



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 04:27 PM UTC

PDB ID : 7DMD / pdb_00007dmd
BMRB ID : 36401
Title : Solution structure of human Aha1 N-terminal domain
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Deposited on : 2020-12-03

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

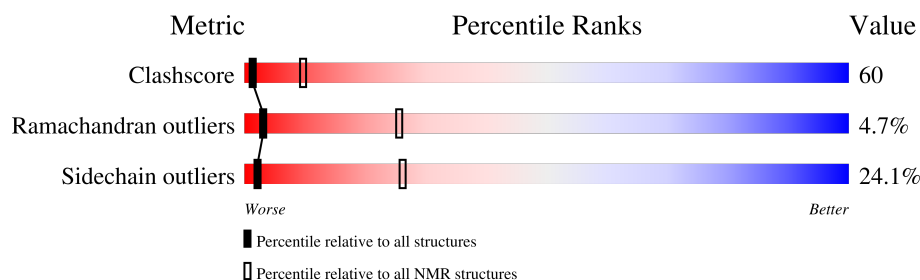
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

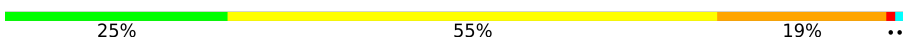
The overall completeness of chemical shifts assignment is 78%.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	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	135	

2 Ensemble composition and analysis

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:29-A:162 (134)	0.56	1

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 2116 atoms, of which 1053 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Activator of 90 kDa heat shock protein ATPase homolog 1.

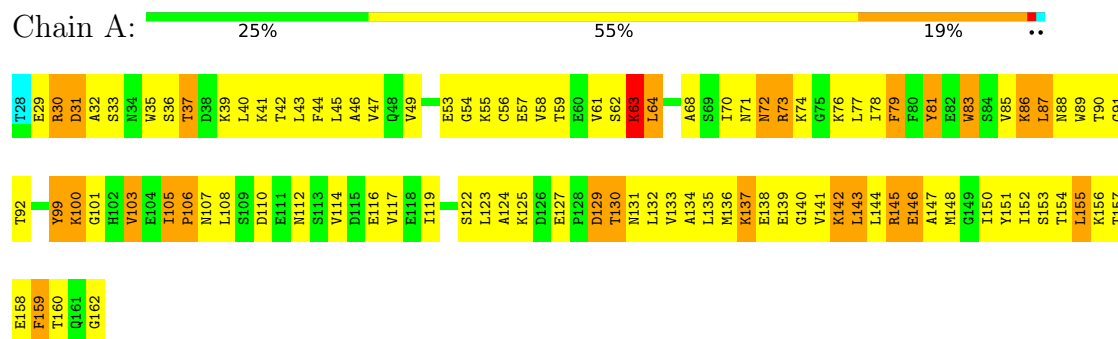
Mol	Chain	Residues	Atoms						Trace
1	A	135	Total	C	H	N	O	S	0
			2116	667	1053	174	219	3	

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: Activator of 90 kDa heat shock protein ATPase homolog 1

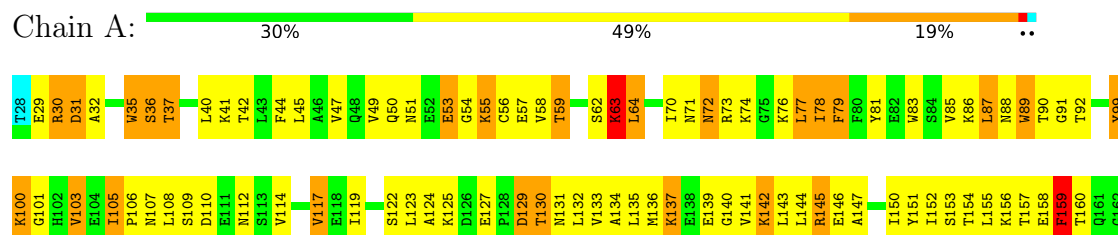


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

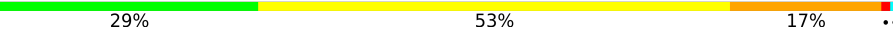
4.2.1 Score per residue for model 1 (medoid)

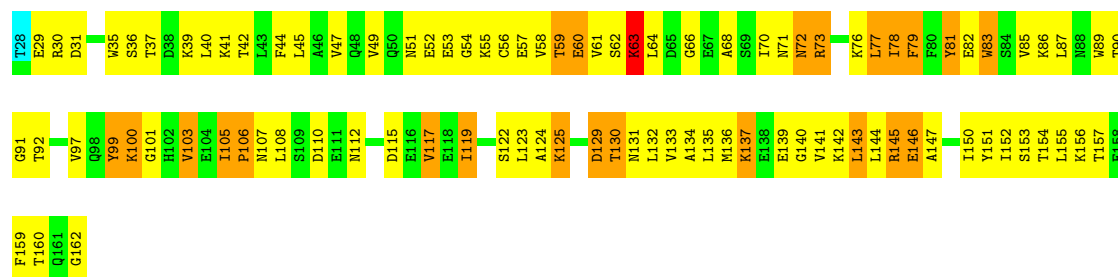
- Molecule 1: Activator of 90 kDa heat shock protein ATPase homolog 1



4.2.2 Score per residue for model 2

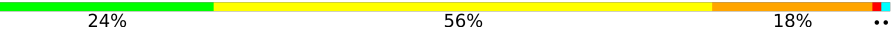
- Molecule 1: Activator of 90 kDa heat shock protein ATPase homolog 1

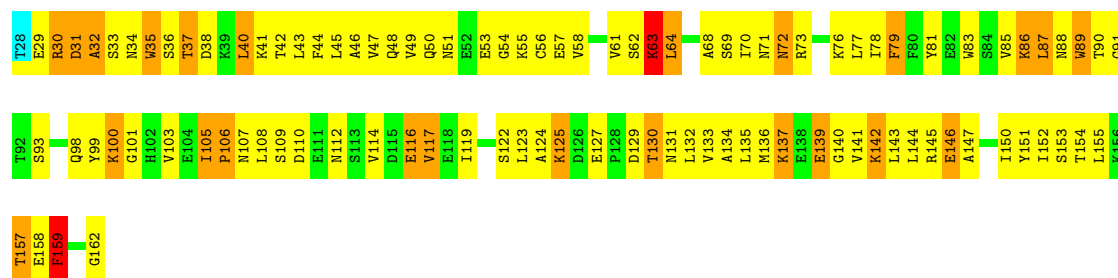
Chain A:  29% 53% 17% ..



4.2.3 Score per residue for model 3

- Molecule 1: Activator of 90 kDa heat shock protein ATPase homolog 1

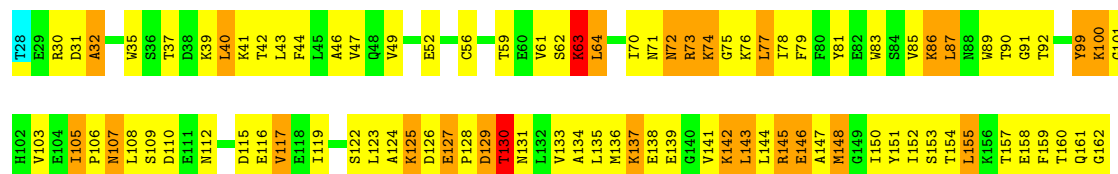
Chain A:  24% 56% 18% ..



4.2.4 Score per residue for model 4

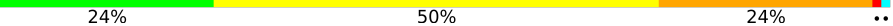
- Molecule 1: Activator of 90 kDa heat shock protein ATPase homolog 1

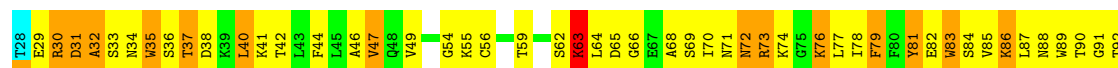
Chain A:  31% 49% 18% ..

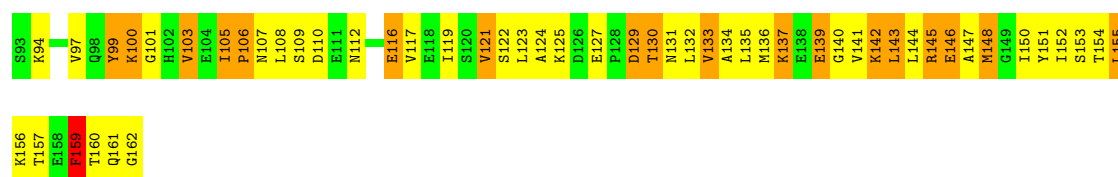


4.2.5 Score per residue for model 5

- Molecule 1: Activator of 90 kDa heat shock protein ATPase homolog 1

Chain A:  24% 50% 24% ..

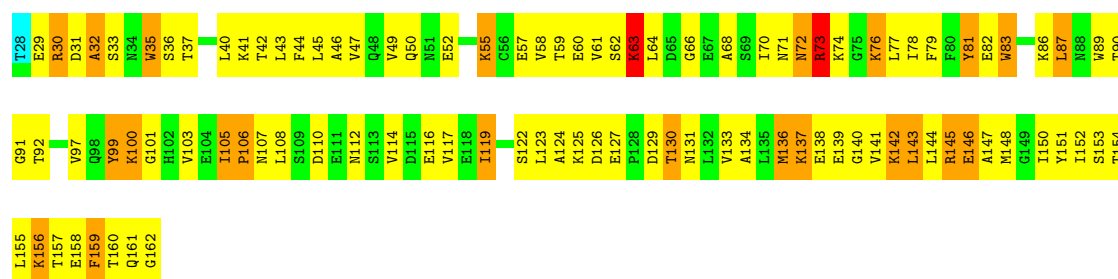




4.2.6 Score per residue for model 6

- Molecule 1: Activator of 90 kDa heat shock protein ATPase homolog 1

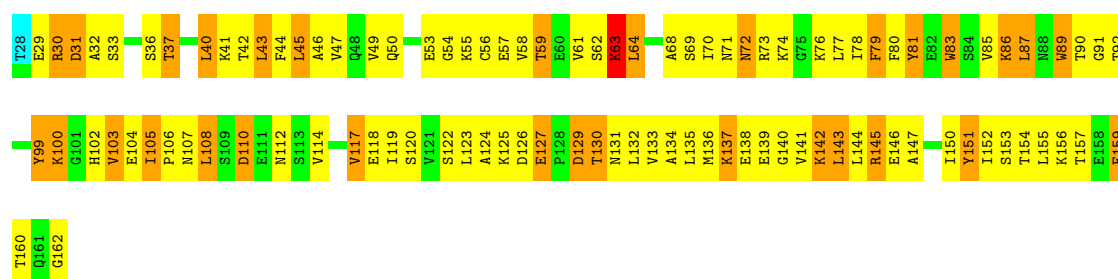
Chain A: 25% 56% 17% **



4.2.7 Score per residue for model 7

- Molecule 1: Activator of 90 kDa heat shock protein ATPase homolog 1

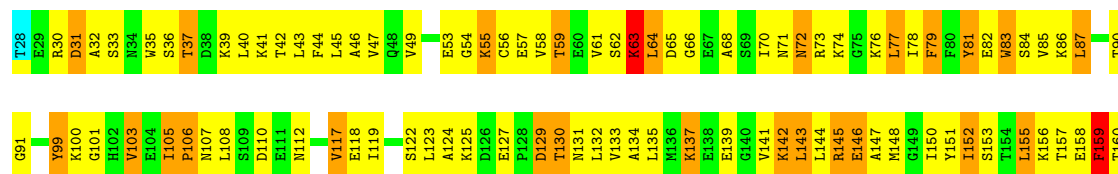
Chain A: 24% 51% 23% **



4.2.8 Score per residue for model 8

- Molecule 1: Activator of 90 kDa heat shock protein ATPase homolog 1

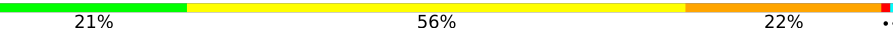
Chain A: 28% 51% 19% **

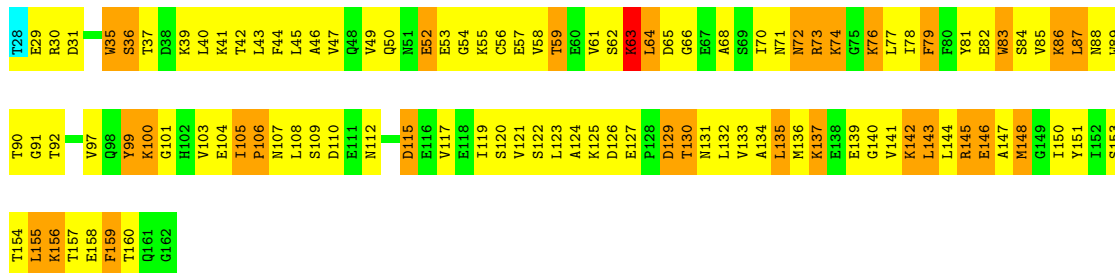


Q161
G162

4.2.9 Score per residue for model 9

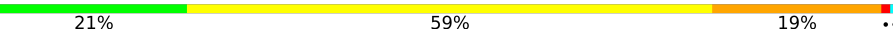
- Molecule 1: Activator of 90 kDa heat shock protein ATPase homolog 1

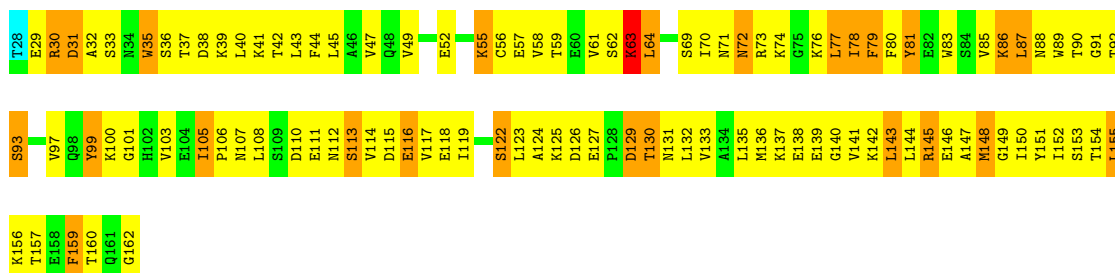
Chain A: 



4.2.10 Score per residue for model 10

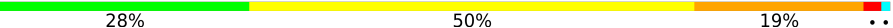
- Molecule 1: Activator of 90 kDa heat shock protein ATPase homolog 1

Chain A: 



4.2.11 Score per residue for model 11

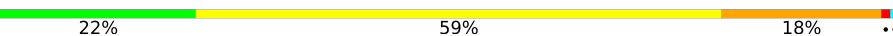
- Molecule 1: Activator of 90 kDa heat shock protein ATPase homolog 1

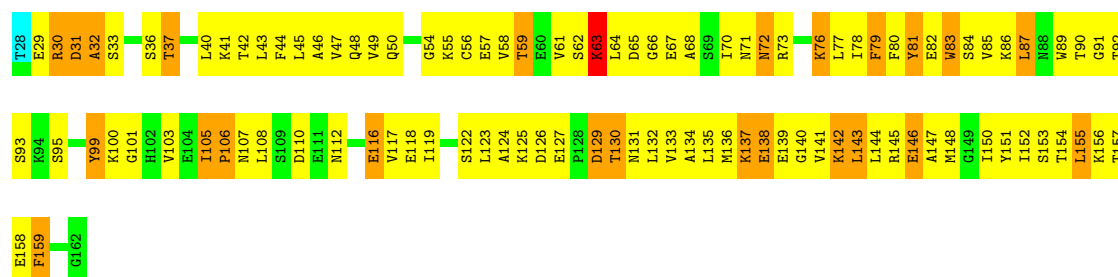
Chain A: 



4.2.12 Score per residue for model 12

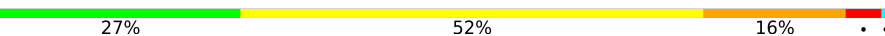
- Molecule 1: Activator of 90 kDa heat shock protein ATPase homolog 1

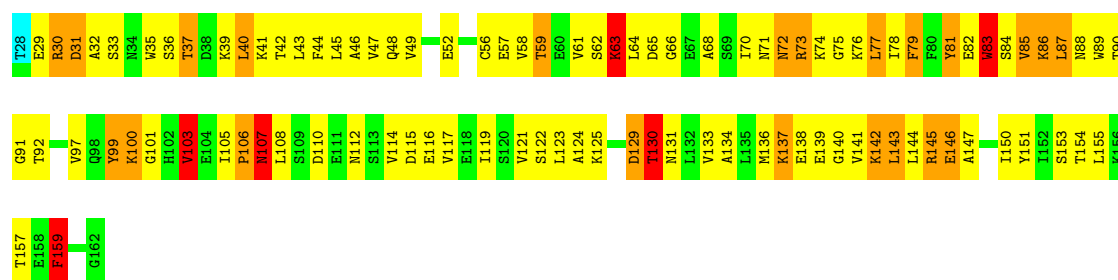
Chain A: 



4.2.13 Score per residue for model 13

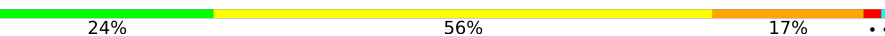
- Molecule 1: Activator of 90 kDa heat shock protein ATPase homolog 1

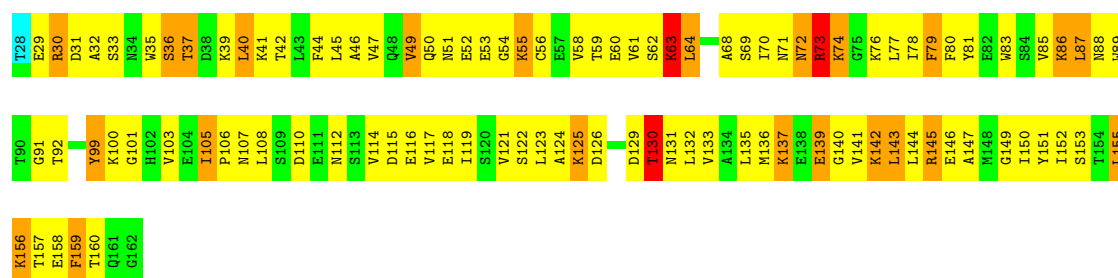
Chain A: 



4.2.14 Score per residue for model 14

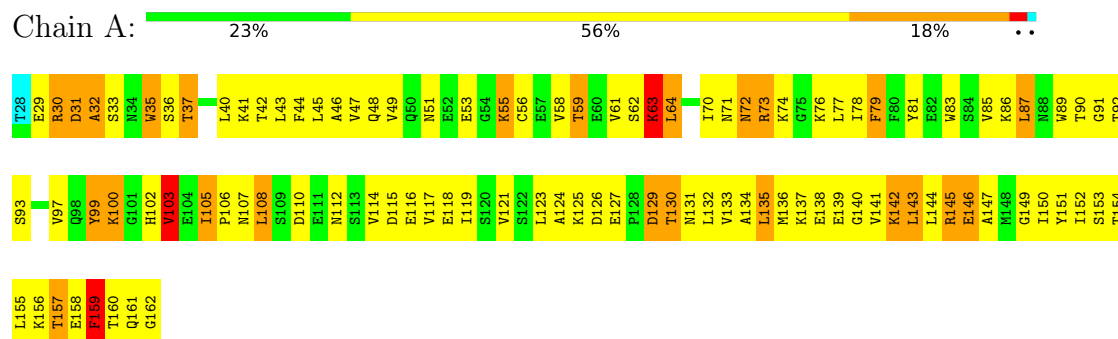
- Molecule 1: Activator of 90 kDa heat shock protein ATPase homolog 1

Chain A: 



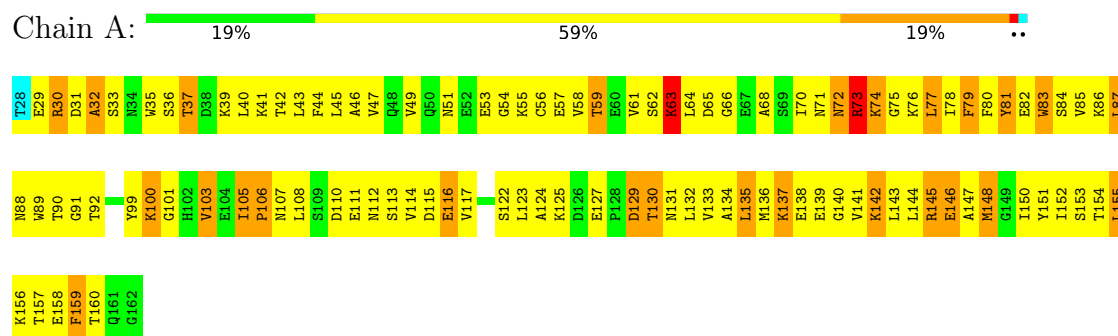
4.2.15 Score per residue for model 15

- Molecule 1: Activator of 90 kDa heat shock protein ATPase homolog 1



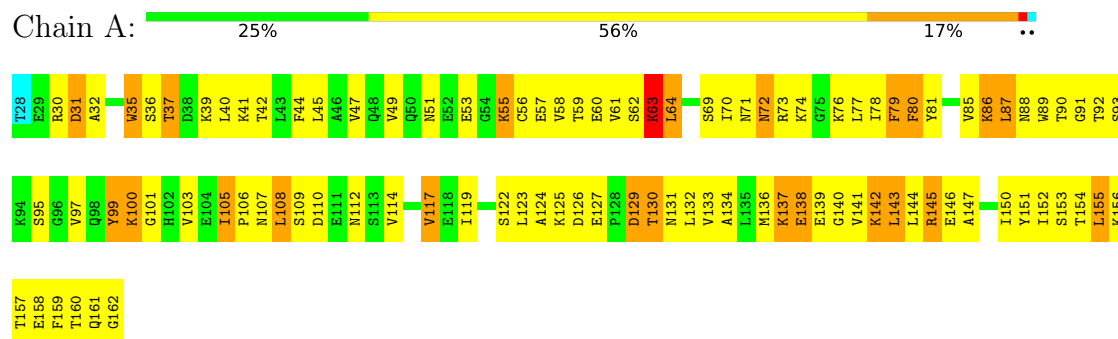
4.2.16 Score per residue for model 16

- Molecule 1: Activator of 90 kDa heat shock protein ATPase homolog 1



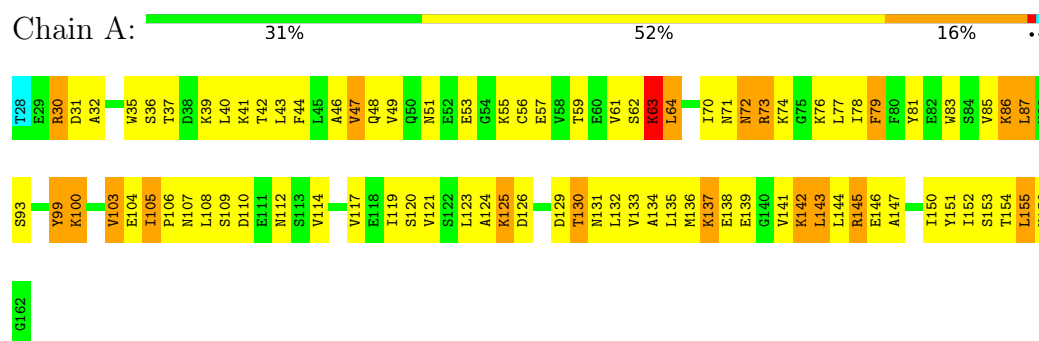
4.2.17 Score per residue for model 17

- Molecule 1: Activator of 90 kDa heat shock protein ATPase homolog 1



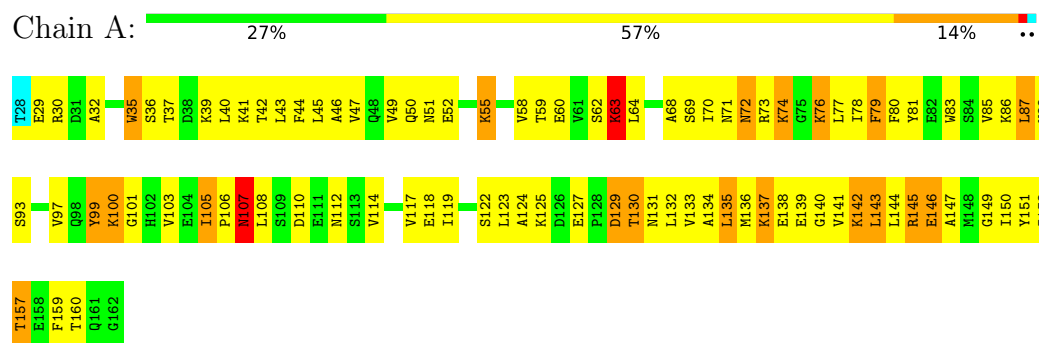
4.2.18 Score per residue for model 18

- Molecule 1: Activator of 90 kDa heat shock protein ATPase homolog 1



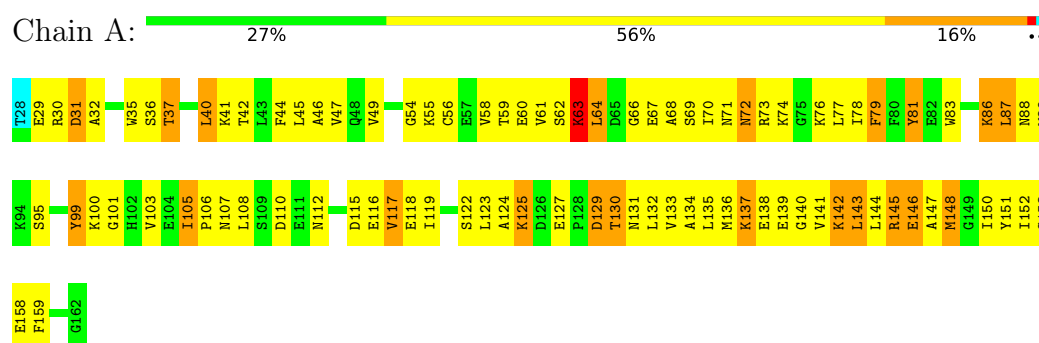
4.2.19 Score per residue for model 19

- Molecule 1: Activator of 90 kDa heat shock protein ATPase homolog 1



4.2.20 Score per residue for model 20

- Molecule 1: Activator of 90 kDa heat shock protein ATPase homolog 1



5 Refinement protocol and experimental data overview

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

Of the 100 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
X-PLOR NIH	refinement	
X-PLOR NIH	structure calculation	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1407
Number of shifts mapped to atoms	1407
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	78%

6 Model quality

6.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.65±0.01	0±0/1071 (0.0± 0.0%)	1.09±0.01	1±0/1443 (0.1± 0.0%)
All	All	0.65	0/21420 (0.0%)	1.09	21/28860 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	2.8±0.4
All	All	0	56

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	159	PHE	CA-CB-CG	-6.38	107.42	113.80	7	19
1	A	76	LYS	N-CA-C	-5.15	106.30	112.59	19	1
1	A	80	PHE	CA-CB-CG	-5.02	108.78	113.80	17	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	73	ARG	Sidechain	20
1	A	30	ARG	Sidechain	18
1	A	145	ARG	Sidechain	18

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	1056	1046	1046	126±13
All	All	21120	20920	20920	2523

