



Full wwPDB NMR Structure Validation Report ⓘ

Mar 30, 2026 – 03:50 PM UTC

PDB ID : 1ZO0 / pdb_00001zo0
Title : NMR structure of antizyme isoform 1 from rat
Authors : Hoffman, D.W.; Hackert, M.L.
Deposited on : 2005-05-12

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

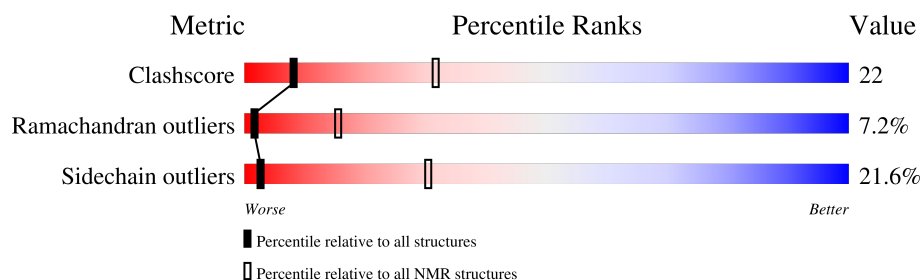
1 Overall quality at a glance

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	126	

2 Ensemble composition and analysis

This entry contains 12 models. Model 11 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:94-A:108, A:113-A:200, A:208-A:219 (115)	1.89	11

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	2, 3, 4, 5, 6, 7, 8, 10, 11
2	1, 9, 12

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 2003 atoms, of which 997 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Ornithine decarboxylase antizyme.

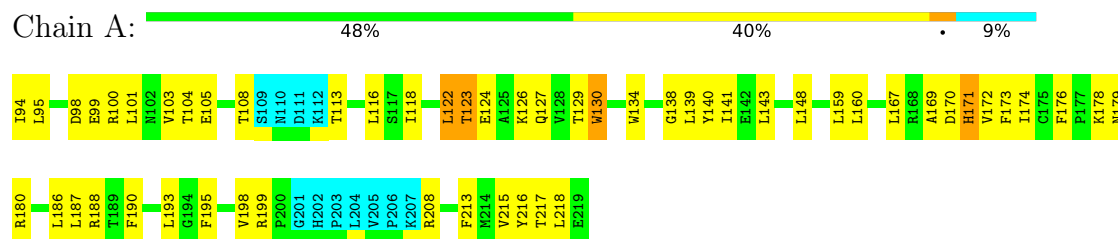
Mol	Chain	Residues	Atoms						Trace
1	A	126	Total	C	H	N	O	S	0
			2003	645	997	171	186	4	

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: Ornithine decarboxylase antizyme

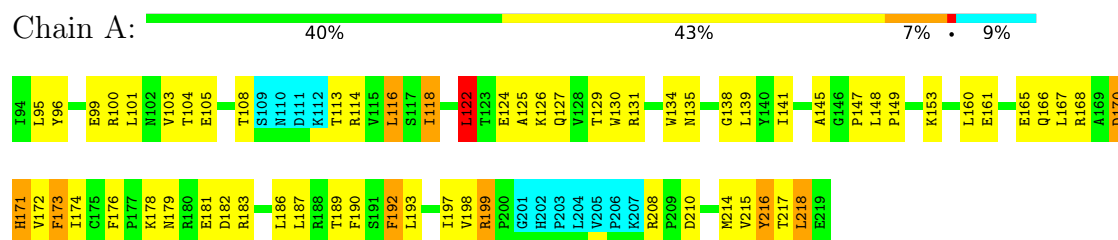


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

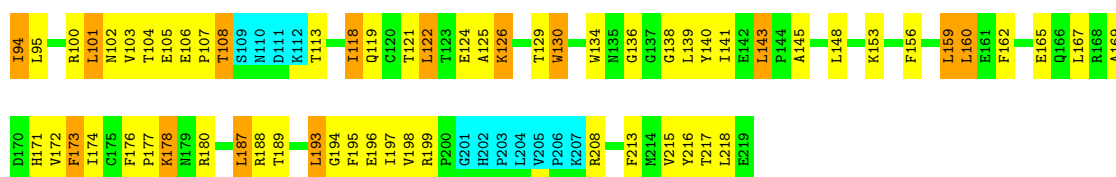
- Molecule 1: Ornithine decarboxylase antizyme



4.2.2 Score per residue for model 2

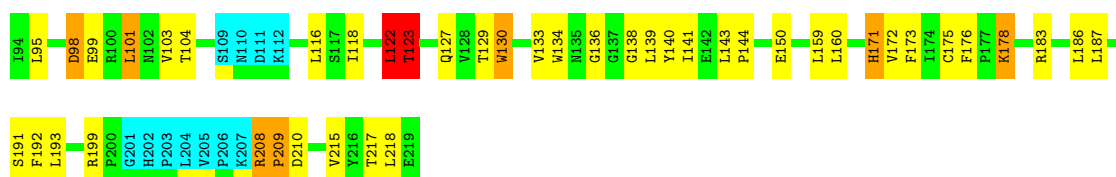
- Molecule 1: Ornithine decarboxylase antizyme





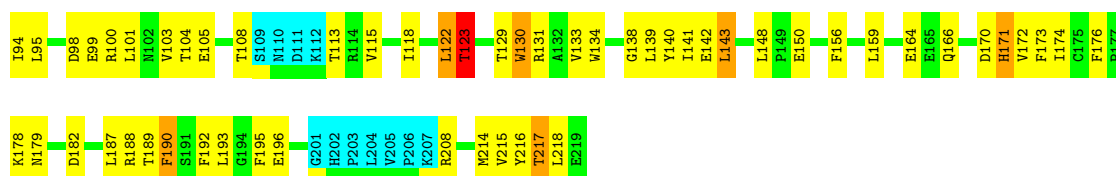
4.2.3 Score per residue for model 3

- Molecule 1: Ornithine decarboxylase antizyme



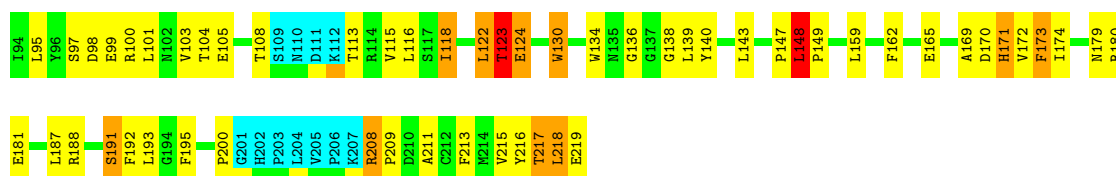
4.2.4 Score per residue for model 4

- Molecule 1: Ornithine decarboxylase antizyme



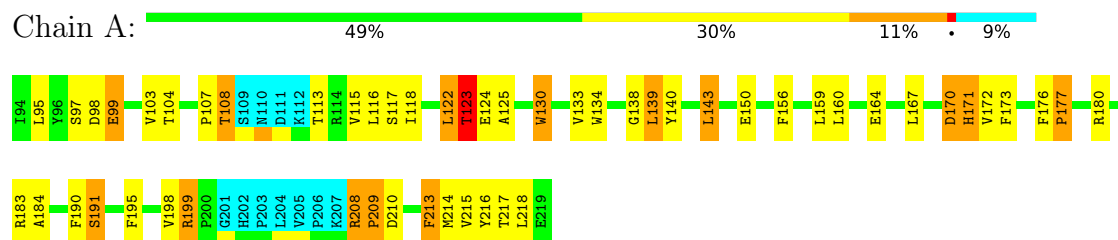
4.2.5 Score per residue for model 5

- Molecule 1: Ornithine decarboxylase antizyme



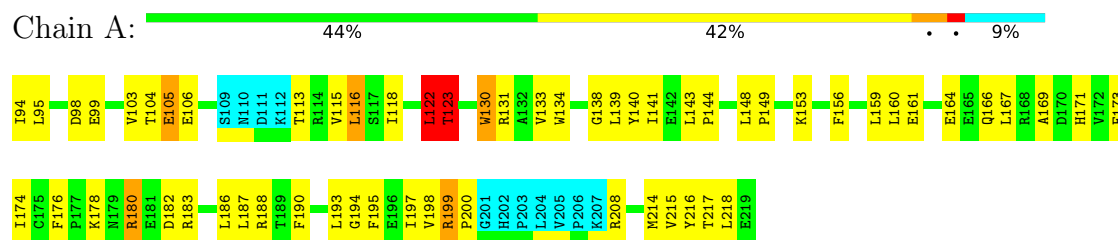
4.2.6 Score per residue for model 6

- Molecule 1: Ornithine decarboxylase antizyme



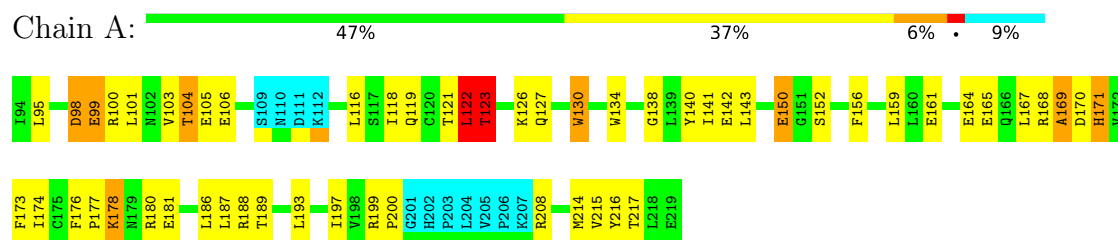
4.2.7 Score per residue for model 7

- Molecule 1: Ornithine decarboxylase antizyme



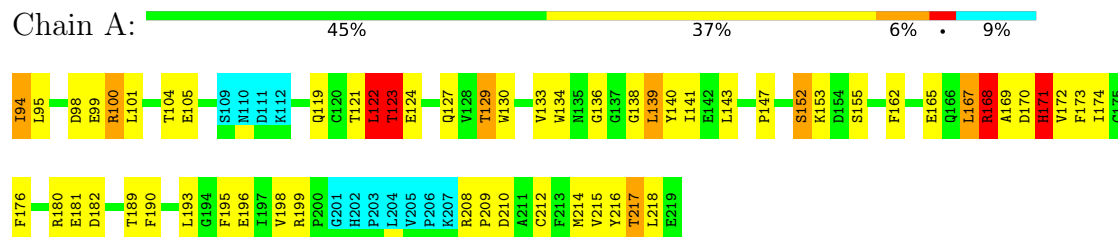
4.2.8 Score per residue for model 8

- Molecule 1: Ornithine decarboxylase antizyme



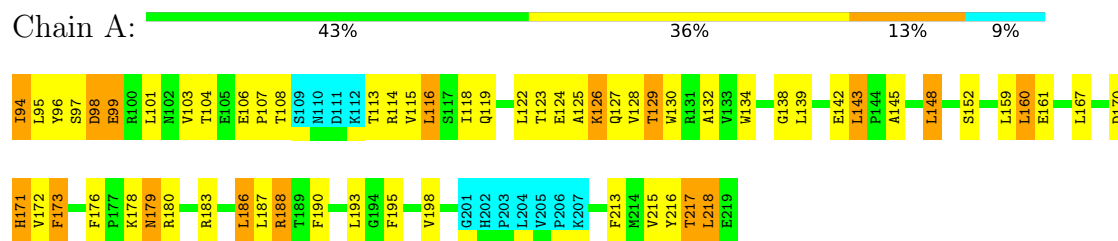
4.2.9 Score per residue for model 9

- Molecule 1: Ornithine decarboxylase antizyme



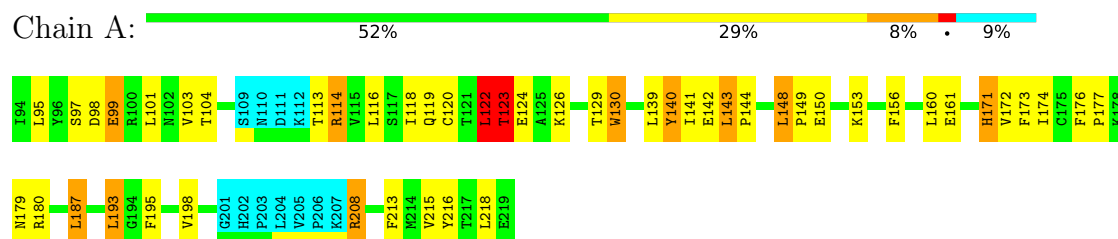
4.2.10 Score per residue for model 10

- Molecule 1: Ornithine decarboxylase antizyme



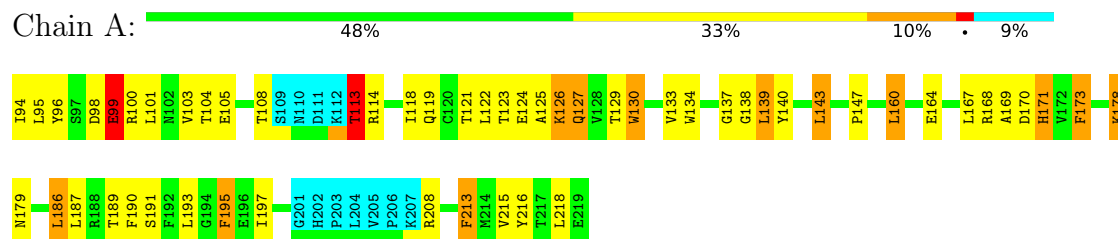
4.2.11 Score per residue for model 11 (medoid)

- Molecule 1: Ornithine decarboxylase antizyme



4.2.12 Score per residue for model 12

- Molecule 1: Ornithine decarboxylase antizyme



5 Refinement protocol and experimental data overview

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

Of the 12 calculated structures, 12 were deposited, based on the following criterion: *all calculated structures submitted*.

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

Software name	Classification	Version
CNS	refinement	1.1

No chemical shift data was provided.

6 Model quality ⓘ

6.1 Standard geometry ⓘ

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	923	911	909	40±6
All	All	11076	10932	10908	483

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 22.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:139:LEU:HD11	1:A:172:VAL:HG13	1.07	1.18	11	2
1:A:173:PHE:CD1	1:A:215:VAL:HG23	0.88	2.04	10	3
1:A:118:ILE:HG21	1:A:159:LEU:HD11	0.87	1.46	4	3
1:A:173:PHE:CE1	1:A:215:VAL:HG23	0.83	2.08	10	2
1:A:143:LEU:HD22	1:A:176:PHE:CD2	0.81	2.10	7	2
1:A:103:VAL:HG22	1:A:118:ILE:HG23	0.80	1.53	10	4
1:A:122:LEU:HA	1:A:126:LYS:O	0.80	1.77	1	2
1:A:103:VAL:HG12	1:A:118:ILE:HG22	0.79	1.55	1	2
1:A:134:TRP:CZ3	1:A:167:LEU:HD21	0.79	2.13	7	1
1:A:134:TRP:CH2	1:A:167:LEU:HD13	0.78	2.13	12	2
1:A:187:LEU:HD11	1:A:197:ILE:HG21	0.78	1.55	2	2
1:A:134:TRP:CZ3	1:A:167:LEU:HD13	0.77	2.14	1	3
1:A:143:LEU:HD13	1:A:176:PHE:CE2	0.77	2.14	7	3
1:A:134:TRP:CZ2	1:A:167:LEU:HD22	0.77	2.15	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:148:LEU:HD23	1:A:186:LEU:HD11	0.76	1.56	10	1
1:A:95:LEU:HB2	1:A:104:THR:HG22	0.76	1.58	1	4
1:A:122:LEU:HB3	1:A:125:ALA:HB3	0.76	1.57	12	2
1:A:108:THR:HG22	1:A:113:THR:O	0.75	1.80	10	2
1:A:101:LEU:HD23	1:A:119:GLN:O	0.74	1.82	2	1
1:A:119:GLN:OE1	1:A:129:THR:HG22	0.73	1.83	10	1
1:A:95:LEU:CB	1:A:104:THR:HG22	0.71	2.15	1	2
1:A:139:LEU:HD11	1:A:172:VAL:HG23	0.71	1.62	3	1
1:A:95:LEU:HD13	1:A:104:THR:OG1	0.70	1.86	12	2
1:A:141:ILE:HD12	1:A:174:ILE:CG1	0.70	2.15	4	1
1:A:133:VAL:HG23	1:A:140:TYR:HB3	0.70	1.61	4	1
1:A:116:LEU:HD23	1:A:117:SER:N	0.69	2.03	6	1
1:A:99:GLU:O	1:A:101:LEU:HD12	0.69	1.86	1	2
1:A:141:ILE:HD11	1:A:174:ILE:HG12	0.69	1.63	2	1
1:A:103:VAL:CG1	1:A:118:ILE:HG22	0.69	2.18	1	2
1:A:171:HIS:CD2	1:A:217:THR:HG23	0.69	2.23	3	4
1:A:108:THR:HG23	1:A:113:THR:O	0.69	1.88	6	1
1:A:187:LEU:CG	1:A:197:ILE:HG21	0.69	2.17	8	1
1:A:139:LEU:CD1	1:A:172:VAL:HG13	0.69	2.14	10	1
1:A:170:ASP:C	1:A:217:THR:HG23	0.69	2.12	8	2
1:A:103:VAL:HG12	1:A:118:ILE:HG23	0.68	1.63	4	1
1:A:141:ILE:HD12	1:A:174:ILE:HG13	0.68	1.64	4	1
1:A:171:HIS:NE2	1:A:217:THR:HG23	0.68	2.04	7	3
1:A:101:LEU:HD12	1:A:119:GLN:O	0.68	1.89	12	2
1:A:103:VAL:CG1	1:A:118:ILE:HG23	0.68	2.19	4	1
1:A:173:PHE:HB3	1:A:215:VAL:HG12	0.68	1.66	5	2
1:A:173:PHE:CD2	1:A:215:VAL:HG23	0.67	2.23	2	1
1:A:139:LEU:HD21	1:A:172:VAL:HG22	0.67	1.67	10	2
1:A:173:PHE:CE2	1:A:215:VAL:HG23	0.67	2.24	2	1
1:A:95:LEU:HA	1:A:104:THR:HG22	0.67	1.65	4	1
1:A:208:ARG:CG	1:A:211:ALA:HB3	0.66	2.21	5	1
1:A:141:ILE:HD11	1:A:174:ILE:CG1	0.66	2.19	2	1
1:A:160:LEU:HD11	1:A:216:TYR:OH	0.66	1.91	12	1
1:A:133:VAL:HG13	1:A:140:TYR:HB2	0.66	1.68	3	2
1:A:143:LEU:HD22	1:A:177:PRO:HD3	0.65	1.68	6	1
1:A:141:ILE:HB	1:A:174:ILE:HG22	0.65	1.67	8	1
1:A:116:LEU:HD22	1:A:132:ALA:O	0.65	1.91	10	1
1:A:139:LEU:O	1:A:172:VAL:HG13	0.65	1.92	9	1
1:A:187:LEU:HG	1:A:197:ILE:HG21	0.65	1.69	8	1
1:A:101:LEU:HD11	1:A:118:ILE:HG13	0.65	1.69	12	1
1:A:130:TRP:CZ3	1:A:159:LEU:HD22	0.64	2.28	5	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:137:GLY:O	1:A:169:ALA:HB1	0.64	1.93	12	1
1:A:187:LEU:CD1	1:A:197:ILE:HG21	0.64	2.23	8	1
1:A:170:ASP:O	1:A:172:VAL:HG23	0.64	1.93	1	2
1:A:116:LEU:N	1:A:116:LEU:HD22	0.63	2.08	7	1
1:A:116:LEU:HD13	1:A:116:LEU:N	0.63	2.09	10	1
1:A:122:LEU:HA	1:A:126:LYS:C	0.63	2.18	1	2
1:A:187:LEU:HD23	1:A:214:MET:SD	0.63	2.33	7	1
1:A:170:ASP:CG	1:A:218:LEU:HD13	0.63	2.19	10	1
1:A:103:VAL:CG1	1:A:116:LEU:HD21	0.62	2.24	6	1
1:A:173:PHE:CZ	1:A:215:VAL:HG21	0.62	2.29	11	2
1:A:187:LEU:HD11	1:A:197:ILE:HD11	0.62	1.71	12	1
1:A:160:LEU:CD1	1:A:172:VAL:HG11	0.62	2.24	1	1
1:A:104:THR:O	1:A:116:LEU:HD13	0.62	1.94	5	1
1:A:164:GLU:HB3	1:A:218:LEU:HD22	0.62	1.72	12	1
1:A:106:GLU:HB3	1:A:115:VAL:HG23	0.61	1.73	7	1
1:A:94:ILE:HD13	1:A:94:ILE:N	0.60	2.11	9	1
1:A:133:VAL:HG13	1:A:140:TYR:CB	0.60	2.26	3	1
1:A:139:LEU:O	1:A:139:LEU:HD12	0.60	1.96	11	1
1:A:159:LEU:HD12	1:A:160:LEU:N	0.60	2.11	10	1
1:A:187:LEU:HD11	1:A:197:ILE:CG2	0.59	2.27	2	2
1:A:141:ILE:HD12	1:A:174:ILE:HG12	0.59	1.75	9	1
1:A:143:LEU:HD13	1:A:144:PRO:HD2	0.59	1.75	11	1
1:A:139:LEU:CD2	1:A:172:VAL:HG22	0.59	2.28	10	1
1:A:218:LEU:O	1:A:218:LEU:HD13	0.58	1.98	2	1
1:A:94:ILE:HG22	1:A:105:GLU:HB2	0.58	1.75	4	1
1:A:101:LEU:HD11	1:A:118:ILE:CG1	0.58	2.29	12	1
1:A:218:LEU:O	1:A:218:LEU:HD23	0.58	1.99	5	1
1:A:103:VAL:HG11	1:A:118:ILE:HD12	0.58	1.75	12	1
1:A:98:ASP:HB3	1:A:101:LEU:HD21	0.57	1.74	10	1
1:A:134:TRP:CH2	1:A:167:LEU:HD22	0.57	2.33	6	1
1:A:122:LEU:CB	1:A:125:ALA:HB3	0.57	2.29	10	2
1:A:173:PHE:CD1	1:A:215:VAL:HG12	0.57	2.34	7	1
1:A:123:THR:HG22	1:A:124:GLU:HG3	0.57	1.75	10	1
1:A:171:HIS:CD2	1:A:217:THR:HG22	0.57	2.35	1	1
1:A:171:HIS:CE1	1:A:217:THR:HG23	0.56	2.34	4	2
1:A:94:ILE:HD12	1:A:96:TYR:OH	0.56	2.00	10	1
1:A:115:VAL:C	1:A:116:LEU:HD13	0.56	2.24	10	1
1:A:134:TRP:CE3	1:A:167:LEU:HD13	0.56	2.35	10	1
1:A:101:LEU:HD21	1:A:118:ILE:HD11	0.56	1.76	12	1
1:A:183:ARG:NH1	1:A:184:ALA:HB2	0.56	2.16	6	1
1:A:95:LEU:HB2	1:A:104:THR:HG23	0.56	1.76	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:130:TRP:HE1	1:A:143:LEU:HD22	0.55	1.61	11	2
1:A:115:VAL:O	1:A:116:LEU:HD22	0.55	2.00	5	1
1:A:100:ARG:C	1:A:101:LEU:HD12	0.55	2.26	9	1
1:A:98:ASP:O	1:A:99:GLU:C	0.55	2.49	6	6
1:A:103:VAL:HG13	1:A:116:LEU:HD21	0.55	1.78	6	1
1:A:141:ILE:HD12	1:A:174:ILE:HG22	0.55	1.79	7	2
1:A:94:ILE:O	1:A:104:THR:HG23	0.55	2.01	7	1
1:A:122:LEU:HD23	1:A:127:GLN:CD	0.55	2.27	1	1
1:A:105:GLU:HA	1:A:116:LEU:HD12	0.54	1.78	1	2
1:A:141:ILE:CB	1:A:174:ILE:HG22	0.54	2.32	8	1
1:A:103:VAL:HG22	1:A:118:ILE:HG22	0.54	1.77	5	1
1:A:208:ARG:N	1:A:209:PRO:CD	0.54	2.70	3	4
1:A:116:LEU:HD22	1:A:116:LEU:H	0.54	1.63	10	1
1:A:121:THR:HG23	1:A:127:GLN:HB3	0.54	1.80	9	2
1:A:134:TRP:CE3	1:A:167:LEU:HD21	0.53	2.38	7	1
1:A:94:ILE:HD11	1:A:107:PRO:HD3	0.53	1.79	2	1
1:A:187:LEU:HD23	1:A:187:LEU:C	0.53	2.28	3	1
1:A:139:LEU:HD12	1:A:167:LEU:HD12	0.53	1.80	12	1
1:A:113:THR:HG22	1:A:135:ASN:HA	0.53	1.79	1	1
1:A:183:ARG:O	1:A:187:LEU:HD12	0.53	2.03	7	1
1:A:141:ILE:HB	1:A:174:ILE:HG23	0.53	1.79	9	1
1:A:122:LEU:HA	1:A:126:LYS:H	0.53	1.63	2	2
1:A:139:LEU:HD12	1:A:139:LEU:C	0.53	2.29	11	1
1:A:140:TYR:O	1:A:141:ILE:HD13	0.52	2.03	11	2
1:A:216:TYR:CD1	1:A:216:TYR:N	0.52	2.76	1	2
1:A:100:ARG:O	1:A:101:LEU:HD12	0.52	2.05	2	1
1:A:143:LEU:HD13	1:A:144:PRO:CD	0.52	2.34	11	1
1:A:139:LEU:HD12	1:A:167:LEU:HD13	0.52	1.81	6	1
1:A:187:LEU:CD1	1:A:197:ILE:HD11	0.52	2.34	12	1
1:A:167:LEU:HD12	1:A:167:LEU:O	0.52	2.04	7	1
1:A:95:LEU:HD23	1:A:95:LEU:N	0.52	2.20	7	2
1:A:173:PHE:CZ	1:A:215:VAL:HG23	0.52	2.39	3	1
1:A:187:LEU:HB3	1:A:214:MET:HE3	0.52	1.80	4	1
1:A:103:VAL:CG1	1:A:118:ILE:HD12	0.52	2.35	12	1
1:A:130:TRP:CH2	1:A:156:PHE:CD1	0.52	2.98	4	2
1:A:95:LEU:HD23	1:A:95:LEU:H	0.52	1.65	1	5
1:A:143:LEU:HD23	1:A:147:PRO:CB	0.52	2.35	9	1
1:A:124:GLU:O	1:A:125:ALA:HB3	0.51	2.06	1	3
1:A:121:THR:HG22	1:A:127:GLN:HB3	0.51	1.82	8	1
1:A:140:TYR:CD1	1:A:173:PHE:CD2	0.51	2.99	8	1
1:A:122:LEU:CA	1:A:126:LYS:O	0.51	2.57	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:140:TYR:CE1	1:A:213:PHE:CZ	0.51	2.99	5	1
1:A:173:PHE:CD1	1:A:213:PHE:CE1	0.51	2.99	12	1
1:A:95:LEU:HB3	1:A:104:THR:HG23	0.51	1.83	6	1
1:A:103:VAL:HG23	1:A:118:ILE:HG13	0.50	1.81	7	1
1:A:130:TRP:CH2	1:A:156:PHE:CE2	0.50	3.00	6	2
1:A:148:LEU:CD2	1:A:186:LEU:HD11	0.50	2.37	7	1
1:A:195:PHE:CE1	1:A:216:TYR:CD2	0.50	2.99	10	1
1:A:103:VAL:HG13	1:A:118:ILE:HG12	0.50	1.83	11	1
1:A:174:ILE:HG23	1:A:216:TYR:OH	0.50	2.06	1	1
1:A:190:PHE:CE1	1:A:195:PHE:CE2	0.50	3.00	9	1
1:A:122:LEU:HD23	1:A:123:THR:N	0.50	2.21	6	1
1:A:195:PHE:CE1	1:A:216:TYR:CE1	0.50	2.99	9	1
1:A:118:ILE:CG2	1:A:159:LEU:HD11	0.50	2.33	7	1
1:A:195:PHE:CD1	1:A:216:TYR:CD1	0.50	3.00	10	2
1:A:134:TRP:CZ3	1:A:138:GLY:C	0.50	2.89	10	11
1:A:164:GLU:CG	1:A:169:ALA:HB3	0.50	2.37	8	1
1:A:103:VAL:HG23	1:A:118:ILE:HG22	0.50	1.83	3	1
1:A:140:TYR:CZ	1:A:173:PHE:CD1	0.50	3.00	6	1
1:A:213:PHE:CD1	1:A:213:PHE:N	0.50	2.79	6	1
1:A:173:PHE:CD1	1:A:213:PHE:CD1	0.50	2.99	12	1
1:A:196:GLU:HB2	1:A:215:VAL:HG23	0.50	1.83	9	1
1:A:119:GLN:OE1	1:A:129:THR:HG23	0.49	2.06	11	1
1:A:147:PRO:O	1:A:148:LEU:HD12	0.49	2.07	5	1
1:A:167:LEU:O	1:A:168:ARG:CB	0.49	2.60	8	2
1:A:171:HIS:HA	1:A:216:TYR:O	0.49	2.07	1	2
1:A:186:LEU:HD13	1:A:190:PHE:CD1	0.49	2.42	12	1
1:A:187:LEU:HD12	1:A:188:ARG:N	0.49	2.21	10	1
1:A:103:VAL:HG23	1:A:118:ILE:CG2	0.49	2.38	3	1
1:A:139:LEU:HD23	1:A:140:TYR:N	0.49	2.22	4	1
1:A:122:LEU:O	1:A:123:THR:C	0.49	2.55	6	8
1:A:171:HIS:CG	1:A:217:THR:HG22	0.49	2.43	1	1
1:A:208:ARG:N	1:A:209:PRO:HD3	0.49	2.22	9	1
1:A:195:PHE:CZ	1:A:216:TYR:CD2	0.49	3.00	10	1
1:A:121:THR:HG22	1:A:127:GLN:CB	0.48	2.38	8	1
1:A:130:TRP:CH2	1:A:156:PHE:CE1	0.48	3.01	8	2
1:A:190:PHE:CD2	1:A:216:TYR:CE2	0.48	3.01	4	1
1:A:139:LEU:HD12	1:A:167:LEU:CD1	0.48	2.39	6	1
1:A:170:ASP:O	1:A:172:VAL:N	0.48	2.47	4	3
1:A:208:ARG:CG	1:A:209:PRO:HD3	0.48	2.39	3	1
1:A:148:LEU:O	1:A:148:LEU:HD23	0.48	2.09	4	1
1:A:138:GLY:HA3	1:A:171:HIS:CD2	0.48	2.43	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:101:LEU:HD23	1:A:101:LEU:N	0.48	2.23	10	2
1:A:173:PHE:CE2	1:A:215:VAL:HG21	0.48	2.44	11	1
1:A:140:TYR:CE1	1:A:173:PHE:CD1	0.47	3.01	6	1
1:A:190:PHE:CD1	1:A:195:PHE:CE2	0.47	3.02	10	1
1:A:159:LEU:C	1:A:159:LEU:HD23	0.47	2.35	8	1
1:A:197:ILE:HD12	1:A:197:ILE:O	0.47	2.09	8	1
1:A:130:TRP:CZ2	1:A:143:LEU:HD21	0.47	2.45	12	1
1:A:148:LEU:HD11	1:A:176:PHE:CD2	0.47	2.45	1	1
1:A:198:VAL:CG1	1:A:213:PHE:CE2	0.47	2.98	6	1
1:A:164:GLU:CD	1:A:218:LEU:HD22	0.47	2.34	7	1
1:A:173:PHE:CE2	1:A:215:VAL:HG12	0.47	2.45	9	1
1:A:148:LEU:HD22	1:A:186:LEU:HD11	0.47	1.85	7	1
1:A:182:ASP:O	1:A:186:LEU:HD12	0.47	2.10	7	1
1:A:171:HIS:CD2	1:A:171:HIS:N	0.47	2.82	10	1
1:A:122:LEU:CA	1:A:126:LYS:H	0.46	2.23	1	2
1:A:100:ARG:HB3	1:A:101:LEU:HD23	0.46	1.87	5	1
1:A:172:VAL:HG22	1:A:216:TYR:O	0.46	2.10	6	1
1:A:143:LEU:CD1	1:A:176:PHE:CZ	0.46	2.99	3	1
1:A:170:ASP:OD1	1:A:218:LEU:HD13	0.46	2.09	10	1
1:A:174:ILE:CG2	1:A:176:PHE:CE2	0.46	2.99	2	1
1:A:103:VAL:CG2	1:A:118:ILE:HG22	0.46	2.40	3	1
1:A:196:GLU:HB2	1:A:215:VAL:HG13	0.46	1.87	4	1
1:A:171:HIS:HB3	1:A:217:THR:HG23	0.46	1.87	5	1
1:A:187:LEU:HD11	1:A:197:ILE:CB	0.46	2.40	8	1
1:A:187:LEU:HD22	1:A:214:MET:CB	0.46	2.41	4	1
1:A:195:PHE:CD1	1:A:196:GLU:N	0.46	2.84	2	1
1:A:188:ARG:O	1:A:192:PHE:HA	0.46	2.10	5	1
1:A:167:LEU:HG	1:A:169:ALA:HB2	0.46	1.87	7	1
1:A:96:TYR:CZ	1:A:103:VAL:CG2	0.46	2.99	1	1
1:A:134:TRP:CZ3	1:A:167:LEU:CD1	0.46	2.99	12	2
1:A:173:PHE:CZ	1:A:215:VAL:CG2	0.46	2.98	3	3
1:A:171:HIS:CG	1:A:217:THR:HG23	0.45	2.46	4	1
1:A:143:LEU:HD13	1:A:176:PHE:CD1	0.45	2.46	6	2
1:A:116:LEU:N	1:A:116:LEU:CD1	0.45	2.78	10	1
1:A:164:GLU:CB	1:A:218:LEU:HD22	0.45	2.39	12	1
1:A:95:LEU:CB	1:A:104:THR:HG23	0.45	2.41	8	2
1:A:218:LEU:HD13	1:A:218:LEU:C	0.45	2.36	2	1
1:A:133:VAL:CG2	1:A:140:TYR:CD1	0.45	2.99	4	1
1:A:123:THR:HG22	1:A:124:GLU:N	0.45	2.26	12	1
1:A:171:HIS:CD2	1:A:217:THR:CG2	0.45	2.99	1	3
1:A:173:PHE:CD1	1:A:173:PHE:N	0.45	2.84	2	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:170:ASP:O	1:A:217:THR:HG23	0.45	2.11	6	1
1:A:133:VAL:HG13	1:A:140:TYR:HB3	0.45	1.87	7	1
1:A:130:TRP:CZ3	1:A:159:LEU:HD13	0.45	2.46	2	1
1:A:195:PHE:CD1	1:A:216:TYR:CB	0.45	2.99	5	2
1:A:173:PHE:CD1	1:A:215:VAL:CG1	0.45	2.99	7	1
1:A:164:GLU:OE2	1:A:218:LEU:HD22	0.45	2.12	7	1
1:A:172:VAL:HG13	1:A:172:VAL:O	0.45	2.12	3	1
1:A:173:PHE:CE2	1:A:215:VAL:CG2	0.45	2.99	3	2
1:A:176:PHE:CD1	1:A:176:PHE:N	0.45	2.84	11	2
1:A:143:LEU:HD22	1:A:176:PHE:HD2	0.45	1.70	9	2
1:A:94:ILE:CG2	1:A:96:TYR:CE2	0.45	3.00	12	1
1:A:148:LEU:CB	1:A:149:PRO:CD	0.45	2.95	5	3
1:A:134:TRP:CH2	1:A:169:ALA:HB2	0.45	2.47	2	2
1:A:170:ASP:O	1:A:171:HIS:HB2	0.45	2.12	8	2
1:A:195:PHE:CE1	1:A:216:TYR:CG	0.45	3.05	10	1
1:A:148:LEU:HD21	1:A:176:PHE:CD2	0.45	2.47	11	1
1:A:171:HIS:CD2	1:A:215:VAL:HG22	0.45	2.47	11	1
1:A:141:ILE:HD12	1:A:174:ILE:CG2	0.45	2.41	1	1
1:A:103:VAL:HG13	1:A:118:ILE:HG13	0.45	1.88	10	1
1:A:139:LEU:HD13	1:A:167:LEU:HD12	0.45	1.88	2	1
1:A:116:LEU:N	1:A:116:LEU:CD2	0.45	2.80	7	1
1:A:198:VAL:CG1	1:A:213:PHE:CZ	0.45	3.00	10	2
1:A:96:TYR:CE2	1:A:103:VAL:CG2	0.44	2.99	1	1
1:A:122:LEU:HD23	1:A:122:LEU:C	0.44	2.37	6	1
1:A:186:LEU:HD13	1:A:190:PHE:CE1	0.44	2.47	12	1
1:A:187:LEU:CD2	1:A:197:ILE:HG21	0.44	2.42	1	1
1:A:215:VAL:HG23	1:A:215:VAL:O	0.44	2.11	5	1
1:A:190:PHE:CD2	1:A:214:MET:CE	0.44	3.00	7	1
1:A:95:LEU:HD12	1:A:96:TYR:N	0.44	2.28	12	1
1:A:140:TYR:CD1	1:A:173:PHE:CE2	0.44	3.05	8	1
1:A:171:HIS:CD2	1:A:215:VAL:CG2	0.44	3.00	8	1
1:A:101:LEU:HD23	1:A:101:LEU:H	0.44	1.73	10	1
1:A:133:VAL:HG23	1:A:140:TYR:HB2	0.44	1.87	6	2
1:A:195:PHE:CD1	1:A:195:PHE:N	0.44	2.85	7	1
1:A:164:GLU:CD	1:A:218:LEU:HD13	0.44	2.38	6	1
1:A:130:TRP:CZ3	1:A:159:LEU:CD2	0.44	3.00	5	1
1:A:191:SER:O	1:A:195:PHE:CD1	0.44	2.71	6	1
1:A:173:PHE:HD1	1:A:215:VAL:HG23	0.44	1.73	4	2
1:A:94:ILE:O	1:A:105:GLU:N	0.44	2.50	2	2
1:A:170:ASP:O	1:A:171:HIS:CG	0.44	2.70	9	1
1:A:187:LEU:HD12	1:A:195:PHE:CZ	0.44	2.48	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:116:LEU:HD22	1:A:116:LEU:N	0.43	2.27	10	1
1:A:139:LEU:CD1	1:A:167:LEU:HD12	0.43	2.43	2	1
1:A:191:SER:O	1:A:192:PHE:CB	0.43	2.66	5	2
1:A:188:ARG:HA	1:A:192:PHE:HA	0.43	1.88	5	1
1:A:115:VAL:C	1:A:116:LEU:HD22	0.43	2.38	5	1
1:A:215:VAL:O	1:A:215:VAL:HG13	0.43	2.13	6	3
1:A:174:ILE:O	1:A:174:ILE:HG23	0.43	2.12	11	1
1:A:98:ASP:O	1:A:101:LEU:HD23	0.43	2.13	3	1
1:A:98:ASP:HB2	1:A:101:LEU:HD21	0.43	1.90	11	1
1:A:119:GLN:CD	1:A:129:THR:HG22	0.43	2.38	10	1
1:A:122:LEU:CB	1:A:126:LYS:N	0.43	2.81	1	1
1:A:170:ASP:O	1:A:171:HIS:CB	0.43	2.66	8	1
1:A:125:ALA:O	1:A:126:LYS:CB	0.43	2.67	10	1
1:A:143:LEU:CD1	1:A:176:PHE:CE2	0.43	3.00	10	1
1:A:183:ARG:CD	1:A:187:LEU:HD23	0.43	2.44	10	1
1:A:164:GLU:OE2	1:A:218:LEU:HD13	0.43	2.14	6	1
1:A:94:ILE:N	1:A:94:ILE:CD1	0.43	2.81	9	1
1:A:120:CYS:SG	1:A:122:LEU:HD21	0.43	2.53	11	1
1:A:183:ARG:HD3	1:A:187:LEU:HD23	0.42	1.89	10	1
1:A:187:LEU:HD12	1:A:195:PHE:HZ	0.42	1.74	12	1
1:A:122:LEU:CA	1:A:126:LYS:C	0.42	2.92	1	1
1:A:98:ASP:N	1:A:101:LEU:O	0.42	2.49	4	1
1:A:160:LEU:O	1:A:160:LEU:HD13	0.42	2.14	2	1
1:A:122:LEU:O	1:A:124:GLU:N	0.42	2.53	5	1
1:A:171:HIS:HB3	1:A:217:THR:HA	0.42	1.92	5	1
1:A:134:TRP:CZ3	1:A:138:GLY:O	0.42	2.73	6	2
1:A:95:LEU:CA	1:A:104:THR:HG23	0.42	2.45	8	1
1:A:193:LEU:HD23	1:A:216:TYR:CE2	0.42	2.49	8	1
1:A:208:ARG:H	1:A:209:PRO:CD	0.42	2.27	3	1
1:A:190:PHE:CD2	1:A:214:MET:HE3	0.42	2.50	7	1
1:A:139:LEU:HD11	1:A:172:VAL:CG1	0.42	2.12	11	1
1:A:187:LEU:HD23	1:A:195:PHE:CE1	0.42	2.50	11	1
1:A:198:VAL:HG12	1:A:199:ARG:N	0.42	2.29	9	4
1:A:139:LEU:C	1:A:139:LEU:HD12	0.42	2.40	3	1
1:A:130:TRP:CH2	1:A:156:PHE:CZ	0.42	3.08	11	1
1:A:140:TYR:CD1	1:A:140:TYR:C	0.42	2.98	4	1
1:A:122:LEU:HD13	1:A:126:LYS:O	0.42	2.15	10	1
1:A:140:TYR:CZ	1:A:142:GLU:CG	0.42	3.03	8	1
1:A:130:TRP:HZ3	1:A:159:LEU:HD22	0.41	1.74	5	2
1:A:191:SER:O	1:A:195:PHE:CG	0.41	2.72	6	1
1:A:190:PHE:O	1:A:195:PHE:CD2	0.41	2.73	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:105:GLU:HG3	1:A:116:LEU:HD23	0.41	1.91	8	1
1:A:143:LEU:HD23	1:A:177:PRO:HD2	0.41	1.91	8	1
1:A:94:ILE:HD11	1:A:105:GLU:O	0.41	2.16	2	1
1:A:130:TRP:HZ3	1:A:159:LEU:HD13	0.41	1.75	2	1
1:A:193:LEU:HD23	1:A:193:LEU:O	0.41	2.15	11	1
1:A:134:TRP:HE3	1:A:139:LEU:HD12	0.41	1.75	1	1
1:A:139:LEU:O	1:A:173:PHE:CZ	0.41	2.73	4	1
1:A:171:HIS:CE1	1:A:173:PHE:CE1	0.41	3.09	8	1
1:A:195:PHE:CD1	1:A:195:PHE:C	0.41	2.98	12	1
1:A:139:LEU:O	1:A:173:PHE:CD2	0.41	2.73	7	1
1:A:190:PHE:CD1	1:A:195:PHE:CD2	0.41	3.08	9	1
1:A:216:TYR:CG	1:A:217:THR:N	0.41	2.88	9	1
1:A:198:VAL:O	1:A:213:PHE:CD1	0.41	2.73	11	1
1:A:195:PHE:CD1	1:A:216:TYR:HB2	0.41	2.51	5	1
1:A:140:TYR:C	1:A:140:TYR:CD1	0.41	2.99	2	1
1:A:138:GLY:HA3	1:A:171:HIS:O	0.41	2.16	12	1
1:A:170:ASP:CA	1:A:217:THR:HG23	0.41	2.45	6	1
1:A:119:GLN:NE2	1:A:129:THR:HG22	0.41	2.31	9	1
1:A:96:TYR:CD1	1:A:96:TYR:N	0.41	2.89	1	1
1:A:143:LEU:C	1:A:143:LEU:HD13	0.41	2.41	2	1
1:A:171:HIS:CE1	1:A:217:THR:CG2	0.41	3.03	4	1
1:A:171:HIS:O	1:A:173:PHE:CD1	0.41	2.73	4	1
1:A:199:ARG:O	1:A:213:PHE:CE1	0.41	2.74	6	1
1:A:143:LEU:HD23	1:A:147:PRO:HB2	0.41	1.92	9	1
1:A:171:HIS:CG	1:A:217:THR:OG1	0.41	2.74	10	1
1:A:130:TRP:CZ2	1:A:156:PHE:CE2	0.41	3.09	2	1
1:A:134:TRP:CE2	1:A:136:GLY:O	0.41	2.74	2	4
1:A:194:GLY:O	1:A:216:TYR:CD1	0.41	2.74	2	1
1:A:171:HIS:CD2	1:A:217:THR:OG1	0.41	2.73	3	3
1:A:191:SER:HB2	1:A:195:PHE:CZ	0.41	2.51	5	1
1:A:104:THR:HG22	1:A:105:GLU:N	0.41	2.31	9	1
1:A:98:ASP:O	1:A:100:ARG:N	0.41	2.53	12	1
1:A:118:ILE:HG23	1:A:118:ILE:O	0.41	2.16	12	1
1:A:216:TYR:CE2	1:A:217:THR:O	0.41	2.74	2	1
1:A:115:VAL:HA	1:A:133:VAL:HG12	0.41	1.91	4	1
1:A:195:PHE:CD1	1:A:195:PHE:O	0.41	2.74	12	1
1:A:194:GLY:O	1:A:216:TYR:CE1	0.40	2.74	2	1
1:A:190:PHE:O	1:A:216:TYR:CD2	0.40	2.74	6	1
1:A:94:ILE:O	1:A:104:THR:HA	0.40	2.15	9	1
1:A:133:VAL:CG1	1:A:140:TYR:CB	0.40	2.99	3	1
1:A:189:THR:O	1:A:192:PHE:CD2	0.40	2.75	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:103:VAL:HG13	1:A:118:ILE:HG22	0.40	1.94	5	1
1:A:191:SER:CB	1:A:195:PHE:CB	0.40	3.00	6	1
1:A:176:PHE:CE1	1:A:214:MET:HE1	0.40	2.51	1	1
1:A:189:THR:O	1:A:192:PHE:CD1	0.40	2.75	1	1
1:A:171:HIS:NE2	1:A:217:THR:CG2	0.40	2.85	4	1
1:A:172:VAL:O	1:A:216:TYR:CE1	0.40	2.74	5	1
1:A:114:ARG:CD	1:A:116:LEU:HD11	0.40	2.46	11	1
1:A:134:TRP:CZ2	1:A:136:GLY:O	0.40	2.75	3	1
1:A:195:PHE:O	1:A:195:PHE:CD1	0.40	2.74	4	1
1:A:216:TYR:CD1	1:A:216:TYR:O	0.40	2.74	11	1

6.3 Torsion angles

6.3.1 Protein backbone

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	113/126 (90%)	90±4 (79±3%)	15±4 (13±3%)	8±1 (7±1%)	2	15
All	All	1356/1512 (90%)	1078 (79%)	181 (13%)	97 (7%)	2	15

All 32 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	122	LEU	10
1	A	171	HIS	9
1	A	123	THR	8
1	A	179	ASN	5
1	A	178	LYS	5
1	A	99	GLU	5
1	A	208	ARG	4
1	A	180	ARG	4
1	A	193	LEU	4
1	A	113	THR	4
1	A	145	ALA	3
1	A	177	PRO	3

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Mol	Chain	Res	Type	Models (Total)
1	A	200	PRO	3
1	A	147	PRO	2
1	A	181	GLU	2
1	A	182	ASP	2
1	A	218	LEU	2
1	A	144	PRO	2
1	A	209	PRO	2
1	A	210	ASP	2
1	A	107	PRO	2
1	A	152	SER	2
1	A	169	ALA	2
1	A	126	LYS	2
1	A	108	THR	1
1	A	148	LEU	1
1	A	191	SER	1
1	A	149	PRO	1
1	A	194	GLY	1
1	A	100	ARG	1
1	A	150	GLU	1
1	A	168	ARG	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	99/109 (91%)	78±4 (78±4%)	21±4 (22±4%)	3	30
All	All	1188/1308 (91%)	931 (78%)	257 (22%)	3	30

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	130	TRP	12
1	A	123	THR	8
1	A	129	THR	7
1	A	178	LYS	7
1	A	193	LEU	7

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Mol	Chain	Res	Type	Models (Total)
1	A	143	LEU	7
1	A	160	LEU	7
1	A	208	ARG	7
1	A	122	LEU	6
1	A	218	LEU	6
1	A	108	THR	5
1	A	153	LYS	5
1	A	161	GLU	5
1	A	165	GLU	5
1	A	173	PHE	5
1	A	186	LEU	5
1	A	199	ARG	5
1	A	188	ARG	5
1	A	98	ASP	5
1	A	150	GLU	5
1	A	180	ARG	5
1	A	114	ARG	4
1	A	116	LEU	4
1	A	126	LYS	4
1	A	148	LEU	4
1	A	189	THR	4
1	A	217	THR	4
1	A	97	SER	4
1	A	99	GLU	4
1	A	139	LEU	4
1	A	171	HIS	4
1	A	100	ARG	3
1	A	118	ILE	3
1	A	131	ARG	3
1	A	166	GLN	3
1	A	168	ARG	3
1	A	170	ASP	3
1	A	94	ILE	3
1	A	106	GLU	3
1	A	162	PHE	3
1	A	187	LEU	3
1	A	213	PHE	3
1	A	127	GLN	3
1	A	142	GLU	3
1	A	105	GLU	3
1	A	124	GLU	3
1	A	214	MET	3

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Mol	Chain	Res	Type	Models (Total)
1	A	183	ARG	2
1	A	190	PHE	2
1	A	210	ASP	2
1	A	101	LEU	2
1	A	95	LEU	2
1	A	104	THR	2
1	A	181	GLU	2
1	A	191	SER	2
1	A	152	SER	2
1	A	179	ASN	2
1	A	192	PHE	1
1	A	216	TYR	1
1	A	102	ASN	1
1	A	121	THR	1
1	A	159	LEU	1
1	A	172	VAL	1
1	A	175	CYS	1
1	A	164	GLU	1
1	A	182	ASP	1
1	A	174	ILE	1
1	A	219	GLU	1
1	A	156	PHE	1
1	A	197	ILE	1
1	A	155	SER	1
1	A	167	LEU	1
1	A	212	CYS	1
1	A	128	VAL	1
1	A	140	TYR	1
1	A	113	THR	1
1	A	195	PHE	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 [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided