



Full wwPDB NMR Structure Validation Report ⓘ

Mar 10, 2026 – 05:07 AM UTC

PDB ID : 1VDJ / pdb_00001vdj
Title : Solution structure of actin-binding domain of troponin in Ca²⁺-bound state
Authors : Murakami, K.; Yumoto, F.; Ohki, S.; Yasunaga, T.; Tanokura, M.; Wakabayashi, T.
Deposited on : 2004-03-22

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

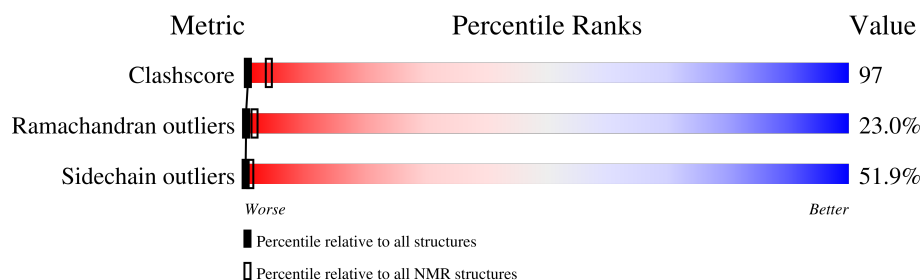
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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

Mol	Chain	Length	Quality of chain
1	A	52	

2 Ensemble composition and analysis

This entry contains 20 models. Model 10 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:141-A:178 (38)	1.21	10

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 4 clusters and 1 single-model cluster was found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 858 atoms, of which 432 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Troponin I, fast skeletal muscle.

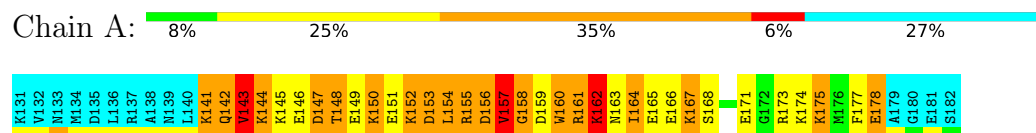
Mol	Chain	Residues	Atoms						Trace
1	A	52	Total	C	H	N	O	S	0
			858	259	432	79	85	3	

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: Troponin I, fast skeletal muscle

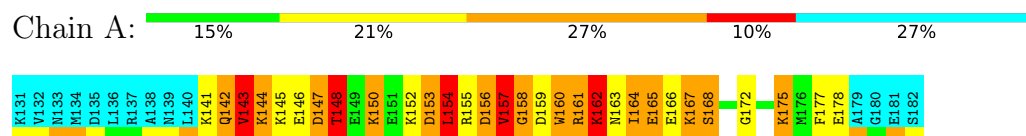


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

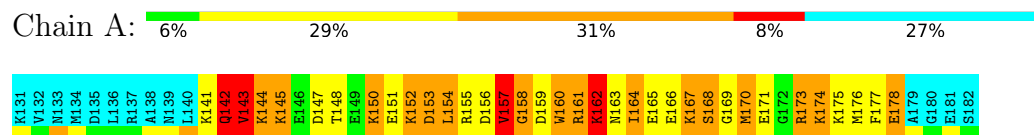
4.2.1 Score per residue for model 1

- Molecule 1: Troponin I, fast skeletal muscle



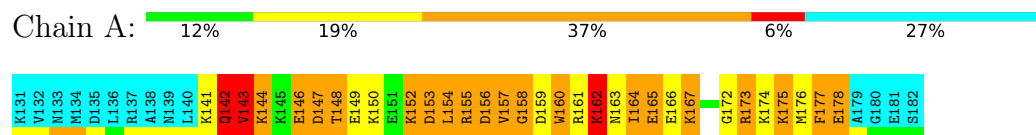
4.2.2 Score per residue for model 2

- Molecule 1: Troponin I, fast skeletal muscle



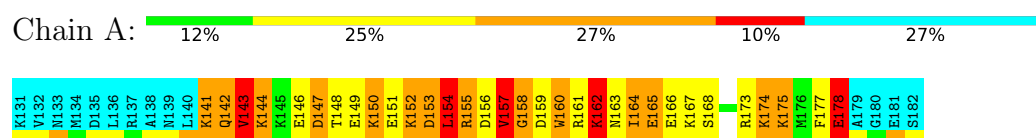
4.2.3 Score per residue for model 3

- Molecule 1: Troponin I, fast skeletal muscle



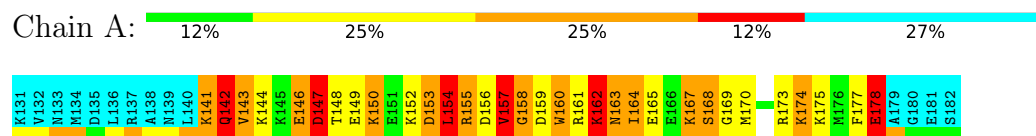
4.2.4 Score per residue for model 4

- Molecule 1: Troponin I, fast skeletal muscle



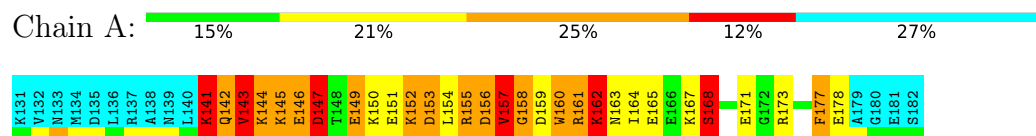
4.2.5 Score per residue for model 5

- Molecule 1: Troponin I, fast skeletal muscle



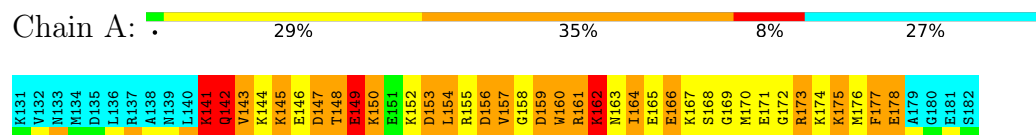
4.2.6 Score per residue for model 6

- Molecule 1: Troponin I, fast skeletal muscle



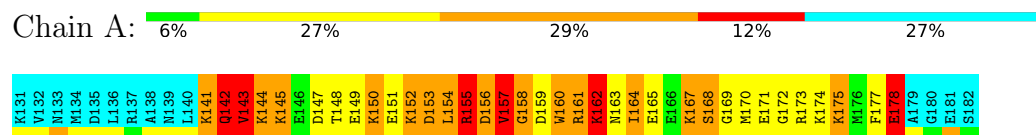
4.2.7 Score per residue for model 7

- Molecule 1: Troponin I, fast skeletal muscle



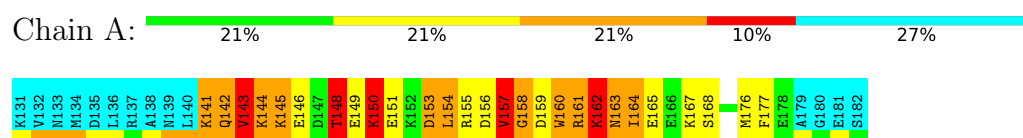
4.2.8 Score per residue for model 8

- Molecule 1: Troponin I, fast skeletal muscle



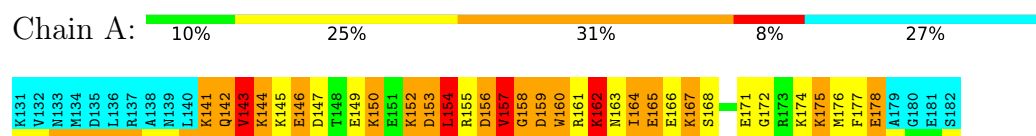
4.2.9 Score per residue for model 9

- Molecule 1: Troponin I, fast skeletal muscle



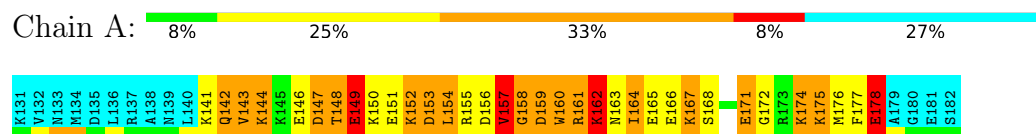
4.2.10 Score per residue for model 10 (medoid)

- Molecule 1: Troponin I, fast skeletal muscle



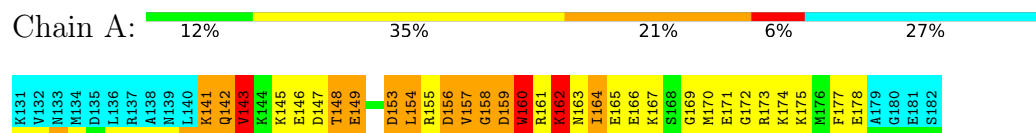
4.2.11 Score per residue for model 11

- Molecule 1: Troponin I, fast skeletal muscle



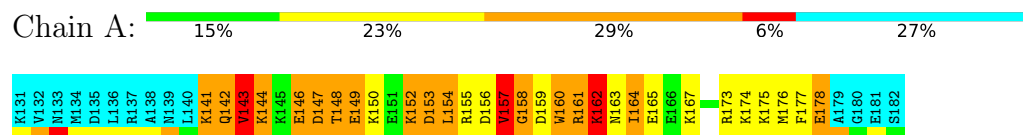
4.2.12 Score per residue for model 12

- Molecule 1: Troponin I, fast skeletal muscle



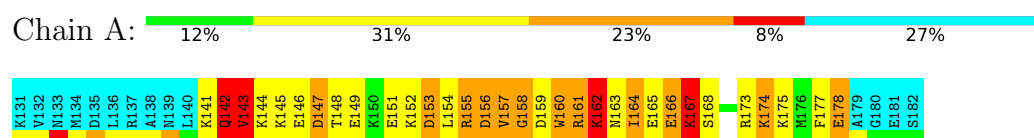
4.2.13 Score per residue for model 13

- Molecule 1: Troponin I, fast skeletal muscle



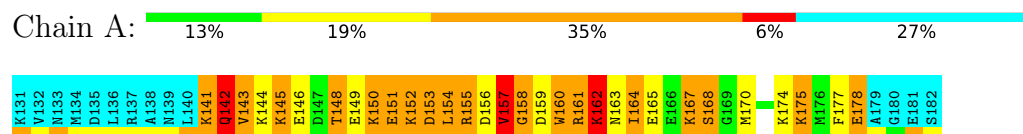
4.2.14 Score per residue for model 14

- Molecule 1: Troponin I, fast skeletal muscle



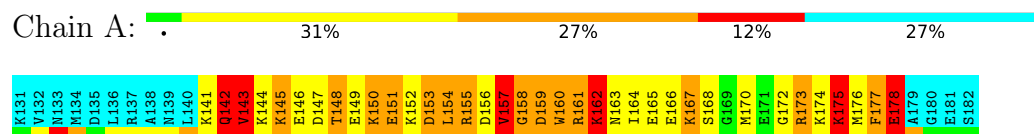
4.2.15 Score per residue for model 15

- Molecule 1: Troponin I, fast skeletal muscle



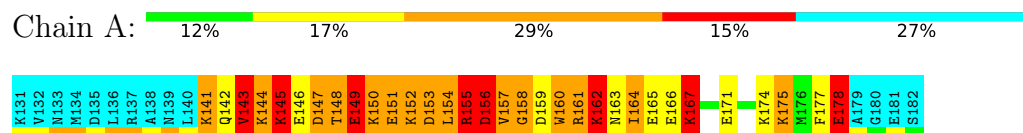
4.2.16 Score per residue for model 16

- Molecule 1: Troponin I, fast skeletal muscle



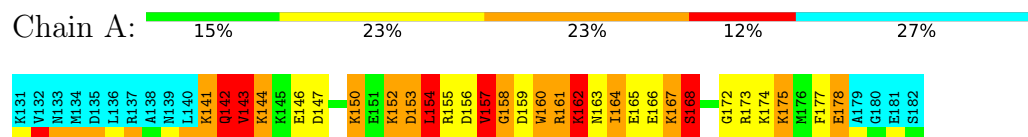
4.2.17 Score per residue for model 17

- Molecule 1: Troponin I, fast skeletal muscle



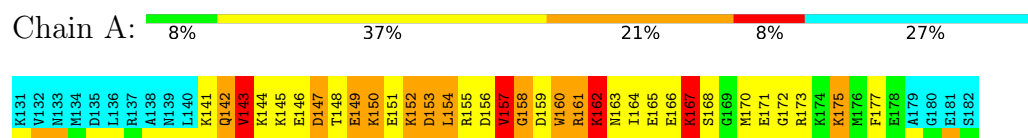
4.2.18 Score per residue for model 18

- Molecule 1: Troponin I, fast skeletal muscle



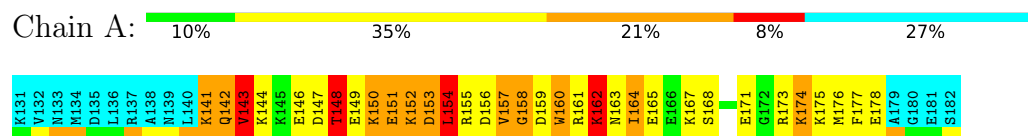
4.2.19 Score per residue for model 19

- Molecule 1: Troponin I, fast skeletal muscle



4.2.20 Score per residue for model 20

- Molecule 1: Troponin I, fast skeletal muscle



5 Refinement protocol and experimental data overview ⓘ

Of the 20 calculated structures, 20 were deposited, based on the following criterion: *target function*.

The authors did not provide any information on software used for structure solution, optimization or refinement.

No chemical shift data was provided.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	322	326	326	63±9
All	All	6440	6520	6520	1255

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 97.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:157:VAL:HG23	1:A:161:ARG:CB	1.04	1.81	19	13
1:A:143:VAL:HG23	1:A:160:TRP:CH2	0.97	1.94	15	18
1:A:143:VAL:HG23	1:A:160:TRP:CZ3	0.95	1.94	6	5
1:A:154:LEU:C	1:A:154:LEU:HD13	0.93	1.89	12	7
1:A:154:LEU:HD13	1:A:154:LEU:N	0.87	1.82	2	3
1:A:157:VAL:HG13	1:A:161:ARG:CB	0.85	2.01	6	7
1:A:157:VAL:HG22	1:A:158:GLY:N	0.84	1.87	11	13
1:A:160:TRP:CZ3	1:A:164:ILE:HG21	0.84	2.07	13	20
1:A:157:VAL:HG23	1:A:161:ARG:HB2	0.83	1.48	10	13
1:A:157:VAL:HG23	1:A:161:ARG:HB3	0.81	1.49	19	11
1:A:143:VAL:HG23	1:A:160:TRP:CE3	0.81	2.11	16	2
1:A:157:VAL:HG12	1:A:158:GLY:N	0.80	1.89	6	7
1:A:142:GLN:C	1:A:154:LEU:HD11	0.78	2.03	9	1
1:A:142:GLN:CA	1:A:154:LEU:HD13	0.76	2.10	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:143:VAL:CG2	1:A:160:TRP:CH2	0.76	2.69	13	12
1:A:157:VAL:HG13	1:A:161:ARG:HB2	0.74	1.59	14	7
1:A:142:GLN:C	1:A:143:VAL:HG12	0.74	2.06	8	8
1:A:153:ASP:C	1:A:154:LEU:HD13	0.73	2.07	2	1
1:A:142:GLN:HA	1:A:154:LEU:HD13	0.73	1.59	6	3
1:A:155:ARG:O	1:A:157:VAL:HG12	0.72	1.84	10	8
1:A:154:LEU:HD22	1:A:155:ARG:N	0.72	1.98	5	3
1:A:148:THR:O	1:A:148:THR:HG23	0.71	1.83	1	1
1:A:154:LEU:C	1:A:154:LEU:CD1	0.71	2.64	12	5
1:A:142:GLN:O	1:A:143:VAL:C	0.71	2.34	13	12
1:A:153:ASP:OD2	1:A:157:VAL:HG21	0.70	1.86	6	1
1:A:141:LYS:HE2	1:A:154:LEU:HD12	0.69	1.63	13	2
1:A:157:VAL:HG22	1:A:161:ARG:HG3	0.69	1.64	6	7
1:A:142:GLN:N	1:A:154:LEU:HD13	0.69	2.03	11	1
1:A:142:GLN:HG3	1:A:143:VAL:HG12	0.69	1.65	6	2
1:A:157:VAL:HG13	1:A:161:ARG:HB3	0.68	1.64	6	6
1:A:143:VAL:HA	1:A:160:TRP:CZ2	0.68	2.23	10	12
1:A:155:ARG:O	1:A:157:VAL:N	0.68	2.26	12	5
1:A:142:GLN:HA	1:A:154:LEU:HD22	0.68	1.64	4	3
1:A:141:LYS:O	1:A:143:VAL:HG12	0.68	1.89	11	1
1:A:154:LEU:N	1:A:154:LEU:CD1	0.68	2.56	2	3
1:A:160:TRP:CZ3	1:A:164:ILE:HG12	0.67	2.25	19	20
1:A:147:ASP:O	1:A:148:THR:HG22	0.66	1.90	1	1
1:A:161:ARG:O	1:A:162:LYS:C	0.66	2.38	6	20
1:A:157:VAL:CG2	1:A:158:GLY:N	0.66	2.59	11	13
1:A:160:TRP:CZ3	1:A:164:ILE:CG2	0.66	2.78	10	20
1:A:160:TRP:CH2	1:A:164:ILE:HG21	0.66	2.26	10	15
1:A:157:VAL:CG1	1:A:158:GLY:N	0.66	2.57	3	7
1:A:153:ASP:OD1	1:A:157:VAL:HG21	0.66	1.90	7	5
1:A:154:LEU:C	1:A:154:LEU:HD22	0.66	2.16	17	1
1:A:142:GLN:CA	1:A:154:LEU:HD22	0.66	2.20	4	1
1:A:143:VAL:HG23	1:A:160:TRP:CZ2	0.65	2.27	7	5
1:A:177:PHE:CD1	1:A:178:GLU:N	0.65	2.64	3	14
1:A:142:GLN:C	1:A:154:LEU:HD12	0.65	2.16	17	1
1:A:157:VAL:CG2	1:A:161:ARG:HB2	0.64	2.22	18	20
1:A:142:GLN:C	1:A:154:LEU:HD22	0.64	2.18	4	1
1:A:159:ASP:O	1:A:160:TRP:C	0.64	2.39	12	20
1:A:154:LEU:HD13	1:A:154:LEU:O	0.64	1.91	3	2
1:A:155:ARG:O	1:A:156:ASP:C	0.64	2.39	8	5
1:A:154:LEU:C	1:A:154:LEU:CD2	0.64	2.70	17	1
1:A:145:LYS:CB	1:A:151:GLU:HA	0.63	2.24	15	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:177:PHE:O	1:A:178:GLU:C	0.63	2.42	3	15
1:A:157:VAL:HG22	1:A:158:GLY:H	0.63	1.53	11	13
1:A:142:GLN:H	1:A:154:LEU:HD13	0.63	1.54	11	1
1:A:157:VAL:HG23	1:A:161:ARG:CG	0.62	2.23	16	2
1:A:143:VAL:N	1:A:154:LEU:HD22	0.62	2.10	4	2
1:A:143:VAL:CG2	1:A:160:TRP:CZ2	0.62	2.83	3	3
1:A:153:ASP:CG	1:A:153:ASP:O	0.62	2.43	20	9
1:A:164:ILE:HD12	1:A:165:GLU:N	0.61	2.10	16	3
1:A:142:GLN:C	1:A:143:VAL:HG13	0.61	2.20	2	1
1:A:156:ASP:O	1:A:158:GLY:N	0.61	2.33	11	9
1:A:148:THR:O	1:A:148:THR:CG2	0.61	2.49	1	1
1:A:156:ASP:O	1:A:157:VAL:C	0.61	2.44	4	11
1:A:154:LEU:N	1:A:154:LEU:HD12	0.61	2.11	10	3
1:A:143:VAL:HG23	1:A:160:TRP:HH2	0.60	1.56	5	5
1:A:157:VAL:O	1:A:158:GLY:C	0.60	2.43	12	20
1:A:161:ARG:O	1:A:165:GLU:N	0.60	2.35	6	20
1:A:154:LEU:O	1:A:155:ARG:C	0.60	2.45	16	4
1:A:153:ASP:OD1	1:A:153:ASP:C	0.60	2.45	9	13
1:A:141:LYS:O	1:A:142:GLN:CG	0.59	2.50	6	1
1:A:148:THR:O	1:A:149:GLU:CG	0.59	2.51	15	1
1:A:162:LYS:C	1:A:162:LYS:CD	0.59	2.76	1	8
1:A:157:VAL:HG22	1:A:161:ARG:HB2	0.59	1.75	12	7
1:A:157:VAL:HG22	1:A:161:ARG:CG	0.59	2.28	6	6
1:A:157:VAL:CG2	1:A:161:ARG:CB	0.58	2.79	20	3
1:A:154:LEU:HD23	1:A:156:ASP:H	0.58	1.58	6	1
1:A:157:VAL:HG12	1:A:158:GLY:H	0.58	1.56	6	7
1:A:143:VAL:HB	1:A:160:TRP:CZ2	0.58	2.33	7	5
1:A:153:ASP:CG	1:A:157:VAL:HG21	0.58	2.23	12	4
1:A:164:ILE:O	1:A:165:GLU:C	0.58	2.47	6	20
1:A:142:GLN:CA	1:A:154:LEU:HG	0.57	2.29	8	2
1:A:142:GLN:O	1:A:154:LEU:HD11	0.57	2.00	9	1
1:A:145:LYS:N	1:A:145:LYS:CD	0.57	2.67	9	1
1:A:161:ARG:O	1:A:163:ASN:N	0.57	2.37	10	20
1:A:146:GLU:O	1:A:148:THR:N	0.57	2.38	5	1
1:A:143:VAL:HG22	1:A:145:LYS:HD2	0.57	1.76	15	1
1:A:142:GLN:HA	1:A:154:LEU:CD1	0.57	2.29	6	2
1:A:143:VAL:HB	1:A:160:TRP:CH2	0.57	2.35	9	3
1:A:141:LYS:O	1:A:142:GLN:C	0.57	2.47	18	5
1:A:155:ARG:O	1:A:157:VAL:CG1	0.56	2.52	19	8
1:A:174:LYS:O	1:A:177:PHE:CD1	0.56	2.58	13	11
1:A:144:LYS:C	1:A:145:LYS:HG3	0.56	2.25	17	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:167:LYS:O	1:A:168:SER:CB	0.56	2.53	15	1
1:A:166:GLU:O	1:A:167:LYS:C	0.56	2.47	16	8
1:A:154:LEU:HD23	1:A:160:TRP:NE1	0.56	2.16	1	1
1:A:154:LEU:HD11	1:A:157:VAL:H	0.56	1.59	3	1
1:A:142:GLN:HA	1:A:154:LEU:CB	0.56	2.31	6	1
1:A:143:VAL:HG22	1:A:143:VAL:O	0.55	2.01	2	4
1:A:142:GLN:C	1:A:143:VAL:CG1	0.55	2.79	2	9
1:A:176:MET:O	1:A:177:PHE:C	0.55	2.50	7	3
1:A:143:VAL:N	1:A:154:LEU:HD12	0.55	2.17	17	1
1:A:145:LYS:CD	1:A:145:LYS:C	0.55	2.80	6	3
1:A:143:VAL:CB	1:A:160:TRP:CH2	0.54	2.90	4	5
1:A:166:GLU:CG	1:A:167:LYS:N	0.54	2.70	11	1
1:A:141:LYS:O	1:A:143:VAL:CG1	0.54	2.54	11	1
1:A:142:GLN:OE1	1:A:154:LEU:HD11	0.54	2.03	15	1
1:A:142:GLN:O	1:A:143:VAL:O	0.54	2.25	7	7
1:A:146:GLU:C	1:A:147:ASP:CG	0.54	2.75	5	1
1:A:148:THR:HG22	1:A:150:LYS:CD	0.54	2.33	1	1
1:A:157:VAL:O	1:A:159:ASP:N	0.54	2.40	9	11
1:A:148:THR:CG2	1:A:149:GLU:N	0.54	2.70	5	1
1:A:151:GLU:N	1:A:151:GLU:CD	0.54	2.66	17	1
1:A:164:ILE:O	1:A:168:SER:N	0.53	2.36	14	4
1:A:157:VAL:CG1	1:A:161:ARG:HB2	0.53	2.32	17	7
1:A:142:GLN:O	1:A:143:VAL:HB	0.53	2.03	11	2
1:A:174:LYS:HA	1:A:177:PHE:CE1	0.53	2.38	2	10
1:A:143:VAL:CB	1:A:160:TRP:CZ2	0.53	2.92	7	3
1:A:159:ASP:O	1:A:161:ARG:N	0.53	2.42	12	4
1:A:144:LYS:CG	1:A:152:LYS:CB	0.53	2.86	8	2
1:A:147:ASP:O	1:A:148:THR:C	0.53	2.51	4	2
1:A:143:VAL:CG2	1:A:160:TRP:CZ3	0.53	2.91	14	3
1:A:154:LEU:H	1:A:154:LEU:HD13	0.53	1.63	17	1
1:A:142:GLN:O	1:A:143:VAL:HG12	0.53	2.03	8	3
1:A:142:GLN:O	1:A:143:VAL:CB	0.53	2.57	11	5
1:A:160:TRP:CH2	1:A:164:ILE:HG12	0.53	2.39	16	5
1:A:142:GLN:HA	1:A:154:LEU:HG	0.53	1.81	8	5
1:A:147:ASP:O	1:A:148:THR:CG2	0.53	2.57	1	2
1:A:154:LEU:HD13	1:A:156:ASP:N	0.53	2.19	10	2
1:A:174:LYS:O	1:A:177:PHE:CE1	0.52	2.62	14	6
1:A:164:ILE:O	1:A:167:LYS:N	0.52	2.43	9	1
1:A:151:GLU:CD	1:A:164:ILE:HD13	0.52	2.29	14	1
1:A:157:VAL:O	1:A:160:TRP:N	0.52	2.43	20	5
1:A:153:ASP:OD2	1:A:161:ARG:CZ	0.52	2.58	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:149:GLU:O	1:A:151:GLU:N	0.52	2.42	9	3
1:A:154:LEU:O	1:A:156:ASP:N	0.52	2.43	16	1
1:A:144:LYS:O	1:A:152:LYS:CB	0.52	2.57	17	1
1:A:153:ASP:HB2	1:A:157:VAL:CG2	0.52	2.34	12	5
1:A:154:LEU:CD1	1:A:160:TRP:CD1	0.52	2.93	8	2
1:A:164:ILE:O	1:A:168:SER:CB	0.52	2.58	16	4
1:A:156:ASP:O	1:A:160:TRP:CD1	0.52	2.63	7	1
1:A:153:ASP:CG	1:A:161:ARG:NE	0.52	2.68	16	1
1:A:141:LYS:CE	1:A:154:LEU:CB	0.52	2.88	7	1
1:A:173:ARG:HD3	1:A:176:MET:HE2	0.51	1.82	2	1
1:A:141:LYS:O	1:A:142:GLN:HG3	0.51	2.05	11	2
1:A:143:VAL:O	1:A:143:VAL:CG2	0.51	2.57	2	1
1:A:165:GLU:CD	1:A:165:GLU:C	0.51	2.79	4	4
1:A:147:ASP:O	1:A:150:LYS:HB2	0.51	2.05	19	1
1:A:153:ASP:OD1	1:A:154:LEU:O	0.51	2.28	15	11
1:A:146:GLU:O	1:A:147:ASP:CB	0.51	2.59	11	4
1:A:154:LEU:CD1	1:A:154:LEU:N	0.51	2.73	5	3
1:A:153:ASP:OD2	1:A:157:VAL:CG2	0.51	2.59	6	1
1:A:147:ASP:O	1:A:148:THR:CB	0.51	2.58	1	5
1:A:166:GLU:C	1:A:168:SER:N	0.51	2.69	14	3
1:A:154:LEU:HD23	1:A:154:LEU:H	0.51	1.66	15	1
1:A:153:ASP:OD1	1:A:157:VAL:CG2	0.51	2.59	3	4
1:A:147:ASP:O	1:A:150:LYS:CG	0.51	2.59	8	2
1:A:165:GLU:CD	1:A:166:GLU:N	0.50	2.69	1	2
1:A:177:PHE:CG	1:A:178:GLU:N	0.50	2.79	13	11
1:A:157:VAL:HG22	1:A:161:ARG:CB	0.50	2.36	8	7
1:A:154:LEU:HD23	1:A:155:ARG:N	0.50	2.21	9	1
1:A:148:THR:O	1:A:150:LYS:CD	0.50	2.59	2	2
1:A:143:VAL:HA	1:A:160:TRP:CE2	0.50	2.41	14	3
1:A:174:LYS:C	1:A:176:MET:N	0.50	2.68	3	3
1:A:155:ARG:C	1:A:157:VAL:HG12	0.50	2.32	19	6
1:A:154:LEU:HD22	1:A:156:ASP:N	0.50	2.21	8	1
1:A:171:GLU:O	1:A:175:LYS:CG	0.50	2.59	11	3
1:A:150:LYS:CG	1:A:150:LYS:O	0.49	2.59	1	1
1:A:141:LYS:CG	1:A:142:GLN:N	0.49	2.75	9	3
1:A:154:LEU:HD22	1:A:155:ARG:H	0.49	1.66	5	1
1:A:165:GLU:C	1:A:165:GLU:CD	0.49	2.80	9	3
1:A:161:ARG:CD	1:A:165:GLU:CG	0.49	2.91	3	1
1:A:141:LYS:O	1:A:143:VAL:N	0.49	2.45	11	1
1:A:151:GLU:OE1	1:A:168:SER:CB	0.49	2.60	15	1
1:A:147:ASP:O	1:A:150:LYS:N	0.49	2.45	19	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:154:LEU:CD1	1:A:154:LEU:H	0.49	2.21	7	2
1:A:142:GLN:O	1:A:142:GLN:CD	0.49	2.56	11	1
1:A:175:LYS:O	1:A:175:LYS:CE	0.49	2.60	16	2
1:A:154:LEU:HD22	1:A:156:ASP:H	0.49	1.67	16	2
1:A:177:PHE:CZ	1:A:178:GLU:O	0.49	2.65	7	1
1:A:154:LEU:HD23	1:A:155:ARG:H	0.49	1.67	9	1
1:A:148:THR:HG22	1:A:149:GLU:N	0.49	2.23	17	3
1:A:151:GLU:O	1:A:151:GLU:CD	0.49	2.56	16	1
1:A:160:TRP:HZ3	1:A:164:ILE:HG21	0.49	1.65	19	1
1:A:144:LYS:C	1:A:145:LYS:CG	0.49	2.86	9	1
1:A:143:VAL:HB	1:A:160:TRP:CD2	0.49	2.43	14	2
1:A:156:ASP:O	1:A:157:VAL:O	0.48	2.31	4	4
1:A:142:GLN:CB	1:A:154:LEU:HD23	0.48	2.39	10	1
1:A:163:ASN:O	1:A:167:LYS:N	0.48	2.47	9	1
1:A:141:LYS:C	1:A:143:VAL:N	0.48	2.69	11	1
1:A:154:LEU:O	1:A:157:VAL:HG12	0.48	2.09	13	1
1:A:143:VAL:HB	1:A:160:TRP:CZ3	0.48	2.43	4	4
1:A:174:LYS:HA	1:A:177:PHE:CD1	0.48	2.44	2	4
1:A:161:ARG:NE	1:A:165:GLU:CG	0.48	2.76	3	1
1:A:144:LYS:O	1:A:145:LYS:CB	0.48	2.61	17	1
1:A:144:LYS:CD	1:A:152:LYS:CB	0.48	2.92	10	2
1:A:166:GLU:O	1:A:170:MET:CG	0.48	2.62	12	1
1:A:161:ARG:C	1:A:163:ASN:N	0.48	2.72	13	20
1:A:177:PHE:O	1:A:178:GLU:O	0.48	2.31	13	9
1:A:148:THR:O	1:A:149:GLU:CB	0.48	2.62	7	1
1:A:153:ASP:O	1:A:153:ASP:OD1	0.47	2.32	10	5
1:A:157:VAL:HA	1:A:160:TRP:CD1	0.47	2.44	9	9
1:A:148:THR:O	1:A:150:LYS:N	0.47	2.47	9	1
1:A:154:LEU:CD2	1:A:155:ARG:N	0.47	2.77	9	1
1:A:153:ASP:OD1	1:A:153:ASP:O	0.47	2.33	4	5
1:A:160:TRP:CE3	1:A:164:ILE:HG12	0.47	2.44	19	7
1:A:172:GLY:O	1:A:175:LYS:CE	0.47	2.62	19	3
1:A:143:VAL:N	1:A:154:LEU:CD2	0.47	2.78	4	1
1:A:151:GLU:CD	1:A:151:GLU:N	0.47	2.72	16	1
1:A:154:LEU:HD13	1:A:154:LEU:H	0.47	1.66	13	2
1:A:144:LYS:CE	1:A:152:LYS:CB	0.47	2.93	11	1
1:A:144:LYS:CG	1:A:152:LYS:HB2	0.47	2.40	8	2
1:A:148:THR:HG23	1:A:149:GLU:H	0.47	1.70	20	1
1:A:141:LYS:O	1:A:142:GLN:O	0.46	2.33	2	4
1:A:144:LYS:HD2	1:A:152:LYS:CB	0.46	2.40	14	3
1:A:154:LEU:CD1	1:A:157:VAL:H	0.46	2.23	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:157:VAL:CB	1:A:161:ARG:HB2	0.46	2.40	6	5
1:A:154:LEU:HD13	1:A:154:LEU:C	0.46	2.35	10	1
1:A:161:ARG:HD3	1:A:165:GLU:CB	0.46	2.40	10	1
1:A:155:ARG:CG	1:A:156:ASP:N	0.46	2.77	11	1
1:A:159:ASP:C	1:A:161:ARG:N	0.46	2.74	12	3
1:A:174:LYS:O	1:A:176:MET:N	0.46	2.48	16	3
1:A:157:VAL:CA	1:A:161:ARG:HB2	0.46	2.41	16	5
1:A:161:ARG:CD	1:A:165:GLU:HB2	0.46	2.40	20	3
1:A:153:ASP:OD1	1:A:157:VAL:HB	0.46	2.10	19	4
1:A:154:LEU:HD21	1:A:156:ASP:CB	0.46	2.41	8	1
1:A:151:GLU:OE1	1:A:168:SER:C	0.46	2.59	19	1
1:A:156:ASP:OD1	1:A:156:ASP:C	0.46	2.59	1	1
1:A:142:GLN:HB2	1:A:154:LEU:CD2	0.46	2.40	10	1
1:A:151:GLU:N	1:A:151:GLU:OE2	0.46	2.49	16	1
1:A:167:LYS:O	1:A:168:SER:C	0.46	2.59	4	3
1:A:174:LYS:O	1:A:175:LYS:C	0.46	2.58	16	3
1:A:155:ARG:C	1:A:157:VAL:H	0.46	2.18	4	3
1:A:163:ASN:O	1:A:167:LYS:CG	0.46	2.64	5	3
1:A:175:LYS:HA	1:A:175:LYS:CE	0.46	2.41	17	2
1:A:146:GLU:C	1:A:147:ASP:OD1	0.45	2.59	13	2
1:A:161:ARG:CD	1:A:165:GLU:CB	0.45	2.93	10	1
1:A:166:GLU:O	1:A:168:SER:N	0.45	2.49	14	2
1:A:142:GLN:HA	1:A:154:LEU:CG	0.45	2.41	3	1
1:A:153:ASP:O	1:A:153:ASP:CG	0.45	2.59	4	1
1:A:145:LYS:HB2	1:A:150:LYS:O	0.45	2.10	17	2
1:A:144:LYS:HG3	1:A:152:LYS:CB	0.45	2.42	5	10
1:A:172:GLY:O	1:A:175:LYS:N	0.45	2.50	10	1
1:A:173:ARG:O	1:A:176:MET:N	0.45	2.49	13	1
1:A:150:LYS:N	1:A:150:LYS:HD2	0.45	2.25	19	1
1:A:145:LYS:HB3	1:A:151:GLU:CB	0.45	2.42	16	1
1:A:151:GLU:CD	1:A:168:SER:CB	0.45	2.90	6	1
1:A:154:LEU:H	1:A:154:LEU:HD12	0.45	1.72	5	2
1:A:153:ASP:OD2	1:A:161:ARG:NE	0.45	2.49	9	2
1:A:143:VAL:HG23	1:A:160:TRP:CD2	0.45	2.47	16	1
1:A:154:LEU:CD1	1:A:156:ASP:HB3	0.45	2.42	16	1
1:A:169:GLY:O	1:A:170:MET:C	0.45	2.59	12	5
1:A:154:LEU:HD23	1:A:156:ASP:N	0.45	2.27	17	1
1:A:146:GLU:O	1:A:147:ASP:CG	0.45	2.60	17	2
1:A:141:LYS:HG2	1:A:154:LEU:CD1	0.45	2.42	11	1
1:A:142:GLN:O	1:A:144:LYS:N	0.45	2.50	17	1
1:A:144:LYS:HG2	1:A:152:LYS:CB	0.44	2.42	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:156:ASP:O	1:A:160:TRP:HD1	0.44	1.94	7	1
1:A:154:LEU:HD23	1:A:160:TRP:CD1	0.44	2.46	1	1
1:A:144:LYS:CE	1:A:152:LYS:HB3	0.44	2.42	2	1
1:A:145:LYS:O	1:A:145:LYS:CD	0.44	2.65	8	1
1:A:142:GLN:CB	1:A:154:LEU:HD13	0.44	2.42	6	1
1:A:168:SER:OG	1:A:169:GLY:N	0.44	2.50	8	1
1:A:162:LYS:HG3	1:A:163:ASN:N	0.44	2.28	20	6
1:A:169:GLY:O	1:A:172:GLY:N	0.44	2.50	8	1
1:A:154:LEU:HD23	1:A:156:ASP:CB	0.44	2.43	13	1
1:A:151:GLU:CD	1:A:168:SER:OG	0.44	2.61	20	1
1:A:153:ASP:CG	1:A:157:VAL:HB	0.44	2.37	19	2
1:A:155:ARG:C	1:A:157:VAL:N	0.44	2.76	4	3
1:A:142:GLN:CG	1:A:142:GLN:O	0.44	2.66	6	1
1:A:141:LYS:CE	1:A:154:LEU:HB2	0.44	2.43	7	1
1:A:143:VAL:H	1:A:154:LEU:HD22	0.44	1.72	15	1
1:A:144:LYS:CG	1:A:152:LYS:HB3	0.44	2.42	3	6
1:A:141:LYS:HE3	1:A:154:LEU:CB	0.44	2.43	7	1
1:A:154:LEU:HD22	1:A:154:LEU:C	0.43	2.38	8	1
1:A:168:SER:O	1:A:172:GLY:N	0.43	2.50	18	1
1:A:147:ASP:C	1:A:148:THR:HG22	0.43	2.38	19	1
1:A:154:LEU:H	1:A:154:LEU:HD22	0.43	1.74	13	3
1:A:146:GLU:HB2	1:A:150:LYS:CB	0.43	2.43	19	1
1:A:153:ASP:OD1	1:A:160:TRP:NE1	0.43	2.51	2	1
1:A:157:VAL:CG2	1:A:161:ARG:HG3	0.43	2.41	8	6
1:A:157:VAL:CG1	1:A:161:ARG:CB	0.43	2.88	6	1
1:A:154:LEU:C	1:A:156:ASP:N	0.43	2.76	16	1
1:A:148:THR:OG1	1:A:149:GLU:N	0.43	2.48	20	1
1:A:155:ARG:O	1:A:156:ASP:CB	0.43	2.66	9	1
1:A:142:GLN:HA	1:A:154:LEU:CD2	0.43	2.42	14	1
1:A:148:THR:HG22	1:A:150:LYS:HD3	0.43	1.91	1	1
1:A:161:ARG:HD3	1:A:165:GLU:CG	0.43	2.43	12	2
1:A:175:LYS:CD	1:A:175:LYS:C	0.43	2.91	4	1
1:A:154:LEU:HD11	1:A:156:ASP:C	0.43	2.39	12	1
1:A:147:ASP:O	1:A:149:GLU:N	0.43	2.45	13	2
1:A:175:LYS:CE	1:A:176:MET:N	0.43	2.81	20	1
1:A:155:ARG:O	1:A:156:ASP:O	0.43	2.37	3	1
1:A:141:LYS:HD2	1:A:144:LYS:CD	0.43	2.44	13	2
1:A:175:LYS:C	1:A:175:LYS:CE	0.43	2.91	4	1
1:A:157:VAL:C	1:A:161:ARG:HB2	0.43	2.39	16	1
1:A:172:GLY:O	1:A:173:ARG:C	0.43	2.62	3	3
1:A:161:ARG:HG2	1:A:165:GLU:CB	0.43	2.44	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:142:GLN:C	1:A:154:LEU:CD1	0.43	2.87	9	1
1:A:141:LYS:CD	1:A:144:LYS:HD3	0.42	2.44	8	3
1:A:144:LYS:HG2	1:A:154:LEU:HD12	0.42	1.89	9	1
1:A:148:THR:O	1:A:150:LYS:HG3	0.42	2.14	15	1
1:A:157:VAL:HA	1:A:161:ARG:HB2	0.42	1.90	15	1
1:A:161:ARG:O	1:A:164:ILE:N	0.42	2.52	6	2
1:A:165:GLU:C	1:A:165:GLU:OE2	0.42	2.62	11	1
1:A:144:LYS:CD	1:A:152:LYS:HB3	0.42	2.44	18	1
1:A:147:ASP:O	1:A:148:THR:HB	0.42	2.15	7	2
1:A:143:VAL:HB	1:A:160:TRP:CE2	0.42	2.49	17	1
1:A:160:TRP:O	1:A:164:ILE:CG1	0.42	2.67	3	1
1:A:149:GLU:O	1:A:150:LYS:CB	0.42	2.68	8	1
1:A:142:GLN:O	1:A:160:TRP:CD1	0.42	2.73	14	1
1:A:142:GLN:C	1:A:154:LEU:HG	0.42	2.39	3	1
1:A:171:GLU:O	1:A:172:GLY:C	0.42	2.62	12	1
1:A:142:GLN:CA	1:A:154:LEU:HD12	0.42	2.44	17	1
1:A:167:LYS:CG	1:A:167:LYS:O	0.42	2.68	8	1
1:A:148:THR:O	1:A:149:GLU:HG2	0.42	2.14	15	1
1:A:154:LEU:HD12	1:A:160:TRP:NE1	0.42	2.30	8	1
1:A:143:VAL:N	1:A:154:LEU:HD11	0.42	2.30	9	1
1:A:148:THR:O	1:A:149:GLU:HG3	0.42	2.14	15	1
1:A:144:LYS:CG	1:A:154:LEU:HD11	0.42	2.44	2	1
1:A:166:GLU:HG3	1:A:167:LYS:N	0.42	2.29	11	1
1:A:147:ASP:C	1:A:149:GLU:N	0.42	2.77	19	1
1:A:142:GLN:CB	1:A:154:LEU:HG	0.41	2.44	16	1
1:A:164:ILE:O	1:A:168:SER:OG	0.41	2.38	2	1
1:A:143:VAL:CG2	1:A:145:LYS:HD3	0.41	2.45	7	1
1:A:146:GLU:CB	1:A:150:LYS:HG3	0.41	2.45	7	1
1:A:167:LYS:O	1:A:168:SER:OG	0.41	2.38	15	1
1:A:142:GLN:HA	1:A:154:LEU:HD12	0.41	1.92	17	1
1:A:142:GLN:HG3	1:A:143:VAL:CG1	0.41	2.45	20	1
1:A:144:LYS:O	1:A:152:LYS:N	0.41	2.53	3	1
1:A:142:GLN:O	1:A:143:VAL:CG1	0.41	2.68	16	2
1:A:143:VAL:HG21	1:A:160:TRP:CH2	0.41	2.50	3	1
1:A:141:LYS:HE2	1:A:154:LEU:CB	0.41	2.45	7	1
1:A:166:GLU:O	1:A:168:SER:O	0.41	2.39	10	2
1:A:156:ASP:C	1:A:157:VAL:CG1	0.41	2.93	11	1
1:A:144:LYS:O	1:A:145:LYS:HB3	0.41	2.16	17	1
1:A:170:MET:C	1:A:172:GLY:N	0.41	2.77	8	1
1:A:173:ARG:O	1:A:174:LYS:C	0.41	2.63	13	2
1:A:141:LYS:CE	1:A:144:LYS:HG2	0.41	2.45	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:144:LYS:O	1:A:152:LYS:O	0.41	2.37	14	1
1:A:174:LYS:CD	1:A:174:LYS:C	0.41	2.94	20	1
1:A:156:ASP:C	1:A:156:ASP:OD1	0.41	2.63	3	1
1:A:144:LYS:O	1:A:144:LYS:HG3	0.41	2.15	9	1
1:A:142:GLN:CB	1:A:154:LEU:CD2	0.41	2.99	10	1
1:A:142:GLN:HB2	1:A:156:ASP:CB	0.41	2.46	14	1
1:A:142:GLN:O	1:A:143:VAL:HG13	0.41	2.14	20	1
1:A:154:LEU:HD11	1:A:156:ASP:O	0.41	2.16	12	1
1:A:153:ASP:CB	1:A:161:ARG:HG3	0.41	2.46	18	1
1:A:150:LYS:CE	1:A:150:LYS:HA	0.41	2.45	19	1
1:A:171:GLU:O	1:A:175:LYS:CB	0.41	2.69	20	1
1:A:145:LYS:C	1:A:145:LYS:HD3	0.41	2.40	16	2
1:A:172:GLY:O	1:A:176:MET:CB	0.41	2.69	11	1
1:A:173:ARG:C	1:A:175:LYS:N	0.41	2.78	12	1
1:A:143:VAL:CA	1:A:154:LEU:HD11	0.41	2.45	13	1
1:A:164:ILE:HA	1:A:167:LYS:CG	0.41	2.46	14	1
1:A:151:GLU:O	1:A:151:GLU:OE1	0.41	2.39	16	1
1:A:148:THR:O	1:A:149:GLU:HB2	0.41	2.15	19	1
1:A:146:GLU:O	1:A:147:ASP:O	0.40	2.39	3	2
1:A:146:GLU:CB	1:A:150:LYS:HB2	0.40	2.46	6	1
1:A:141:LYS:HG2	1:A:142:GLN:N	0.40	2.31	7	1
1:A:142:GLN:HB2	1:A:154:LEU:HD22	0.40	1.93	19	1
1:A:153:ASP:HB2	1:A:164:ILE:HD11	0.40	1.94	5	1
1:A:146:GLU:C	1:A:147:ASP:O	0.40	2.65	1	1
1:A:154:LEU:HD11	1:A:157:VAL:N	0.40	2.31	3	1
1:A:144:LYS:HE2	1:A:152:LYS:CB	0.40	2.47	11	1
1:A:165:GLU:OE2	1:A:165:GLU:O	0.40	2.40	11	1
1:A:143:VAL:CG2	1:A:145:LYS:HD2	0.40	2.46	15	1
1:A:142:GLN:NE2	1:A:154:LEU:HD21	0.40	2.32	9	1
1:A:141:LYS:HG3	1:A:154:LEU:CD2	0.40	2.47	14	1
1:A:148:THR:O	1:A:149:GLU:HB3	0.40	2.16	14	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	38/52 (73%)	16±2 (42±6%)	13±3 (35±8%)	9±2 (23±4%)	0 2
All	All	760/1040 (73%)	319 (42%)	266 (35%)	175 (23%)	0 2

All 22 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	143	VAL	20
1	A	162	LYS	20
1	A	158	GLY	19
1	A	157	VAL	14
1	A	178	GLU	14
1	A	142	GLN	13
1	A	147	ASP	10
1	A	141	LYS	9
1	A	154	LEU	9
1	A	150	LYS	7
1	A	167	LYS	6
1	A	168	SER	6
1	A	156	ASP	6
1	A	148	THR	5
1	A	149	GLU	5
1	A	155	ARG	4
1	A	163	ASN	2
1	A	177	PHE	2
1	A	146	GLU	1
1	A	160	TRP	1
1	A	175	LYS	1
1	A	145	LYS	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	35/46 (76%)	17±2 (48±6%)	18±2 (52±6%)	0 1
All	All	700/920 (76%)	337 (48%)	363 (52%)	0 1

All 34 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	153	ASP	20
1	A	157	VAL	20
1	A	160	TRP	20
1	A	162	LYS	20
1	A	164	ILE	17
1	A	143	VAL	16
1	A	175	LYS	16
1	A	142	GLN	15
1	A	150	LYS	15
1	A	154	LEU	15
1	A	167	LYS	15
1	A	161	ARG	14
1	A	152	LYS	14
1	A	144	LYS	13
1	A	145	LYS	13
1	A	173	ARG	12
1	A	146	GLU	11
1	A	141	LYS	10
1	A	148	THR	9
1	A	155	ARG	9
1	A	149	GLU	8
1	A	171	GLU	6
1	A	174	LYS	6
1	A	178	GLU	6
1	A	147	ASP	6
1	A	151	GLU	6
1	A	168	SER	5
1	A	159	ASP	5
1	A	156	ASP	4
1	A	165	GLU	4
1	A	170	MET	4
1	A	166	GLU	4
1	A	177	PHE	3
1	A	176	MET	2

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided