE:HG23	0.49	2.08	13	8
1:A:38:CYS:CB	1:A:143:LEU:HD12	0.49	2.37	12	1
1:A:44:PRO:CD	1:A:76:TYR:CZ	0.49	2.95	13	3
1:A:124:LEU:CD2	1:A:147:ILE:HD13	0.49	2.29	5	1
1:A:89:PHE:CE1	1:A:130:ILE:HD12	0.49	2.43	14	1
1:A:34:CYS:O	1:A:48:LEU:O	0.49	2.30	5	11
1:A:104:ILE:O	1:A:104:ILE:HG12	0.49	2.08	14	20
1:A:89:PHE:CZ	1:A:91:ILE:HG13	0.49	2.42	4	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:89:PHE:CD1	1:A:89:PHE:C	0.49	2.86	13	3
1:A:72:PRO:O	1:A:77:HIS:HB2	0.49	2.08	16	18
1:A:65:VAL:CG1	1:A:91:ILE:O	0.48	2.61	6	19
1:A:143:LEU:C	1:A:143:LEU:HD13	0.48	2.29	16	3
1:A:40:THR:HG21	1:A:142:SER:OG	0.48	2.07	20	5
1:A:100:LEU:HD23	1:A:122:GLN:O	0.48	2.08	4	2
1:A:36:VAL:HG22	1:A:46:ARG:O	0.48	2.08	5	1
1:A:116:VAL:HG22	1:A:117:GLU:N	0.48	2.23	5	7
1:A:81:ILE:O	1:A:86:ASN:OD1	0.48	2.31	9	2
1:A:30:GLU:O	1:A:52:ILE:HD12	0.48	2.08	20	1
1:A:44:PRO:CG	1:A:76:TYR:CE1	0.48	2.97	20	6
1:A:49:SER:O	1:A:66:TRP:HZ2	0.48	1.92	11	10
1:A:46:ARG:CG	1:A:76:TYR:CE2	0.48	2.96	8	1
1:A:101:LEU:CD1	1:A:145:ILE:HD13	0.48	2.38	8	1
1:A:67:THR:HB	1:A:74:CYS:HB3	0.48	1.86	9	17
1:A:44:PRO:CG	1:A:76:TYR:CZ	0.48	2.97	6	3
1:A:42:GLN:HE22	1:A:143:LEU:HD11	0.48	1.67	14	1
1:A:68:PHE:CD2	1:A:89:PHE:CE2	0.48	3.01	16	1
1:A:40:THR:CG2	1:A:142:SER:CB	0.48	2.92	19	5
1:A:89:PHE:CE1	1:A:130:ILE:CD1	0.48	2.97	11	5
1:A:103:ASP:OD1	1:A:109:THR:HG21	0.48	2.09	19	3
1:A:42:GLN:CG	1:A:141:LEU:HD12	0.48	2.38	11	2
1:A:65:VAL:HG22	1:A:92:LEU:CD2	0.48	2.38	17	1
1:A:43:ILE:HG23	1:A:44:PRO:HD2	0.47	1.86	1	3
1:A:42:GLN:HB2	1:A:43:ILE:HD12	0.47	1.86	4	2
1:A:124:LEU:HD11	1:A:147:ILE:HD12	0.47	1.84	14	1
1:A:43:ILE:CG2	1:A:76:TYR:CD1	0.47	2.97	15	1
1:A:76:TYR:CE1	1:A:78:LEU:HD13	0.47	2.44	17	1
1:A:67:THR:HB	1:A:74:CYS:CB	0.47	2.39	9	7
1:A:88:HIS:NE2	1:A:132:VAL:HB	0.47	2.24	14	17
1:A:101:LEU:O	1:A:122:GLN:N	0.47	2.48	1	20
1:A:81:ILE:CB	1:A:85:SER:HB2	0.47	2.40	18	6
1:A:124:LEU:HD11	1:A:147:ILE:CG1	0.47	2.39	12	3
1:A:37:ILE:N	1:A:144:VAL:O	0.47	2.48	12	2
1:A:81:ILE:HD12	1:A:85:SER:HB2	0.47	1.86	10	2
1:A:143:LEU:HD13	1:A:143:LEU:C	0.47	2.30	13	1
1:A:124:LEU:O	1:A:124:LEU:HD13	0.47	2.09	15	1
1:A:72:PRO:O	1:A:73:ALA:HB2	0.47	2.10	9	20
1:A:36:VAL:HG21	1:A:68:PHE:HZ	0.47	1.68	5	2
1:A:71:ASN:ND2	1:A:76:TYR:O	0.47	2.48	11	1
1:A:66:TRP:HB2	1:A:91:ILE:HB	0.47	1.87	8	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:89:PHE:CZ	1:A:91:ILE:CD1	0.47	2.98	17	2
1:A:123:LEU:HD13	1:A:123:LEU:C	0.47	2.30	12	3
1:A:67:THR:O	1:A:75:ASP:CB	0.47	2.63	17	3
1:A:84:LEU:N	1:A:84:LEU:CD1	0.47	2.78	9	5
1:A:68:PHE:HE2	1:A:91:ILE:HD11	0.47	1.68	10	1
1:A:36:VAL:HG11	1:A:68:PHE:HZ	0.47	1.70	3	2
1:A:110:TRP:O	1:A:130:ILE:CG2	0.47	2.63	1	20
1:A:33:VAL:HG23	1:A:49:SER:CA	0.47	2.39	20	2
1:A:32:ILE:HG22	1:A:32:ILE:O	0.46	2.09	7	1
1:A:40:THR:HG21	1:A:142:SER:HB3	0.46	1.87	4	2
1:A:89:PHE:CZ	1:A:130:ILE:CD1	0.46	2.98	6	1
1:A:142:SER:O	1:A:143:LEU:HD22	0.46	2.10	2	1
1:A:36:VAL:HG12	1:A:145:ILE:CG1	0.46	2.41	13	1
1:A:86:ASN:OD1	1:A:86:ASN:N	0.46	2.47	1	5
1:A:89:PHE:CE1	1:A:90:GLN:O	0.46	2.68	10	9
1:A:33:VAL:HG21	1:A:93:LEU:HG	0.46	1.86	19	2
1:A:68:PHE:CE1	1:A:75:ASP:OD2	0.46	2.69	9	9
1:A:88:HIS:CD2	1:A:132:VAL:HG11	0.46	2.45	16	5
1:A:48:LEU:CD1	1:A:66:TRP:CD1	0.46	2.97	11	3
1:A:48:LEU:HG	1:A:66:TRP:CG	0.46	2.45	2	1
1:A:124:LEU:N	1:A:124:LEU:CD1	0.46	2.78	15	5
1:A:83:ARG:C	1:A:84:LEU:HD13	0.46	2.30	9	6
1:A:93:LEU:HD12	1:A:99:LEU:HD12	0.46	1.86	11	1
1:A:33:VAL:HG23	1:A:49:SER:C	0.46	2.31	20	2
1:A:93:LEU:HD22	1:A:93:LEU:C	0.46	2.31	17	4
1:A:43:ILE:CG2	1:A:76:TYR:CG	0.46	2.99	4	5
1:A:91:ILE:HG22	1:A:93:LEU:CD2	0.46	2.41	8	1
1:A:89:PHE:CD2	1:A:103:ASP:HA	0.46	2.46	18	2
1:A:71:ASN:C	1:A:73:ALA:N	0.45	2.70	17	3
1:A:81:ILE:N	1:A:81:ILE:CD1	0.45	2.79	6	3
1:A:70:ARG:CD	1:A:86:ASN:HB3	0.45	2.41	11	1
1:A:40:THR:CG2	1:A:142:SER:HB2	0.45	2.40	20	5
1:A:84:LEU:HD22	1:A:84:LEU:N	0.45	2.24	14	1
1:A:118:LYS:O	1:A:120:SER:N	0.45	2.50	3	1
1:A:147:ILE:N	1:A:147:ILE:CD1	0.45	2.79	11	1
1:A:129:GLU:HB2	1:A:144:VAL:HG22	0.45	1.88	18	1
1:A:34:CYS:O	1:A:48:LEU:N	0.45	2.50	14	7
1:A:40:THR:OG1	1:A:142:SER:O	0.45	2.35	14	4
1:A:92:LEU:N	1:A:100:LEU:O	0.45	2.48	13	10
1:A:69:GLY:CA	1:A:86:ASN:O	0.45	2.65	14	8
1:A:80:ASN:C	1:A:81:ILE:HD12	0.45	2.31	16	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:93:LEU:HD23	1:A:99:LEU:HD23	0.45	1.88	19	1
1:A:48:LEU:N	1:A:48:LEU:HD12	0.45	2.25	2	1
1:A:64:LYS:O	1:A:66:TRP:CZ3	0.45	2.70	8	1
1:A:42:GLN:CG	1:A:141:LEU:HD22	0.45	2.40	15	1
1:A:49:SER:O	1:A:66:TRP:CH2	0.45	2.70	5	5
1:A:93:LEU:CD1	1:A:99:LEU:HD12	0.45	2.41	11	1
1:A:78:LEU:N	1:A:78:LEU:CD1	0.45	2.80	15	1
1:A:68:PHE:CE2	1:A:75:ASP:OD2	0.45	2.70	11	6
1:A:48:LEU:HG	1:A:66:TRP:CD1	0.45	2.47	10	2
1:A:33:VAL:HG22	1:A:93:LEU:HD13	0.45	1.89	11	1
1:A:118:LYS:O	1:A:119:ASN:C	0.44	2.55	3	14
1:A:124:LEU:O	1:A:124:LEU:HD22	0.44	2.12	15	1
1:A:50:ALA:HB2	1:A:93:LEU:HD22	0.44	1.89	1	2
1:A:44:PRO:HD2	1:A:76:TYR:CZ	0.44	2.47	7	3
1:A:43:ILE:HG21	1:A:76:TYR:CG	0.44	2.47	18	2
1:A:36:VAL:HG13	1:A:143:LEU:CD1	0.44	2.37	16	1
1:A:92:LEU:HD22	1:A:121:ASN:HD21	0.44	1.70	6	2
1:A:129:GLU:HA	1:A:143:LEU:O	0.44	2.13	7	10
1:A:65:VAL:CG2	1:A:91:ILE:O	0.44	2.65	8	1
1:A:42:GLN:CD	1:A:141:LEU:HD12	0.44	2.32	9	3
1:A:43:ILE:HG23	1:A:76:TYR:CD2	0.44	2.48	2	3
1:A:47:ASP:C	1:A:48:LEU:HD23	0.44	2.33	4	1
1:A:88:HIS:NE2	1:A:105:SER:OG	0.44	2.49	6	3
1:A:68:PHE:CE2	1:A:91:ILE:HD11	0.44	2.48	10	1
1:A:66:TRP:N	1:A:91:ILE:O	0.44	2.48	18	13
1:A:89:PHE:CG	1:A:90:GLN:N	0.44	2.85	15	3
1:A:141:LEU:HD22	1:A:141:LEU:N	0.44	2.28	13	2
1:A:70:ARG:CD	1:A:86:ASN:CB	0.44	2.95	11	1
1:A:33:VAL:CG2	1:A:93:LEU:CD1	0.44	2.95	1	1
1:A:38:CYS:HB2	1:A:43:ILE:O	0.44	2.13	12	2
1:A:124:LEU:HD13	1:A:124:LEU:O	0.44	2.13	19	2
1:A:125:SER:O	1:A:147:ILE:CD1	0.43	2.66	6	3
1:A:134:VAL:HG12	1:A:135:GLY:N	0.43	2.28	7	10
1:A:81:ILE:CG1	1:A:85:SER:CB	0.43	2.96	5	1
1:A:48:LEU:HD11	1:A:91:ILE:CD1	0.43	2.38	15	1
1:A:81:ILE:O	1:A:86:ASN:CG	0.43	2.57	1	3
1:A:129:GLU:CG	1:A:143:LEU:O	0.43	2.67	5	3
1:A:123:LEU:C	1:A:123:LEU:HD13	0.43	2.33	18	1
1:A:110:TRP:N	1:A:131:THR:O	0.43	2.49	16	8
1:A:68:PHE:CZ	1:A:75:ASP:OD2	0.43	2.71	12	8
1:A:66:TRP:O	1:A:91:ILE:N	0.43	2.43	9	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:111:LEU:C	1:A:111:LEU:HD12	0.43	2.34	13	11
1:A:89:PHE:CZ	1:A:91:ILE:CG1	0.43	3.02	4	2
1:A:32:ILE:HD13	1:A:48:LEU:C	0.43	2.33	4	1
1:A:73:ALA:HA	1:A:76:TYR:C	0.43	2.33	9	6
1:A:76:TYR:CE1	1:A:77:HIS:O	0.43	2.72	19	3
1:A:44:PRO:CD	1:A:76:TYR:CE2	0.43	3.01	13	1
1:A:88:HIS:NE2	1:A:132:VAL:CG1	0.43	2.82	8	9
1:A:33:VAL:O	1:A:34:CYS:SG	0.43	2.76	4	1
1:A:88:HIS:NE2	1:A:132:VAL:HG11	0.43	2.29	8	3
1:A:38:CYS:SG	1:A:43:ILE:HD12	0.43	2.54	6	1
1:A:33:VAL:HG22	1:A:50:ALA:HB3	0.43	1.91	7	2
1:A:33:VAL:CG2	1:A:50:ALA:CB	0.43	2.97	20	2
1:A:92:LEU:O	1:A:99:LEU:HD12	0.43	2.13	7	1
1:A:101:LEU:HD11	1:A:145:ILE:HD13	0.43	1.89	8	1
1:A:87:LYS:O	1:A:104:ILE:CG1	0.43	2.66	9	2
1:A:33:VAL:HG13	1:A:99:LEU:HD11	0.43	1.90	15	1
1:A:31:ASN:HA	1:A:52:ILE:HD12	0.43	1.90	9	3
1:A:92:LEU:CD1	1:A:121:ASN:ND2	0.43	2.82	17	1
1:A:33:VAL:HG22	1:A:50:ALA:CB	0.43	2.43	20	1
1:A:120:SER:OG	1:A:122:GLN:NE2	0.43	2.52	19	4
1:A:131:THR:CG2	1:A:140:ILE:HG23	0.43	2.44	7	4
1:A:101:LEU:N	1:A:122:GLN:O	0.42	2.49	7	4
1:A:125:SER:O	1:A:147:ILE:HD13	0.42	2.13	3	1
1:A:92:LEU:O	1:A:100:LEU:O	0.42	2.37	8	2
1:A:50:ALA:CB	1:A:93:LEU:CD2	0.42	2.98	1	2
1:A:66:TRP:O	1:A:90:GLN:CG	0.42	2.67	3	1
1:A:84:LEU:N	1:A:84:LEU:HD23	0.42	2.28	17	2
1:A:38:CYS:HB3	1:A:143:LEU:HD12	0.42	1.90	12	1
1:A:36:VAL:CG2	1:A:48:LEU:CD2	0.42	2.97	2	1
1:A:67:THR:O	1:A:75:ASP:HB3	0.42	2.13	14	3
1:A:110:TRP:HB2	1:A:131:THR:O	0.42	2.14	19	1
1:A:110:TRP:CH2	1:A:115:LYS:NZ	0.42	2.87	9	1
1:A:44:PRO:O	1:A:76:TYR:CE2	0.42	2.72	8	1
1:A:32:ILE:O	1:A:148:ASN:ND2	0.42	2.53	8	4
1:A:68:PHE:CE1	1:A:75:ASP:OD1	0.42	2.73	7	6
1:A:73:ALA:HA	1:A:77:HIS:N	0.42	2.30	17	2
1:A:68:PHE:CZ	1:A:75:ASP:CG	0.42	2.93	6	5
1:A:68:PHE:CE2	1:A:91:ILE:CD1	0.42	3.03	10	1
1:A:71:ASN:O	1:A:73:ALA:N	0.42	2.52	17	1
1:A:92:LEU:O	1:A:100:LEU:N	0.42	2.50	20	1
1:A:103:ASP:O	1:A:119:ASN:N	0.42	2.53	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:VAL:HG12	1:A:48:LEU:HD21	0.42	1.91	3	1
1:A:134:VAL:CG1	1:A:135:GLY:N	0.42	2.83	6	9
1:A:35:ARG:HH11	1:A:37:ILE:HD11	0.42	1.74	20	1
1:A:130:ILE:N	1:A:143:LEU:O	0.41	2.52	15	2
1:A:110:TRP:O	1:A:131:THR:N	0.41	2.52	12	3
1:A:33:VAL:CG1	1:A:99:LEU:HD21	0.41	2.45	17	1
1:A:89:PHE:HA	1:A:104:ILE:H	0.41	1.75	12	4
1:A:69:GLY:O	1:A:71:ASN:ND2	0.41	2.54	11	1
1:A:143:LEU:N	1:A:143:LEU:CD1	0.41	2.83	17	3
1:A:99:LEU:HD12	1:A:124:LEU:HG	0.41	1.92	19	1
1:A:92:LEU:CD2	1:A:121:ASN:ND2	0.41	2.82	20	1
1:A:36:VAL:HG13	1:A:145:ILE:HG13	0.41	1.93	20	1
1:A:99:LEU:N	1:A:99:LEU:CD1	0.41	2.84	20	1
1:A:99:LEU:CD1	1:A:124:LEU:HD22	0.41	2.20	4	1
1:A:81:ILE:HB	1:A:85:SER:CB	0.41	2.46	19	2
1:A:43:ILE:CG2	1:A:44:PRO:HD2	0.41	2.46	16	1
1:A:68:PHE:CE2	1:A:75:ASP:OD1	0.41	2.74	9	2
1:A:44:PRO:HG3	1:A:76:TYR:CZ	0.41	2.50	16	1
1:A:76:TYR:CE2	1:A:78:LEU:HB3	0.41	2.51	16	2
1:A:68:PHE:HD2	1:A:89:PHE:CD2	0.41	2.34	10	1
1:A:70:ARG:N	1:A:86:ASN:HA	0.41	2.29	11	1
1:A:69:GLY:N	1:A:78:LEU:HD21	0.41	2.31	12	1
1:A:48:LEU:HD22	1:A:75:ASP:OD1	0.41	2.16	14	1
1:A:40:THR:HG21	1:A:142:SER:CA	0.41	2.46	17	1
1:A:48:LEU:CD1	1:A:91:ILE:CD1	0.41	2.99	5	1
1:A:133:GLY:O	1:A:139:ASP:O	0.41	2.40	15	3
1:A:93:LEU:CD2	1:A:99:LEU:HD22	0.41	2.40	12	1
1:A:70:ARG:CD	1:A:86:ASN:CG	0.41	2.89	15	2
1:A:89:PHE:N	1:A:104:ILE:O	0.41	2.50	19	1
1:A:36:VAL:HG13	1:A:48:LEU:CD1	0.40	2.36	13	1
1:A:84:LEU:N	1:A:84:LEU:HD22	0.40	2.30	20	1
1:A:44:PRO:HG2	1:A:76:TYR:CE1	0.40	2.51	6	1
1:A:32:ILE:HA	1:A:49:SER:HB3	0.40	1.93	7	1
1:A:76:TYR:C	1:A:76:TYR:CD1	0.40	2.94	19	1
1:A:76:TYR:CD1	1:A:77:HIS:N	0.40	2.88	19	1
1:A:33:VAL:HG11	1:A:93:LEU:CD2	0.40	2.47	20	1
1:A:84:LEU:O	1:A:85:SER:HB2	0.40	2.16	6	2
1:A:81:ILE:HD13	1:A:85:SER:CB	0.40	2.41	12	1
1:A:81:ILE:HG13	1:A:85:SER:CB	0.40	2.47	5	1
1:A:132:VAL:O	1:A:141:LEU:HD12	0.40	2.17	4	1
1:A:92:LEU:HD13	1:A:121:ASN:CG	0.40	2.37	6	2

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	108/164 (66%)	91±1 (85±1%)	11±1 (10±1%)	6±1 (5±1%)	3 23
All	All	2160/3280 (66%)	1827 (85%)	215 (10%)	118 (5%)	3 23

All 11 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	73	ALA	20
1	A	85	SER	20
1	A	87	LYS	20
1	A	86	ASN	17
1	A	119	ASN	17
1	A	33	VAL	10
1	A	63	LYS	4
1	A	45	ILE	3
1	A	83	ARG	3
1	A	79	GLY	3
1	A	42	GLN	1

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	97/149 (65%)	72±3 (74±3%)	25±3 (26±3%)	2 24
All	All	1940/2980 (65%)	1444 (74%)	496 (26%)	2 24

All 61 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	32	ILE	20
1	A	74	CYS	20
1	A	84	LEU	20
1	A	89	PHE	20
1	A	104	ILE	20
1	A	115	LYS	20
1	A	125	SER	20
1	A	92	LEU	19
1	A	111	LEU	19
1	A	145	ILE	19
1	A	33	VAL	18
1	A	49	SER	18
1	A	85	SER	16
1	A	46	ARG	15
1	A	51	ASP	13
1	A	48	LEU	11
1	A	93	LEU	11
1	A	38	CYS	9
1	A	78	LEU	9
1	A	99	LEU	8
1	A	114	GLN	8
1	A	87	LYS	8
1	A	83	ARG	7
1	A	86	ASN	7
1	A	138	SER	7
1	A	82	SER	7
1	A	137	GLU	7
1	A	63	LYS	7
1	A	70	ARG	7
1	A	150	LYS	7
1	A	126	GLN	7
1	A	124	LEU	7
1	A	35	ARG	6
1	A	142	SER	6
1	A	40	THR	5
1	A	42	GLN	5
1	A	30	GLU	4
1	A	149	ASP	4
1	A	47	ASP	4
1	A	139	ASP	4
1	A	43	ILE	4
1	A	117	GLU	4
1	A	129	GLU	4

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Mol	Chain	Res	Type	Models (Total)
1	A	71	ASN	4
1	A	100	LEU	4
1	A	80	ASN	3
1	A	101	LEU	3
1	A	143	LEU	2
1	A	64	LYS	2
1	A	118	LYS	2
1	A	119	ASN	2
1	A	123	LEU	2
1	A	146	PHE	2
1	A	148	ASN	2
1	A	81	ILE	1
1	A	130	ILE	1
1	A	90	GLN	1
1	A	39	THR	1
1	A	76	TYR	1
1	A	120	SER	1
1	A	141	LEU	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