



Full wwPDB NMR Structure Validation Report ⓘ

Mar 8, 2026 – 03:49 AM UTC

PDB ID : 2N7H / pdb_00002n7h
BMRB ID : 25334
Title : Hybrid structure of the Type 1 Pilus of Uropathogenic E.coli
Authors : Habenstein, B.; Loquet, A.; Giller, K.; Vasa, S.; Becker, S.; Habeck, M.; Lange, A.
Deposited on : 2015-09-11

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

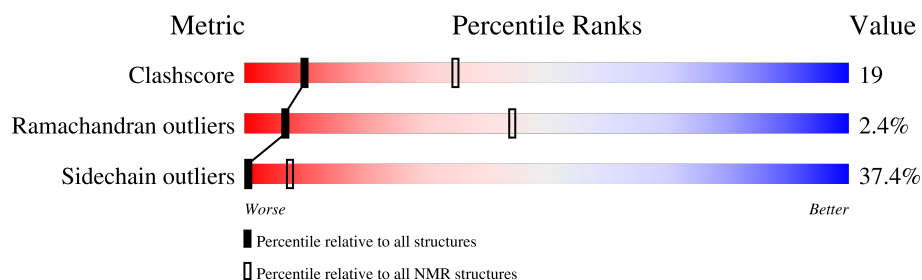
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLID-STATE NMR

The overall completeness of chemical shifts assignment is 7%.

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	160	50% 42% 6% ..
1	B	160	47% 46% 6% .
1	C	160	48% 46% 6% .
1	D	160	46% 49% 5% .
1	E	160	46% 48% 6% .
1	F	160	51% 43% 6% .

2 Ensemble composition and analysis

This entry contains 10 models. Model 3 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:2-A:159, B:1-B:159, C:1-C:159, D:1-D:159, E:1-E:159, F:1-F:159 (953)	0.90	3

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

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

The models can be grouped into 2 clusters and 2 single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 8, 10
2	7, 9
Single-model clusters	5; 6

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 13074 atoms, of which 6402 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called FimA.

Mol	Chain	Residues	Atoms						Trace
1	A	159	Total	C	H	N	O	S	0
			2179	680	1067	196	234	2	
1	B	159	Total	C	H	N	O	S	0
			2179	680	1067	196	234	2	
1	C	159	Total	C	H	N	O	S	0
			2179	680	1067	196	234	2	
1	D	159	Total	C	H	N	O	S	0
			2179	680	1067	196	234	2	
1	E	159	Total	C	H	N	O	S	0
			2179	680	1067	196	234	2	
1	F	159	Total	C	H	N	O	S	0
			2179	680	1067	196	234	2	

There are 6 discrepancies between the modelled and reference sequences:

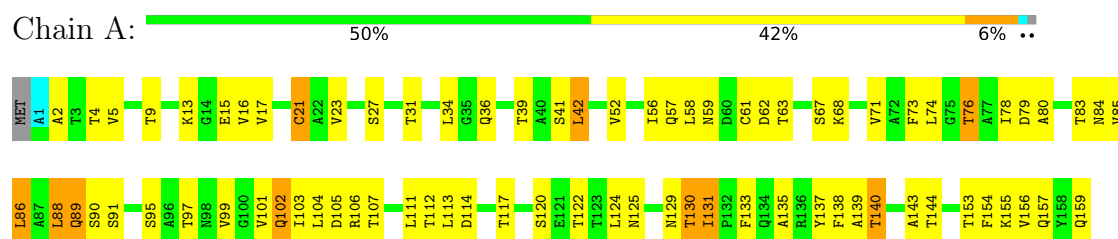
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	expression tag	UNP Q547G4
B	0	MET	-	expression tag	UNP Q547G4
C	0	MET	-	expression tag	UNP Q547G4
D	0	MET	-	expression tag	UNP Q547G4
E	0	MET	-	expression tag	UNP Q547G4
F	0	MET	-	expression tag	UNP Q547G4

4 Residue-property plots

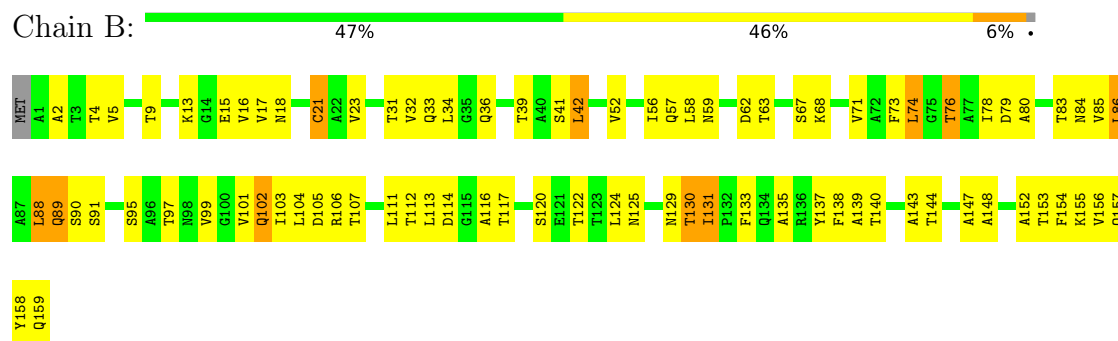
4.1 Average score per residue in the NMR ensemble

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.

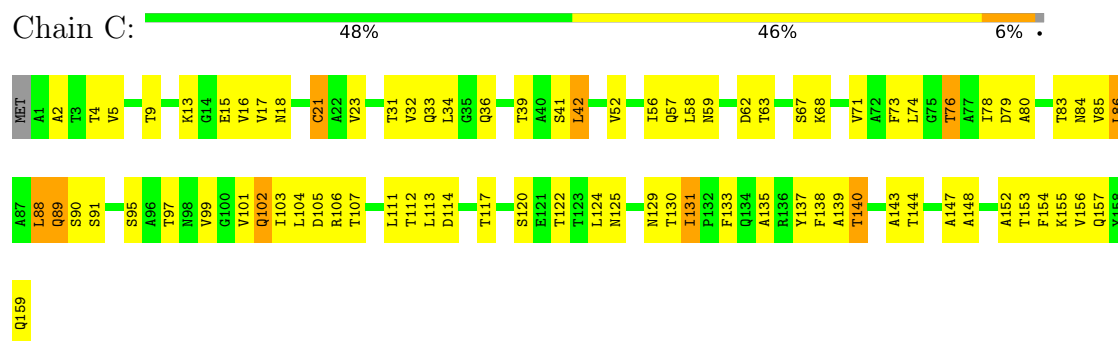
• Molecule 1: FimA



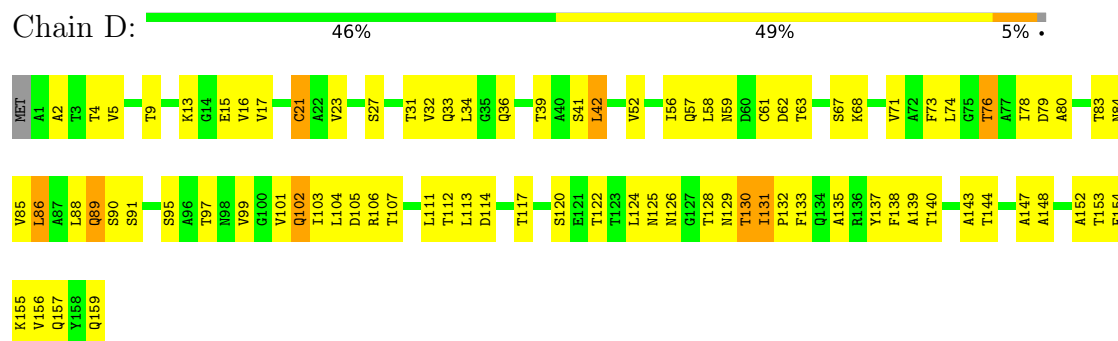
• Molecule 1: FimA



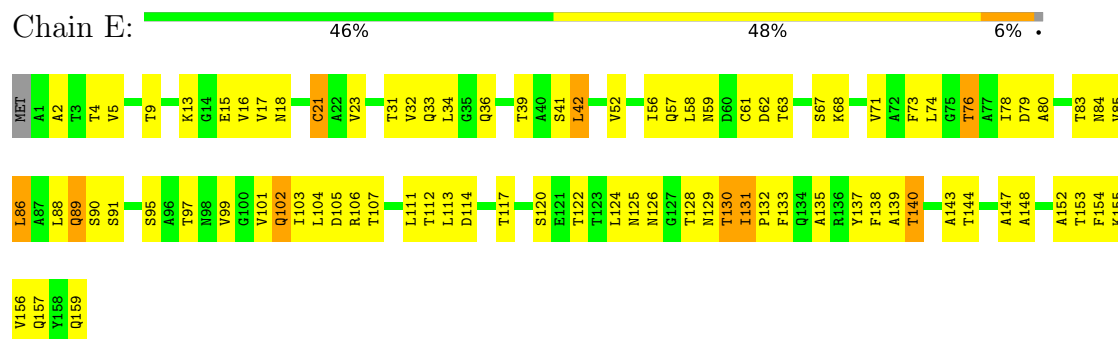
• Molecule 1: FimA



• Molecule 1: FimA



• Molecule 1: FimA



• Molecule 1: FimA

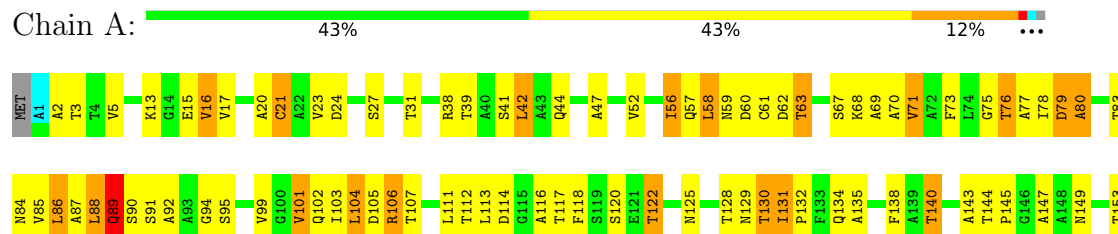


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

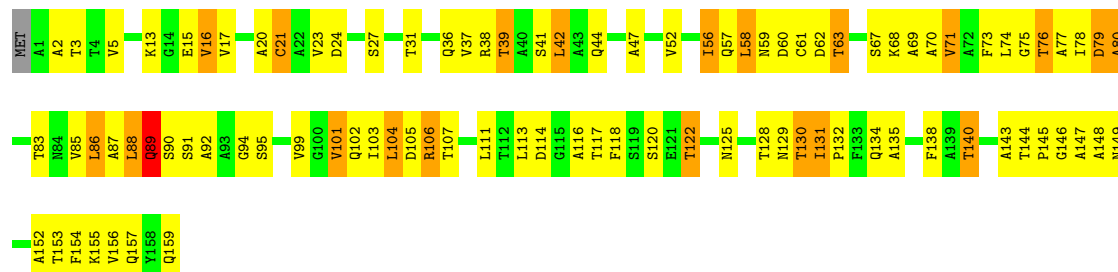
• Molecule 1: FimA



F154
K155
V156
Q157
Y158
Q159

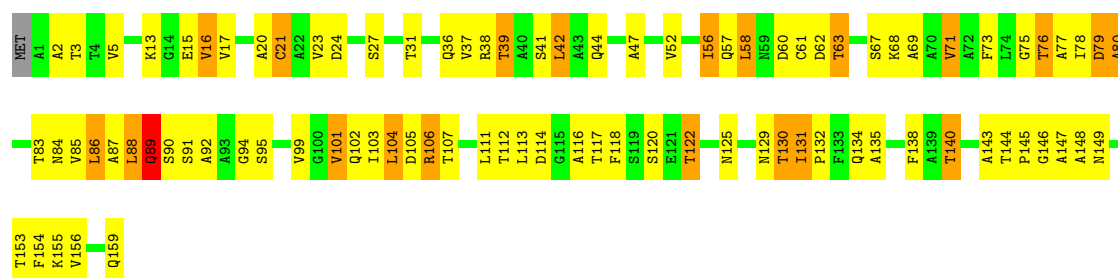
• Molecule 1: FimA

Chain B: 41% 46% 12% ..



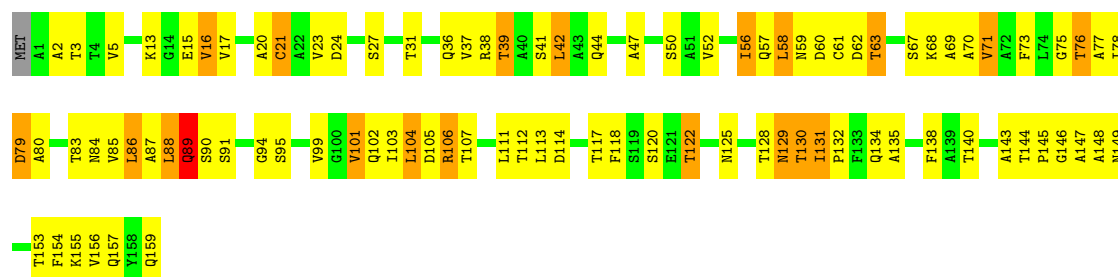
• Molecule 1: FimA

Chain C: 43% 43% 12% ..



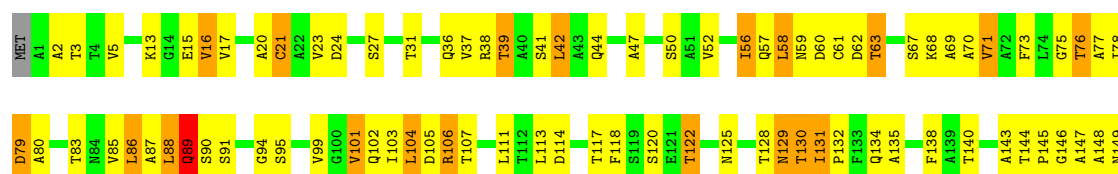
• Molecule 1: FimA

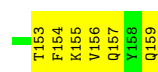
Chain D: 41% 46% 12% ..



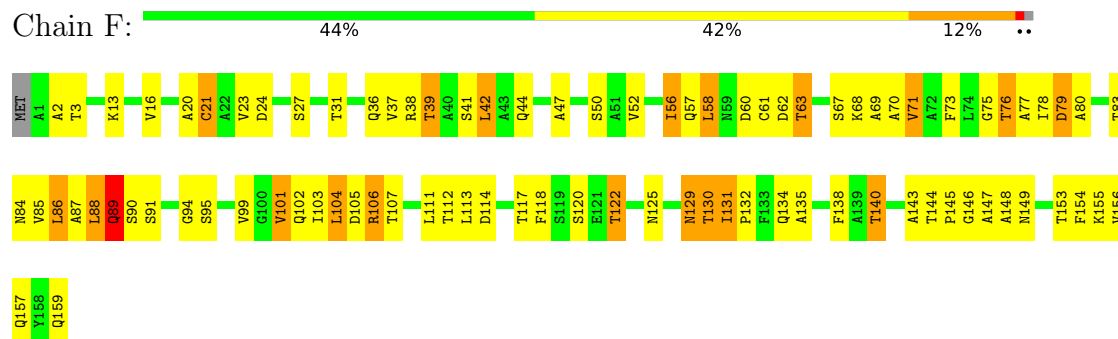
• Molecule 1: FimA

Chain E: 42% 44% 12% ..



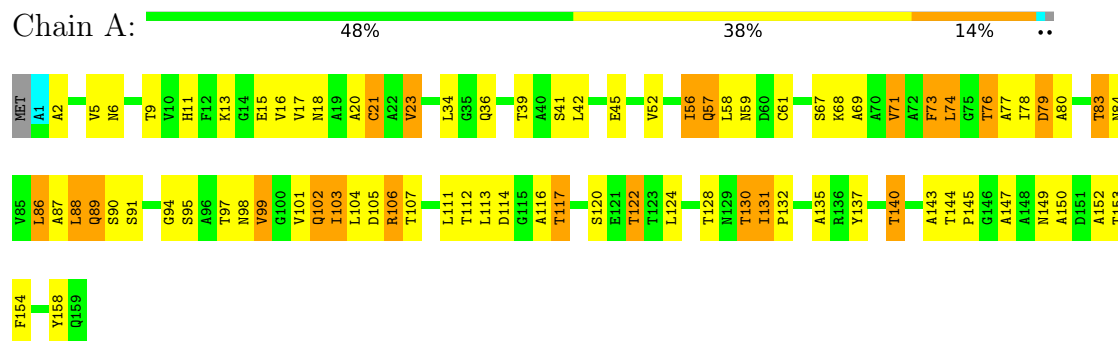


• Molecule 1: FimA

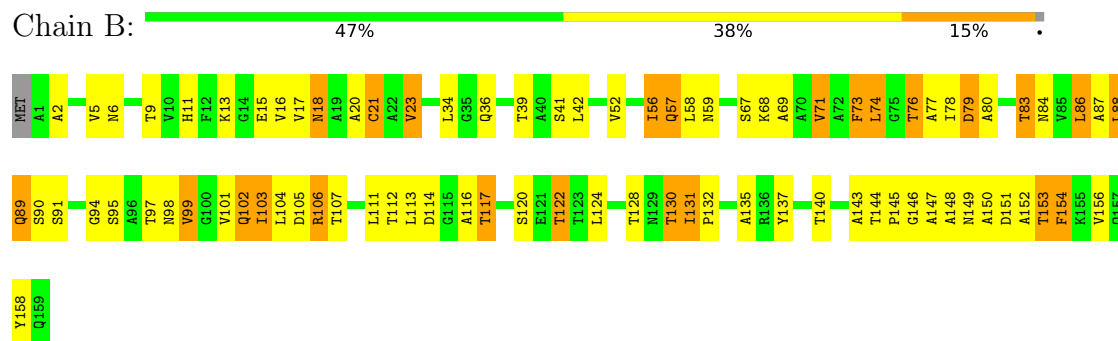


4.2.2 Score per residue for model 2

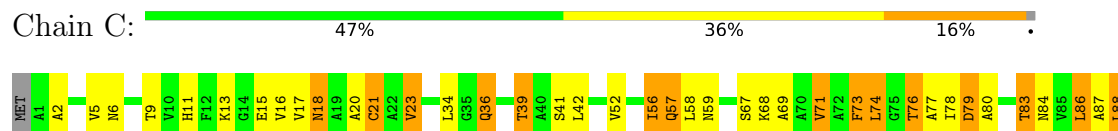
• Molecule 1: FimA

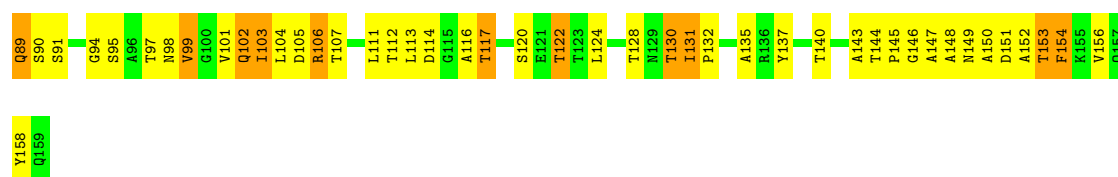


• Molecule 1: FimA



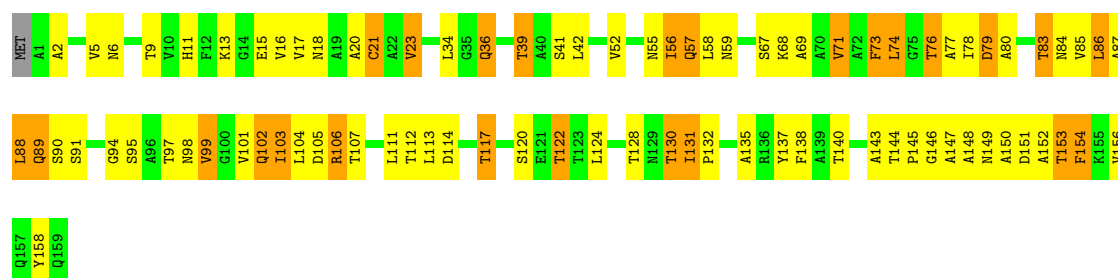
• Molecule 1: FimA





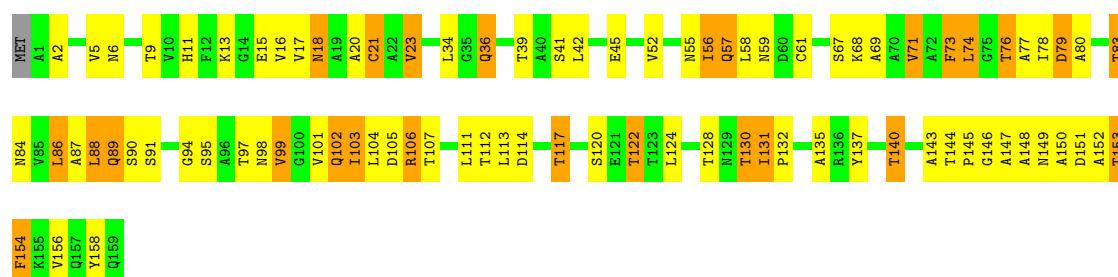
• Molecule 1: FimA

Chain D: 46% 38% 16%



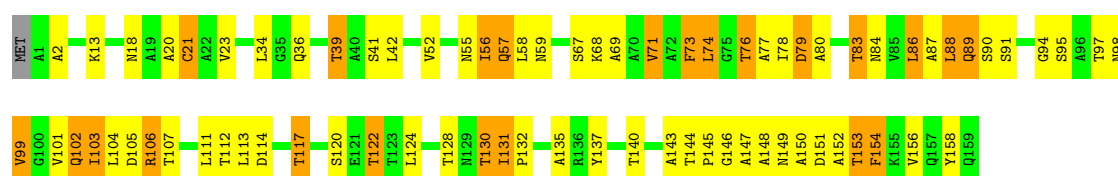
• Molecule 1: FimA

Chain E: 46% 38% 16%



• Molecule 1: FimA

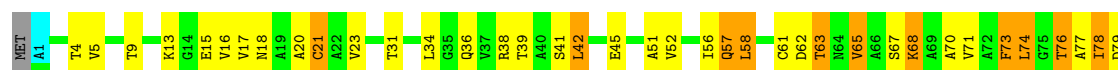
Chain F: 51% 34% 14%

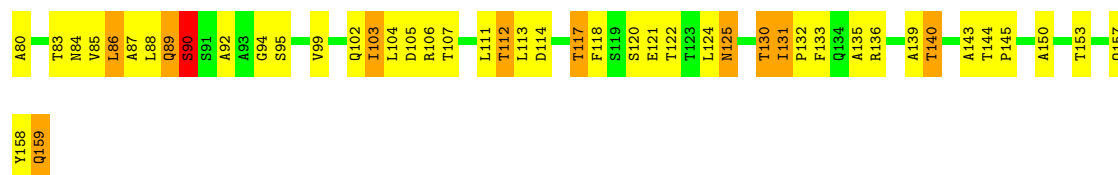


4.2.3 Score per residue for model 3 (medoid)

• Molecule 1: FimA

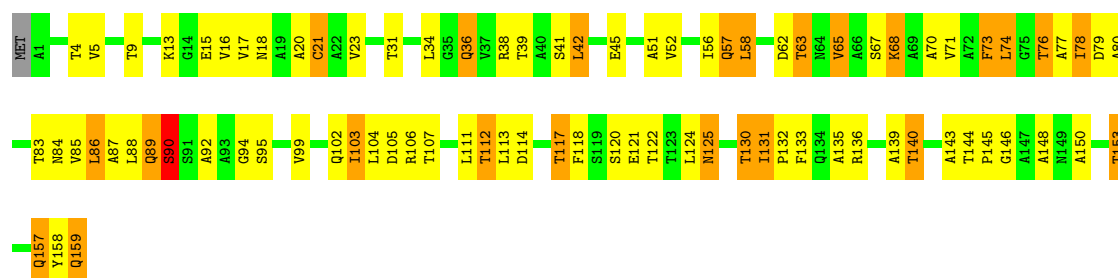
Chain A: 46% 39% 13% ...





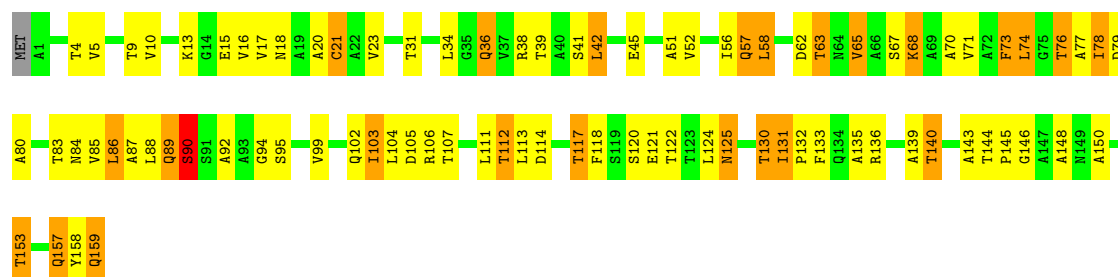
• Molecule 1: FimA

Chain B: 46% 38% 15% ..