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 60.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:70:ILE:HD12	1:A:77:LEU:HD11	1.08	1.26	18	13
1:A:150:ILE:HD12	1:A:151:TYR:N	0.96	1.76	1	20
1:A:99:TYR:CD1	1:A:123:LEU:HD21	0.93	1.99	3	6
1:A:121:VAL:HG11	1:A:137:LYS:NZ	0.92	1.79	14	1
1:A:130:THR:O	1:A:133:VAL:HG12	0.92	1.65	14	19
1:A:121:VAL:HG11	1:A:137:LYS:HZ1	0.90	1.25	14	1
1:A:70:ILE:HD12	1:A:77:LEU:HD21	0.89	1.43	8	4
1:A:77:LEU:N	1:A:77:LEU:HD13	0.88	1.84	13	1
1:A:99:TYR:CD2	1:A:123:LEU:HD21	0.87	2.04	11	8
1:A:77:LEU:HD23	1:A:77:LEU:N	0.87	1.85	4	2
1:A:155:LEU:HD12	1:A:155:LEU:O	0.86	1.71	17	7
1:A:71:ASN:O	1:A:77:LEU:HD12	0.85	1.71	17	13
1:A:66:GLY:N	1:A:83:TRP:NE1	0.84	2.24	11	1
1:A:56:CYS:SG	1:A:136:MET:HE3	0.82	2.14	17	5
1:A:99:TYR:OH	1:A:132:LEU:HD13	0.82	1.75	16	8
1:A:86:LYS:C	1:A:87:LEU:HD23	0.81	1.99	14	13
1:A:123:LEU:HD13	1:A:136:MET:HE1	0.80	1.49	1	2
1:A:56:CYS:SG	1:A:136:MET:HE1	0.80	2.16	3	3
1:A:155:LEU:HD12	1:A:155:LEU:C	0.80	2.01	8	7
1:A:70:ILE:HD13	1:A:155:LEU:HD11	0.80	1.52	8	3
1:A:129:ASP:O	1:A:131:ASN:N	0.80	2.15	18	20
1:A:40:LEU:CD1	1:A:150:ILE:HD11	0.79	2.06	20	7
1:A:148:MET:O	1:A:152:ILE:HD12	0.78	1.77	5	3
1:A:114:VAL:O	1:A:117:VAL:HG22	0.77	1.79	6	3
1:A:89:TRP:CD1	1:A:123:LEU:HD12	0.77	2.14	18	9
1:A:70:ILE:CD1	1:A:77:LEU:HD11	0.76	2.11	3	13
1:A:108:LEU:HD22	1:A:108:LEU:N	0.76	1.95	13	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:44:PHE:O	1:A:47:VAL:HG23	0.75	1.82	10	17
1:A:75:GLY:H	1:A:77:LEU:HD21	0.75	1.41	4	2
1:A:155:LEU:C	1:A:155:LEU:HD23	0.74	2.07	7	8
1:A:66:GLY:N	1:A:83:TRP:CE3	0.74	2.55	20	1
1:A:114:VAL:O	1:A:117:VAL:HG13	0.74	1.82	6	3
1:A:64:LEU:C	1:A:83:TRP:NE1	0.73	2.46	11	1
1:A:105:ILE:HG22	1:A:119:ILE:HG23	0.73	1.58	11	17
1:A:98:GLN:C	1:A:100:LYS:HZ1	0.73	1.92	3	1
1:A:79:PHE:N	1:A:79:PHE:CD2	0.72	2.55	10	10
1:A:76:LYS:H	1:A:77:LEU:HD23	0.72	1.43	16	2
1:A:79:PHE:CD1	1:A:79:PHE:N	0.72	2.57	7	9
1:A:100:LYS:H	1:A:100:LYS:HZ2	0.71	1.27	15	2
1:A:79:PHE:CE1	1:A:151:TYR:CE2	0.71	2.78	6	1
1:A:45:LEU:C	1:A:58:VAL:HG11	0.71	2.11	3	14
1:A:64:LEU:H	1:A:64:LEU:HD23	0.71	1.46	14	6
1:A:129:ASP:N	1:A:129:ASP:OD1	0.70	2.24	5	9
1:A:40:LEU:CD2	1:A:147:ALA:HB1	0.70	2.16	8	6
1:A:153:SER:O	1:A:157:THR:HG23	0.70	1.86	13	2
1:A:81:TYR:CE2	1:A:151:TYR:CE1	0.70	2.80	3	5
1:A:43:LEU:HD23	1:A:146:GLU:OE2	0.70	1.87	16	4
1:A:70:ILE:HD12	1:A:77:LEU:CD1	0.69	2.15	20	10
1:A:87:LEU:HD23	1:A:87:LEU:N	0.69	2.02	18	13
1:A:64:LEU:HD12	1:A:64:LEU:O	0.69	1.88	2	2
1:A:64:LEU:HD12	1:A:83:TRP:CZ3	0.69	2.23	7	1
1:A:68:ALA:N	1:A:83:TRP:HE1	0.69	1.86	20	1
1:A:73:ARG:HA	1:A:77:LEU:HD12	0.68	1.64	13	1
1:A:73:ARG:HA	1:A:77:LEU:HD22	0.68	1.65	4	2
1:A:76:LYS:N	1:A:77:LEU:HD23	0.68	2.04	16	2
1:A:35:TRP:CD1	1:A:154:THR:HG22	0.68	2.23	10	6
1:A:65:ASP:C	1:A:83:TRP:CD1	0.67	2.72	11	1
1:A:81:TYR:CD2	1:A:82:GLU:N	0.67	2.63	13	4
1:A:75:GLY:H	1:A:77:LEU:HD11	0.67	1.48	13	1
1:A:55:LYS:O	1:A:132:LEU:HD11	0.67	1.89	17	10
1:A:79:PHE:CE2	1:A:156:LYS:NZ	0.67	2.62	9	2
1:A:89:TRP:CZ3	1:A:136:MET:SD	0.66	2.88	9	1
1:A:123:LEU:C	1:A:123:LEU:HD13	0.66	2.15	14	1
1:A:125:LYS:N	1:A:125:LYS:HE3	0.66	2.05	11	1
1:A:89:TRP:CZ2	1:A:136:MET:SD	0.66	2.88	1	2
1:A:99:TYR:CE1	1:A:129:ASP:CG	0.66	2.74	2	9
1:A:36:SER:O	1:A:40:LEU:HD12	0.66	1.91	5	5
1:A:43:LEU:HD23	1:A:146:GLU:OE1	0.66	1.91	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:62:SER:O	1:A:63:LYS:HB3	0.65	1.92	1	20
1:A:89:TRP:CH2	1:A:136:MET:SD	0.65	2.89	9	2
1:A:40:LEU:CD2	1:A:150:ILE:HD11	0.65	2.20	17	2
1:A:70:ILE:HG21	1:A:156:LYS:NZ	0.65	2.07	18	2
1:A:76:LYS:N	1:A:77:LEU:HD13	0.65	2.06	13	1
1:A:129:ASP:OD2	1:A:129:ASP:N	0.65	2.29	19	6
1:A:83:TRP:CD1	1:A:83:TRP:C	0.65	2.75	14	1
1:A:153:SER:O	1:A:157:THR:HG22	0.64	1.92	6	18
1:A:99:TYR:CE2	1:A:129:ASP:CG	0.64	2.76	15	6
1:A:89:TRP:CE3	1:A:136:MET:CE	0.64	2.80	18	1
1:A:89:TRP:NE1	1:A:123:LEU:HD12	0.64	2.07	3	14
1:A:66:GLY:N	1:A:83:TRP:CD1	0.64	2.65	11	1
1:A:40:LEU:O	1:A:44:PHE:CG	0.64	2.51	12	17
1:A:56:CYS:SG	1:A:136:MET:SD	0.64	2.96	7	5
1:A:81:TYR:CD2	1:A:81:TYR:N	0.64	2.66	10	3
1:A:142:LYS:O	1:A:145:ARG:N	0.64	2.31	10	20
1:A:144:LEU:O	1:A:147:ALA:N	0.64	2.31	2	19
1:A:31:ASP:OD1	1:A:69:SER:N	0.64	2.30	20	1
1:A:40:LEU:HD23	1:A:147:ALA:HB1	0.63	1.68	8	1
1:A:105:ILE:HD12	1:A:117:VAL:HG11	0.63	1.68	10	6
1:A:123:LEU:CD2	1:A:136:MET:SD	0.63	2.87	17	1
1:A:114:VAL:O	1:A:117:VAL:HG23	0.63	1.93	10	5
1:A:64:LEU:H	1:A:64:LEU:CD2	0.62	2.06	4	4
1:A:80:PHE:N	1:A:80:PHE:CD2	0.62	2.65	17	1
1:A:32:ALA:HB1	1:A:35:TRP:CD1	0.62	2.30	15	3
1:A:77:LEU:HD23	1:A:77:LEU:H	0.62	1.49	4	2
1:A:108:LEU:CD2	1:A:108:LEU:N	0.62	2.63	19	12
1:A:70:ILE:CG2	1:A:156:LYS:HZ1	0.62	2.06	18	1
1:A:91:GLY:O	1:A:99:TYR:CE1	0.62	2.53	12	8
1:A:123:LEU:CD1	1:A:136:MET:HE1	0.62	2.24	9	2
1:A:136:MET:O	1:A:140:GLY:N	0.62	2.32	15	14
1:A:144:LEU:O	1:A:147:ALA:HB3	0.62	1.94	10	12
1:A:36:SER:OG	1:A:40:LEU:HD22	0.62	1.94	2	1
1:A:40:LEU:O	1:A:44:PHE:CD1	0.62	2.53	10	12
1:A:115:ASP:OD1	1:A:116:GLU:N	0.62	2.32	14	2
1:A:64:LEU:O	1:A:83:TRP:NE1	0.62	2.33	11	1
1:A:76:LYS:H	1:A:77:LEU:HD13	0.62	1.52	13	1
1:A:123:LEU:HD13	1:A:136:MET:CE	0.62	2.25	9	2
1:A:155:LEU:C	1:A:155:LEU:CD1	0.62	2.71	8	9
1:A:30:ARG:O	1:A:159:PHE:CZ	0.61	2.53	5	7
1:A:35:TRP:CD1	1:A:158:GLU:OE1	0.61	2.53	16	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:70:ILE:HD11	1:A:159:PHE:CD2	0.61	2.29	4	4
1:A:99:TYR:HH	1:A:132:LEU:HD13	0.61	1.53	12	5
1:A:35:TRP:NE1	1:A:158:GLU:OE2	0.61	2.33	18	4
1:A:55:LYS:O	1:A:55:LYS:NZ	0.61	2.33	14	1
1:A:43:LEU:HD22	1:A:146:GLU:OE2	0.61	1.94	6	3
1:A:55:LYS:NZ	1:A:136:MET:CE	0.61	2.63	14	1
1:A:115:ASP:OD2	1:A:141:VAL:HG12	0.61	1.95	2	1
1:A:89:TRP:CE3	1:A:136:MET:SD	0.61	2.93	9	1
1:A:40:LEU:O	1:A:44:PHE:CD2	0.61	2.54	13	5
1:A:91:GLY:O	1:A:99:TYR:CE2	0.61	2.53	10	12
1:A:30:ARG:O	1:A:159:PHE:CE1	0.61	2.53	7	10
1:A:44:PHE:HB2	1:A:61:VAL:HG11	0.61	1.71	2	1
1:A:99:TYR:CE1	1:A:129:ASP:OD1	0.61	2.54	17	4
1:A:108:LEU:N	1:A:108:LEU:CD2	0.61	2.64	13	8
1:A:99:TYR:CD1	1:A:129:ASP:CG	0.61	2.79	9	4
1:A:150:ILE:CD1	1:A:151:TYR:N	0.61	2.64	12	19
1:A:77:LEU:HD13	1:A:77:LEU:H	0.61	1.50	13	1
1:A:66:GLY:C	1:A:83:TRP:CE2	0.61	2.79	20	1
1:A:114:VAL:O	1:A:117:VAL:HG12	0.61	1.95	1	4
1:A:31:ASP:OD2	1:A:68:ALA:HB1	0.61	1.96	9	1
1:A:64:LEU:C	1:A:83:TRP:HE1	0.61	2.01	11	1
1:A:30:ARG:O	1:A:159:PHE:CE2	0.60	2.54	1	4
1:A:99:TYR:CE1	1:A:129:ASP:OD2	0.60	2.54	19	2
1:A:35:TRP:NE1	1:A:158:GLU:OE1	0.60	2.34	3	6
1:A:35:TRP:NE1	1:A:158:GLU:CD	0.60	2.60	9	3
1:A:88:ASN:OD1	1:A:89:TRP:N	0.60	2.34	16	4
1:A:70:ILE:CD1	1:A:77:LEU:HD21	0.60	2.24	8	1
1:A:124:ALA:O	1:A:127:GLU:N	0.60	2.34	11	1
1:A:125:LYS:H	1:A:125:LYS:CD	0.60	2.08	11	2
1:A:148:MET:SD	1:A:152:ILE:HD13	0.60	2.35	20	1
1:A:99:TYR:CG	1:A:129:ASP:OD1	0.60	2.55	1	6
1:A:91:GLY:C	1:A:99:TYR:CE2	0.60	2.80	10	9
1:A:91:GLY:O	1:A:99:TYR:CZ	0.60	2.55	8	6
1:A:99:TYR:CG	1:A:129:ASP:OD2	0.60	2.55	5	7
1:A:80:PHE:CE1	1:A:111:GLU:CD	0.60	2.80	16	1
1:A:35:TRP:CE2	1:A:158:GLU:OE1	0.60	2.55	20	1
1:A:50:GLN:NE2	1:A:139:GLU:OE1	0.60	2.35	19	1
1:A:36:SER:OG	1:A:151:TYR:CE2	0.60	2.55	15	3
1:A:71:ASN:O	1:A:72:ASN:O	0.60	2.20	2	20
1:A:43:LEU:HD22	1:A:146:GLU:OE1	0.60	1.96	11	3
1:A:99:TYR:CE2	1:A:123:LEU:HD21	0.59	2.32	6	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:140:GLY:O	1:A:143:LEU:N	0.59	2.35	14	10
1:A:148:MET:SD	1:A:148:MET:O	0.59	2.60	10	4
1:A:81:TYR:C	1:A:81:TYR:CD1	0.59	2.80	5	2
1:A:59:THR:HG22	1:A:90:THR:OG1	0.59	1.97	15	9
1:A:80:PHE:CD1	1:A:111:GLU:OE1	0.59	2.55	16	1
1:A:99:TYR:CD2	1:A:129:ASP:OD1	0.59	2.55	19	3
1:A:99:TYR:CD1	1:A:129:ASP:OD1	0.59	2.54	7	6
1:A:123:LEU:O	1:A:124:ALA:HB3	0.59	1.96	11	17
1:A:99:TYR:CZ	1:A:129:ASP:CG	0.59	2.80	12	9
1:A:31:ASP:O	1:A:33:SER:N	0.59	2.35	6	8
1:A:90:THR:HG23	1:A:100:LYS:HG3	0.59	1.73	3	13
1:A:72:ASN:O	1:A:76:LYS:C	0.59	2.45	2	20
1:A:81:TYR:CD2	1:A:81:TYR:C	0.59	2.81	2	4
1:A:99:TYR:CD2	1:A:129:ASP:OD2	0.59	2.54	17	2
1:A:81:TYR:OH	1:A:156:LYS:NZ	0.59	2.36	14	1
1:A:130:THR:O	1:A:133:VAL:N	0.59	2.33	14	2
1:A:81:TYR:CE1	1:A:108:LEU:O	0.59	2.55	12	3
1:A:99:TYR:CE2	1:A:129:ASP:OD2	0.59	2.56	4	2
1:A:157:THR:O	1:A:162:GLY:N	0.59	2.36	8	6
1:A:99:TYR:CZ	1:A:132:LEU:HD21	0.59	2.32	3	1
1:A:99:TYR:CD1	1:A:129:ASP:OD2	0.59	2.55	20	6
1:A:81:TYR:CD1	1:A:81:TYR:C	0.59	2.81	8	2
1:A:36:SER:O	1:A:40:LEU:N	0.59	2.36	14	6
1:A:122:SER:C	1:A:125:LYS:HZ3	0.59	2.05	4	1
1:A:148:MET:SD	1:A:148:MET:C	0.59	2.86	9	4
1:A:55:LYS:NZ	1:A:57:GLU:OE2	0.59	2.35	8	2
1:A:115:ASP:OD2	1:A:116:GLU:N	0.59	2.36	4	2
1:A:59:THR:OG1	1:A:88:ASN:ND2	0.59	2.36	14	2
1:A:29:GLU:OE2	1:A:73:ARG:NE	0.59	2.35	6	1
1:A:50:GLN:NE2	1:A:139:GLU:OE2	0.59	2.35	7	2
1:A:137:LYS:O	1:A:141:VAL:CG2	0.59	2.51	7	15
1:A:40:LEU:HD13	1:A:64:LEU:HD13	0.59	1.75	8	1
1:A:65:ASP:CA	1:A:83:TRP:HE1	0.59	2.11	11	1
1:A:29:GLU:O	1:A:70:ILE:N	0.58	2.36	12	4
1:A:38:ASP:O	1:A:42:THR:HG23	0.58	1.97	10	1
1:A:54:GLY:HA2	1:A:132:LEU:HD12	0.58	1.74	16	7
1:A:112:ASN:ND2	1:A:116:GLU:OE1	0.58	2.36	10	2
1:A:40:LEU:HD11	1:A:151:TYR:CD2	0.58	2.33	15	1
1:A:87:LEU:O	1:A:88:ASN:ND2	0.58	2.36	17	2
1:A:110:ASP:OD1	1:A:151:TYR:CE1	0.58	2.56	11	1
1:A:67:GLU:C	1:A:83:TRP:NE1	0.58	2.61	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:110:ASP:C	1:A:112:ASN:H	0.58	2.05	11	17
1:A:35:TRP:CE2	1:A:158:GLU:OE2	0.58	2.56	14	2
1:A:83:TRP:CZ2	1:A:151:TYR:OH	0.58	2.52	7	1
1:A:93:SER:N	1:A:99:TYR:OH	0.58	2.36	17	4
1:A:48:GLN:HE21	1:A:50:GLN:NE2	0.58	1.96	12	1
1:A:55:LYS:NZ	1:A:57:GLU:OE1	0.58	2.37	17	1
1:A:81:TYR:CE2	1:A:110:ASP:CG	0.58	2.82	11	1
1:A:41:LYS:CG	1:A:42:THR:N	0.58	2.67	18	20
1:A:44:PHE:HB3	1:A:61:VAL:HG21	0.58	1.73	7	10
1:A:33:SER:O	1:A:37:THR:HG22	0.58	1.98	7	6
1:A:29:GLU:OE2	1:A:72:ASN:N	0.58	2.36	16	1
1:A:47:VAL:HG11	1:A:56:CYS:SG	0.58	2.39	2	12
1:A:61:VAL:HG13	1:A:87:LEU:HB3	0.58	1.76	3	15
1:A:79:PHE:CD2	1:A:79:PHE:C	0.57	2.80	6	1
1:A:70:ILE:HG21	1:A:156:LYS:HZ1	0.57	1.58	18	1
1:A:110:ASP:C	1:A:112:ASN:N	0.57	2.61	20	20
1:A:91:GLY:O	1:A:99:TYR:CD2	0.57	2.58	19	7
1:A:108:LEU:N	1:A:108:LEU:HD22	0.57	2.15	20	12
1:A:64:LEU:O	1:A:64:LEU:CD1	0.57	2.52	2	2
1:A:45:LEU:O	1:A:58:VAL:HG11	0.57	2.00	11	10
1:A:155:LEU:HD22	1:A:156:LYS:HZ3	0.57	1.59	7	1
1:A:92:THR:C	1:A:99:TYR:HH	0.57	2.07	12	2
1:A:29:GLU:N	1:A:70:ILE:O	0.57	2.37	6	5
1:A:65:ASP:C	1:A:83:TRP:NE1	0.57	2.63	11	1
1:A:124:ALA:O	1:A:127:GLU:O	0.57	2.22	11	14
1:A:91:GLY:O	1:A:99:TYR:CD1	0.57	2.58	4	6
1:A:77:LEU:N	1:A:77:LEU:CD1	0.57	2.59	13	1
1:A:110:ASP:OD2	1:A:151:TYR:CE2	0.57	2.57	20	1
1:A:81:TYR:CD1	1:A:82:GLU:N	0.57	2.72	16	3
1:A:66:GLY:O	1:A:83:TRP:CH2	0.57	2.57	20	1
1:A:97:VAL:O	1:A:99:TYR:CE1	0.57	2.58	17	7
1:A:123:LEU:O	1:A:133:VAL:CG2	0.57	2.53	14	3
1:A:31:ASP:OD2	1:A:155:LEU:CD1	0.57	2.53	7	1
1:A:55:LYS:O	1:A:56:CYS:SG	0.56	2.63	9	3
1:A:89:TRP:CE2	1:A:136:MET:SD	0.56	2.98	9	2
1:A:152:ILE:CD1	1:A:152:ILE:N	0.56	2.68	10	8
1:A:55:LYS:NZ	1:A:92:THR:OG1	0.56	2.36	6	2
1:A:153:SER:O	1:A:157:THR:CG2	0.56	2.53	7	19
1:A:36:SER:OG	1:A:151:TYR:CZ	0.56	2.58	17	4
1:A:105:ILE:O	1:A:105:ILE:HD12	0.56	2.00	13	1
1:A:67:GLU:C	1:A:83:TRP:HE1	0.56	2.07	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:92:THR:C	1:A:99:TYR:OH	0.56	2.48	19	14
1:A:83:TRP:O	1:A:106:PRO:O	0.56	2.24	9	8
1:A:107:ASN:HD22	1:A:107:ASN:C	0.56	2.08	19	2
1:A:81:TYR:CE1	1:A:151:TYR:CE1	0.56	2.93	15	1
1:A:59:THR:O	1:A:60:GLU:CB	0.56	2.53	2	1
1:A:123:LEU:C	1:A:123:LEU:HD23	0.56	2.25	18	8
1:A:56:CYS:SG	1:A:139:GLU:OE1	0.56	2.63	5	1
1:A:123:LEU:HD13	1:A:136:MET:SD	0.56	2.41	11	3
1:A:99:TYR:CE1	1:A:123:LEU:HD21	0.56	2.35	12	3
1:A:55:LYS:C	1:A:56:CYS:SG	0.56	2.88	9	3
1:A:29:GLU:CB	1:A:70:ILE:O	0.56	2.54	3	1
1:A:89:TRP:CD1	1:A:89:TRP:N	0.56	2.73	11	3
1:A:66:GLY:O	1:A:83:TRP:CZ2	0.56	2.58	20	1
1:A:105:ILE:CG1	1:A:105:ILE:O	0.56	2.54	3	18
1:A:107:ASN:C	1:A:107:ASN:ND2	0.56	2.61	19	2
1:A:44:PHE:CD2	1:A:87:LEU:HD13	0.56	2.36	18	3
1:A:70:ILE:CG2	1:A:156:LYS:NZ	0.56	2.69	10	1
1:A:64:LEU:HD23	1:A:64:LEU:N	0.55	2.16	4	4
1:A:142:LYS:O	1:A:145:ARG:CB	0.55	2.54	1	16
1:A:89:TRP:CD2	1:A:136:MET:SD	0.55	2.99	9	1
1:A:155:LEU:HD23	1:A:155:LEU:O	0.55	2.01	2	10
1:A:62:SER:O	1:A:63:LYS:CB	0.55	2.55	18	19
1:A:114:VAL:O	1:A:117:VAL:CG1	0.55	2.54	1	4
1:A:55:LYS:CE	1:A:92:THR:H	0.55	2.14	14	1
1:A:31:ASP:OD2	1:A:31:ASP:N	0.55	2.35	20	1
1:A:121:VAL:HG21	1:A:137:LYS:NZ	0.55	2.16	5	2
1:A:152:ILE:O	1:A:156:LYS:CG	0.55	2.54	7	4
1:A:123:LEU:HD13	1:A:124:ALA:N	0.55	2.16	14	1
1:A:132:LEU:HD21	1:A:136:MET:SD	0.55	2.41	2	2
1:A:91:GLY:C	1:A:99:TYR:CE1	0.55	2.84	4	5
1:A:32:ALA:HB3	1:A:155:LEU:HG	0.55	1.79	6	4
1:A:135:LEU:HD21	1:A:139:GLU:OE1	0.55	2.02	18	4
1:A:89:TRP:CD2	1:A:136:MET:HE1	0.55	2.37	17	1
1:A:75:GLY:H	1:A:77:LEU:CD2	0.55	2.14	4	2
1:A:155:LEU:C	1:A:155:LEU:CD2	0.55	2.80	7	8
1:A:93:SER:CB	1:A:99:TYR:OH	0.55	2.55	10	1
1:A:122:SER:C	1:A:125:LYS:NZ	0.55	2.65	4	1
1:A:114:VAL:O	1:A:117:VAL:CG2	0.55	2.55	10	8
1:A:132:LEU:HD21	1:A:136:MET:HE3	0.55	1.78	15	1
1:A:148:MET:O	1:A:152:ILE:CD1	0.54	2.55	5	3
1:A:143:LEU:CD1	1:A:146:GLU:CD	0.54	2.81	15	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:44:PHE:CE2	1:A:144:LEU:HD22	0.54	2.38	7	1
1:A:68:ALA:HB2	1:A:83:TRP:CZ3	0.54	2.37	7	1
1:A:32:ALA:H	1:A:155:LEU:HD13	0.54	1.62	20	6
1:A:144:LEU:O	1:A:147:ALA:CB	0.54	2.55	10	7
1:A:83:TRP:N	1:A:83:TRP:CD1	0.54	2.75	7	3
1:A:123:LEU:O	1:A:124:ALA:CB	0.54	2.55	11	14
1:A:40:LEU:HD12	1:A:150:ILE:HD11	0.54	1.76	20	2
1:A:152:ILE:N	1:A:152:ILE:HD12	0.54	2.17	14	8
1:A:82:GLU:O	1:A:83:TRP:CD1	0.54	2.61	9	6
1:A:89:TRP:N	1:A:89:TRP:CD1	0.54	2.75	3	6
1:A:135:LEU:HD21	1:A:139:GLU:CD	0.54	2.27	2	10
1:A:97:VAL:O	1:A:99:TYR:CE2	0.54	2.61	5	2
1:A:40:LEU:HD22	1:A:150:ILE:HD11	0.54	1.79	17	1
1:A:123:LEU:HD23	1:A:124:ALA:N	0.54	2.17	16	6
1:A:47:VAL:CG1	1:A:56:CYS:SG	0.54	2.96	17	11
1:A:93:SER:CB	1:A:99:TYR:HH	0.54	2.15	10	1
1:A:64:LEU:C	1:A:83:TRP:CD1	0.54	2.86	11	1
1:A:72:ASN:O	1:A:77:LEU:CA	0.54	2.56	16	5
1:A:43:LEU:C	1:A:43:LEU:HD12	0.54	2.28	7	1
1:A:152:ILE:CG1	1:A:153:SER:N	0.53	2.71	8	1
1:A:67:GLU:O	1:A:67:GLU:CG	0.53	2.55	12	1
1:A:99:TYR:OH	1:A:129:ASP:OD2	0.53	2.26	18	1
1:A:68:ALA:N	1:A:83:TRP:NE1	0.53	2.55	20	1
1:A:79:PHE:CE1	1:A:156:LYS:NZ	0.53	2.76	2	1
1:A:124:ALA:O	1:A:125:LYS:C	0.53	2.52	11	1
1:A:39:LYS:O	1:A:43:LEU:HD13	0.53	2.02	8	4
1:A:81:TYR:CE2	1:A:108:LEU:O	0.53	2.62	5	3
1:A:31:ASP:OD2	1:A:31:ASP:O	0.53	2.26	3	3
1:A:119:ILE:HD13	1:A:141:VAL:HG11	0.53	1.80	2	2
1:A:99:TYR:CD2	1:A:129:ASP:CG	0.53	2.86	5	3
1:A:77:LEU:HD23	1:A:156:LYS:HD2	0.53	1.78	17	4
1:A:70:ILE:HD13	1:A:155:LEU:HD21	0.53	1.79	7	1
1:A:64:LEU:H	1:A:64:LEU:HD12	0.53	1.64	15	1
1:A:131:ASN:O	1:A:134:ALA:HB3	0.53	2.04	3	2
1:A:118:GLU:OE1	1:A:118:GLU:N	0.53	2.40	20	1
1:A:56:CYS:SG	1:A:136:MET:CE	0.53	2.96	7	6
1:A:63:LYS:HG2	1:A:64:LEU:N	0.53	2.18	11	16
1:A:127:GLU:O	1:A:129:ASP:N	0.53	2.42	4	1
1:A:69:SER:O	1:A:80:PHE:O	0.53	2.27	7	4
1:A:31:ASP:O	1:A:31:ASP:OD1	0.53	2.27	13	9
1:A:45:LEU:HA	1:A:58:VAL:HG21	0.53	1.81	13	14

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:150:ILE:O	1:A:154:THR:N	0.53	2.42	4	18
1:A:89:TRP:CZ3	1:A:136:MET:HE2	0.53	2.39	2	2
1:A:35:TRP:CZ2	1:A:158:GLU:OE1	0.53	2.62	9	1
1:A:35:TRP:HE1	1:A:158:GLU:CD	0.53	2.12	3	3
1:A:150:ILE:HD12	1:A:150:ILE:C	0.53	2.29	20	17
1:A:55:LYS:HZ2	1:A:92:THR:CB	0.53	2.17	10	1
1:A:108:LEU:HD12	1:A:118:GLU:OE1	0.53	2.04	20	1
1:A:87:LEU:N	1:A:87:LEU:CD2	0.52	2.71	20	5
1:A:83:TRP:HE1	1:A:85:VAL:CG1	0.52	2.17	14	1
1:A:133:VAL:O	1:A:137:LYS:CE	0.52	2.56	14	1
1:A:81:TYR:N	1:A:109:SER:OG	0.52	2.41	1	2
1:A:70:ILE:HD12	1:A:77:LEU:CD2	0.52	2.27	8	1
1:A:117:VAL:HG12	1:A:118:GLU:N	0.52	2.19	15	5
1:A:77:LEU:HD22	1:A:77:LEU:O	0.52	2.04	13	1
1:A:125:LYS:HE3	1:A:133:VAL:HG11	0.52	1.81	3	2
1:A:43:LEU:HD23	1:A:146:GLU:CD	0.52	2.29	4	4
1:A:104:GLU:O	1:A:120:SER:CB	0.52	2.58	18	3
1:A:70:ILE:HD11	1:A:159:PHE:CG	0.52	2.40	18	1
1:A:152:ILE:HG13	1:A:156:LYS:HZ3	0.52	1.65	2	1
1:A:99:TYR:OH	1:A:129:ASP:OD1	0.52	2.27	14	2
1:A:64:LEU:HD12	1:A:85:VAL:HG11	0.52	1.81	13	1
1:A:89:TRP:CZ3	1:A:136:MET:HE3	0.52	2.39	18	1
1:A:52:GLU:O	1:A:92:THR:O	0.52	2.27	19	7
1:A:64:LEU:HA	1:A:85:VAL:HG12	0.52	1.82	17	4
1:A:65:ASP:N	1:A:83:TRP:CD1	0.52	2.77	11	1
1:A:121:VAL:CG1	1:A:137:LYS:NZ	0.52	2.67	14	1
1:A:122:SER:O	1:A:125:LYS:NZ	0.52	2.43	4	1
1:A:73:ARG:CB	1:A:77:LEU:HD13	0.52	2.34	11	3
1:A:138:GLU:CD	1:A:138:GLU:O	0.52	2.53	17	2
1:A:44:PHE:CB	1:A:61:VAL:HG11	0.52	2.34	2	2
1:A:110:ASP:OD2	1:A:151:TYR:CD2	0.52	2.62	4	2
1:A:31:ASP:OD1	1:A:68:ALA:O	0.52	2.28	13	5
1:A:40:LEU:HD21	1:A:151:TYR:CE1	0.52	2.40	7	1
1:A:43:LEU:HD22	1:A:146:GLU:CD	0.52	2.29	12	1
1:A:93:SER:CB	1:A:129:ASP:OD2	0.52	2.57	18	1
1:A:66:GLY:C	1:A:83:TRP:CD2	0.52	2.87	20	1
1:A:85:VAL:HG22	1:A:105:ILE:HG12	0.52	1.82	18	8
1:A:123:LEU:HD23	1:A:123:LEU:C	0.51	2.30	16	2
1:A:57:GLU:N	1:A:90:THR:O	0.51	2.43	11	4
1:A:55:LYS:HZ3	1:A:91:GLY:HA2	0.51	1.64	14	1
1:A:45:LEU:HA	1:A:58:VAL:HG11	0.51	1.82	19	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:116:GLU:O	1:A:116:GLU:CD	0.51	2.53	16	3
1:A:76:LYS:H	1:A:77:LEU:CD2	0.51	2.18	16	2
1:A:68:ALA:HB2	1:A:83:TRP:CE3	0.51	2.40	7	1
1:A:138:GLU:CD	1:A:138:GLU:C	0.51	2.78	12	2
1:A:123:LEU:C	1:A:123:LEU:CD1	0.51	2.84	14	1
1:A:29:GLU:O	1:A:70:ILE:O	0.51	2.29	5	14
1:A:74:LYS:N	1:A:160:THR:OG1	0.51	2.43	4	7
1:A:115:ASP:OD1	1:A:115:ASP:C	0.51	2.54	9	1
1:A:105:ILE:O	1:A:105:ILE:CG1	0.51	2.58	19	2
1:A:32:ALA:CB	1:A:35:TRP:CD1	0.51	2.94	15	3
1:A:72:ASN:O	1:A:76:LYS:O	0.51	2.29	6	9
1:A:59:THR:OG1	1:A:88:ASN:CG	0.51	2.54	14	1
1:A:70:ILE:HG22	1:A:79:PHE:HA	0.51	1.83	9	7
1:A:88:ASN:OD1	1:A:101:GLY:O	0.51	2.29	16	4
1:A:52:GLU:N	1:A:52:GLU:CD	0.51	2.69	9	1
1:A:64:LEU:CD2	1:A:64:LEU:H	0.51	2.18	17	1
1:A:51:ASN:OD1	1:A:52:GLU:N	0.51	2.43	19	1
1:A:150:ILE:HD12	1:A:151:TYR:CA	0.51	2.35	19	15
1:A:31:ASP:OD1	1:A:68:ALA:HB1	0.51	2.06	20	2
1:A:48:GLN:HE21	1:A:50:GLN:HE22	0.51	1.48	12	1
1:A:33:SER:O	1:A:36:SER:OG	0.51	2.28	14	1
1:A:117:VAL:O	1:A:119:ILE:CD1	0.51	2.59	4	2
1:A:65:ASP:O	1:A:84:SER:O	0.50	2.29	8	6
1:A:68:ALA:HB2	1:A:83:TRP:CD1	0.50	2.41	19	1
1:A:103:VAL:CG2	1:A:103:VAL:O	0.50	2.59	2	1
1:A:50:GLN:OE1	1:A:139:GLU:OE1	0.50	2.29	1	2
1:A:79:PHE:O	1:A:110:ASP:OD1	0.50	2.30	20	1
1:A:103:VAL:O	1:A:103:VAL:HG23	0.50	2.06	2	1
1:A:123:LEU:O	1:A:133:VAL:HG23	0.50	2.06	14	3
1:A:123:LEU:C	1:A:125:LYS:H	0.50	2.14	4	2
1:A:83:TRP:CH2	1:A:151:TYR:OH	0.50	2.58	15	1
1:A:36:SER:O	1:A:37:THR:C	0.50	2.54	14	5
1:A:64:LEU:O	1:A:64:LEU:CG	0.50	2.60	6	2
1:A:29:GLU:OE1	1:A:73:ARG:NH2	0.50	2.45	11	1
1:A:73:ARG:CA	1:A:77:LEU:HD12	0.50	2.37	13	1
1:A:64:LEU:HD12	1:A:64:LEU:C	0.50	2.31	2	2
1:A:48:GLN:O	1:A:56:CYS:O	0.50	2.29	18	4
1:A:81:TYR:O	1:A:109:SER:OG	0.50	2.29	3	6
1:A:87:LEU:O	1:A:88:ASN:OD1	0.50	2.30	19	4
1:A:117:VAL:HG13	1:A:118:GLU:N	0.50	2.21	8	3
1:A:117:VAL:CG1	1:A:118:GLU:N	0.50	2.74	15	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:129:ASP:O	1:A:130:THR:C	0.50	2.54	14	13
1:A:140:GLY:O	1:A:141:VAL:C	0.50	2.55	14	9
1:A:57:GLU:O	1:A:90:THR:N	0.50	2.45	6	10
1:A:135:LEU:HD21	1:A:139:GLU:OE2	0.50	2.06	8	5
1:A:127:GLU:C	1:A:129:ASP:H	0.50	2.15	4	1
1:A:80:PHE:CE1	1:A:111:GLU:OE1	0.50	2.64	16	1
1:A:99:TYR:CD1	1:A:99:TYR:O	0.49	2.65	3	1
1:A:116:GLU:CD	1:A:116:GLU:C	0.49	2.79	3	3
1:A:31:ASP:OD1	1:A:31:ASP:C	0.49	2.54	7	4
1:A:29:GLU:OE1	1:A:72:ASN:OD1	0.49	2.30	16	1
1:A:81:TYR:CB	1:A:83:TRP:NE1	0.49	2.75	10	2
1:A:130:THR:O	1:A:131:ASN:C	0.49	2.54	14	3
1:A:40:LEU:HD22	1:A:64:LEU:HD23	0.49	1.84	6	1
1:A:100:LYS:HZ2	1:A:100:LYS:N	0.49	2.00	15	2
1:A:126:ASP:CG	1:A:127:GLU:OE2	0.49	2.55	15	1
1:A:72:ASN:O	1:A:77:LEU:HA	0.49	2.07	10	14
1:A:98:GLN:C	1:A:100:LYS:NZ	0.49	2.66	3	1
1:A:71:ASN:OD1	1:A:76:LYS:O	0.49	2.30	4	1
1:A:39:LYS:O	1:A:43:LEU:N	0.49	2.42	10	3
1:A:79:PHE:O	1:A:110:ASP:OD2	0.49	2.30	11	1
1:A:125:LYS:HZ2	1:A:126:ASP:CG	0.49	2.15	14	1
1:A:104:GLU:O	1:A:120:SER:N	0.49	2.45	18	1
1:A:81:TYR:CE2	1:A:151:TYR:CD1	0.49	3.00	4	1
1:A:71:ASN:O	1:A:72:ASN:C	0.49	2.55	1	19
1:A:31:ASP:OD2	1:A:68:ALA:O	0.49	2.31	6	5
1:A:50:GLN:OE1	1:A:139:GLU:CD	0.49	2.55	6	1
1:A:77:LEU:N	1:A:77:LEU:CD2	0.49	2.59	16	1
1:A:134:ALA:O	1:A:137:LYS:CB	0.49	2.60	15	10
1:A:34:ASN:O	1:A:38:ASP:CG	0.49	2.56	5	2
1:A:81:TYR:CE2	1:A:83:TRP:N	0.49	2.81	13	3
1:A:68:ALA:N	1:A:83:TRP:CE3	0.49	2.81	11	1
1:A:54:GLY:CA	1:A:135:LEU:CD2	0.49	2.90	14	1
1:A:30:ARG:NH1	1:A:33:SER:OG	0.49	2.45	15	1
1:A:89:TRP:CE3	1:A:136:MET:HE2	0.49	2.42	10	2
1:A:126:ASP:C	1:A:127:GLU:OE1	0.49	2.56	12	3
1:A:37:THR:O	1:A:41:LYS:CG	0.49	2.61	20	3
1:A:153:SER:O	1:A:157:THR:OG1	0.49	2.29	13	2
1:A:31:ASP:O	1:A:31:ASP:OD2	0.49	2.31	11	2
1:A:46:ALA:O	1:A:47:VAL:C	0.49	2.56	12	16
1:A:134:ALA:O	1:A:137:LYS:CE	0.49	2.61	11	6
1:A:31:ASP:OD1	1:A:31:ASP:O	0.49	2.30	9	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:126:ASP:O	1:A:127:GLU:OE1	0.49	2.30	7	2
1:A:99:TYR:OH	1:A:132:LEU:HD11	0.49	2.08	11	1
1:A:125:LYS:N	1:A:125:LYS:CE	0.49	2.75	11	1
1:A:49:VAL:O	1:A:50:GLN:NE2	0.49	2.46	14	1
1:A:157:THR:O	1:A:161:GLN:CA	0.49	2.61	8	3
1:A:126:ASP:C	1:A:127:GLU:CD	0.49	2.81	9	4
1:A:66:GLY:H	1:A:83:TRP:NE1	0.49	2.01	11	1
1:A:126:ASP:O	1:A:127:GLU:CD	0.48	2.56	12	1
1:A:55:LYS:CE	1:A:55:LYS:C	0.48	2.86	14	1
1:A:126:ASP:C	1:A:127:GLU:OE2	0.48	2.56	15	2
1:A:105:ILE:O	1:A:105:ILE:CD1	0.48	2.61	13	1
1:A:157:THR:CG2	1:A:158:GLU:N	0.48	2.76	16	6
1:A:31:ASP:OD2	1:A:68:ALA:C	0.48	2.56	20	3
1:A:31:ASP:CG	1:A:68:ALA:HB3	0.48	2.33	8	1
1:A:30:ARG:NH2	1:A:33:SER:OG	0.48	2.45	15	1
1:A:142:LYS:O	1:A:143:LEU:C	0.48	2.56	10	17
1:A:40:LEU:HD13	1:A:64:LEU:HD21	0.48	1.85	15	1
1:A:113:SER:OG	1:A:116:GLU:OE2	0.48	2.31	10	1
1:A:99:TYR:CD2	1:A:99:TYR:O	0.48	2.66	11	1
1:A:139:GLU:O	1:A:143:LEU:N	0.48	2.46	15	4
1:A:55:LYS:HD3	1:A:92:THR:H	0.48	1.66	14	1
1:A:93:SER:CA	1:A:99:TYR:OH	0.48	2.61	17	1
1:A:32:ALA:HB2	1:A:159:PHE:CE2	0.48	2.44	7	1
1:A:115:ASP:O	1:A:115:ASP:OD1	0.48	2.31	13	2
1:A:137:LYS:N	1:A:137:LYS:HE2	0.48	2.23	14	1
1:A:99:TYR:CE2	1:A:129:ASP:OD1	0.48	2.66	15	2
1:A:93:SER:OG	1:A:129:ASP:OD2	0.48	2.30	18	1
1:A:156:LYS:O	1:A:160:THR:HG22	0.48	2.08	15	2
1:A:157:THR:OG1	1:A:162:GLY:OXT	0.48	2.31	10	1
1:A:39:LYS:NZ	1:A:154:THR:OG1	0.48	2.36	16	2
1:A:50:GLN:NE2	1:A:139:GLU:CD	0.48	2.72	7	1
1:A:83:TRP:CD1	1:A:83:TRP:H	0.48	2.26	7	1
1:A:54:GLY:CA	1:A:135:LEU:HD22	0.48	2.38	2	1
1:A:99:TYR:CZ	1:A:129:ASP:OD2	0.48	2.67	4	1
1:A:132:LEU:O	1:A:133:VAL:C	0.48	2.55	5	1
1:A:124:ALA:HB1	1:A:130:THR:N	0.48	2.23	11	2
1:A:68:ALA:HB1	1:A:81:TYR:CD2	0.48	2.44	14	2
1:A:125:LYS:HD3	1:A:125:LYS:H	0.48	1.69	18	2
1:A:135:LEU:O	1:A:139:GLU:N	0.47	2.47	3	4
1:A:64:LEU:HD12	1:A:85:VAL:CG1	0.47	2.39	13	1
1:A:60:GLU:O	1:A:88:ASN:OD1	0.47	2.32	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:29:GLU:OE2	1:A:71:ASN:C	0.47	2.56	16	1
1:A:108:LEU:CB	1:A:117:VAL:HG13	0.47	2.39	5	2
1:A:126:ASP:OD1	1:A:126:ASP:O	0.47	2.32	6	1
1:A:39:LYS:O	1:A:42:THR:OG1	0.47	2.30	10	1
1:A:63:LYS:C	1:A:63:LYS:CD	0.47	2.87	19	2
1:A:59:THR:CG2	1:A:89:TRP:C	0.47	2.87	2	2
1:A:35:TRP:CZ2	1:A:158:GLU:OE2	0.47	2.67	4	2
1:A:81:TYR:CB	1:A:83:TRP:HE1	0.47	2.23	1	1
1:A:79:PHE:CE2	1:A:152:ILE:HD11	0.47	2.45	2	1
1:A:99:TYR:CZ	1:A:132:LEU:CD2	0.47	2.97	3	2
1:A:99:TYR:N	1:A:100:LYS:NZ	0.47	2.62	3	1
1:A:135:LEU:C	1:A:137:LYS:N	0.47	2.70	15	3
1:A:73:ARG:CA	1:A:77:LEU:HD22	0.47	2.39	4	2
1:A:64:LEU:HD13	1:A:151:TYR:OH	0.47	2.10	7	1
1:A:44:PHE:CB	1:A:61:VAL:HG21	0.47	2.39	20	2
1:A:76:LYS:H	1:A:77:LEU:CD1	0.47	2.21	13	1
1:A:55:LYS:CD	1:A:92:THR:H	0.47	2.22	14	1
1:A:29:GLU:N	1:A:29:GLU:CD	0.47	2.72	16	1
1:A:62:SER:OG	1:A:86:LYS:O	0.47	2.31	5	2
1:A:42:THR:O	1:A:46:ALA:N	0.47	2.48	18	1
1:A:55:LYS:O	1:A:99:TYR:OH	0.47	2.30	3	1
1:A:138:GLU:O	1:A:142:LYS:CD	0.47	2.63	16	5
1:A:73:ARG:H	1:A:73:ARG:CD	0.47	2.23	9	1
1:A:37:THR:O	1:A:41:LYS:CB	0.47	2.63	11	2
1:A:73:ARG:CG	1:A:77:LEU:HD13	0.47	2.40	11	1
1:A:83:TRP:CH2	1:A:110:ASP:OD1	0.47	2.68	14	1
1:A:53:GLU:O	1:A:53:GLU:CD	0.46	2.58	2	1
1:A:64:LEU:H	1:A:64:LEU:CD1	0.46	2.21	15	1
1:A:81:TYR:CZ	1:A:110:ASP:OD2	0.46	2.67	7	1
1:A:155:LEU:HD22	1:A:156:LYS:NZ	0.46	2.26	7	1
1:A:103:VAL:HG22	1:A:103:VAL:O	0.46	2.10	15	2
1:A:123:LEU:HD23	1:A:124:ALA:CB	0.46	2.41	4	1
1:A:100:LYS:CE	1:A:100:LYS:N	0.46	2.79	9	6
1:A:36:SER:O	1:A:40:LEU:CG	0.46	2.63	12	2
1:A:31:ASP:C	1:A:31:ASP:OD1	0.46	2.55	17	1
1:A:36:SER:C	1:A:40:LEU:HD12	0.46	2.35	8	3
1:A:101:GLY:CA	1:A:122:SER:O	0.46	2.63	11	17
1:A:32:ALA:O	1:A:36:SER:OG	0.46	2.31	7	1
1:A:37:THR:O	1:A:41:LYS:HB3	0.46	2.10	20	4
1:A:91:GLY:C	1:A:99:TYR:CZ	0.46	2.94	16	2
1:A:55:LYS:HE2	1:A:92:THR:H	0.46	1.70	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:90:THR:HG23	1:A:100:LYS:CG	0.46	2.40	3	1
1:A:43:LEU:HD23	1:A:146:GLU:CG	0.46	2.40	8	5
1:A:39:LYS:O	1:A:40:LEU:C	0.46	2.59	14	4
1:A:155:LEU:CD2	1:A:155:LEU:C	0.46	2.88	18	2
1:A:65:ASP:CA	1:A:83:TRP:NE1	0.46	2.78	11	1
1:A:146:GLU:O	1:A:149:GLY:N	0.46	2.49	19	2
1:A:36:SER:OG	1:A:40:LEU:CD1	0.46	2.63	1	1
1:A:40:LEU:HD11	1:A:150:ILE:HD11	0.46	1.87	19	3
1:A:40:LEU:O	1:A:44:PHE:N	0.46	2.49	19	3
1:A:73:ARG:CD	1:A:73:ARG:N	0.45	2.79	6	2
1:A:51:ASN:C	1:A:53:GLU:N	0.45	2.72	18	9
1:A:73:ARG:HB3	1:A:77:LEU:HD13	0.45	1.88	6	5
1:A:73:ARG:CD	1:A:73:ARG:H	0.45	2.24	6	1
1:A:35:TRP:CD1	1:A:158:GLU:OE2	0.45	2.69	9	1
1:A:93:SER:OG	1:A:99:TYR:OH	0.45	2.27	10	1
1:A:69:SER:OG	1:A:80:PHE:CE1	0.45	2.66	17	1
1:A:62:SER:CB	1:A:86:LYS:O	0.45	2.64	1	2
1:A:144:LEU:O	1:A:145:ARG:C	0.45	2.59	20	7
1:A:50:GLN:H	1:A:55:LYS:HA	0.45	1.71	14	2
1:A:130:THR:O	1:A:133:VAL:CG1	0.45	2.64	5	2
1:A:138:GLU:O	1:A:142:LYS:CB	0.45	2.65	6	3
1:A:81:TYR:CE2	1:A:110:ASP:OD2	0.45	2.70	7	1
1:A:126:ASP:CB	1:A:127:GLU:OE2	0.45	2.64	9	1
1:A:42:THR:OG1	1:A:43:LEU:N	0.45	2.49	10	1
1:A:55:LYS:HZ2	1:A:136:MET:CE	0.45	2.24	14	1
1:A:64:LEU:CB	1:A:83:TRP:CE3	0.45	3.00	1	2
1:A:134:ALA:O	1:A:137:LYS:CG	0.45	2.65	7	9
1:A:31:ASP:O	1:A:31:ASP:CG	0.45	2.59	6	5
1:A:161:GLN:O	1:A:162:GLY:C	0.45	2.58	6	4
1:A:45:LEU:HD21	1:A:61:VAL:H	0.45	1.71	11	2
1:A:138:GLU:O	1:A:142:LYS:HD3	0.45	2.12	4	10
1:A:151:TYR:O	1:A:155:LEU:CB	0.45	2.64	11	3
1:A:40:LEU:HD13	1:A:150:ILE:HD11	0.45	1.86	20	1
1:A:55:LYS:NZ	1:A:92:THR:CB	0.45	2.79	10	1
1:A:99:TYR:OH	1:A:132:LEU:CD1	0.45	2.65	11	1
1:A:55:LYS:C	1:A:55:LYS:CD	0.45	2.90	14	1
1:A:64:LEU:HD22	1:A:83:TRP:CZ2	0.45	2.46	15	1
1:A:113:SER:HG	1:A:116:GLU:CD	0.45	2.20	10	1
1:A:53:GLU:CG	1:A:54:GLY:N	0.45	2.80	16	2
1:A:79:PHE:CB	1:A:81:TYR:OH	0.45	2.65	10	2
1:A:132:LEU:O	1:A:135:LEU:N	0.45	2.50	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:143:LEU:CD1	1:A:146:GLU:OE1	0.45	2.65	5	1
1:A:112:ASN:CB	1:A:116:GLU:OE1	0.45	2.65	12	1
1:A:40:LEU:HD11	1:A:151:TYR:CE2	0.45	2.47	15	1
1:A:152:ILE:O	1:A:156:LYS:HG2	0.44	2.12	7	1
1:A:151:TYR:CE2	1:A:155:LEU:HD12	0.44	2.47	9	1
1:A:157:THR:OG1	1:A:162:GLY:C	0.44	2.60	10	1
1:A:32:ALA:O	1:A:155:LEU:CD2	0.44	2.64	11	1
1:A:134:ALA:O	1:A:137:LYS:N	0.44	2.50	18	4
1:A:45:LEU:CA	1:A:58:VAL:HG11	0.44	2.41	17	6
1:A:36:SER:O	1:A:40:LEU:CD1	0.44	2.66	9	4
1:A:99:TYR:OH	1:A:129:ASP:CB	0.44	2.65	14	1
1:A:123:LEU:HD23	1:A:124:ALA:HB2	0.44	1.88	4	1
1:A:135:LEU:HD12	1:A:138:GLU:OE2	0.44	2.11	7	1
1:A:55:LYS:NZ	1:A:91:GLY:HA2	0.44	2.28	14	1
1:A:30:ARG:HH12	1:A:33:SER:CB	0.44	2.25	15	1
1:A:66:GLY:CA	1:A:83:TRP:CD2	0.44	3.00	20	1
1:A:157:THR:O	1:A:161:GLN:N	0.44	2.50	4	2
1:A:149:GLY:O	1:A:153:SER:OG	0.44	2.34	10	2
1:A:93:SER:C	1:A:95:SER:N	0.44	2.75	17	3
1:A:143:LEU:HD12	1:A:146:GLU:OE2	0.44	2.11	12	1
1:A:75:GLY:H	1:A:77:LEU:CD1	0.44	2.21	13	1
1:A:89:TRP:CD1	1:A:89:TRP:H	0.44	2.29	11	3
1:A:32:ALA:N	1:A:155:LEU:HD13	0.44	2.27	4	2
1:A:56:CYS:SG	1:A:136:MET:CG	0.44	3.04	5	1
1:A:40:LEU:HD13	1:A:64:LEU:CD1	0.44	2.41	8	1
1:A:65:ASP:N	1:A:83:TRP:NE1	0.44	2.65	11	1
1:A:88:ASN:OD1	1:A:88:ASN:O	0.44	2.36	1	1
1:A:85:VAL:HG12	1:A:105:ILE:HG12	0.44	1.89	1	1
1:A:89:TRP:C	1:A:89:TRP:CD1	0.44	2.94	2	1
1:A:81:TYR:O	1:A:109:SER:CB	0.44	2.66	18	2
1:A:66:GLY:CA	1:A:83:TRP:CB	0.44	2.95	5	8
1:A:126:ASP:CB	1:A:127:GLU:OE1	0.44	2.65	10	1
1:A:135:LEU:CD2	1:A:139:GLU:OE2	0.44	2.66	8	1
1:A:104:GLU:O	1:A:120:SER:OG	0.44	2.30	9	1
1:A:63:LYS:C	1:A:85:VAL:HG23	0.43	2.38	1	1
1:A:133:VAL:O	1:A:134:ALA:C	0.43	2.61	5	1
1:A:148:MET:O	1:A:152:ILE:HD13	0.43	2.12	11	1
1:A:125:LYS:CE	1:A:126:ASP:H	0.43	2.25	4	1
1:A:37:THR:O	1:A:41:LYS:N	0.43	2.47	7	1
1:A:56:CYS:SG	1:A:136:MET:HE2	0.43	2.52	15	2
1:A:31:ASP:OD1	1:A:151:TYR:OH	0.43	2.35	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:32:ALA:H	1:A:155:LEU:HD21	0.43	1.72	19	3
1:A:55:LYS:O	1:A:55:LYS:CE	0.43	2.67	14	1
1:A:53:GLU:CD	1:A:53:GLU:C	0.43	2.86	2	1
1:A:101:GLY:N	1:A:123:LEU:HD23	0.43	2.28	14	1
1:A:143:LEU:CD1	1:A:146:GLU:OE2	0.43	2.67	15	1
1:A:125:LYS:NZ	1:A:133:VAL:HG11	0.43	2.28	20	1
1:A:152:ILE:HD12	1:A:152:ILE:N	0.43	2.27	17	1
1:A:135:LEU:CD2	1:A:139:GLU:OE1	0.43	2.67	20	1
1:A:31:ASP:CB	1:A:70:ILE:HG23	0.43	2.44	13	4
1:A:103:VAL:O	1:A:103:VAL:HG22	0.43	2.14	8	4
1:A:102:HIS:C	1:A:103:VAL:HG12	0.43	2.39	7	2
1:A:125:LYS:N	1:A:125:LYS:CD	0.43	2.81	11	1
1:A:132:LEU:HD23	1:A:133:VAL:N	0.43	2.28	12	1
1:A:59:THR:HG1	1:A:88:ASN:CG	0.43	2.22	14	1
1:A:68:ALA:CA	1:A:83:TRP:HE1	0.43	2.26	20	1
1:A:108:LEU:CD1	1:A:118:GLU:OE1	0.43	2.67	20	1
1:A:77:LEU:HD12	1:A:160:THR:HB	0.43	1.89	1	1
1:A:124:ALA:HB1	1:A:129:ASP:HB2	0.43	1.90	4	1
1:A:54:GLY:O	1:A:135:LEU:CD2	0.43	2.65	5	1
1:A:115:ASP:CB	1:A:141:VAL:O	0.43	2.67	20	1
1:A:100:LYS:HB2	1:A:100:LYS:HZ2	0.43	1.74	6	2
1:A:31:ASP:OD2	1:A:68:ALA:HB3	0.43	2.14	3	1
1:A:85:VAL:HG22	1:A:87:LEU:CD2	0.43	2.44	3	1
1:A:105:ILE:O	1:A:106:PRO:O	0.43	2.37	11	2
1:A:125:LYS:N	1:A:125:LYS:HE2	0.43	2.29	4	1
1:A:41:LYS:O	1:A:45:LEU:HD12	0.43	2.14	7	1
1:A:39:LYS:O	1:A:43:LEU:CD1	0.43	2.67	8	1
1:A:38:ASP:O	1:A:42:THR:CG2	0.43	2.66	10	1
1:A:70:ILE:CG2	1:A:156:LYS:HZ3	0.43	2.27	10	1
1:A:77:LEU:O	1:A:77:LEU:CD2	0.43	2.66	13	1
1:A:161:GLN:O	1:A:162:GLY:O	0.43	2.37	15	1
1:A:81:TYR:CD1	1:A:81:TYR:O	0.43	2.72	20	1
1:A:53:GLU:O	1:A:132:LEU:HD12	0.42	2.14	2	1
1:A:152:ILE:HG22	1:A:153:SER:N	0.42	2.29	4	1
1:A:90:THR:HG22	1:A:91:GLY:N	0.42	2.29	12	2
1:A:144:LEU:N	1:A:144:LEU:HD23	0.42	2.29	10	2
1:A:99:TYR:CZ	1:A:132:LEU:HD22	0.42	2.49	11	1
1:A:150:ILE:CG1	1:A:151:TYR:N	0.42	2.82	12	1
1:A:72:ASN:O	1:A:77:LEU:N	0.42	2.52	17	1
1:A:110:ASP:OD1	1:A:110:ASP:N	0.42	2.52	20	1
1:A:81:TYR:OH	1:A:83:TRP:O	0.42	2.34	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:63:LYS:O	1:A:63:LYS:CE	0.42	2.68	3	6
1:A:32:ALA:HB2	1:A:159:PHE:CE1	0.42	2.50	6	1
1:A:50:GLN:OE1	1:A:139:GLU:OE2	0.42	2.37	6	1
1:A:89:TRP:CH2	1:A:103:VAL:CG1	0.42	3.03	1	1
1:A:61:VAL:HG13	1:A:87:LEU:HD22	0.42	1.92	4	1
1:A:77:LEU:H	1:A:77:LEU:CD2	0.42	2.20	4	1
1:A:121:VAL:CG2	1:A:137:LYS:NZ	0.42	2.82	5	1
1:A:127:GLU:C	1:A:129:ASP:N	0.42	2.78	4	1
1:A:40:LEU:HD22	1:A:64:LEU:HD22	0.42	1.91	18	1
1:A:64:LEU:CD2	1:A:64:LEU:N	0.42	2.81	14	2
1:A:82:GLU:O	1:A:83:TRP:CB	0.42	2.67	9	6
1:A:81:TYR:CD1	1:A:81:TYR:N	0.42	2.86	18	3
1:A:55:LYS:O	1:A:136:MET:SD	0.42	2.78	6	1
1:A:124:ALA:HB1	1:A:130:THR:H	0.42	1.74	10	2
1:A:40:LEU:O	1:A:44:PHE:CB	0.42	2.68	10	1
1:A:59:THR:HG23	1:A:89:TRP:CA	0.42	2.44	15	1
1:A:126:ASP:O	1:A:126:ASP:OD2	0.42	2.36	18	2
1:A:40:LEU:HG	1:A:147:ALA:HB1	0.42	1.91	20	1
1:A:140:GLY:C	1:A:142:LYS:N	0.42	2.75	14	6
1:A:160:THR:HG23	1:A:162:GLY:N	0.42	2.30	17	2
1:A:29:GLU:OE2	1:A:29:GLU:N	0.42	2.53	16	1
1:A:71:ASN:CB	1:A:78:ILE:HD11	0.42	2.45	1	2
1:A:70:ILE:HD11	1:A:159:PHE:CD1	0.42	2.50	3	2
1:A:29:GLU:O	1:A:69:SER:OG	0.42	2.31	5	1
1:A:83:TRP:O	1:A:106:PRO:C	0.42	2.63	6	1
1:A:105:ILE:CG2	1:A:119:ILE:HG23	0.42	2.42	14	1
1:A:81:TYR:N	1:A:81:TYR:CD1	0.42	2.85	1	1
1:A:135:LEU:CD2	1:A:139:GLU:CD	0.42	2.93	3	1
1:A:83:TRP:O	1:A:83:TRP:CE3	0.42	2.73	18	2
1:A:115:ASP:O	1:A:115:ASP:OD2	0.42	2.38	10	1
1:A:35:TRP:N	1:A:35:TRP:CE3	0.42	2.88	15	1
1:A:63:LYS:CE	1:A:63:LYS:C	0.41	2.93	3	1
1:A:77:LEU:HD23	1:A:78:ILE:N	0.41	2.30	10	1
1:A:136:MET:O	1:A:140:GLY:CA	0.41	2.69	9	1
1:A:89:TRP:CD1	1:A:89:TRP:C	0.41	2.94	6	2
1:A:79:PHE:O	1:A:111:GLU:CB	0.41	2.68	10	1
1:A:150:ILE:O	1:A:151:TYR:C	0.41	2.61	17	1
1:A:56:CYS:C	1:A:57:GLU:CG	0.41	2.93	18	1
1:A:40:LEU:CD2	1:A:40:LEU:N	0.41	2.84	3	1
1:A:68:ALA:CB	1:A:83:TRP:CZ3	0.41	3.04	7	1
1:A:112:ASN:OD1	1:A:113:SER:N	0.41	2.52	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:41:LYS:HG3	1:A:42:THR:N	0.41	2.31	14	2
1:A:51:ASN:O	1:A:55:LYS:N	0.41	2.54	14	1
1:A:63:LYS:CE	1:A:63:LYS:O	0.41	2.69	18	3
1:A:80:PHE:CD1	1:A:80:PHE:N	0.41	2.86	14	1
1:A:93:SER:CB	1:A:129:ASP:OD1	0.41	2.68	3	1
1:A:72:ASN:O	1:A:77:LEU:HB3	0.41	2.15	16	2
1:A:127:GLU:CD	1:A:127:GLU:N	0.41	2.79	9	1
1:A:132:LEU:C	1:A:132:LEU:HD23	0.41	2.41	20	1
1:A:35:TRP:CE3	1:A:35:TRP:N	0.41	2.89	8	1
1:A:64:LEU:CB	1:A:83:TRP:CD1	0.41	3.04	11	1
1:A:132:LEU:HD23	1:A:132:LEU:C	0.41	2.40	12	1
1:A:31:ASP:OD1	1:A:68:ALA:C	0.41	2.63	13	1
1:A:123:LEU:C	1:A:125:LYS:N	0.41	2.79	4	1
1:A:81:TYR:CE1	1:A:83:TRP:N	0.41	2.88	16	2
1:A:152:ILE:N	1:A:152:ILE:CD1	0.41	2.84	7	1
1:A:31:ASP:OD1	1:A:68:ALA:HB3	0.41	2.15	8	1
1:A:44:PHE:CD1	1:A:44:PHE:N	0.41	2.88	12	1
1:A:92:THR:O	1:A:99:TYR:OH	0.41	2.37	12	1
1:A:99:TYR:CZ	1:A:129:ASP:OD1	0.41	2.73	12	1
1:A:100:LYS:N	1:A:100:LYS:CE	0.41	2.84	16	1
1:A:31:ASP:HB2	1:A:155:LEU:HD11	0.41	1.92	18	1
1:A:88:ASN:OD1	1:A:88:ASN:C	0.41	2.63	1	1
1:A:42:THR:C	1:A:44:PHE:N	0.41	2.75	10	1
1:A:45:LEU:CD2	1:A:61:VAL:H	0.40	2.30	3	1
1:A:41:LYS:HG2	1:A:42:THR:N	0.40	2.31	11	2
1:A:73:ARG:H	1:A:73:ARG:HD3	0.40	1.75	9	1
1:A:125:LYS:HE3	1:A:125:LYS:N	0.40	2.31	14	1
1:A:132:LEU:CD2	1:A:136:MET:SD	0.40	3.09	2	1
1:A:99:TYR:CE1	1:A:132:LEU:HD21	0.40	2.51	3	1
1:A:65:ASP:N	1:A:83:TRP:HE1	0.40	2.14	11	1
1:A:148:MET:O	1:A:152:ILE:CG1	0.40	2.70	16	1
1:A:107:ASN:OD1	1:A:107:ASN:C	0.40	2.65	4	1
1:A:80:PHE:N	1:A:80:PHE:CD1	0.40	2.88	12	1
1:A:155:LEU:HD23	1:A:155:LEU:C	0.40	2.40	14	1
1:A:59:THR:HG23	1:A:89:TRP:HA	0.40	1.94	17	1
1:A:41:LYS:O	1:A:45:LEU:CD1	0.40	2.69	7	1
1:A:55:LYS:HD2	1:A:92:THR:H	0.40	1.77	7	1
1:A:42:THR:O	1:A:45:LEU:N	0.40	2.55	10	1
1:A:125:LYS:HG2	1:A:126:ASP:N	0.40	2.32	14	1
1:A:114:VAL:HG21	1:A:144:LEU:O	0.40	2.17	18	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	133/135 (99%)	111±2 (83±1%)	16±2 (12±2%)	6±1 (5±1%)	3	25
All	All	2660/2700 (99%)	2213 (83%)	321 (12%)	126 (5%)	3	25

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	63	LYS	20
1	A	72	ASN	20
1	A	106	PRO	20
1	A	130	THR	20
1	A	107	ASN	19
1	A	32	ALA	10
1	A	83	TRP	8
1	A	60	GLU	5
1	A	103	VAL	2
1	A	128	PRO	1
1	A	124	ALA	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	119/120 (99%)	90±3 (76±3%)	29±3 (24±3%)	2	26
All	All	2380/2400 (99%)	1807 (76%)	573 (24%)	2	26

All 66 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	37	THR	20
1	A	49	VAL	20
1	A	63	LYS	20
1	A	78	ILE	20
1	A	87	LEU	20
1	A	100	LYS	20
1	A	103	VAL	20
1	A	125	LYS	20
1	A	143	LEU	20
1	A	146	GLU	20
1	A	105	ILE	19
1	A	137	LYS	19
1	A	79	PHE	18
1	A	142	LYS	18
1	A	86	LYS	18
1	A	99	TYR	17
1	A	74	LYS	16
1	A	129	ASP	16
1	A	59	THR	15
1	A	64	LEU	13
1	A	155	LEU	12
1	A	31	ASP	11
1	A	35	TRP	11
1	A	55	LYS	10
1	A	117	VAL	10
1	A	81	TYR	10
1	A	148	MET	9
1	A	85	VAL	8
1	A	116	GLU	8
1	A	156	LYS	8
1	A	77	LEU	7
1	A	159	PHE	7
1	A	73	ARG	7
1	A	40	LEU	7
1	A	53	GLU	5
1	A	160	THR	5
1	A	121	VAL	5
1	A	135	LEU	5
1	A	89	TRP	4
1	A	119	ILE	4
1	A	139	GLU	4
1	A	157	THR	4
1	A	76	LYS	4

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Mol	Chain	Res	Type	Models (Total)
1	A	36	SER	3
1	A	127	GLU	3
1	A	130	THR	3
1	A	83	TRP	3
1	A	108	LEU	3
1	A	47	VAL	2
1	A	122	SER	2
1	A	113	SER	2
1	A	138	GLU	2
1	A	107	ASN	2
1	A	132	LEU	2
1	A	69	SER	1
1	A	94	LYS	1
1	A	133	VAL	1
1	A	136	MET	1
1	A	43	LEU	1
1	A	45	LEU	1
1	A	110	ASP	1
1	A	151	TYR	1
1	A	152	ILE	1
1	A	52	GLU	1
1	A	115	ASP	1
1	A	93	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 oligosaccharides in this entry.

6.6 Ligand geometry ⓘ

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

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

7.1 Chemical shift list 1

File name: `working_cs.cif`

Chemical shift list name: *starch_output*

7.1.1 Bookkeeping

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

Total number of shifts	1407
Number of shifts mapped to atoms	1407
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	132	-0.17 ± 0.11	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	124	0.10 ± 0.12	None needed (< 0.5 ppm)
$^{13}\text{C}'$	122	0.25 ± 0.15	None needed (< 0.5 ppm)
^{15}N	129	0.18 ± 0.32	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 78%, i.e. 1396 atoms were assigned a chemical shift out of a possible 1799. 0 out of 25 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	643/675 (95%)	263/275 (96%)	252/268 (94%)	128/132 (97%)
Sidechain	749/1014 (74%)	486/654 (74%)	263/326 (81%)	0/34 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	4/110 (4%)	2/54 (4%)	0/52 (0%)	2/4 (50%)
Overall	1396/1799 (78%)	751/983 (76%)	515/646 (80%)	130/170 (76%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 78%, i.e. 1406 atoms were assigned a chemical shift out of a possible 1810. 0 out of 25 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	647/680 (95%)	264/277 (95%)	254/270 (94%)	129/133 (97%)
Sidechain	755/1020 (74%)	490/658 (74%)	265/328 (81%)	0/34 (0%)
Aromatic	4/110 (4%)	2/54 (4%)	0/52 (0%)	2/4 (50%)
Overall	1406/1810 (78%)	756/989 (76%)	519/650 (80%)	131/171 (77%)

7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots [i](#)

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

Random coil index (RCI) for chain A:

