



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 08:25 PM UTC

PDB ID : 1QW1 / pdb_00001qw1
Title : Solution Structure of the C-Terminal Domain of DtxR residues 110-226
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Deposited on : 2003-08-29

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ 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

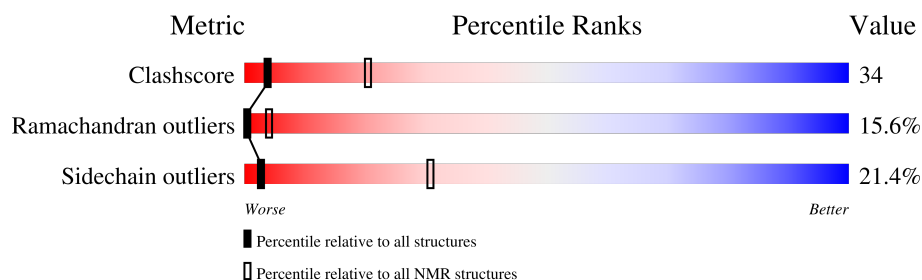
1 Overall quality at a glance

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	121	43% 42% 10% • •

2 Ensemble composition and analysis

This entry contains 14 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:111-A:226 (116)	1.86	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, 2, 3, 4, 5, 6, 9, 10, 11, 12, 13, 14
2	7, 8

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1874 atoms, of which 938 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Diphtheria toxin repressor.

Mol	Chain	Residues	Atoms						Trace
1	A	121	Total	C	H	N	O	S	0
			1874	577	938	168	189	2	

There are 4 discrepancies between the modelled and reference sequences:

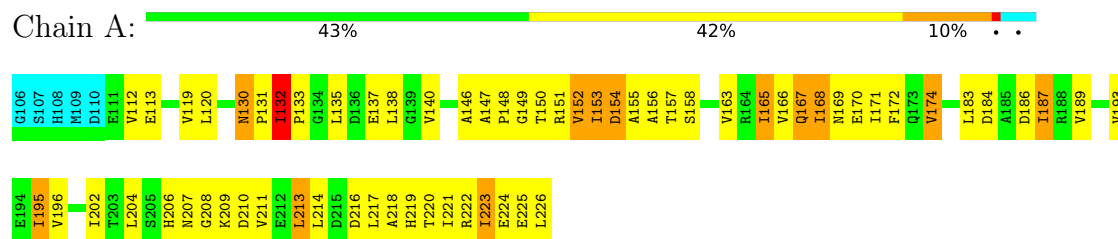
Chain	Residue	Modelled	Actual	Comment	Reference
A	106	GLY	-	cloning artifact	UNP P33120
A	107	SER	-	cloning artifact	UNP P33120
A	108	HIS	-	cloning artifact	UNP P33120
A	109	MET	-	cloning artifact	UNP P33120

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: Diphtheria toxin repressor

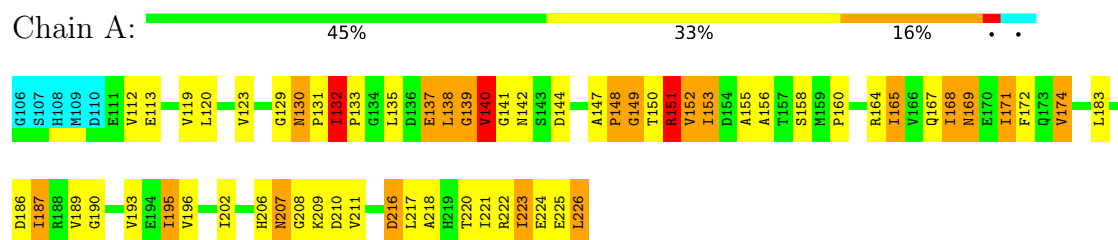


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

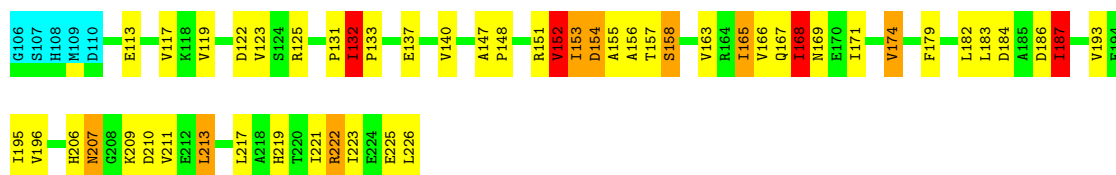
- Molecule 1: Diphtheria toxin repressor



4.2.2 Score per residue for model 2

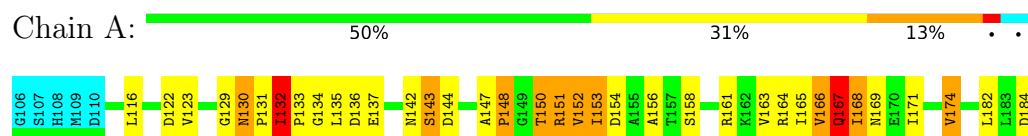
- Molecule 1: Diphtheria toxin repressor





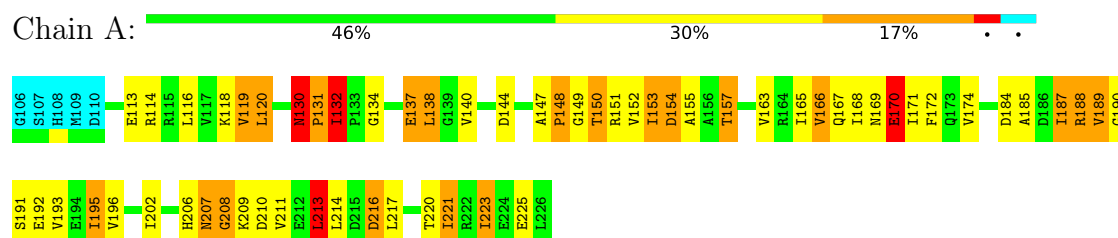
4.2.3 Score per residue for model 3

- Molecule 1: Diphtheria toxin repressor



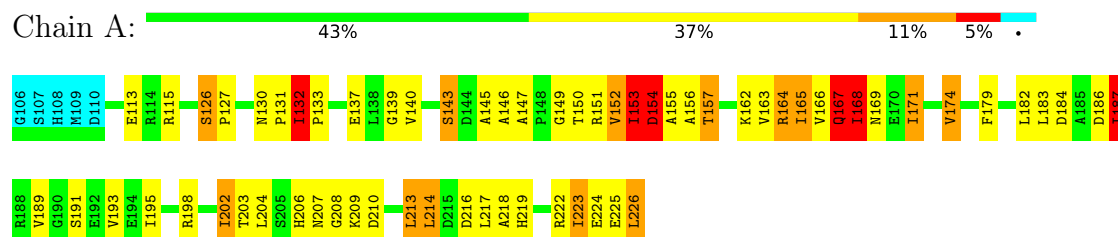
4.2.4 Score per residue for model 4

- Molecule 1: Diphtheria toxin repressor



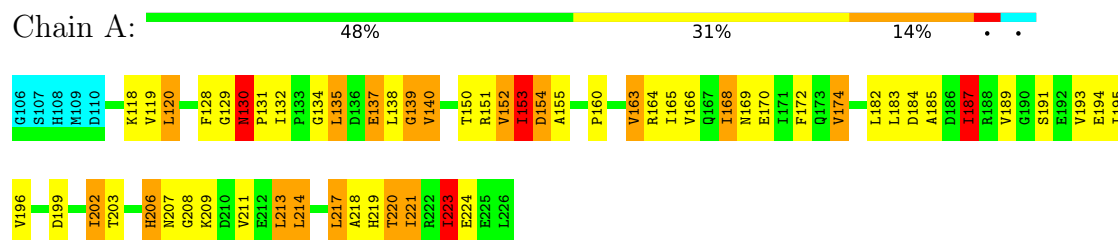
4.2.5 Score per residue for model 5

- Molecule 1: Diphtheria toxin repressor



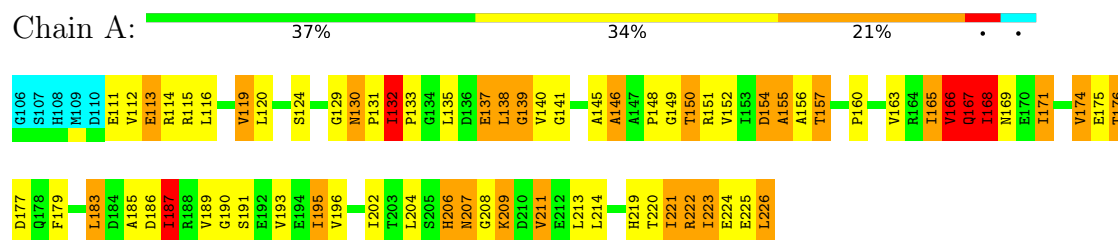
4.2.6 Score per residue for model 6

- Molecule 1: Diphtheria toxin repressor



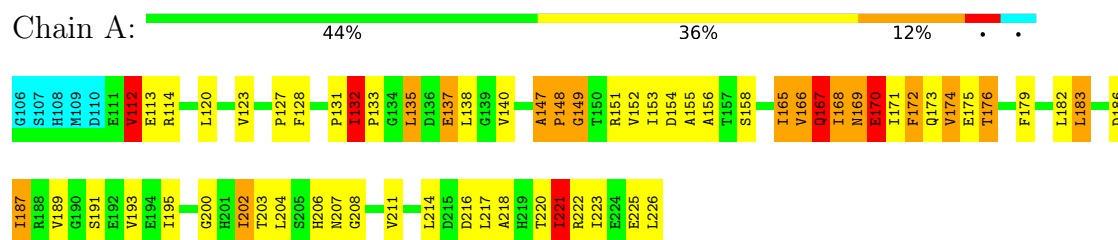
4.2.7 Score per residue for model 7

- Molecule 1: Diphtheria toxin repressor



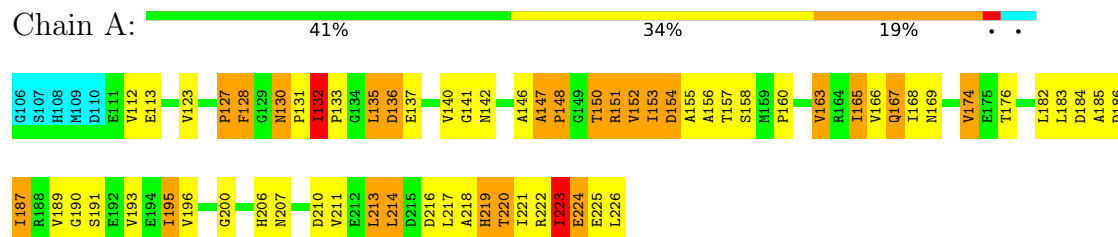
4.2.8 Score per residue for model 8

- Molecule 1: Diphtheria toxin repressor



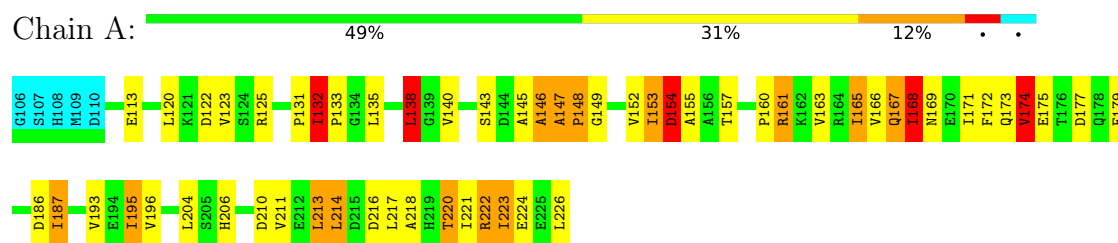
4.2.9 Score per residue for model 9

- Molecule 1: Diphtheria toxin repressor



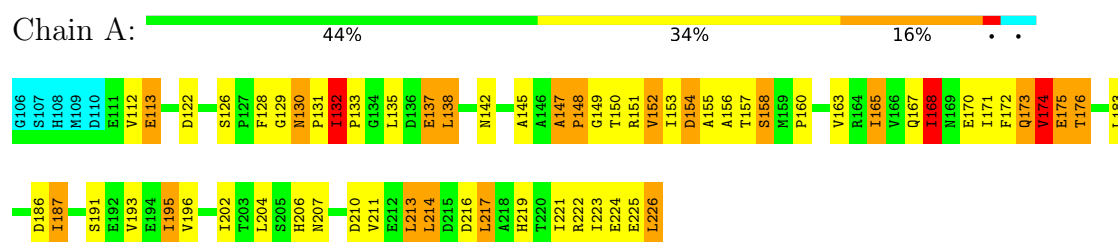
4.2.10 Score per residue for model 10

- Molecule 1: Diphtheria toxin repressor



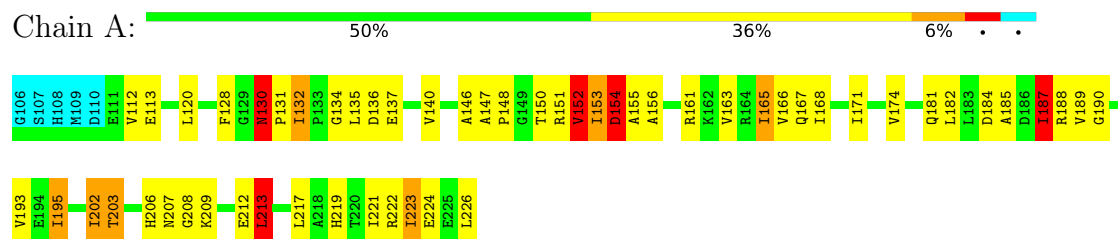
4.2.11 Score per residue for model 11

- Molecule 1: Diphtheria toxin repressor



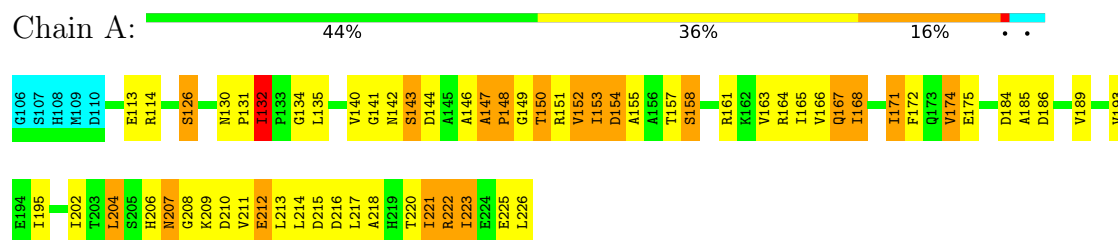
4.2.12 Score per residue for model 12

- Molecule 1: Diphtheria toxin repressor



4.2.13 Score per residue for model 13

- Molecule 1: Diphtheria toxin repressor



4.2.14 Score per residue for model 14

● Molecule 1: Diphtheria toxin repressor

Chain A:

46%

32%

13%



5 Refinement protocol and experimental data overview ⓘ

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

Of the 60 calculated structures, 14 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
CNS	refinement	1.0

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	900	907	904	62±12
All	All	12600	12698	12656	861

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:152:VAL:HG11	1:A:218:ALA:HB1	1.07	1.26	10	2
1:A:163:VAL:HG13	1:A:195:ILE:HD11	0.93	1.38	12	1
1:A:147:ALA:HB1	1:A:148:PRO:HD2	0.83	1.50	10	4
1:A:165:ILE:HD11	1:A:168:ILE:HG12	0.83	1.48	12	1
1:A:152:VAL:HG22	1:A:223:ILE:CD1	0.83	2.03	7	1
1:A:135:LEU:O	1:A:137:GLU:N	0.83	2.12	9	1
1:A:152:VAL:HG22	1:A:221:ILE:HG12	0.81	1.52	6	1
1:A:165:ILE:HA	1:A:223:ILE:HG23	0.81	1.52	14	4
1:A:217:LEU:O	1:A:221:ILE:HD13	0.80	1.75	4	1
1:A:221:ILE:HG22	1:A:223:ILE:HD11	0.80	1.51	4	2
1:A:150:THR:O	1:A:223:ILE:HD13	0.80	1.77	4	1
1:A:165:ILE:HD11	1:A:168:ILE:CG1	0.80	2.07	12	2
1:A:152:VAL:HG13	1:A:202:ILE:HD11	0.80	1.52	11	1
1:A:220:THR:O	1:A:221:ILE:HD12	0.79	1.76	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:151:ARG:HB2	1:A:223:ILE:HG21	0.78	1.55	13	3
1:A:193:VAL:HG12	1:A:206:HIS:CD2	0.78	2.14	1	5
1:A:132:ILE:N	1:A:187:ILE:HD13	0.75	1.96	14	2
1:A:165:ILE:HG12	1:A:223:ILE:HD12	0.75	1.58	14	1
1:A:112:VAL:HB	1:A:202:ILE:HG22	0.74	1.58	7	1
1:A:132:ILE:HG23	1:A:132:ILE:O	0.74	1.81	12	2
1:A:165:ILE:HD13	1:A:166:VAL:N	0.74	1.98	12	5
1:A:214:LEU:O	1:A:218:ALA:HB3	0.74	1.83	5	3
1:A:132:ILE:N	1:A:133:PRO:CD	0.73	2.50	1	6
1:A:151:ARG:CB	1:A:223:ILE:HG21	0.73	2.13	9	1
1:A:134:GLY:O	1:A:221:ILE:HD11	0.73	1.84	4	2
1:A:135:LEU:CB	1:A:217:LEU:HD22	0.73	2.13	6	1
1:A:137:GLU:O	1:A:168:ILE:HG22	0.73	1.84	7	1
1:A:185:ALA:HB3	1:A:187:ILE:HD11	0.72	1.58	6	2
1:A:151:ARG:O	1:A:153:ILE:HD13	0.72	1.84	3	1
1:A:221:ILE:HB	1:A:223:ILE:HD11	0.72	1.62	1	3
1:A:135:LEU:CB	1:A:217:LEU:HD12	0.72	2.15	11	1
1:A:155:ALA:HB1	1:A:226:LEU:HD21	0.71	1.61	10	1
1:A:153:ILE:HD13	1:A:219:HIS:O	0.71	1.86	11	2
1:A:221:ILE:HG23	1:A:222:ARG:N	0.71	2.00	7	1
1:A:138:LEU:HD13	1:A:139:GLY:N	0.71	2.01	7	1
1:A:150:THR:O	1:A:153:ILE:HG22	0.71	1.86	14	1
1:A:150:THR:O	1:A:153:ILE:HD11	0.70	1.86	3	1
1:A:165:ILE:O	1:A:165:ILE:HG23	0.70	1.86	7	3
1:A:195:ILE:HD12	1:A:196:VAL:N	0.70	2.02	9	1
1:A:151:ARG:N	1:A:155:ALA:HB2	0.69	2.01	4	2
1:A:168:ILE:HG22	1:A:221:ILE:HG23	0.69	1.62	10	1
1:A:204:LEU:HD23	1:A:213:LEU:HD22	0.69	1.63	10	2
1:A:147:ALA:HB1	1:A:148:PRO:CD	0.69	2.17	10	4
1:A:193:VAL:HG12	1:A:206:HIS:CG	0.69	2.22	8	6
1:A:132:ILE:O	1:A:132:ILE:HD13	0.69	1.88	7	4
1:A:167:GLN:O	1:A:168:ILE:HD13	0.69	1.88	11	3
1:A:151:ARG:O	1:A:153:ILE:HG22	0.69	1.87	2	1
1:A:165:ILE:HA	1:A:222:ARG:O	0.68	1.88	7	4
1:A:153:ILE:HG23	1:A:218:ALA:O	0.68	1.88	8	2
1:A:168:ILE:HG22	1:A:221:ILE:HG21	0.68	1.65	9	1
1:A:155:ALA:HB1	1:A:195:ILE:HD13	0.68	1.65	7	1
1:A:156:ALA:HB2	1:A:195:ILE:HG21	0.68	1.66	12	1
1:A:138:LEU:O	1:A:220:THR:HG23	0.68	1.88	10	1
1:A:185:ALA:CB	1:A:187:ILE:HD11	0.68	2.18	14	2
1:A:163:VAL:CG1	1:A:195:ILE:HD11	0.68	2.18	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:163:VAL:HB	1:A:223:ILE:HG22	0.67	1.65	3	2
1:A:156:ALA:HB2	1:A:202:ILE:HA	0.67	1.66	7	1
1:A:151:ARG:CB	1:A:220:THR:HG22	0.67	2.20	8	1
1:A:139:GLY:O	1:A:140:VAL:HG23	0.67	1.88	1	1
1:A:132:ILE:HD11	1:A:221:ILE:HG21	0.67	1.66	7	1
1:A:167:GLN:C	1:A:168:ILE:HD13	0.67	2.15	1	2
1:A:186:ASP:C	1:A:187:ILE:HD13	0.67	2.14	2	1
1:A:131:PRO:O	1:A:132:ILE:HB	0.66	1.89	1	8
1:A:225:GLU:C	1:A:226:LEU:HD23	0.66	2.15	5	1
1:A:130:ASN:ND2	1:A:211:VAL:HG22	0.66	2.04	4	1
1:A:202:ILE:HD13	1:A:203:THR:N	0.66	2.04	5	4
1:A:154:ASP:O	1:A:157:THR:HG22	0.66	1.91	4	3
1:A:204:LEU:HD12	1:A:213:LEU:HD22	0.65	1.68	14	1
1:A:217:LEU:N	1:A:217:LEU:HD13	0.65	2.04	11	1
1:A:147:ALA:O	1:A:149:GLY:N	0.65	2.29	1	2
1:A:187:ILE:HD12	1:A:187:ILE:N	0.65	2.07	14	2
1:A:129:GLY:O	1:A:130:ASN:O	0.65	2.15	1	5
1:A:131:PRO:O	1:A:132:ILE:CB	0.65	2.45	1	7
1:A:147:ALA:HB3	1:A:148:PRO:HD3	0.65	1.69	11	6
1:A:218:ALA:HA	1:A:221:ILE:HD11	0.65	1.68	3	1
1:A:155:ALA:HA	1:A:226:LEU:HD22	0.65	1.68	5	1
1:A:150:THR:CG2	1:A:155:ALA:HB2	0.64	2.22	1	1
1:A:213:LEU:HD23	1:A:218:ALA:HB2	0.64	1.68	10	2
1:A:182:LEU:HD13	1:A:182:LEU:O	0.64	1.92	2	1
1:A:150:THR:HG23	1:A:223:ILE:HB	0.64	1.69	14	1
1:A:168:ILE:HG22	1:A:221:ILE:CG2	0.63	2.23	9	2
1:A:131:PRO:O	1:A:185:ALA:HB1	0.63	1.94	4	1
1:A:143:SER:OG	1:A:153:ILE:HG23	0.63	1.93	5	1
1:A:152:VAL:CG1	1:A:202:ILE:HD11	0.63	2.23	11	2
1:A:130:ASN:CB	1:A:131:PRO:CD	0.63	2.77	4	1
1:A:164:ARG:O	1:A:223:ILE:HG23	0.63	1.93	13	1
1:A:132:ILE:HD12	1:A:222:ARG:HD2	0.63	1.71	13	1
1:A:140:VAL:C	1:A:220:THR:HG21	0.63	2.18	10	1
1:A:202:ILE:HD11	1:A:214:LEU:C	0.63	2.18	14	1
1:A:151:ARG:H	1:A:155:ALA:HB2	0.62	1.54	13	2
1:A:133:PRO:O	1:A:187:ILE:HG21	0.62	1.93	5	1
1:A:222:ARG:C	1:A:223:ILE:HD13	0.62	2.20	14	1
1:A:134:GLY:HA3	1:A:221:ILE:HG21	0.62	1.71	3	2
1:A:152:VAL:HG13	1:A:223:ILE:CG1	0.62	2.24	3	1
1:A:165:ILE:HG22	1:A:191:SER:O	0.62	1.93	7	4
1:A:187:ILE:HD13	1:A:222:ARG:NH1	0.62	2.10	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:131:PRO:HA	1:A:187:ILE:HG21	0.62	1.70	12	1
1:A:195:ILE:CG2	1:A:204:LEU:HD23	0.62	2.25	14	1
1:A:163:VAL:HG23	1:A:193:VAL:HG23	0.62	1.72	2	1
1:A:151:ARG:O	1:A:153:ILE:N	0.62	2.33	2	5
1:A:220:THR:O	1:A:220:THR:HG23	0.62	1.93	9	1
1:A:151:ARG:O	1:A:152:VAL:HG12	0.62	1.95	14	2
1:A:221:ILE:CG2	1:A:223:ILE:HD11	0.62	2.25	14	1
1:A:143:SER:CB	1:A:153:ILE:HG23	0.61	2.25	5	1
1:A:206:HIS:O	1:A:207:ASN:C	0.61	2.43	1	6
1:A:155:ALA:CB	1:A:226:LEU:HD21	0.61	2.25	10	1
1:A:165:ILE:CG1	1:A:189:VAL:HG23	0.61	2.26	6	1
1:A:223:ILE:HG22	1:A:224:GLU:H	0.61	1.55	14	1
1:A:152:VAL:HG13	1:A:223:ILE:CD1	0.60	2.25	3	1
1:A:139:GLY:CA	1:A:217:LEU:HD13	0.60	2.26	5	1
1:A:168:ILE:HG21	1:A:220:THR:O	0.60	1.96	7	1
1:A:152:VAL:HG13	1:A:218:ALA:HB1	0.60	1.71	8	1
1:A:150:THR:HG21	1:A:226:LEU:HD22	0.60	1.73	9	1
1:A:149:GLY:O	1:A:163:VAL:HG12	0.60	1.95	7	1
1:A:166:VAL:O	1:A:167:GLN:CB	0.60	2.50	10	3
1:A:139:GLY:O	1:A:140:VAL:CB	0.59	2.49	1	1
1:A:164:ARG:O	1:A:223:ILE:HA	0.59	1.96	3	4
1:A:223:ILE:HD12	1:A:223:ILE:N	0.59	2.11	4	6
1:A:135:LEU:HB2	1:A:217:LEU:HD22	0.59	1.73	6	1
1:A:155:ALA:CB	1:A:195:ILE:HD13	0.59	2.26	7	1
1:A:221:ILE:CG2	1:A:222:ARG:N	0.59	2.64	7	2
1:A:139:GLY:O	1:A:140:VAL:CG2	0.59	2.50	1	1
1:A:150:THR:HG23	1:A:155:ALA:HB2	0.59	1.75	1	1
1:A:151:ARG:HD2	1:A:153:ILE:HD11	0.59	1.72	8	1
1:A:133:PRO:HB2	1:A:182:LEU:HD23	0.59	1.74	8	1
1:A:153:ILE:HD13	1:A:219:HIS:CE1	0.59	2.33	12	1
1:A:145:ALA:O	1:A:146:ALA:HB3	0.59	1.97	7	2
1:A:179:PHE:CZ	1:A:182:LEU:HD12	0.58	2.32	2	1
1:A:138:LEU:C	1:A:138:LEU:HD22	0.58	2.23	7	1
1:A:152:VAL:HG23	1:A:223:ILE:HD11	0.58	1.73	5	1
1:A:152:VAL:HG23	1:A:195:ILE:HG21	0.58	1.75	14	1
1:A:151:ARG:HA	1:A:163:VAL:HG11	0.58	1.75	4	1
1:A:149:GLY:HA2	1:A:163:VAL:HB	0.58	1.75	7	1
1:A:138:LEU:HD12	1:A:221:ILE:HD11	0.58	1.73	11	1
1:A:165:ILE:HD13	1:A:223:ILE:HG23	0.58	1.74	3	1
1:A:138:LEU:HB3	1:A:221:ILE:HG22	0.58	1.75	6	1
1:A:135:LEU:HD22	1:A:179:PHE:CD2	0.58	2.33	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:187:ILE:HD12	1:A:222:ARG:NH2	0.58	2.13	8	1
1:A:152:VAL:HG13	1:A:223:ILE:HG12	0.58	1.75	3	1
1:A:213:LEU:HB3	1:A:218:ALA:HB2	0.58	1.76	6	1
1:A:213:LEU:HA	1:A:217:LEU:HD23	0.58	1.75	11	1
1:A:174:VAL:HG22	1:A:183:LEU:HD11	0.58	1.74	11	1
1:A:221:ILE:HG22	1:A:223:ILE:CD1	0.58	2.29	7	3
1:A:221:ILE:HG23	1:A:222:ARG:H	0.58	1.58	7	1
1:A:167:GLN:CA	1:A:222:ARG:HB3	0.58	2.29	13	1
1:A:165:ILE:CD1	1:A:189:VAL:HG12	0.58	2.28	14	1
1:A:135:LEU:HB2	1:A:217:LEU:HD12	0.58	1.73	11	1
1:A:153:ILE:O	1:A:154:ASP:CB	0.58	2.52	13	5
1:A:153:ILE:HD13	1:A:153:ILE:N	0.57	2.14	13	1
1:A:186:ASP:O	1:A:187:ILE:C	0.57	2.47	2	4
1:A:163:VAL:HG22	1:A:193:VAL:O	0.57	1.98	5	5
1:A:156:ALA:HB2	1:A:195:ILE:HD11	0.57	1.76	9	1
1:A:151:ARG:O	1:A:152:VAL:CG2	0.57	2.53	3	1
1:A:135:LEU:HB3	1:A:217:LEU:HD22	0.57	1.75	6	1
1:A:150:THR:C	1:A:155:ALA:HB2	0.57	2.24	9	1
1:A:163:VAL:CG2	1:A:193:VAL:HG23	0.57	2.29	2	4
1:A:160:PRO:HB3	1:A:226:LEU:HD22	0.57	1.76	1	1
1:A:225:GLU:C	1:A:226:LEU:HD12	0.57	2.23	11	1
1:A:193:VAL:HG12	1:A:206:HIS:ND1	0.57	2.14	8	2
1:A:128:PHE:O	1:A:211:VAL:HG13	0.57	1.99	8	1
1:A:165:ILE:HD12	1:A:189:VAL:HA	0.57	1.77	9	2
1:A:156:ALA:HB2	1:A:195:ILE:CD1	0.56	2.30	2	3
1:A:150:THR:OG1	1:A:155:ALA:N	0.56	2.37	9	1
1:A:165:ILE:HD11	1:A:168:ILE:HG23	0.56	1.76	9	1
1:A:152:VAL:HG22	1:A:221:ILE:CG1	0.56	2.28	6	1
1:A:132:ILE:HG21	1:A:193:VAL:HG21	0.56	1.77	9	1
1:A:168:ILE:HD13	1:A:187:ILE:CD1	0.56	2.29	10	1
1:A:151:ARG:C	1:A:152:VAL:HG23	0.56	2.25	6	3
1:A:174:VAL:O	1:A:174:VAL:HG13	0.56	2.00	13	8
1:A:167:GLN:O	1:A:222:ARG:HB3	0.56	2.00	13	3
1:A:151:ARG:CB	1:A:163:VAL:HG21	0.56	2.30	4	1
1:A:138:LEU:HD22	1:A:138:LEU:O	0.56	2.00	7	1
1:A:130:ASN:CB	1:A:131:PRO:HD2	0.56	2.31	6	2
1:A:166:VAL:O	1:A:167:GLN:C	0.56	2.48	5	1
1:A:134:GLY:HA3	1:A:221:ILE:HD13	0.56	1.77	3	1
1:A:167:GLN:O	1:A:222:ARG:CG	0.56	2.53	7	1
1:A:168:ILE:HD13	1:A:187:ILE:HD12	0.56	1.77	10	1
1:A:152:VAL:HG11	1:A:221:ILE:HD12	0.56	1.76	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:133:PRO:HG3	1:A:211:VAL:HG11	0.56	1.76	8	1
1:A:165:ILE:HG23	1:A:222:ARG:HG3	0.56	1.77	13	2
1:A:166:VAL:O	1:A:189:VAL:HG22	0.56	1.99	6	1
1:A:152:VAL:HG21	1:A:218:ALA:HB1	0.56	1.77	13	1
1:A:171:ILE:O	1:A:172:PHE:C	0.56	2.49	1	1
1:A:225:GLU:O	1:A:226:LEU:C	0.55	2.49	5	4
1:A:152:VAL:O	1:A:154:ASP:N	0.55	2.39	2	4
1:A:163:VAL:HB	1:A:223:ILE:O	0.55	2.00	6	1
1:A:135:LEU:HB3	1:A:217:LEU:HD12	0.55	1.77	11	1
1:A:156:ALA:O	1:A:157:THR:HG23	0.55	2.01	14	3
1:A:165:ILE:HD11	1:A:168:ILE:HD11	0.55	1.79	4	1
1:A:130:ASN:CB	1:A:131:PRO:HD3	0.55	2.31	12	1
1:A:132:ILE:N	1:A:133:PRO:HD3	0.55	2.15	1	5
1:A:147:ALA:HB3	1:A:148:PRO:CD	0.55	2.31	11	6
1:A:175:GLU:O	1:A:176:THR:HG23	0.55	2.00	8	2
1:A:131:PRO:O	1:A:132:ILE:C	0.55	2.49	13	1
1:A:152:VAL:CG1	1:A:218:ALA:HB1	0.55	2.32	8	3
1:A:149:GLY:O	1:A:153:ILE:HG23	0.55	2.02	4	1
1:A:214:LEU:N	1:A:214:LEU:HD23	0.55	2.17	5	1
1:A:120:LEU:HG	1:A:217:LEU:HD21	0.55	1.78	6	1
1:A:150:THR:HG21	1:A:224:GLU:HB2	0.55	1.79	6	1
1:A:204:LEU:CD2	1:A:213:LEU:HD22	0.55	2.31	5	2
1:A:186:ASP:O	1:A:187:ILE:O	0.55	2.25	3	5
1:A:152:VAL:CG2	1:A:221:ILE:HG23	0.55	2.32	6	1
1:A:179:PHE:CD1	1:A:182:LEU:HD22	0.54	2.37	8	2
1:A:132:ILE:O	1:A:132:ILE:CG2	0.54	2.53	12	1
1:A:221:ILE:HD11	1:A:223:ILE:HG12	0.54	1.79	6	1
1:A:187:ILE:HD12	1:A:222:ARG:HH22	0.54	1.61	8	1
1:A:174:VAL:CG1	1:A:174:VAL:O	0.54	2.54	10	1
1:A:152:VAL:H	1:A:223:ILE:HD13	0.54	1.61	12	1
1:A:195:ILE:CG2	1:A:204:LEU:HD13	0.54	2.33	5	2
1:A:225:GLU:O	1:A:226:LEU:HD23	0.54	2.03	5	1
1:A:168:ILE:HG13	1:A:187:ILE:HD12	0.54	1.79	1	1
1:A:165:ILE:HD13	1:A:165:ILE:C	0.54	2.27	9	1
1:A:169:ASN:OD1	1:A:187:ILE:HD11	0.54	2.03	9	1
1:A:165:ILE:O	1:A:165:ILE:CG2	0.54	2.56	7	4
1:A:158:SER:O	1:A:226:LEU:HD22	0.53	2.03	11	1
1:A:173:GLN:O	1:A:174:VAL:HG12	0.53	2.03	11	1
1:A:168:ILE:HD12	1:A:169:ASN:N	0.53	2.18	9	1
1:A:187:ILE:HG13	1:A:187:ILE:O	0.53	2.03	1	3
1:A:152:VAL:HG22	1:A:223:ILE:HD13	0.53	1.76	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:151:ARG:HB2	1:A:221:ILE:HB	0.53	1.79	11	1
1:A:153:ILE:HG21	1:A:220:THR:HA	0.53	1.81	9	1
1:A:217:LEU:O	1:A:221:ILE:HD11	0.53	2.04	9	1
1:A:167:GLN:O	1:A:168:ILE:HB	0.53	2.03	8	2
1:A:132:ILE:O	1:A:168:ILE:HG21	0.53	2.04	12	1
1:A:168:ILE:CD1	1:A:187:ILE:HD12	0.53	2.32	9	1
1:A:155:ALA:HA	1:A:226:LEU:HD23	0.53	1.81	12	1
1:A:151:ARG:O	1:A:152:VAL:HG22	0.53	2.04	3	1
1:A:131:PRO:CB	1:A:187:ILE:HA	0.53	2.34	1	2
1:A:152:VAL:HG11	1:A:218:ALA:CB	0.53	2.34	6	2
1:A:119:VAL:HG13	1:A:120:LEU:N	0.53	2.18	7	1
1:A:195:ILE:HD12	1:A:204:LEU:HD22	0.53	1.81	7	1
1:A:138:LEU:O	1:A:140:VAL:N	0.53	2.42	1	2
1:A:151:ARG:HB3	1:A:220:THR:HG22	0.52	1.80	8	1
1:A:149:GLY:O	1:A:226:LEU:N	0.52	2.43	7	1
1:A:167:GLN:O	1:A:168:ILE:CB	0.52	2.58	8	3
1:A:138:LEU:HD22	1:A:216:ASP:O	0.52	2.05	14	2
1:A:138:LEU:HD22	1:A:217:LEU:O	0.52	2.04	1	1
1:A:167:GLN:CB	1:A:222:ARG:HA	0.52	2.34	8	2
1:A:146:ALA:HB3	1:A:222:ARG:NE	0.52	2.18	9	1
1:A:152:VAL:HG13	1:A:223:ILE:HD13	0.52	1.80	3	1
1:A:148:PRO:O	1:A:224:GLU:HB2	0.52	2.03	7	1
1:A:186:ASP:O	1:A:187:ILE:HG23	0.52	2.04	14	1
1:A:189:VAL:O	1:A:189:VAL:HG13	0.52	2.04	7	3
1:A:145:ALA:O	1:A:146:ALA:CB	0.52	2.57	7	2
1:A:174:VAL:HG11	1:A:183:LEU:CD2	0.52	2.35	8	1
1:A:137:GLU:HG2	1:A:168:ILE:HD11	0.52	1.81	11	1
1:A:174:VAL:O	1:A:174:VAL:HG22	0.52	2.05	1	2
1:A:152:VAL:CG2	1:A:223:ILE:HD11	0.52	2.35	10	2
1:A:165:ILE:CG1	1:A:223:ILE:HD12	0.52	2.33	14	1
1:A:171:ILE:HD11	1:A:189:VAL:HG12	0.52	1.80	8	1
1:A:213:LEU:O	1:A:214:LEU:HD22	0.52	2.04	10	1
1:A:212:GLU:O	1:A:213:LEU:C	0.52	2.53	12	3
1:A:138:LEU:HD21	1:A:216:ASP:O	0.51	2.04	1	1
1:A:156:ALA:HB2	1:A:195:ILE:HG12	0.51	1.81	3	1
1:A:202:ILE:O	1:A:202:ILE:HG23	0.51	2.06	13	1
1:A:222:ARG:C	1:A:223:ILE:HD12	0.51	2.31	8	2
1:A:160:PRO:N	1:A:226:LEU:HD13	0.51	2.21	10	1
1:A:130:ASN:OD1	1:A:211:VAL:HG22	0.51	2.05	6	1
1:A:152:VAL:CB	1:A:218:ALA:HB1	0.51	2.36	1	1
1:A:166:VAL:HA	1:A:189:VAL:HG13	0.51	1.83	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:221:ILE:HG22	1:A:222:ARG:N	0.51	2.21	11	2
1:A:206:HIS:O	1:A:208:GLY:N	0.51	2.44	12	8
1:A:149:GLY:HA2	1:A:163:VAL:CB	0.51	2.36	7	1
1:A:166:VAL:HG13	1:A:190:GLY:HA2	0.51	1.83	7	1
1:A:129:GLY:O	1:A:130:ASN:CG	0.51	2.54	1	5
1:A:163:VAL:CG2	1:A:194:GLU:HA	0.51	2.36	6	1
1:A:152:VAL:HG23	1:A:223:ILE:CD1	0.50	2.36	5	1
1:A:123:VAL:HG13	1:A:123:VAL:O	0.50	2.06	9	1
1:A:130:ASN:O	1:A:185:ALA:HB1	0.50	2.06	12	1
1:A:152:VAL:CG2	1:A:195:ILE:HG21	0.50	2.35	14	1
1:A:165:ILE:HD12	1:A:189:VAL:HG12	0.50	1.83	14	1
1:A:132:ILE:H	1:A:187:ILE:HG22	0.50	1.65	5	3
1:A:132:ILE:HG23	1:A:165:ILE:CD1	0.50	2.37	3	1
1:A:155:ALA:HA	1:A:226:LEU:HD21	0.50	1.82	1	1
1:A:149:GLY:HA3	1:A:224:GLU:C	0.50	2.32	7	1
1:A:222:ARG:O	1:A:223:ILE:HD13	0.50	2.06	14	1
1:A:151:ARG:HG3	1:A:163:VAL:HG21	0.50	1.82	4	1
1:A:165:ILE:HG23	1:A:190:GLY:H	0.50	1.67	9	3
1:A:167:GLN:O	1:A:222:ARG:CA	0.50	2.59	7	2
1:A:152:VAL:HG22	1:A:204:LEU:HD11	0.50	1.82	13	1
1:A:147:ALA:N	1:A:148:PRO:HD2	0.50	2.22	12	2
1:A:165:ILE:HD11	1:A:168:ILE:CD1	0.50	2.37	1	2
1:A:135:LEU:HD13	1:A:176:THR:HG21	0.50	1.84	8	1
1:A:130:ASN:HB2	1:A:131:PRO:HD2	0.50	1.83	14	1
1:A:195:ILE:CG1	1:A:196:VAL:N	0.50	2.75	6	6
1:A:226:LEU:HD23	1:A:226:LEU:N	0.50	2.21	2	1
1:A:202:ILE:HD13	1:A:202:ILE:C	0.50	2.31	8	4
1:A:154:ASP:O	1:A:155:ALA:C	0.50	2.55	7	2
1:A:151:ARG:CD	1:A:221:ILE:O	0.50	2.60	1	1
1:A:160:PRO:HA	1:A:226:LEU:HD22	0.50	1.83	10	1
1:A:150:THR:HG21	1:A:155:ALA:HB2	0.50	1.83	12	1
1:A:147:ALA:HB1	1:A:225:GLU:CB	0.49	2.37	4	1
1:A:131:PRO:C	1:A:132:ILE:CG1	0.49	2.85	9	2
1:A:152:VAL:HG21	1:A:218:ALA:HA	0.49	1.84	6	1
1:A:135:LEU:O	1:A:138:LEU:HD12	0.49	2.08	7	1
1:A:175:GLU:O	1:A:176:THR:O	0.49	2.30	7	1
1:A:168:ILE:O	1:A:169:ASN:O	0.49	2.30	8	1
1:A:219:HIS:O	1:A:220:THR:HG23	0.49	2.07	3	1
1:A:151:ARG:O	1:A:152:VAL:C	0.49	2.55	1	1
1:A:132:ILE:HG21	1:A:187:ILE:HG23	0.49	1.84	4	1
1:A:119:VAL:HG22	1:A:120:LEU:H	0.49	1.67	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:150:THR:O	1:A:151:ARG:C	0.49	2.54	9	1
1:A:150:THR:HG22	1:A:224:GLU:O	0.49	2.06	12	2
1:A:160:PRO:CA	1:A:226:LEU:HD13	0.49	2.38	10	1
1:A:151:ARG:CG	1:A:220:THR:HA	0.49	2.37	1	1
1:A:151:ARG:C	1:A:153:ILE:HD13	0.49	2.31	3	1
1:A:195:ILE:HD11	1:A:202:ILE:HG13	0.49	1.83	3	2
1:A:167:GLN:N	1:A:222:ARG:CB	0.49	2.75	8	2
1:A:168:ILE:O	1:A:168:ILE:HG22	0.49	2.07	13	1
1:A:183:LEU:HD13	1:A:183:LEU:O	0.49	2.08	8	2
1:A:152:VAL:HG12	1:A:202:ILE:HD13	0.49	1.84	13	1
1:A:138:LEU:CD2	1:A:216:ASP:O	0.48	2.61	1	1
1:A:151:ARG:NE	1:A:193:VAL:HG21	0.48	2.23	4	1
1:A:132:ILE:HD13	1:A:132:ILE:C	0.48	2.33	7	2
1:A:153:ILE:O	1:A:154:ASP:HB2	0.48	2.07	9	2
1:A:213:LEU:HD12	1:A:213:LEU:O	0.48	2.08	12	1
1:A:217:LEU:N	1:A:217:LEU:CD1	0.48	2.76	11	1
1:A:168:ILE:HD13	1:A:168:ILE:N	0.48	2.23	7	1
1:A:151:ARG:HB2	1:A:220:THR:HG22	0.48	1.85	8	1
1:A:217:LEU:O	1:A:221:ILE:CG1	0.48	2.60	11	1
1:A:187:ILE:HD13	1:A:187:ILE:C	0.48	2.33	12	1
1:A:151:ARG:HG2	1:A:219:HIS:O	0.48	2.09	2	1
1:A:165:ILE:HG23	1:A:222:ARG:O	0.48	2.08	3	1
1:A:147:ALA:N	1:A:148:PRO:CD	0.48	2.77	12	1
1:A:219:HIS:HD2	1:A:220:THR:HG23	0.48	1.69	7	1
1:A:165:ILE:HD11	1:A:168:ILE:HD13	0.48	1.85	1	1
1:A:150:THR:CG2	1:A:224:GLU:CB	0.47	2.92	6	1
1:A:186:ASP:O	1:A:187:ILE:HG13	0.47	2.08	7	1
1:A:165:ILE:O	1:A:166:VAL:HG13	0.47	2.10	8	1
1:A:165:ILE:CA	1:A:223:ILE:HG23	0.47	2.34	14	2
1:A:168:ILE:HD12	1:A:221:ILE:HA	0.47	1.85	8	1
1:A:132:ILE:HD11	1:A:189:VAL:N	0.47	2.23	13	1
1:A:219:HIS:C	1:A:219:HIS:CD2	0.47	2.93	6	1
1:A:221:ILE:O	1:A:223:ILE:HD12	0.47	2.10	9	1
1:A:137:GLU:O	1:A:138:LEU:C	0.47	2.57	11	2
1:A:150:THR:HG21	1:A:225:GLU:HA	0.47	1.86	13	1
1:A:167:GLN:O	1:A:222:ARG:CB	0.47	2.63	1	4
1:A:112:VAL:CB	1:A:202:ILE:HG22	0.47	2.36	7	1
1:A:186:ASP:O	1:A:187:ILE:HG12	0.47	2.10	11	1
1:A:208:GLY:O	1:A:209:LYS:HG3	0.47	2.09	1	5
1:A:131:PRO:C	1:A:133:PRO:HD2	0.47	2.35	3	1
1:A:119:VAL:CG1	1:A:120:LEU:N	0.47	2.78	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:150:THR:HG21	1:A:224:GLU:CB	0.47	2.39	6	1
1:A:221:ILE:HG13	1:A:223:ILE:HD11	0.47	1.85	6	1
1:A:138:LEU:O	1:A:220:THR:OG1	0.47	2.31	1	1
1:A:118:LYS:HB3	1:A:214:LEU:HD21	0.47	1.86	6	2
1:A:141:GLY:C	1:A:168:ILE:HD12	0.47	2.35	7	1
1:A:165:ILE:HD13	1:A:222:ARG:O	0.47	2.10	13	1
1:A:189:VAL:HG23	1:A:189:VAL:O	0.47	2.09	1	1
1:A:152:VAL:HG22	1:A:221:ILE:HB	0.47	1.87	2	1
1:A:195:ILE:HG22	1:A:204:LEU:HD22	0.47	1.87	5	1
1:A:112:VAL:HG23	1:A:113:GLU:N	0.47	2.25	1	2
1:A:179:PHE:CE1	1:A:217:LEU:HD21	0.47	2.45	8	1
1:A:139:GLY:O	1:A:140:VAL:HB	0.46	2.08	1	1
1:A:155:ALA:O	1:A:226:LEU:HD11	0.46	2.10	10	1
1:A:131:PRO:C	1:A:133:PRO:CD	0.46	2.88	3	1
1:A:214:LEU:HD12	1:A:216:ASP:HB2	0.46	1.87	5	1
1:A:221:ILE:HG22	1:A:223:ILE:CG1	0.46	2.41	7	1
1:A:158:SER:C	1:A:226:LEU:HD22	0.46	2.34	11	1
1:A:140:VAL:HG12	1:A:141:GLY:N	0.46	2.23	1	1
1:A:170:GLU:O	1:A:172:PHE:N	0.46	2.48	8	3
1:A:132:ILE:HB	1:A:193:VAL:HG11	0.46	1.87	11	1
1:A:153:ILE:CG1	1:A:153:ILE:O	0.46	2.64	11	1
1:A:160:PRO:HA	1:A:226:LEU:HD23	0.46	1.86	11	1
1:A:129:GLY:C	1:A:130:ASN:CG	0.46	2.83	1	2
1:A:156:ALA:HB2	1:A:195:ILE:HD12	0.46	1.86	5	1
1:A:150:THR:N	1:A:224:GLU:O	0.46	2.49	7	1
1:A:117:VAL:HG23	1:A:119:VAL:HG23	0.46	1.88	2	1
1:A:151:ARG:C	1:A:152:VAL:CG2	0.46	2.89	2	3
1:A:150:THR:O	1:A:151:ARG:CB	0.46	2.64	3	1
1:A:155:ALA:C	1:A:226:LEU:HD21	0.46	2.36	1	1
1:A:165:ILE:CD1	1:A:223:ILE:HG23	0.46	2.41	3	1
1:A:135:LEU:HD23	1:A:182:LEU:CD2	0.46	2.41	12	1
1:A:152:VAL:HG21	1:A:221:ILE:HG23	0.46	1.87	6	1
1:A:179:PHE:C	1:A:179:PHE:CD1	0.46	2.93	7	1
1:A:132:ILE:O	1:A:151:ARG:NH2	0.46	2.49	11	1
1:A:166:VAL:O	1:A:167:GLN:HB2	0.46	2.10	14	1
1:A:165:ILE:HG23	1:A:191:SER:H	0.46	1.71	4	1
1:A:134:GLY:HA3	1:A:137:GLU:HG2	0.46	1.87	6	1
1:A:220:THR:C	1:A:221:ILE:HD13	0.46	2.36	8	1
1:A:187:ILE:HG12	1:A:187:ILE:O	0.46	2.09	2	1
1:A:165:ILE:HD13	1:A:167:GLN:H	0.46	1.70	5	1
1:A:150:THR:HG22	1:A:155:ALA:CA	0.45	2.41	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:163:VAL:CG2	1:A:223:ILE:CG2	0.45	2.94	7	1
1:A:160:PRO:HA	1:A:226:LEU:HD12	0.45	1.87	9	1
1:A:135:LEU:HD12	1:A:136:ASP:N	0.45	2.27	12	1
1:A:151:ARG:CG	1:A:163:VAL:HG21	0.45	2.41	9	2
1:A:130:ASN:O	1:A:131:PRO:C	0.45	2.59	14	1
1:A:149:GLY:HA3	1:A:224:GLU:HA	0.45	1.89	5	1
1:A:165:ILE:O	1:A:190:GLY:N	0.45	2.50	7	1
1:A:131:PRO:HA	1:A:187:ILE:CG2	0.45	2.41	12	1
1:A:158:SER:HB3	1:A:226:LEU:HD13	0.45	1.87	11	1
1:A:152:VAL:N	1:A:223:ILE:HD13	0.45	2.26	12	1
1:A:147:ALA:HB1	1:A:225:GLU:HB2	0.45	1.89	4	1
1:A:132:ILE:CG1	1:A:193:VAL:HG11	0.45	2.42	11	1
1:A:138:LEU:HB3	1:A:221:ILE:HD12	0.45	1.88	14	1
1:A:151:ARG:O	1:A:153:ILE:CD1	0.45	2.63	3	1
1:A:167:GLN:HA	1:A:189:VAL:HG11	0.45	1.89	9	1
1:A:138:LEU:HD21	1:A:216:ASP:C	0.45	2.36	4	1
1:A:155:ALA:CA	1:A:226:LEU:HD21	0.45	2.41	1	2
1:A:132:ILE:N	1:A:132:ILE:HD13	0.45	2.27	3	1
1:A:165:ILE:CD1	1:A:168:ILE:HD11	0.45	2.42	4	1
1:A:149:GLY:CA	1:A:224:GLU:HA	0.45	2.41	5	1
1:A:152:VAL:HG22	1:A:204:LEU:CD1	0.45	2.42	13	1
1:A:151:ARG:O	1:A:152:VAL:HG23	0.44	2.12	2	1
1:A:151:ARG:C	1:A:152:VAL:HG22	0.44	2.37	3	1
1:A:138:LEU:HD13	1:A:138:LEU:C	0.44	2.37	7	1
1:A:149:GLY:CA	1:A:225:GLU:N	0.44	2.81	7	1
1:A:186:ASP:O	1:A:187:ILE:CG1	0.44	2.65	3	1
1:A:155:ALA:HA	1:A:226:LEU:HD13	0.44	1.88	2	1
1:A:146:ALA:O	1:A:147:ALA:HB2	0.44	2.13	5	1
1:A:112:VAL:HG13	1:A:113:GLU:H	0.44	1.72	8	1
1:A:137:GLU:CD	1:A:168:ILE:HD13	0.44	2.37	14	1
1:A:152:VAL:HA	1:A:155:ALA:HB3	0.44	1.89	1	1
1:A:155:ALA:HB1	1:A:195:ILE:HG21	0.44	1.89	6	1
1:A:187:ILE:HD13	1:A:188:ARG:N	0.44	2.27	12	1
1:A:165:ILE:HG22	1:A:191:SER:N	0.44	2.27	11	2
1:A:167:GLN:O	1:A:222:ARG:HA	0.44	2.13	7	1
1:A:221:ILE:HG22	1:A:222:ARG:H	0.44	1.72	9	1
1:A:163:VAL:HG23	1:A:193:VAL:C	0.44	2.37	6	1
1:A:134:GLY:N	1:A:168:ILE:CG2	0.44	2.81	12	1
1:A:151:ARG:CB	1:A:221:ILE:HB	0.44	2.43	14	1
1:A:164:ARG:O	1:A:223:ILE:CA	0.44	2.66	3	2
1:A:164:ARG:HB2	1:A:224:GLU:HB2	0.44	1.90	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:165:ILE:HG23	1:A:191:SER:N	0.44	2.28	4	1
1:A:195:ILE:CD1	1:A:202:ILE:HD11	0.44	2.43	4	1
1:A:153:ILE:O	1:A:153:ILE:CG1	0.44	2.66	5	1
1:A:169:ASN:HB2	1:A:189:VAL:HG21	0.44	1.89	7	1
1:A:149:GLY:HA2	1:A:221:ILE:O	0.44	2.13	11	1
1:A:221:ILE:HG13	1:A:223:ILE:CD1	0.43	2.44	6	1
1:A:154:ASP:O	1:A:156:ALA:N	0.43	2.51	7	1
1:A:173:GLN:O	1:A:174:VAL:HG23	0.43	2.13	8	1
1:A:138:LEU:C	1:A:138:LEU:HD23	0.43	2.38	11	1
1:A:132:ILE:HG23	1:A:165:ILE:HD12	0.43	1.90	3	1
1:A:151:ARG:HB2	1:A:163:VAL:HG21	0.43	1.90	4	1
1:A:151:ARG:HE	1:A:193:VAL:HG21	0.43	1.72	4	1
1:A:165:ILE:CG1	1:A:168:ILE:HD11	0.43	2.42	4	1
1:A:168:ILE:HD12	1:A:168:ILE:N	0.43	2.27	4	1
1:A:149:GLY:HA2	1:A:163:VAL:CA	0.43	2.44	7	1
1:A:130:ASN:N	1:A:185:ALA:CB	0.43	2.80	13	1
1:A:133:PRO:HB3	1:A:213:LEU:HD11	0.43	1.90	14	1
1:A:165:ILE:O	1:A:166:VAL:CG2	0.43	2.66	3	1
1:A:152:VAL:HG11	1:A:213:LEU:HD22	0.43	1.89	4	1
1:A:135:LEU:HD23	1:A:179:PHE:CZ	0.43	2.48	10	1
1:A:128:PHE:HB3	1:A:182:LEU:HD12	0.43	1.90	12	1
1:A:134:GLY:CA	1:A:221:ILE:HG21	0.43	2.43	13	1
1:A:132:ILE:HG22	1:A:133:PRO:HD3	0.43	1.91	7	2
1:A:147:ALA:O	1:A:148:PRO:C	0.43	2.61	1	4
1:A:168:ILE:HB	1:A:189:VAL:HG21	0.43	1.90	6	1
1:A:204:LEU:O	1:A:211:VAL:HG23	0.43	2.14	8	1
1:A:165:ILE:HG23	1:A:190:GLY:N	0.43	2.28	12	2
1:A:132:ILE:HD12	1:A:222:ARG:CD	0.43	2.42	13	1
1:A:165:ILE:O	1:A:190:GLY:CA	0.43	2.66	1	2
1:A:187:ILE:H	1:A:187:ILE:HD12	0.43	1.73	6	1
1:A:135:LEU:O	1:A:136:ASP:C	0.43	2.62	9	1
1:A:165:ILE:HD11	1:A:168:ILE:CG2	0.43	2.43	9	1
1:A:167:GLN:C	1:A:222:ARG:HB3	0.43	2.38	13	1
1:A:187:ILE:O	1:A:187:ILE:CG1	0.43	2.66	2	4
1:A:137:GLU:O	1:A:168:ILE:HD13	0.43	2.14	8	1
1:A:133:PRO:CB	1:A:213:LEU:HD11	0.43	2.43	14	1
1:A:163:VAL:HG23	1:A:193:VAL:CG2	0.43	2.44	4	1
1:A:150:THR:HG22	1:A:225:GLU:CA	0.43	2.43	5	1
1:A:153:ILE:HD12	1:A:219:HIS:CE1	0.43	2.49	5	1
1:A:213:LEU:HD23	1:A:218:ALA:CB	0.43	2.40	5	1
1:A:165:ILE:HA	1:A:223:ILE:HA	0.43	1.91	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:132:ILE:CD1	1:A:221:ILE:HG21	0.43	2.41	7	1
1:A:185:ALA:O	1:A:186:ASP:CB	0.43	2.67	7	2
1:A:187:ILE:O	1:A:187:ILE:HG13	0.43	2.14	8	1
1:A:127:PRO:C	1:A:128:PHE:CG	0.43	2.97	9	1
1:A:132:ILE:CD1	1:A:193:VAL:HG11	0.43	2.43	9	1
1:A:160:PRO:HA	1:A:226:LEU:HD13	0.43	1.91	10	1
1:A:151:ARG:HD2	1:A:204:LEU:HD11	0.43	1.91	14	1
1:A:151:ARG:HB3	1:A:153:ILE:CG2	0.43	2.44	1	1
1:A:175:GLU:O	1:A:176:THR:CG2	0.43	2.67	7	1
1:A:151:ARG:CA	1:A:155:ALA:HB2	0.43	2.44	9	1
1:A:131:PRO:HA	1:A:187:ILE:HD12	0.43	1.90	12	1
1:A:132:ILE:HG21	1:A:222:ARG:CZ	0.43	2.44	13	1
1:A:202:ILE:HG23	1:A:214:LEU:HA	0.43	1.90	13	1
1:A:221:ILE:CG2	1:A:223:ILE:CD1	0.43	2.96	14	1
1:A:140:VAL:O	1:A:168:ILE:HG23	0.43	2.14	7	1
1:A:147:ALA:CB	1:A:148:PRO:CD	0.43	2.92	8	4
1:A:195:ILE:C	1:A:195:ILE:HD12	0.43	2.39	14	1
1:A:120:LEU:HD21	1:A:135:LEU:HD11	0.43	1.90	1	1
1:A:131:PRO:O	1:A:132:ILE:CG2	0.43	2.67	1	1
1:A:188:ARG:O	1:A:189:VAL:C	0.43	2.62	4	1
1:A:195:ILE:HG23	1:A:204:LEU:HD13	0.43	1.90	5	2
1:A:134:GLY:HA3	1:A:137:GLU:CG	0.43	2.44	6	1
1:A:165:ILE:HG12	1:A:189:VAL:HG23	0.43	1.90	6	1
1:A:149:GLY:HA3	1:A:224:GLU:N	0.43	2.29	7	1
1:A:149:GLY:C	1:A:163:VAL:HG12	0.43	2.39	7	1
1:A:173:GLN:O	1:A:174:VAL:CG2	0.43	2.66	8	1
1:A:217:LEU:N	1:A:217:LEU:CD2	0.43	2.82	13	1
1:A:192:GLU:O	1:A:206:HIS:CE1	0.42	2.72	4	1
1:A:195:ILE:O	1:A:196:VAL:HG13	0.42	2.14	1	1
1:A:166:VAL:O	1:A:166:VAL:HG12	0.42	2.14	5	1
1:A:226:LEU:O	1:A:226:LEU:CG	0.42	2.66	5	1
1:A:132:ILE:HG21	1:A:193:VAL:CG2	0.42	2.43	9	1
1:A:150:THR:N	1:A:224:GLU:C	0.42	2.77	7	1
1:A:112:VAL:HG13	1:A:113:GLU:N	0.42	2.30	11	2
1:A:131:PRO:CA	1:A:187:ILE:HD12	0.42	2.43	12	1
1:A:132:ILE:CG2	1:A:133:PRO:HD3	0.42	2.45	11	3
1:A:158:SER:HB3	1:A:226:LEU:HD11	0.42	1.91	2	1
1:A:168:ILE:HD13	1:A:189:VAL:HB	0.42	1.91	4	1
1:A:132:ILE:CB	1:A:133:PRO:HD3	0.42	2.43	9	1
1:A:195:ILE:HG22	1:A:204:LEU:HD23	0.42	1.89	14	1
1:A:137:GLU:O	1:A:169:ASN:CB	0.42	2.68	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:130:ASN:HB3	1:A:131:PRO:CD	0.42	2.44	4	1
1:A:132:ILE:H	1:A:187:ILE:HD13	0.42	1.72	6	1
1:A:156:ALA:HB2	1:A:195:ILE:CG2	0.42	2.42	12	1
1:A:131:PRO:O	1:A:132:ILE:CG1	0.42	2.67	3	1
1:A:168:ILE:HG22	1:A:169:ASN:N	0.42	2.30	5	1
1:A:165:ILE:C	1:A:165:ILE:CD1	0.42	2.92	9	1
1:A:196:VAL:O	1:A:196:VAL:HG23	0.42	2.15	11	1
1:A:132:ILE:O	1:A:132:ILE:HG23	0.42	2.15	14	1
1:A:150:THR:CG2	1:A:151:ARG:N	0.42	2.83	3	1
1:A:143:SER:HB3	1:A:153:ILE:HG23	0.42	1.91	5	1
1:A:163:VAL:CB	1:A:223:ILE:O	0.42	2.68	6	1
1:A:151:ARG:HB2	1:A:153:ILE:CD1	0.42	2.45	3	1
1:A:222:ARG:C	1:A:223:ILE:HG13	0.42	2.39	3	1
1:A:163:VAL:CG2	1:A:194:GLU:CA	0.42	2.97	6	1
1:A:150:THR:C	1:A:224:GLU:O	0.42	2.62	7	1
1:A:137:GLU:CG	1:A:168:ILE:HD11	0.42	2.45	11	1
1:A:135:LEU:O	1:A:217:LEU:HG	0.42	2.14	13	1
1:A:131:PRO:CG	1:A:193:VAL:HG12	0.42	2.45	14	1
1:A:153:ILE:HD13	1:A:218:ALA:O	0.42	2.14	14	1
1:A:143:SER:HA	1:A:153:ILE:CG1	0.42	2.45	3	1
1:A:150:THR:OG1	1:A:151:ARG:N	0.42	2.53	6	1
1:A:163:VAL:CG1	1:A:223:ILE:O	0.42	2.68	6	1
1:A:155:ALA:HB3	1:A:195:ILE:HD13	0.41	1.91	6	1
1:A:217:LEU:HD23	1:A:217:LEU:N	0.41	2.30	6	1
1:A:221:ILE:C	1:A:223:ILE:HD12	0.41	2.40	8	1
1:A:150:THR:O	1:A:152:VAL:N	0.41	2.52	4	1
1:A:221:ILE:CG1	1:A:223:ILE:HD11	0.41	2.45	6	1
1:A:169:ASN:ND2	1:A:189:VAL:HG11	0.41	2.30	7	1
1:A:158:SER:O	1:A:226:LEU:HD13	0.41	2.14	11	1
1:A:149:GLY:HA3	1:A:225:GLU:N	0.41	2.30	7	1
1:A:149:GLY:HA2	1:A:222:ARG:HA	0.41	1.91	11	1
1:A:135:LEU:O	1:A:217:LEU:CG	0.41	2.68	13	1
1:A:158:SER:HB2	1:A:226:LEU:HD12	0.41	1.93	13	1
1:A:152:VAL:HB	1:A:218:ALA:HB1	0.41	1.90	1	1
1:A:151:ARG:NH1	1:A:152:VAL:HG13	0.41	2.30	9	1
1:A:213:LEU:CA	1:A:217:LEU:HD23	0.41	2.44	11	1
1:A:165:ILE:C	1:A:166:VAL:HG23	0.41	2.41	3	1
1:A:195:ILE:HD12	1:A:196:VAL:H	0.41	1.74	4	1
1:A:135:LEU:HD22	1:A:179:PHE:CG	0.41	2.50	8	1
1:A:151:ARG:O	1:A:152:VAL:CG1	0.41	2.67	11	2
1:A:130:ASN:OD1	1:A:211:VAL:HG13	0.41	2.15	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:155:ALA:HA	1:A:226:LEU:HD11	0.41	1.92	11	1
1:A:131:PRO:O	1:A:132:ILE:HG12	0.41	2.15	3	1
1:A:223:ILE:N	1:A:223:ILE:CD1	0.41	2.79	4	1
1:A:164:ARG:H	1:A:224:GLU:CB	0.41	2.28	5	1
1:A:226:LEU:O	1:A:226:LEU:HG	0.41	2.16	5	1
1:A:138:LEU:HB2	1:A:220:THR:HG23	0.41	1.92	6	1
1:A:113:GLU:O	1:A:115:ARG:N	0.41	2.53	7	1
1:A:163:VAL:CB	1:A:223:ILE:HG22	0.41	2.43	7	1
1:A:167:GLN:H	1:A:222:ARG:CB	0.41	2.28	8	1
1:A:140:VAL:HG13	1:A:141:GLY:N	0.41	2.31	13	1
1:A:156:ALA:HB2	1:A:195:ILE:HD13	0.41	1.93	2	1
1:A:158:SER:O	1:A:226:LEU:HD11	0.41	2.16	8	1
1:A:174:VAL:CG2	1:A:183:LEU:HD21	0.41	2.45	11	1
1:A:151:ARG:O	1:A:218:ALA:HB1	0.41	2.15	14	1
1:A:138:LEU:CD2	1:A:217:LEU:O	0.41	2.68	1	1
1:A:168:ILE:HD13	1:A:187:ILE:HG12	0.41	1.93	2	1
1:A:138:LEU:HD12	1:A:139:GLY:N	0.41	2.31	6	1
1:A:150:THR:HB	1:A:224:GLU:HB3	0.41	1.92	6	1
1:A:219:HIS:CD2	1:A:220:THR:HG22	0.41	2.51	6	1
1:A:152:VAL:O	1:A:202:ILE:CD1	0.41	2.69	7	1
1:A:149:GLY:C	1:A:150:THR:HG22	0.41	2.40	14	1
1:A:151:ARG:HG3	1:A:220:THR:HA	0.41	1.92	1	1
1:A:225:GLU:C	1:A:226:LEU:CD2	0.41	2.91	5	1
1:A:167:GLN:C	1:A:222:ARG:CB	0.40	2.94	1	1
1:A:165:ILE:HG12	1:A:222:ARG:O	0.40	2.16	7	1
1:A:150:THR:O	1:A:151:ARG:HB2	0.40	2.16	3	1
1:A:139:GLY:HA3	1:A:217:LEU:HD13	0.40	1.93	5	1
1:A:150:THR:HA	1:A:153:ILE:O	0.40	2.17	9	1
1:A:153:ILE:O	1:A:153:ILE:HG23	0.40	2.15	10	1
1:A:151:ARG:CD	1:A:193:VAL:HG21	0.40	2.46	13	1
1:A:165:ILE:HD12	1:A:189:VAL:CB	0.40	2.46	14	1
1:A:150:THR:O	1:A:155:ALA:HB2	0.40	2.17	9	1
1:A:132:ILE:CB	1:A:193:VAL:HG11	0.40	2.46	11	1
1:A:150:THR:HG21	1:A:224:GLU:C	0.40	2.41	14	1
1:A:134:GLY:CA	1:A:137:GLU:HG2	0.40	2.46	6	1
1:A:132:ILE:H	1:A:133:PRO:CD	0.40	2.29	11	1
1:A:165:ILE:HG23	1:A:222:ARG:CG	0.40	2.44	13	1
1:A:135:LEU:HD23	1:A:135:LEU:C	0.40	2.41	14	1
1:A:151:ARG:HB2	1:A:221:ILE:CG2	0.40	2.47	14	1
1:A:112:VAL:HB	1:A:202:ILE:HD12	0.40	1.93	1	1
1:A:151:ARG:HD3	1:A:221:ILE:O	0.40	2.16	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:150:THR:O	1:A:153:ILE:CD1	0.40	2.67	3	1
1:A:186:ASP:C	1:A:187:ILE:HG23	0.40	2.41	7	1
1:A:174:VAL:O	1:A:174:VAL:CG1	0.40	2.69	11	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	115/121 (95%)	68±4 (59±4%)	29±4 (25±4%)	18±3 (16±3%)	0	4
All	All	1610/1694 (95%)	957 (59%)	402 (25%)	251 (16%)	0	4

All 66 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	174	VAL	14
1	A	187	ILE	13
1	A	132	ILE	11
1	A	154	ASP	11
1	A	207	ASN	10
1	A	213	LEU	10
1	A	130	ASN	9
1	A	148	PRO	9
1	A	168	ILE	9
1	A	167	GLN	8
1	A	140	VAL	7
1	A	152	VAL	7
1	A	169	ASN	7
1	A	157	THR	7
1	A	166	VAL	6
1	A	153	ILE	5
1	A	171	ILE	5
1	A	147	ALA	5
1	A	172	PHE	5

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Mol	Chain	Res	Type	Models (Total)
1	A	144	ASP	4
1	A	149	GLY	4
1	A	161	ARG	4
1	A	170	GLU	4
1	A	146	ALA	4
1	A	139	GLY	3
1	A	151	ARG	3
1	A	120	LEU	3
1	A	138	LEU	3
1	A	127	PRO	3
1	A	128	PHE	3
1	A	150	THR	3
1	A	142	ASN	2
1	A	156	ALA	2
1	A	209	LYS	2
1	A	114	ARG	2
1	A	131	PRO	2
1	A	189	VAL	2
1	A	208	GLY	2
1	A	126	SER	2
1	A	143	SER	2
1	A	145	ALA	2
1	A	160	PRO	2
1	A	223	ILE	2
1	A	155	ALA	2
1	A	123	VAL	2
1	A	200	GLY	2
1	A	220	THR	2
1	A	122	ASP	2
1	A	125	ARG	1
1	A	116	LEU	1
1	A	113	GLU	1
1	A	199	ASP	1
1	A	124	SER	1
1	A	176	THR	1
1	A	112	VAL	1
1	A	221	ILE	1
1	A	136	ASP	1
1	A	141	GLY	1
1	A	173	GLN	1
1	A	214	LEU	1
1	A	137	GLU	1

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Mol	Chain	Res	Type	Models (Total)
1	A	158	SER	1
1	A	186	ASP	1
1	A	216	ASP	1
1	A	115	ARG	1
1	A	119	VAL	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	101/105 (96%)	79±3 (79±3%)	22±3 (21±3%)	3	31
All	All	1414/1470 (96%)	1112 (79%)	302 (21%)	3	31

All 77 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	132	ILE	12
1	A	223	ILE	11
1	A	137	GLU	10
1	A	165	ILE	10
1	A	171	ILE	10
1	A	195	ILE	10
1	A	210	ASP	10
1	A	211	VAL	9
1	A	184	ASP	9
1	A	214	LEU	9
1	A	154	ASP	8
1	A	153	ILE	7
1	A	168	ILE	7
1	A	183	LEU	7
1	A	221	ILE	7
1	A	216	ASP	6
1	A	226	LEU	6
1	A	113	GLU	6
1	A	152	VAL	6
1	A	187	ILE	6

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Mol	Chain	Res	Type	Models (Total)
1	A	158	SER	5
1	A	224	GLU	5
1	A	217	LEU	5
1	A	222	ARG	5
1	A	150	THR	5
1	A	167	GLN	5
1	A	130	ASN	5
1	A	119	VAL	4
1	A	213	LEU	4
1	A	135	LEU	4
1	A	202	ILE	4
1	A	175	GLU	4
1	A	123	VAL	3
1	A	138	LEU	3
1	A	143	SER	3
1	A	182	LEU	3
1	A	116	LEU	3
1	A	166	VAL	3
1	A	126	SER	3
1	A	120	LEU	3
1	A	176	THR	3
1	A	142	ASN	3
1	A	140	VAL	2
1	A	164	ARG	2
1	A	122	ASP	2
1	A	136	ASP	2
1	A	188	ARG	2
1	A	219	HIS	2
1	A	170	GLU	2
1	A	163	VAL	2
1	A	206	HIS	2
1	A	220	THR	2
1	A	177	ASP	2
1	A	209	LYS	2
1	A	114	ARG	2
1	A	225	GLU	2
1	A	174	VAL	2
1	A	212	GLU	2
1	A	151	ARG	1
1	A	115	ARG	1
1	A	162	LYS	1
1	A	198	ARG	1

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Mol	Chain	Res	Type	Models (Total)
1	A	111	GLU	1
1	A	207	ASN	1
1	A	112	VAL	1
1	A	125	ARG	1
1	A	161	ARG	1
1	A	169	ASN	1
1	A	173	GLN	1
1	A	181	GLN	1
1	A	203	THR	1
1	A	204	LEU	1
1	A	215	ASP	1
1	A	157	THR	1
1	A	178	GLN	1
1	A	192	GLU	1
1	A	201	HIS	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 ⓘ

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided