



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 05:46 PM UTC

PDB ID : 2L7B / pdb_00002l7b
BMRB ID : 15744
Title : NMR Structure of full length apoE3
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Deposited on : 2010-12-07

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

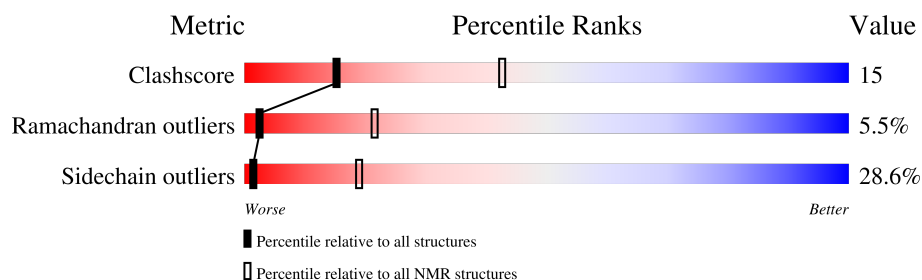
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

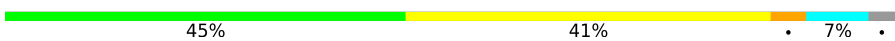
The overall completeness of chemical shifts assignment is 67%.

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	307	

2 Ensemble composition and analysis

This entry contains 20 models. Model 9 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:3-A:181, A:186-A:200, A:209-A:281, A:287-A:296 (277)	0.92	9

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 5 clusters and 3 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4792 atoms, of which 2396 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Apolipoprotein E.

Mol	Chain	Residues	Atoms						Trace
1	A	299	Total	C	H	N	O	S	0
			4792	1464	2396	459	465	8	

There are 13 discrepancies between the modelled and reference sequences:

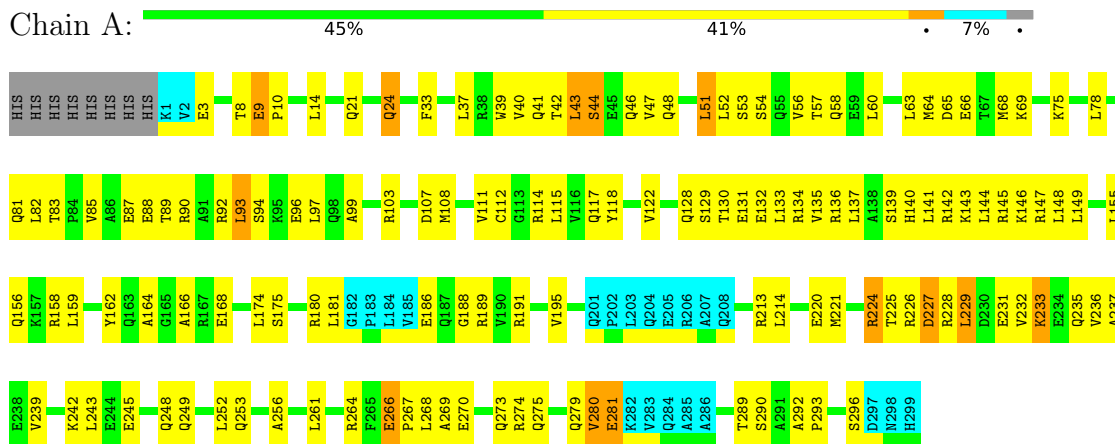
Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	HIS	-	expression tag	UNP P02649
A	-6	HIS	-	expression tag	UNP P02649
A	-5	HIS	-	expression tag	UNP P02649
A	-4	HIS	-	expression tag	UNP P02649
A	-3	HIS	-	expression tag	UNP P02649
A	-2	HIS	-	expression tag	UNP P02649
A	-1	HIS	-	expression tag	UNP P02649
A	0	HIS	-	expression tag	UNP P02649
A	257	ALA	PHE	engineered mutation	UNP P02649
A	264	ARG	TRP	engineered mutation	UNP P02649
A	269	ALA	VAL	engineered mutation	UNP P02649
A	279	GLN	LEU	engineered mutation	UNP P02649
A	287	GLU	VAL	engineered mutation	UNP P02649

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: Apolipoprotein E

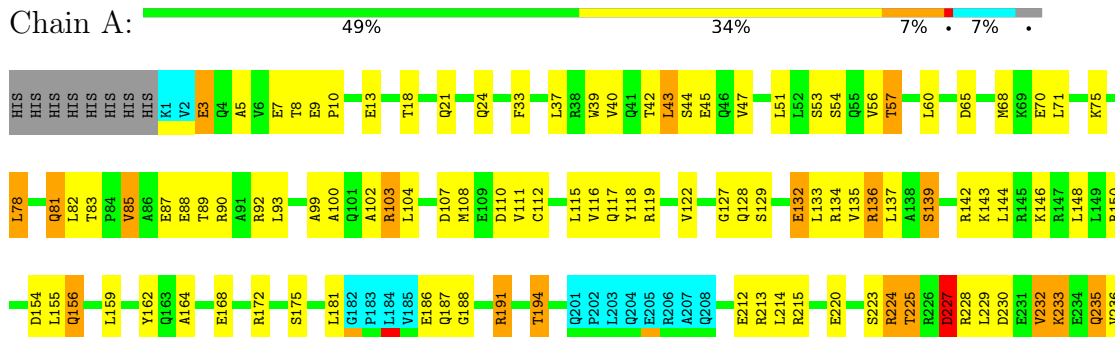


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

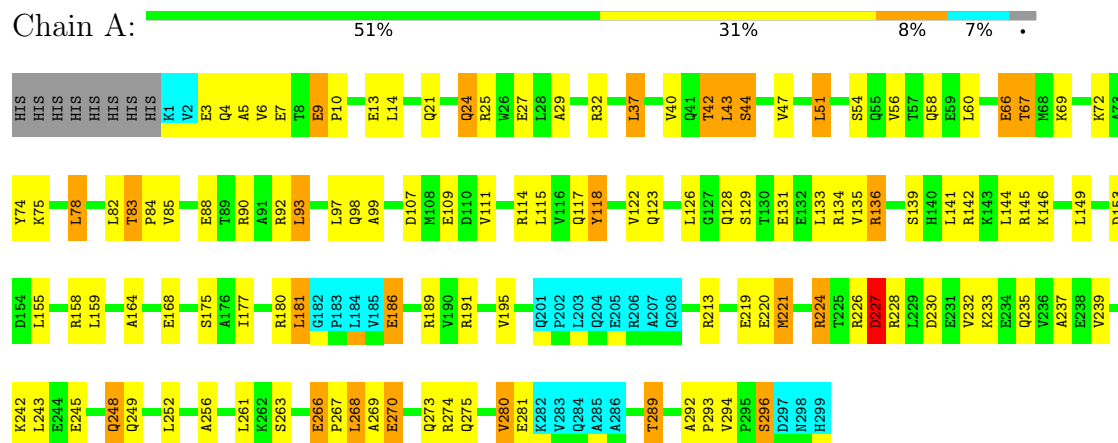
- Molecule 1: Apolipoprotein E





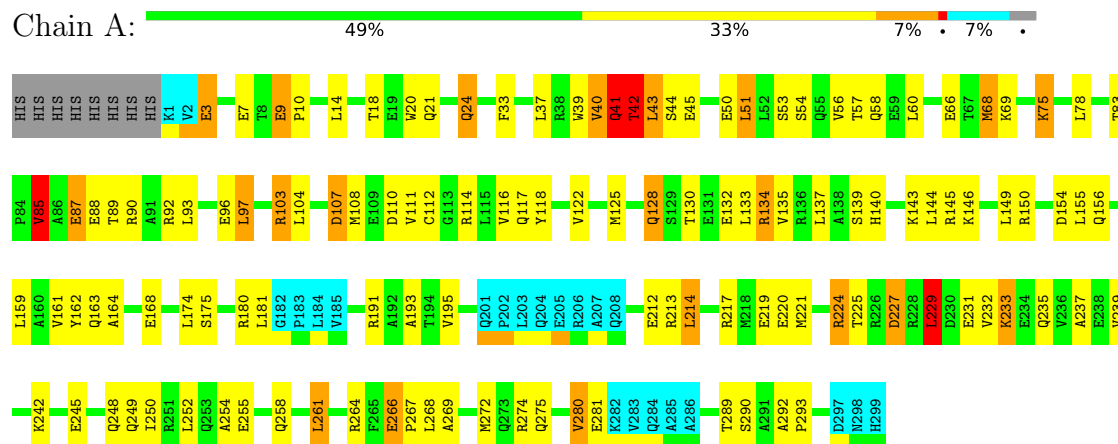
4.2.2 Score per residue for model 2

- Molecule 1: Apolipoprotein E



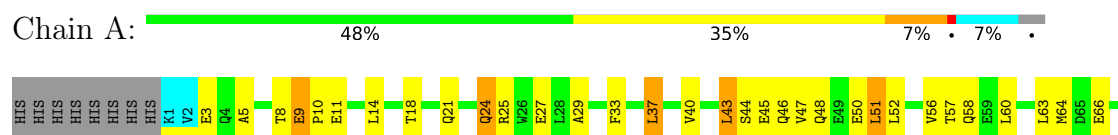
4.2.3 Score per residue for model 3

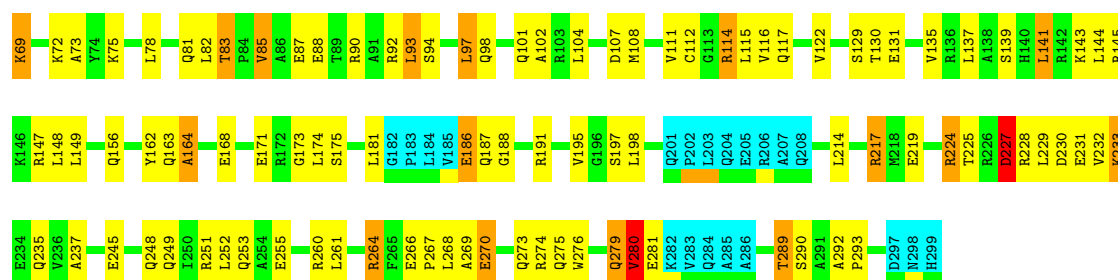
- Molecule 1: Apolipoprotein E



4.2.4 Score per residue for model 4

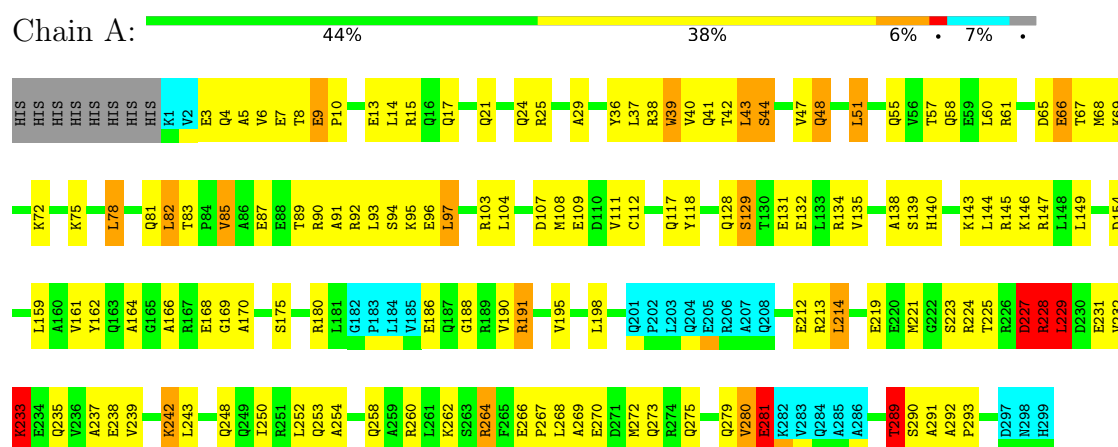
- Molecule 1: Apolipoprotein E





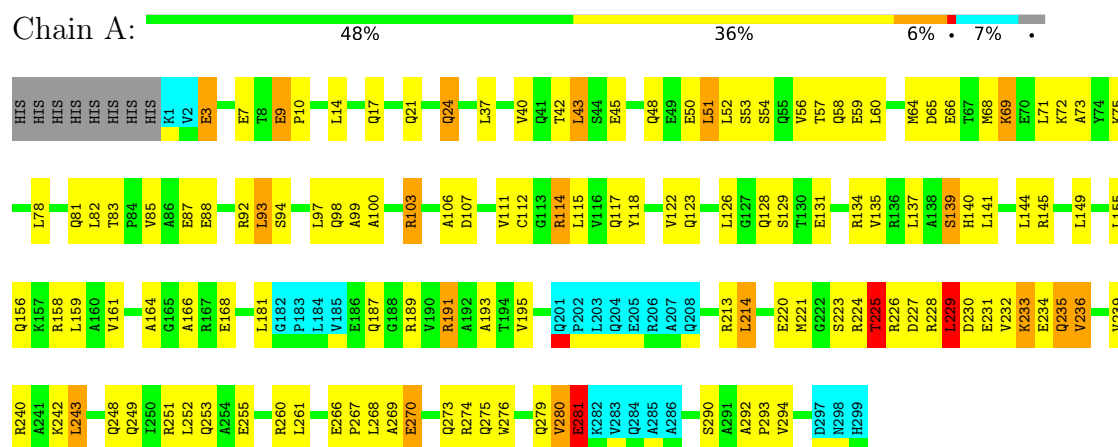
4.2.5 Score per residue for model 5

- Molecule 1: Apolipoprotein E



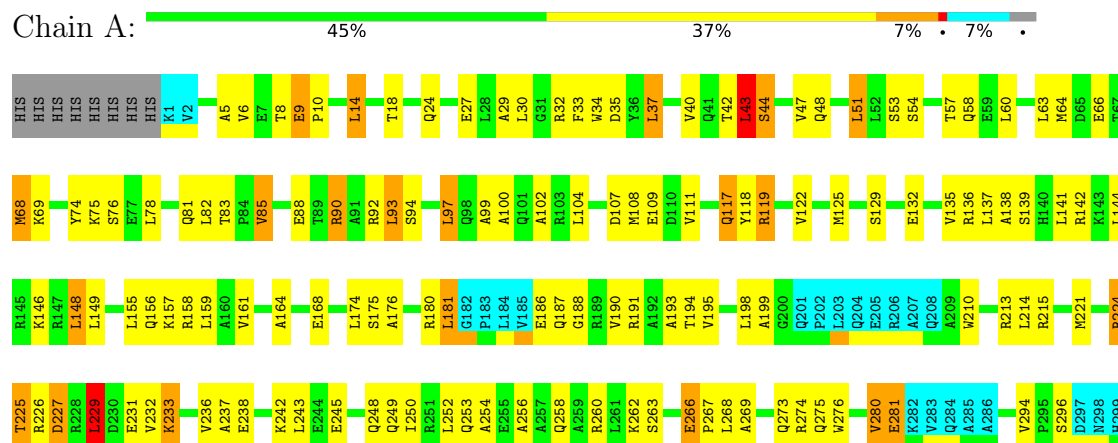
4.2.6 Score per residue for model 6

- Molecule 1: Apolipoprotein E



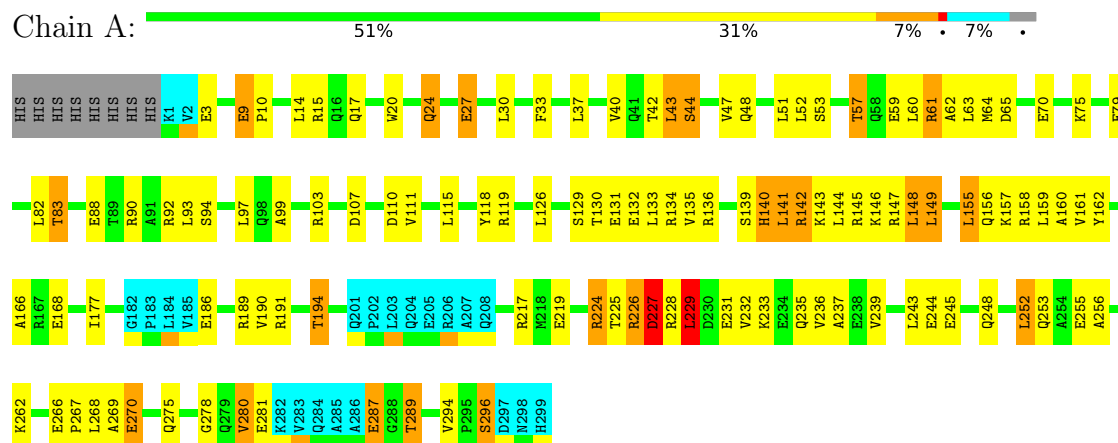
4.2.7 Score per residue for model 7

• Molecule 1: Apolipoprotein E



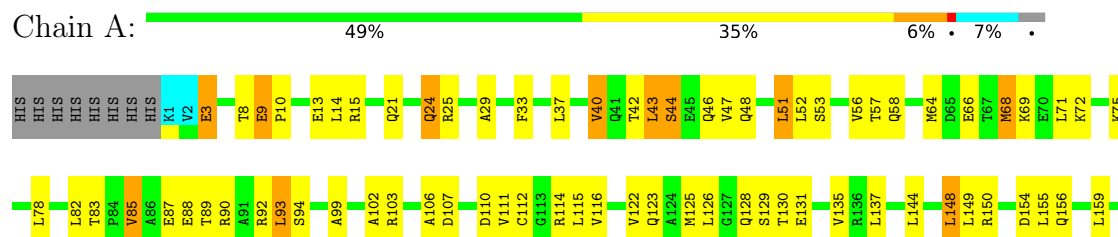
4.2.8 Score per residue for model 8

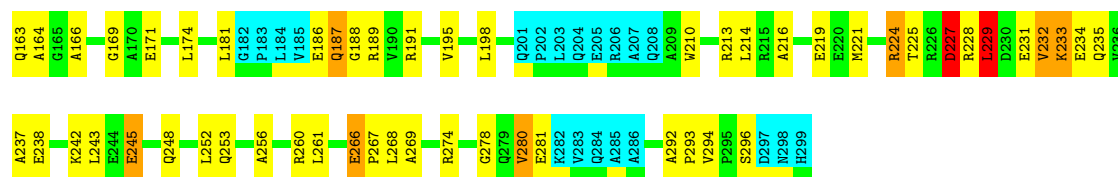
• Molecule 1: Apolipoprotein E



4.2.9 Score per residue for model 9 (medoid)

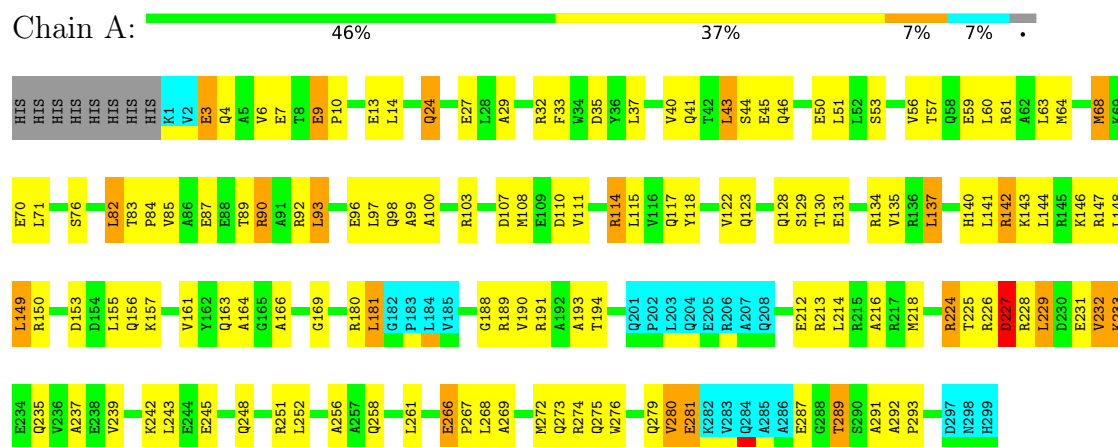
• Molecule 1: Apolipoprotein E





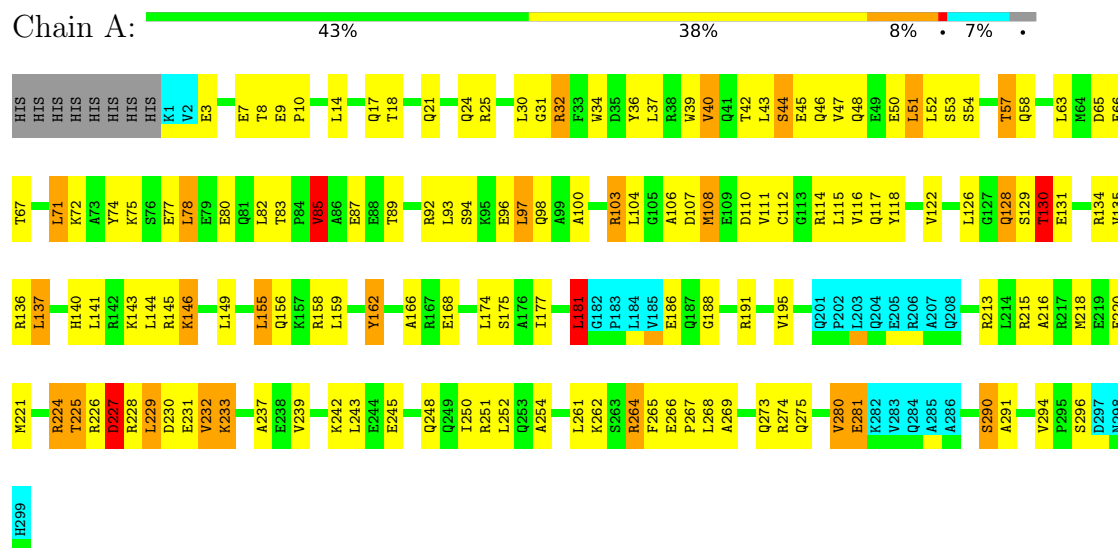
4.2.10 Score per residue for model 10

- Molecule 1: Apolipoprotein E



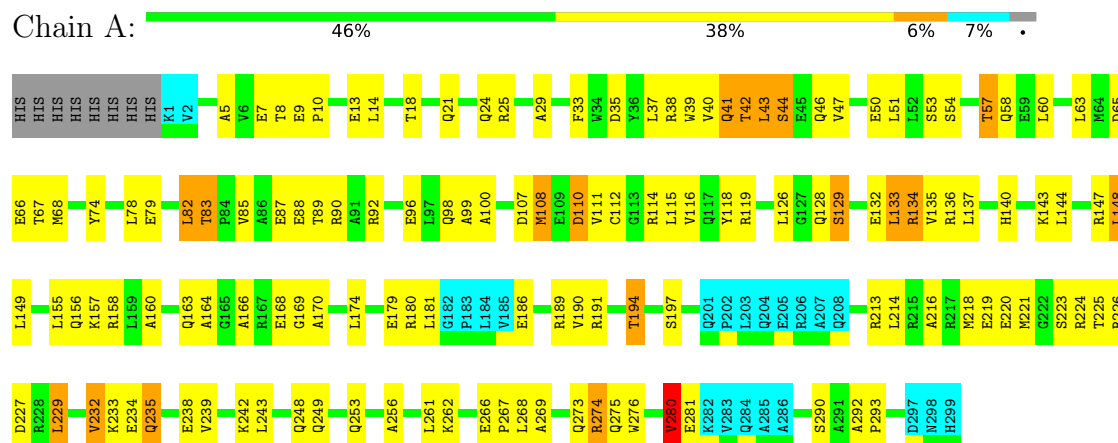
4.2.11 Score per residue for model 11

- Molecule 1: Apolipoprotein E



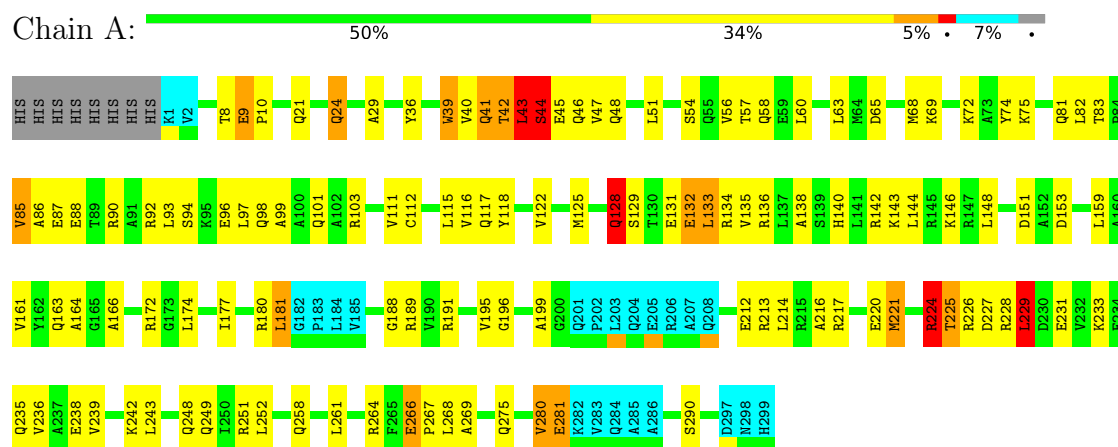
4.2.12 Score per residue for model 12

- Molecule 1: Apolipoprotein E



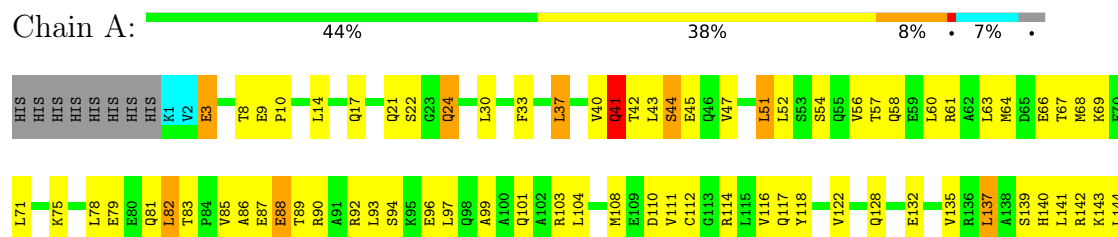
4.2.13 Score per residue for model 13

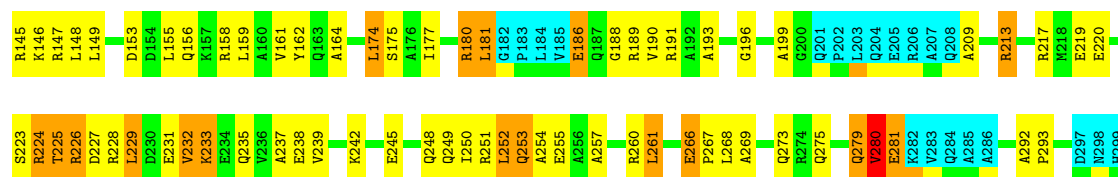
- Molecule 1: Apolipoprotein E



4.2.14 Score per residue for model 14

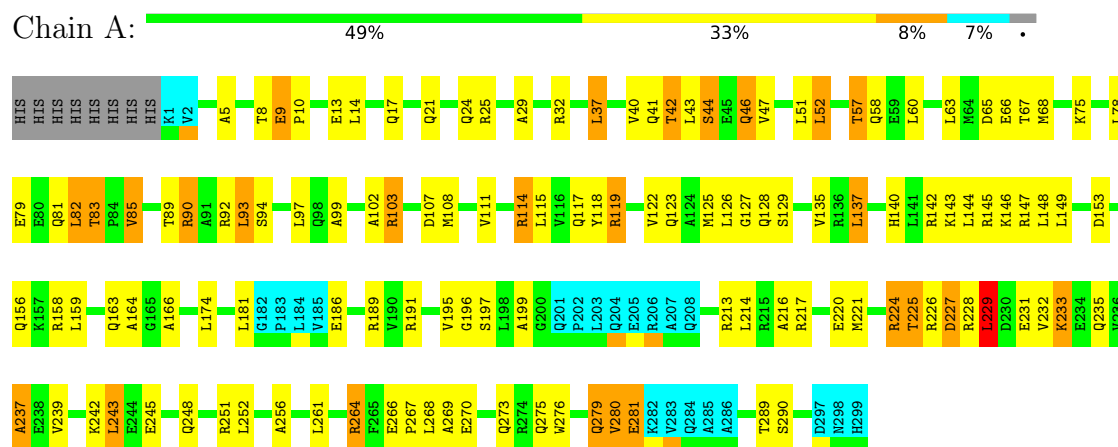
- Molecule 1: Apolipoprotein E





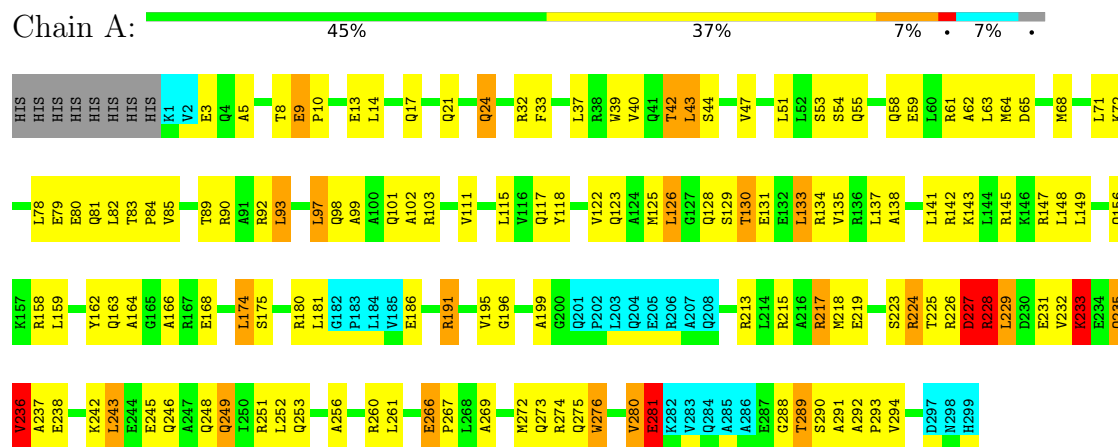
4.2.15 Score per residue for model 15

- Molecule 1: Apolipoprotein E



4.2.16 Score per residue for model 16

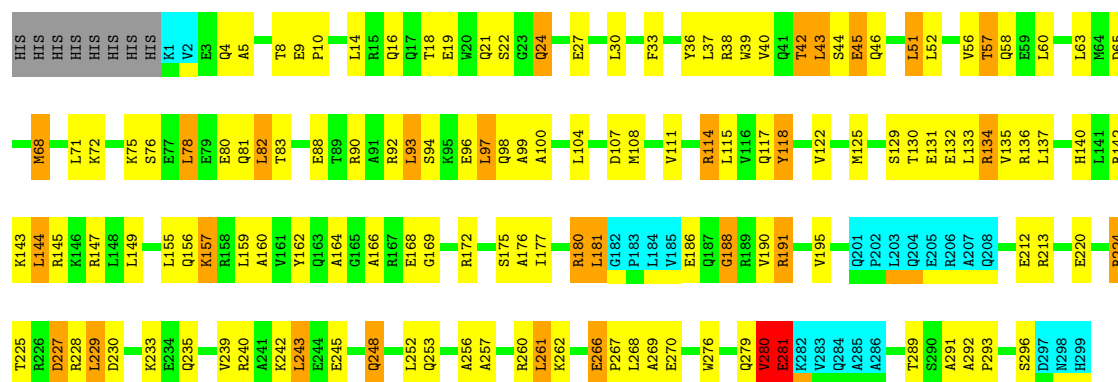
- Molecule 1: Apolipoprotein E



4.2.17 Score per residue for model 17

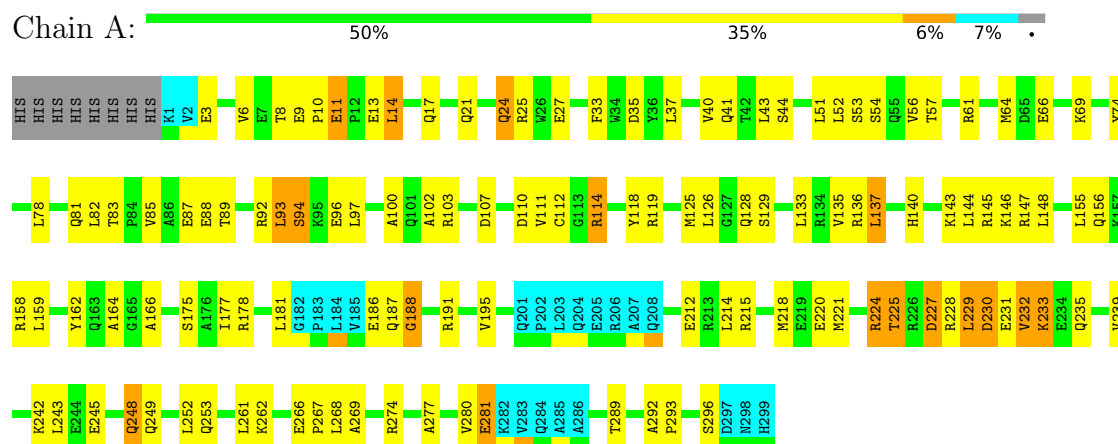
- Molecule 1: Apolipoprotein E





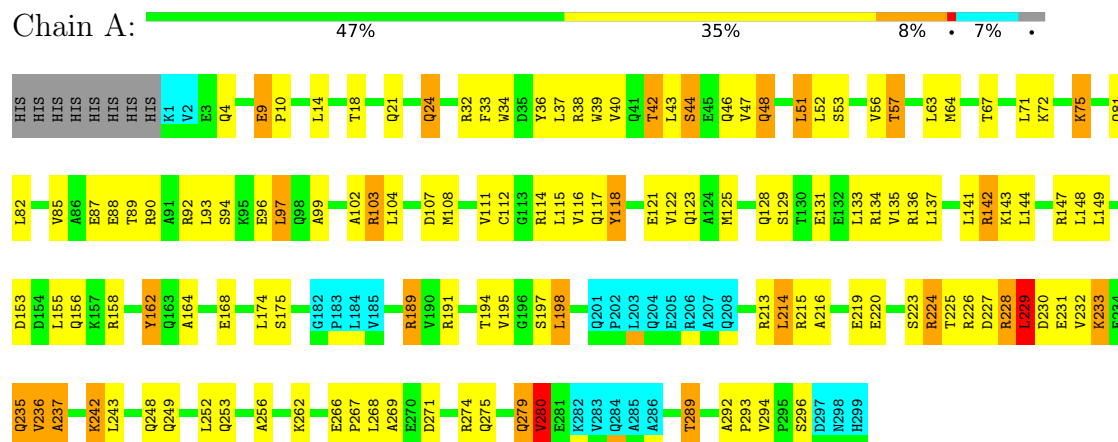
4.2.18 Score per residue for model 18

- Molecule 1: Apolipoprotein E



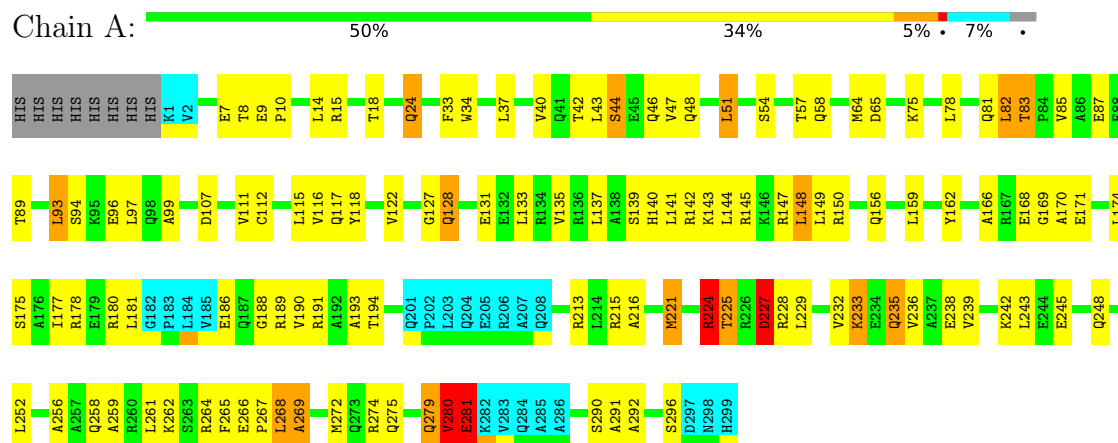
4.2.19 Score per residue for model 19

- Molecule 1: Apolipoprotein E



4.2.20 Score per residue for model 20

● Molecule 1: Apolipoprotein E



5 Refinement protocol and experimental data overview

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

Of the 20 calculated structures, 20 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
CYANA	structure solution	
ProcheckNMR	geometry optimization	
ProcheckNMR	refinement	
CNS	geometry optimization	
CNS	refinement	

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	2810
Number of shifts mapped to atoms	2810
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	67%

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	2226	2221	2221	66±7
All	All	44520	44420	44420	1323

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 15.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:78:LEU:HD13	1:A:159:LEU:HD22	0.99	1.35	2	2
1:A:51:LEU:HD13	1:A:122:VAL:HG11	0.96	1.35	2	4
1:A:111:VAL:HG22	1:A:144:LEU:HD21	0.95	1.34	7	13
1:A:243:LEU:HD23	1:A:294:VAL:HG22	0.93	1.35	16	1
1:A:243:LEU:HD21	1:A:294:VAL:HG23	0.86	1.48	9	3
1:A:43:LEU:HD12	1:A:137:LEU:HD21	0.83	1.49	20	2
1:A:71:LEU:HD22	1:A:104:LEU:HD23	0.82	1.50	11	1
1:A:82:LEU:HD13	1:A:93:LEU:HD22	0.81	1.51	10	2
1:A:82:LEU:HD13	1:A:93:LEU:HD21	0.79	1.52	9	2
1:A:64:MET:HE3	1:A:190:VAL:HG13	0.79	1.54	14	2
1:A:51:LEU:HD21	1:A:122:VAL:HG11	0.75	1.59	4	1
1:A:14:LEU:HD22	1:A:149:LEU:HD21	0.74	1.60	14	9
1:A:149:LEU:HD23	1:A:280:VAL:HG12	0.73	1.58	4	3
1:A:104:LEU:HD11	1:A:108:MET:HE2	0.73	1.58	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:43:LEU:HD22	1:A:47:VAL:HG23	0.71	1.61	20	2
1:A:78:LEU:HD22	1:A:159:LEU:HD23	0.71	1.62	20	2
1:A:68:MET:HE2	1:A:190:VAL:HG11	0.70	1.61	5	1
1:A:82:LEU:HD21	1:A:93:LEU:HD13	0.70	1.64	4	1
1:A:51:LEU:HD11	1:A:118:TYR:CE2	0.70	2.21	15	6
1:A:268:LEU:O	1:A:269:ALA:HB3	0.69	1.87	20	1
1:A:104:LEU:HD11	1:A:108:MET:HE3	0.69	1.62	4	5
1:A:99:ALA:HB1	1:A:256:ALA:HB2	0.69	1.64	15	6
1:A:100:ALA:HB1	1:A:155:LEU:HD12	0.69	1.63	12	5
1:A:40:VAL:HG11	1:A:141:LEU:HD11	0.69	1.63	11	5
1:A:83:THR:HG22	1:A:161:VAL:HG12	0.68	1.65	3	5
1:A:51:LEU:HD21	1:A:118:TYR:CE2	0.68	2.23	1	7
1:A:40:VAL:HG22	1:A:56:VAL:HG12	0.68	1.63	17	1
1:A:51:LEU:HD21	1:A:118:TYR:CD2	0.68	2.24	11	5
1:A:42:THR:HG22	1:A:217:ARG:HD3	0.67	1.67	14	2
1:A:46:GLN:HG3	1:A:216:ALA:HB3	0.67	1.65	13	4
1:A:33:PHE:CE2	1:A:37:LEU:HD22	0.67	2.24	16	3
1:A:81:GLN:O	1:A:82:LEU:HD13	0.67	1.90	15	3
1:A:131:GLU:O	1:A:135:VAL:HG13	0.66	1.90	13	3
1:A:42:THR:C	1:A:43:LEU:HD22	0.66	2.15	19	1
1:A:51:LEU:HD11	1:A:118:TYR:CZ	0.66	2.25	10	7
1:A:85:VAL:HG11	1:A:89:THR:HG21	0.66	1.66	3	3
1:A:140:HIS:CE1	1:A:239:VAL:HG23	0.66	2.26	5	3
1:A:135:VAL:HG21	1:A:232:VAL:CG2	0.66	2.21	20	11
1:A:239:VAL:HG12	1:A:243:LEU:HD22	0.65	1.66	12	3
1:A:82:LEU:HD21	1:A:169:GLY:C	0.65	2.16	10	1
1:A:33:PHE:CZ	1:A:148:LEU:HD13	0.65	2.27	20	2
1:A:82:LEU:HD12	1:A:93:LEU:HD13	0.65	1.67	8	1
1:A:36:TYR:O	1:A:40:VAL:HG23	0.65	1.92	13	3
1:A:8:THR:HG21	1:A:280:VAL:HG12	0.65	1.68	20	1
1:A:36:TYR:CD2	1:A:63:LEU:HD11	0.65	2.27	19	1
1:A:40:VAL:HG21	1:A:60:LEU:HD11	0.64	1.69	5	3
1:A:43:LEU:HD11	1:A:226:ARG:HB3	0.64	1.68	8	1
1:A:33:PHE:CZ	1:A:37:LEU:HD22	0.64	2.27	20	1
1:A:131:GLU:O	1:A:135:VAL:HG23	0.64	1.91	9	10
1:A:8:THR:HG22	1:A:280:VAL:HG23	0.64	1.68	11	3
1:A:82:LEU:HD12	1:A:93:LEU:HD23	0.64	1.69	11	1
1:A:3:GLU:O	1:A:6:VAL:HG12	0.64	1.92	5	1
1:A:90:ARG:HA	1:A:93:LEU:HD23	0.64	1.69	7	1
1:A:33:PHE:HB2	1:A:63:LEU:HD11	0.64	1.70	12	1
1:A:93:LEU:HD13	1:A:162:TYR:CZ	0.64	2.27	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:37:LEU:O	1:A:40:VAL:HG12	0.64	1.93	15	16
1:A:81:GLN:O	1:A:82:LEU:HD23	0.64	1.93	1	6
1:A:48:GLN:HA	1:A:51:LEU:HD23	0.64	1.70	5	5
1:A:81:GLN:C	1:A:82:LEU:HD22	0.63	2.18	13	2
1:A:181:LEU:HD11	1:A:186:GLU:OE1	0.63	1.93	11	1
1:A:8:THR:HG21	1:A:149:LEU:CD2	0.63	2.23	14	4
1:A:140:HIS:CE1	1:A:239:VAL:HG13	0.63	2.29	10	5
1:A:33:PHE:CZ	1:A:148:LEU:HD22	0.63	2.29	12	1
1:A:102:ALA:HB3	1:A:252:LEU:HD21	0.63	1.69	1	3
1:A:79:GLU:OE2	1:A:174:LEU:HD12	0.63	1.94	12	3
1:A:43:LEU:HD13	1:A:221:MET:CB	0.63	2.23	13	1
1:A:51:LEU:HD13	1:A:122:VAL:HG21	0.63	1.70	1	6
1:A:82:LEU:HD21	1:A:170:ALA:HA	0.63	1.71	5	3
1:A:27:GLU:OE1	1:A:30:LEU:HD11	0.63	1.94	17	1
1:A:10:PRO:O	1:A:11:GLU:C	0.62	2.41	18	1
1:A:107:ASP:O	1:A:111:VAL:HG23	0.62	1.94	17	15
1:A:3:GLU:OE2	1:A:289:THR:HG23	0.62	1.94	3	3
1:A:125:MET:HE2	1:A:128:GLN:CD	0.62	2.19	18	3
1:A:248:GLN:OE1	1:A:252:LEU:HD11	0.62	1.95	6	7
1:A:42:THR:HG22	1:A:221:MET:CG	0.62	2.24	11	4
1:A:81:GLN:C	1:A:82:LEU:HD23	0.62	2.20	18	6
1:A:93:LEU:HD12	1:A:162:TYR:CE1	0.62	2.30	18	1
1:A:83:THR:HG22	1:A:161:VAL:CG1	0.62	2.25	10	6
1:A:139:SER:OG	1:A:229:LEU:HD13	0.62	1.94	6	2
1:A:78:LEU:HD12	1:A:162:TYR:HB2	0.62	1.72	1	1
1:A:268:LEU:O	1:A:269:ALA:CB	0.62	2.48	20	1
1:A:85:VAL:HG11	1:A:89:THR:HG22	0.61	1.71	19	3
1:A:133:LEU:HD23	1:A:235:GLN:CG	0.61	2.25	1	1
1:A:125:MET:HE2	1:A:128:GLN:OE1	0.61	1.96	18	2
1:A:42:THR:HG22	1:A:221:MET:HG2	0.61	1.71	7	2
1:A:83:THR:O	1:A:166:ALA:HB2	0.61	1.95	11	11
1:A:40:VAL:HG23	1:A:56:VAL:HB	0.61	1.70	14	2
1:A:82:LEU:HD11	1:A:169:GLY:C	0.61	2.21	17	2
1:A:46:GLN:CG	1:A:216:ALA:HB3	0.61	2.25	11	6
1:A:280:VAL:HG13	1:A:281:GLU:CD	0.61	2.21	15	2
1:A:280:VAL:HG22	1:A:281:GLU:HG3	0.61	1.73	18	5
1:A:81:GLN:C	1:A:82:LEU:HD13	0.61	2.20	15	2
1:A:228:ARG:C	1:A:229:LEU:HD12	0.60	2.20	8	2
1:A:138:ALA:HB3	1:A:228:ARG:O	0.60	1.96	16	2
1:A:142:ARG:CZ	1:A:229:LEU:HD11	0.60	2.25	1	3
1:A:43:LEU:HD22	1:A:47:VAL:CG2	0.60	2.27	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:74:TYR:CD2	1:A:159:LEU:HD11	0.60	2.32	13	1
1:A:114:ARG:NH2	1:A:137:LEU:HD12	0.60	2.11	6	4
1:A:191:ARG:O	1:A:195:VAL:HG23	0.60	1.96	15	13
1:A:132:GLU:O	1:A:135:VAL:HG22	0.60	1.97	13	5
1:A:264:ARG:NH1	1:A:268:LEU:HD21	0.60	2.12	5	4
1:A:266:GLU:HB2	1:A:267:PRO:HD3	0.60	1.72	6	9
1:A:135:VAL:HG21	1:A:232:VAL:HG21	0.60	1.74	19	6
1:A:33:PHE:HA	1:A:63:LEU:HD23	0.60	1.74	16	2
1:A:112:CYS:O	1:A:116:VAL:HG23	0.60	1.97	3	9
1:A:187:GLN:CD	1:A:190:VAL:HG13	0.60	2.21	7	1
1:A:139:SER:HB2	1:A:229:LEU:HD23	0.59	1.74	8	2
1:A:82:LEU:CD1	1:A:93:LEU:HD23	0.59	2.26	11	1
1:A:117:GLN:NE2	1:A:237:ALA:HB1	0.59	2.12	15	1
1:A:75:LYS:HD2	1:A:159:LEU:HD11	0.59	1.74	1	1
1:A:135:VAL:HG21	1:A:232:VAL:HB	0.59	1.73	12	2
1:A:111:VAL:CG2	1:A:144:LEU:HD21	0.59	2.25	4	7
1:A:37:LEU:HD11	1:A:145:ARG:HG2	0.59	1.74	11	7
1:A:111:VAL:O	1:A:115:LEU:HD23	0.59	1.97	13	6
1:A:40:VAL:HG23	1:A:56:VAL:CG2	0.59	2.26	18	2
1:A:60:LEU:HD13	1:A:111:VAL:CG1	0.59	2.28	14	8
1:A:82:LEU:HD22	1:A:93:LEU:HD13	0.59	1.74	2	1
1:A:8:THR:CG2	1:A:280:VAL:HG12	0.59	2.28	20	1
1:A:60:LEU:HD22	1:A:111:VAL:HG11	0.59	1.71	2	5
1:A:5:ALA:O	1:A:8:THR:HG22	0.59	1.97	12	5
1:A:42:THR:HG23	1:A:217:ARG:HG3	0.59	1.73	3	1
1:A:82:LEU:CD2	1:A:93:LEU:HD13	0.59	2.26	4	1
1:A:46:GLN:HG2	1:A:216:ALA:HB3	0.59	1.74	15	2
1:A:82:LEU:HD22	1:A:162:TYR:CZ	0.59	2.33	19	1
1:A:43:LEU:HD11	1:A:137:LEU:HD22	0.59	1.75	9	1
1:A:243:LEU:HD23	1:A:296:SER:HA	0.59	1.75	19	2
1:A:44:SER:O	1:A:47:VAL:HG12	0.58	1.98	15	15
1:A:82:LEU:HD13	1:A:93:LEU:CD2	0.58	2.26	9	4
1:A:43:LEU:HD12	1:A:137:LEU:CD2	0.58	2.24	20	1
1:A:82:LEU:HD22	1:A:93:LEU:CD1	0.58	2.28	1	2
1:A:267:PRO:HG2	1:A:268:LEU:HD23	0.58	1.75	11	15
1:A:82:LEU:CD2	1:A:166:ALA:HB3	0.58	2.27	11	2
1:A:280:VAL:HG12	1:A:281:GLU:HG3	0.58	1.75	16	2
1:A:75:LYS:HA	1:A:78:LEU:HD23	0.58	1.74	11	1
1:A:135:VAL:HG11	1:A:232:VAL:HB	0.58	1.73	1	1
1:A:258:GLN:HA	1:A:261:LEU:HD12	0.58	1.74	1	1
1:A:93:LEU:HD11	1:A:173:GLY:HA2	0.58	1.75	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:135:VAL:HG11	1:A:232:VAL:HG23	0.58	1.74	19	1
1:A:227:ASP:O	1:A:229:LEU:N	0.58	2.37	5	2
1:A:187:GLN:NE2	1:A:190:VAL:HG13	0.58	2.12	7	1
1:A:71:LEU:HD11	1:A:155:LEU:HD21	0.58	1.75	10	3
1:A:71:LEU:HD13	1:A:104:LEU:HD22	0.58	1.75	17	2
1:A:102:ALA:HB3	1:A:252:LEU:CD2	0.58	2.28	9	7
1:A:42:THR:HG22	1:A:221:MET:HG3	0.58	1.75	20	3
1:A:75:LYS:HE3	1:A:97:LEU:HD21	0.58	1.75	3	1
1:A:149:LEU:HD23	1:A:280:VAL:CG1	0.58	2.29	4	2
1:A:140:HIS:NE2	1:A:239:VAL:HG13	0.58	2.13	6	3
1:A:74:TYR:CE1	1:A:159:LEU:HD13	0.58	2.33	11	1
1:A:156:GLN:HA	1:A:159:LEU:HD12	0.58	1.75	20	1
1:A:32:ARG:HB3	1:A:63:LEU:HD22	0.58	1.75	11	1
1:A:99:ALA:CB	1:A:256:ALA:HB2	0.58	2.28	9	12
1:A:139:SER:CB	1:A:229:LEU:HD23	0.57	2.29	8	1
1:A:264:ARG:NE	1:A:268:LEU:HD21	0.57	2.13	3	1
1:A:30:LEU:HD13	1:A:34:TRP:CH2	0.57	2.33	11	2
1:A:155:LEU:O	1:A:155:LEU:HD13	0.57	1.99	3	3
1:A:78:LEU:HD22	1:A:159:LEU:CD2	0.57	2.28	20	2
1:A:14:LEU:HD12	1:A:149:LEU:HD21	0.57	1.75	2	1
1:A:75:LYS:HD3	1:A:97:LEU:HD21	0.57	1.77	19	2
1:A:157:LYS:O	1:A:161:VAL:HG23	0.57	1.99	7	1
1:A:71:LEU:HD11	1:A:155:LEU:CD2	0.57	2.30	19	2
1:A:180:ARG:O	1:A:181:LEU:HD22	0.57	2.00	10	3
1:A:71:LEU:HD11	1:A:155:LEU:HD22	0.57	1.77	1	2
1:A:232:VAL:O	1:A:233:LYS:C	0.57	2.48	15	10
1:A:64:MET:HE3	1:A:190:VAL:CG1	0.57	2.27	14	1
1:A:180:ARG:HG3	1:A:181:LEU:HD22	0.57	1.76	16	1
1:A:83:THR:HG21	1:A:266:GLU:CD	0.57	2.24	2	1
1:A:14:LEU:HD13	1:A:149:LEU:CD1	0.56	2.30	6	1
1:A:40:VAL:O	1:A:42:THR:HG23	0.56	2.00	14	1
1:A:3:GLU:O	1:A:6:VAL:HG22	0.56	2.00	18	1
1:A:60:LEU:HD22	1:A:111:VAL:CG1	0.56	2.30	2	1
1:A:250:ILE:O	1:A:254:ALA:HB2	0.56	2.01	11	5
1:A:75:LYS:CE	1:A:159:LEU:HD11	0.56	2.30	9	1
1:A:33:PHE:CE2	1:A:148:LEU:HD22	0.56	2.36	20	2
1:A:181:LEU:HD21	1:A:186:GLU:OE2	0.56	2.01	12	1
1:A:37:LEU:HD12	1:A:145:ARG:HG2	0.56	1.76	15	2
1:A:32:ARG:CD	1:A:63:LEU:HD22	0.56	2.30	15	1
1:A:78:LEU:HD23	1:A:159:LEU:HD22	0.56	1.77	15	1
1:A:210:TRP:CZ2	1:A:214:LEU:HD22	0.56	2.36	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:114:ARG:NH1	1:A:137:LEU:HD13	0.56	2.15	19	1
1:A:68:MET:CE	1:A:190:VAL:HG11	0.56	2.30	5	1
1:A:40:VAL:HG23	1:A:56:VAL:HG21	0.56	1.78	3	1
1:A:8:THR:HG21	1:A:149:LEU:HD23	0.56	1.75	9	2
1:A:84:PRO:HD3	1:A:164:ALA:HB3	0.56	1.77	16	2
1:A:67:THR:HB	1:A:108:MET:HE1	0.56	1.77	11	1
1:A:21:GLN:CG	1:A:160:ALA:HB2	0.56	2.31	17	2
1:A:75:LYS:NZ	1:A:97:LEU:HD22	0.55	2.15	6	2
1:A:39:TRP:NE1	1:A:214:LEU:HD21	0.55	2.16	13	1
1:A:8:THR:HG22	1:A:280:VAL:CG2	0.55	2.31	15	1
1:A:243:LEU:HD21	1:A:293:PRO:HA	0.55	1.78	6	1
1:A:111:VAL:HA	1:A:144:LEU:HD21	0.55	1.78	1	3
1:A:228:ARG:C	1:A:229:LEU:HD23	0.55	2.26	16	8
1:A:75:LYS:HE2	1:A:159:LEU:HD11	0.55	1.78	9	1
1:A:180:ARG:HG2	1:A:181:LEU:HD23	0.55	1.76	7	1
1:A:18:THR:HG22	1:A:156:GLN:HG3	0.55	1.77	12	3
1:A:29:ALA:HB3	1:A:70:GLU:OE2	0.55	2.01	10	1
1:A:33:PHE:CE2	1:A:148:LEU:HD13	0.55	2.37	20	1
1:A:135:VAL:HG21	1:A:232:VAL:HG23	0.55	1.78	14	4
1:A:103:ARG:NH1	1:A:252:LEU:HD13	0.55	2.17	19	3
1:A:267:PRO:O	1:A:268:LEU:HD23	0.55	2.02	13	2
1:A:248:GLN:OE1	1:A:252:LEU:HD21	0.55	2.00	11	6
1:A:100:ALA:HB1	1:A:155:LEU:HD23	0.55	1.77	7	1
1:A:141:LEU:HD23	1:A:145:ARG:NH2	0.55	2.16	14	1
1:A:103:ARG:HG2	1:A:252:LEU:HD22	0.54	1.76	3	3
1:A:50:GLU:OE2	1:A:56:VAL:HG13	0.54	2.02	4	1
1:A:47:VAL:HG22	1:A:118:TYR:OH	0.54	2.02	19	1
1:A:118:TYR:O	1:A:122:VAL:HG22	0.54	2.01	1	1
1:A:149:LEU:HD23	1:A:280:VAL:HG13	0.54	1.78	7	1
1:A:110:ASP:HB3	1:A:144:LEU:HD13	0.54	1.78	12	3
1:A:75:LYS:HD3	1:A:97:LEU:HD23	0.54	1.77	14	1
1:A:83:THR:HG22	1:A:161:VAL:HG11	0.54	1.80	5	1
1:A:18:THR:HG23	1:A:156:GLN:HG3	0.54	1.78	19	1
1:A:60:LEU:HD12	1:A:115:LEU:HD21	0.54	1.79	17	1
1:A:18:THR:HG22	1:A:156:GLN:HG2	0.54	1.77	1	1
1:A:140:HIS:CE1	1:A:239:VAL:HG22	0.54	2.38	18	2
1:A:51:LEU:HD22	1:A:119:ARG:CA	0.54	2.33	15	1
1:A:82:LEU:HD12	1:A:169:GLY:C	0.54	2.27	9	1
1:A:45:GLU:HA	1:A:130:THR:HG21	0.54	1.78	10	3
1:A:93:LEU:HD23	1:A:94:SER:N	0.54	2.18	18	1
1:A:233:LYS:HB2	1:A:236:VAL:HG22	0.54	1.78	7	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:155:LEU:HD23	1:A:159:LEU:HD22	0.54	1.80	8	1
1:A:257:ALA:O	1:A:261:LEU:HD13	0.54	2.02	17	2
1:A:140:HIS:NE2	1:A:144:LEU:HD12	0.54	2.17	17	1
1:A:51:LEU:HD22	1:A:122:VAL:HG21	0.54	1.78	16	1
1:A:191:ARG:O	1:A:194:THR:HG22	0.54	2.03	20	6
1:A:140:HIS:NE2	1:A:239:VAL:HG22	0.54	2.18	12	3
1:A:33:PHE:CE1	1:A:148:LEU:HD13	0.54	2.38	12	1
1:A:264:ARG:HH11	1:A:268:LEU:HD21	0.53	1.63	5	4
1:A:39:TRP:CD1	1:A:214:LEU:HD11	0.53	2.37	13	1
1:A:224:ARG:O	1:A:225:THR:HG22	0.53	2.03	14	3
1:A:140:HIS:NE2	1:A:239:VAL:HG23	0.53	2.17	14	1
1:A:144:LEU:HD13	1:A:242:LYS:HE2	0.53	1.80	19	1
1:A:104:LEU:HD11	1:A:108:MET:CE	0.53	2.32	4	2
1:A:51:LEU:HD21	1:A:118:TYR:CZ	0.53	2.38	16	1
1:A:224:ARG:O	1:A:225:THR:C	0.53	2.51	7	3
1:A:236:VAL:HG22	1:A:236:VAL:O	0.53	2.04	13	2
1:A:97:LEU:HD22	1:A:177:ILE:HG22	0.53	1.79	11	1
1:A:266:GLU:HB2	1:A:267:PRO:CD	0.53	2.33	6	7
1:A:280:VAL:HG13	1:A:281:GLU:HG3	0.53	1.81	15	3
1:A:51:LEU:CD1	1:A:122:VAL:HG11	0.53	2.33	17	2
1:A:101:GLN:OE1	1:A:177:ILE:HD12	0.53	2.03	13	1
1:A:33:PHE:HA	1:A:63:LEU:HD13	0.53	1.80	8	3
1:A:33:PHE:CE1	1:A:37:LEU:HD23	0.53	2.39	19	1
1:A:139:SER:HB2	1:A:229:LEU:HD22	0.53	1.81	7	2
1:A:33:PHE:CE2	1:A:148:LEU:HD21	0.53	2.39	7	1
1:A:142:ARG:NH2	1:A:229:LEU:HD11	0.53	2.19	13	2
1:A:40:VAL:HG13	1:A:56:VAL:HG11	0.53	1.81	17	1
1:A:133:LEU:HD12	1:A:134:ARG:N	0.53	2.19	17	1
1:A:155:LEU:HD23	1:A:155:LEU:O	0.53	2.03	14	3
1:A:33:PHE:CE2	1:A:60:LEU:HD22	0.53	2.38	3	1
1:A:126:LEU:C	1:A:126:LEU:HD13	0.53	2.30	16	1
1:A:74:TYR:O	1:A:78:LEU:HD12	0.52	2.04	2	1
1:A:83:THR:HG21	1:A:266:GLU:OE2	0.52	2.03	2	2
1:A:233:LYS:HB3	1:A:236:VAL:HG22	0.52	1.80	6	1
1:A:146:LYS:HG2	1:A:280:VAL:HG21	0.52	1.80	11	1
1:A:118:TYR:CZ	1:A:122:VAL:HG21	0.52	2.39	20	1
1:A:290:SER:O	1:A:291:ALA:HB3	0.52	2.04	20	1
1:A:68:MET:HB2	1:A:108:MET:HE1	0.52	1.81	14	2
1:A:8:THR:HG21	1:A:149:LEU:HD21	0.52	1.80	12	1
1:A:78:LEU:O	1:A:78:LEU:HD13	0.52	2.05	16	1
1:A:144:LEU:HD12	1:A:242:LYS:HE3	0.52	1.81	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:78:LEU:CD1	1:A:159:LEU:HD22	0.52	2.24	2	1
1:A:93:LEU:HD12	1:A:93:LEU:O	0.52	2.04	17	3
1:A:252:LEU:HD13	1:A:253:GLN:N	0.52	2.20	14	1
1:A:33:PHE:CE2	1:A:148:LEU:HD23	0.52	2.40	1	1
1:A:280:VAL:O	1:A:281:GLU:C	0.52	2.53	8	2
1:A:43:LEU:HD21	1:A:226:ARG:HB2	0.52	1.79	8	1
1:A:78:LEU:HD21	1:A:97:LEU:HD11	0.52	1.81	11	1
1:A:279:GLN:O	1:A:280:VAL:HG13	0.52	2.04	17	5
1:A:22:SER:OG	1:A:30:LEU:HD21	0.52	2.03	14	1
1:A:14:LEU:HD12	1:A:14:LEU:O	0.52	2.03	18	1
1:A:114:ARG:CZ	1:A:137:LEU:HD12	0.52	2.34	6	1
1:A:133:LEU:HD23	1:A:234:GLU:O	0.52	2.05	12	1
1:A:93:LEU:HD12	1:A:162:TYR:CZ	0.52	2.39	18	1
1:A:40:VAL:HG13	1:A:141:LEU:HD21	0.52	1.82	19	3
1:A:43:LEU:HD13	1:A:221:MET:HB2	0.52	1.80	13	1
1:A:99:ALA:HB1	1:A:252:LEU:CD2	0.52	2.35	14	1
1:A:97:LEU:HD23	1:A:101:GLN:HG2	0.51	1.80	4	2
1:A:268:LEU:HD12	1:A:270:GLU:HG2	0.51	1.81	5	4
1:A:243:LEU:CD2	1:A:294:VAL:HG22	0.51	2.24	16	1
1:A:90:ARG:NH1	1:A:91:ALA:HB2	0.51	2.21	5	1
1:A:51:LEU:HD22	1:A:119:ARG:HA	0.51	1.82	15	2
1:A:103:ARG:NH1	1:A:252:LEU:HD23	0.51	2.20	8	1
1:A:82:LEU:CB	1:A:93:LEU:HD22	0.51	2.35	20	1
1:A:37:LEU:C	1:A:37:LEU:HD13	0.51	2.31	2	8
1:A:85:VAL:HG21	1:A:89:THR:HG21	0.51	1.82	15	5
1:A:82:LEU:HD12	1:A:93:LEU:HD22	0.51	1.83	6	1
1:A:82:LEU:CD1	1:A:93:LEU:HD13	0.51	2.35	8	1
1:A:42:THR:HG22	1:A:217:ARG:CD	0.51	2.35	15	2
1:A:11:GLU:HB2	1:A:14:LEU:HD23	0.51	1.83	18	1
1:A:118:TYR:CE2	1:A:122:VAL:HG21	0.51	2.41	20	1
1:A:51:LEU:HD22	1:A:122:VAL:HB	0.51	1.82	2	1
1:A:229:LEU:HB2	1:A:291:ALA:HB3	0.51	1.83	17	2
1:A:60:LEU:HA	1:A:63:LEU:HD12	0.51	1.82	17	2
1:A:110:ASP:CB	1:A:144:LEU:HD13	0.51	2.35	12	1
1:A:146:LYS:HD3	1:A:280:VAL:HG21	0.51	1.82	2	2
1:A:180:ARG:HG3	1:A:181:LEU:HD23	0.51	1.81	2	1
1:A:40:VAL:HG22	1:A:56:VAL:HB	0.51	1.81	13	1
1:A:74:TYR:CE2	1:A:159:LEU:HD11	0.51	2.41	13	1
1:A:57:THR:HG23	1:A:115:LEU:HB2	0.51	1.83	8	3
1:A:43:LEU:HD22	1:A:137:LEU:HD21	0.51	1.83	7	1
1:A:85:VAL:HG11	1:A:89:THR:CG2	0.51	2.36	1	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:42:THR:O	1:A:43:LEU:HD12	0.51	2.06	13	2
1:A:112:CYS:SG	1:A:193:ALA:HB1	0.50	2.45	14	2
1:A:51:LEU:CD2	1:A:122:VAL:HG11	0.50	2.33	4	1
1:A:14:LEU:HD12	1:A:149:LEU:HD11	0.50	1.82	10	1
1:A:102:ALA:CB	1:A:252:LEU:HD21	0.50	2.35	1	1
1:A:47:VAL:O	1:A:51:LEU:HD12	0.50	2.06	2	1
1:A:103:ARG:NH2	1:A:106:ALA:HB3	0.50	2.21	11	2
1:A:118:TYR:O	1:A:122:VAL:HG23	0.50	2.06	11	7
1:A:99:ALA:HB1	1:A:252:LEU:O	0.50	2.07	17	3
1:A:52:LEU:HD12	1:A:52:LEU:O	0.50	2.06	15	2
1:A:280:VAL:HG13	1:A:281:GLU:CG	0.50	2.37	15	1
1:A:214:LEU:HD13	1:A:214:LEU:O	0.50	2.07	6	3
1:A:29:ALA:HB1	1:A:67:THR:OG1	0.50	2.07	12	3
1:A:48:GLN:HB2	1:A:130:THR:HG22	0.50	1.83	4	1
1:A:135:VAL:HG11	1:A:232:VAL:N	0.50	2.22	18	6
1:A:40:VAL:O	1:A:41:GLN:C	0.50	2.55	13	2
1:A:99:ALA:HB3	1:A:256:ALA:HB2	0.50	1.83	19	2
1:A:40:VAL:HG22	1:A:56:VAL:CG1	0.50	2.36	17	1
1:A:29:ALA:HB2	1:A:66:GLU:HG2	0.49	1.83	5	4
1:A:14:LEU:HD22	1:A:149:LEU:CD2	0.49	2.36	6	1
1:A:51:LEU:HD12	1:A:51:LEU:O	0.49	2.07	6	1
1:A:18:THR:HG21	1:A:34:TRP:CH2	0.49	2.42	7	1
1:A:51:LEU:CD1	1:A:122:VAL:HG21	0.49	2.36	7	2
1:A:78:LEU:HD22	1:A:159:LEU:HD13	0.49	1.83	7	1
1:A:210:TRP:NE1	1:A:214:LEU:HD12	0.49	2.20	9	1
1:A:78:LEU:HD11	1:A:163:GLN:HA	0.49	1.84	12	1
1:A:142:ARG:NH2	1:A:229:LEU:HD21	0.49	2.22	19	2
1:A:194:THR:O	1:A:198:LEU:HD12	0.49	2.07	19	1
1:A:43:LEU:HD23	1:A:217:ARG:CG	0.49	2.37	16	2
1:A:75:LYS:HE3	1:A:97:LEU:HD23	0.49	1.84	8	1
1:A:239:VAL:HG13	1:A:243:LEU:HD23	0.49	1.82	8	1
1:A:40:VAL:HG23	1:A:56:VAL:HG11	0.49	1.83	1	1
1:A:82:LEU:HD22	1:A:93:LEU:HD11	0.49	1.83	1	1
1:A:43:LEU:HD22	1:A:134:ARG:NH2	0.49	2.22	12	1
1:A:79:GLU:HA	1:A:82:LEU:HD11	0.49	1.83	15	1
1:A:228:ARG:O	1:A:229:LEU:C	0.49	2.55	14	7
1:A:266:GLU:N	1:A:267:PRO:HD2	0.49	2.22	4	20
1:A:9:GLU:CB	1:A:10:PRO:CD	0.49	2.91	18	19
1:A:51:LEU:HD22	1:A:122:VAL:CG1	0.49	2.38	9	2
1:A:99:ALA:O	1:A:252:LEU:HD23	0.49	2.08	1	1
1:A:103:ARG:HH11	1:A:252:LEU:HD13	0.49	1.68	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:82:LEU:HD22	1:A:82:LEU:N	0.49	2.22	15	3
1:A:83:THR:CG2	1:A:161:VAL:HG11	0.49	2.37	8	1
1:A:82:LEU:HD11	1:A:169:GLY:HA3	0.49	1.84	20	2
1:A:135:VAL:HG13	1:A:230:ASP:N	0.49	2.23	18	3
1:A:43:LEU:HD23	1:A:217:ARG:HG2	0.49	1.83	4	1
1:A:85:VAL:HG13	1:A:266:GLU:OE2	0.49	2.07	11	1
1:A:71:LEU:HD23	1:A:104:LEU:HD22	0.49	1.85	14	1
1:A:9:GLU:N	1:A:10:PRO:HD2	0.48	2.23	3	20
1:A:33:PHE:HA	1:A:63:LEU:HD12	0.48	1.83	4	1
1:A:43:LEU:HD11	1:A:225:THR:HB	0.48	1.84	6	1
1:A:71:LEU:HD13	1:A:104:LEU:CD2	0.48	2.37	11	2
1:A:118:TYR:CE2	1:A:137:LEU:HD13	0.48	2.42	16	2
1:A:114:ARG:NH1	1:A:137:LEU:HD12	0.48	2.22	4	1
1:A:8:THR:OG1	1:A:14:LEU:HD21	0.48	2.08	5	1
1:A:108:MET:SD	1:A:190:VAL:HG11	0.48	2.47	12	1
1:A:128:GLN:HG3	1:A:133:LEU:HD11	0.48	1.82	20	2
1:A:58:GLN:OE1	1:A:198:LEU:HD23	0.48	2.07	5	1
1:A:85:VAL:HG12	1:A:87:GLU:H	0.48	1.68	9	2
1:A:41:GLN:O	1:A:42:THR:C	0.48	2.55	12	1
1:A:140:HIS:CE1	1:A:144:LEU:HD22	0.48	2.43	8	1
1:A:75:LYS:HE2	1:A:97:LEU:HD11	0.48	1.85	19	1
1:A:135:VAL:HG23	1:A:230:ASP:H	0.48	1.69	1	1
1:A:118:TYR:CE1	1:A:122:VAL:HG21	0.48	2.44	6	1
1:A:210:TRP:HE1	1:A:214:LEU:HD12	0.48	1.68	9	1
1:A:64:MET:HE3	1:A:108:MET:O	0.48	2.09	10	1
1:A:37:LEU:HD11	1:A:145:ARG:CG	0.48	2.39	18	2
1:A:39:TRP:O	1:A:42:THR:HG22	0.48	2.09	16	1
1:A:5:ALA:HB2	1:A:142:ARG:O	0.48	2.08	17	1
1:A:39:TRP:NE1	1:A:214:LEU:HD11	0.48	2.23	1	2
1:A:14:LEU:CD1	1:A:149:LEU:HD21	0.48	2.39	10	3
1:A:8:THR:OG1	1:A:149:LEU:HD21	0.48	2.08	4	2
1:A:21:GLN:HG3	1:A:160:ALA:HB2	0.48	1.84	17	2
1:A:82:LEU:HD13	1:A:93:LEU:HD13	0.47	1.86	18	2
1:A:33:PHE:CE1	1:A:60:LEU:HD23	0.47	2.44	10	1
1:A:155:LEU:HD13	1:A:155:LEU:C	0.47	2.34	17	3
1:A:266:GLU:CB	1:A:267:PRO:CD	0.47	2.93	19	14
1:A:133:LEU:HD23	1:A:235:GLN:HG3	0.47	1.86	1	1
1:A:190:VAL:O	1:A:193:ALA:HB3	0.47	2.10	7	3
1:A:292:ALA:HB1	1:A:293:PRO:HD2	0.47	1.87	1	14
1:A:135:VAL:HG13	1:A:230:ASP:H	0.47	1.69	2	4
1:A:83:THR:HG23	1:A:162:TYR:CD1	0.47	2.44	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:56:VAL:O	1:A:60:LEU:HD12	0.47	2.10	10	1
1:A:196:GLY:O	1:A:199:ALA:HB3	0.47	2.09	15	4
1:A:243:LEU:HD23	1:A:296:SER:C	0.47	2.34	2	1
1:A:142:ARG:CZ	1:A:229:LEU:HD21	0.47	2.40	10	1
1:A:149:LEU:HD23	1:A:150:ARG:N	0.47	2.24	10	1
1:A:121:GLU:OE2	1:A:237:ALA:HB3	0.47	2.09	19	1
1:A:37:LEU:HD21	1:A:145:ARG:HG2	0.47	1.87	17	2
1:A:227:ASP:C	1:A:228:ARG:CG	0.47	2.87	5	2
1:A:195:VAL:O	1:A:199:ALA:HB2	0.47	2.08	7	1
1:A:214:LEU:C	1:A:214:LEU:HD13	0.47	2.35	15	2
1:A:64:MET:HE1	1:A:112:CYS:HB2	0.47	1.86	18	1
1:A:43:LEU:HD11	1:A:220:GLU:CG	0.47	2.40	3	1
1:A:14:LEU:CD2	1:A:149:LEU:HD21	0.47	2.40	7	2
1:A:94:SER:HA	1:A:176:ALA:HB2	0.47	1.87	7	2
1:A:89:THR:HG23	1:A:90:ARG:HE	0.47	1.70	15	1
1:A:8:THR:OG1	1:A:14:LEU:HD11	0.47	2.09	5	1
1:A:56:VAL:CG2	1:A:115:LEU:HD11	0.47	2.40	6	2
1:A:243:LEU:HD12	1:A:294:VAL:O	0.47	2.10	8	1
1:A:83:THR:HG23	1:A:85:VAL:HG23	0.47	1.86	11	1
1:A:43:LEU:HD11	1:A:226:ARG:CB	0.46	2.39	8	1
1:A:114:ARG:HH22	1:A:137:LEU:HD12	0.46	1.71	10	3
1:A:79:GLU:CD	1:A:174:LEU:HD12	0.46	2.34	12	1
1:A:37:LEU:O	1:A:37:LEU:HD22	0.46	2.11	2	1
1:A:99:ALA:HB1	1:A:252:LEU:HD22	0.46	1.85	14	1
1:A:33:PHE:CZ	1:A:37:LEU:HD23	0.46	2.45	19	1
1:A:83:THR:HG22	1:A:84:PRO:HD2	0.46	1.87	2	1
1:A:27:GLU:OE2	1:A:30:LEU:HD11	0.46	2.10	8	1
1:A:135:VAL:HG11	1:A:232:VAL:CG2	0.46	2.41	8	1
1:A:231:GLU:CA	1:A:291:ALA:HB2	0.46	2.41	11	1
1:A:155:LEU:O	1:A:159:LEU:HD23	0.46	2.11	18	1
1:A:227:ASP:O	1:A:228:ARG:C	0.46	2.58	14	15
1:A:82:LEU:HG	1:A:166:ALA:HB3	0.46	1.87	20	4
1:A:136:ARG:CD	1:A:239:VAL:HG21	0.46	2.40	1	1
1:A:57:THR:HA	1:A:115:LEU:HD23	0.46	1.86	11	1
1:A:261:LEU:HD12	1:A:272:MET:HG2	0.46	1.88	3	1
1:A:111:VAL:HG22	1:A:144:LEU:CD2	0.46	2.40	11	1
1:A:111:VAL:O	1:A:115:LEU:HD13	0.46	2.11	4	1
1:A:93:LEU:CD2	1:A:97:LEU:HD13	0.46	2.40	5	1
1:A:268:LEU:HD11	1:A:271:ASP:HB2	0.46	1.87	19	1
1:A:231:GLU:H	1:A:291:ALA:HB2	0.46	1.69	10	1
1:A:75:LYS:HD2	1:A:97:LEU:HD11	0.46	1.87	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:149:LEU:CD2	1:A:280:VAL:HG13	0.46	2.41	7	1
1:A:60:LEU:HD13	1:A:111:VAL:HG12	0.46	1.88	12	1
1:A:78:LEU:C	1:A:78:LEU:HD13	0.46	2.36	14	1
1:A:75:LYS:CD	1:A:177:ILE:HD12	0.46	2.41	17	1
1:A:264:ARG:HE	1:A:268:LEU:HD21	0.45	1.69	3	1
1:A:248:GLN:O	1:A:252:LEU:HD12	0.45	2.11	6	1
1:A:64:MET:HE3	1:A:190:VAL:HG12	0.45	1.88	7	1
1:A:57:THR:HG23	1:A:115:LEU:HB3	0.45	1.88	15	2
1:A:51:LEU:HD13	1:A:122:VAL:CG1	0.45	2.41	17	1
1:A:43:LEU:HD12	1:A:47:VAL:HG23	0.45	1.89	19	1
1:A:136:ARG:HH11	1:A:239:VAL:HG21	0.45	1.70	2	1
1:A:68:MET:HE1	1:A:190:VAL:CG1	0.45	2.41	17	1
1:A:82:LEU:HD13	1:A:93:LEU:HD11	0.45	1.88	16	1
1:A:228:ARG:O	1:A:229:LEU:HD23	0.45	2.11	5	1
1:A:107:ASP:HB3	1:A:148:LEU:HD12	0.45	1.87	8	1
1:A:74:TYR:CE2	1:A:78:LEU:HD11	0.45	2.47	18	1
1:A:43:LEU:HD23	1:A:221:MET:HA	0.45	1.88	3	1
1:A:82:LEU:HB2	1:A:166:ALA:HB3	0.45	1.86	6	1
1:A:144:LEU:HD23	1:A:144:LEU:O	0.45	2.11	6	1
1:A:43:LEU:HD13	1:A:137:LEU:HD23	0.45	1.89	7	1
1:A:112:CYS:HB2	1:A:193:ALA:HB1	0.45	1.89	6	1
1:A:68:MET:CB	1:A:108:MET:HE1	0.45	2.42	10	1
1:A:74:TYR:CE1	1:A:159:LEU:HD22	0.45	2.47	11	1
1:A:140:HIS:HE1	1:A:239:VAL:HG13	0.45	1.72	12	1
1:A:71:LEU:HD23	1:A:104:LEU:CD2	0.45	2.41	14	1
1:A:288:GLY:O	1:A:289:THR:HG23	0.45	2.11	16	1
1:A:64:MET:HE2	1:A:108:MET:C	0.45	2.35	19	1
1:A:261:LEU:HD23	1:A:272:MET:HG2	0.45	1.87	1	1
1:A:18:THR:HG23	1:A:156:GLN:NE2	0.45	2.27	3	1
1:A:100:ALA:CB	1:A:155:LEU:HD12	0.45	2.40	12	1
1:A:96:GLU:HG3	1:A:259:ALA:HB3	0.45	1.89	20	1
1:A:117:GLN:OE1	1:A:237:ALA:HB1	0.45	2.11	1	1
1:A:51:LEU:HD11	1:A:118:TYR:OH	0.45	2.11	16	2
1:A:117:GLN:CD	1:A:237:ALA:HB1	0.45	2.37	7	2
1:A:37:LEU:HA	1:A:60:LEU:HD21	0.45	1.89	8	2
1:A:40:VAL:HA	1:A:56:VAL:HG11	0.45	1.88	2	1
1:A:110:ASP:HB3	1:A:144:LEU:HD12	0.45	1.89	9	1
1:A:78:LEU:HD23	1:A:159:LEU:CD2	0.45	2.42	15	1
1:A:59:GLU:O	1:A:63:LEU:HD13	0.45	2.12	16	1
1:A:82:LEU:HD21	1:A:166:ALA:HB3	0.45	1.88	8	1
1:A:63:LEU:C	1:A:63:LEU:HD13	0.45	2.37	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:78:LEU:HD13	1:A:78:LEU:C	0.45	2.36	16	1
1:A:268:LEU:HD23	1:A:270:GLU:HG3	0.44	1.87	2	1
1:A:93:LEU:HD21	1:A:97:LEU:HD13	0.44	1.88	5	1
1:A:239:VAL:HG22	1:A:243:LEU:CD1	0.44	2.42	5	1
1:A:188:GLY:O	1:A:189:ARG:C	0.44	2.60	10	1
1:A:128:GLN:CG	1:A:133:LEU:HD11	0.44	2.42	13	1
1:A:78:LEU:HD13	1:A:159:LEU:HG	0.44	1.89	9	1
1:A:78:LEU:HD12	1:A:78:LEU:O	0.44	2.11	11	1
1:A:274:ARG:HH21	1:A:275:GLN:NE2	0.44	2.10	12	1
1:A:132:GLU:CA	1:A:232:VAL:HG11	0.44	2.43	14	1
1:A:18:THR:HG23	1:A:156:GLN:OE1	0.44	2.13	17	1
1:A:243:LEU:CG	1:A:294:VAL:HG23	0.44	2.43	2	1
1:A:93:LEU:O	1:A:93:LEU:HD23	0.44	2.12	8	1
1:A:157:LYS:O	1:A:160:ALA:HB3	0.44	2.12	8	2
1:A:8:THR:HG21	1:A:149:LEU:HD22	0.44	1.89	14	1
1:A:78:LEU:HD11	1:A:162:TYR:HB3	0.44	1.87	14	1
1:A:236:VAL:O	1:A:237:ALA:HB3	0.44	2.13	16	1
1:A:14:LEU:O	1:A:18:THR:HG23	0.44	2.12	20	2
1:A:40:VAL:HG13	1:A:141:LEU:CD2	0.44	2.43	10	2
1:A:68:MET:HE2	1:A:186:GLU:HG3	0.44	1.89	16	1
1:A:11:GLU:CB	1:A:14:LEU:HD23	0.44	2.43	18	1
1:A:56:VAL:HG23	1:A:115:LEU:HD13	0.44	1.89	19	1
1:A:243:LEU:HD21	1:A:294:VAL:CG2	0.44	2.43	2	1
1:A:14:LEU:HD13	1:A:149:LEU:HD21	0.44	1.89	3	1
1:A:61:ARG:HA	1:A:64:MET:HE3	0.44	1.90	18	1
1:A:64:MET:HE3	1:A:112:CYS:SG	0.44	2.52	20	1
1:A:39:TRP:HE1	1:A:214:LEU:HD11	0.44	1.72	1	1
1:A:129:SER:O	1:A:130:THR:HG23	0.44	2.12	11	1
1:A:229:LEU:HD12	1:A:229:LEU:O	0.44	2.13	19	1
1:A:280:VAL:C	1:A:281:GLU:HG3	0.44	2.38	8	2
1:A:75:LYS:HZ3	1:A:97:LEU:HD22	0.44	1.73	6	1
1:A:133:LEU:HD23	1:A:235:GLN:NE2	0.44	2.27	19	1
1:A:137:LEU:O	1:A:137:LEU:HD23	0.44	2.12	9	3
1:A:132:GLU:HA	1:A:232:VAL:HG11	0.44	1.88	14	2
1:A:122:VAL:HG13	1:A:128:GLN:CD	0.44	2.37	20	2
1:A:146:LYS:CG	1:A:280:VAL:HG21	0.44	2.42	11	1
1:A:42:THR:HG21	1:A:47:VAL:HG21	0.44	1.89	13	1
1:A:180:ARG:HD2	1:A:181:LEU:HD23	0.44	1.90	17	1
1:A:33:PHE:CE1	1:A:148:LEU:HD22	0.44	2.48	18	1
1:A:107:ASP:CB	1:A:148:LEU:HD13	0.44	2.43	19	1
1:A:291:ALA:O	1:A:292:ALA:HB3	0.44	2.13	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:61:ARG:HH11	1:A:62:ALA:HB2	0.43	1.72	8	2
1:A:43:LEU:C	1:A:43:LEU:HD13	0.43	2.38	17	1
1:A:82:LEU:HB3	1:A:93:LEU:HD22	0.43	1.90	20	1
1:A:85:VAL:HG12	1:A:87:GLU:HG2	0.43	1.90	5	2
1:A:138:ALA:HB3	1:A:229:LEU:CD2	0.43	2.44	13	2
1:A:57:THR:HG23	1:A:115:LEU:CB	0.43	2.43	12	1
1:A:57:THR:CA	1:A:115:LEU:HD23	0.43	2.43	17	1
1:A:34:TRP:CZ3	1:A:149:LEU:HD13	0.43	2.48	19	1
1:A:89:THR:HG21	1:A:266:GLU:OE1	0.43	2.13	3	2
1:A:75:LYS:CE	1:A:177:ILE:HG22	0.43	2.43	2	1
1:A:243:LEU:HD23	1:A:296:SER:CA	0.43	2.43	19	2
1:A:99:ALA:HB2	1:A:255:GLU:HB2	0.43	1.90	6	1
1:A:214:LEU:HD23	1:A:214:LEU:O	0.43	2.13	9	1
1:A:90:ARG:O	1:A:93:LEU:HD23	0.43	2.13	10	1
1:A:14:LEU:HD11	1:A:34:TRP:CH2	0.43	2.48	20	1
1:A:114:ARG:CD	1:A:115:LEU:HD12	0.43	2.43	4	1
1:A:78:LEU:HD12	1:A:162:TYR:CD2	0.43	2.47	5	1
1:A:46:GLN:CD	1:A:216:ALA:HB3	0.43	2.39	9	2
1:A:68:MET:HE2	1:A:69:LYS:N	0.43	2.28	9	1
1:A:246:GLN:HE22	1:A:249:GLN:NE2	0.43	2.12	16	1
1:A:14:LEU:CD1	1:A:149:LEU:HD11	0.43	2.42	19	1
1:A:40:VAL:CG1	1:A:141:LEU:HD21	0.43	2.44	7	2
1:A:102:ALA:CB	1:A:252:LEU:HD13	0.43	2.44	7	1
1:A:181:LEU:HD11	1:A:186:GLU:CD	0.43	2.38	15	1
1:A:218:MET:HA	1:A:221:MET:HE3	0.43	1.91	18	1
1:A:32:ARG:HB3	1:A:63:LEU:HD11	0.43	1.91	10	1
1:A:107:ASP:O	1:A:144:LEU:HD11	0.43	2.14	1	1
1:A:40:VAL:O	1:A:43:LEU:HD21	0.43	2.14	2	1
1:A:85:VAL:HG21	1:A:266:GLU:OE1	0.43	2.14	7	3
1:A:82:LEU:HD23	1:A:162:TYR:CD2	0.42	2.49	4	1
1:A:100:ALA:CB	1:A:155:LEU:HD23	0.42	2.43	17	2
1:A:224:ARG:O	1:A:225:THR:CG2	0.42	2.67	13	2
1:A:135:VAL:HG23	1:A:230:ASP:N	0.42	2.28	1	1
1:A:264:ARG:C	1:A:267:PRO:HD2	0.42	2.39	4	2
1:A:122:VAL:HG13	1:A:128:GLN:NE2	0.42	2.28	11	1
1:A:40:VAL:HG23	1:A:56:VAL:CB	0.42	2.41	14	2
1:A:112:CYS:O	1:A:116:VAL:HG12	0.42	2.13	20	1
1:A:14:LEU:O	1:A:18:THR:HG22	0.42	2.14	7	1
1:A:29:ALA:HB2	1:A:66:GLU:CG	0.42	2.44	7	1
1:A:75:LYS:CE	1:A:97:LEU:HD21	0.42	2.42	3	1
1:A:51:LEU:HD22	1:A:122:VAL:HG11	0.42	1.90	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:29:ALA:HA	1:A:63:LEU:HD12	0.42	1.90	13	1
1:A:235:GLN:O	1:A:236:VAL:C	0.42	2.62	13	2
1:A:141:LEU:HD23	1:A:145:ARG:NH1	0.42	2.30	16	1
1:A:103:ARG:N	1:A:252:LEU:HD22	0.42	2.29	19	1
1:A:139:SER:N	1:A:229:LEU:HD22	0.42	2.29	3	1
1:A:68:MET:HE1	1:A:186:GLU:OE1	0.42	2.14	7	1
1:A:59:GLU:O	1:A:63:LEU:HD12	0.42	2.14	8	1
1:A:3:GLU:OE1	1:A:289:THR:HG23	0.42	2.15	10	1
1:A:43:LEU:CD1	1:A:137:LEU:HD21	0.42	2.36	11	1
1:A:68:MET:SD	1:A:108:MET:HE1	0.42	2.54	3	1
1:A:100:ALA:HB1	1:A:155:LEU:HG	0.42	1.92	11	1
1:A:78:LEU:HD11	1:A:162:TYR:HB2	0.42	1.92	20	1
1:A:51:LEU:HD11	1:A:118:TYR:CD2	0.42	2.50	8	1
1:A:33:PHE:CZ	1:A:148:LEU:HD11	0.42	2.50	9	1
1:A:150:ARG:HB3	1:A:280:VAL:HG11	0.42	1.90	3	1
1:A:141:LEU:HD23	1:A:145:ARG:HD3	0.42	1.92	4	1
1:A:106:ALA:HB1	1:A:245:GLU:OE2	0.42	2.14	9	1
1:A:125:MET:HE1	1:A:234:GLU:CG	0.42	2.45	9	1
1:A:33:PHE:CB	1:A:63:LEU:HD11	0.42	2.42	12	1
1:A:82:LEU:CD1	1:A:93:LEU:HD22	0.41	2.44	4	2
1:A:162:TYR:CD1	1:A:162:TYR:C	0.41	2.96	11	1
1:A:71:LEU:CD1	1:A:104:LEU:HD22	0.41	2.44	17	1
1:A:177:ILE:HD11	1:A:180:ARG:NH2	0.41	2.29	20	1
1:A:249:GLN:HA	1:A:252:LEU:HD12	0.41	1.92	3	1
1:A:133:LEU:HD12	1:A:133:LEU:C	0.41	2.40	17	1
1:A:41:GLN:NE2	1:A:134:ARG:HH12	0.41	2.13	3	1
1:A:78:LEU:CD2	1:A:159:LEU:HD13	0.41	2.45	7	1
1:A:8:THR:OG1	1:A:14:LEU:HD23	0.41	2.15	12	1
1:A:83:THR:HG22	1:A:93:LEU:CD2	0.41	2.45	16	1
1:A:136:ARG:NH1	1:A:239:VAL:HG21	0.41	2.29	17	1
1:A:229:LEU:HD12	1:A:291:ALA:H	0.41	1.76	5	1
1:A:228:ARG:O	1:A:229:LEU:CB	0.41	2.68	19	1
1:A:14:LEU:HD12	1:A:15:ARG:N	0.41	2.31	8	2
1:A:40:VAL:CG1	1:A:141:LEU:HD11	0.41	2.45	8	1
1:A:78:LEU:HD11	1:A:162:TYR:CB	0.41	2.46	16	1
1:A:130:THR:HA	1:A:133:LEU:HD12	0.41	1.91	16	1
1:A:235:GLN:C	1:A:236:VAL:HG23	0.41	2.39	16	1
1:A:210:TRP:CH2	1:A:214:LEU:HD22	0.41	2.50	7	1
1:A:30:LEU:HD12	1:A:31:GLY:N	0.41	2.29	11	1
1:A:42:THR:HG22	1:A:221:MET:SD	0.41	2.55	11	1
1:A:14:LEU:HD13	1:A:149:LEU:HG	0.41	1.92	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:14:LEU:HD13	1:A:149:LEU:HD13	0.41	1.91	6	1
1:A:83:THR:HG22	1:A:93:LEU:HD22	0.41	1.93	16	1
1:A:14:LEU:HD11	1:A:34:TRP:HH2	0.41	1.76	20	1
1:A:48:GLN:CB	1:A:130:THR:HG22	0.41	2.45	4	1
1:A:136:ARG:HD2	1:A:239:VAL:HG21	0.41	1.92	8	2
1:A:144:LEU:C	1:A:144:LEU:HD23	0.41	2.41	3	1
1:A:69:LYS:O	1:A:73:ALA:HB2	0.41	2.15	4	2
1:A:149:LEU:CD2	1:A:280:VAL:HG22	0.41	2.46	6	1
1:A:233:LYS:O	1:A:235:GLN:N	0.41	2.54	6	1
1:A:90:ARG:CA	1:A:93:LEU:HD23	0.41	2.42	7	1
1:A:209:ALA:HB3	1:A:213:ARG:HG3	0.41	1.92	14	1
1:A:181:LEU:HD22	1:A:186:GLU:H	0.41	1.76	20	1
1:A:267:PRO:C	1:A:268:LEU:HD23	0.41	2.40	20	1
1:A:83:THR:HG23	1:A:161:VAL:HG11	0.41	1.93	8	1
1:A:129:SER:O	1:A:133:LEU:HD12	0.41	2.15	8	1
1:A:228:ARG:O	1:A:229:LEU:HD12	0.41	2.15	8	1
1:A:71:LEU:CD2	1:A:104:LEU:HD23	0.41	2.34	11	1
1:A:265:PHE:HA	1:A:269:ALA:HB2	0.41	1.93	20	1
1:A:243:LEU:CD2	1:A:294:VAL:HG23	0.40	2.46	2	1
1:A:68:MET:HG3	1:A:104:LEU:HD21	0.40	1.92	3	1
1:A:135:VAL:HG21	1:A:232:VAL:CB	0.40	2.46	3	1
1:A:163:GLN:O	1:A:164:ALA:C	0.40	2.61	4	1
1:A:100:ALA:HB3	1:A:155:LEU:HD23	0.40	1.92	17	1
1:A:266:GLU:N	1:A:267:PRO:CD	0.40	2.85	4	1
1:A:75:LYS:HE2	1:A:97:LEU:HD21	0.40	1.94	5	1
1:A:48:GLN:HA	1:A:51:LEU:HD12	0.40	1.93	7	1
1:A:64:MET:HE3	1:A:187:GLN:OE1	0.40	2.16	9	1
1:A:14:LEU:HD13	1:A:149:LEU:CD2	0.40	2.46	3	1
1:A:43:LEU:HD12	1:A:43:LEU:C	0.40	2.41	3	1
1:A:126:LEU:HD13	1:A:126:LEU:O	0.40	2.15	16	1
1:A:239:VAL:HG22	1:A:243:LEU:HD22	0.40	1.93	17	1
1:A:43:LEU:HD13	1:A:43:LEU:C	0.40	2.41	1	1
1:A:132:GLU:O	1:A:135:VAL:HG12	0.40	2.17	1	1
1:A:232:VAL:O	1:A:232:VAL:HG12	0.40	2.17	15	1
1:A:280:VAL:O	1:A:281:GLU:CB	0.40	2.68	18	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	277/307 (90%)	216±5 (78±2%)	46±6 (17±2%)	15±2 (6±1%)	2	21
All	All	5540/6140 (90%)	4310 (78%)	923 (17%)	307 (6%)	2	21

All 43 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	24	GLN	20
1	A	224	ARG	20
1	A	269	ALA	20
1	A	280	VAL	19
1	A	227	ASP	17
1	A	164	ALA	15
1	A	229	LEU	15
1	A	225	THR	13
1	A	237	ALA	11
1	A	85	VAL	10
1	A	188	GLY	10
1	A	281	GLU	10
1	A	44	SER	10
1	A	231	GLU	10
1	A	232	VAL	8
1	A	42	THR	8
1	A	43	LEU	7
1	A	233	LYS	7
1	A	87	GLU	6
1	A	189	ARG	6
1	A	41	GLN	6
1	A	88	GLU	6
1	A	296	SER	5
1	A	3	GLU	5
1	A	129	SER	5
1	A	186	GLU	4
1	A	236	VAL	4

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Mol	Chain	Res	Type	Models (Total)
1	A	127	GLY	3
1	A	128	GLN	3
1	A	130	THR	3
1	A	289	THR	3
1	A	226	ARG	3
1	A	228	ARG	2
1	A	278	GLY	2
1	A	290	SER	2
1	A	86	ALA	2
1	A	288	GLY	1
1	A	234	GLU	1
1	A	287	GLU	1
1	A	181	LEU	1
1	A	235	GLN	1
1	A	126	LEU	1
1	A	291	ALA	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	227/253 (90%)	162±7 (71±3%)	65±7 (29±3%)	1	19
All	All	4540/5060 (90%)	3243 (71%)	1297 (29%)	1	19

All 188 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	92	ARG	19
1	A	57	THR	18
1	A	233	LYS	18
1	A	242	LYS	18
1	A	213	ARG	17
1	A	235	GLN	17
1	A	143	LYS	16
1	A	90	ARG	15
1	A	93	LEU	15

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Mol	Chain	Res	Type	Models (Total)
1	A	261	LEU	15
1	A	275	GLN	15
1	A	21	GLN	14
1	A	168	GLU	14
1	A	274	ARG	14
1	A	24	GLN	14
1	A	58	GLN	14
1	A	97	LEU	14
1	A	117	GLN	14
1	A	245	GLU	14
1	A	103	ARG	13
1	A	134	ARG	13
1	A	175	SER	13
1	A	224	ARG	13
1	A	253	GLN	13
1	A	281	GLU	13
1	A	9	GLU	13
1	A	43	LEU	13
1	A	54	SER	12
1	A	128	GLN	12
1	A	129	SER	12
1	A	227	ASP	12
1	A	51	LEU	12
1	A	229	LEU	12
1	A	94	SER	12
1	A	147	ARG	12
1	A	53	SER	11
1	A	65	ASP	11
1	A	220	GLU	11
1	A	243	LEU	11
1	A	114	ARG	11
1	A	158	ARG	11
1	A	181	LEU	11
1	A	273	GLN	11
1	A	174	LEU	11
1	A	148	LEU	11
1	A	68	MET	10
1	A	146	LYS	10
1	A	156	GLN	10
1	A	266	GLU	10
1	A	72	LYS	10
1	A	219	GLU	10

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Mol	Chain	Res	Type	Models (Total)
1	A	226	ARG	10
1	A	248	GLN	10
1	A	249	GLN	10
1	A	96	GLU	10
1	A	7	GLU	9
1	A	13	GLU	9
1	A	83	THR	9
1	A	88	GLU	9
1	A	225	THR	9
1	A	290	SER	9
1	A	66	GLU	9
1	A	69	LYS	9
1	A	98	GLN	9
1	A	289	THR	9
1	A	262	LYS	9
1	A	78	LEU	8
1	A	136	ARG	8
1	A	25	ARG	8
1	A	126	LEU	8
1	A	251	ARG	8
1	A	260	ARG	8
1	A	279	GLN	8
1	A	17	GLN	8
1	A	238	GLU	8
1	A	3	GLU	7
1	A	45	GLU	7
1	A	186	GLU	7
1	A	212	GLU	7
1	A	215	ARG	7
1	A	223	SER	7
1	A	123	GLN	7
1	A	142	ARG	7
1	A	221	MET	7
1	A	39	TRP	7
1	A	44	SER	7
1	A	214	LEU	7
1	A	52	LEU	7
1	A	276	TRP	7
1	A	280	VAL	7
1	A	82	LEU	7
1	A	110	ASP	6
1	A	119	ARG	6

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Mol	Chain	Res	Type	Models (Total)
1	A	139	SER	6
1	A	191	ARG	6
1	A	264	ARG	6
1	A	27	GLU	6
1	A	133	LEU	6
1	A	153	ASP	6
1	A	270	GLU	6
1	A	163	GLN	6
1	A	258	GLN	6
1	A	48	GLN	6
1	A	137	LEU	6
1	A	42	THR	5
1	A	272	MET	5
1	A	4	GLN	5
1	A	32	ARG	5
1	A	37	LEU	5
1	A	50	GLU	5
1	A	75	LYS	5
1	A	87	GLU	5
1	A	125	MET	5
1	A	159	LEU	5
1	A	180	ARG	5
1	A	154	ASP	4
1	A	67	THR	4
1	A	118	TYR	4
1	A	41	GLN	4
1	A	85	VAL	4
1	A	255	GLU	4
1	A	187	GLN	4
1	A	197	SER	4
1	A	198	LEU	4
1	A	217	ARG	4
1	A	38	ARG	4
1	A	61	ARG	4
1	A	35	ASP	4
1	A	218	MET	4
1	A	132	GLU	3
1	A	172	ARG	3
1	A	194	THR	3
1	A	109	GLU	3
1	A	40	VAL	3
1	A	231	GLU	3

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Mol	Chain	Res	Type	Models (Total)
1	A	46	GLN	3
1	A	64	MET	3
1	A	171	GLU	3
1	A	228	ARG	3
1	A	76	SER	3
1	A	130	THR	3
1	A	162	TYR	3
1	A	177	ILE	3
1	A	189	ARG	3
1	A	296	SER	3
1	A	157	LYS	3
1	A	80	GLU	3
1	A	108	MET	3
1	A	230	ASP	3
1	A	70	GLU	2
1	A	81	GLN	2
1	A	150	ARG	2
1	A	263	SER	2
1	A	268	LEU	2
1	A	20	TRP	2
1	A	107	ASP	2
1	A	11	GLU	2
1	A	141	LEU	2
1	A	15	ARG	2
1	A	55	GLN	2
1	A	59	GLU	2
1	A	240	ARG	2
1	A	14	LEU	2
1	A	74	TYR	2
1	A	149	LEU	2
1	A	155	LEU	2
1	A	252	LEU	2
1	A	71	LEU	2
1	A	144	LEU	2
1	A	178	ARG	2
1	A	95	LYS	1
1	A	112	CYS	1
1	A	6	VAL	1
1	A	79	GLU	1
1	A	140	HIS	1
1	A	244	GLU	1
1	A	287	GLU	1

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Mol	Chain	Res	Type	Models (Total)
1	A	36	TYR	1
1	A	77	GLU	1
1	A	265	PHE	1
1	A	179	GLU	1
1	A	151	ASP	1
1	A	101	GLN	1
1	A	236	VAL	1
1	A	16	GLN	1
1	A	19	GLU	1
1	A	22	SER	1
1	A	8	THR	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 [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation [i](#)

The completeness of assignment taking into account all chemical shift lists is 67% for the well-defined parts and 67% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping [i](#)

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	2810
Number of shifts mapped to atoms	2810
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	298	0.26 ± 0.14	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	281	0.79 ± 0.05	Should be checked
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	289	-1.11 ± 0.10	Should be applied

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 67%, i.e. 2617 atoms were assigned a chemical shift out of a possible 3914. 0 out of 51 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	1094/1389 (79%)	546/564 (97%)	277/554 (50%)	271/271 (100%)
Sidechain	1523/2390 (64%)	917/1532 (60%)	606/718 (84%)	0/140 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	0/135 (0%)	0/66 (0%)	0/62 (0%)	0/7 (0%)
Overall	2617/3914 (67%)	1463/2162 (68%)	883/1334 (66%)	271/418 (65%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 67%, i.e. 2810 atoms were assigned a chemical shift out of a possible 4219. 0 out of 56 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	1171/1496 (78%)	584/607 (96%)	298/598 (50%)	289/291 (99%)
Sidechain	1639/2581 (64%)	987/1655 (60%)	652/776 (84%)	0/150 (0%)
Aromatic	0/142 (0%)	0/70 (0%)	0/64 (0%)	0/8 (0%)
Overall	2810/4219 (67%)	1571/2332 (67%)	950/1438 (66%)	289/449 (64%)

7.1.4 Statistically unusual chemical shifts ⓘ

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots ⓘ

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:

