



Full wwPDB NMR Structure Validation Report ⓘ

Mar 25, 2026 – 12:05 AM UTC

PDB ID : 8GBD / pdb_00008gbd
BMRB ID : 51834
Title : Homo sapiens Zalpha mutant - P193A
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Deposited on : 2023-02-25

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

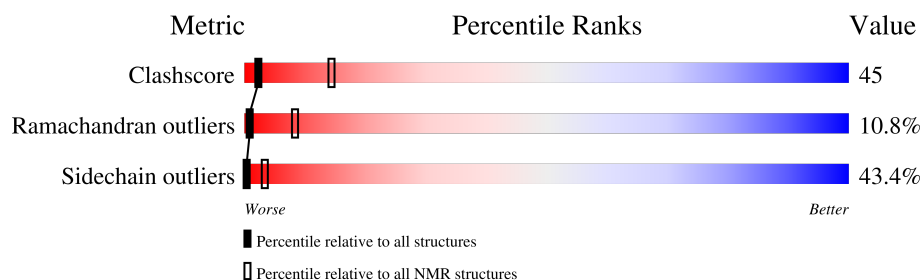
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 64%.

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	84	

2 Ensemble composition and analysis

This entry contains 20 models. Model 16 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:140-A:198 (59)	0.48	16

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 3 clusters. No single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1010 atoms, of which 523 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Double-stranded RNA-specific adenosine deaminase.

Mol	Chain	Residues	Atoms					Trace
1	A	63	Total	C	H	N	O	0
			1010	311	523	86	90	

There are 22 discrepancies between the modelled and reference sequences:

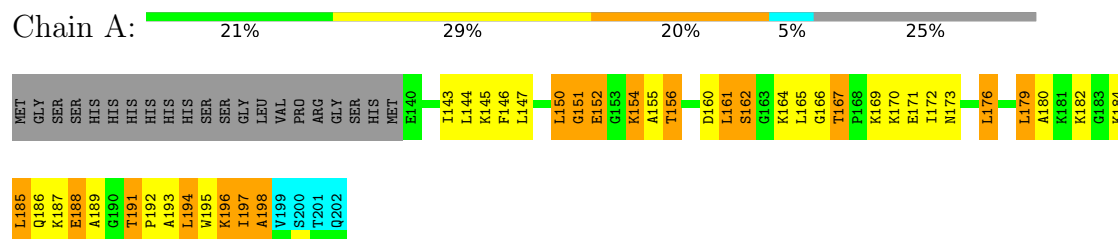
Chain	Residue	Modelled	Actual	Comment	Reference
A	119	MET	-	initiating methionine	UNP P55265
A	120	GLY	-	expression tag	UNP P55265
A	121	SER	-	expression tag	UNP P55265
A	122	SER	-	expression tag	UNP P55265
A	123	HIS	-	expression tag	UNP P55265
A	124	HIS	-	expression tag	UNP P55265
A	125	HIS	-	expression tag	UNP P55265
A	126	HIS	-	expression tag	UNP P55265
A	127	HIS	-	expression tag	UNP P55265
A	128	HIS	-	expression tag	UNP P55265
A	129	SER	-	expression tag	UNP P55265
A	130	SER	-	expression tag	UNP P55265
A	131	GLY	-	expression tag	UNP P55265
A	132	LEU	-	expression tag	UNP P55265
A	133	VAL	-	expression tag	UNP P55265
A	134	PRO	-	expression tag	UNP P55265
A	135	ARG	-	expression tag	UNP P55265
A	136	GLY	-	expression tag	UNP P55265
A	137	SER	-	expression tag	UNP P55265
A	138	HIS	-	expression tag	UNP P55265
A	139	MET	-	expression tag	UNP P55265
A	193	ALA	PRO	engineered mutation	UNP P55265

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: Double-stranded RNA-specific adenosine deaminase

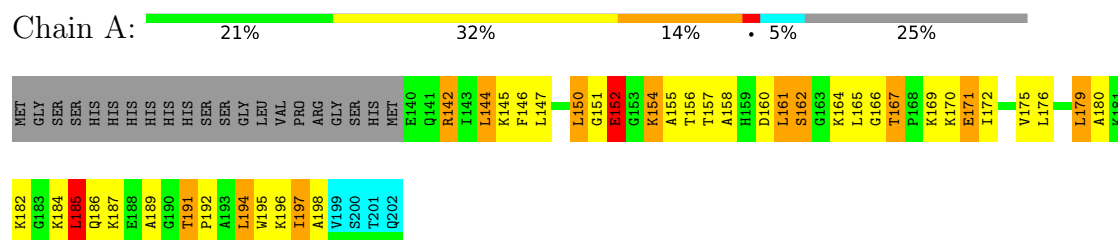


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

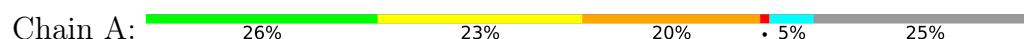
4.2.1 Score per residue for model 1

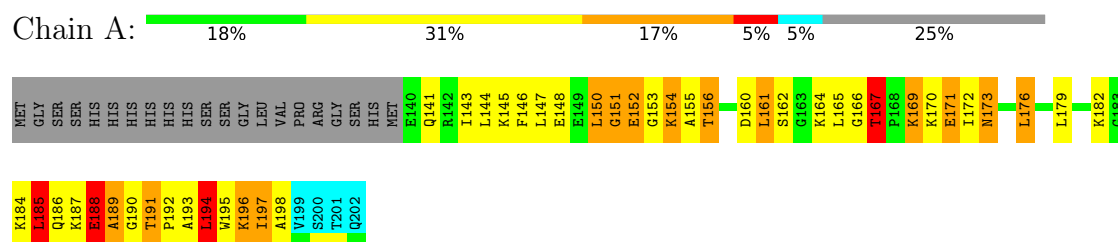
- Molecule 1: Double-stranded RNA-specific adenosine deaminase



4.2.2 Score per residue for model 2

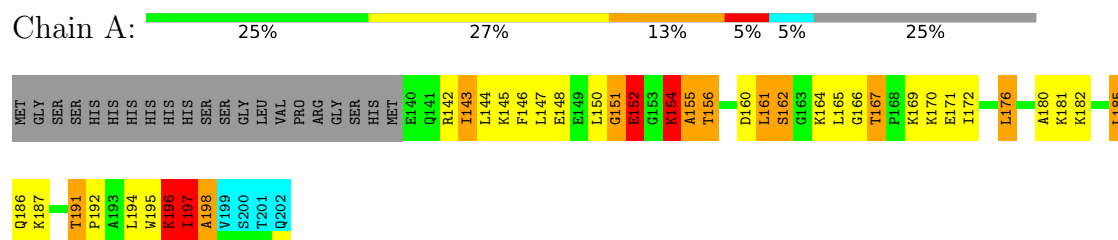
- Molecule 1: Double-stranded RNA-specific adenosine deaminase





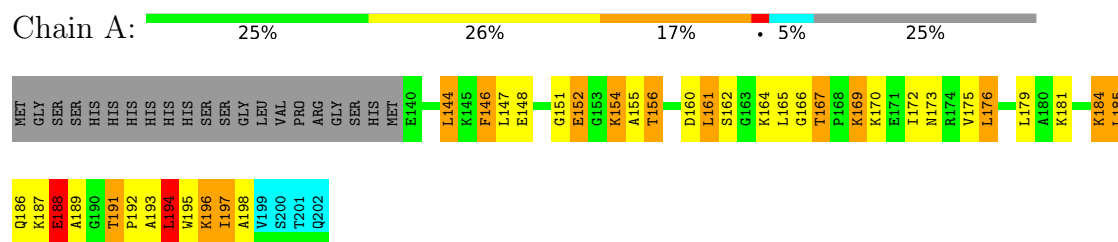
4.2.7 Score per residue for model 7

- Molecule 1: Double-stranded RNA-specific adenosine deaminase



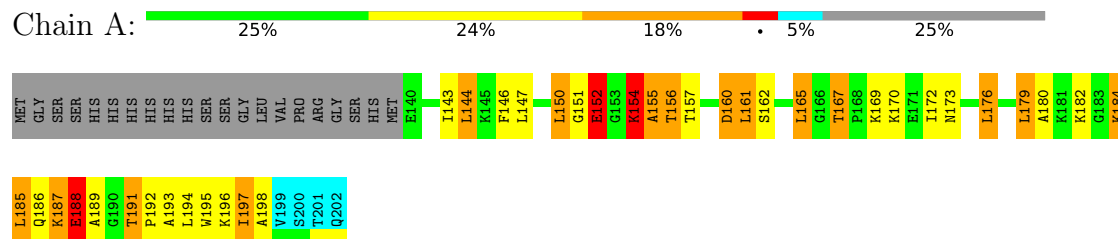
4.2.8 Score per residue for model 8

- Molecule 1: Double-stranded RNA-specific adenosine deaminase



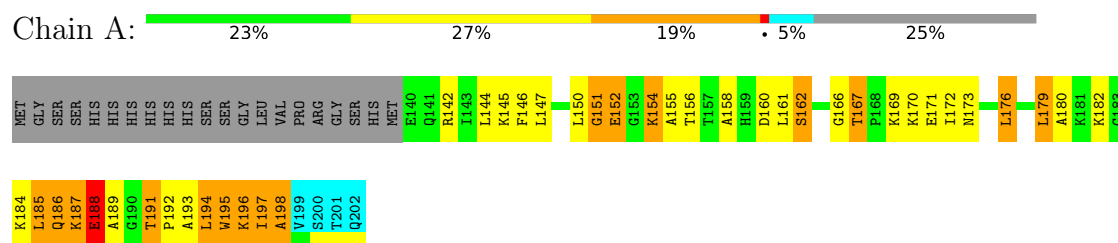
4.2.9 Score per residue for model 9

- Molecule 1: Double-stranded RNA-specific adenosine deaminase



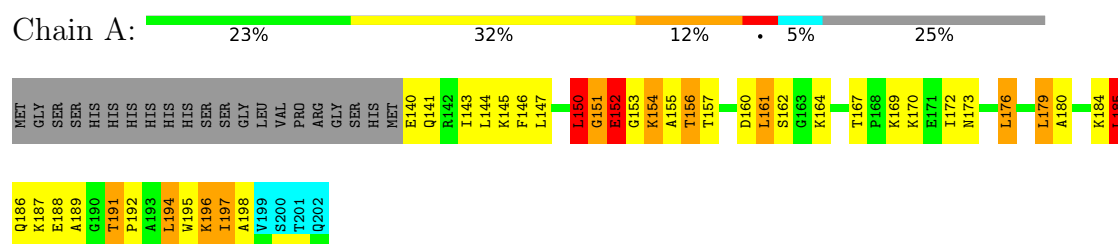
4.2.10 Score per residue for model 10

- Molecule 1: Double-stranded RNA-specific adenosine deaminase



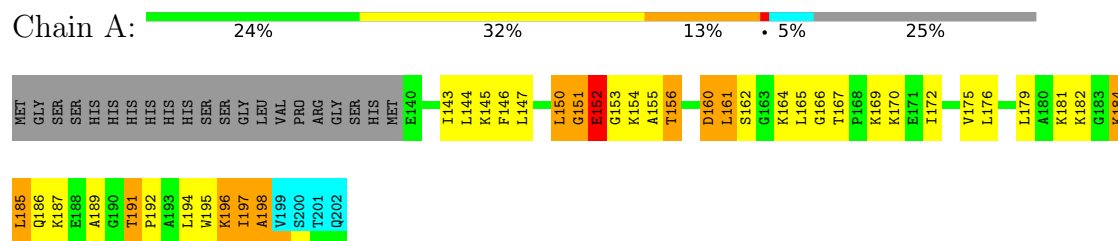
4.2.11 Score per residue for model 11

- Molecule 1: Double-stranded RNA-specific adenosine deaminase



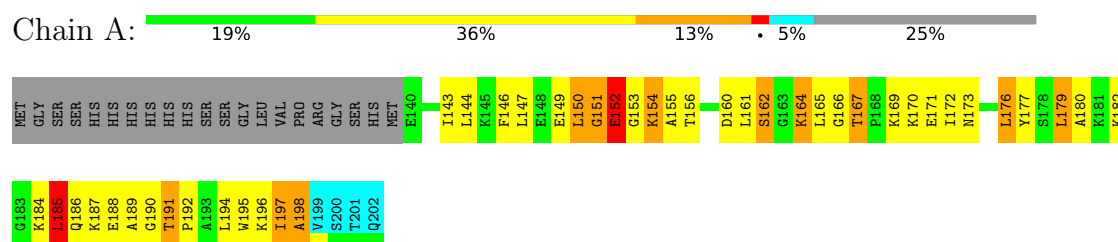
4.2.12 Score per residue for model 12

- Molecule 1: Double-stranded RNA-specific adenosine deaminase



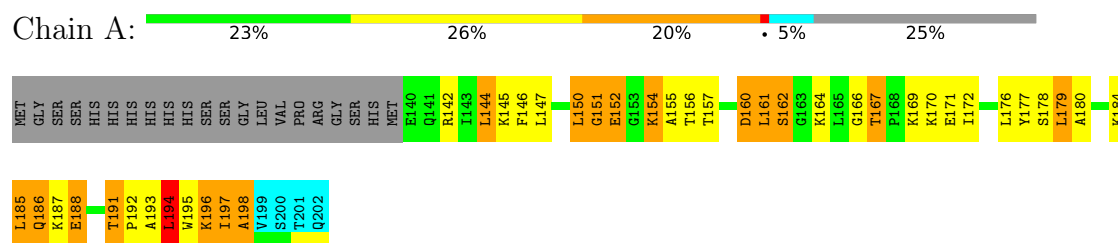
4.2.13 Score per residue for model 13

- Molecule 1: Double-stranded RNA-specific adenosine deaminase



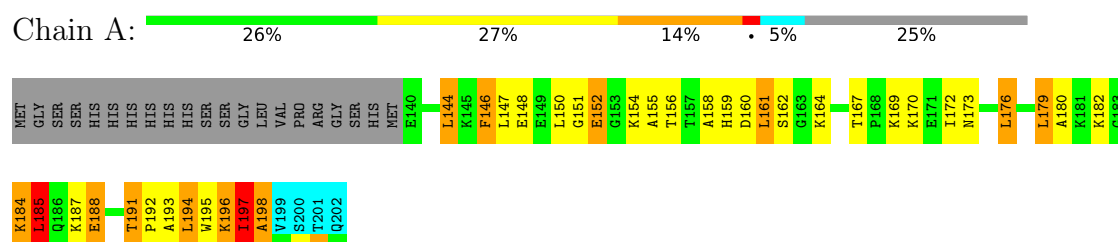
4.2.14 Score per residue for model 14

- Molecule 1: Double-stranded RNA-specific adenosine deaminase



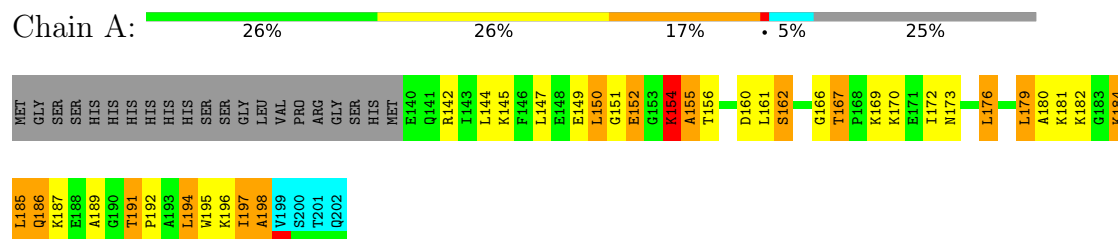
4.2.15 Score per residue for model 15

- Molecule 1: Double-stranded RNA-specific adenosine deaminase



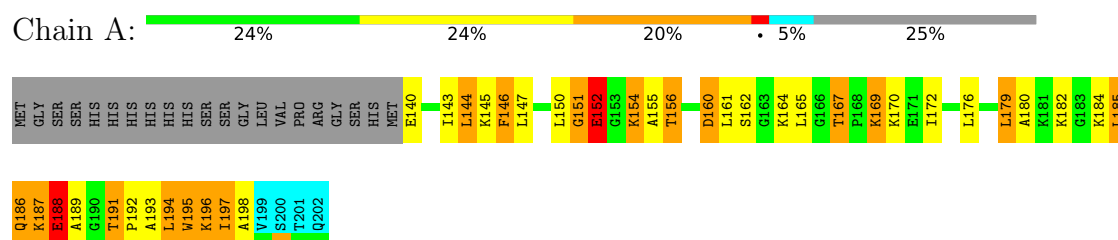
4.2.16 Score per residue for model 16 (medoid)

- Molecule 1: Double-stranded RNA-specific adenosine deaminase



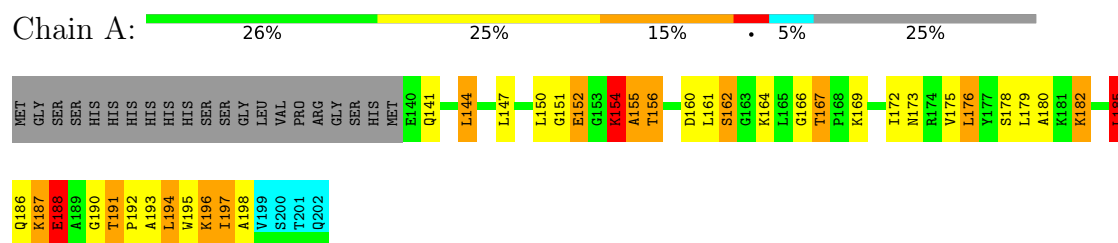
4.2.17 Score per residue for model 17

- Molecule 1: Double-stranded RNA-specific adenosine deaminase



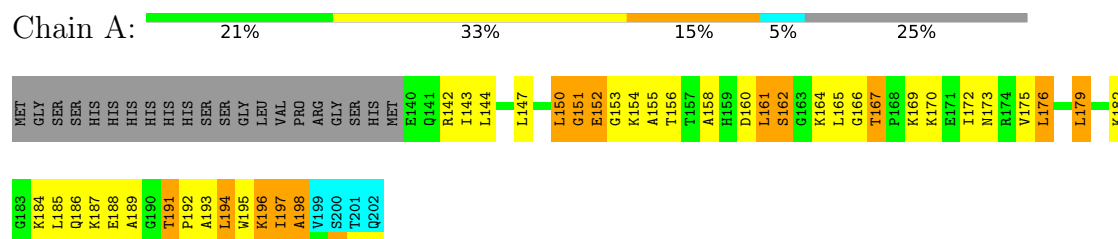
4.2.18 Score per residue for model 18

- Molecule 1: Double-stranded RNA-specific adenosine deaminase



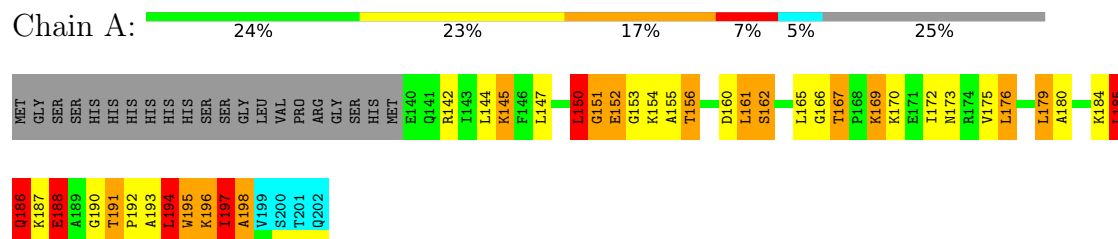
4.2.19 Score per residue for model 19

- Molecule 1: Double-stranded RNA-specific adenosine deaminase



4.2.20 Score per residue for model 20

- Molecule 1: Double-stranded RNA-specific adenosine deaminase



5 Refinement protocol and experimental data overview

The models were refined using the following method: *na*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CYANA	structure calculation	3.98.13

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	562
Number of shifts mapped to atoms	555
Number of unparsed shifts	0
Number of shifts with mapping errors	7
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	64%

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	458	494	493	43±8
All	All	9160	9880	9860	862

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 45.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:179:LEU:C	1:A:179:LEU:HD22	1.17	1.65	4	1
1:A:179:LEU:HD21	1:A:185:LEU:HD22	0.95	1.39	9	4
1:A:188:GLU:CD	1:A:193:ALA:HB3	0.90	1.91	20	4
1:A:188:GLU:OE2	1:A:193:ALA:HB3	0.90	1.64	10	2
1:A:188:GLU:OE1	1:A:193:ALA:HB3	0.90	1.65	4	4
1:A:179:LEU:HD13	1:A:180:ALA:N	0.89	1.83	4	1
1:A:155:ALA:HB1	1:A:194:LEU:HD13	0.87	1.47	16	3
1:A:194:LEU:HD12	1:A:195:TRP:N	0.86	1.85	3	3
1:A:188:GLU:CD	1:A:188:GLU:N	0.84	2.33	17	8
1:A:179:LEU:HD23	1:A:184:LYS:CG	0.82	2.03	4	1
1:A:179:LEU:C	1:A:179:LEU:CD2	0.81	2.42	4	1
1:A:185:LEU:C	1:A:185:LEU:HD12	0.81	2.01	7	1
1:A:179:LEU:HD13	1:A:180:ALA:H	0.80	1.33	4	1
1:A:176:LEU:C	1:A:176:LEU:HD12	0.78	2.04	13	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:155:ALA:HB1	1:A:194:LEU:HG	0.78	1.56	1	9
1:A:188:GLU:CD	1:A:188:GLU:H	0.77	1.87	17	8
1:A:179:LEU:HD22	1:A:179:LEU:O	0.76	1.80	4	1
1:A:185:LEU:HD22	1:A:186:GLN:N	0.75	1.97	2	4
1:A:179:LEU:HD21	1:A:185:LEU:CB	0.75	2.11	4	1
1:A:185:LEU:O	1:A:185:LEU:HD13	0.74	1.83	2	1
1:A:155:ALA:CB	1:A:194:LEU:HD13	0.73	2.12	16	4
1:A:151:GLY:O	1:A:152:GLU:C	0.72	2.33	3	20
1:A:179:LEU:HD23	1:A:180:ALA:N	0.72	1.99	10	8
1:A:176:LEU:HD21	1:A:195:TRP:NE1	0.71	2.00	1	1
1:A:161:LEU:HD12	1:A:161:LEU:O	0.71	1.85	15	2
1:A:188:GLU:HG2	1:A:194:LEU:N	0.71	2.00	18	10
1:A:150:LEU:HD21	1:A:154:LYS:O	0.70	1.86	13	7
1:A:176:LEU:HD13	1:A:195:TRP:CZ3	0.70	2.21	20	4
1:A:185:LEU:HD13	1:A:185:LEU:C	0.69	2.13	2	1
1:A:176:LEU:HD11	1:A:195:TRP:CE2	0.69	2.22	4	3
1:A:188:GLU:OE2	1:A:194:LEU:O	0.69	2.11	9	5
1:A:179:LEU:HD11	1:A:185:LEU:HD13	0.69	1.64	13	4
1:A:175:VAL:HG22	1:A:179:LEU:HD23	0.69	1.64	20	1
1:A:197:ILE:O	1:A:198:ALA:C	0.68	2.35	7	19
1:A:179:LEU:HD22	1:A:180:ALA:N	0.68	2.01	4	1
1:A:185:LEU:HD13	1:A:186:GLN:O	0.68	1.86	10	5
1:A:180:ALA:HB2	1:A:185:LEU:HD12	0.68	1.66	2	1
1:A:150:LEU:HD11	1:A:154:LYS:HG2	0.68	1.66	2	1
1:A:191:THR:CB	1:A:192:PRO:CD	0.68	2.72	20	20
1:A:188:GLU:CG	1:A:194:LEU:O	0.68	2.42	5	4
1:A:176:LEU:HD13	1:A:195:TRP:CH2	0.68	2.23	9	6
1:A:179:LEU:CD2	1:A:185:LEU:HD22	0.67	2.17	13	4
1:A:173:ASN:HA	1:A:176:LEU:HD23	0.67	1.66	10	11
1:A:176:LEU:HD11	1:A:195:TRP:NE1	0.67	2.05	7	2
1:A:157:THR:O	1:A:161:LEU:HD22	0.67	1.88	11	2
1:A:188:GLU:OE2	1:A:190:GLY:O	0.67	2.12	20	2
1:A:188:GLU:OE1	1:A:194:LEU:O	0.67	2.12	10	5
1:A:158:ALA:HA	1:A:161:LEU:HD12	0.66	1.67	1	3
1:A:188:GLU:OE2	1:A:188:GLU:C	0.66	2.38	20	3
1:A:155:ALA:HB1	1:A:194:LEU:HD22	0.66	1.65	6	1
1:A:161:LEU:HD11	1:A:172:ILE:CD1	0.66	2.21	15	1
1:A:188:GLU:HG3	1:A:194:LEU:O	0.66	1.91	5	4
1:A:194:LEU:HG	1:A:195:TRP:N	0.66	2.04	14	4
1:A:191:THR:OG1	1:A:192:PRO:HD3	0.65	1.91	18	9
1:A:158:ALA:HA	1:A:161:LEU:HD23	0.64	1.69	15	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:157:THR:HG23	1:A:194:LEU:CD1	0.64	2.22	9	1
1:A:166:GLY:O	1:A:167:THR:C	0.64	2.41	6	12
1:A:179:LEU:HD23	1:A:184:LYS:HG2	0.64	1.68	4	1
1:A:150:LEU:HD12	1:A:154:LYS:HE3	0.63	1.71	14	1
1:A:147:LEU:CD1	1:A:197:ILE:HD13	0.62	2.23	17	2
1:A:176:LEU:HD13	1:A:176:LEU:C	0.62	2.18	1	2
1:A:194:LEU:C	1:A:195:TRP:CG	0.62	2.77	10	7
1:A:179:LEU:CD1	1:A:185:LEU:HD22	0.62	2.25	11	1
1:A:150:LEU:HD13	1:A:154:LYS:HG3	0.62	1.71	18	1
1:A:176:LEU:HD11	1:A:195:TRP:CH2	0.62	2.30	5	1
1:A:172:ILE:HD13	1:A:172:ILE:O	0.62	1.94	4	1
1:A:188:GLU:HG3	1:A:194:LEU:HD23	0.62	1.69	5	4
1:A:176:LEU:HD21	1:A:195:TRP:CD1	0.62	2.29	1	1
1:A:155:ALA:HB1	1:A:194:LEU:CD2	0.61	2.25	8	6
1:A:188:GLU:CD	1:A:194:LEU:O	0.61	2.42	6	8
1:A:176:LEU:HD11	1:A:195:TRP:CZ2	0.61	2.29	5	1
1:A:179:LEU:HD12	1:A:184:LYS:HE3	0.61	1.71	16	1
1:A:179:LEU:HD12	1:A:185:LEU:HD22	0.61	1.72	11	1
1:A:160:ASP:C	1:A:161:LEU:HD23	0.61	2.20	9	2
1:A:180:ALA:HB1	1:A:187:LYS:CE	0.61	2.25	11	4
1:A:155:ALA:HB1	1:A:194:LEU:HD23	0.61	1.72	9	2
1:A:176:LEU:HD11	1:A:195:TRP:CZ3	0.61	2.31	14	1
1:A:156:THR:HG22	1:A:160:ASP:HB2	0.60	1.71	11	3
1:A:194:LEU:HD23	1:A:194:LEU:C	0.60	2.22	18	3
1:A:179:LEU:HD13	1:A:185:LEU:HD13	0.60	1.71	11	1
1:A:155:ALA:HB1	1:A:194:LEU:CG	0.60	2.26	1	6
1:A:155:ALA:CB	1:A:194:LEU:HD12	0.60	2.27	14	2
1:A:194:LEU:C	1:A:194:LEU:HD23	0.60	2.22	20	1
1:A:156:THR:OG1	1:A:161:LEU:HD21	0.60	1.97	1	1
1:A:176:LEU:HA	1:A:179:LEU:HD22	0.60	1.72	9	9
1:A:144:LEU:HD12	1:A:144:LEU:C	0.59	2.22	6	12
1:A:188:GLU:N	1:A:188:GLU:OE2	0.59	2.35	6	3
1:A:185:LEU:HD11	1:A:195:TRP:HB3	0.59	1.75	9	3
1:A:162:SER:HA	1:A:167:THR:HG23	0.59	1.73	4	14
1:A:176:LEU:HD21	1:A:195:TRP:CH2	0.59	2.32	14	2
1:A:150:LEU:HD11	1:A:154:LYS:CG	0.59	2.28	2	2
1:A:180:ALA:HB2	1:A:185:LEU:HD21	0.59	1.72	7	1
1:A:164:LYS:HG3	1:A:165:LEU:HD22	0.59	1.74	5	1
1:A:179:LEU:HD12	1:A:182:LYS:HD2	0.59	1.74	18	1
1:A:146:PHE:CE2	1:A:150:LEU:HD21	0.59	2.32	10	1
1:A:185:LEU:HD11	1:A:195:TRP:CD1	0.58	2.31	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:179:LEU:HD21	1:A:185:LEU:HB3	0.58	1.75	4	1
1:A:176:LEU:HD23	1:A:177:TYR:CE2	0.58	2.33	14	1
1:A:179:LEU:HD23	1:A:184:LYS:HG3	0.58	1.74	4	1
1:A:194:LEU:C	1:A:195:TRP:CD1	0.58	2.81	10	2
1:A:150:LEU:HD22	1:A:154:LYS:CB	0.58	2.29	18	1
1:A:179:LEU:HD23	1:A:180:ALA:H	0.57	1.60	10	9
1:A:179:LEU:CD1	1:A:180:ALA:N	0.57	2.65	4	1
1:A:147:LEU:HD13	1:A:197:ILE:HD13	0.57	1.77	17	1
1:A:180:ALA:HB1	1:A:187:LYS:HD3	0.57	1.77	20	3
1:A:179:LEU:HD13	1:A:184:LYS:NZ	0.57	2.15	8	1
1:A:147:LEU:C	1:A:147:LEU:HD12	0.57	2.25	6	19
1:A:161:LEU:HD21	1:A:172:ILE:CG1	0.56	2.30	4	2
1:A:144:LEU:O	1:A:144:LEU:HD12	0.56	2.00	8	7
1:A:150:LEU:HD12	1:A:151:GLY:N	0.56	2.15	16	2
1:A:191:THR:OG1	1:A:192:PRO:CD	0.56	2.53	18	12
1:A:188:GLU:HG2	1:A:194:LEU:CB	0.56	2.30	17	6
1:A:180:ALA:HB1	1:A:187:LYS:HG2	0.56	1.76	3	3
1:A:179:LEU:HG	1:A:185:LEU:HB3	0.56	1.78	16	8
1:A:180:ALA:HB2	1:A:185:LEU:CD2	0.56	2.31	7	6
1:A:194:LEU:O	1:A:195:TRP:CD2	0.55	2.58	9	3
1:A:191:THR:CB	1:A:192:PRO:HD3	0.55	2.30	20	9
1:A:180:ALA:HB1	1:A:187:LYS:CD	0.55	2.32	14	5
1:A:150:LEU:HD12	1:A:151:GLY:H	0.55	1.61	4	2
1:A:188:GLU:CG	1:A:194:LEU:N	0.55	2.68	20	3
1:A:150:LEU:HD11	1:A:154:LYS:CD	0.55	2.30	19	1
1:A:144:LEU:HD12	1:A:145:LYS:N	0.55	2.16	20	3
1:A:175:VAL:HG22	1:A:179:LEU:HD22	0.55	1.78	19	2
1:A:146:PHE:CZ	1:A:161:LEU:HD11	0.55	2.36	8	1
1:A:150:LEU:C	1:A:150:LEU:HD12	0.55	2.26	3	9
1:A:144:LEU:HD13	1:A:144:LEU:O	0.54	2.01	2	1
1:A:155:ALA:HB2	1:A:196:LYS:CD	0.54	2.33	6	1
1:A:155:ALA:HB1	1:A:194:LEU:CD1	0.54	2.31	18	1
1:A:150:LEU:HD21	1:A:154:LYS:HB3	0.54	1.80	3	1
1:A:179:LEU:HD22	1:A:184:LYS:HD3	0.54	1.77	8	1
1:A:155:ALA:CB	1:A:194:LEU:CD1	0.54	2.86	20	1
1:A:188:GLU:N	1:A:188:GLU:OE1	0.54	2.39	10	2
1:A:150:LEU:HD22	1:A:154:LYS:HB3	0.54	1.78	18	1
1:A:179:LEU:HD21	1:A:185:LEU:N	0.53	2.17	4	1
1:A:146:PHE:O	1:A:150:LEU:HG	0.53	2.03	10	3
1:A:179:LEU:HD12	1:A:184:LYS:HE2	0.53	1.79	3	2
1:A:161:LEU:HD11	1:A:172:ILE:HD13	0.53	1.79	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:179:LEU:HD12	1:A:184:LYS:HD2	0.53	1.80	9	2
1:A:165:LEU:O	1:A:166:GLY:C	0.53	2.52	12	4
1:A:175:VAL:HG22	1:A:179:LEU:CD2	0.53	2.34	19	2
1:A:143:ILE:HG23	1:A:144:LEU:HD23	0.53	1.80	19	1
1:A:188:GLU:CG	1:A:194:LEU:HD23	0.53	2.34	14	2
1:A:157:THR:HG23	1:A:194:LEU:HD12	0.53	1.80	9	1
1:A:176:LEU:HD13	1:A:176:LEU:O	0.52	2.04	1	2
1:A:185:LEU:HD21	1:A:195:TRP:CE3	0.52	2.39	9	3
1:A:169:LYS:HA	1:A:172:ILE:HG22	0.52	1.80	16	18
1:A:179:LEU:HD12	1:A:184:LYS:CE	0.52	2.33	16	2
1:A:150:LEU:HD13	1:A:154:LYS:HD2	0.52	1.80	10	2
1:A:176:LEU:HD21	1:A:195:TRP:CZ3	0.52	2.39	12	1
1:A:194:LEU:O	1:A:195:TRP:CG	0.52	2.63	4	5
1:A:160:ASP:OD2	1:A:161:LEU:HD23	0.52	2.04	12	1
1:A:164:LYS:O	1:A:165:LEU:HD23	0.52	2.04	12	2
1:A:151:GLY:O	1:A:153:GLY:N	0.52	2.42	11	8
1:A:176:LEU:CD2	1:A:185:LEU:HD21	0.52	2.34	1	1
1:A:179:LEU:CD1	1:A:185:LEU:HD13	0.52	2.35	11	1
1:A:185:LEU:HD21	1:A:195:TRP:CD1	0.51	2.41	3	3
1:A:179:LEU:HD21	1:A:185:LEU:HD12	0.51	1.82	17	3
1:A:147:LEU:HD12	1:A:148:GLU:N	0.51	2.20	15	3
1:A:179:LEU:HD22	1:A:184:LYS:HD2	0.51	1.80	12	1
1:A:147:LEU:HD12	1:A:147:LEU:C	0.51	2.30	15	1
1:A:155:ALA:HB1	1:A:194:LEU:HD12	0.51	1.80	14	2
1:A:195:TRP:CD2	1:A:195:TRP:C	0.51	2.88	3	1
1:A:156:THR:OG1	1:A:161:LEU:HD23	0.51	2.06	8	1
1:A:176:LEU:HD13	1:A:195:TRP:HE1	0.50	1.65	16	1
1:A:176:LEU:C	1:A:176:LEU:CD1	0.50	2.80	9	9
1:A:156:THR:HG22	1:A:160:ASP:CB	0.50	2.36	11	2
1:A:144:LEU:HD13	1:A:144:LEU:C	0.50	2.30	2	1
1:A:146:PHE:CE2	1:A:165:LEU:HD22	0.50	2.41	6	1
1:A:188:GLU:OE1	1:A:188:GLU:C	0.50	2.54	14	1
1:A:185:LEU:HD22	1:A:185:LEU:C	0.50	2.30	2	4
1:A:146:PHE:CZ	1:A:161:LEU:HD21	0.50	2.41	8	1
1:A:194:LEU:CG	1:A:195:TRP:N	0.50	2.74	14	4
1:A:176:LEU:HD11	1:A:195:TRP:CE3	0.50	2.42	14	1
1:A:194:LEU:CD1	1:A:196:LYS:CG	0.50	2.90	19	1
1:A:150:LEU:HD11	1:A:154:LYS:O	0.50	2.06	11	3
1:A:156:THR:HG22	1:A:160:ASP:HB3	0.50	1.84	7	2
1:A:179:LEU:CD2	1:A:185:LEU:CB	0.50	2.89	4	1
1:A:155:ALA:HA	1:A:195:TRP:O	0.49	2.07	3	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:180:ALA:HB1	1:A:187:LYS:CG	0.49	2.37	18	4
1:A:188:GLU:OE2	1:A:188:GLU:CA	0.49	2.59	18	3
1:A:185:LEU:HD12	1:A:186:GLN:N	0.49	2.21	7	1
1:A:188:GLU:CG	1:A:193:ALA:HB3	0.49	2.37	18	4
1:A:176:LEU:HD22	1:A:185:LEU:HD21	0.49	1.84	1	1
1:A:195:TRP:C	1:A:196:LYS:HG3	0.49	2.32	10	2
1:A:191:THR:HB	1:A:192:PRO:HD3	0.49	1.85	20	4
1:A:148:GLU:OE1	1:A:197:ILE:HD12	0.49	2.07	7	1
1:A:175:VAL:HG22	1:A:179:LEU:HD11	0.49	1.84	12	1
1:A:140:GLU:O	1:A:144:LEU:HD23	0.49	2.08	17	1
1:A:154:LYS:O	1:A:155:ALA:HB2	0.49	2.08	18	3
1:A:155:ALA:HB2	1:A:196:LYS:HE3	0.48	1.85	10	1
1:A:179:LEU:HD13	1:A:184:LYS:HZ3	0.48	1.67	8	1
1:A:185:LEU:HD22	1:A:186:GLN:H	0.48	1.68	3	1
1:A:146:PHE:CE1	1:A:161:LEU:HD11	0.48	2.43	8	1
1:A:180:ALA:HB1	1:A:187:LYS:HE2	0.48	1.85	14	2
1:A:161:LEU:HD12	1:A:161:LEU:C	0.48	2.34	4	1
1:A:169:LYS:O	1:A:172:ILE:HG22	0.48	2.08	6	2
1:A:179:LEU:HD11	1:A:185:LEU:HB3	0.48	1.86	4	1
1:A:155:ALA:HB3	1:A:194:LEU:HD13	0.48	1.85	2	1
1:A:156:THR:N	1:A:194:LEU:HD22	0.48	2.24	2	1
1:A:188:GLU:HB2	1:A:193:ALA:HB1	0.48	1.86	15	1
1:A:191:THR:HB	1:A:192:PRO:CD	0.48	2.38	16	2
1:A:185:LEU:C	1:A:185:LEU:CD1	0.48	2.72	7	2
1:A:187:LYS:O	1:A:188:GLU:O	0.48	2.32	9	6
1:A:179:LEU:HD22	1:A:184:LYS:CD	0.47	2.39	12	1
1:A:179:LEU:HD11	1:A:185:LEU:HB2	0.47	1.86	15	3
1:A:180:ALA:HB2	1:A:185:LEU:HD23	0.47	1.86	13	3
1:A:195:TRP:O	1:A:195:TRP:CE3	0.47	2.67	3	2
1:A:161:LEU:HD22	1:A:164:LYS:HD3	0.47	1.86	8	1
1:A:191:THR:HG23	1:A:192:PRO:CD	0.47	2.39	12	9
1:A:196:LYS:O	1:A:197:ILE:C	0.47	2.55	7	10
1:A:180:ALA:N	1:A:185:LEU:HD23	0.47	2.25	5	2
1:A:188:GLU:O	1:A:190:GLY:N	0.47	2.47	3	2
1:A:147:LEU:O	1:A:150:LEU:HD11	0.47	2.10	4	1
1:A:197:ILE:CG1	1:A:198:ALA:N	0.47	2.77	9	9
1:A:161:LEU:O	1:A:165:LEU:HD12	0.47	2.09	12	1
1:A:161:LEU:HD21	1:A:172:ILE:HG13	0.47	1.86	4	1
1:A:191:THR:O	1:A:195:TRP:CZ2	0.47	2.67	12	1
1:A:150:LEU:HD13	1:A:154:LYS:HG2	0.47	1.86	16	1
1:A:175:VAL:HG22	1:A:179:LEU:HG	0.47	1.86	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:176:LEU:HD12	1:A:176:LEU:O	0.47	2.10	18	6
1:A:175:VAL:HA	1:A:178:SER:OG	0.46	2.11	4	2
1:A:188:GLU:OE1	1:A:190:GLY:O	0.46	2.33	6	1
1:A:161:LEU:HD21	1:A:172:ILE:HD11	0.46	1.87	4	2
1:A:171:GLU:O	1:A:175:VAL:HG12	0.46	2.11	5	2
1:A:155:ALA:HB2	1:A:196:LYS:HD3	0.46	1.87	6	1
1:A:150:LEU:C	1:A:150:LEU:HD23	0.46	2.35	18	1
1:A:150:LEU:HD22	1:A:154:LYS:NZ	0.46	2.26	10	1
1:A:179:LEU:HD11	1:A:185:LEU:CB	0.45	2.41	15	2
1:A:179:LEU:HD21	1:A:185:LEU:CD2	0.45	2.34	15	2
1:A:188:GLU:CB	1:A:194:LEU:HG	0.45	2.42	11	1
1:A:176:LEU:HD21	1:A:195:TRP:CE2	0.45	2.47	1	1
1:A:161:LEU:HD21	1:A:172:ILE:CD1	0.45	2.41	4	1
1:A:160:ASP:C	1:A:161:LEU:HD13	0.45	2.36	11	1
1:A:179:LEU:HD22	1:A:184:LYS:CE	0.45	2.42	12	1
1:A:191:THR:N	1:A:192:PRO:HD2	0.45	2.27	2	8
1:A:188:GLU:HB2	1:A:194:LEU:CD2	0.45	2.42	3	1
1:A:188:GLU:HG2	1:A:194:LEU:HB2	0.44	1.88	6	1
1:A:185:LEU:HD21	1:A:195:TRP:HE3	0.44	1.72	9	2
1:A:156:THR:HB	1:A:161:LEU:HD21	0.44	1.88	7	6
1:A:179:LEU:HD23	1:A:185:LEU:CB	0.44	2.42	18	2
1:A:155:ALA:HB2	1:A:196:LYS:HG2	0.44	1.90	17	2
1:A:169:LYS:C	1:A:171:GLU:N	0.44	2.76	6	1
1:A:191:THR:C	1:A:193:ALA:H	0.43	2.21	20	3
1:A:185:LEU:HD11	1:A:195:TRP:HD1	0.43	1.72	1	1
1:A:160:ASP:CG	1:A:161:LEU:HD23	0.43	2.38	14	1
1:A:144:LEU:HD22	1:A:147:LEU:HD11	0.43	1.89	2	1
1:A:191:THR:HG22	1:A:192:PRO:N	0.43	2.28	19	2
1:A:150:LEU:HD22	1:A:154:LYS:HD2	0.43	1.89	16	1
1:A:179:LEU:HD11	1:A:185:LEU:HG	0.43	1.88	14	2
1:A:194:LEU:C	1:A:194:LEU:CD2	0.43	2.87	18	3
1:A:144:LEU:CD2	1:A:147:LEU:HD11	0.43	2.44	2	1
1:A:185:LEU:CD2	1:A:195:TRP:CD1	0.43	3.02	2	1
1:A:180:ALA:HB1	1:A:187:LYS:HE3	0.43	1.87	11	1
1:A:180:ALA:CB	1:A:185:LEU:HD12	0.43	2.42	2	1
1:A:185:LEU:CD1	1:A:186:GLN:O	0.43	2.66	17	2
1:A:176:LEU:HD12	1:A:176:LEU:C	0.42	2.38	18	1
1:A:142:ARG:HE	1:A:165:LEU:HD22	0.42	1.74	20	1
1:A:165:LEU:HB2	1:A:167:THR:HG22	0.42	1.91	2	4
1:A:185:LEU:CD2	1:A:196:LYS:O	0.42	2.67	17	1
1:A:142:ARG:HE	1:A:165:LEU:HD21	0.42	1.73	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:184:LYS:O	1:A:184:LYS:CG	0.42	2.67	12	2
1:A:188:GLU:CD	1:A:194:LEU:H	0.42	2.23	9	4
1:A:144:LEU:C	1:A:144:LEU:CD1	0.42	2.92	6	2
1:A:188:GLU:OE1	1:A:188:GLU:CA	0.42	2.67	14	1
1:A:188:GLU:CG	1:A:193:ALA:CB	0.42	2.97	18	1
1:A:172:ILE:HG23	1:A:173:ASN:ND2	0.42	2.29	20	1
1:A:150:LEU:HD23	1:A:154:LYS:HG3	0.42	1.90	9	2
1:A:188:GLU:HB2	1:A:193:ALA:CB	0.42	2.43	15	1
1:A:150:LEU:HD11	1:A:154:LYS:HE2	0.42	1.90	6	1
1:A:155:ALA:HB2	1:A:196:LYS:CG	0.42	2.44	10	1
1:A:179:LEU:CG	1:A:185:LEU:HB3	0.42	2.45	15	1
1:A:179:LEU:HD13	1:A:185:LEU:CB	0.42	2.44	20	1
1:A:186:GLN:C	1:A:187:LYS:HG3	0.42	2.39	5	1
1:A:175:VAL:O	1:A:179:LEU:HG	0.42	2.15	20	2
1:A:176:LEU:HD12	1:A:177:TYR:N	0.42	2.30	13	1
1:A:142:ARG:CD	1:A:165:LEU:HD21	0.42	2.43	3	1
1:A:169:LYS:O	1:A:173:ASN:CG	0.42	2.63	6	1
1:A:157:THR:HG22	1:A:194:LEU:CD1	0.42	2.44	1	1
1:A:185:LEU:HD23	1:A:195:TRP:CD1	0.42	2.50	2	1
1:A:195:TRP:C	1:A:196:LYS:CG	0.42	2.93	6	1
1:A:179:LEU:HD11	1:A:185:LEU:CD1	0.42	2.41	13	1
1:A:156:THR:HG21	1:A:160:ASP:CG	0.42	2.40	17	1
1:A:191:THR:OG1	1:A:192:PRO:N	0.42	2.53	18	1
1:A:194:LEU:HD12	1:A:194:LEU:HA	0.42	1.78	1	1
1:A:161:LEU:HD12	1:A:172:ILE:HD11	0.41	1.92	6	1
1:A:144:LEU:O	1:A:144:LEU:HD22	0.41	2.15	2	1
1:A:143:ILE:O	1:A:147:LEU:HD23	0.41	2.15	7	1
1:A:186:GLN:HE21	1:A:194:LEU:HD11	0.41	1.76	16	1
1:A:188:GLU:OE2	1:A:188:GLU:N	0.41	2.53	18	1
1:A:142:ARG:O	1:A:146:PHE:CD1	0.41	2.74	4	1
1:A:157:THR:O	1:A:161:LEU:HG	0.41	2.15	14	1
1:A:193:ALA:O	1:A:194:LEU:HB3	0.41	2.14	19	1
1:A:179:LEU:HG	1:A:185:LEU:CB	0.41	2.46	3	1
1:A:189:ALA:O	1:A:193:ALA:HB2	0.41	2.15	3	2
1:A:194:LEU:HD12	1:A:195:TRP:CA	0.41	2.45	3	1
1:A:176:LEU:HD21	1:A:195:TRP:CZ2	0.41	2.51	4	1
1:A:155:ALA:HB2	1:A:196:LYS:NZ	0.41	2.31	8	1
1:A:150:LEU:HD12	1:A:154:LYS:CE	0.41	2.42	14	1
1:A:188:GLU:CG	1:A:193:ALA:HB1	0.41	2.45	19	2
1:A:179:LEU:CD2	1:A:180:ALA:N	0.41	2.77	4	1
1:A:179:LEU:HD23	1:A:185:LEU:HB2	0.41	1.93	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:176:LEU:O	1:A:179:LEU:HD23	0.41	2.16	13	3
1:A:142:ARG:HD3	1:A:165:LEU:HD22	0.41	1.93	1	1
1:A:150:LEU:HD12	1:A:150:LEU:O	0.41	2.16	9	1
1:A:191:THR:O	1:A:195:TRP:CH2	0.40	2.74	1	1
1:A:155:ALA:HB2	1:A:196:LYS:HE2	0.40	1.93	18	1
1:A:169:LYS:C	1:A:171:GLU:H	0.40	2.23	6	1
1:A:157:THR:O	1:A:160:ASP:N	0.40	2.50	14	1
1:A:160:ASP:OD1	1:A:160:ASP:C	0.40	2.64	14	1
1:A:179:LEU:HB2	1:A:184:LYS:CD	0.40	2.46	16	1
1:A:179:LEU:N	1:A:179:LEU:CD1	0.40	2.84	19	1
1:A:188:GLU:HG3	1:A:194:LEU:CD2	0.40	2.43	18	1
1:A:165:LEU:HD12	1:A:165:LEU:O	0.40	2.16	8	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	58/84 (69%)	44±2 (77±4%)	7±2 (13±4%)	6±1 (11±2%)	1	8
All	All	1160/1680 (69%)	889 (77%)	146 (13%)	125 (11%)	1	8

All 14 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	152	GLU	20
1	A	197	ILE	20
1	A	189	ALA	14
1	A	151	GLY	13
1	A	198	ALA	10
1	A	185	LEU	9
1	A	188	GLU	9
1	A	194	LEU	8
1	A	150	LEU	7
1	A	154	LYS	6

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Mol	Chain	Res	Type	Models (Total)
1	A	155	ALA	5
1	A	186	GLN	2
1	A	167	THR	1
1	A	196	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	47/69 (68%)	27±2 (57±5%)	20±2 (43±5%)	0 3
All	All	940/1380 (68%)	532 (57%)	408 (43%)	0 3

All 40 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	185	LEU	20
1	A	191	THR	20
1	A	161	LEU	19
1	A	167	THR	19
1	A	170	LYS	19
1	A	156	THR	19
1	A	196	LYS	18
1	A	186	GLN	17
1	A	154	LYS	16
1	A	162	SER	16
1	A	184	LYS	16
1	A	176	LEU	15
1	A	179	LEU	14
1	A	160	ASP	13
1	A	187	LYS	13
1	A	164	LYS	12
1	A	182	LYS	12
1	A	194	LEU	12
1	A	188	GLU	12
1	A	146	PHE	11
1	A	145	LYS	10

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Mol	Chain	Res	Type	Models (Total)
1	A	150	LEU	10
1	A	152	GLU	10
1	A	143	ILE	9
1	A	171	GLU	8
1	A	144	LEU	7
1	A	142	ARG	5
1	A	169	LYS	5
1	A	195	TRP	5
1	A	181	LYS	4
1	A	140	GLU	3
1	A	165	LEU	3
1	A	141	GLN	3
1	A	197	ILE	3
1	A	174	ARG	2
1	A	172	ILE	2
1	A	173	ASN	2
1	A	149	GLU	2
1	A	178	SER	1
1	A	159	HIS	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 64% for the well-defined parts and 64% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chemical_shifts_1*

7.1.1 Bookkeeping

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

Total number of shifts	562
Number of shifts mapped to atoms	555
Number of unparsed shifts	0
Number of shifts with mapping errors	7
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	4

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. All 7 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	138	HIS	HA	4.548	0.000	1
1	A	138	HIS	HB2	3.337	0.000	.
1	A	139	MET	H	8.416	0.000	1
1	A	139	MET	HA	4.239	0.000	1
1	A	139	MET	CA	57.613	0.000	1
1	A	139	MET	CB	31.848	0.000	1
1	A	139	MET	N	119.682	0.000	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	64	-0.26 $\pm$ 0.18	None needed (< 0.5 ppm)

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Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\beta$	58	-0.25 ± 0.19	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	62	0.52 ± 0.33	None needed (imprecise)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 64%, i.e. 529 atoms were assigned a chemical shift out of a possible 824. 0 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	233/297 (78%)	117/122 (96%)	59/118 (50%)	57/57 (100%)
Sidechain	294/489 (60%)	198/317 (62%)	93/153 (61%)	3/19 (16%)
Aromatic	2/38 (5%)	1/19 (5%)	0/17 (0%)	1/2 (50%)
Overall	529/824 (64%)	316/458 (69%)	152/288 (53%)	61/78 (78%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 64%, i.e. 555 atoms were assigned a chemical shift out of a possible 873. 0 out of 11 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	247/317 (78%)	123/130 (95%)	63/126 (50%)	61/61 (100%)
Sidechain	306/518 (59%)	205/336 (61%)	97/162 (60%)	4/20 (20%)
Aromatic	2/38 (5%)	1/19 (5%)	0/17 (0%)	1/2 (50%)
Overall	555/873 (64%)	329/485 (68%)	160/305 (52%)	66/83 (80%)

7.1.4 Statistically unusual chemical shifts [i](#)

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	176	LEU	HB3	-0.98	-0.26 – 3.31	-7.0
1	A	187	LYS	HG3	-0.10	0.04 – 2.67	-5.5
1	A	175	VAL	CG1	28.79	14.71 – 28.29	5.4
1	A	187	LYS	HB2	0.55	0.58 – 2.97	-5.2

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

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

Random coil index (RCI) for chain A:

