



Full wwPDB NMR Structure Validation Report ⓘ

Mar 1, 2026 – 10:22 AM UTC

PDB ID : 1Q8X / pdb_00001q8x
Title : NMR structure of human cofilin
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Deposited on : 2003-08-22

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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
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)	:	2.49

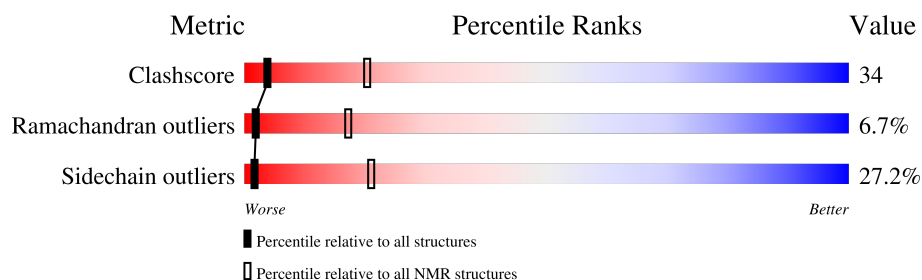
1 Overall quality at a glance

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	166	

2 Ensemble composition and analysis

This entry contains 20 models. Model 6 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:5-A:166 (162)	0.82	6

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 3 clusters and 3 single-model clusters were found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 2642 atoms, of which 1346 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Cofilin, non-muscle isoform.

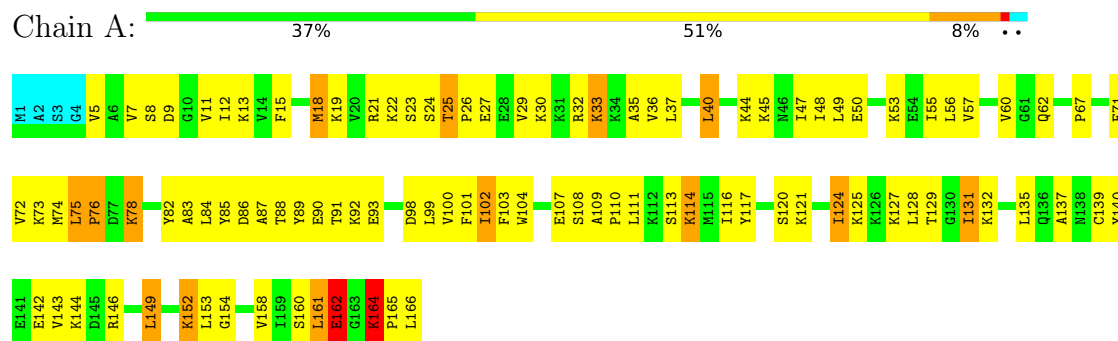
Mol	Chain	Residues	Atoms						Trace
1	A	166	Total	C	H	N	O	S	0
			2642	826	1346	211	251	8	

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: Cofilin, non-muscle isoform

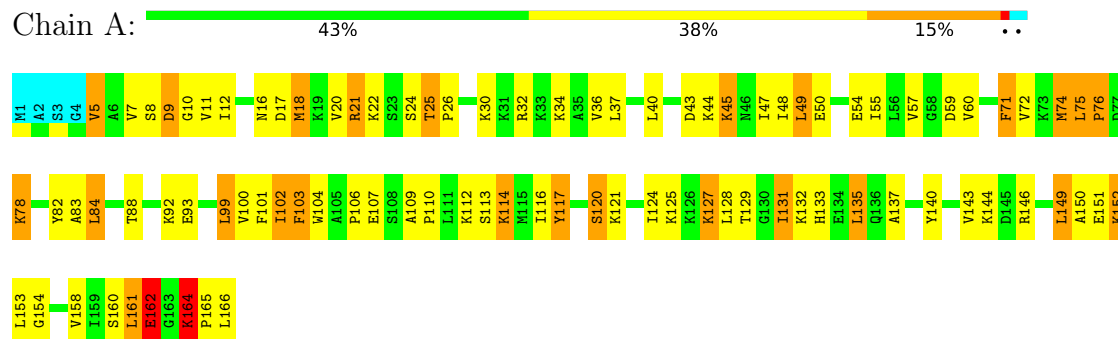


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

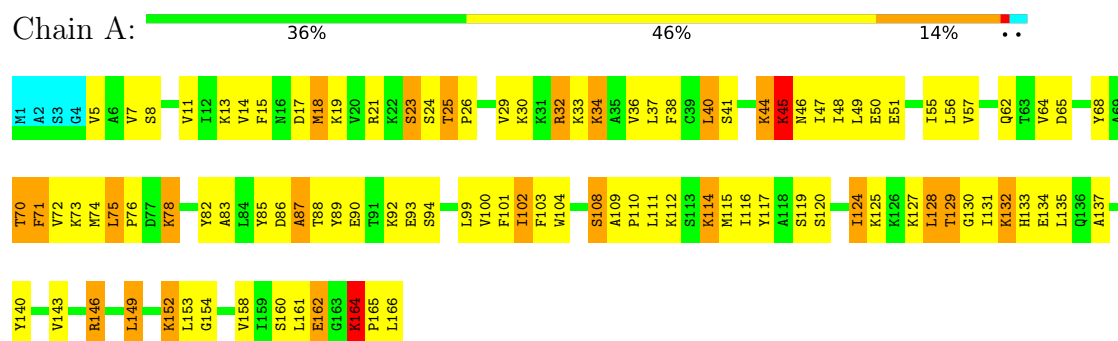
4.2.1 Score per residue for model 1

- Molecule 1: Cofilin, non-muscle isoform



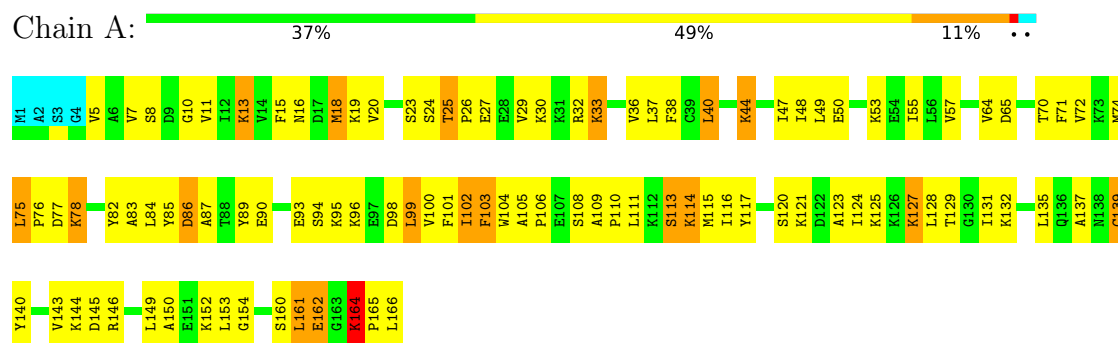
4.2.2 Score per residue for model 2

- Molecule 1: Cofilin, non-muscle isoform



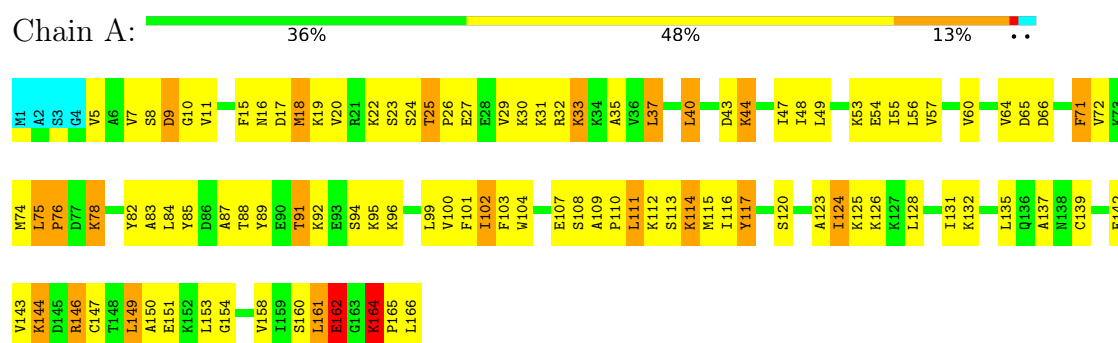
4.2.3 Score per residue for model 3

- Molecule 1: Cofilin, non-muscle isoform



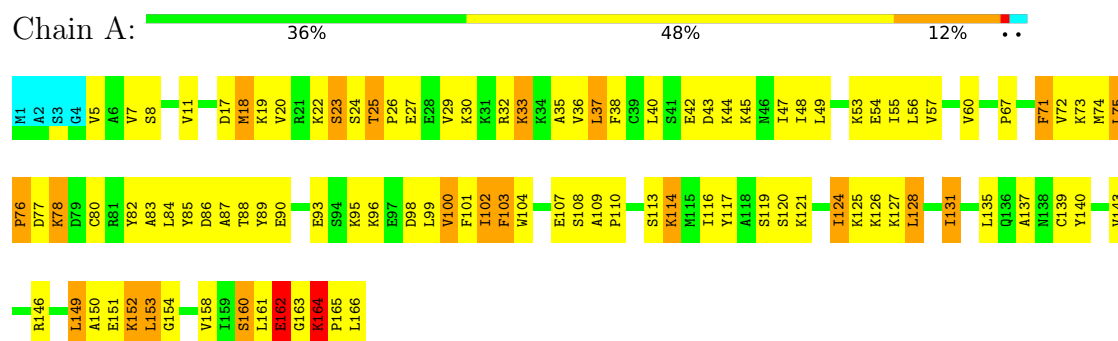
4.2.4 Score per residue for model 4

- Molecule 1: Cofilin, non-muscle isoform



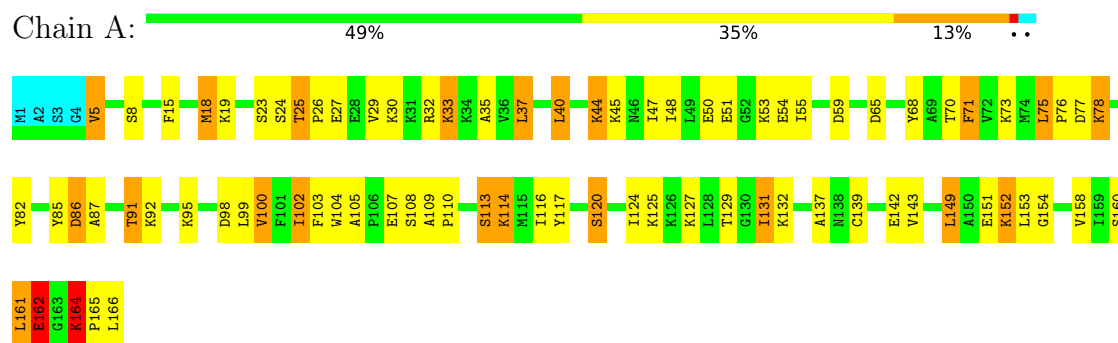
4.2.5 Score per residue for model 5

- Molecule 1: Cofilin, non-muscle isoform



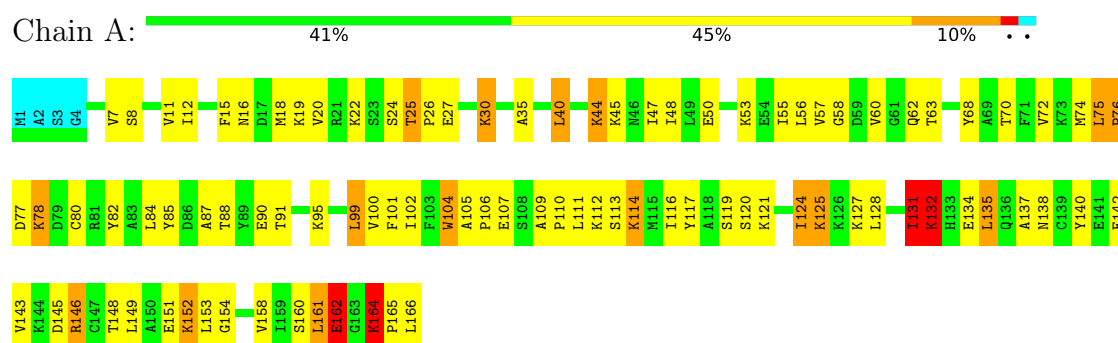
4.2.6 Score per residue for model 6 (medoid)

- Molecule 1: Cofilin, non-muscle isoform



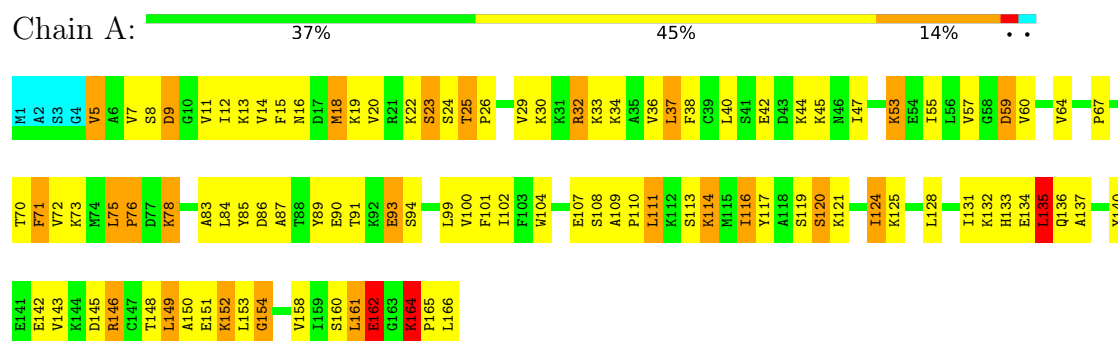
4.2.7 Score per residue for model 7

- Molecule 1: Cofilin, non-muscle isoform



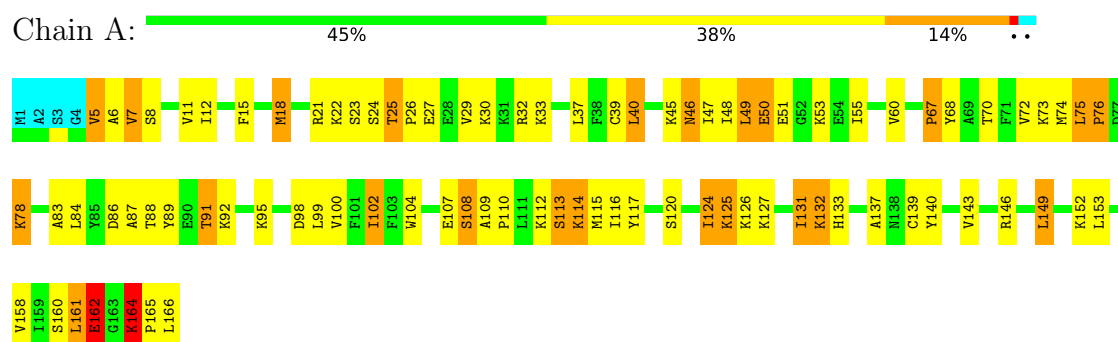
4.2.8 Score per residue for model 8

- Molecule 1: Cofilin, non-muscle isoform



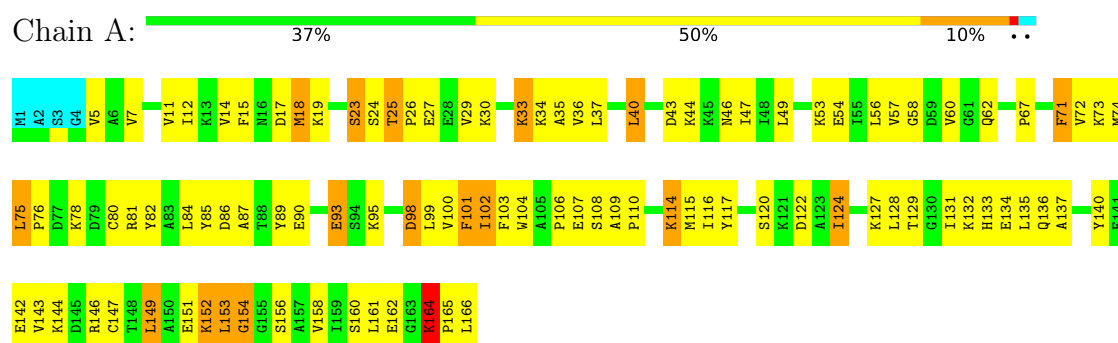
4.2.9 Score per residue for model 9

- Molecule 1: Cofilin, non-muscle isoform



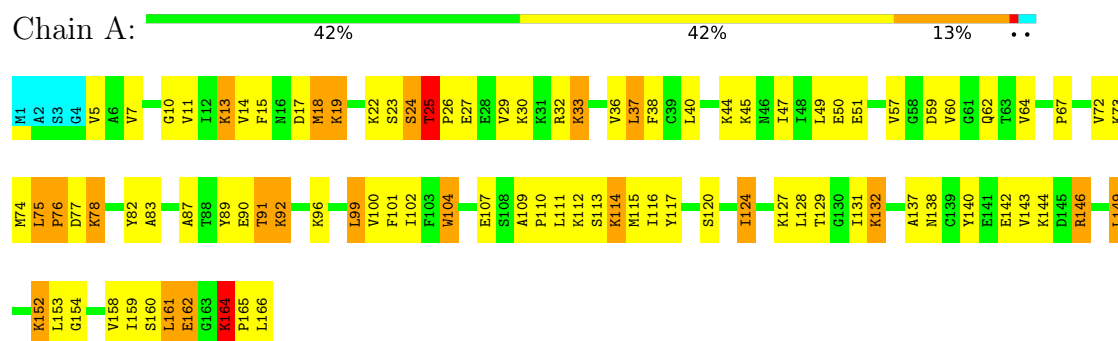
4.2.10 Score per residue for model 10

- Molecule 1: Cofilin, non-muscle isoform



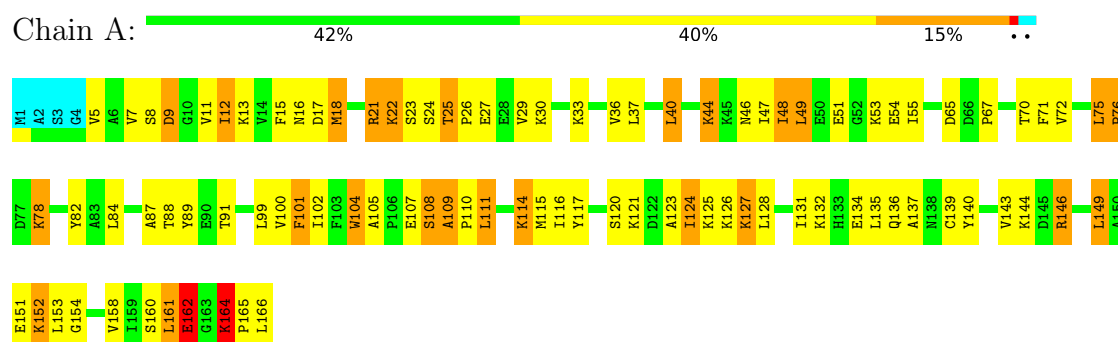
4.2.11 Score per residue for model 11

- Molecule 1: Cofilin, non-muscle isoform



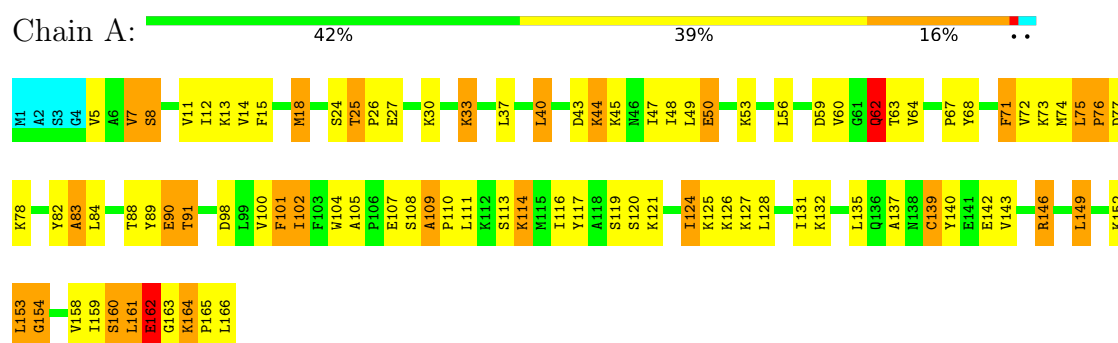
4.2.12 Score per residue for model 12

- Molecule 1: Cofilin, non-muscle isoform



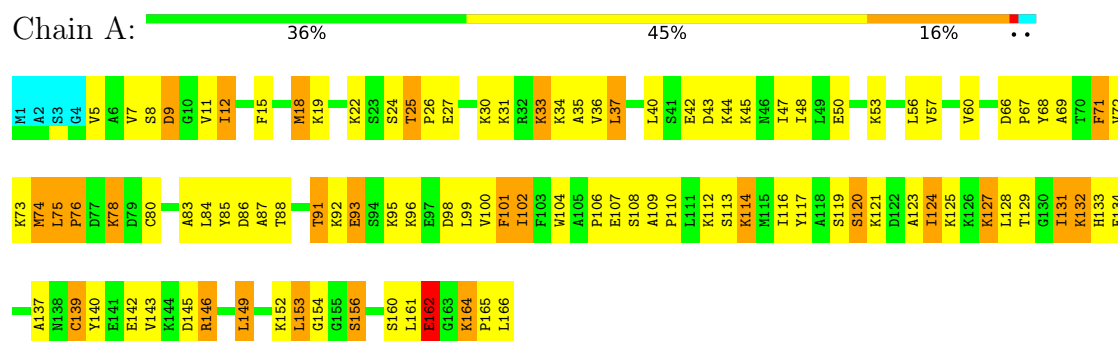
4.2.13 Score per residue for model 13

- Molecule 1: Cofilin, non-muscle isoform



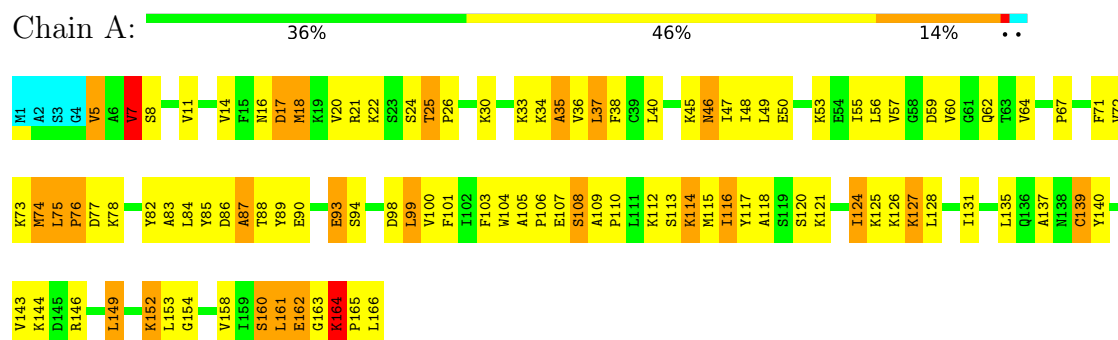
4.2.14 Score per residue for model 14

- Molecule 1: Cofilin, non-muscle isoform



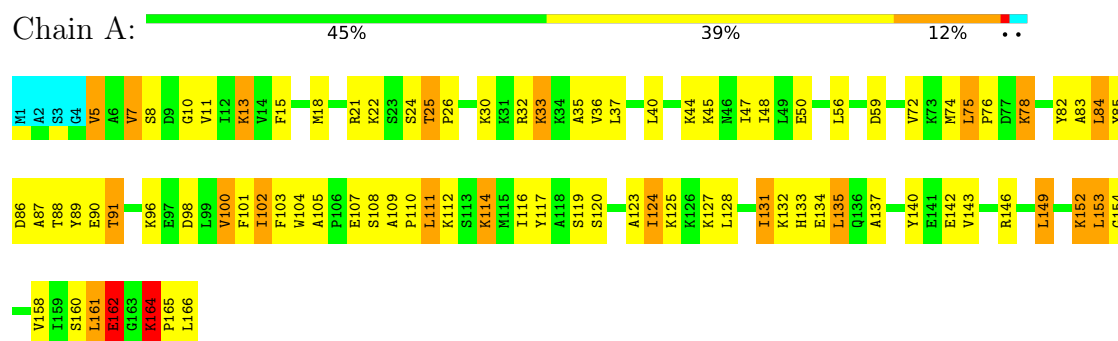
4.2.15 Score per residue for model 15

- Molecule 1: Cofilin, non-muscle isoform



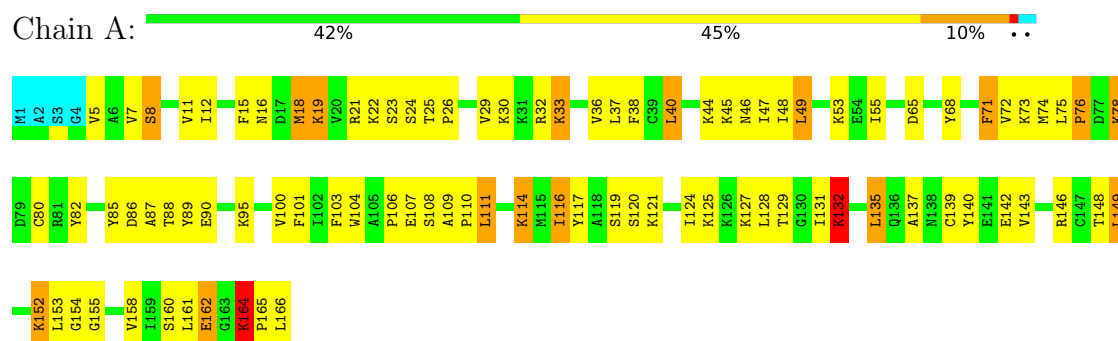
4.2.16 Score per residue for model 16

- Molecule 1: Cofilin, non-muscle isoform



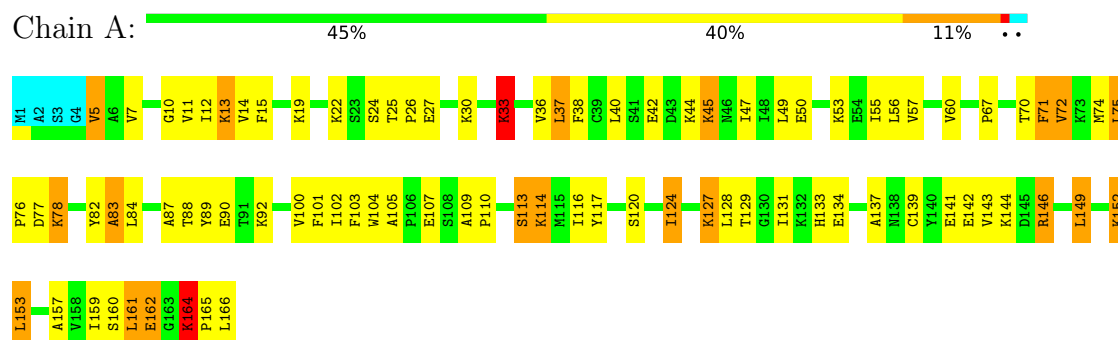
4.2.17 Score per residue for model 17

- Molecule 1: Cofilin, non-muscle isoform



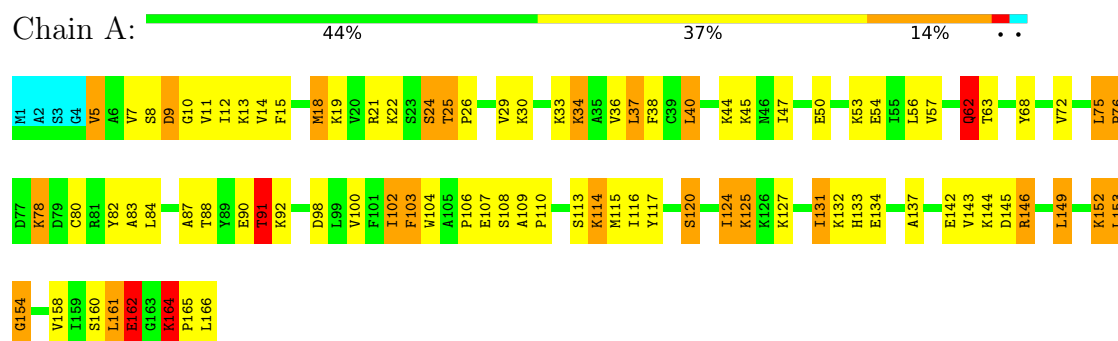
4.2.18 Score per residue for model 18

- Molecule 1: Cofilin, non-muscle isoform



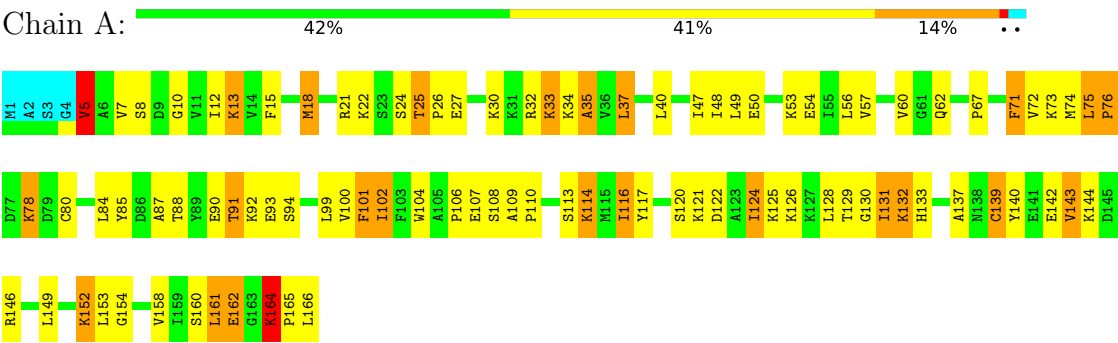
4.2.19 Score per residue for model 19

- Molecule 1: Cofilin, non-muscle isoform



4.2.20 Score per residue for model 20

- Molecule 1: Cofilin, non-muscle isoform



5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CYANA	structure solution	1.1
CYANA	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	1273	1322	1321	89±12
All	All	25460	26440	26420	1778

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 34.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:100:VAL:HG21	1:A:149:LEU:HD21	1.09	1.20	10	1
1:A:100:VAL:HG11	1:A:149:LEU:HD21	1.05	1.18	12	2
1:A:87:ALA:HB2	1:A:149:LEU:HD12	1.01	1.27	18	11
1:A:55:ILE:HD13	1:A:70:THR:HG23	1.01	1.30	8	3
1:A:47:ILE:HG21	1:A:124:ILE:HD12	0.87	1.45	20	12
1:A:89:TYR:CD1	1:A:153:LEU:HD22	0.86	2.05	2	6
1:A:135:LEU:HD22	1:A:149:LEU:HD22	0.85	1.45	1	3
1:A:89:TYR:CD1	1:A:153:LEU:HD13	0.84	2.08	3	7
1:A:12:ILE:HD11	1:A:127:LYS:CD	0.84	2.02	13	2
1:A:153:LEU:HD12	1:A:158:VAL:HG21	0.83	1.49	13	1
1:A:12:ILE:HD12	1:A:127:LYS:CG	0.83	2.04	14	1
1:A:15:PHE:CE1	1:A:128:LEU:HD22	0.82	2.10	18	2
1:A:153:LEU:CD1	1:A:158:VAL:HG21	0.82	2.05	13	10
1:A:37:LEU:HD22	1:A:74:MET:HE3	0.81	1.52	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:109:ALA:HB1	1:A:110:PRO:HD2	0.81	1.53	17	20
1:A:87:ALA:HB2	1:A:149:LEU:CD1	0.81	2.06	18	9
1:A:37:LEU:HD23	1:A:74:MET:HE3	0.80	1.50	15	1
1:A:105:ALA:HB2	1:A:117:TYR:CE1	0.80	2.12	15	8
1:A:12:ILE:HD11	1:A:127:LYS:HD3	0.80	1.53	18	2
1:A:8:SER:OG	1:A:48:ILE:HG22	0.80	1.77	15	2
1:A:135:LEU:CD2	1:A:148:THR:HG22	0.80	2.07	8	2
1:A:15:PHE:CZ	1:A:131:ILE:HD12	0.79	2.11	6	9
1:A:109:ALA:HB3	1:A:114:LYS:HG3	0.79	1.52	16	19
1:A:120:SER:O	1:A:124:ILE:HG22	0.78	1.78	20	4
1:A:55:ILE:CD1	1:A:70:THR:HG23	0.78	2.08	8	2
1:A:44:LYS:O	1:A:116:ILE:HD13	0.77	1.77	2	5
1:A:146:ARG:CD	1:A:161:LEU:HD22	0.77	2.09	10	3
1:A:153:LEU:HD13	1:A:158:VAL:HG21	0.77	1.57	10	2
1:A:154:GLY:O	1:A:158:VAL:HG23	0.77	1.80	13	16
1:A:87:ALA:CB	1:A:149:LEU:HD12	0.76	2.10	18	10
1:A:137:ALA:HB3	1:A:143:VAL:HG22	0.76	1.58	18	17
1:A:161:LEU:HD13	1:A:161:LEU:O	0.76	1.81	17	10
1:A:146:ARG:HG3	1:A:161:LEU:HD22	0.76	1.55	5	4
1:A:84:LEU:HD22	1:A:99:LEU:HD11	0.76	1.56	5	2
1:A:67:PRO:O	1:A:70:THR:HG22	0.76	1.80	8	2
1:A:89:TYR:CE1	1:A:153:LEU:HD22	0.76	2.16	9	3
1:A:153:LEU:HD12	1:A:154:GLY:N	0.76	1.96	2	8
1:A:47:ILE:HD11	1:A:120:SER:OG	0.75	1.80	13	5
1:A:71:PHE:CE2	1:A:102:ILE:HG21	0.74	2.17	5	8
1:A:100:VAL:HG21	1:A:149:LEU:CD2	0.74	2.09	10	1
1:A:12:ILE:HD12	1:A:127:LYS:HG3	0.74	1.59	14	1
1:A:35:ALA:HB2	1:A:85:TYR:CD2	0.74	2.18	14	7
1:A:88:THR:HG23	1:A:162:GLU:HG2	0.73	1.58	7	6
1:A:109:ALA:HB3	1:A:114:LYS:CG	0.73	2.13	16	5
1:A:60:VAL:HG21	1:A:162:GLU:OE2	0.73	1.84	15	1
1:A:101:PHE:CE2	1:A:128:LEU:HD11	0.73	2.19	7	15
1:A:139:CYS:O	1:A:143:VAL:HG12	0.72	1.83	20	1
1:A:68:TYR:OH	1:A:149:LEU:HD23	0.72	1.84	2	5
1:A:60:VAL:HG22	1:A:67:PRO:HD3	0.72	1.60	10	1
1:A:149:LEU:HD13	1:A:149:LEU:O	0.71	1.85	3	7
1:A:84:LEU:HD21	1:A:131:ILE:HD11	0.71	1.60	19	6
1:A:72:VAL:HG11	1:A:144:LYS:HB2	0.71	1.62	19	4
1:A:85:TYR:O	1:A:100:VAL:HG12	0.71	1.85	2	1
1:A:5:VAL:HG11	1:A:120:SER:HB2	0.71	1.61	12	5
1:A:72:VAL:HG11	1:A:144:LYS:CD	0.71	2.15	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:40:LEU:CD2	1:A:47:ILE:HD13	0.71	2.16	13	7
1:A:109:ALA:HB3	1:A:114:LYS:HG2	0.71	1.61	3	1
1:A:47:ILE:CG2	1:A:124:ILE:HD12	0.70	2.15	2	3
1:A:37:LEU:CD2	1:A:74:MET:HE3	0.70	2.15	1	1
1:A:18:MET:SD	1:A:99:LEU:HD11	0.70	2.26	12	2
1:A:162:GLU:HB2	1:A:165:PRO:HG3	0.70	1.62	5	20
1:A:8:SER:HB3	1:A:48:ILE:HG22	0.70	1.63	7	6
1:A:8:SER:HB2	1:A:48:ILE:HG22	0.70	1.63	3	8
1:A:59:ASP:HB3	1:A:64:VAL:HG21	0.70	1.63	15	3
1:A:72:VAL:HG22	1:A:143:VAL:HG12	0.70	1.63	10	4
1:A:18:MET:HE1	1:A:84:LEU:O	0.70	1.86	13	2
1:A:104:TRP:CZ3	1:A:143:VAL:HG21	0.70	2.22	10	13
1:A:87:ALA:HB1	1:A:161:LEU:HD11	0.70	1.63	11	3
1:A:57:VAL:O	1:A:60:VAL:HG23	0.69	1.86	14	6
1:A:8:SER:CB	1:A:48:ILE:HG22	0.69	2.17	12	12
1:A:100:VAL:HG11	1:A:152:LYS:HG2	0.69	1.64	6	3
1:A:89:TYR:CE1	1:A:153:LEU:HD13	0.69	2.22	15	3
1:A:75:LEU:HD22	1:A:143:VAL:HG11	0.69	1.63	1	6
1:A:137:ALA:HB1	1:A:142:GLU:HB2	0.69	1.64	18	13
1:A:18:MET:HE3	1:A:33:LYS:CG	0.69	2.17	4	1
1:A:135:LEU:HD12	1:A:149:LEU:HD22	0.69	1.62	3	4
1:A:60:VAL:HG22	1:A:67:PRO:HG2	0.69	1.64	20	1
1:A:87:ALA:HB3	1:A:153:LEU:HD21	0.68	1.63	8	3
1:A:40:LEU:HD13	1:A:44:LYS:HG3	0.68	1.66	12	1
1:A:23:SER:CB	1:A:29:VAL:HG12	0.68	2.19	10	6
1:A:100:VAL:HG12	1:A:133:HIS:HB2	0.68	1.64	1	5
1:A:18:MET:HE3	1:A:84:LEU:O	0.67	1.89	15	5
1:A:111:LEU:O	1:A:111:LEU:HD23	0.67	1.89	11	3
1:A:18:MET:HE1	1:A:86:ASP:HB2	0.67	1.67	9	2
1:A:59:ASP:CB	1:A:64:VAL:HG21	0.67	2.20	15	1
1:A:75:LEU:HD22	1:A:104:TRP:CD1	0.67	2.25	16	1
1:A:111:LEU:HD11	1:A:115:MET:HE2	0.66	1.67	2	1
1:A:5:VAL:CG1	1:A:47:ILE:HD11	0.66	2.21	20	1
1:A:106:PRO:HG2	1:A:109:ALA:HB2	0.66	1.67	10	9
1:A:100:VAL:HG12	1:A:133:HIS:CB	0.66	2.20	1	4
1:A:16:ASN:O	1:A:20:VAL:HG22	0.66	1.89	3	3
1:A:47:ILE:HG21	1:A:124:ILE:CD1	0.66	2.21	4	4
1:A:87:ALA:HB1	1:A:153:LEU:HD11	0.65	1.68	17	4
1:A:72:VAL:HG21	1:A:144:LYS:HD3	0.65	1.66	4	2
1:A:62:GLN:OE1	1:A:63:THR:HG22	0.65	1.91	13	1
1:A:18:MET:O	1:A:99:LEU:HD21	0.65	1.91	14	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:87:ALA:HB2	1:A:149:LEU:HD11	0.65	1.68	3	2
1:A:139:CYS:O	1:A:143:VAL:HG23	0.65	1.91	12	9
1:A:149:LEU:HD22	1:A:152:LYS:HE2	0.65	1.67	10	1
1:A:102:ILE:HD11	1:A:149:LEU:HD21	0.64	1.68	16	2
1:A:87:ALA:HB3	1:A:149:LEU:CD1	0.64	2.21	5	1
1:A:134:GLU:O	1:A:135:LEU:HD12	0.64	1.92	8	1
1:A:5:VAL:HG13	1:A:47:ILE:HG12	0.64	1.69	15	1
1:A:146:ARG:CG	1:A:161:LEU:HD22	0.64	2.23	2	2
1:A:75:LEU:HD13	1:A:104:TRP:CE2	0.64	2.28	12	5
1:A:20:VAL:HG23	1:A:22:LYS:HG2	0.64	1.68	5	1
1:A:104:TRP:CH2	1:A:143:VAL:HG11	0.64	2.27	20	1
1:A:150:ALA:HB2	1:A:161:LEU:HD23	0.64	1.69	1	3
1:A:72:VAL:HG22	1:A:140:TYR:CE2	0.64	2.26	9	4
1:A:100:VAL:HG11	1:A:152:LYS:CG	0.64	2.23	6	3
1:A:18:MET:HE2	1:A:33:LYS:HG3	0.64	1.68	14	1
1:A:128:LEU:HD12	1:A:131:ILE:HG21	0.64	1.70	3	1
1:A:84:LEU:HD22	1:A:99:LEU:CD1	0.63	2.24	9	2
1:A:5:VAL:HG13	1:A:123:ALA:CB	0.63	2.24	3	5
1:A:5:VAL:CG1	1:A:40:LEU:HD11	0.63	2.23	17	2
1:A:84:LEU:HD22	1:A:99:LEU:HD22	0.63	1.71	7	1
1:A:49:LEU:N	1:A:49:LEU:HD13	0.63	2.09	9	2
1:A:75:LEU:HD13	1:A:104:TRP:CD1	0.63	2.28	19	3
1:A:5:VAL:HG11	1:A:40:LEU:HD21	0.63	1.71	17	1
1:A:36:VAL:HG23	1:A:38:PHE:CE1	0.63	2.29	19	3
1:A:57:VAL:O	1:A:60:VAL:HG12	0.63	1.94	4	4
1:A:7:VAL:HG13	1:A:11:VAL:HG21	0.62	1.69	8	14
1:A:161:LEU:N	1:A:166:LEU:HB2	0.62	2.09	6	13
1:A:100:VAL:HG21	1:A:149:LEU:HD11	0.62	1.72	8	1
1:A:100:VAL:HG11	1:A:149:LEU:CD2	0.62	2.10	12	1
1:A:7:VAL:HG21	1:A:127:LYS:HG3	0.62	1.70	11	6
1:A:75:LEU:HD12	1:A:143:VAL:HG11	0.62	1.71	9	4
1:A:60:VAL:HG22	1:A:67:PRO:HG3	0.62	1.71	14	1
1:A:12:ILE:HD12	1:A:127:LYS:HG2	0.62	1.72	14	1
1:A:15:PHE:CE1	1:A:131:ILE:HD12	0.62	2.29	7	3
1:A:75:LEU:CD2	1:A:143:VAL:HG11	0.61	2.24	2	6
1:A:18:MET:HE1	1:A:86:ASP:OD2	0.61	1.95	17	1
1:A:84:LEU:HD21	1:A:131:ILE:CD1	0.61	2.25	5	9
1:A:10:GLY:HA2	1:A:13:LYS:HB2	0.61	1.70	19	6
1:A:84:LEU:HD11	1:A:131:ILE:CD1	0.61	2.25	20	1
1:A:18:MET:HE1	1:A:86:ASP:OD1	0.61	1.96	10	4
1:A:100:VAL:CG2	1:A:149:LEU:HD21	0.61	2.13	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:7:VAL:HG13	1:A:11:VAL:CG2	0.61	2.26	8	5
1:A:84:LEU:HB3	1:A:99:LEU:HD11	0.61	1.72	4	1
1:A:153:LEU:HD11	1:A:158:VAL:HG21	0.61	1.72	4	2
1:A:72:VAL:HG12	1:A:140:TYR:CE2	0.61	2.30	8	11
1:A:40:LEU:CD1	1:A:47:ILE:HD13	0.61	2.26	15	1
1:A:37:LEU:HD21	1:A:75:LEU:CD1	0.61	2.25	4	1
1:A:32:ARG:NH1	1:A:57:VAL:HG11	0.61	2.10	2	2
1:A:5:VAL:HG21	1:A:47:ILE:CD1	0.61	2.26	18	2
1:A:71:PHE:CZ	1:A:75:LEU:HD11	0.61	2.31	15	12
1:A:135:LEU:CD1	1:A:149:LEU:HD22	0.61	2.26	3	3
1:A:5:VAL:HG11	1:A:120:SER:CB	0.61	2.25	3	4
1:A:25:THR:HG22	1:A:26:PRO:HD3	0.60	1.73	20	18
1:A:153:LEU:HD21	1:A:161:LEU:CD2	0.60	2.26	14	2
1:A:60:VAL:HG23	1:A:67:PRO:HG3	0.60	1.73	15	3
1:A:15:PHE:CD1	1:A:84:LEU:HD13	0.60	2.32	10	2
1:A:75:LEU:HD13	1:A:104:TRP:NE1	0.60	2.12	11	5
1:A:18:MET:CE	1:A:99:LEU:HD11	0.60	2.26	8	1
1:A:150:ALA:HB2	1:A:161:LEU:CD2	0.60	2.25	8	2
1:A:88:THR:HG23	1:A:162:GLU:CG	0.59	2.26	7	3
1:A:40:LEU:HD22	1:A:47:ILE:HD13	0.59	1.74	13	2
1:A:89:TYR:HE1	1:A:153:LEU:HD22	0.59	1.58	3	2
1:A:86:ASP:OD2	1:A:99:LEU:HD13	0.59	1.97	6	1
1:A:33:LYS:HA	1:A:56:LEU:HD23	0.59	1.74	18	9
1:A:146:ARG:HD2	1:A:161:LEU:HD22	0.59	1.72	3	3
1:A:57:VAL:HG22	1:A:57:VAL:O	0.59	1.97	3	2
1:A:18:MET:HE2	1:A:33:LYS:O	0.59	1.98	3	2
1:A:135:LEU:HD13	1:A:149:LEU:HD22	0.59	1.75	16	2
1:A:87:ALA:HB1	1:A:153:LEU:HD22	0.59	1.74	18	1
1:A:7:VAL:HG13	1:A:47:ILE:HB	0.59	1.73	15	1
1:A:5:VAL:HG22	1:A:47:ILE:HG12	0.58	1.74	8	8
1:A:11:VAL:HG21	1:A:47:ILE:HG22	0.58	1.75	11	6
1:A:72:VAL:HG11	1:A:144:LYS:HD3	0.58	1.75	11	1
1:A:34:LYS:HE3	1:A:88:THR:HG22	0.58	1.73	14	1
1:A:15:PHE:CD1	1:A:128:LEU:HD22	0.58	2.33	18	2
1:A:109:ALA:HB1	1:A:110:PRO:CD	0.58	2.29	6	13
1:A:104:TRP:CZ3	1:A:143:VAL:HG11	0.58	2.34	20	1
1:A:72:VAL:HG22	1:A:140:TYR:CD2	0.57	2.34	16	3
1:A:5:VAL:HG21	1:A:47:ILE:HD11	0.57	1.75	10	4
1:A:5:VAL:HG13	1:A:123:ALA:HB3	0.57	1.75	3	2
1:A:72:VAL:HG21	1:A:144:LYS:HB2	0.57	1.76	12	4
1:A:87:ALA:HB1	1:A:153:LEU:CD2	0.57	2.28	18	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:37:LEU:HD11	1:A:75:LEU:CD1	0.57	2.28	6	4
1:A:60:VAL:HG13	1:A:67:PRO:HG3	0.57	1.76	11	2
1:A:60:VAL:HG22	1:A:67:PRO:CG	0.57	2.29	14	1
1:A:5:VAL:O	1:A:5:VAL:HG12	0.57	1.98	20	2
1:A:7:VAL:HG22	1:A:47:ILE:HB	0.57	1.74	19	5
1:A:99:LEU:C	1:A:99:LEU:HD13	0.57	2.24	5	1
1:A:89:TYR:HB2	1:A:158:VAL:HG13	0.57	1.76	13	2
1:A:14:VAL:HB	1:A:49:LEU:HD13	0.57	1.77	2	6
1:A:135:LEU:HD22	1:A:149:LEU:CD2	0.56	2.24	17	2
1:A:14:VAL:CB	1:A:49:LEU:HD13	0.56	2.30	10	5
1:A:153:LEU:C	1:A:153:LEU:HD12	0.56	2.26	4	1
1:A:84:LEU:HD21	1:A:131:ILE:HD13	0.56	1.76	5	2
1:A:60:VAL:HG21	1:A:162:GLU:OE1	0.56	2.01	1	1
1:A:88:THR:HG23	1:A:88:THR:O	0.56	2.00	15	11
1:A:116:ILE:O	1:A:120:SER:N	0.56	2.37	16	17
1:A:18:MET:SD	1:A:99:LEU:HD21	0.56	2.40	3	1
1:A:25:THR:HG22	1:A:26:PRO:CD	0.56	2.30	12	5
1:A:103:PHE:HB2	1:A:135:LEU:O	0.56	1.99	2	1
1:A:18:MET:HE3	1:A:33:LYS:HG3	0.56	1.76	4	3
1:A:128:LEU:N	1:A:128:LEU:HD23	0.56	2.15	2	1
1:A:40:LEU:HD23	1:A:117:TYR:CE1	0.56	2.35	4	2
1:A:12:ILE:N	1:A:12:ILE:HD12	0.56	2.15	20	2
1:A:60:VAL:HG22	1:A:67:PRO:CD	0.56	2.30	10	1
1:A:49:LEU:HD12	1:A:49:LEU:O	0.56	2.01	12	1
1:A:5:VAL:HG12	1:A:45:LYS:C	0.56	2.24	17	1
1:A:75:LEU:N	1:A:76:PRO:HD3	0.56	2.15	19	18
1:A:161:LEU:H	1:A:166:LEU:HB2	0.56	1.61	6	15
1:A:18:MET:HE3	1:A:33:LYS:O	0.56	2.00	17	4
1:A:131:ILE:HG23	1:A:131:ILE:O	0.56	2.01	4	4
1:A:18:MET:SD	1:A:99:LEU:HD13	0.56	2.41	9	1
1:A:72:VAL:HG12	1:A:140:TYR:CD2	0.56	2.36	3	8
1:A:15:PHE:CD2	1:A:128:LEU:HD22	0.56	2.36	8	2
1:A:12:ILE:HD13	1:A:127:LYS:HB3	0.56	1.77	17	1
1:A:160:SER:HA	1:A:166:LEU:CB	0.55	2.32	2	20
1:A:37:LEU:HD12	1:A:83:ALA:HB2	0.55	1.77	8	4
1:A:100:VAL:HG21	1:A:135:LEU:HD12	0.55	1.77	15	3
1:A:59:ASP:HB2	1:A:64:VAL:HG21	0.55	1.77	13	1
1:A:5:VAL:HG11	1:A:40:LEU:HD11	0.55	1.78	17	1
1:A:84:LEU:HD22	1:A:99:LEU:CG	0.54	2.32	9	1
1:A:36:VAL:O	1:A:83:ALA:HB1	0.54	2.03	14	2
1:A:32:ARG:O	1:A:56:LEU:HD22	0.54	2.02	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:62:GLN:HG3	1:A:63:THR:HG22	0.54	1.78	7	1
1:A:11:VAL:HA	1:A:49:LEU:HD12	0.54	1.78	9	2
1:A:37:LEU:HD21	1:A:71:PHE:CE2	0.54	2.37	12	1
1:A:87:ALA:HB1	1:A:153:LEU:HD23	0.54	1.80	2	1
1:A:18:MET:HE1	1:A:99:LEU:HD11	0.54	1.79	8	1
1:A:111:LEU:O	1:A:111:LEU:HD13	0.54	2.03	8	3
1:A:84:LEU:HD22	1:A:99:LEU:HD21	0.54	1.78	4	1
1:A:87:ALA:CB	1:A:153:LEU:HD11	0.54	2.33	9	2
1:A:164:LYS:N	1:A:165:PRO:HD2	0.54	2.18	5	20
1:A:18:MET:O	1:A:99:LEU:HD22	0.54	2.02	8	1
1:A:49:LEU:HD22	1:A:49:LEU:O	0.54	2.03	9	2
1:A:82:TYR:CE1	1:A:117:TYR:CE2	0.53	2.96	7	9
1:A:160:SER:HA	1:A:166:LEU:HB2	0.53	1.79	14	18
1:A:55:ILE:HD11	1:A:74:MET:HE2	0.53	1.80	15	4
1:A:164:LYS:HG3	1:A:165:PRO:N	0.53	2.19	6	20
1:A:87:ALA:HB3	1:A:149:LEU:HD11	0.53	1.79	5	1
1:A:72:VAL:HG11	1:A:144:LYS:HD2	0.53	1.78	11	1
1:A:101:PHE:HB2	1:A:131:ILE:HD13	0.53	1.79	18	1
1:A:40:LEU:HD23	1:A:117:TYR:CD1	0.53	2.38	4	2
1:A:82:TYR:O	1:A:83:ALA:HB2	0.53	2.04	13	5
1:A:23:SER:HB3	1:A:29:VAL:HG12	0.53	1.80	5	4
1:A:12:ILE:HD12	1:A:127:LYS:HD3	0.53	1.79	12	1
1:A:137:ALA:CB	1:A:143:VAL:HG22	0.53	2.33	2	7
1:A:18:MET:HE3	1:A:33:LYS:HG2	0.53	1.80	4	1
1:A:40:LEU:HD22	1:A:44:LYS:HA	0.53	1.80	12	1
1:A:7:VAL:CG1	1:A:11:VAL:HG21	0.53	2.32	15	1
1:A:82:TYR:CD2	1:A:124:ILE:HD13	0.53	2.39	2	1
1:A:75:LEU:N	1:A:76:PRO:CD	0.53	2.72	19	16
1:A:12:ILE:HD11	1:A:127:LYS:HD2	0.53	1.75	13	1
1:A:5:VAL:HG13	1:A:47:ILE:HD11	0.53	1.79	20	1
1:A:100:VAL:O	1:A:100:VAL:HG13	0.53	2.04	12	6
1:A:60:VAL:HG12	1:A:60:VAL:O	0.53	2.04	11	1
1:A:36:VAL:HG23	1:A:36:VAL:O	0.52	2.05	1	2
1:A:37:LEU:HD21	1:A:75:LEU:HD11	0.52	1.81	4	1
1:A:135:LEU:HD11	1:A:152:LYS:NZ	0.52	2.19	10	1
1:A:31:LYS:O	1:A:56:LEU:HD22	0.52	2.04	14	2
1:A:37:LEU:HD12	1:A:74:MET:HE3	0.52	1.80	4	1
1:A:114:LYS:NZ	1:A:118:ALA:HB2	0.52	2.19	15	1
1:A:149:LEU:HD13	1:A:152:LYS:HD2	0.52	1.80	2	2
1:A:40:LEU:HD12	1:A:44:LYS:HA	0.52	1.81	17	3
1:A:116:ILE:HG22	1:A:116:ILE:O	0.52	2.05	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:89:TYR:CG	1:A:153:LEU:HD22	0.52	2.40	5	1
1:A:160:SER:C	1:A:166:LEU:HD12	0.52	2.29	7	4
1:A:131:ILE:HG23	1:A:132:LYS:H	0.52	1.64	7	1
1:A:88:THR:HG23	1:A:162:GLU:CD	0.52	2.29	14	1
1:A:87:ALA:CB	1:A:149:LEU:HD11	0.52	2.35	3	1
1:A:71:PHE:CZ	1:A:102:ILE:HG21	0.52	2.39	10	5
1:A:153:LEU:HD12	1:A:154:GLY:H	0.52	1.64	10	1
1:A:146:ARG:HG2	1:A:161:LEU:CB	0.52	2.35	13	4
1:A:60:VAL:HG21	1:A:162:GLU:CD	0.52	2.29	15	1
1:A:66:ASP:HB3	1:A:69:ALA:HB3	0.51	1.82	14	1
1:A:89:TYR:CD2	1:A:153:LEU:HD13	0.51	2.40	18	1
1:A:18:MET:HE1	1:A:86:ASP:CB	0.51	2.36	5	1
1:A:76:PRO:O	1:A:104:TRP:NE1	0.51	2.43	3	16
1:A:72:VAL:HG22	1:A:143:VAL:CG1	0.51	2.34	8	4
1:A:153:LEU:HD21	1:A:161:LEU:HD21	0.51	1.80	14	3
1:A:82:TYR:CZ	1:A:117:TYR:CD2	0.51	2.97	6	6
1:A:40:LEU:HD22	1:A:44:LYS:CA	0.51	2.34	12	1
1:A:105:ALA:HB2	1:A:117:TYR:HE1	0.51	1.58	3	3
1:A:48:ILE:HD12	1:A:48:ILE:C	0.51	2.30	9	4
1:A:149:LEU:HA	1:A:152:LYS:HE2	0.51	1.80	10	1
1:A:20:VAL:HG23	1:A:22:LYS:CG	0.51	2.36	5	1
1:A:85:TYR:O	1:A:100:VAL:HG22	0.51	2.05	17	1
1:A:82:TYR:CE1	1:A:103:PHE:CE2	0.51	2.99	1	1
1:A:101:PHE:CE1	1:A:103:PHE:CE1	0.51	2.99	2	1
1:A:37:LEU:HD11	1:A:75:LEU:HD12	0.51	1.82	4	2
1:A:60:VAL:HG13	1:A:67:PRO:HD3	0.51	1.83	9	1
1:A:59:ASP:CG	1:A:64:VAL:HG21	0.51	2.31	15	1
1:A:5:VAL:O	1:A:5:VAL:HG13	0.50	2.06	2	4
1:A:114:LYS:HZ1	1:A:118:ALA:HB2	0.50	1.66	15	1
1:A:149:LEU:HD22	1:A:152:LYS:CE	0.50	2.36	10	1
1:A:84:LEU:HD23	1:A:101:PHE:N	0.50	2.22	12	2
1:A:86:ASP:OD1	1:A:99:LEU:HD12	0.50	2.05	15	1
1:A:82:TYR:CD1	1:A:117:TYR:CE2	0.50	2.99	3	4
1:A:68:TYR:CD2	1:A:85:TYR:CZ	0.50	3.00	7	1
1:A:8:SER:O	1:A:9:ASP:CB	0.50	2.59	8	4
1:A:25:THR:O	1:A:29:VAL:HG22	0.50	2.05	19	2
1:A:135:LEU:HD21	1:A:148:THR:HG22	0.50	1.79	8	1
1:A:146:ARG:HG3	1:A:161:LEU:HD13	0.50	1.83	10	1
1:A:75:LEU:CD2	1:A:104:TRP:CD1	0.49	2.95	16	4
1:A:82:TYR:CE2	1:A:117:TYR:CZ	0.49	3.01	2	1
1:A:100:VAL:HG11	1:A:152:LYS:CB	0.49	2.36	11	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:75:LEU:HD13	1:A:104:TRP:CG	0.49	2.43	16	3
1:A:146:ARG:HG3	1:A:161:LEU:HG	0.49	1.83	11	8
1:A:82:TYR:CE1	1:A:117:TYR:CD2	0.49	3.00	13	4
1:A:14:VAL:CG2	1:A:36:VAL:HG11	0.49	2.37	19	2
1:A:82:TYR:CE2	1:A:117:TYR:CE2	0.49	3.00	10	2
1:A:23:SER:HB2	1:A:29:VAL:HG12	0.49	1.84	10	5
1:A:75:LEU:HD23	1:A:104:TRP:CD2	0.49	2.43	1	1
1:A:5:VAL:HG13	1:A:47:ILE:CD1	0.49	2.37	20	1
1:A:82:TYR:CZ	1:A:117:TYR:CE2	0.49	3.00	10	3
1:A:82:TYR:CD2	1:A:117:TYR:CE2	0.49	3.01	2	1
1:A:37:LEU:HD11	1:A:75:LEU:HD11	0.49	1.84	5	1
1:A:84:LEU:CD2	1:A:99:LEU:HD11	0.49	2.33	5	1
1:A:75:LEU:CD1	1:A:104:TRP:CG	0.49	2.96	16	3
1:A:146:ARG:O	1:A:161:LEU:HD13	0.49	2.08	10	1
1:A:104:TRP:CH2	1:A:143:VAL:HG21	0.49	2.43	12	1
1:A:25:THR:CB	1:A:26:PRO:CD	0.49	2.91	13	20
1:A:7:VAL:HG11	1:A:127:LYS:HG3	0.49	1.84	15	1
1:A:146:ARG:HG2	1:A:165:PRO:HB2	0.49	1.84	14	7
1:A:154:GLY:C	1:A:158:VAL:HG23	0.49	2.32	8	1
1:A:149:LEU:CD1	1:A:152:LYS:HZ2	0.49	2.20	11	1
1:A:5:VAL:HG13	1:A:40:LEU:HD11	0.49	1.85	9	1
1:A:159:ILE:HG23	1:A:160:SER:N	0.49	2.22	13	1
1:A:15:PHE:HE2	1:A:131:ILE:HD12	0.49	1.67	14	1
1:A:100:VAL:HG23	1:A:100:VAL:O	0.49	2.06	10	1
1:A:84:LEU:HD23	1:A:101:PHE:HA	0.48	1.83	8	2
1:A:135:LEU:HD23	1:A:148:THR:HG22	0.48	1.83	8	1
1:A:11:VAL:CG2	1:A:47:ILE:HG22	0.48	2.36	11	3
1:A:110:PRO:O	1:A:114:LYS:HB2	0.48	2.08	3	3
1:A:72:VAL:HG21	1:A:144:LYS:CB	0.48	2.38	12	2
1:A:8:SER:HG	1:A:48:ILE:HG22	0.48	1.66	15	1
1:A:15:PHE:CE1	1:A:84:LEU:HD13	0.48	2.43	10	1
1:A:55:ILE:HD13	1:A:70:THR:HB	0.48	1.85	6	2
1:A:27:GLU:O	1:A:27:GLU:CG	0.48	2.61	13	11
1:A:75:LEU:CD1	1:A:104:TRP:CE2	0.48	2.96	12	3
1:A:104:TRP:HA	1:A:104:TRP:CE3	0.48	2.43	12	3
1:A:131:ILE:HG23	1:A:132:LYS:N	0.48	2.24	17	1
1:A:140:TYR:HA	1:A:143:VAL:HG13	0.48	1.85	20	1
1:A:152:LYS:CE	1:A:153:LEU:HD23	0.48	2.38	8	1
1:A:25:THR:HB	1:A:26:PRO:CD	0.48	2.38	18	12
1:A:149:LEU:HD13	1:A:149:LEU:C	0.48	2.33	3	1
1:A:161:LEU:N	1:A:166:LEU:HD12	0.48	2.24	13	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:161:LEU:O	1:A:161:LEU:CD1	0.48	2.61	13	6
1:A:37:LEU:HD21	1:A:75:LEU:HD23	0.48	1.84	19	1
1:A:40:LEU:HD22	1:A:44:LYS:C	0.47	2.34	12	1
1:A:72:VAL:CG1	1:A:140:TYR:CD2	0.47	2.97	1	9
1:A:37:LEU:HD11	1:A:75:LEU:CD2	0.47	2.39	11	1
1:A:47:ILE:HD12	1:A:82:TYR:CE2	0.47	2.44	15	1
1:A:99:LEU:HD22	1:A:100:VAL:N	0.47	2.24	5	1
1:A:71:PHE:CE2	1:A:75:LEU:CD2	0.47	2.97	17	11
1:A:71:PHE:CE1	1:A:75:LEU:CD1	0.47	2.97	1	3
1:A:103:PHE:CE2	1:A:121:LYS:CB	0.47	2.97	3	2
1:A:104:TRP:CZ3	1:A:143:VAL:CG2	0.47	2.97	16	12
1:A:35:ALA:CB	1:A:85:TYR:CD2	0.47	2.98	4	4
1:A:68:TYR:CD1	1:A:146:ARG:NH2	0.47	2.83	7	2
1:A:47:ILE:O	1:A:48:ILE:HG23	0.47	2.10	17	2
1:A:101:PHE:CE2	1:A:128:LEU:CD1	0.47	2.97	4	13
1:A:72:VAL:CG2	1:A:140:TYR:CD2	0.47	2.97	11	5
1:A:72:VAL:HG21	1:A:144:LYS:CA	0.47	2.40	10	1
1:A:82:TYR:HB3	1:A:101:PHE:CE1	0.47	2.44	13	1
1:A:84:LEU:HD23	1:A:100:VAL:C	0.47	2.35	16	3
1:A:5:VAL:HG13	1:A:47:ILE:CG1	0.47	2.40	20	2
1:A:46:ASN:O	1:A:48:ILE:HG23	0.47	2.10	15	1
1:A:82:TYR:CE1	1:A:103:PHE:CE1	0.47	3.03	19	1
1:A:35:ALA:HB3	1:A:55:ILE:HB	0.47	1.85	15	2
1:A:149:LEU:HD11	1:A:152:LYS:NZ	0.46	2.25	19	1
1:A:152:LYS:CD	1:A:152:LYS:C	0.46	2.88	17	5
1:A:160:SER:CA	1:A:166:LEU:HB2	0.46	2.40	18	7
1:A:7:VAL:HG22	1:A:47:ILE:CG1	0.46	2.40	18	1
1:A:37:LEU:HD13	1:A:74:MET:HE3	0.46	1.87	20	1
1:A:92:LYS:HD2	1:A:157:ALA:HB1	0.46	1.85	18	1
1:A:18:MET:HE2	1:A:36:VAL:HG13	0.46	1.86	1	2
1:A:110:PRO:O	1:A:113:SER:N	0.46	2.47	3	1
1:A:62:GLN:OE1	1:A:63:THR:HG23	0.46	2.10	19	1
1:A:162:GLU:HB2	1:A:165:PRO:CG	0.46	2.39	9	14
1:A:77:ASP:O	1:A:77:ASP:CG	0.46	2.59	15	6
1:A:32:ARG:O	1:A:57:VAL:HG13	0.46	2.10	8	1
1:A:71:PHE:CZ	1:A:75:LEU:CD1	0.46	2.99	2	5
1:A:152:LYS:C	1:A:152:LYS:HD3	0.46	2.35	7	1
1:A:34:LYS:HB2	1:A:57:VAL:HG12	0.46	1.87	8	1
1:A:10:GLY:C	1:A:49:LEU:HD22	0.46	2.36	4	2
1:A:100:VAL:HG13	1:A:152:LYS:NZ	0.46	2.26	8	1
1:A:112:LYS:O	1:A:115:MET:HE2	0.46	2.11	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:15:PHE:CE1	1:A:131:ILE:CD1	0.46	2.99	12	3
1:A:90:GLU:CB	1:A:159:ILE:HD11	0.46	2.40	11	1
1:A:104:TRP:CZ3	1:A:143:VAL:CG1	0.46	2.99	20	1
1:A:153:LEU:HD12	1:A:153:LEU:C	0.46	2.36	1	2
1:A:35:ALA:HB2	1:A:85:TYR:CG	0.46	2.45	6	1
1:A:40:LEU:HD23	1:A:46:ASN:O	0.46	2.11	12	1
1:A:90:GLU:HB3	1:A:159:ILE:HD11	0.46	1.87	18	1
1:A:71:PHE:HE2	1:A:102:ILE:HG21	0.45	1.71	1	1
1:A:15:PHE:CZ	1:A:131:ILE:CD1	0.45	2.99	13	4
1:A:89:TYR:CE1	1:A:153:LEU:CB	0.45	2.99	10	1
1:A:83:ALA:HB3	1:A:102:ILE:HB	0.45	1.86	13	1
1:A:37:LEU:HG	1:A:83:ALA:HB2	0.45	1.88	1	1
1:A:55:ILE:HD12	1:A:70:THR:CG2	0.45	2.41	2	1
1:A:37:LEU:HD23	1:A:83:ALA:HB2	0.45	1.88	13	2
1:A:44:LYS:NZ	1:A:116:ILE:HD13	0.45	2.25	7	1
1:A:11:VAL:HG21	1:A:47:ILE:CG2	0.45	2.40	11	2
1:A:149:LEU:HD12	1:A:152:LYS:HZ2	0.45	1.72	11	1
1:A:160:SER:OG	1:A:166:LEU:HB2	0.45	2.10	11	2
1:A:34:LYS:NZ	1:A:60:VAL:HG22	0.45	2.26	20	1
1:A:5:VAL:HG13	1:A:5:VAL:O	0.45	2.11	3	3
1:A:37:LEU:CD2	1:A:71:PHE:CE2	0.45	3.00	12	1
1:A:71:PHE:CZ	1:A:75:LEU:CD2	0.45	3.00	17	1
1:A:84:LEU:CD2	1:A:131:ILE:HD11	0.45	2.36	3	2
1:A:12:ILE:HD11	1:A:127:LYS:HB2	0.45	1.89	10	1
1:A:71:PHE:CE1	1:A:75:LEU:HD11	0.45	2.47	2	3
1:A:152:LYS:HZ2	1:A:153:LEU:HD21	0.45	1.72	3	1
1:A:117:TYR:O	1:A:121:LYS:N	0.45	2.49	20	9
1:A:12:ILE:N	1:A:12:ILE:CD1	0.45	2.80	20	2
1:A:68:TYR:CD1	1:A:85:TYR:CE2	0.45	3.05	17	1
1:A:36:VAL:HG23	1:A:38:PHE:CZ	0.45	2.47	8	2
1:A:85:TYR:CD1	1:A:86:ASP:N	0.45	2.85	3	5
1:A:137:ALA:HB1	1:A:142:GLU:CB	0.45	2.41	10	2
1:A:12:ILE:CD1	1:A:128:LEU:HD23	0.45	2.42	17	1
1:A:103:PHE:N	1:A:135:LEU:O	0.45	2.50	4	2
1:A:36:VAL:CG2	1:A:38:PHE:CE2	0.45	2.99	15	1
1:A:84:LEU:HD21	1:A:101:PHE:CD2	0.45	2.46	18	1
1:A:40:LEU:HD21	1:A:47:ILE:CD1	0.44	2.41	7	2
1:A:49:LEU:N	1:A:49:LEU:CD1	0.44	2.80	9	1
1:A:15:PHE:CZ	1:A:19:LYS:CG	0.44	3.00	11	2
1:A:15:PHE:CE1	1:A:19:LYS:CG	0.44	3.00	17	1
1:A:72:VAL:HA	1:A:75:LEU:CB	0.44	2.43	5	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:71:PHE:CD2	1:A:75:LEU:HD13	0.44	2.48	10	1
1:A:11:VAL:N	1:A:49:LEU:HD22	0.44	2.28	4	1
1:A:40:LEU:HD12	1:A:44:LYS:C	0.44	2.38	6	1
1:A:113:SER:HA	1:A:116:ILE:HD12	0.44	1.90	18	2
1:A:55:ILE:CD1	1:A:70:THR:HG22	0.44	2.42	7	2
1:A:5:VAL:HG21	1:A:120:SER:HB2	0.44	1.90	20	2
1:A:44:LYS:O	1:A:116:ILE:HD12	0.44	2.12	12	1
1:A:80:CYS:HG	1:A:117:TYR:CB	0.44	2.26	20	2
1:A:37:LEU:HD21	1:A:75:LEU:HD12	0.44	1.88	15	1
1:A:101:PHE:HD2	1:A:131:ILE:HD13	0.44	1.72	1	1
1:A:47:ILE:HG21	1:A:124:ILE:HD13	0.44	1.90	4	1
1:A:99:LEU:HD23	1:A:100:VAL:H	0.44	1.73	11	1
1:A:55:ILE:HD11	1:A:74:MET:CE	0.44	2.42	17	1
1:A:60:VAL:HG22	1:A:67:PRO:HB3	0.44	1.88	18	1
1:A:75:LEU:CD2	1:A:143:VAL:HG21	0.44	2.43	20	1
1:A:78:LYS:N	1:A:78:LYS:CD	0.43	2.81	3	7
1:A:100:VAL:HG21	1:A:135:LEU:CD1	0.43	2.43	2	1
1:A:83:ALA:O	1:A:102:ILE:N	0.43	2.51	9	3
1:A:55:ILE:HD13	1:A:70:THR:CG2	0.43	2.21	8	1
1:A:68:TYR:CD2	1:A:146:ARG:CD	0.43	3.01	14	2
1:A:117:TYR:C	1:A:117:TYR:CD1	0.43	2.96	16	1
1:A:131:ILE:O	1:A:132:LYS:CB	0.43	2.66	17	1
1:A:135:LEU:HD22	1:A:148:THR:CG2	0.43	2.43	7	1
1:A:84:LEU:HD11	1:A:101:PHE:CD2	0.43	2.48	15	1
1:A:34:LYS:N	1:A:55:ILE:O	0.43	2.51	8	2
1:A:72:VAL:CG1	1:A:140:TYR:CG	0.43	3.01	14	1
1:A:15:PHE:CD1	1:A:128:LEU:CD2	0.43	3.01	18	1
1:A:37:LEU:CD2	1:A:71:PHE:CE1	0.43	3.01	10	1
1:A:82:TYR:CD2	1:A:117:TYR:CZ	0.43	3.06	2	2
1:A:36:VAL:O	1:A:38:PHE:CE1	0.43	2.72	18	4
1:A:124:ILE:O	1:A:127:LYS:CG	0.43	2.67	10	1
1:A:78:LYS:CD	1:A:78:LYS:N	0.43	2.82	11	10
1:A:37:LEU:HD12	1:A:83:ALA:CB	0.43	2.43	5	1
1:A:160:SER:OG	1:A:161:LEU:N	0.43	2.52	13	4
1:A:75:LEU:HD13	1:A:104:TRP:CD2	0.43	2.49	16	2
1:A:64:VAL:HG12	1:A:65:ASP:N	0.43	2.29	3	3
1:A:60:VAL:HG23	1:A:67:PRO:CD	0.43	2.44	8	1
1:A:20:VAL:HG12	1:A:21:ARG:N	0.43	2.29	1	2
1:A:48:ILE:HD12	1:A:49:LEU:O	0.43	2.13	12	1
1:A:12:ILE:O	1:A:16:ASN:N	0.43	2.51	17	1
1:A:25:THR:HB	1:A:26:PRO:HD2	0.43	1.91	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:9:ASP:CG	1:A:10:GLY:N	0.43	2.77	1	1
1:A:37:LEU:HD22	1:A:74:MET:CE	0.43	2.37	1	1
1:A:100:VAL:HG13	1:A:102:ILE:HG13	0.43	1.91	2	1
1:A:15:PHE:CD1	1:A:84:LEU:CD1	0.43	3.01	10	2
1:A:72:VAL:CG2	1:A:140:TYR:CE2	0.43	3.01	7	1
1:A:149:LEU:O	1:A:152:LYS:CD	0.43	2.67	10	3
1:A:89:TYR:CG	1:A:153:LEU:HD13	0.43	2.48	11	1
1:A:90:GLU:C	1:A:159:ILE:CG2	0.43	2.92	13	1
1:A:131:ILE:O	1:A:133:HIS:N	0.43	2.52	20	1
1:A:15:PHE:HZ	1:A:131:ILE:HD12	0.42	1.70	4	2
1:A:91:THR:O	1:A:93:GLU:N	0.42	2.51	14	1
1:A:149:LEU:O	1:A:153:LEU:HD23	0.42	2.13	18	1
1:A:40:LEU:N	1:A:117:TYR:CE1	0.42	2.87	2	1
1:A:82:TYR:CG	1:A:117:TYR:CE2	0.42	3.07	2	1
1:A:87:ALA:HB3	1:A:152:LYS:NZ	0.42	2.29	3	2
1:A:37:LEU:HD13	1:A:74:MET:CE	0.42	2.44	18	2
1:A:111:LEU:HD13	1:A:111:LEU:O	0.42	2.14	12	1
1:A:89:TYR:CB	1:A:158:VAL:HG13	0.42	2.44	13	1
1:A:40:LEU:HD12	1:A:45:LYS:N	0.42	2.29	15	1
1:A:75:LEU:HG	1:A:104:TRP:CD1	0.42	2.50	17	1
1:A:82:TYR:CE1	1:A:103:PHE:CD1	0.42	3.08	19	2
1:A:100:VAL:HG12	1:A:133:HIS:HB3	0.42	1.90	16	1
1:A:99:LEU:HD23	1:A:100:VAL:N	0.42	2.29	11	1
1:A:77:ASP:OD2	1:A:108:SER:CB	0.42	2.68	15	1
1:A:75:LEU:O	1:A:104:TRP:CZ2	0.42	2.73	3	1
1:A:87:ALA:CB	1:A:152:LYS:CE	0.42	2.98	3	1
1:A:160:SER:OG	1:A:163:GLY:N	0.42	2.53	5	3
1:A:8:SER:CB	1:A:48:ILE:CG2	0.42	2.96	9	3
1:A:68:TYR:CG	1:A:146:ARG:CZ	0.42	3.02	13	1
1:A:18:MET:O	1:A:99:LEU:HD11	0.42	2.14	1	1
1:A:75:LEU:HD23	1:A:104:TRP:CE2	0.42	2.50	1	1
1:A:44:LYS:O	1:A:116:ILE:HG21	0.42	2.14	3	1
1:A:57:VAL:O	1:A:57:VAL:CG2	0.42	2.68	3	1
1:A:14:VAL:CG1	1:A:49:LEU:HD22	0.42	2.45	13	1
1:A:38:PHE:CZ	1:A:84:LEU:HD12	0.42	2.50	18	1
1:A:74:MET:C	1:A:76:PRO:HD3	0.42	2.40	1	4
1:A:7:VAL:CG1	1:A:11:VAL:CG2	0.42	2.98	4	5
1:A:164:LYS:CB	1:A:165:PRO:CD	0.42	2.97	10	8
1:A:25:THR:HG22	1:A:26:PRO:HD2	0.42	1.91	5	2
1:A:72:VAL:CG2	1:A:140:TYR:CG	0.42	3.02	5	1
1:A:100:VAL:CG1	1:A:152:LYS:CD	0.42	2.98	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:127:LYS:O	1:A:129:THR:HG23	0.42	2.14	6	1
1:A:135:LEU:HD11	1:A:152:LYS:HZ3	0.42	1.74	10	1
1:A:24:SER:O	1:A:29:VAL:HG13	0.42	2.15	19	2
1:A:84:LEU:HD21	1:A:101:PHE:HD2	0.42	1.73	18	1
1:A:44:LYS:C	1:A:116:ILE:HG21	0.42	2.40	3	1
1:A:19:LYS:HG3	1:A:20:VAL:HG13	0.42	1.91	4	1
1:A:161:LEU:O	1:A:162:GLU:CB	0.42	2.67	11	1
1:A:40:LEU:HD21	1:A:47:ILE:HD13	0.41	1.91	3	1
1:A:89:TYR:CD2	1:A:158:VAL:HG22	0.41	2.49	9	1
1:A:49:LEU:N	1:A:49:LEU:HD23	0.41	2.31	1	1
1:A:45:LYS:O	1:A:46:ASN:ND2	0.41	2.54	2	2
1:A:5:VAL:CG1	1:A:46:ASN:N	0.41	2.83	9	1
1:A:57:VAL:HG23	1:A:58:GLY:N	0.41	2.30	10	1
1:A:15:PHE:CE2	1:A:131:ILE:HD12	0.41	2.50	14	1
1:A:37:LEU:HD23	1:A:74:MET:CE	0.41	2.45	14	1
1:A:80:CYS:O	1:A:117:TYR:CE1	0.41	2.73	14	1
1:A:7:VAL:HG12	1:A:11:VAL:CG2	0.41	2.45	15	1
1:A:18:MET:HE1	1:A:99:LEU:HD21	0.41	1.92	20	1
1:A:124:ILE:HG23	1:A:125:LYS:N	0.41	2.30	9	5
1:A:72:VAL:HA	1:A:75:LEU:HB2	0.41	1.92	5	3
1:A:146:ARG:NE	1:A:165:PRO:CB	0.41	2.84	9	1
1:A:104:TRP:O	1:A:117:TYR:CE2	0.41	2.74	7	1
1:A:49:LEU:HD13	1:A:49:LEU:H	0.41	1.73	9	1
1:A:113:SER:O	1:A:117:TYR:CE1	0.41	2.73	9	1
1:A:87:ALA:HB3	1:A:149:LEU:HD12	0.41	1.93	11	1
1:A:89:TYR:CZ	1:A:96:LYS:CB	0.41	3.03	16	1
1:A:10:GLY:CA	1:A:13:LYS:HB2	0.41	2.44	19	1
1:A:14:VAL:HG11	1:A:38:PHE:CE2	0.41	2.51	19	1
1:A:104:TRP:CZ3	1:A:137:ALA:O	0.41	2.74	2	1
1:A:71:PHE:CZ	1:A:102:ILE:CG2	0.41	3.04	10	1
1:A:159:ILE:CG2	1:A:160:SER:N	0.41	2.83	13	1
1:A:164:LYS:CG	1:A:165:PRO:HD3	0.41	2.46	18	3
1:A:135:LEU:CD1	1:A:152:LYS:CG	0.41	2.98	1	1
1:A:7:VAL:HG12	1:A:8:SER:N	0.41	2.30	9	3
1:A:100:VAL:HG13	1:A:100:VAL:O	0.41	2.16	7	1
1:A:135:LEU:HD12	1:A:149:LEU:CD2	0.41	2.46	10	1
1:A:90:GLU:C	1:A:159:ILE:HG22	0.41	2.41	13	1
1:A:89:TYR:CE2	1:A:96:LYS:CD	0.41	3.03	16	1
1:A:100:VAL:CG1	1:A:152:LYS:CE	0.41	2.98	18	1
1:A:130:GLY:O	1:A:132:LYS:N	0.41	2.54	20	1
1:A:16:ASN:OD1	1:A:17:ASP:N	0.41	2.54	1	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:101:PHE:HE2	1:A:128:LEU:HD12	0.41	1.75	2	1
1:A:150:ALA:HA	1:A:153:LEU:HD12	0.41	1.92	3	1
1:A:25:THR:CG2	1:A:26:PRO:CD	0.41	2.99	6	2
1:A:30:LYS:O	1:A:58:GLY:N	0.41	2.54	7	1
1:A:7:VAL:HG11	1:A:11:VAL:HB	0.41	1.92	12	1
1:A:8:SER:HB2	1:A:48:ILE:HG23	0.41	1.92	17	1
1:A:5:VAL:CG1	1:A:123:ALA:HB3	0.41	2.46	3	1
1:A:25:THR:O	1:A:29:VAL:HG13	0.41	2.16	3	1
1:A:80:CYS:O	1:A:117:TYR:CZ	0.41	2.74	19	4
1:A:150:ALA:HA	1:A:153:LEU:HD21	0.41	1.93	5	1
1:A:60:VAL:O	1:A:60:VAL:HG22	0.41	2.16	7	1
1:A:14:VAL:HG21	1:A:36:VAL:HG11	0.41	1.92	8	1
1:A:98:ASP:OD2	1:A:133:HIS:CD2	0.41	2.74	10	1
1:A:116:ILE:O	1:A:117:TYR:C	0.41	2.64	18	1
1:A:34:LYS:HE2	1:A:88:THR:HG22	0.41	1.92	19	1
1:A:91:THR:HG23	1:A:92:LYS:H	0.41	1.76	19	1
1:A:84:LEU:HD11	1:A:131:ILE:HD13	0.41	1.93	20	1
1:A:132:LYS:O	1:A:133:HIS:CG	0.41	2.73	2	2
1:A:6:ALA:O	1:A:7:VAL:O	0.41	2.39	9	1
1:A:89:TYR:CE1	1:A:153:LEU:HB2	0.41	2.51	10	1
1:A:5:VAL:CG2	1:A:47:ILE:CD1	0.41	2.99	11	1
1:A:105:ALA:CB	1:A:117:TYR:CE1	0.41	3.00	16	1
1:A:10:GLY:O	1:A:13:LYS:N	0.41	2.54	19	1
1:A:99:LEU:N	1:A:99:LEU:HD12	0.40	2.31	2	1
1:A:33:LYS:CD	1:A:36:VAL:CG1	0.40	3.00	10	1
1:A:60:VAL:HG11	1:A:162:GLU:CD	0.40	2.41	11	2
1:A:89:TYR:CE2	1:A:96:LYS:HB2	0.40	2.51	16	1
1:A:37:LEU:HD13	1:A:74:MET:HE1	0.40	1.92	1	1
1:A:101:PHE:CE1	1:A:103:PHE:CZ	0.40	3.10	2	1
1:A:88:THR:CG2	1:A:162:GLU:CG	0.40	2.98	5	1
1:A:40:LEU:HD13	1:A:44:LYS:HA	0.40	1.94	12	1
1:A:117:TYR:CD1	1:A:117:TYR:C	0.40	2.99	12	1
1:A:75:LEU:CD1	1:A:104:TRP:CD1	0.40	3.05	17	1
1:A:146:ARG:HG3	1:A:161:LEU:CG	0.40	2.46	19	1
1:A:25:THR:CB	1:A:26:PRO:HD2	0.40	2.47	6	1
1:A:131:ILE:CG1	1:A:132:LYS:N	0.40	2.83	7	1
1:A:149:LEU:CA	1:A:152:LYS:HE2	0.40	2.46	10	1
1:A:152:LYS:CD	1:A:153:LEU:N	0.40	2.84	12	3
1:A:68:TYR:CE2	1:A:143:VAL:O	0.40	2.74	14	1
1:A:149:LEU:CD1	1:A:152:LYS:HZ3	0.40	2.29	5	1
1:A:152:LYS:CD	1:A:153:LEU:CD2	0.40	2.99	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:80:CYS:SG	1:A:117:TYR:CG	0.40	3.14	10	1
1:A:161:LEU:O	1:A:161:LEU:HD13	0.40	2.15	12	1
1:A:5:VAL:CG1	1:A:123:ALA:CB	0.40	3.00	16	1
1:A:15:PHE:CZ	1:A:19:LYS:HG3	0.40	2.52	17	1
1:A:25:THR:CG2	1:A:26:PRO:HD2	0.40	2.47	6	1
1:A:146:ARG:CD	1:A:165:PRO:HB2	0.40	2.46	10	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	161/166 (97%)	116±5 (72±3%)	34±5 (21±3%)	11±3 (7±2%)	2	17
All	All	3220/3320 (97%)	2324 (72%)	681 (21%)	215 (7%)	2	17

All 38 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	24	SER	20
1	A	164	LYS	20
1	A	102	ILE	18
1	A	162	GLU	16
1	A	76	PRO	14
1	A	71	PHE	12
1	A	132	LYS	12
1	A	91	THR	11
1	A	5	VAL	9
1	A	22	LYS	6
1	A	21	ARG	6
1	A	7	VAL	6
1	A	93	GLU	5
1	A	154	GLY	5
1	A	9	ASP	5
1	A	101	PHE	5

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Mol	Chain	Res	Type	Models (Total)
1	A	108	SER	4
1	A	35	ALA	4
1	A	45	LYS	3
1	A	129	THR	3
1	A	131	ILE	3
1	A	116	ILE	3
1	A	62	GLN	3
1	A	87	ALA	2
1	A	67	PRO	2
1	A	50	GLU	2
1	A	92	LYS	2
1	A	109	ALA	2
1	A	83	ALA	2
1	A	33	LYS	2
1	A	32	ARG	1
1	A	41	SER	1
1	A	130	GLY	1
1	A	53	LYS	1
1	A	135	LEU	1
1	A	25	THR	1
1	A	156	SER	1
1	A	155	GLY	1

6.3.2 Protein sidechains ⓘ

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	142/144 (99%)	103±4 (73±3%)	39±4 (27±3%)	2	21
All	All	2840/2880 (99%)	2068 (73%)	772 (27%)	2	21

All 101 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	30	LYS	20
1	A	78	LYS	20
1	A	114	LYS	20

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Mol	Chain	Res	Type	Models (Total)
1	A	124	ILE	20
1	A	75	LEU	19
1	A	18	MET	18
1	A	25	THR	18
1	A	107	GLU	18
1	A	149	LEU	18
1	A	152	LYS	18
1	A	164	LYS	18
1	A	40	LEU	16
1	A	53	LYS	16
1	A	113	SER	15
1	A	125	LYS	15
1	A	161	LEU	15
1	A	162	GLU	15
1	A	108	SER	15
1	A	50	GLU	14
1	A	33	LYS	14
1	A	45	LYS	13
1	A	37	LEU	13
1	A	44	LYS	12
1	A	19	LYS	12
1	A	73	LYS	12
1	A	90	GLU	12
1	A	127	LYS	11
1	A	32	ARG	10
1	A	146	ARG	10
1	A	98	ASP	10
1	A	74	MET	9
1	A	13	LYS	9
1	A	132	LYS	9
1	A	95	LYS	9
1	A	22	LYS	9
1	A	91	THR	9
1	A	54	GLU	8
1	A	103	PHE	8
1	A	112	LYS	8
1	A	131	ILE	8
1	A	151	GLU	8
1	A	119	SER	8
1	A	134	GLU	8
1	A	92	LYS	7
1	A	129	THR	7

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Mol	Chain	Res	Type	Models (Total)
1	A	23	SER	7
1	A	93	GLU	7
1	A	115	MET	7
1	A	139	CYS	7
1	A	111	LEU	7
1	A	126	LYS	7
1	A	153	LEU	7
1	A	12	ILE	6
1	A	43	ASP	6
1	A	49	LEU	6
1	A	62	GLN	6
1	A	94	SER	6
1	A	34	LYS	5
1	A	99	LEU	5
1	A	120	SER	5
1	A	135	LEU	5
1	A	17	ASP	5
1	A	51	GLU	5
1	A	96	LYS	5
1	A	145	ASP	5
1	A	59	ASP	4
1	A	100	VAL	4
1	A	42	GLU	4
1	A	21	ARG	3
1	A	160	SER	3
1	A	65	ASP	3
1	A	104	TRP	3
1	A	136	GLN	3
1	A	46	ASN	3
1	A	9	ASP	2
1	A	84	LEU	2
1	A	117	TYR	2
1	A	128	LEU	2
1	A	86	ASP	2
1	A	144	LYS	2
1	A	147	CYS	2
1	A	56	LEU	2
1	A	77	ASP	2
1	A	138	ASN	2
1	A	5	VAL	2
1	A	27	GLU	2
1	A	122	ASP	2

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Mol	Chain	Res	Type	Models (Total)
1	A	156	SER	2
1	A	8	SER	2
1	A	121	LYS	1
1	A	70	THR	1
1	A	66	ASP	1
1	A	80	CYS	1
1	A	39	CYS	1
1	A	81	ARG	1
1	A	48	ILE	1
1	A	7	VAL	1
1	A	116	ILE	1
1	A	72	VAL	1
1	A	141	GLU	1
1	A	143	VAL	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 oligosaccharides 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

No chemical shift data were provided