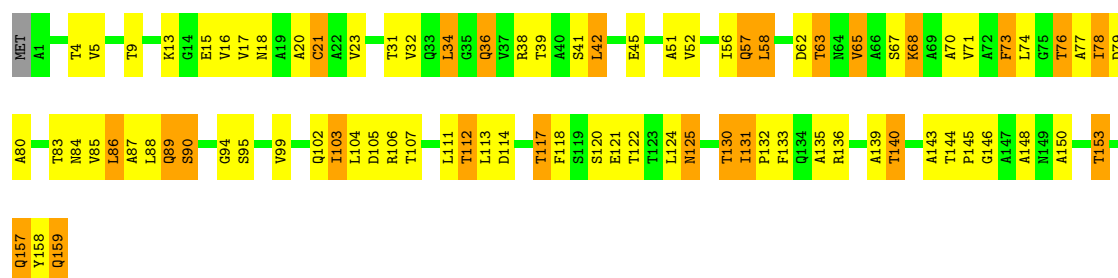
• Molecule 1: FimA

Chain C: 46% 38% 15% ..



• Molecule 1: FimA

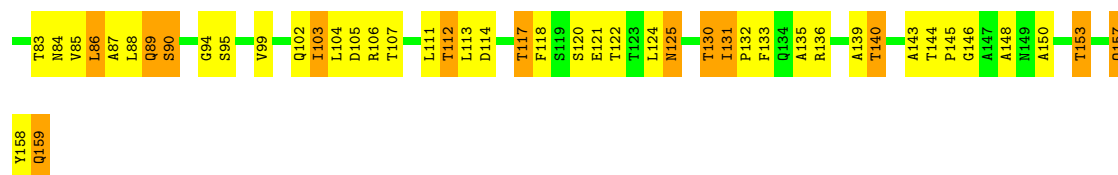
Chain D: 46% 38% 16% .



• Molecule 1: FimA

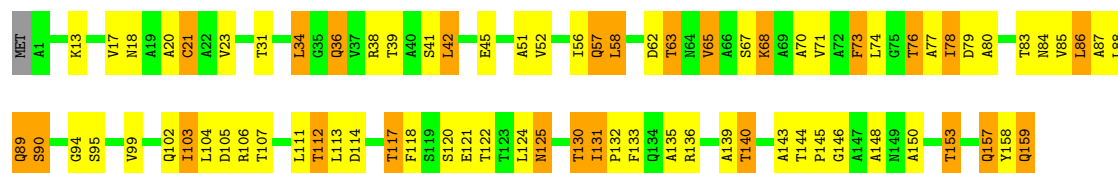
Chain E: 47% 37% 16% .





- Molecule 1: FimA

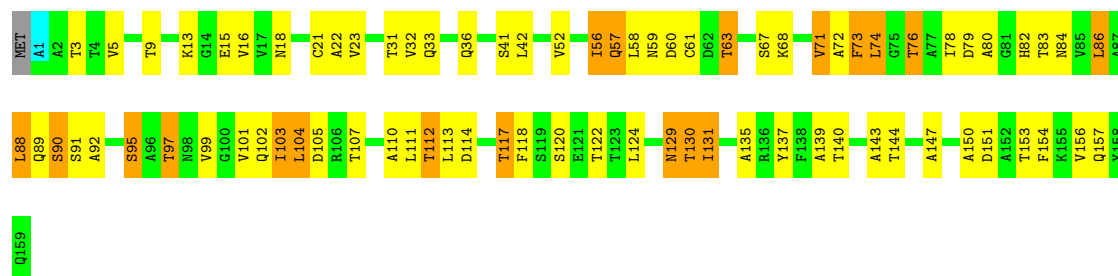
Chain F: 50% 34% 16%



4.2.4 Score per residue for model 4

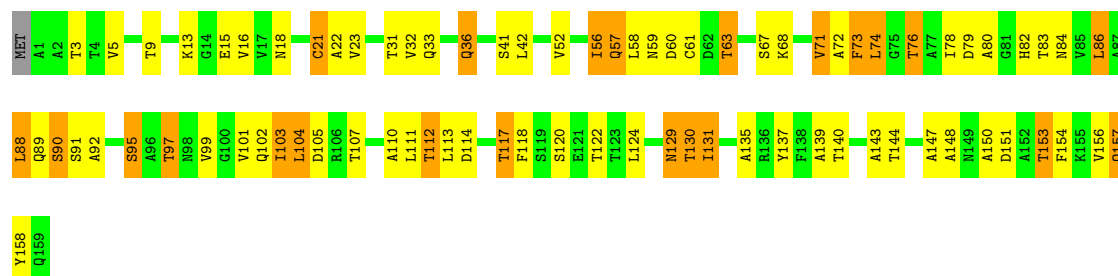
- Molecule 1: FimA

Chain A: 50% 37% 12%



- Molecule 1: FimA

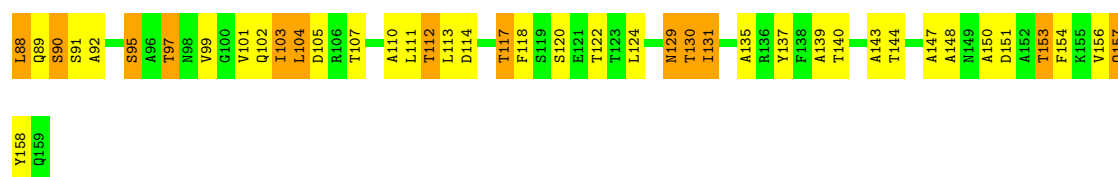
Chain B: 49% 36% 14%



- Molecule 1: FimA

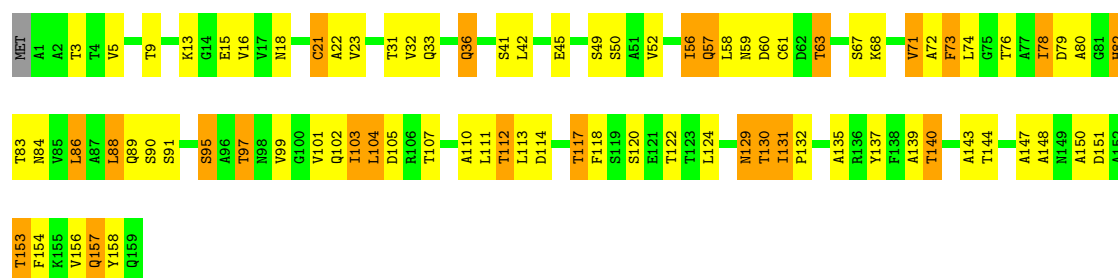
Chain C: 49% 34% 16%





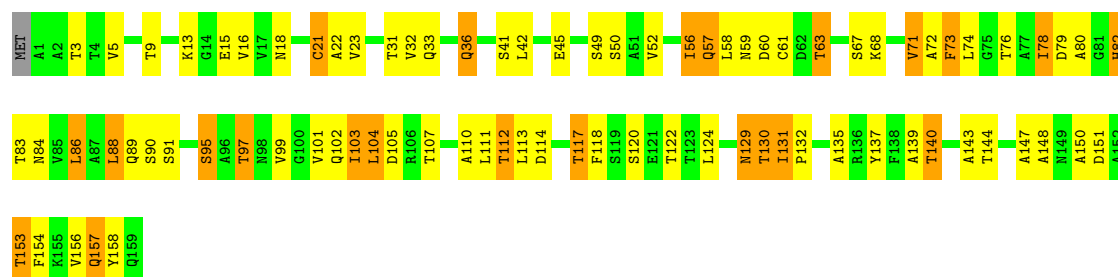
• Molecule 1: FimA

Chain D: 48% 38% 14%



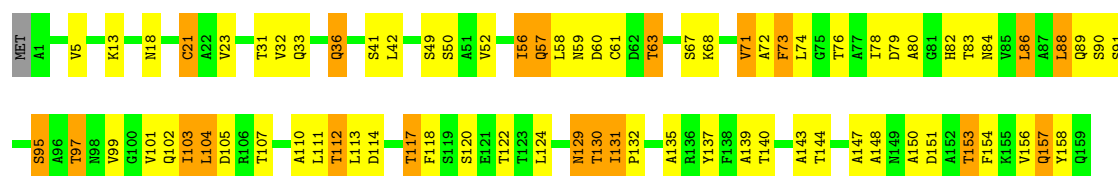
• Molecule 1: FimA

Chain E: 48% 38% 14%



• Molecule 1: FimA

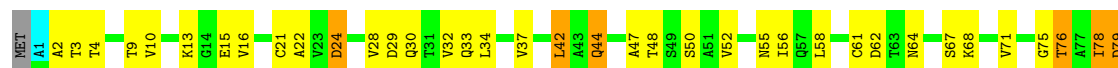
Chain F: 51% 36% 12%



4.2.5 Score per residue for model 5

• Molecule 1: FimA

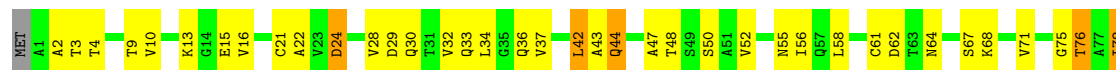
Chain A: 51% 41% 8%





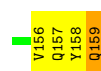
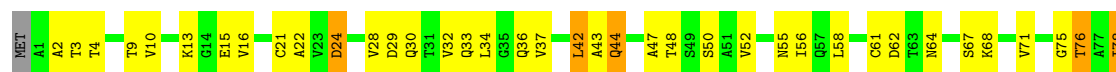
- Molecule 1: FimA

Chain B:  48% 44% 8%



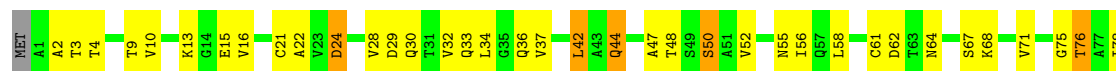
- Molecule 1: FimA

Chain C:  47% 43% 9%

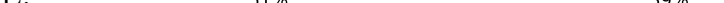


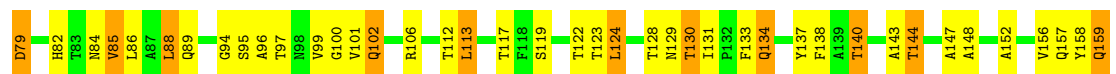
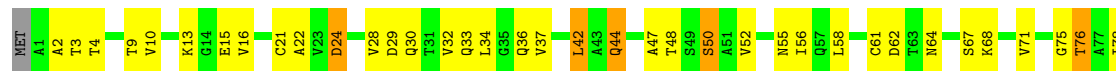
- Molecule 1: FimA

Chain D: 51% 38% 11%

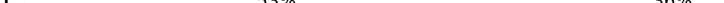


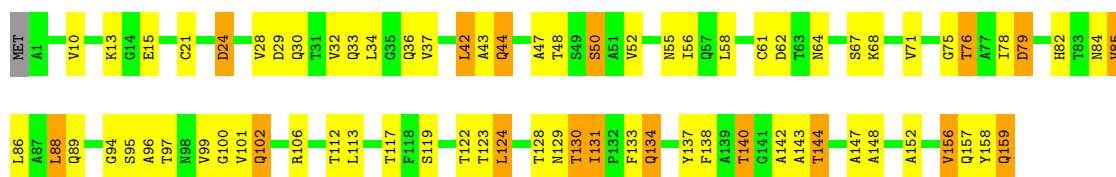
- Molecule 1: FimA

Chain E:  51% 39% 10%



- Molecule 1: FimA

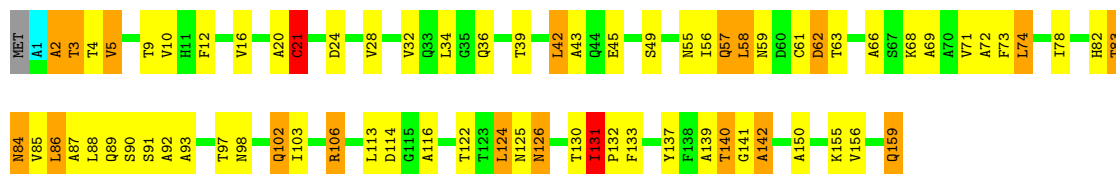
Chain F:  53% 36% 11%



4.2.6 Score per residue for model 6

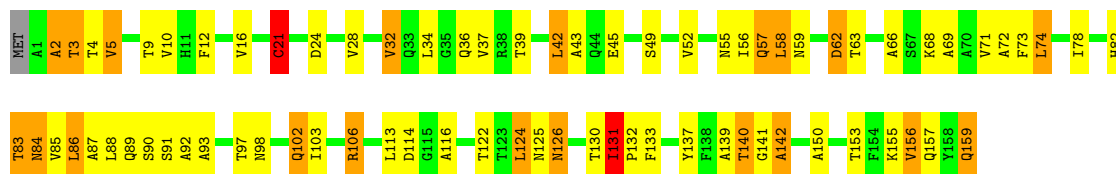
• Molecule 1: FimA

Chain A: 53% 33% 11% ...



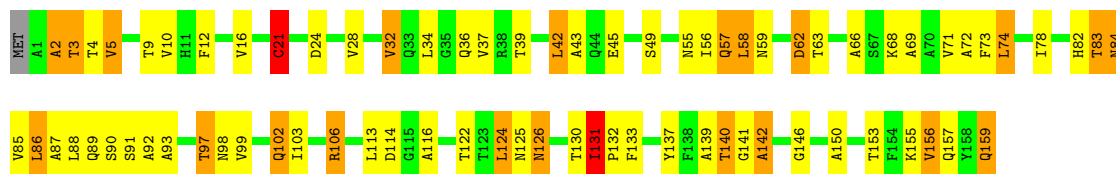
• Molecule 1: FimA

Chain B: 52% 33% 12% ..



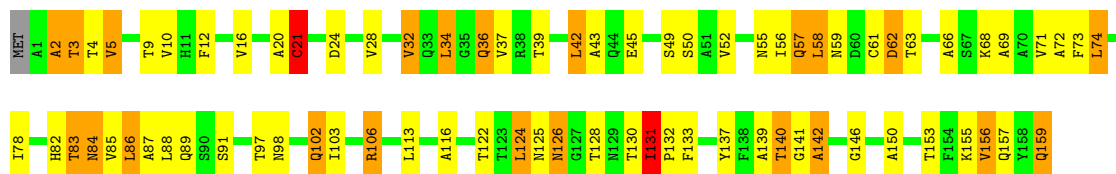
• Molecule 1: FimA

Chain C: 52% 33% 13% ..



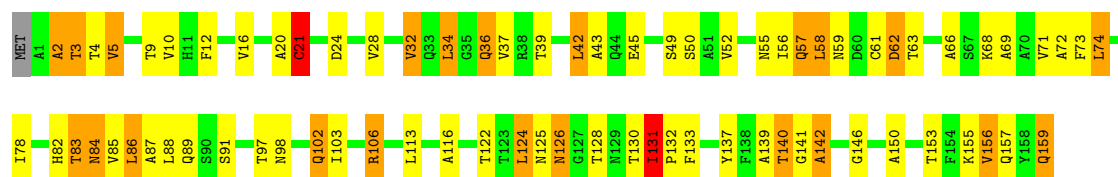
• Molecule 1: FimA

Chain D: 52% 32% 14% ..



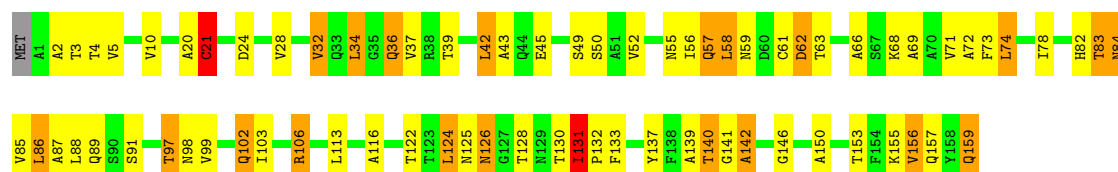
• Molecule 1: FimA

Chain E: 52% 32% 14% ..



• Molecule 1: FimA

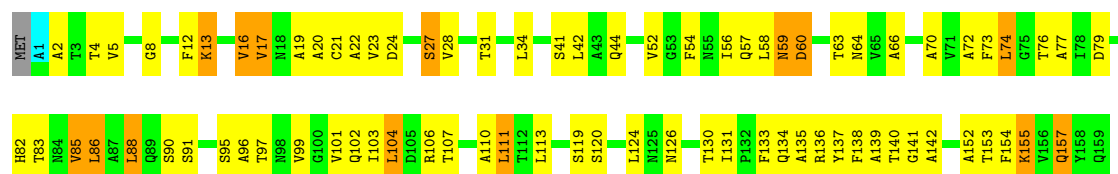
Chain F: 53% 32% 12% ..



4.2.7 Score per residue for model 7

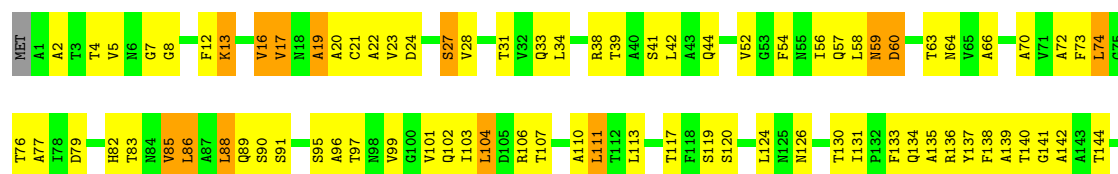
• Molecule 1: FimA

Chain A: 49% 41% 9% ..



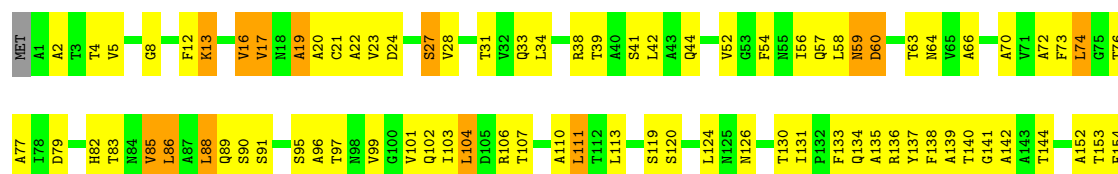
• Molecule 1: FimA

Chain B: 45% 45% 9% ..



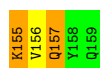
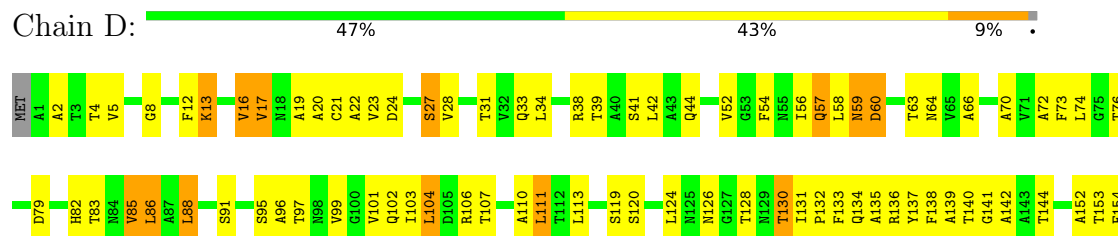
• Molecule 1: FimA

Chain C: 46% 44% 9% ..

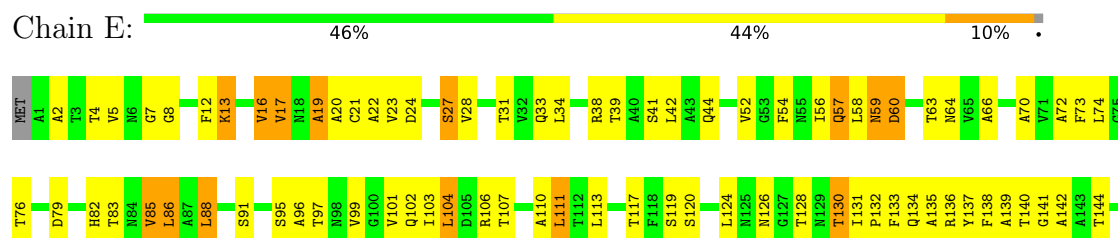




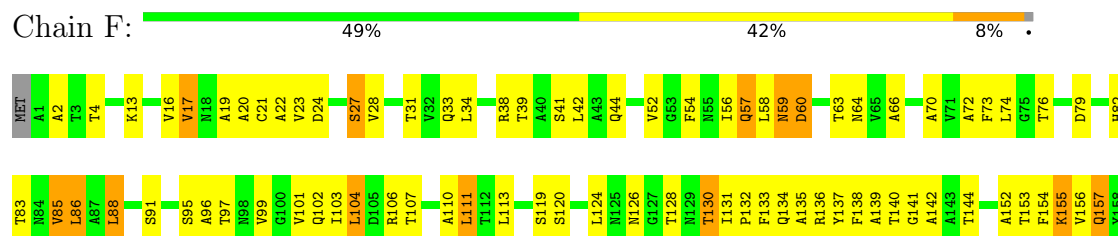
• Molecule 1: FimA



• Molecule 1: FimA

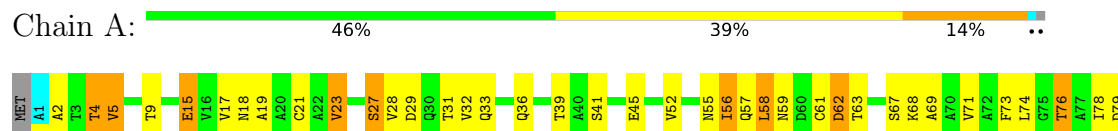


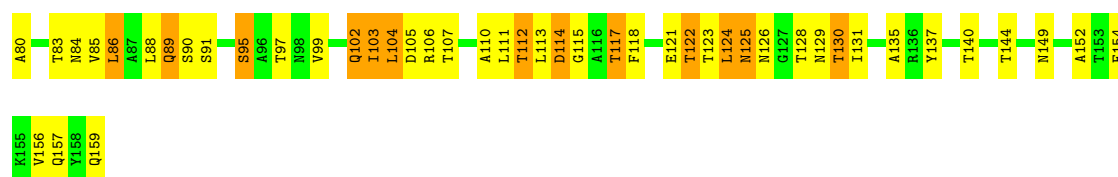
• Molecule 1: FimA



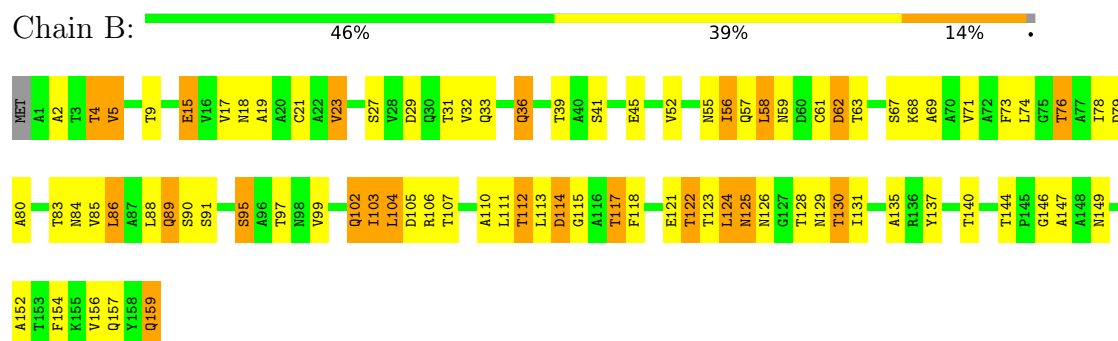
4.2.8 Score per residue for model 8

• Molecule 1: FimA

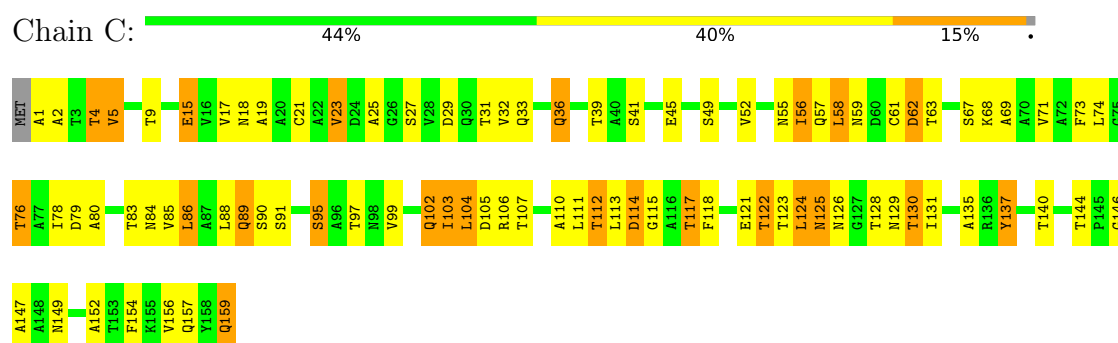




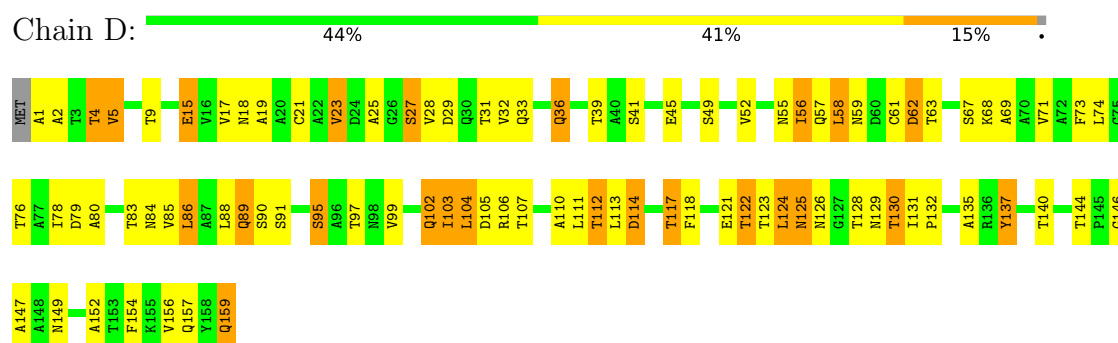
• Molecule 1: FimA



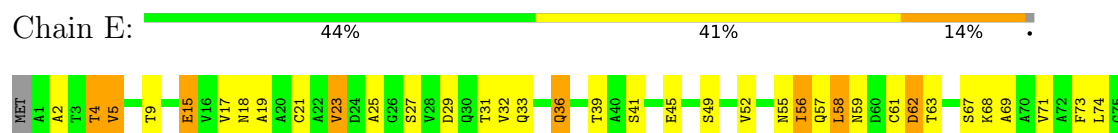
• Molecule 1: FimA

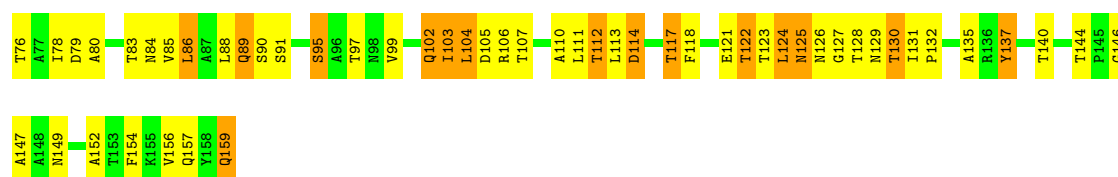


• Molecule 1: FimA



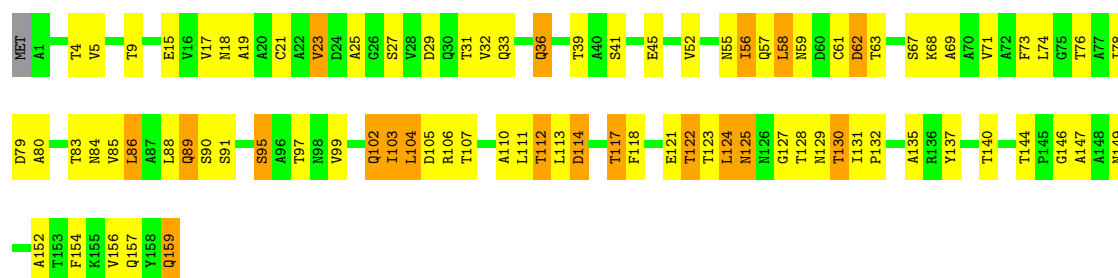
• Molecule 1: FimA





• Molecule 1: FimA

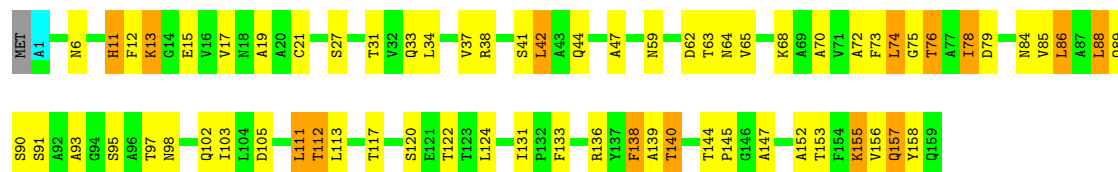
Chain F: 46% 41% 12%



4.2.9 Score per residue for model 9

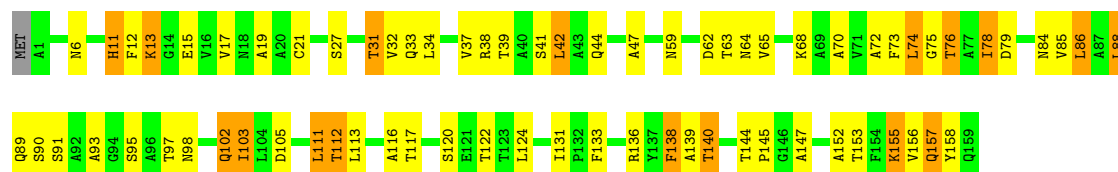
• Molecule 1: FimA

Chain A: 56% 34% 9%



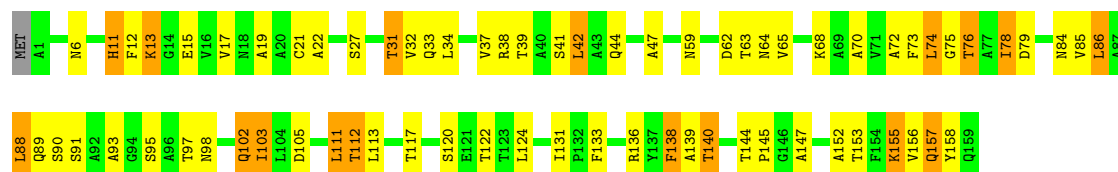
• Molecule 1: FimA

Chain B: 55% 34% 11%



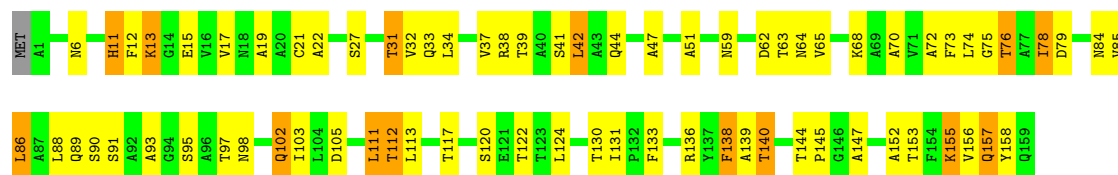
• Molecule 1: FimA

Chain C: 55% 34% 11%



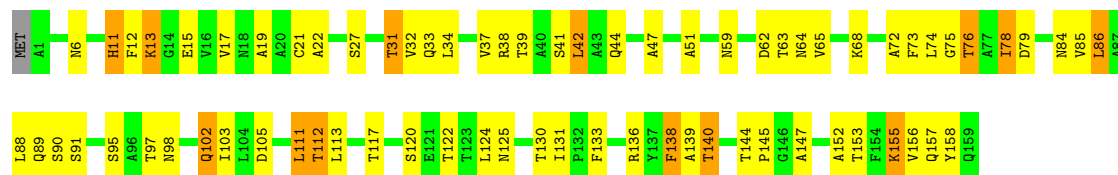
- Molecule 1: FimA

Chain D: 



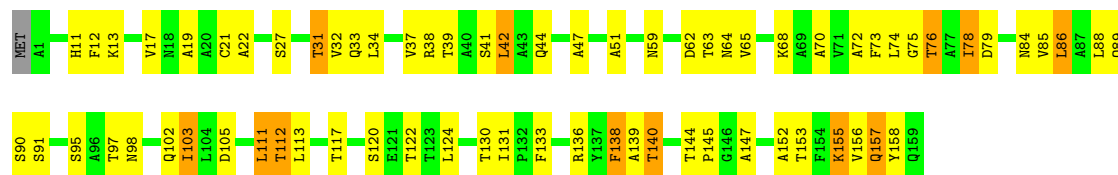
- Molecule 1: FimA

Chain E: 



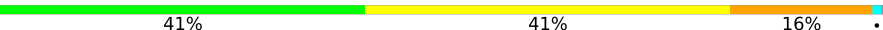
- Molecule 1: FimA

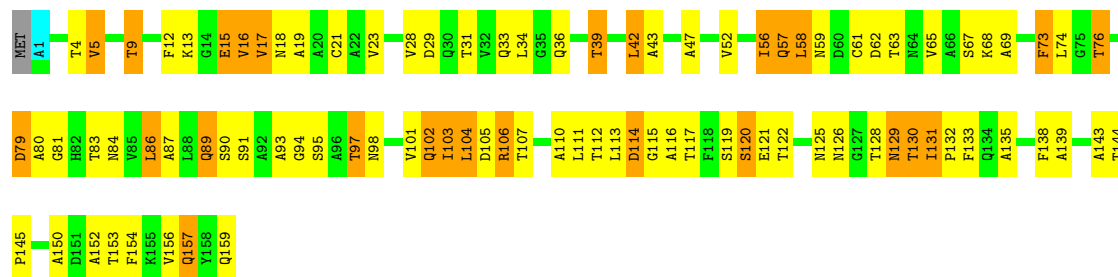
Chain F: 



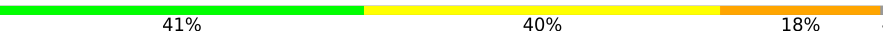
4.2.10 Score per residue for model 10

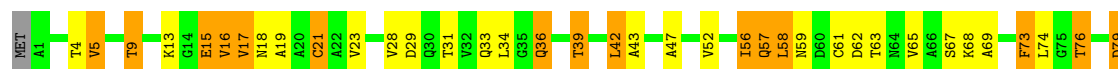
- Molecule 1: FimA

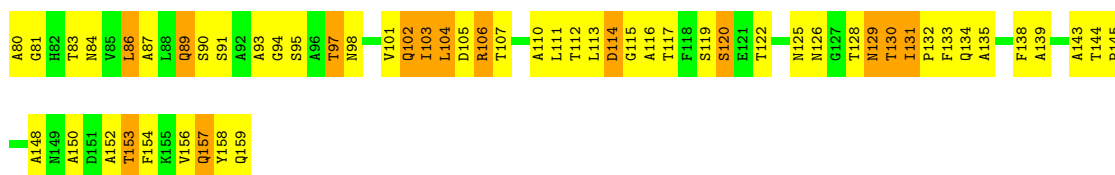
Chain A: 



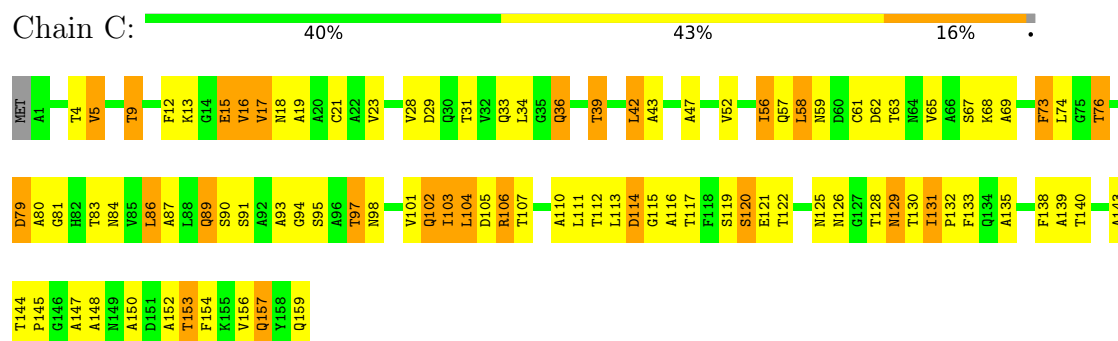
- Molecule 1: FimA

Chain B: 

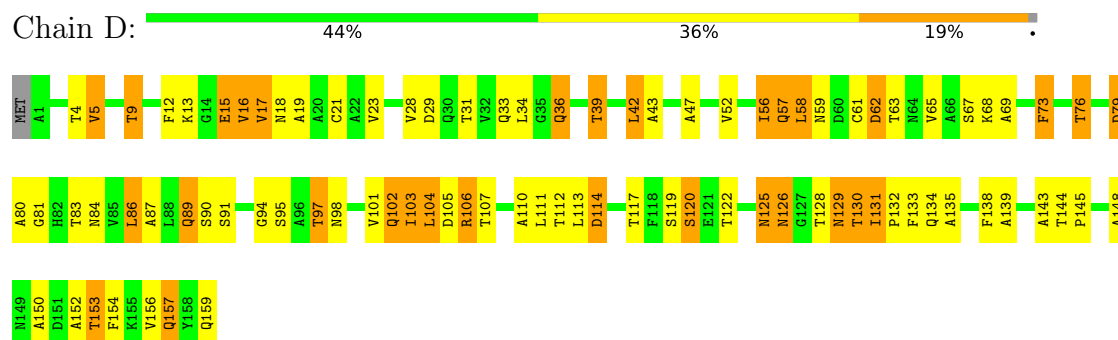




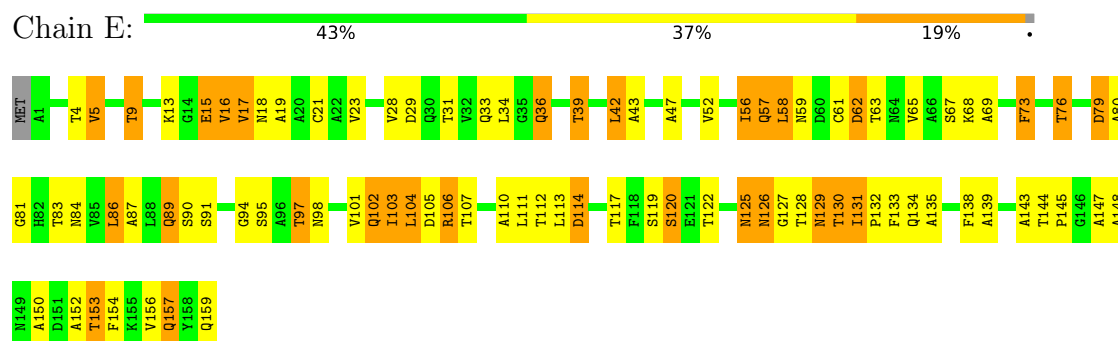
• Molecule 1: FimA



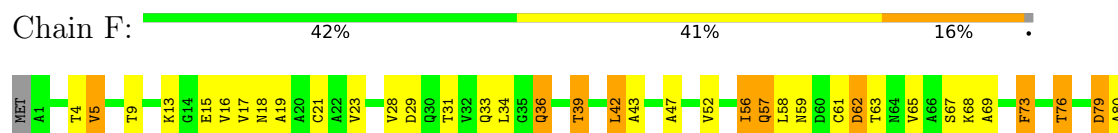
• Molecule 1: FimA



• Molecule 1: FimA



• Molecule 1: FimA



A148	A149	A150	A151	A152	T153	F154	F155	V156	Q157	V158	Q159		G81	H82	T83	N84	V85	L86	A87	L88	Q89	S90	S91		G94	S95	A96	T97	N98		V101	Q102	T103	L104	D105	R106	T107		A110	L111	T112	L113	D114		T117	F118	S119	S120	E121	T122		M125	M126	G127	T128	M129	T130	I131	P132	F133	Q134	A135		F138	A139	T140		A143	T144	P145	G146	A147
------	------	------	------	------	------	------	------	------	------	------	------	--	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	--	-----	-----	-----	-----	-----	--	------	------	------	------	------	------	------	--	------	------	------	------	------	--	------	------	------	------	------	------	--	------	------	------	------	------	------	------	------	------	------	------	--	------	------	------	--	------	------	------	------	------

5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics*.

Of the 1100 calculated structures, 10 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
ISD	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	800
Number of shifts mapped to atoms	800
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	7%

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.32±0.01	0±0/1119 (0.0± 0.0%)	0.64±0.01	1±0/1529 (0.0± 0.0%)
1	B	0.32±0.01	0±0/1124 (0.0± 0.0%)	0.64±0.01	1±0/1536 (0.0± 0.0%)
1	C	0.32±0.01	0±0/1124 (0.0± 0.0%)	0.64±0.01	1±0/1536 (0.0± 0.0%)
1	D	0.32±0.01	0±0/1124 (0.0± 0.0%)	0.64±0.01	1±0/1536 (0.0± 0.0%)
1	E	0.32±0.01	0±0/1124 (0.0± 0.0%)	0.64±0.01	1±0/1536 (0.0± 0.0%)
1	F	0.32±0.01	0±0/1124 (0.0± 0.0%)	0.64±0.01	1±0/1536 (0.0± 0.0%)
All	All	0.32	0/67390 (0.0%)	0.64	42/92090 (0.0%)

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	C	131	ILE	N-CA-C	7.12	114.04	107.56	10	7
1	F	131	ILE	N-CA-C	7.12	114.04	107.56	10	7
1	E	131	ILE	N-CA-C	7.11	114.03	107.56	10	7
1	D	131	ILE	N-CA-C	7.11	114.03	107.56	10	7
1	A	131	ILE	N-CA-C	7.09	114.01	107.56	10	7
1	B	131	ILE	N-CA-C	7.05	113.97	107.56	10	7

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	1107	1062	1070	46±11
1	B	1112	1067	1077	56±11
1	C	1112	1067	1077	56±11
1	D	1112	1067	1077	56±12
1	E	1112	1067	1077	56±12
1	F	1112	1067	1077	46±9
All	All	66670	63970	64526	2552

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 19.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:112:THR:HG23	1:B:117:THR:HG21	0.90	1.44	4	3
1:A:112:THR:HG23	1:A:117:THR:HG21	0.89	1.44	4	3
1:A:21:CYS:HG	1:A:61:CYS:HG	0.88	0.97	6	4
1:C:112:THR:HG23	1:C:117:THR:HG21	0.88	1.44	4	3
1:E:112:THR:HG23	1:E:117:THR:HG21	0.87	1.45	4	3
1:F:112:THR:HG23	1:F:117:THR:HG21	0.87	1.44	4	3
1:C:9:THR:HG22	1:D:153:THR:HG23	0.87	1.46	3	3
1:D:9:THR:HG22	1:E:153:THR:HG23	0.85	1.46	3	3
1:D:112:THR:HG23	1:D:117:THR:HG21	0.85	1.44	4	3
1:C:21:CYS:HG	1:C:61:CYS:HG	0.85	0.99	1	1
1:E:9:THR:HG22	1:F:153:THR:HG23	0.84	1.46	3	3
1:A:9:THR:HG22	1:B:153:THR:HG23	0.84	1.46	3	3
1:B:86:LEU:HD22	1:B:150:ALA:HB1	0.83	1.50	6	5
1:E:86:LEU:HD22	1:E:150:ALA:HB1	0.83	1.50	6	5
1:F:86:LEU:HD22	1:F:150:ALA:HB1	0.83	1.50	6	5
1:A:86:LEU:HD22	1:A:150:ALA:HB1	0.83	1.50	6	5
1:E:21:CYS:HG	1:E:61:CYS:HG	0.83	0.95	1	2
1:B:9:THR:HG22	1:C:153:THR:HG23	0.83	1.46	3	3
1:C:86:LEU:HD22	1:C:150:ALA:HB1	0.83	1.50	6	5
1:B:21:CYS:HG	1:B:61:CYS:HG	0.81	0.94	1	1
1:D:21:CYS:HG	1:D:61:CYS:HG	0.81	0.95	1	1
1:D:86:LEU:HD22	1:D:150:ALA:HB1	0.80	1.50	6	5
1:A:74:LEU:HD21	1:D:130:THR:HG21	0.80	1.53	4	3
1:B:74:LEU:HD21	1:E:130:THR:HG21	0.79	1.53	4	3
1:C:79:ASP:CB	1:C:140:THR:HG21	0.79	2.08	5	1
1:F:79:ASP:CB	1:F:140:THR:HG21	0.78	2.08	5	1
1:D:79:ASP:CB	1:D:140:THR:HG21	0.78	2.08	5	1
1:A:79:ASP:CB	1:A:140:THR:HG21	0.78	2.08	5	1
1:C:74:LEU:HD21	1:F:130:THR:HG21	0.78	1.53	4	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:E:79:ASP:CB	1:E:140:THR:HG21	0.77	2.08	5	1
1:F:79:ASP:HB3	1:F:140:THR:HG21	0.77	1.56	5	1
1:B:79:ASP:CB	1:B:140:THR:HG21	0.77	2.08	5	1
1:C:79:ASP:HB3	1:C:140:THR:HG21	0.77	1.56	5	1
1:E:104:LEU:HD12	1:E:110:ALA:HB2	0.77	1.56	8	2
1:B:104:LEU:HD12	1:B:110:ALA:HB2	0.77	1.56	8	2
1:D:79:ASP:HB3	1:D:140:THR:HG21	0.77	1.56	5	1
1:D:104:LEU:HD12	1:D:110:ALA:HB2	0.77	1.56	8	1
1:A:79:ASP:HB3	1:A:140:THR:HG21	0.77	1.56	5	1
1:E:112:THR:CG2	1:E:117:THR:HG21	0.76	2.10	4	3
1:B:112:THR:CG2	1:B:117:THR:HG21	0.76	2.10	4	3
1:E:79:ASP:HB3	1:E:140:THR:HG21	0.76	1.56	5	1
1:A:112:THR:CG2	1:A:117:THR:HG21	0.76	2.10	4	3
1:C:104:LEU:HD12	1:C:110:ALA:HB2	0.76	1.56	8	2
1:F:104:LEU:HD12	1:F:110:ALA:HB2	0.76	1.56	8	1
1:F:112:THR:CG2	1:F:117:THR:HG21	0.75	2.10	4	2
1:D:112:THR:CG2	1:D:117:THR:HG21	0.75	2.10	4	3
1:B:5:VAL:HG21	1:C:17:VAL:HG12	0.75	1.58	3	2
1:E:5:VAL:HG21	1:F:17:VAL:HG12	0.75	1.57	3	2
1:A:104:LEU:HD12	1:A:110:ALA:HB2	0.75	1.56	8	2
1:C:112:THR:CG2	1:C:117:THR:HG21	0.75	2.10	4	3
1:B:86:LEU:HD12	1:B:113:LEU:HD22	0.75	1.59	10	1
1:E:86:LEU:HD12	1:E:113:LEU:HD22	0.75	1.59	10	1
1:B:79:ASP:HB3	1:B:140:THR:HG21	0.74	1.56	5	1
1:C:5:VAL:HG21	1:D:17:VAL:HG12	0.74	1.58	3	2
1:D:5:VAL:HG21	1:E:17:VAL:HG12	0.74	1.58	3	2
1:F:86:LEU:HD12	1:F:113:LEU:HD22	0.74	1.59	10	1
1:D:69:ALA:HB2	1:D:124:LEU:HD13	0.74	1.60	8	1
1:C:86:LEU:HD12	1:C:113:LEU:HD22	0.73	1.59	10	1
1:A:5:VAL:HG21	1:B:17:VAL:HG12	0.73	1.58	3	2
1:E:69:ALA:HB2	1:E:124:LEU:HD13	0.73	1.60	8	1
1:A:90:SER:HA	1:D:52:VAL:HG13	0.73	1.60	6	1
1:E:144:THR:CG2	1:E:145:PRO:CD	0.73	2.67	2	4
1:F:144:THR:CG2	1:F:145:PRO:CD	0.73	2.67	2	4
1:D:86:LEU:HD12	1:D:113:LEU:HD22	0.73	1.59	10	1
1:A:69:ALA:HB2	1:A:124:LEU:HD13	0.73	1.60	8	1
1:B:144:THR:CG2	1:B:145:PRO:CD	0.72	2.67	2	4
1:B:69:ALA:HB2	1:B:124:LEU:HD13	0.72	1.60	8	1
1:A:86:LEU:HD12	1:A:113:LEU:HD22	0.72	1.59	10	1
1:A:144:THR:CG2	1:A:145:PRO:CD	0.72	2.67	2	4
1:F:21:CYS:HG	1:F:61:CYS:HG	0.72	0.73	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:F:69:ALA:HB2	1:F:124:LEU:HD13	0.72	1.60	8	1
1:C:69:ALA:HB2	1:C:124:LEU:HD13	0.72	1.60	8	1
1:C:90:SER:HA	1:F:52:VAL:HG13	0.72	1.60	6	1
1:D:144:THR:CG2	1:D:145:PRO:CD	0.72	2.67	2	4
1:C:144:THR:CG2	1:C:145:PRO:CD	0.71	2.67	2	4
1:B:90:SER:HA	1:E:52:VAL:HG13	0.71	1.60	6	1
1:D:84:ASN:HA	1:D:112:THR:HA	0.70	1.64	8	6
1:F:84:ASN:HA	1:F:112:THR:HA	0.70	1.64	8	6
1:A:84:ASN:HA	1:A:112:THR:HA	0.70	1.64	8	6
1:C:84:ASN:HA	1:C:112:THR:HA	0.70	1.64	8	6
1:E:16:VAL:HG23	1:F:148:ALA:HB2	0.69	1.64	4	5
1:B:16:VAL:HG23	1:C:148:ALA:HB2	0.69	1.64	4	5
1:B:15:GLU:CG	1:C:146:GLY:O	0.69	2.41	3	3
1:E:15:GLU:CG	1:F:146:GLY:O	0.69	2.41	3	3
1:C:16:VAL:HG23	1:D:148:ALA:HB2	0.68	1.65	4	5
1:A:57:GLN:HA	1:A:130:THR:HG23	0.68	1.65	4	5
1:A:16:VAL:HG23	1:B:148:ALA:HB2	0.68	1.65	4	5
1:D:16:VAL:HG23	1:E:148:ALA:HB2	0.68	1.64	4	5
1:F:72:ALA:HB3	1:F:155:LYS:HB3	0.68	1.66	7	2
1:C:15:GLU:CG	1:D:146:GLY:O	0.68	2.41	3	3
1:D:15:GLU:CG	1:E:146:GLY:O	0.68	2.41	3	3
1:A:15:GLU:CG	1:B:146:GLY:O	0.68	2.41	3	3
1:D:57:GLN:HA	1:D:130:THR:HG23	0.67	1.65	4	4
1:F:57:GLN:HA	1:F:130:THR:HG23	0.67	1.65	4	4
1:E:84:ASN:HA	1:E:112:THR:HA	0.67	1.64	8	5
1:C:72:ALA:HB3	1:C:155:LYS:HB3	0.67	1.66	7	2
1:C:57:GLN:HA	1:C:130:THR:HG23	0.67	1.65	4	4
1:B:84:ASN:HA	1:B:112:THR:HA	0.67	1.64	8	5
1:D:93:ALA:HB1	1:F:22:ALA:HB1	0.67	1.67	9	1
1:D:144:THR:CG2	1:D:145:PRO:HD2	0.67	2.20	2	4
1:C:93:ALA:HB1	1:E:22:ALA:HB1	0.67	1.67	9	1
1:A:144:THR:CG2	1:A:145:PRO:HD2	0.67	2.20	2	4
1:C:144:THR:CG2	1:C:145:PRO:HD2	0.67	2.20	2	4
1:A:93:ALA:HB1	1:C:22:ALA:HB1	0.67	1.67	9	1
1:F:42:LEU:O	1:F:143:ALA:HB2	0.67	1.90	10	4
1:B:42:LEU:O	1:B:143:ALA:HB2	0.66	1.90	10	4
1:B:57:GLN:HA	1:B:130:THR:HG23	0.66	1.65	4	5
1:E:42:LEU:O	1:E:143:ALA:HB2	0.66	1.90	10	4
1:E:57:GLN:HA	1:E:130:THR:HG23	0.66	1.65	4	4
1:C:42:LEU:O	1:C:143:ALA:HB2	0.66	1.90	10	4
1:F:105:ASP:HB3	1:F:107:THR:HG22	0.66	1.68	2	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:21:CYS:SG	1:B:58:LEU:HB3	0.66	2.31	5	2
1:C:21:CYS:SG	1:C:58:LEU:HB3	0.66	2.31	5	2
1:C:105:ASP:HB3	1:C:107:THR:HG22	0.66	1.68	2	6
1:E:21:CYS:SG	1:E:58:LEU:HB3	0.66	2.31	5	2
1:F:21:CYS:SG	1:F:58:LEU:HB3	0.66	2.31	5	2
1:F:144:THR:CG2	1:F:145:PRO:HD2	0.66	2.20	2	4
1:A:105:ASP:HB3	1:A:107:THR:HG22	0.66	1.68	2	6
1:B:52:VAL:HG22	1:B:135:ALA:O	0.65	1.91	1	4
1:B:93:ALA:HB1	1:D:22:ALA:HB1	0.65	1.67	9	1
1:D:105:ASP:HB3	1:D:107:THR:HG22	0.65	1.68	2	6
1:B:144:THR:CG2	1:B:145:PRO:HD2	0.65	2.20	2	4
1:B:72:ALA:HB3	1:B:155:LYS:HB3	0.65	1.66	7	2
1:A:17:VAL:O	1:B:39:THR:HG22	0.65	1.92	1	1
1:A:21:CYS:SG	1:A:58:LEU:HB3	0.65	2.31	5	2
1:C:52:VAL:HG22	1:C:135:ALA:O	0.65	1.91	1	4
1:E:144:THR:CG2	1:E:145:PRO:HD2	0.65	2.20	2	4
1:C:17:VAL:O	1:D:39:THR:HG22	0.65	1.92	1	1
1:A:52:VAL:HG22	1:A:135:ALA:O	0.65	1.91	1	4
1:D:72:ALA:HB3	1:D:155:LYS:HB3	0.65	1.66	7	2
1:A:42:LEU:O	1:A:143:ALA:HB2	0.65	1.91	10	4
1:D:21:CYS:SG	1:D:58:LEU:HB3	0.65	2.31	5	2
1:F:71:VAL:HG11	1:F:131:ILE:HG21	0.65	1.69	1	5
1:A:72:ALA:HB3	1:A:155:LYS:HB3	0.65	1.66	7	2
1:E:72:ALA:HB3	1:E:155:LYS:HB3	0.65	1.66	7	2
1:D:17:VAL:O	1:E:39:THR:HG22	0.65	1.92	1	1
1:E:52:VAL:HG22	1:E:135:ALA:O	0.65	1.91	1	4
1:F:52:VAL:HG22	1:F:135:ALA:O	0.65	1.91	1	4
1:E:105:ASP:HB3	1:E:107:THR:HG22	0.64	1.68	2	6
1:E:144:THR:HG23	1:E:145:PRO:CD	0.64	2.22	2	3
1:B:71:VAL:HG11	1:B:131:ILE:HG21	0.64	1.69	1	5
1:B:105:ASP:HB3	1:B:107:THR:HG22	0.64	1.68	2	6
1:F:144:THR:HG23	1:F:145:PRO:CD	0.64	2.23	2	3
1:C:144:THR:HG23	1:C:145:PRO:CD	0.64	2.23	2	3
1:D:52:VAL:HG22	1:D:135:ALA:O	0.64	1.91	1	4
1:A:44:GLN:HG3	1:A:47:ALA:HB2	0.64	1.70	5	1
1:A:71:VAL:HG11	1:A:131:ILE:HG21	0.64	1.70	3	3
1:B:144:THR:HG23	1:B:145:PRO:CD	0.64	2.23	2	3
1:C:71:VAL:HG11	1:C:131:ILE:HG21	0.64	1.69	1	3
1:D:42:LEU:O	1:D:143:ALA:HB2	0.64	1.90	10	4
1:E:17:VAL:O	1:F:39:THR:HG22	0.64	1.92	1	1
1:B:44:GLN:HG3	1:B:47:ALA:HB2	0.64	1.70	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:95:SER:HA	1:A:147:ALA:HB3	0.64	1.69	1	5
1:F:44:GLN:HG3	1:F:47:ALA:HB2	0.64	1.70	5	1
1:B:15:GLU:O	1:C:36:GLN:HA	0.64	1.93	2	6
1:A:56:ILE:HB	1:A:131:ILE:HD12	0.64	1.70	7	1
1:A:144:THR:HG23	1:A:145:PRO:CD	0.64	2.23	2	3
1:D:71:VAL:HG11	1:D:131:ILE:HG21	0.64	1.69	1	4
1:E:71:VAL:HG11	1:E:131:ILE:HG21	0.64	1.69	3	5
1:E:44:GLN:HG3	1:E:47:ALA:HB2	0.64	1.70	5	1
1:A:69:ALA:HB2	1:A:124:LEU:HD12	0.64	1.70	6	1
1:D:15:GLU:O	1:E:36:GLN:HA	0.64	1.93	2	6
1:B:69:ALA:HB2	1:B:124:LEU:HD12	0.64	1.71	6	1
1:B:17:VAL:O	1:C:39:THR:HG22	0.63	1.92	1	1
1:C:95:SER:HA	1:C:147:ALA:HB3	0.63	1.69	1	5
1:E:95:SER:HA	1:E:147:ALA:HB3	0.63	1.69	1	5
1:D:69:ALA:HB2	1:D:124:LEU:HD12	0.63	1.71	6	1
1:E:69:ALA:HB2	1:E:124:LEU:HD12	0.63	1.70	6	1
1:C:9:THR:HG23	1:D:153:THR:HG23	0.63	1.69	10	1
1:D:9:THR:HG23	1:E:153:THR:HG23	0.63	1.69	10	1
1:D:95:SER:HA	1:D:147:ALA:HB3	0.63	1.69	1	5
1:F:69:ALA:HB2	1:F:124:LEU:HD12	0.63	1.70	6	1
1:B:95:SER:HA	1:B:147:ALA:HB3	0.63	1.69	1	5
1:E:15:GLU:O	1:F:36:GLN:HA	0.63	1.93	2	6
1:C:44:GLN:HG3	1:C:47:ALA:HB2	0.63	1.70	5	1
1:D:44:GLN:HG3	1:D:47:ALA:HB2	0.63	1.70	5	1
1:A:9:THR:HG23	1:B:153:THR:HG23	0.63	1.69	10	1
1:B:9:THR:HG23	1:C:153:THR:HG23	0.63	1.69	10	1
1:A:15:GLU:O	1:B:36:GLN:HA	0.63	1.93	2	6
1:A:82:HIS:HB3	1:A:85:VAL:HB	0.63	1.70	6	1
1:C:69:ALA:HB2	1:C:124:LEU:HD12	0.63	1.71	6	1
1:C:63:THR:HG23	1:C:124:LEU:O	0.63	1.94	4	1
1:D:82:HIS:HB3	1:D:85:VAL:HB	0.62	1.70	6	1
1:C:56:ILE:HB	1:C:131:ILE:HD12	0.62	1.70	7	1
1:E:9:THR:HG23	1:F:153:THR:HG23	0.62	1.69	10	1
1:C:15:GLU:O	1:D:36:GLN:HA	0.62	1.93	2	6
1:F:95:SER:HA	1:F:147:ALA:HB3	0.62	1.69	1	5
1:D:56:ILE:HB	1:D:131:ILE:HD12	0.62	1.70	7	1
1:B:12:PHE:HB3	1:C:34:LEU:HD21	0.62	1.70	7	1
1:C:12:PHE:HB3	1:D:34:LEU:HD21	0.62	1.70	7	1
1:C:82:HIS:HB3	1:C:85:VAL:HB	0.62	1.70	6	1
1:C:15:GLU:HG3	1:D:146:GLY:O	0.62	1.94	3	4
1:B:56:ILE:HB	1:B:131:ILE:HD12	0.62	1.70	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:15:GLU:HG3	1:C:146:GLY:O	0.62	1.94	3	4
1:B:102:GLN:O	1:B:135:ALA:HA	0.62	1.95	4	5
1:C:75:GLY:HA3	1:C:113:LEU:HD22	0.62	1.72	1	1
1:C:102:GLN:O	1:C:135:ALA:HA	0.62	1.95	4	5
1:E:102:GLN:O	1:E:135:ALA:HA	0.62	1.94	4	5
1:A:104:LEU:HA	1:A:110:ALA:HA	0.62	1.72	4	4
1:A:12:PHE:HB3	1:B:34:LEU:HD21	0.62	1.70	7	1
1:F:56:ILE:HB	1:F:131:ILE:HD12	0.62	1.70	7	1
1:C:88:LEU:HD12	1:F:51:ALA:O	0.62	1.95	9	1
1:D:63:THR:HG23	1:D:124:LEU:O	0.62	1.94	4	1
1:D:12:PHE:HB3	1:E:34:LEU:HD21	0.62	1.70	7	1
1:A:102:GLN:O	1:A:135:ALA:HA	0.62	1.94	4	5
1:D:75:GLY:HA3	1:D:113:LEU:HD22	0.62	1.72	1	1
1:C:17:VAL:HG11	1:D:36:GLN:NE2	0.62	2.10	2	3
1:A:63:THR:HG23	1:A:124:LEU:O	0.62	1.94	4	1
1:B:63:THR:HG23	1:B:124:LEU:O	0.62	1.94	4	1
1:F:63:THR:HG23	1:F:124:LEU:O	0.62	1.94	4	1
1:E:56:ILE:HB	1:E:131:ILE:HD12	0.62	1.70	7	1
1:D:144:THR:HG23	1:D:145:PRO:CD	0.62	2.23	2	3
1:F:75:GLY:HA3	1:F:113:LEU:HD22	0.62	1.72	1	1
1:A:17:VAL:O	1:B:39:THR:HG23	0.62	1.95	7	2
1:E:12:PHE:HB3	1:F:34:LEU:HD21	0.62	1.70	7	1
1:D:17:VAL:HG11	1:E:36:GLN:NE2	0.62	2.10	2	3
1:A:17:VAL:HG11	1:B:36:GLN:NE2	0.61	2.10	2	3
1:E:63:THR:HG23	1:E:124:LEU:O	0.61	1.94	4	1
1:A:75:GLY:HA3	1:A:113:LEU:HD22	0.61	1.72	1	1
1:B:82:HIS:HB3	1:B:85:VAL:HB	0.61	1.70	6	1
1:D:15:GLU:HG3	1:E:146:GLY:O	0.61	1.94	3	4
1:D:104:LEU:HA	1:D:110:ALA:HA	0.61	1.72	4	4
1:E:17:VAL:O	1:F:39:THR:HG23	0.61	1.95	7	2
1:B:61:CYS:SG	1:B:129:ASN:HB2	0.61	2.35	4	3
1:E:82:HIS:HB3	1:E:85:VAL:HB	0.61	1.70	6	1
1:A:88:LEU:HD12	1:D:51:ALA:O	0.61	1.95	9	1
1:B:17:VAL:HG11	1:C:36:GLN:NE2	0.61	2.10	2	3
1:D:102:GLN:O	1:D:135:ALA:HA	0.61	1.94	4	5
1:E:75:GLY:HA3	1:E:113:LEU:HD22	0.61	1.72	1	1
1:E:15:GLU:HG3	1:F:146:GLY:O	0.61	1.94	3	4
1:A:61:CYS:SG	1:A:129:ASN:HB2	0.61	2.36	4	3
1:B:17:VAL:O	1:C:39:THR:HG23	0.61	1.95	7	2
1:A:15:GLU:HG3	1:B:146:GLY:O	0.61	1.94	3	4
1:F:61:CYS:SG	1:F:129:ASN:HB2	0.61	2.36	4	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:88:LEU:HD12	1:E:51:ALA:O	0.61	1.95	9	1
1:B:112:THR:HG22	1:B:117:THR:HG21	0.61	1.73	10	1
1:E:112:THR:HG22	1:E:117:THR:HG21	0.61	1.73	10	1
1:D:16:VAL:HG13	1:E:37:VAL:HG13	0.61	1.73	1	1
1:B:104:LEU:HA	1:B:110:ALA:HA	0.61	1.72	4	3
1:E:104:LEU:HA	1:E:110:ALA:HA	0.61	1.72	4	3
1:E:17:VAL:HG11	1:F:36:GLN:NE2	0.61	2.10	2	3
1:D:61:CYS:SG	1:D:129:ASN:HB2	0.61	2.36	4	3
1:A:42:LEU:CB	1:A:139:ALA:HB2	0.61	2.26	6	1
1:F:82:HIS:HB3	1:F:85:VAL:HB	0.61	1.70	6	1
1:D:42:LEU:CB	1:D:139:ALA:HB2	0.60	2.26	6	1
1:F:102:GLN:O	1:F:135:ALA:HA	0.60	1.95	4	5
1:E:16:VAL:CG1	1:F:144:THR:O	0.60	2.49	3	2
1:C:61:CYS:SG	1:C:129:ASN:HB2	0.60	2.36	4	3
1:B:55:ASN:HA	1:B:131:ILE:O	0.60	1.96	6	1
1:C:42:LEU:CB	1:C:139:ALA:HB2	0.60	2.26	6	1
1:E:55:ASN:HA	1:E:131:ILE:O	0.60	1.96	6	1
1:D:17:VAL:O	1:E:39:THR:HG23	0.60	1.95	7	2
1:B:16:VAL:CG1	1:C:144:THR:O	0.60	2.49	3	2
1:C:16:VAL:CG1	1:D:144:THR:O	0.60	2.50	3	2
1:E:5:VAL:HG21	1:F:17:VAL:CG1	0.60	2.26	3	1
1:C:104:LEU:HA	1:C:110:ALA:HA	0.60	1.72	4	3
1:E:91:SER:HB2	1:E:95:SER:HB2	0.60	1.73	10	2
1:A:16:VAL:CG1	1:B:144:THR:O	0.60	2.49	3	2
1:B:5:VAL:HG21	1:C:17:VAL:CG1	0.60	2.27	3	1
1:D:55:ASN:HA	1:D:131:ILE:O	0.60	1.96	6	1
1:B:42:LEU:CB	1:B:139:ALA:HB2	0.60	2.26	6	1
1:C:5:VAL:HG21	1:D:17:VAL:CG1	0.60	2.27	3	1
1:C:90:SER:HA	1:F:52:VAL:HB	0.60	1.74	4	1
1:E:61:CYS:SG	1:E:129:ASN:HB2	0.60	2.36	4	3
1:B:75:GLY:HA3	1:B:113:LEU:HD22	0.60	1.72	1	1
1:F:42:LEU:CB	1:F:139:ALA:HB2	0.60	2.26	6	1
1:B:91:SER:HB2	1:B:95:SER:HB2	0.60	1.73	10	2
1:B:90:SER:HA	1:E:52:VAL:HB	0.60	1.74	4	1
1:C:17:VAL:O	1:D:39:THR:HG23	0.60	1.95	7	2
1:F:104:LEU:HA	1:F:110:ALA:HA	0.59	1.72	4	3
1:F:55:ASN:HA	1:F:131:ILE:O	0.59	1.96	6	1
1:A:91:SER:HB2	1:A:95:SER:HB2	0.59	1.73	10	2
1:D:16:VAL:CG1	1:E:144:THR:O	0.59	2.50	3	2
1:A:5:VAL:HG21	1:B:17:VAL:CG1	0.59	2.27	3	1
1:E:42:LEU:CB	1:E:139:ALA:HB2	0.59	2.26	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:D:91:SER:HB2	1:D:95:SER:HB2	0.59	1.72	10	2
1:F:91:SER:HB2	1:F:95:SER:HB2	0.59	1.73	10	2
1:A:16:VAL:HG13	1:B:37:VAL:HG13	0.59	1.73	1	1
1:E:97:THR:H	1:E:144:THR:HB	0.59	1.58	4	2
1:A:55:ASN:HA	1:A:131:ILE:O	0.59	1.96	6	1
1:F:112:THR:HG22	1:F:117:THR:HG21	0.59	1.73	10	1
1:E:86:LEU:HG	1:E:113:LEU:HD13	0.59	1.75	2	3
1:D:5:VAL:HG21	1:E:17:VAL:CG1	0.59	2.27	3	1
1:A:97:THR:H	1:A:144:THR:HB	0.59	1.58	4	2
1:C:91:SER:HB2	1:C:95:SER:HB2	0.59	1.73	10	2
1:B:86:LEU:HG	1:B:113:LEU:HD13	0.59	1.75	2	3
1:E:3:THR:O	1:F:157:GLN:HA	0.59	1.98	4	2
1:C:55:ASN:HA	1:C:131:ILE:O	0.59	1.96	6	1
1:C:85:VAL:HA	1:C:102:GLN:HA	0.59	1.74	7	2
1:C:16:VAL:HG13	1:D:37:VAL:HG13	0.59	1.73	1	1
1:A:3:THR:O	1:B:157:GLN:HA	0.59	1.98	4	2
1:B:97:THR:H	1:B:144:THR:HB	0.59	1.58	4	2
1:D:97:THR:H	1:D:144:THR:HB	0.59	1.58	4	2
1:C:112:THR:HG22	1:C:117:THR:HG21	0.59	1.73	10	1
1:A:78:ILE:HB	1:A:87:ALA:HA	0.59	1.75	6	1
1:D:78:ILE:HB	1:D:87:ALA:HA	0.59	1.75	6	1
1:B:16:VAL:HG13	1:C:37:VAL:HG13	0.58	1.73	1	1
1:B:5:VAL:HG23	1:C:156:VAL:HG23	0.58	1.75	10	5
1:C:3:THR:O	1:D:157:GLN:HA	0.58	1.98	4	2
1:D:85:VAL:HA	1:D:102:GLN:HA	0.58	1.74	7	2
1:F:85:VAL:HA	1:F:102:GLN:HA	0.58	1.74	7	2
1:A:112:THR:HG22	1:A:117:THR:HG21	0.58	1.73	10	1
1:C:77:ALA:O	1:C:87:ALA:HB2	0.58	1.98	1	3
1:C:97:THR:H	1:C:144:THR:HB	0.58	1.58	4	2
1:A:85:VAL:HA	1:A:102:GLN:HA	0.58	1.74	7	2
1:E:86:LEU:HD21	1:E:152:ALA:HB2	0.58	1.75	9	2
1:F:77:ALA:O	1:F:87:ALA:HB2	0.58	1.98	1	3
1:F:86:LEU:HG	1:F:113:LEU:HD13	0.58	1.75	2	3
1:B:77:ALA:O	1:B:87:ALA:HB2	0.58	1.98	1	3
1:B:144:THR:HG23	1:B:145:PRO:HD2	0.58	1.76	2	3
1:C:144:THR:HG23	1:C:145:PRO:HD2	0.58	1.76	2	3
1:B:3:THR:O	1:C:157:GLN:HA	0.58	1.98	4	2
1:D:3:THR:O	1:E:157:GLN:HA	0.58	1.98	4	2
1:A:86:LEU:HD21	1:A:152:ALA:HB2	0.58	1.75	9	2
1:D:112:THR:HG22	1:D:117:THR:HG21	0.58	1.73	10	1
1:E:16:VAL:HG13	1:F:37:VAL:HG13	0.58	1.73	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:42:LEU:HD23	1:C:99:VAL:HG13	0.58	1.75	2	1
1:E:5:VAL:HG23	1:F:156:VAL:HG23	0.58	1.75	10	5
1:E:78:ILE:HB	1:E:87:ALA:HA	0.58	1.75	6	1
1:D:86:LEU:HD21	1:D:152:ALA:HB2	0.58	1.75	9	2
1:D:77:ALA:O	1:D:87:ALA:HB2	0.58	1.98	1	3
1:D:42:LEU:HD23	1:D:99:VAL:HG13	0.58	1.75	2	1
1:B:86:LEU:HD21	1:B:152:ALA:HB2	0.58	1.75	9	2
1:C:86:LEU:HG	1:C:113:LEU:HD13	0.58	1.75	2	3
1:E:77:ALA:O	1:E:87:ALA:HB2	0.58	1.99	1	3
1:A:42:LEU:HD23	1:A:99:VAL:HG13	0.58	1.75	2	1
1:A:90:SER:HA	1:D:52:VAL:HB	0.58	1.74	4	2
1:D:23:VAL:HA	1:D:58:LEU:HG	0.58	1.76	8	3
1:D:144:THR:HG23	1:D:145:PRO:HD2	0.58	1.76	2	3
1:C:111:LEU:HD21	1:C:117:THR:O	0.58	1.99	8	2
1:F:52:VAL:HG22	1:F:135:ALA:HB3	0.58	1.76	4	3
1:B:78:ILE:HB	1:B:87:ALA:HA	0.58	1.75	6	1
1:A:77:ALA:O	1:A:87:ALA:HB2	0.57	1.98	1	3
1:F:42:LEU:HD23	1:F:99:VAL:HG13	0.57	1.75	2	1
1:B:73:PHE:HD2	1:B:103:ILE:HD13	0.57	1.59	10	1
1:C:73:PHE:HD2	1:C:103:ILE:HD13	0.57	1.59	10	1
1:F:73:PHE:HD2	1:F:103:ILE:HD13	0.57	1.59	10	1
1:A:23:VAL:HA	1:A:58:LEU:HG	0.57	1.76	8	3
1:E:52:VAL:HG22	1:E:135:ALA:HB3	0.57	1.76	4	3
1:F:97:THR:H	1:F:144:THR:HB	0.57	1.58	4	2
1:E:73:PHE:HD2	1:E:103:ILE:HD13	0.57	1.59	10	1
1:A:86:LEU:HG	1:A:113:LEU:HD13	0.57	1.75	2	3
1:D:86:LEU:HG	1:D:113:LEU:HD13	0.57	1.75	2	3
1:E:23:VAL:HA	1:E:58:LEU:HG	0.57	1.76	8	3
1:A:111:LEU:HD21	1:A:117:THR:O	0.57	1.99	8	2
1:B:42:LEU:HD23	1:B:99:VAL:HG13	0.57	1.75	2	1
1:E:42:LEU:HD23	1:E:99:VAL:HG13	0.57	1.75	2	1
1:B:85:VAL:HA	1:B:102:GLN:HA	0.57	1.74	7	2
1:A:73:PHE:HD2	1:A:103:ILE:HD13	0.57	1.59	10	1
1:D:76:THR:O	1:D:86:LEU:HA	0.57	2.00	10	5
1:A:5:VAL:HG23	1:B:156:VAL:HG23	0.57	1.75	10	5
1:C:5:VAL:HG23	1:D:156:VAL:HG23	0.57	1.75	10	5
1:F:111:LEU:HD21	1:F:117:THR:O	0.57	1.99	8	2
1:E:106:ARG:HG3	1:E:132:PRO:HG2	0.57	1.77	2	4
1:E:16:VAL:HG11	1:F:144:THR:O	0.57	2.00	5	4
1:B:111:LEU:HD21	1:B:117:THR:O	0.57	1.99	8	2
1:B:52:VAL:HG22	1:B:135:ALA:HB3	0.57	1.77	4	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:4:THR:HG21	1:E:127:GLY:HA2	0.57	1.75	8	2
1:A:144:THR:HG23	1:A:145:PRO:HD2	0.57	1.76	2	3
1:B:23:VAL:HA	1:B:58:LEU:HG	0.57	1.76	8	3
1:B:106:ARG:HG3	1:B:132:PRO:HG2	0.57	1.77	2	4
1:D:52:VAL:HG22	1:D:135:ALA:HB3	0.57	1.76	4	3
1:E:13:LYS:HG2	1:F:33:GLN:HA	0.57	1.77	7	1
1:D:73:PHE:HD2	1:D:103:ILE:HD13	0.57	1.59	10	1
1:D:106:ARG:HG3	1:D:132:PRO:HG2	0.57	1.77	2	4
1:E:144:THR:HG23	1:E:145:PRO:HD2	0.57	1.76	2	3
1:E:111:LEU:HD21	1:E:117:THR:O	0.57	1.99	8	2
1:E:85:VAL:HA	1:E:102:GLN:HA	0.57	1.74	7	2
1:A:13:LYS:HG2	1:B:33:GLN:HA	0.57	1.77	7	1
1:B:74:LEU:HD11	1:E:57:GLN:HG2	0.57	1.77	7	1
1:A:76:THR:O	1:A:86:LEU:HA	0.56	2.00	10	5
1:A:106:ARG:HG3	1:A:132:PRO:HG2	0.56	1.77	2	4
1:F:23:VAL:HA	1:F:58:LEU:HG	0.56	1.76	8	3
1:A:16:VAL:HG11	1:B:144:THR:O	0.56	2.00	5	4
1:C:78:ILE:HB	1:C:87:ALA:HA	0.56	1.75	6	1
1:C:23:VAL:HA	1:C:58:LEU:HG	0.56	1.77	8	3
1:C:74:LEU:HD11	1:F:57:GLN:HG2	0.56	1.77	7	1
1:A:88:LEU:HG	1:A:95:SER:HB3	0.56	1.78	4	4
1:F:144:THR:HG23	1:F:145:PRO:HD2	0.56	1.76	2	3
1:D:111:LEU:HD21	1:D:117:THR:O	0.56	1.99	8	2
1:C:86:LEU:HD21	1:C:152:ALA:HB2	0.56	1.75	9	2
1:C:16:VAL:HG11	1:D:144:THR:O	0.56	2.00	5	4
1:F:78:ILE:HB	1:F:87:ALA:HA	0.56	1.75	6	1
1:D:13:LYS:HG2	1:E:33:GLN:HA	0.56	1.77	7	1
1:B:4:THR:HG21	1:F:127:GLY:HA2	0.56	1.75	8	2
1:C:86:LEU:HD11	1:C:152:ALA:HB2	0.56	1.78	8	1
1:D:88:LEU:HG	1:D:95:SER:HB3	0.56	1.78	4	4
1:D:5:VAL:HG23	1:E:156:VAL:HG23	0.56	1.75	10	5
1:D:16:VAL:HG11	1:E:144:THR:O	0.56	2.00	5	4
1:B:45:GLU:HA	1:B:140:THR:O	0.56	2.01	8	2
1:C:74:LEU:HD12	1:F:130:THR:OG1	0.56	2.01	9	2
1:F:86:LEU:HD21	1:F:152:ALA:HB2	0.56	1.75	9	2
1:F:86:LEU:HD11	1:F:152:ALA:HB2	0.56	1.78	8	1
1:A:76:THR:HA	1:D:132:PRO:HB3	0.56	1.77	4	4
1:C:23:VAL:HG12	1:D:36:GLN:HB2	0.56	1.78	2	1
1:A:45:GLU:HA	1:A:140:THR:O	0.56	2.01	8	2
1:C:52:VAL:HG22	1:C:135:ALA:HB3	0.56	1.76	4	3
1:B:76:THR:O	1:B:86:LEU:HA	0.56	2.00	10	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:76:THR:O	1:C:86:LEU:HA	0.56	2.00	10	5
1:E:76:THR:O	1:E:86:LEU:HA	0.56	2.00	10	5
1:D:45:GLU:HA	1:D:140:THR:O	0.56	2.01	8	3
1:F:45:GLU:HA	1:F:140:THR:O	0.56	2.01	8	2
1:F:76:THR:O	1:F:86:LEU:HA	0.56	2.00	10	5
1:A:74:LEU:HD12	1:D:130:THR:OG1	0.56	2.01	9	2
1:B:13:LYS:HG2	1:C:33:GLN:HA	0.56	1.77	7	1
1:C:45:GLU:HA	1:C:140:THR:O	0.56	2.01	8	2
1:A:74:LEU:HD11	1:A:155:LYS:HG2	0.56	1.78	6	1
1:C:74:LEU:HD11	1:C:155:LYS:HG2	0.56	1.78	6	1
1:B:16:VAL:HG11	1:C:144:THR:O	0.56	2.00	5	4
1:D:74:LEU:HD11	1:D:155:LYS:HG2	0.56	1.78	6	1
1:A:74:LEU:HD11	1:D:57:GLN:HG2	0.56	1.77	7	1
1:D:88:LEU:HD22	1:D:96:ALA:O	0.56	2.01	7	1
1:E:88:LEU:HG	1:E:95:SER:HB3	0.55	1.78	4	4
1:F:74:LEU:HD11	1:F:155:LYS:HG2	0.55	1.78	6	1
1:B:74:LEU:HD12	1:E:130:THR:OG1	0.55	2.01	9	2
1:F:88:LEU:HD22	1:F:96:ALA:O	0.55	2.01	7	1
1:C:56:ILE:O	1:C:56:ILE:HG23	0.55	2.02	4	5
1:B:88:LEU:HD22	1:B:96:ALA:O	0.55	2.01	7	1
1:C:13:LYS:HG2	1:D:33:GLN:HA	0.55	1.77	7	1
1:B:76:THR:HA	1:E:132:PRO:HB3	0.55	1.77	4	4
1:B:88:LEU:HG	1:B:95:SER:HB3	0.55	1.78	4	4
1:C:88:LEU:HG	1:C:95:SER:HB3	0.55	1.78	4	4
1:C:106:ARG:HG3	1:C:132:PRO:HG2	0.55	1.77	2	4
1:F:56:ILE:HG23	1:F:56:ILE:O	0.55	2.02	4	5
1:F:104:LEU:HD13	1:F:134:GLN:NE2	0.55	2.17	1	1
1:E:45:GLU:HA	1:E:140:THR:O	0.55	2.01	8	3
1:E:88:LEU:HD22	1:E:96:ALA:O	0.55	2.01	7	1
1:A:9:THR:HG22	1:B:153:THR:CG2	0.55	2.30	2	1
1:A:52:VAL:HG22	1:A:135:ALA:HB3	0.55	1.76	4	3
1:D:86:LEU:HD11	1:D:152:ALA:HB2	0.55	1.78	8	1
1:D:4:THR:HG23	1:E:157:GLN:HG3	0.55	1.79	8	2
1:B:56:ILE:HG23	1:B:56:ILE:O	0.55	2.02	4	5
1:E:56:ILE:HG23	1:E:56:ILE:O	0.55	2.02	4	5
1:D:84:ASN:HA	1:D:113:LEU:HD13	0.55	1.79	9	1
1:F:106:ARG:HG3	1:F:132:PRO:HG2	0.55	1.77	2	4
1:B:104:LEU:HD13	1:B:134:GLN:NE2	0.55	2.17	1	1
1:C:104:LEU:HD13	1:C:134:GLN:NE2	0.55	2.17	1	1
1:F:88:LEU:HG	1:F:95:SER:HB3	0.55	1.78	4	4
1:B:74:LEU:HD11	1:B:155:LYS:HG2	0.55	1.78	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:86:LEU:HD11	1:A:152:ALA:HB2	0.55	1.78	8	1
1:A:84:ASN:HA	1:A:113:LEU:HD13	0.55	1.79	9	1
1:A:104:LEU:HD13	1:A:134:GLN:NE2	0.55	2.17	1	1
1:B:9:THR:HG22	1:C:153:THR:CG2	0.55	2.31	2	1
1:E:23:VAL:HG12	1:F:36:GLN:HB2	0.55	1.78	2	1
1:B:4:THR:HG23	1:C:157:GLN:HG3	0.55	1.79	8	2
1:E:74:LEU:HD11	1:E:155:LYS:HG2	0.55	1.79	6	1
1:B:84:ASN:HA	1:B:113:LEU:HD13	0.55	1.79	9	1
1:E:104:LEU:HD13	1:E:134:GLN:NE2	0.54	2.17	1	1
1:A:88:LEU:HD22	1:A:96:ALA:O	0.54	2.01	7	1
1:C:88:LEU:HD22	1:C:96:ALA:O	0.54	2.01	7	1
1:E:84:ASN:HA	1:E:113:LEU:HD13	0.54	1.79	9	1
1:C:76:THR:HA	1:F:132:PRO:HB3	0.54	1.77	4	4
1:D:104:LEU:HD13	1:D:134:GLN:NE2	0.54	2.17	1	1
1:B:23:VAL:HG12	1:C:36:GLN:HB2	0.54	1.78	2	1
1:A:4:THR:HG23	1:B:157:GLN:HG3	0.54	1.79	8	2
1:E:42:LEU:HD23	1:E:139:ALA:HB2	0.54	1.79	4	2
1:E:70:ALA:HB3	1:E:157:GLN:HB3	0.54	1.80	7	2
1:A:23:VAL:HG12	1:B:36:GLN:HB2	0.54	1.78	2	1
1:D:42:LEU:HD23	1:D:139:ALA:HB2	0.54	1.79	4	2
1:A:56:ILE:HG21	1:A:154:PHE:CZ	0.54	2.38	7	1
1:D:23:VAL:HG12	1:E:36:GLN:HB2	0.54	1.78	2	1
1:C:4:THR:HG23	1:D:157:GLN:HG3	0.54	1.79	8	2
1:C:78:ILE:CG2	1:C:85:VAL:HB	0.54	2.33	3	2
1:D:56:ILE:HG21	1:D:154:PHE:CZ	0.54	2.38	7	1
1:E:4:THR:HG23	1:F:157:GLN:HG3	0.54	1.79	8	2
1:D:73:PHE:CD2	1:D:103:ILE:HD13	0.54	2.38	10	1
1:D:70:ALA:HB3	1:D:157:GLN:HB3	0.54	1.80	7	3
1:C:56:ILE:HG21	1:C:154:PHE:CZ	0.54	2.38	7	1
1:F:56:ILE:HG21	1:F:154:PHE:CZ	0.54	2.38	7	1
1:E:131:ILE:HD11	1:E:156:VAL:HG12	0.54	1.80	10	2
1:D:59:ASN:HA	1:D:128:THR:HA	0.54	1.80	8	3
1:F:78:ILE:CG2	1:F:85:VAL:HB	0.54	2.33	3	2
1:A:113:LEU:N	1:A:113:LEU:HD12	0.54	2.18	7	1
1:B:86:LEU:HD11	1:B:152:ALA:HB2	0.54	1.78	8	1
1:A:73:PHE:CD2	1:A:103:ILE:HD13	0.54	2.38	10	1
1:B:80:ALA:HB1	1:E:105:ASP:O	0.54	2.03	1	1
1:F:42:LEU:HD23	1:F:139:ALA:HB2	0.54	1.79	4	2
1:B:43:ALA:HA	1:B:142:ALA:HA	0.54	1.80	6	2
1:B:113:LEU:N	1:B:113:LEU:HD12	0.54	2.18	7	1
1:B:70:ALA:HB3	1:B:157:GLN:HB3	0.54	1.80	7	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:59:ASN:HA	1:C:128:THR:HA	0.54	1.80	8	3
1:B:42:LEU:HD23	1:B:139:ALA:HB2	0.54	1.79	4	2
1:B:78:ILE:CG2	1:B:85:VAL:HB	0.54	2.33	3	2
1:E:78:ILE:CG2	1:E:85:VAL:HB	0.54	2.33	3	2
1:D:43:ALA:HA	1:D:142:ALA:HA	0.54	1.80	6	1
1:F:113:LEU:N	1:F:113:LEU:HD12	0.54	2.18	7	1
1:E:86:LEU:HD11	1:E:152:ALA:HB2	0.54	1.78	8	1
1:D:56:ILE:HG23	1:D:56:ILE:O	0.54	2.02	4	5
1:A:42:LEU:HD23	1:A:139:ALA:HB2	0.54	1.79	4	2
1:D:78:ILE:CG2	1:D:85:VAL:HB	0.54	2.33	3	2
1:C:84:ASN:HA	1:C:113:LEU:HD13	0.54	1.79	9	1
1:A:56:ILE:HG23	1:A:56:ILE:O	0.53	2.02	4	5
1:A:70:ALA:HB3	1:A:157:GLN:HB3	0.53	1.80	7	3
1:A:80:ALA:HB1	1:D:105:ASP:O	0.53	2.03	1	1
1:E:59:ASN:HA	1:E:128:THR:HA	0.53	1.80	8	3
1:C:42:LEU:HD23	1:C:139:ALA:HB2	0.53	1.79	4	2
1:D:113:LEU:N	1:D:113:LEU:HD12	0.53	2.18	7	1
1:D:131:ILE:HD11	1:D:156:VAL:HG12	0.53	1.80	10	2
1:F:84:ASN:HA	1:F:113:LEU:HD13	0.53	1.79	9	1
1:B:11:HIS:HA	1:C:151:ASP:OD1	0.53	2.03	2	1
1:D:9:THR:HG22	1:E:153:THR:CG2	0.53	2.30	2	1
1:E:20:ALA:HB1	1:E:124:LEU:CD2	0.53	2.34	3	1
1:E:42:LEU:HB3	1:E:143:ALA:HB2	0.53	1.80	4	1
1:B:90:SER:HA	1:E:52:VAL:CG1	0.53	2.33	6	1
1:B:72:ALA:HB3	1:B:155:LYS:CB	0.53	2.33	7	1
1:E:73:PHE:CD2	1:E:103:ILE:HD13	0.53	2.38	10	1
1:C:80:ALA:HB1	1:F:105:ASP:O	0.53	2.03	1	1
1:A:82:HIS:O	1:A:84:ASN:N	0.53	2.42	6	1
1:B:82:HIS:O	1:B:84:ASN:N	0.53	2.42	6	1
1:C:90:SER:HA	1:F:52:VAL:CG1	0.53	2.33	6	1
1:F:72:ALA:HB3	1:F:155:LYS:CB	0.53	2.33	7	1
1:F:69:ALA:HB3	1:F:122:THR:O	0.53	2.04	2	1
1:D:82:HIS:O	1:D:84:ASN:N	0.53	2.42	6	1
1:A:72:ALA:HB3	1:A:155:LYS:CB	0.53	2.33	7	1
1:B:56:ILE:HG21	1:B:154:PHE:CZ	0.53	2.38	7	1
1:D:72:ALA:HB3	1:D:155:LYS:CB	0.53	2.33	7	1
1:E:56:ILE:HG21	1:E:154:PHE:CZ	0.53	2.38	7	1
1:E:72:ALA:HB3	1:E:155:LYS:CB	0.53	2.33	7	1
1:B:73:PHE:CD2	1:B:103:ILE:HD13	0.53	2.38	10	1
1:C:73:PHE:CD2	1:C:103:ILE:HD13	0.53	2.38	10	1
1:F:73:PHE:CD2	1:F:103:ILE:HD13	0.53	2.38	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:ALA:HB1	1:A:124:LEU:CD2	0.53	2.34	3	1
1:D:20:ALA:HB1	1:D:124:LEU:CD2	0.53	2.34	3	1
1:D:102:GLN:HB2	1:D:138:PHE:CD1	0.53	2.39	5	1
1:A:155:LYS:NZ	1:D:128:THR:HG21	0.53	2.19	7	1
1:F:70:ALA:HB3	1:F:157:GLN:HB3	0.53	1.80	7	3
1:B:20:ALA:HB1	1:B:124:LEU:CD2	0.53	2.34	3	1
1:C:72:ALA:HB3	1:C:155:LYS:CB	0.53	2.33	7	1
1:C:113:LEU:HD12	1:C:113:LEU:N	0.53	2.18	7	1
1:B:69:ALA:HB3	1:B:122:THR:O	0.53	2.04	2	1
1:A:78:ILE:CG2	1:A:85:VAL:HB	0.53	2.33	3	2
1:D:42:LEU:HB3	1:D:143:ALA:HB2	0.53	1.80	4	1
1:B:102:GLN:HB2	1:B:138:PHE:CD1	0.53	2.39	5	1
1:E:102:GLN:HB2	1:E:138:PHE:CD1	0.53	2.39	5	1
1:E:82:HIS:O	1:E:84:ASN:N	0.53	2.42	6	1
1:B:19:ALA:O	1:B:65:VAL:HG21	0.53	2.04	10	1
1:A:11:HIS:HA	1:B:151:ASP:OD1	0.53	2.03	2	1
1:C:69:ALA:HB3	1:C:122:THR:O	0.53	2.04	2	1
1:B:116:ALA:HB2	1:E:129:ASN:HA	0.53	1.80	5	1
1:E:43:ALA:HA	1:E:142:ALA:HA	0.53	1.80	6	1
1:C:155:LYS:NZ	1:F:128:THR:HG21	0.53	2.19	7	1
1:E:19:ALA:O	1:E:65:VAL:HG21	0.53	2.04	10	1
1:C:43:ALA:HA	1:C:142:ALA:HA	0.53	1.80	6	2
1:C:116:ALA:HB2	1:F:129:ASN:HA	0.53	1.80	5	1
1:F:43:ALA:HA	1:F:142:ALA:HA	0.53	1.80	6	2
1:F:102:GLN:HB2	1:F:138:PHE:CD1	0.53	2.39	5	1
1:C:70:ALA:HB3	1:C:157:GLN:HB3	0.53	1.80	7	2
1:B:59:ASN:HA	1:B:128:THR:HA	0.53	1.80	8	3
1:E:11:HIS:HA	1:F:151:ASP:OD1	0.53	2.03	2	1
1:C:42:LEU:HB3	1:C:143:ALA:HB2	0.53	1.80	4	1
1:B:158:TYR:C	1:B:159:GLN:HG3	0.52	2.30	3	1
1:C:19:ALA:HA	1:D:38:ARG:HG2	0.52	1.80	7	1
1:D:19:ALA:HA	1:E:38:ARG:HG2	0.52	1.80	7	1
1:E:113:LEU:HD12	1:E:113:LEU:N	0.52	2.18	7	1
1:C:9:THR:HG22	1:D:153:THR:CG2	0.52	2.30	2	1
1:E:69:ALA:HB3	1:E:122:THR:O	0.52	2.04	2	1
1:A:42:LEU:HB3	1:A:143:ALA:HB2	0.52	1.80	4	1
1:A:102:GLN:HB2	1:A:138:PHE:CD1	0.52	2.39	5	1
1:A:131:ILE:HD11	1:A:156:VAL:HG12	0.52	1.80	10	2
1:C:11:HIS:HA	1:D:151:ASP:OD1	0.52	2.03	2	1
1:D:11:HIS:HA	1:E:151:ASP:OD1	0.52	2.04	2	1
1:D:70:ALA:HB1	1:D:118:PHE:HB3	0.52	1.81	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:85:VAL:HB	1:A:100:GLY:HA3	0.52	1.82	5	1
1:C:102:GLN:HB2	1:C:138:PHE:CD1	0.52	2.39	5	1
1:A:43:ALA:HA	1:A:142:ALA:HA	0.52	1.80	6	1
1:A:90:SER:HA	1:D:52:VAL:CG1	0.52	2.33	6	1
1:B:155:LYS:NZ	1:E:128:THR:HG21	0.52	2.19	7	1
1:F:131:ILE:HD11	1:F:156:VAL:HG12	0.52	1.80	10	1
1:C:70:ALA:HB1	1:C:118:PHE:HB3	0.52	1.81	3	1
1:B:19:ALA:HA	1:C:38:ARG:HG2	0.52	1.80	7	1
1:E:71:VAL:CG1	1:E:131:ILE:HG21	0.52	2.35	1	1
1:A:78:ILE:O	1:D:134:GLN:HG2	0.52	2.05	5	1
1:A:59:ASN:HA	1:A:128:THR:HA	0.52	1.80	8	3
1:A:69:ALA:HB3	1:A:122:THR:O	0.52	2.04	2	1
1:E:9:THR:HG22	1:F:153:THR:CG2	0.52	2.30	2	1
1:A:70:ALA:HB1	1:A:118:PHE:HB3	0.52	1.81	3	1
1:C:158:TYR:C	1:C:159:GLN:HG3	0.52	2.30	3	1
1:B:42:LEU:HB3	1:B:143:ALA:HB2	0.52	1.80	4	1
1:F:82:HIS:O	1:F:84:ASN:N	0.52	2.42	6	1
1:C:6:ASN:HA	1:D:155:LYS:HE2	0.52	1.81	9	1
1:A:19:ALA:O	1:A:65:VAL:HG21	0.52	2.04	10	1
1:D:69:ALA:HB3	1:D:122:THR:O	0.52	2.04	2	1
1:A:19:ALA:HA	1:B:38:ARG:HG2	0.52	1.81	7	1
1:E:19:ALA:HA	1:F:38:ARG:HG2	0.52	1.80	7	1
1:C:19:ALA:O	1:C:65:VAL:HG21	0.52	2.04	10	1
1:F:19:ALA:O	1:F:65:VAL:HG21	0.52	2.04	10	1
1:B:71:VAL:CG1	1:B:131:ILE:HG21	0.52	2.35	1	1
1:A:158:TYR:C	1:A:159:GLN:HG3	0.52	2.30	3	1
1:C:20:ALA:HB1	1:C:124:LEU:CD2	0.52	2.34	3	1
1:A:116:ALA:HB2	1:D:129:ASN:HA	0.52	1.80	5	1
1:B:78:ILE:O	1:E:134:GLN:HG2	0.52	2.05	5	1
1:C:82:HIS:O	1:C:84:ASN:N	0.52	2.42	6	1
1:B:131:ILE:HD11	1:B:156:VAL:HG12	0.52	1.80	10	2
1:A:6:ASN:HA	1:B:155:LYS:HE2	0.52	1.81	9	1
1:D:39:THR:HA	1:D:143:ALA:HB3	0.52	1.82	3	1
1:C:131:ILE:HD11	1:C:156:VAL:HG12	0.52	1.80	10	1
1:D:19:ALA:O	1:D:65:VAL:HG21	0.52	2.04	10	1
1:F:20:ALA:HB1	1:F:124:LEU:CD2	0.52	2.34	3	1
1:F:42:LEU:HB3	1:F:143:ALA:HB2	0.52	1.80	4	1
1:C:101:VAL:HG22	1:C:137:TYR:CE1	0.52	2.41	5	1
1:C:71:VAL:CG1	1:C:131:ILE:HG21	0.51	2.35	1	1
1:F:71:VAL:CG1	1:F:131:ILE:HG21	0.51	2.35	1	1
1:F:59:ASN:HA	1:F:128:THR:HA	0.51	1.80	8	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:F:158:TYR:C	1:F:159:GLN:HG3	0.51	2.30	3	1
1:D:101:VAL:HG22	1:D:137:TYR:CE1	0.51	2.41	5	1
1:E:85:VAL:HB	1:E:100:GLY:HA3	0.51	1.82	5	1
1:F:70:ALA:HB1	1:F:118:PHE:HB3	0.51	1.81	3	1
1:B:88:LEU:HB3	1:B:148:ALA:HA	0.51	1.83	5	1
1:B:83:THR:HG21	1:B:114:ASP:OD1	0.51	2.05	8	1
1:A:71:VAL:CG1	1:A:131:ILE:HG21	0.51	2.35	1	1
1:A:101:VAL:HG22	1:A:137:TYR:CE1	0.51	2.40	5	1
1:C:78:ILE:O	1:F:134:GLN:HG2	0.51	2.05	5	1
1:C:85:VAL:HB	1:C:100:GLY:HA3	0.51	1.82	5	1
1:C:83:THR:HG21	1:C:114:ASP:OD1	0.51	2.05	8	1
1:C:86:LEU:HD23	1:C:87:ALA:N	0.51	2.21	10	1
1:E:39:THR:HA	1:E:143:ALA:HB3	0.51	1.81	3	1
1:A:24:ASP:O	1:A:28:VAL:HG23	0.51	2.06	6	3
1:F:24:ASP:O	1:F:28:VAL:HG23	0.51	2.06	6	3
1:F:101:VAL:HG22	1:F:137:TYR:CE1	0.51	2.41	5	1
1:F:39:THR:HA	1:F:143:ALA:HB3	0.51	1.82	3	1
1:B:48:THR:HA	1:B:137:TYR:O	0.51	2.06	5	1
1:D:48:THR:HA	1:D:137:TYR:O	0.51	2.06	5	1
1:F:83:THR:HG21	1:F:114:ASP:OD1	0.51	2.05	8	1
1:D:6:ASN:HA	1:E:155:LYS:HE2	0.51	1.82	9	1
1:B:5:VAL:HG23	1:C:156:VAL:HG22	0.51	1.83	1	1
1:D:71:VAL:CG1	1:D:131:ILE:HG21	0.51	2.35	1	1
1:E:158:TYR:C	1:E:159:GLN:HG3	0.51	2.30	3	1
1:E:101:VAL:HG22	1:E:137:TYR:CE1	0.51	2.41	5	1
1:E:15:GLU:HB3	1:F:36:GLN:HG3	0.51	1.83	8	1
1:F:112:THR:HB	1:F:117:THR:HG21	0.51	1.82	9	1
1:C:144:THR:HG22	1:C:145:PRO:CD	0.51	2.36	2	1
1:A:48:THR:HA	1:A:137:TYR:O	0.51	2.06	5	1
1:B:85:VAL:HB	1:B:100:GLY:HA3	0.51	1.82	5	1
1:C:124:LEU:HG	1:C:129:ASN:ND2	0.51	2.21	5	1
1:E:88:LEU:HB3	1:E:148:ALA:HA	0.51	1.83	5	1
1:F:85:VAL:HB	1:F:100:GLY:HA3	0.51	1.82	5	1
1:D:83:THR:HG21	1:D:114:ASP:OD1	0.51	2.05	8	1
1:E:83:THR:HG21	1:E:114:ASP:OD1	0.51	2.05	8	1
1:E:6:ASN:HA	1:F:155:LYS:HE2	0.51	1.81	9	1
1:E:70:ALA:HB1	1:E:118:PHE:HB3	0.51	1.81	3	1
1:B:90:SER:O	1:E:52:VAL:HG22	0.51	2.06	5	1
1:D:24:ASP:O	1:D:28:VAL:HG23	0.51	2.06	6	3
1:A:83:THR:HG21	1:A:114:ASP:OD1	0.51	2.05	8	1
1:D:91:SER:HA	1:F:25:ALA:HB2	0.51	1.83	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:112:THR:HB	1:A:117:THR:HG21	0.51	1.82	9	1
1:B:6:ASN:HA	1:C:155:LYS:HE2	0.51	1.82	9	1
1:B:112:THR:HB	1:B:117:THR:HG21	0.51	1.82	9	1
1:E:86:LEU:HD23	1:E:87:ALA:N	0.51	2.21	10	1
1:E:91:SER:O	1:E:95:SER:HB2	0.50	2.06	4	3
1:D:144:THR:HG22	1:D:145:PRO:CD	0.50	2.36	2	1
1:C:22:ALA:HA	1:D:36:GLN:HB2	0.50	1.84	5	1
1:C:90:SER:O	1:F:52:VAL:HG22	0.50	2.06	5	1
1:D:85:VAL:HB	1:D:100:GLY:HA3	0.50	1.82	5	1
1:E:124:LEU:HG	1:E:129:ASN:ND2	0.50	2.21	5	1
1:B:114:ASP:O	1:E:130:THR:O	0.50	2.28	6	1
1:C:45:GLU:N	1:C:141:GLY:HA2	0.50	2.22	6	1
1:A:91:SER:HA	1:C:25:ALA:HB2	0.50	1.83	8	1
1:D:86:LEU:HD23	1:D:87:ALA:N	0.50	2.21	10	1
1:B:39:THR:HA	1:B:143:ALA:HB3	0.50	1.81	3	1
1:B:62:ASP:OD2	1:B:65:VAL:HG23	0.50	2.07	3	1
1:E:45:GLU:N	1:E:141:GLY:HA2	0.50	2.22	6	1
1:C:112:THR:HB	1:C:117:THR:HG21	0.50	1.82	9	1
1:B:86:LEU:HD23	1:B:87:ALA:N	0.50	2.21	10	1
1:D:158:TYR:C	1:D:159:GLN:HG3	0.50	2.30	3	1
1:A:114:ASP:O	1:D:130:THR:O	0.50	2.28	6	1
1:C:114:ASP:O	1:F:130:THR:O	0.50	2.28	6	1
1:F:69:ALA:CB	1:F:124:LEU:HD13	0.50	2.36	8	1
1:A:86:LEU:HD23	1:A:87:ALA:N	0.50	2.21	10	1
1:B:15:GLU:HB3	1:C:36:GLN:HG3	0.50	1.83	8	2
1:B:101:VAL:HG22	1:B:137:TYR:CE1	0.50	2.41	5	1
1:D:124:LEU:HG	1:D:129:ASN:ND2	0.50	2.21	5	1
1:E:48:THR:HA	1:E:137:TYR:O	0.50	2.06	5	1
1:F:86:LEU:HD23	1:F:87:ALA:N	0.50	2.21	10	1
1:C:91:SER:O	1:C:95:SER:HB2	0.50	2.06	4	3
1:B:24:ASP:O	1:B:28:VAL:HG23	0.50	2.06	6	3
1:D:45:GLU:N	1:D:141:GLY:HA2	0.50	2.22	6	1
1:D:112:THR:HB	1:D:117:THR:HG21	0.50	1.82	9	1
1:A:91:SER:O	1:A:95:SER:HB2	0.50	2.07	4	3
1:B:15:GLU:HG2	1:C:146:GLY:O	0.50	2.07	3	1
1:C:39:THR:HA	1:C:143:ALA:HB3	0.50	1.81	3	1
1:A:124:LEU:HG	1:A:129:ASN:ND2	0.50	2.21	5	1
1:F:48:THR:HA	1:F:137:TYR:O	0.50	2.06	5	1
1:E:112:THR:HB	1:E:117:THR:HG21	0.50	1.82	9	1
1:A:5:VAL:HG23	1:B:156:VAL:HG22	0.50	1.83	1	1
1:A:39:THR:HA	1:A:143:ALA:HB3	0.50	1.81	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:D:62:ASP:OD2	1:D:65:VAL:HG23	0.50	2.07	3	1
1:C:88:LEU:HB3	1:C:148:ALA:HA	0.50	1.83	5	1
1:A:45:GLU:N	1:A:141:GLY:HA2	0.50	2.22	6	1
1:E:5:VAL:HG23	1:F:156:VAL:HG22	0.50	1.83	1	1
1:E:62:ASP:OD2	1:E:65:VAL:HG23	0.50	2.07	3	1
1:A:22:ALA:HA	1:B:36:GLN:HB2	0.50	1.83	5	1
1:A:15:GLU:HB3	1:B:36:GLN:HG3	0.50	1.83	8	1
1:B:91:SER:HA	1:D:25:ALA:HB2	0.50	1.83	8	1
1:B:91:SER:O	1:B:95:SER:HB2	0.50	2.07	4	2
1:B:124:LEU:HG	1:B:129:ASN:ND2	0.50	2.21	5	1
1:D:22:ALA:HA	1:E:36:GLN:HB2	0.50	1.83	5	1
1:F:124:LEU:HG	1:F:129:ASN:ND2	0.50	2.21	5	1
1:C:24:ASP:O	1:C:28:VAL:HG23	0.49	2.06	6	3
1:C:91:SER:HA	1:E:25:ALA:HB2	0.49	1.83	8	1
1:F:91:SER:O	1:F:95:SER:HB2	0.49	2.06	4	3
1:A:9:THR:CG2	1:B:153:THR:HG23	0.49	2.31	3	1
1:C:48:THR:HA	1:C:137:TYR:O	0.49	2.06	5	1
1:D:88:LEU:HB3	1:D:148:ALA:HA	0.49	1.83	5	1
1:E:22:ALA:HA	1:F:36:GLN:HB2	0.49	1.83	5	1
1:B:42:LEU:HD21	1:B:137:TYR:HB3	0.49	1.83	2	1
1:B:144:THR:HG22	1:B:145:PRO:CD	0.49	2.36	2	1
1:D:42:LEU:HD21	1:D:137:TYR:HB3	0.49	1.83	2	1
1:E:42:LEU:HD21	1:E:137:TYR:HB3	0.49	1.83	2	1
1:F:144:THR:HG22	1:F:145:PRO:CD	0.49	2.36	2	1
1:A:90:SER:O	1:D:52:VAL:HG22	0.49	2.06	5	1
1:E:24:ASP:O	1:E:28:VAL:HG23	0.49	2.06	6	3
1:F:39:THR:HA	1:F:42:LEU:HD12	0.49	1.84	6	1
1:A:17:VAL:HG21	1:A:21:CYS:O	0.49	2.07	7	1
1:B:4:THR:HG21	1:F:127:GLY:CA	0.49	2.37	8	1
1:F:69:ALA:HA	1:F:157:GLN:O	0.49	2.08	10	1
1:B:70:ALA:HB1	1:B:118:PHE:HB3	0.49	1.81	3	1
1:C:9:THR:CG2	1:D:153:THR:HG23	0.49	2.31	3	1
1:E:15:GLU:HG2	1:F:146:GLY:O	0.49	2.07	3	1
1:C:39:THR:HA	1:C:42:LEU:HD12	0.49	1.85	6	1
1:C:19:ALA:O	1:C:62:ASP:HB2	0.49	2.08	8	1
1:A:69:ALA:HA	1:A:157:GLN:O	0.49	2.08	10	1
1:D:69:ALA:HA	1:D:157:GLN:O	0.49	2.08	10	1
1:E:5:VAL:HG23	1:F:156:VAL:CG2	0.49	2.38	1	1
1:E:21:CYS:HB2	1:E:158:TYR:CE1	0.49	2.43	2	3
1:F:21:CYS:HB2	1:F:158:TYR:CE1	0.49	2.43	2	3
1:D:57:GLN:HA	1:D:130:THR:HG22	0.49	1.84	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:F:45:GLU:N	1:F:141:GLY:HA2	0.49	2.22	6	1
1:D:73:PHE:HB2	1:D:111:LEU:HD11	0.49	1.84	7	1
1:B:69:ALA:HA	1:B:157:GLN:O	0.49	2.08	10	1
1:A:5:VAL:HG23	1:B:156:VAL:CG2	0.49	2.38	1	1
1:F:42:LEU:HD21	1:F:137:TYR:HB3	0.49	1.83	2	1
1:A:62:ASP:OD2	1:A:65:VAL:HG23	0.49	2.07	3	1
1:D:9:THR:CG2	1:E:153:THR:HG23	0.49	2.31	3	1
1:C:71:VAL:O	1:C:118:PHE:HA	0.49	2.08	4	1
1:F:88:LEU:HB3	1:F:148:ALA:HA	0.49	1.83	5	1
1:B:45:GLU:N	1:B:141:GLY:HA2	0.49	2.22	6	1
1:D:72:ALA:HB1	1:D:116:ALA:HA	0.49	1.85	6	1
1:C:17:VAL:HG21	1:C:21:CYS:O	0.49	2.07	7	1
1:E:17:VAL:HG21	1:E:21:CYS:O	0.49	2.07	7	1
1:F:19:ALA:O	1:F:62:ASP:HB2	0.49	2.08	8	1
1:C:5:VAL:HG23	1:D:156:VAL:CG2	0.49	2.38	1	1
1:C:62:ASP:OD2	1:C:65:VAL:HG23	0.49	2.07	3	1
1:E:71:VAL:O	1:E:118:PHE:HA	0.49	2.08	4	1
1:F:71:VAL:O	1:F:118:PHE:HA	0.49	2.08	4	1
1:D:19:ALA:O	1:D:62:ASP:HB2	0.49	2.08	8	1
1:C:69:ALA:HA	1:C:157:GLN:O	0.49	2.08	10	1
1:B:21:CYS:HB2	1:B:158:TYR:CE1	0.49	2.43	2	3
1:C:15:GLU:HG2	1:D:146:GLY:O	0.49	2.07	3	1
1:F:62:ASP:OD2	1:F:65:VAL:HG23	0.49	2.07	3	1
1:D:71:VAL:O	1:D:118:PHE:HA	0.49	2.08	4	1
1:B:22:ALA:HA	1:C:36:GLN:HB2	0.49	1.83	5	1
1:B:72:ALA:HB1	1:B:116:ALA:HA	0.49	1.84	6	1
1:C:57:GLN:HA	1:C:130:THR:HG22	0.49	1.84	6	1
1:A:73:PHE:HB2	1:A:111:LEU:HD11	0.49	1.84	7	1
1:E:69:ALA:CB	1:E:124:LEU:HD13	0.49	2.36	8	1
1:B:56:ILE:HG21	1:B:131:ILE:HD12	0.49	1.85	10	1
1:E:56:ILE:HG21	1:E:131:ILE:HD12	0.49	1.85	10	1
1:E:69:ALA:HA	1:E:157:GLN:O	0.49	2.08	10	1
1:C:5:VAL:HG23	1:D:156:VAL:HG22	0.49	1.83	1	1
1:A:144:THR:HG22	1:A:145:PRO:CD	0.49	2.36	2	1
1:C:21:CYS:HB2	1:C:158:TYR:CE1	0.49	2.43	2	3
1:B:56:ILE:O	1:B:58:LEU:HD12	0.49	2.08	5	1
1:E:56:ILE:O	1:E:58:LEU:HD12	0.49	2.08	5	1
1:A:39:THR:HA	1:A:42:LEU:HD12	0.49	1.85	6	1
1:D:39:THR:HA	1:D:42:LEU:HD12	0.49	1.85	6	1
1:D:56:ILE:O	1:D:130:THR:HA	0.49	2.08	6	1
1:D:15:GLU:HB3	1:E:36:GLN:HG3	0.49	1.83	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:D:69:ALA:CB	1:D:124:LEU:HD13	0.49	2.36	8	1
1:B:5:VAL:HG23	1:C:156:VAL:CG2	0.49	2.38	1	1
1:B:69:ALA:HB3	1:B:122:THR:HB	0.49	1.85	1	2
1:D:5:VAL:HG23	1:E:156:VAL:CG2	0.49	2.38	1	1
1:D:91:SER:O	1:D:95:SER:HB2	0.49	2.07	4	3
1:A:42:LEU:HD21	1:A:137:TYR:HB3	0.49	1.83	2	1
1:E:144:THR:HG22	1:E:145:PRO:CD	0.49	2.36	2	1
1:A:88:LEU:HB3	1:A:148:ALA:HA	0.49	1.83	5	1
1:A:56:ILE:O	1:A:130:THR:HA	0.49	2.08	6	1
1:A:19:ALA:O	1:A:62:ASP:HB2	0.49	2.08	8	1
1:E:19:ALA:O	1:E:62:ASP:HB2	0.49	2.08	8	1
1:A:79:ASP:O	1:A:81:GLY:N	0.49	2.46	10	1
1:C:79:ASP:O	1:C:81:GLY:N	0.49	2.46	10	1
1:A:21:CYS:HB2	1:A:158:TYR:CE1	0.48	2.43	2	2
1:C:42:LEU:HB2	1:C:139:ALA:HB2	0.48	1.84	6	1
1:A:20:ALA:O	1:A:124:LEU:HD21	0.48	2.08	3	2
1:B:20:ALA:O	1:B:124:LEU:HD21	0.48	2.08	3	2
1:A:15:GLU:HG2	1:B:146:GLY:O	0.48	2.07	3	1
1:A:103:ILE:HD12	1:A:111:LEU:HB3	0.48	1.86	3	1
1:C:15:GLU:HB3	1:D:36:GLN:HG3	0.48	1.83	8	2
1:A:56:ILE:O	1:A:58:LEU:HD12	0.48	2.08	5	1
1:F:57:GLN:HA	1:F:130:THR:HG22	0.48	1.84	6	1
1:B:79:ASP:O	1:B:81:GLY:N	0.48	2.46	10	1
1:F:56:ILE:HG21	1:F:131:ILE:HD12	0.48	1.85	10	1
1:F:79:ASP:O	1:F:81:GLY:N	0.48	2.46	10	1
1:D:5:VAL:HG23	1:E:156:VAL:HG22	0.48	1.83	1	1
1:D:15:GLU:HG2	1:E:146:GLY:O	0.48	2.07	3	1
1:C:56:ILE:O	1:C:58:LEU:HD12	0.48	2.08	5	1
1:D:56:ILE:O	1:D:58:LEU:HD12	0.48	2.08	5	1
1:C:16:VAL:HA	1:D:37:VAL:O	0.48	2.09	6	1
1:D:16:VAL:HA	1:E:37:VAL:O	0.48	2.09	6	1
1:D:42:LEU:HB2	1:D:139:ALA:HB2	0.48	1.84	6	1
1:D:17:VAL:HG21	1:D:21:CYS:O	0.48	2.07	7	1
1:D:78:ILE:HG23	1:D:79:ASP:N	0.48	2.24	1	2
1:D:20:ALA:O	1:D:124:LEU:HD21	0.48	2.08	3	2
1:F:20:ALA:O	1:F:124:LEU:HD21	0.48	2.08	3	2
1:D:103:ILE:HD12	1:D:111:LEU:HB3	0.48	1.86	3	1
1:B:71:VAL:O	1:B:118:PHE:HA	0.48	2.08	4	1
1:A:16:VAL:HA	1:B:37:VAL:O	0.48	2.09	6	1
1:A:4:THR:HG21	1:E:127:GLY:CA	0.48	2.37	8	1
1:D:79:ASP:O	1:D:81:GLY:N	0.48	2.46	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:D:21:CYS:HB2	1:D:158:TYR:CE1	0.48	2.43	2	3
1:B:3:THR:OG1	1:C:158:TYR:HB2	0.48	2.09	5	1
1:F:56:ILE:O	1:F:58:LEU:HD12	0.48	2.08	5	1
1:B:42:LEU:HB2	1:B:139:ALA:HB2	0.48	1.84	6	1
1:C:56:ILE:O	1:C:130:THR:HA	0.48	2.08	6	1
1:B:73:PHE:HB2	1:B:111:LEU:HD11	0.48	1.84	7	1
1:E:144:THR:HB	1:E:145:PRO:CD	0.48	2.39	9	1
1:C:56:ILE:HG21	1:C:131:ILE:HD12	0.48	1.85	10	1
1:C:20:ALA:O	1:C:124:LEU:HD21	0.48	2.08	3	2
1:C:42:LEU:HD21	1:C:137:TYR:HB3	0.48	1.83	2	1
1:A:57:GLN:HA	1:A:130:THR:HG22	0.48	1.84	6	1
1:A:72:ALA:HB1	1:A:116:ALA:HA	0.48	1.85	6	1
1:F:73:PHE:HB2	1:F:111:LEU:HD11	0.48	1.84	7	1
1:C:144:THR:HB	1:C:145:PRO:CD	0.48	2.39	9	1
1:A:69:ALA:HB3	1:A:122:THR:HB	0.48	1.85	1	2
1:E:78:ILE:HG23	1:E:79:ASP:N	0.48	2.24	1	2
1:C:103:ILE:HD12	1:C:111:LEU:HB3	0.48	1.86	3	1
1:A:71:VAL:O	1:A:118:PHE:HA	0.48	2.08	4	1
1:A:42:LEU:HB2	1:A:139:ALA:HB2	0.48	1.84	6	1
1:B:57:GLN:HA	1:B:130:THR:HG22	0.48	1.84	6	1
1:C:72:ALA:HB1	1:C:116:ALA:HA	0.48	1.85	6	1
1:E:39:THR:HA	1:E:42:LEU:HD12	0.48	1.84	6	1
1:E:57:GLN:HA	1:E:130:THR:HG22	0.48	1.84	6	1
1:E:72:ALA:HB1	1:E:116:ALA:HA	0.48	1.84	6	1
1:B:17:VAL:HG21	1:B:21:CYS:O	0.48	2.07	7	1
1:F:17:VAL:HG21	1:F:21:CYS:O	0.48	2.07	7	1
1:F:144:THR:HB	1:F:145:PRO:CD	0.48	2.39	9	1
1:C:3:THR:OG1	1:D:158:TYR:HB2	0.48	2.09	5	1
1:D:3:THR:OG1	1:E:158:TYR:HB2	0.48	2.09	5	1
1:B:39:THR:HA	1:B:42:LEU:HD12	0.48	1.84	6	1
1:E:20:ALA:O	1:E:124:LEU:HD21	0.48	2.08	3	2
1:C:12:PHE:HA	1:D:32:VAL:O	0.48	2.09	6	1
1:B:78:ILE:HG23	1:B:79:ASP:N	0.48	2.24	1	2
1:C:78:ILE:HG23	1:C:79:ASP:N	0.48	2.24	1	2
1:A:3:THR:HB	1:B:158:TYR:CD2	0.48	2.44	4	1
1:E:56:ILE:O	1:E:130:THR:HA	0.48	2.08	6	1
1:F:42:LEU:HB2	1:F:139:ALA:HB2	0.48	1.84	6	1
1:A:34:LEU:N	1:A:34:LEU:HD22	0.48	2.24	7	1
1:D:34:LEU:N	1:D:34:LEU:HD22	0.48	2.24	7	1
1:E:73:PHE:HB2	1:E:111:LEU:HD11	0.48	1.84	7	1
1:D:20:ALA:O	1:D:61:CYS:HA	0.47	2.09	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:F:103:ILE:HD12	1:F:111:LEU:HB3	0.47	1.86	3	1
1:E:16:VAL:HA	1:F:37:VAL:O	0.47	2.09	6	1
1:F:56:ILE:O	1:F:130:THR:HA	0.47	2.08	6	1
1:B:19:ALA:O	1:B:62:ASP:HB2	0.47	2.08	8	1
1:B:144:THR:HB	1:B:145:PRO:CD	0.47	2.39	9	1
1:B:74:LEU:O	1:B:152:ALA:HA	0.47	2.09	2	3
1:B:3:THR:HB	1:C:158:TYR:CD2	0.47	2.45	4	1
1:B:56:ILE:O	1:B:130:THR:HA	0.47	2.08	6	1
1:E:42:LEU:HB2	1:E:139:ALA:HB2	0.47	1.84	6	1
1:A:144:THR:HB	1:A:145:PRO:CD	0.47	2.39	9	1
1:E:79:ASP:O	1:E:81:GLY:N	0.47	2.46	10	1
1:A:74:LEU:O	1:A:152:ALA:HA	0.47	2.09	2	2
1:A:23:VAL:HA	1:A:58:LEU:HA	0.47	1.86	3	1
1:A:3:THR:OG1	1:B:158:TYR:HB2	0.47	2.09	5	1
1:F:72:ALA:HB1	1:F:116:ALA:HA	0.47	1.85	6	1
1:C:73:PHE:HB2	1:C:111:LEU:HD11	0.47	1.84	7	1
1:A:20:ALA:O	1:A:61:CYS:HA	0.47	2.09	1	2
1:F:74:LEU:O	1:F:152:ALA:HA	0.47	2.09	2	2
1:E:3:THR:OG1	1:F:158:TYR:HB2	0.47	2.09	5	1
1:E:55:ASN:OD1	1:E:130:THR:HG21	0.47	2.10	8	1
1:D:144:THR:HB	1:D:145:PRO:CD	0.47	2.39	9	1
1:A:47:ALA:HB3	1:A:139:ALA:HB3	0.47	1.86	10	1
1:A:155:LYS:HE2	1:D:128:THR:HG21	0.47	1.87	6	1
1:A:71:VAL:HG21	1:A:131:ILE:CG2	0.47	2.40	8	1
1:E:71:VAL:HG21	1:E:131:ILE:CG2	0.47	2.40	8	1
1:F:71:VAL:HG21	1:F:131:ILE:CG2	0.47	2.40	8	1
1:D:15:GLU:HG2	1:E:147:ALA:HA	0.47	1.87	9	1
1:D:74:LEU:O	1:D:152:ALA:HA	0.47	2.09	2	2
1:D:23:VAL:HA	1:D:58:LEU:HA	0.47	1.86	3	1
1:E:103:ILE:HD12	1:E:111:LEU:HB3	0.47	1.86	3	1
1:B:16:VAL:HA	1:C:37:VAL:O	0.47	2.09	6	1
1:D:12:PHE:HA	1:E:32:VAL:O	0.47	2.09	6	1
1:A:55:ASN:OD1	1:A:130:THR:HG21	0.47	2.10	8	1
1:B:71:VAL:HG21	1:B:131:ILE:CG2	0.47	2.40	8	1
1:D:47:ALA:HB3	1:D:139:ALA:HB3	0.47	1.86	10	1
1:B:20:ALA:O	1:B:61:CYS:HA	0.47	2.09	1	1
1:E:69:ALA:HB3	1:E:122:THR:HB	0.47	1.85	1	2
1:E:118:PHE:CZ	1:E:155:LYS:HB3	0.47	2.45	1	1
1:F:20:ALA:O	1:F:61:CYS:HA	0.47	2.09	1	2
1:F:78:ILE:HG23	1:F:79:ASP:N	0.47	2.24	1	2
1:B:9:THR:CG2	1:C:153:THR:HG23	0.47	2.31	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:52:VAL:HG13	1:A:135:ALA:O	0.47	2.10	10	2
1:B:52:VAL:HG13	1:B:135:ALA:O	0.47	2.10	4	2
1:C:3:THR:HB	1:D:158:TYR:CD2	0.47	2.44	4	1
1:C:52:VAL:HG13	1:C:135:ALA:O	0.47	2.10	10	2
1:D:52:VAL:HG13	1:D:135:ALA:O	0.47	2.10	4	2
1:C:34:LEU:N	1:C:34:LEU:HD22	0.47	2.24	7	1
1:E:34:LEU:N	1:E:34:LEU:HD22	0.47	2.24	7	1
1:C:71:VAL:HG21	1:C:131:ILE:CG2	0.47	2.40	8	1
1:C:85:VAL:HG22	1:C:102:GLN:HB2	0.47	1.87	8	1
1:F:85:VAL:HG22	1:F:102:GLN:HB2	0.47	1.87	8	1
1:A:56:ILE:HG21	1:A:131:ILE:HD12	0.47	1.85	10	1
1:A:78:ILE:HG23	1:A:79:ASP:N	0.47	2.24	1	2
1:B:118:PHE:CZ	1:B:155:LYS:HB3	0.47	2.45	1	1
1:C:69:ALA:HB3	1:C:122:THR:HB	0.47	1.85	1	2
1:E:97:THR:O	1:E:98:ASN:HB2	0.47	2.10	10	2
1:E:23:VAL:CA	1:E:58:LEU:HG	0.47	2.40	3	2
1:A:72:ALA:HA	1:A:111:LEU:HD21	0.47	1.86	4	1
1:D:3:THR:HB	1:E:158:TYR:CD2	0.47	2.44	4	1
1:E:3:THR:HB	1:F:158:TYR:CD2	0.47	2.44	4	1
1:E:12:PHE:HA	1:F:32:VAL:O	0.47	2.09	6	1
1:E:5:VAL:CG2	1:F:17:VAL:HG12	0.47	2.40	8	1
1:D:56:ILE:HG21	1:D:131:ILE:HD12	0.47	1.85	10	1
1:B:79:ASP:HB2	1:B:140:THR:HG21	0.47	1.86	5	2
1:B:116:ALA:HB3	1:E:129:ASN:OD1	0.47	2.10	1	1
1:B:6:ASN:OD1	1:C:154:PHE:O	0.47	2.33	2	1
1:B:97:THR:O	1:B:98:ASN:HB2	0.47	2.10	10	2
1:C:97:THR:O	1:C:98:ASN:HB2	0.47	2.10	10	2
1:E:6:ASN:OD1	1:F:154:PHE:O	0.47	2.33	2	1
1:E:74:LEU:O	1:E:152:ALA:HA	0.47	2.09	2	2
1:B:103:ILE:HD12	1:B:111:LEU:HB3	0.47	1.86	3	1
1:D:23:VAL:CA	1:D:58:LEU:HG	0.47	2.40	3	2
1:E:52:VAL:HG13	1:E:135:ALA:O	0.47	2.10	4	2
1:C:32:VAL:HG11	1:C:52:VAL:HG11	0.47	1.87	5	1
1:F:37:VAL:CG1	1:F:42:LEU:HD21	0.47	2.40	5	1
1:B:2:ALA:HB2	1:C:159:GLN:HG3	0.47	1.87	6	1
1:F:82:HIS:NE2	1:F:139:ALA:O	0.47	2.48	7	1
1:C:55:ASN:OD1	1:C:130:THR:HG21	0.47	2.10	8	1
1:E:47:ALA:HB3	1:E:139:ALA:HB3	0.47	1.86	10	1
1:A:6:ASN:OD1	1:B:154:PHE:O	0.47	2.33	2	1
1:A:97:THR:O	1:A:98:ASN:HB2	0.47	2.10	10	2
1:D:6:ASN:OD1	1:E:154:PHE:O	0.47	2.33	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:F:97:THR:O	1:F:98:ASN:HB2	0.47	2.10	10	2
1:A:23:VAL:CA	1:A:58:LEU:HG	0.47	2.40	3	2
1:B:23:VAL:CA	1:B:58:LEU:HG	0.47	2.40	3	2
1:E:23:VAL:HA	1:E:58:LEU:HA	0.47	1.86	3	1
1:F:52:VAL:HG13	1:F:135:ALA:O	0.47	2.10	10	2
1:E:44:GLN:CG	1:E:47:ALA:HB2	0.47	2.40	5	1
1:D:16:VAL:HB	1:E:144:THR:O	0.47	2.10	7	1
1:A:97:THR:O	1:A:99:VAL:HG23	0.47	2.10	8	1
1:B:5:VAL:CG2	1:C:17:VAL:HG12	0.47	2.40	8	1
1:C:69:ALA:CB	1:C:124:LEU:HD13	0.47	2.36	8	1
1:E:97:THR:O	1:E:99:VAL:HG23	0.47	2.10	8	1
1:F:55:ASN:OD1	1:F:130:THR:HG21	0.47	2.10	8	1
1:C:6:ASN:OD1	1:D:154:PHE:O	0.46	2.33	2	1
1:A:44:GLN:CG	1:A:47:ALA:HB2	0.46	2.40	5	1
1:C:115:GLY:HA3	1:F:130:THR:OG1	0.46	2.10	5	3
1:D:44:GLN:CG	1:D:47:ALA:HB2	0.46	2.41	5	1
1:C:2:ALA:HB2	1:D:159:GLN:HG3	0.46	1.87	6	1
1:B:34:LEU:N	1:B:34:LEU:HD22	0.46	2.24	7	1
1:F:34:LEU:HD22	1:F:34:LEU:N	0.46	2.24	7	1
1:A:15:GLU:HG2	1:B:147:ALA:HA	0.46	1.86	9	1
1:B:23:VAL:HA	1:B:58:LEU:HA	0.46	1.86	3	1
1:C:72:ALA:HA	1:C:111:LEU:HD21	0.46	1.87	4	1
1:F:72:ALA:HA	1:F:111:LEU:HD21	0.46	1.87	4	1
1:B:37:VAL:CG1	1:B:42:LEU:HD21	0.46	2.40	5	1
1:C:37:VAL:CG1	1:C:42:LEU:HD21	0.46	2.41	5	1
1:B:12:PHE:HA	1:C:32:VAL:O	0.46	2.09	6	1
1:B:68:LYS:HB3	1:B:159:GLN:HB3	0.46	1.87	6	1
1:C:155:LYS:HE2	1:F:128:THR:HG21	0.46	1.87	6	1
1:D:2:ALA:HB2	1:E:159:GLN:HG3	0.46	1.87	6	1
1:A:82:HIS:NE2	1:A:139:ALA:O	0.46	2.48	7	1
1:B:55:ASN:OD1	1:B:130:THR:HG21	0.46	2.10	8	1
1:D:5:VAL:CG2	1:E:17:VAL:HG12	0.46	2.40	8	1
1:E:15:GLU:HG2	1:F:147:ALA:HA	0.46	1.87	9	1
1:E:20:ALA:O	1:E:61:CYS:HA	0.46	2.09	1	2
1:F:69:ALA:HB3	1:F:122:THR:HB	0.46	1.85	1	2
1:D:97:THR:O	1:D:98:ASN:HB2	0.46	2.10	10	2
1:B:2:ALA:H	1:C:159:GLN:HA	0.46	1.70	6	3
1:B:44:GLN:CG	1:B:47:ALA:HB2	0.46	2.40	5	1
1:D:37:VAL:CG1	1:D:42:LEU:HD21	0.46	2.41	5	1
1:A:12:PHE:HA	1:B:32:VAL:O	0.46	2.09	6	1
1:C:92:ALA:HB3	1:F:34:LEU:HD21	0.46	1.87	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:56:ILE:CB	1:B:131:ILE:HD12	0.46	2.40	7	1
1:E:82:HIS:NE2	1:E:139:ALA:O	0.46	2.48	7	1
1:D:55:ASN:OD1	1:D:130:THR:HG21	0.46	2.10	8	1
1:B:47:ALA:HB3	1:B:139:ALA:HB3	0.46	1.86	10	1
1:E:114:ASP:HB2	1:E:117:THR:OG1	0.46	2.11	10	1
1:C:20:ALA:O	1:C:61:CYS:HA	0.46	2.09	1	1
1:D:63:THR:HG23	1:D:125:ASN:HA	0.46	1.87	1	2
1:A:92:ALA:HA	1:D:50:SER:O	0.46	2.11	4	1
1:B:32:VAL:HG11	1:B:52:VAL:HG11	0.46	1.87	5	1
1:E:37:VAL:CG1	1:E:42:LEU:HD21	0.46	2.41	5	1
1:E:79:ASP:HB2	1:E:140:THR:HG21	0.46	1.86	5	1
1:F:32:VAL:HG11	1:F:52:VAL:HG11	0.46	1.87	5	1
1:D:5:VAL:HG12	1:F:146:GLY:HA2	0.46	1.87	6	1
1:E:56:ILE:CB	1:E:131:ILE:HD12	0.46	2.40	7	1
1:C:5:VAL:CG2	1:D:17:VAL:HG12	0.46	2.40	8	1
1:D:85:VAL:HG22	1:D:102:GLN:HB2	0.46	1.87	8	1
1:A:63:THR:HG23	1:A:125:ASN:HA	0.46	1.87	1	2
1:C:116:ALA:HB3	1:F:129:ASN:OD1	0.46	2.10	1	1
1:D:69:ALA:HB3	1:D:122:THR:HB	0.46	1.85	1	2
1:F:118:PHE:CZ	1:F:155:LYS:HB3	0.46	2.45	1	1
1:A:37:VAL:CG1	1:A:42:LEU:HD21	0.46	2.41	5	1
1:C:5:VAL:HG12	1:E:146:GLY:HA2	0.46	1.87	6	1
1:E:68:LYS:HB3	1:E:159:GLN:HB3	0.46	1.87	6	1
1:A:16:VAL:HB	1:B:144:THR:O	0.46	2.10	7	1
1:A:116:ALA:HB3	1:D:129:ASN:OD1	0.46	2.10	1	1
1:C:118:PHE:CZ	1:C:155:LYS:HB3	0.46	2.45	1	1
1:C:74:LEU:O	1:C:152:ALA:HA	0.46	2.09	2	2
1:C:92:ALA:HA	1:F:50:SER:O	0.46	2.11	4	1
1:A:115:GLY:HA3	1:D:130:THR:OG1	0.46	2.10	5	3
1:C:58:LEU:HD11	1:C:131:ILE:HG13	0.46	1.87	6	1
1:D:68:LYS:HB3	1:D:159:GLN:HB3	0.46	1.87	6	1
1:F:68:LYS:HB3	1:F:159:GLN:HB3	0.46	1.87	6	1
1:B:16:VAL:HB	1:C:144:THR:O	0.46	2.10	7	1
1:A:5:VAL:CG2	1:B:17:VAL:HG12	0.46	2.40	8	1
1:B:111:LEU:HD11	1:B:117:THR:HG22	0.46	1.88	8	1
1:D:71:VAL:HG21	1:D:131:ILE:CG2	0.46	2.40	8	1
1:E:111:LEU:HD11	1:E:117:THR:HG22	0.46	1.88	8	1
1:C:75:GLY:C	1:C:113:LEU:HD23	0.46	2.36	9	1
1:A:21:CYS:HB3	1:A:58:LEU:HD23	0.46	1.88	3	1
1:C:21:CYS:HB3	1:C:58:LEU:HD23	0.46	1.88	3	1
1:A:21:CYS:SG	1:A:58:LEU:HB2	0.46	2.51	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:103:ILE:HD12	1:A:113:LEU:HD11	0.46	1.88	6	1
1:D:21:CYS:SG	1:D:58:LEU:HB2	0.46	2.51	6	1
1:B:34:LEU:HD21	1:B:101:VAL:CG2	0.46	2.41	10	1
1:B:21:CYS:HB3	1:B:58:LEU:HD23	0.46	1.88	3	1
1:E:21:CYS:HB3	1:E:58:LEU:HD23	0.46	1.88	3	1
1:F:21:CYS:HB3	1:F:58:LEU:HD23	0.46	1.88	3	1
1:A:22:ALA:HB1	1:B:36:GLN:O	0.46	2.11	4	1
1:D:72:ALA:HA	1:D:111:LEU:HD21	0.46	1.86	4	1
1:C:44:GLN:CG	1:C:47:ALA:HB2	0.46	2.40	5	1
1:F:44:GLN:CG	1:F:47:ALA:HB2	0.46	2.41	5	1
1:E:2:ALA:HB2	1:F:159:GLN:HG3	0.46	1.87	6	1
1:F:58:LEU:HD11	1:F:131:ILE:HG13	0.46	1.87	6	1
1:D:82:HIS:NE2	1:D:139:ALA:O	0.46	2.48	7	1
1:E:16:VAL:HB	1:F:144:THR:O	0.46	2.10	7	1
1:B:15:GLU:HG2	1:C:147:ALA:HA	0.46	1.86	9	1
1:D:75:GLY:C	1:D:113:LEU:HD23	0.46	2.36	9	1
1:E:75:GLY:C	1:E:113:LEU:HD23	0.46	2.36	9	1
1:F:75:GLY:C	1:F:113:LEU:HD23	0.46	2.36	9	1
1:A:34:LEU:HD21	1:A:101:VAL:CG2	0.46	2.41	10	1
1:A:114:ASP:HB2	1:A:117:THR:OG1	0.46	2.11	10	1
1:B:16:VAL:CG2	1:C:148:ALA:HB2	0.46	2.41	10	2
1:C:63:THR:HG23	1:C:125:ASN:HA	0.46	1.87	1	2
1:C:23:VAL:CA	1:C:58:LEU:HG	0.46	2.40	3	2
1:B:92:ALA:HA	1:E:50:SER:O	0.46	2.11	4	1
1:F:97:THR:N	1:F:144:THR:HB	0.46	2.26	4	1
1:C:21:CYS:SG	1:C:58:LEU:HB2	0.46	2.51	6	1
1:E:103:ILE:HD12	1:E:113:LEU:HD11	0.46	1.88	6	1
1:F:21:CYS:SG	1:F:58:LEU:HB2	0.46	2.51	6	1
1:A:111:LEU:HD11	1:A:117:THR:HG22	0.46	1.88	8	1
1:D:111:LEU:HD11	1:D:117:THR:HG22	0.46	1.88	8	1
1:F:97:THR:O	1:F:99:VAL:HG23	0.46	2.10	8	1
1:B:75:GLY:C	1:B:113:LEU:HD23	0.46	2.36	9	1
1:C:114:ASP:HB2	1:C:117:THR:OG1	0.46	2.11	10	1
1:D:34:LEU:HD21	1:D:101:VAL:CG2	0.46	2.41	10	1
1:F:34:LEU:HD21	1:F:101:VAL:CG2	0.46	2.41	10	1
1:C:16:VAL:CG2	1:D:148:ALA:HB2	0.46	2.41	10	2
1:C:23:VAL:HA	1:C:58:LEU:HA	0.46	1.86	3	1
1:C:86:LEU:HD11	1:C:151:ASP:C	0.46	2.36	4	1
1:A:2:ALA:HB2	1:B:159:GLN:HG3	0.46	1.87	6	1
1:A:5:VAL:HG12	1:C:146:GLY:HA2	0.46	1.87	6	1
1:A:58:LEU:HD11	1:A:131:ILE:HG13	0.46	1.87	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:D:97:THR:O	1:D:99:VAL:HG23	0.46	2.10	8	1
1:A:39:THR:O	1:A:43:ALA:HB2	0.46	2.11	10	1
1:B:39:THR:O	1:B:43:ALA:HB2	0.46	2.11	10	1
1:D:39:THR:O	1:D:43:ALA:HB2	0.46	2.11	10	1
1:E:34:LEU:HD21	1:E:101:VAL:CG2	0.46	2.41	10	1
1:E:39:THR:O	1:E:43:ALA:HB2	0.46	2.11	10	1
1:F:39:THR:O	1:F:43:ALA:HB2	0.46	2.11	10	1
1:B:63:THR:HG23	1:B:125:ASN:HA	0.45	1.87	1	2
1:D:21:CYS:HB3	1:D:58:LEU:HD23	0.45	1.88	3	1
1:F:23:VAL:CA	1:F:58:LEU:HG	0.45	2.40	3	2
1:F:86:LEU:HD11	1:F:151:ASP:C	0.45	2.36	4	1
1:A:92:ALA:HB3	1:D:34:LEU:HD21	0.45	1.87	6	1
1:E:58:LEU:HD11	1:E:131:ILE:HG13	0.45	1.87	6	1
1:C:15:GLU:HG2	1:D:147:ALA:HA	0.45	1.87	9	1
1:B:114:ASP:HB2	1:B:117:THR:OG1	0.45	2.11	10	1
1:D:16:VAL:CG2	1:E:148:ALA:HB2	0.45	2.41	10	2
1:E:9:THR:CG2	1:F:153:THR:HG23	0.45	2.31	3	1
1:C:76:THR:H	1:C:86:LEU:HD12	0.45	1.71	5	1
1:E:32:VAL:HG11	1:E:52:VAL:HG11	0.45	1.87	5	1
1:D:58:LEU:HD11	1:D:131:ILE:HG13	0.45	1.87	6	1
1:D:66:ALA:HB1	1:D:159:GLN:O	0.45	2.11	6	1
1:E:86:LEU:HG	1:E:113:LEU:CD2	0.45	2.41	6	1
1:C:16:VAL:HB	1:D:144:THR:O	0.45	2.10	7	1
1:A:85:VAL:HG22	1:A:102:GLN:HB2	0.45	1.87	8	1
1:B:56:ILE:HG22	1:B:131:ILE:HB	0.45	1.89	8	1
1:B:97:THR:O	1:B:99:VAL:HG23	0.45	2.10	8	1
1:C:13:LYS:HD3	1:D:31:THR:HG22	0.45	1.89	9	1
1:E:6:ASN:CA	1:F:155:LYS:HE2	0.45	2.41	9	1
1:A:16:VAL:CG2	1:B:148:ALA:HB2	0.45	2.41	10	2
1:E:16:VAL:CG2	1:F:148:ALA:HB2	0.45	2.41	10	2
1:B:72:ALA:HA	1:B:111:LEU:HD21	0.45	1.86	4	1
1:E:22:ALA:HB1	1:F:36:GLN:O	0.45	2.11	4	1
1:B:115:GLY:HA3	1:E:130:THR:OG1	0.45	2.10	5	3
1:B:5:VAL:HG12	1:D:146:GLY:HA2	0.45	1.87	6	1
1:B:155:LYS:HE2	1:E:128:THR:HG21	0.45	1.87	6	1
1:B:82:HIS:NE2	1:B:139:ALA:O	0.45	2.48	7	1
1:C:97:THR:O	1:C:99:VAL:HG23	0.45	2.10	8	1
1:C:111:LEU:HD11	1:C:117:THR:HG22	0.45	1.88	8	1
1:F:56:ILE:HG22	1:F:131:ILE:HB	0.45	1.89	8	1
1:F:111:LEU:HD11	1:F:117:THR:HG22	0.45	1.88	8	1
1:A:13:LYS:HD3	1:B:31:THR:HG22	0.45	1.89	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:D:6:ASN:CA	1:E:155:LYS:HE2	0.45	2.41	9	1
1:D:13:LYS:HD3	1:E:31:THR:HG22	0.45	1.89	9	1
1:A:91:SER:CB	1:A:95:SER:HB2	0.45	2.42	10	1
1:F:114:ASP:HB2	1:F:117:THR:OG1	0.45	2.11	10	1
1:F:68:LYS:HE3	1:F:121:GLU:HB3	0.45	1.89	3	1
1:E:86:LEU:HD11	1:E:151:ASP:C	0.45	2.36	4	1
1:F:75:GLY:HA3	1:F:113:LEU:HD11	0.45	1.88	5	1
1:A:86:LEU:HG	1:A:113:LEU:CD2	0.45	2.42	6	1
1:B:58:LEU:HD11	1:B:131:ILE:HG13	0.45	1.87	6	1
1:D:86:LEU:HG	1:D:113:LEU:CD2	0.45	2.42	6	1
1:E:56:ILE:HG22	1:E:131:ILE:HB	0.45	1.89	8	1
1:F:17:VAL:HG11	1:F:158:TYR:CE2	0.45	2.47	9	1
1:C:34:LEU:HD21	1:C:101:VAL:CG2	0.45	2.41	10	1
1:D:91:SER:CB	1:D:95:SER:HB2	0.45	2.42	10	1
1:F:63:THR:HG23	1:F:125:ASN:HA	0.45	1.89	3	2
1:E:144:THR:HG22	1:E:145:PRO:HD2	0.45	1.88	2	1
1:A:86:LEU:HD11	1:A:151:ASP:C	0.45	2.36	4	1
1:C:97:THR:N	1:C:144:THR:HB	0.45	2.26	4	1
1:D:2:ALA:H	1:E:159:GLN:HA	0.45	1.70	6	3
1:D:32:VAL:HG11	1:D:52:VAL:HG11	0.45	1.87	5	1
1:B:86:LEU:HG	1:B:113:LEU:CD2	0.45	2.42	6	1
1:C:66:ALA:HB1	1:C:159:GLN:O	0.45	2.11	6	1
1:F:66:ALA:HB1	1:F:159:GLN:O	0.45	2.11	6	1
1:C:52:VAL:HG23	1:C:54:PHE:CD1	0.45	2.47	7	1
1:B:85:VAL:HG22	1:B:102:GLN:HB2	0.45	1.87	8	1
1:C:56:ILE:HG22	1:C:131:ILE:HB	0.45	1.89	8	1
1:A:116:ALA:O	1:D:125:ASN:HB3	0.45	2.12	10	1
1:D:144:THR:HG22	1:D:145:PRO:HD2	0.45	1.88	2	1
1:D:68:LYS:HE3	1:D:121:GLU:HB3	0.45	1.89	3	1
1:F:23:VAL:HA	1:F:58:LEU:HA	0.45	1.86	3	1
1:D:86:LEU:HD11	1:D:151:ASP:C	0.45	2.36	4	1
1:A:32:VAL:HG11	1:A:52:VAL:HG11	0.45	1.87	5	1
1:A:75:GLY:HA3	1:A:113:LEU:HD11	0.45	1.88	5	1
1:C:2:ALA:H	1:D:159:GLN:HA	0.45	1.70	6	3
1:E:2:ALA:H	1:F:159:GLN:HA	0.45	1.72	5	3
1:A:66:ALA:HB1	1:A:159:GLN:O	0.45	2.11	6	1
1:A:68:LYS:HB3	1:A:159:GLN:HB3	0.45	1.87	6	1
1:A:90:SER:O	1:D:52:VAL:HG12	0.45	2.12	7	1
1:D:52:VAL:HG23	1:D:54:PHE:CD1	0.45	2.47	7	1
1:C:6:ASN:CA	1:D:155:LYS:HE2	0.45	2.41	9	1
1:A:118:PHE:CZ	1:A:155:LYS:HB3	0.45	2.45	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:D:118:PHE:CZ	1:D:155:LYS:HB3	0.45	2.45	1	1
1:D:22:ALA:HB1	1:E:36:GLN:O	0.45	2.11	4	1
1:E:72:ALA:HA	1:E:111:LEU:HD21	0.45	1.87	4	1
1:D:79:ASP:HB2	1:D:140:THR:HG21	0.45	1.86	5	1
1:B:98:ASN:HA	1:B:140:THR:HB	0.45	1.89	6	1
1:C:98:ASN:HA	1:C:140:THR:HB	0.45	1.88	6	1
1:E:85:VAL:HG22	1:E:102:GLN:HB2	0.45	1.87	8	1
1:A:75:GLY:C	1:A:113:LEU:HD23	0.45	2.36	9	1
1:E:13:LYS:HD3	1:F:31:THR:HG22	0.45	1.89	9	1
1:C:47:ALA:HB3	1:C:139:ALA:HB3	0.45	1.86	10	1
1:C:22:ALA:HB1	1:D:36:GLN:O	0.45	2.11	4	1
1:D:97:THR:N	1:D:144:THR:HB	0.45	2.26	4	1
1:C:68:LYS:HB3	1:C:159:GLN:HB3	0.45	1.87	6	1
1:F:98:ASN:HA	1:F:140:THR:HB	0.45	1.89	6	1
1:F:103:ILE:HD12	1:F:113:LEU:HD11	0.45	1.88	6	1
1:A:52:VAL:HG23	1:A:54:PHE:CD1	0.45	2.47	7	1
1:D:8:GLY:N	1:E:154:PHE:CE1	0.45	2.85	7	1
1:B:6:ASN:CA	1:C:155:LYS:HE2	0.45	2.41	9	1
1:C:47:ALA:O	1:C:138:PHE:HA	0.45	2.12	9	1
1:C:39:THR:O	1:C:43:ALA:HB2	0.45	2.11	10	1
1:C:68:LYS:HE3	1:C:121:GLU:HB3	0.45	1.89	3	1
1:B:22:ALA:HB1	1:C:36:GLN:O	0.45	2.11	4	1
1:B:86:LEU:HD11	1:B:151:ASP:C	0.45	2.36	4	1
1:B:9:THR:HG23	1:C:152:ALA:O	0.45	2.12	5	1
1:A:92:ALA:HA	1:D:50:SER:HB2	0.45	1.89	6	1
1:B:92:ALA:HB3	1:E:34:LEU:HD21	0.45	1.87	6	1
1:C:86:LEU:HG	1:C:113:LEU:CD2	0.45	2.41	6	1
1:A:8:GLY:N	1:B:154:PHE:CE1	0.45	2.85	7	1
1:D:23:VAL:HG13	1:D:27:SER:HB3	0.45	1.89	7	1
1:A:105:ASP:OD2	1:A:111:LEU:HD22	0.45	2.12	8	1
1:C:105:ASP:OD2	1:C:111:LEU:HD22	0.45	2.12	8	1
1:A:6:ASN:CA	1:B:155:LYS:HE2	0.45	2.41	9	1
1:B:13:LYS:HD3	1:C:31:THR:HG22	0.45	1.89	9	1
1:F:47:ALA:HB3	1:F:139:ALA:HB3	0.45	1.86	10	1
1:E:85:VAL:HG11	1:E:138:PHE:HB3	0.45	1.89	1	1
1:B:103:ILE:HG12	1:B:113:LEU:HG	0.45	1.89	8	2
1:A:2:ALA:H	1:B:159:GLN:HA	0.45	1.70	6	3
1:A:76:THR:H	1:A:86:LEU:HD12	0.45	1.71	5	1
1:E:9:THR:HG23	1:F:152:ALA:O	0.45	2.12	5	1
1:B:66:ALA:HB1	1:B:159:GLN:O	0.45	2.11	6	1
1:D:103:ILE:HD12	1:D:113:LEU:HD11	0.45	1.88	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:E:86:LEU:HG	1:E:113:LEU:HD21	0.45	1.89	6	1
1:B:52:VAL:HG23	1:B:54:PHE:CD1	0.45	2.47	7	1
1:B:90:SER:O	1:E:52:VAL:HG12	0.45	2.12	7	1
1:F:52:VAL:HG23	1:F:54:PHE:CD1	0.45	2.47	7	1
1:E:17:VAL:HG11	1:E:158:TYR:CE2	0.45	2.46	9	1
1:B:44:GLN:HB2	1:B:47:ALA:HB2	0.44	1.89	1	1
1:D:44:GLN:HB2	1:D:47:ALA:HB2	0.44	1.89	1	1
1:D:85:VAL:HG11	1:D:138:PHE:HB3	0.44	1.89	1	1
1:F:103:ILE:HG12	1:F:113:LEU:HG	0.44	1.89	8	2
1:F:144:THR:HG22	1:F:145:PRO:HD2	0.44	1.88	2	1
1:C:75:GLY:HA3	1:C:113:LEU:HD11	0.44	1.88	5	1
1:D:9:THR:HG23	1:E:152:ALA:O	0.44	2.12	5	1
1:B:86:LEU:HG	1:B:113:LEU:HD21	0.44	1.89	6	1
1:F:86:LEU:HG	1:F:113:LEU:CD2	0.44	2.42	6	1
1:B:8:GLY:N	1:C:154:PHE:CE1	0.44	2.85	7	1
1:D:42:LEU:HB3	1:D:139:ALA:HB2	0.44	1.89	9	2
1:E:8:GLY:N	1:F:154:PHE:CE1	0.44	2.85	7	1
1:E:22:ALA:HB3	1:E:59:ASN:O	0.44	2.13	7	1
1:F:23:VAL:HG13	1:F:27:SER:HB3	0.44	1.89	7	1
1:A:56:ILE:HG22	1:A:131:ILE:HB	0.44	1.89	8	1
1:B:69:ALA:CB	1:B:124:LEU:HD13	0.44	2.36	8	1
1:D:56:ILE:HG22	1:D:131:ILE:HB	0.44	1.89	8	1
1:B:91:SER:CB	1:B:95:SER:HB2	0.44	2.42	10	1
1:C:91:SER:CB	1:C:95:SER:HB2	0.44	2.42	10	1
1:E:73:PHE:CB	1:E:103:ILE:HD13	0.44	2.42	2	1
1:C:92:ALA:O	1:F:49:SER:HB3	0.44	2.13	4	1
1:C:4:THR:HG22	1:D:157:GLN:HB2	0.44	1.90	5	1
1:B:103:ILE:HD12	1:B:113:LEU:HD11	0.44	1.88	6	1
1:E:66:ALA:HB1	1:E:159:GLN:O	0.44	2.11	6	1
1:A:22:ALA:HB3	1:A:59:ASN:O	0.44	2.13	7	1
1:B:22:ALA:HB3	1:B:59:ASN:O	0.44	2.13	7	1
1:C:8:GLY:N	1:D:154:PHE:CE1	0.44	2.85	7	1
1:E:52:VAL:HG23	1:E:54:PHE:CD1	0.44	2.47	7	1
1:F:56:ILE:CB	1:F:131:ILE:HD12	0.44	2.40	7	1
1:F:105:ASP:OD2	1:F:111:LEU:HD22	0.44	2.12	8	1
1:A:17:VAL:HG11	1:A:158:TYR:CE2	0.44	2.47	9	1
1:B:11:HIS:O	1:C:32:VAL:HB	0.44	2.13	9	1
1:B:17:VAL:HG11	1:B:158:TYR:CE2	0.44	2.47	9	1
1:D:114:ASP:HB2	1:D:117:THR:OG1	0.44	2.11	10	1
1:E:91:SER:CB	1:E:95:SER:HB2	0.44	2.42	10	1
1:A:44:GLN:HB2	1:A:47:ALA:HB2	0.44	1.89	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:85:VAL:HG11	1:B:138:PHE:HB3	0.44	1.89	1	1
1:E:44:GLN:HB2	1:E:47:ALA:HB2	0.44	1.89	1	1
1:F:44:GLN:HB2	1:F:47:ALA:HB2	0.44	1.89	1	1
1:B:92:ALA:O	1:E:49:SER:HB3	0.44	2.12	4	1
1:E:76:THR:H	1:E:86:LEU:HD12	0.44	1.71	5	1
1:E:98:ASN:HA	1:E:140:THR:HB	0.44	1.89	6	1
1:C:42:LEU:HB3	1:C:139:ALA:HB2	0.44	1.89	9	2
1:D:22:ALA:HB3	1:D:59:ASN:O	0.44	2.13	7	1
1:D:56:ILE:CB	1:D:131:ILE:HD12	0.44	2.40	7	1
1:D:105:ASP:OD2	1:D:111:LEU:HD22	0.44	2.12	8	1
1:F:47:ALA:O	1:F:138:PHE:HA	0.44	2.12	9	1
1:A:79:ASP:HB2	1:A:140:THR:HG21	0.44	1.86	5	2
1:C:44:GLN:HB2	1:C:47:ALA:HB2	0.44	1.89	1	1
1:E:68:LYS:HE3	1:E:121:GLU:HB3	0.44	1.89	3	1
1:D:76:THR:H	1:D:86:LEU:HD12	0.44	1.71	5	1
1:B:21:CYS:SG	1:B:58:LEU:HB2	0.44	2.51	6	1
1:E:23:VAL:HG13	1:E:27:SER:HB3	0.44	1.89	7	1
1:E:105:ASP:OD2	1:E:111:LEU:HD22	0.44	2.12	8	1
1:C:11:HIS:O	1:D:32:VAL:HB	0.44	2.13	9	1
1:C:17:VAL:HG11	1:C:158:TYR:CE2	0.44	2.47	9	1
1:D:11:HIS:O	1:E:32:VAL:HB	0.44	2.13	9	1
1:D:17:VAL:HG11	1:D:158:TYR:CE2	0.44	2.47	9	1
1:C:73:PHE:CB	1:C:103:ILE:HD13	0.44	2.42	2	1
1:C:102:GLN:HG2	1:C:103:ILE:N	0.44	2.28	4	1
1:A:9:THR:HG23	1:B:152:ALA:O	0.44	2.12	5	1
1:B:76:THR:H	1:B:86:LEU:HD12	0.44	1.71	5	1
1:D:4:THR:HG22	1:E:157:GLN:HB2	0.44	1.90	5	1
1:D:75:GLY:HA3	1:D:113:LEU:HD11	0.44	1.88	5	1
1:E:9:THR:HA	1:F:153:THR:HG22	0.44	1.90	6	1
1:F:86:LEU:HG	1:F:113:LEU:HD21	0.44	1.89	6	1
1:A:69:ALA:CB	1:A:124:LEU:HD13	0.44	2.36	8	1
1:D:47:ALA:O	1:D:138:PHE:HA	0.44	2.12	9	1
1:F:73:PHE:CB	1:F:103:ILE:HD13	0.44	2.42	2	1
1:A:68:LYS:HE3	1:A:121:GLU:HB3	0.44	1.89	3	1
1:A:92:ALA:O	1:D:49:SER:HB3	0.44	2.13	4	1
1:A:102:GLN:HG2	1:A:103:ILE:N	0.44	2.28	4	1
1:B:102:GLN:HG2	1:B:103:ILE:N	0.44	2.28	4	1
1:D:102:GLN:HG2	1:D:103:ILE:N	0.44	2.28	4	1
1:E:102:GLN:HG2	1:E:103:ILE:N	0.44	2.28	4	1
1:A:98:ASN:HA	1:A:140:THR:HB	0.44	1.89	6	1
1:D:98:ASN:HA	1:D:140:THR:HB	0.44	1.89	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:E:21:CYS:SG	1:E:58:LEU:HB2	0.44	2.51	6	1
1:F:118:PHE:CD1	1:F:157:GLN:HB2	0.44	2.48	8	1
1:B:116:ALA:O	1:E:125:ASN:HB3	0.44	2.12	10	1
1:F:91:SER:CB	1:F:95:SER:HB2	0.44	2.42	10	1
1:E:63:THR:HG23	1:E:125:ASN:HA	0.44	1.87	1	2
1:C:116:ALA:HB2	1:F:128:THR:C	0.44	2.38	2	1
1:C:103:ILE:HD12	1:C:113:LEU:HD11	0.44	1.88	6	1
1:D:9:THR:HA	1:E:153:THR:HG22	0.44	1.90	6	1
1:A:42:LEU:HB3	1:A:139:ALA:HB2	0.44	1.89	9	2
1:A:56:ILE:CB	1:A:131:ILE:HD12	0.44	2.40	7	1
1:C:77:ALA:H	1:F:132:PRO:HB3	0.44	1.73	7	1
1:C:90:SER:O	1:F:52:VAL:HG12	0.44	2.12	7	1
1:B:105:ASP:OD2	1:B:111:LEU:HD22	0.44	2.12	8	1
1:C:118:PHE:CD1	1:C:157:GLN:HB2	0.44	2.48	8	1
1:E:47:ALA:O	1:E:138:PHE:HA	0.44	2.12	9	1
1:A:16:VAL:O	1:B:145:PRO:HA	0.44	2.13	10	1
1:C:16:VAL:O	1:D:145:PRO:HA	0.44	2.13	10	1
1:B:89:GLN:CG	1:B:149:ASN:HB2	0.44	2.42	2	1
1:C:89:GLN:CG	1:C:149:ASN:HB2	0.44	2.43	2	1
1:E:89:GLN:CG	1:E:149:ASN:HB2	0.44	2.43	2	1
1:F:89:GLN:CG	1:F:149:ASN:HB2	0.44	2.43	2	1
1:B:68:LYS:HE3	1:B:121:GLU:HB3	0.44	1.89	3	1
1:D:51:ALA:CA	1:D:136:ARG:HB3	0.44	2.43	3	1
1:C:86:LEU:HG	1:C:113:LEU:HD21	0.44	1.89	6	1
1:E:42:LEU:HB3	1:E:139:ALA:HB2	0.44	1.89	9	2
1:A:118:PHE:CD1	1:A:157:GLN:HB2	0.44	2.48	8	1
1:D:118:PHE:CD1	1:D:157:GLN:HB2	0.44	2.48	8	1
1:B:47:ALA:O	1:B:138:PHE:HA	0.44	2.12	9	1
1:E:11:HIS:O	1:F:32:VAL:HB	0.44	2.13	9	1
1:F:73:PHE:CB	1:F:111:LEU:HD11	0.44	2.43	9	1
1:D:89:GLN:CG	1:D:149:ASN:HB2	0.44	2.43	2	1
1:D:51:ALA:HA	1:D:136:ARG:HB3	0.44	1.90	3	1
1:B:75:GLY:HA3	1:B:113:LEU:HD11	0.44	1.88	5	1
1:C:23:VAL:HG13	1:C:27:SER:HB3	0.44	1.89	7	1
1:A:11:HIS:O	1:B:32:VAL:HB	0.44	2.13	9	1
1:C:98:ASN:HA	1:C:140:THR:OG1	0.44	2.13	9	1
1:E:73:PHE:CB	1:E:111:LEU:HD11	0.44	2.43	9	1
1:C:116:ALA:O	1:F:125:ASN:HB3	0.44	2.12	10	1
1:A:103:ILE:HG12	1:A:113:LEU:HG	0.43	1.89	8	2
1:D:73:PHE:CB	1:D:103:ILE:HD13	0.43	2.42	2	1
1:F:39:THR:OG1	1:F:143:ALA:O	0.43	2.33	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:97:THR:N	1:A:144:THR:HB	0.43	2.26	4	1
1:A:4:THR:HG22	1:B:157:GLN:HB2	0.43	1.90	5	1
1:F:76:THR:H	1:F:86:LEU:HD12	0.43	1.71	5	1
1:A:93:ALA:HB3	1:D:36:GLN:O	0.43	2.13	6	2
1:B:93:ALA:HB3	1:E:36:GLN:O	0.43	2.13	10	2
1:A:98:ASN:HA	1:A:140:THR:OG1	0.43	2.13	9	1
1:C:73:PHE:CB	1:C:111:LEU:HD11	0.43	2.43	9	1
1:F:105:ASP:HB2	1:F:111:LEU:HB2	0.43	1.91	1	2
1:A:51:ALA:CA	1:A:136:ARG:HB3	0.43	2.43	3	1
1:B:51:ALA:CA	1:B:136:ARG:HB3	0.43	2.43	3	1
1:E:51:ALA:HA	1:E:136:ARG:HB3	0.43	1.90	3	1
1:F:51:ALA:CA	1:F:136:ARG:HB3	0.43	2.43	3	1
1:C:9:THR:HG23	1:D:152:ALA:O	0.43	2.12	5	1
1:E:75:GLY:HA3	1:E:113:LEU:HD11	0.43	1.88	5	1
1:B:42:LEU:HB3	1:B:139:ALA:HB2	0.43	1.89	9	2
1:C:61:CYS:HB3	1:C:125:ASN:O	0.43	2.13	8	1
1:E:55:ASN:OD1	1:E:130:THR:CG2	0.43	2.66	8	1
1:D:98:ASN:HA	1:D:140:THR:OG1	0.43	2.13	9	1
1:F:98:ASN:HA	1:F:140:THR:OG1	0.43	2.13	9	1
1:B:16:VAL:O	1:C:145:PRO:HA	0.43	2.13	10	1
1:C:85:VAL:HG11	1:C:138:PHE:HB3	0.43	1.89	1	1
1:C:105:ASP:HB2	1:C:111:LEU:HB2	0.43	1.91	1	2
1:D:105:ASP:HB2	1:D:111:LEU:HB2	0.43	1.91	1	2
1:F:85:VAL:HG11	1:F:138:PHE:HB3	0.43	1.89	1	1
1:A:73:PHE:CB	1:A:103:ILE:HD13	0.43	2.42	2	2
1:B:73:PHE:CB	1:B:103:ILE:HD13	0.43	2.42	2	1
1:F:102:GLN:HG2	1:F:103:ILE:N	0.43	2.28	4	1
1:B:9:THR:HA	1:C:153:THR:HG22	0.43	1.90	6	1
1:B:92:ALA:HA	1:E:50:SER:HB2	0.43	1.89	6	1
1:C:93:ALA:HB3	1:F:36:GLN:O	0.43	2.13	6	2
1:B:74:LEU:HD11	1:E:57:GLN:HG3	0.43	1.89	10	1
1:D:16:VAL:O	1:E:145:PRO:HA	0.43	2.13	10	1
1:E:16:VAL:O	1:F:145:PRO:HA	0.43	2.13	10	1
1:B:77:ALA:HB2	1:B:83:THR:HG23	0.43	1.90	2	1
1:B:116:ALA:HB2	1:E:128:THR:C	0.43	2.38	2	1
1:C:5:VAL:CG1	1:E:146:GLY:HA2	0.43	2.44	6	1
1:A:23:VAL:HG13	1:A:27:SER:HB3	0.43	1.89	7	1
1:B:77:ALA:H	1:E:132:PRO:HB3	0.43	1.73	7	1
1:C:22:ALA:HB3	1:C:59:ASN:O	0.43	2.13	7	1
1:C:82:HIS:NE2	1:C:139:ALA:O	0.43	2.48	7	1
1:B:73:PHE:CB	1:B:111:LEU:HD11	0.43	2.43	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:73:PHE:CD1	1:A:152:ALA:HB1	0.43	2.49	2	1
1:C:73:PHE:CD1	1:C:152:ALA:HB1	0.43	2.49	2	1
1:E:77:ALA:HB2	1:E:83:THR:HG23	0.43	1.90	2	1
1:E:103:ILE:HG12	1:E:113:LEU:HG	0.43	1.89	8	2
1:A:51:ALA:HA	1:A:136:ARG:HB3	0.43	1.90	3	1
1:E:51:ALA:CA	1:E:136:ARG:HB3	0.43	2.43	3	1
1:C:63:THR:HA	1:C:66:ALA:O	0.43	2.14	7	1
1:A:61:CYS:HB3	1:A:125:ASN:O	0.43	2.13	8	1
1:E:61:CYS:HB3	1:E:125:ASN:O	0.43	2.13	8	1
1:A:47:ALA:O	1:A:138:PHE:HA	0.43	2.12	9	1
1:D:6:ASN:CB	1:E:155:LYS:HE2	0.43	2.44	9	1
1:A:89:GLN:CG	1:A:149:ASN:HB2	0.43	2.43	2	1
1:A:116:ALA:HB2	1:D:128:THR:C	0.43	2.38	2	1
1:C:103:ILE:HG12	1:C:113:LEU:HG	0.43	1.89	8	2
1:E:73:PHE:CD1	1:E:152:ALA:HB1	0.43	2.49	2	1
1:A:106:ARG:CZ	1:A:132:PRO:HG2	0.43	2.44	6	1
1:C:92:ALA:HA	1:F:50:SER:HB2	0.43	1.89	6	1
1:D:5:VAL:CG1	1:F:146:GLY:HA2	0.43	2.44	6	1
1:D:106:ARG:CZ	1:D:132:PRO:HG2	0.43	2.44	6	1
1:A:77:ALA:H	1:D:132:PRO:HB3	0.43	1.73	7	1
1:B:23:VAL:HG13	1:B:27:SER:HB3	0.43	1.89	7	1
1:F:42:LEU:HB3	1:F:139:ALA:HB2	0.43	1.89	9	2
1:A:55:ASN:OD1	1:A:130:THR:CG2	0.43	2.66	8	1
1:B:55:ASN:OD1	1:B:130:THR:CG2	0.43	2.66	8	1
1:F:55:ASN:OD1	1:F:130:THR:CG2	0.43	2.66	8	1
1:A:6:ASN:CB	1:B:155:LYS:HE2	0.43	2.44	9	1
1:B:98:ASN:HA	1:B:140:THR:OG1	0.43	2.13	9	1
1:B:84:ASN:HB3	1:B:102:GLN:HG2	0.43	1.91	5	1
1:E:99:VAL:HB	1:E:143:ALA:HB1	0.43	1.90	5	1
1:A:86:LEU:HG	1:A:113:LEU:HD21	0.43	1.89	6	1
1:F:63:THR:HA	1:F:66:ALA:O	0.43	2.14	7	1
1:B:61:CYS:HB3	1:B:125:ASN:O	0.43	2.14	8	1
1:C:55:ASN:OD1	1:C:130:THR:CG2	0.43	2.66	8	1
1:D:107:THR:HB	1:D:120:SER:HA	0.43	1.91	10	1
1:A:85:VAL:HG11	1:A:138:PHE:HB3	0.43	1.89	1	1
1:D:73:PHE:CD1	1:D:152:ALA:HB1	0.43	2.49	2	1
1:F:73:PHE:CD1	1:F:152:ALA:HB1	0.43	2.49	2	1
1:C:51:ALA:CA	1:C:136:ARG:HB3	0.43	2.43	3	1
1:C:9:THR:HA	1:D:153:THR:HG22	0.43	1.90	6	1
1:D:86:LEU:HG	1:D:113:LEU:HD21	0.43	1.89	6	1
1:A:74:LEU:HD11	1:D:57:GLN:HG3	0.43	1.89	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:E:107:THR:HB	1:E:120:SER:HA	0.43	1.91	10	1
1:A:105:ASP:HB2	1:A:111:LEU:HB2	0.43	1.91	1	2
1:B:73:PHE:CD1	1:B:152:ALA:HB1	0.43	2.49	2	1
1:C:17:VAL:HG11	1:D:36:GLN:HE21	0.43	1.74	2	1
1:B:99:VAL:HB	1:B:143:ALA:HB1	0.43	1.90	5	1
1:B:63:THR:HA	1:B:66:ALA:O	0.43	2.14	7	1
1:B:155:LYS:HZ2	1:E:128:THR:HG21	0.43	1.74	7	1
1:F:22:ALA:HB3	1:F:59:ASN:O	0.43	2.13	7	1
1:D:15:GLU:HG3	1:E:147:ALA:HA	0.43	1.91	8	2
1:A:107:THR:HB	1:A:120:SER:HA	0.43	1.91	10	1
1:C:74:LEU:HD11	1:F:57:GLN:HG3	0.43	1.89	10	1
1:B:92:ALA:HB3	1:E:34:LEU:HB3	0.43	1.91	3	1
1:A:9:THR:HA	1:B:153:THR:HG22	0.43	1.90	6	1
1:E:106:ARG:CZ	1:E:132:PRO:HG2	0.43	2.44	6	1
1:B:118:PHE:CD1	1:B:157:GLN:HB2	0.43	2.48	8	1
1:C:59:ASN:CA	1:C:128:THR:HG23	0.43	2.44	8	1
1:D:55:ASN:OD1	1:D:130:THR:CG2	0.43	2.66	8	1
1:E:15:GLU:HG3	1:F:147:ALA:HA	0.43	1.91	8	2
1:A:89:GLN:HG3	1:A:149:ASN:HB2	0.42	1.91	1	1
1:F:89:GLN:HG3	1:F:149:ASN:HB2	0.42	1.91	1	1
1:A:144:THR:HG22	1:A:145:PRO:HD2	0.42	1.88	2	1
1:B:74:LEU:HD21	1:E:55:ASN:OD1	0.42	2.14	2	1
1:C:77:ALA:HB2	1:C:83:THR:HG23	0.42	1.90	2	1
1:B:97:THR:N	1:B:144:THR:HB	0.42	2.26	4	1
1:A:5:VAL:CG1	1:C:146:GLY:HA2	0.42	2.44	6	1
1:C:106:ARG:CZ	1:C:132:PRO:HG2	0.42	2.44	6	1
1:F:61:CYS:HB3	1:F:125:ASN:O	0.42	2.13	8	1
1:E:6:ASN:CB	1:F:155:LYS:HE2	0.42	2.44	9	1
1:B:92:ALA:O	1:E:50:SER:HB3	0.42	2.14	1	1
1:E:59:ASN:CA	1:E:128:THR:HG23	0.42	2.44	8	2
1:A:74:LEU:HD21	1:D:55:ASN:OD1	0.42	2.14	2	1
1:F:51:ALA:HA	1:F:136:ARG:HB3	0.42	1.90	3	1
1:B:4:THR:HG22	1:C:157:GLN:HB2	0.42	1.90	5	1
1:B:106:ARG:CZ	1:B:132:PRO:HG2	0.42	2.44	6	1
1:F:106:ARG:CZ	1:F:132:PRO:HG2	0.42	2.44	6	1
1:D:17:VAL:HG13	1:E:36:GLN:HG2	0.42	1.91	8	1
1:A:73:PHE:CB	1:A:111:LEU:HD11	0.42	2.44	9	1
1:D:73:PHE:CB	1:D:111:LEU:HD11	0.42	2.44	9	1
1:D:56:ILE:CG2	1:D:131:ILE:HD12	0.42	2.44	10	1
1:B:89:GLN:HG3	1:B:149:ASN:HB2	0.42	1.91	1	1
1:B:17:VAL:HG11	1:C:36:GLN:HE21	0.42	1.74	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:144:THR:HG22	1:B:145:PRO:HD2	0.42	1.88	2	1
1:A:92:ALA:HB3	1:D:34:LEU:HB3	0.42	1.91	3	1
1:B:51:ALA:HA	1:B:136:ARG:HB3	0.42	1.90	3	1
1:B:90:SER:C	1:E:52:VAL:HG12	0.42	2.39	3	1
1:C:90:SER:C	1:F:52:VAL:HG12	0.42	2.39	3	1
1:A:131:ILE:CD1	1:A:156:VAL:HG12	0.42	2.44	4	1
1:C:92:ALA:HA	1:F:50:SER:HB3	0.42	1.91	5	1
1:D:99:VAL:HB	1:D:143:ALA:HB1	0.42	1.91	5	1
1:B:62:ASP:HA	1:B:126:ASN:OD1	0.42	2.15	6	2
1:F:62:ASP:HA	1:F:126:ASN:OD1	0.42	2.15	6	2
1:A:17:VAL:HG23	1:B:38:ARG:HA	0.42	1.92	7	1
1:B:17:VAL:HG23	1:C:38:ARG:HA	0.42	1.91	7	1
1:E:63:THR:HA	1:E:66:ALA:O	0.42	2.14	7	1
1:E:118:PHE:CD1	1:E:157:GLN:HB2	0.42	2.48	8	1
1:B:6:ASN:CB	1:C:155:LYS:HE2	0.42	2.44	9	1
1:B:4:THR:O	1:B:5:VAL:HG13	0.42	2.14	10	1
1:B:59:ASN:CA	1:B:128:THR:HG23	0.42	2.44	8	2
1:E:17:VAL:HG11	1:F:36:GLN:HE21	0.42	1.74	2	1
1:E:97:THR:N	1:E:144:THR:HB	0.42	2.26	4	1
1:F:131:ILE:CD1	1:F:156:VAL:HG12	0.42	2.45	4	1
1:A:99:VAL:HB	1:A:143:ALA:HB1	0.42	1.90	5	1
1:B:92:ALA:HA	1:E:50:SER:HB3	0.42	1.91	5	1
1:E:17:VAL:HG23	1:F:38:ARG:HA	0.42	1.92	7	1
1:C:15:GLU:HG3	1:D:147:ALA:HA	0.42	1.91	8	1
1:B:86:LEU:CD1	1:B:152:ALA:HB2	0.42	2.45	10	1
1:F:56:ILE:CG2	1:F:131:ILE:HD12	0.42	2.44	10	1
1:B:105:ASP:HB2	1:B:111:LEU:HB2	0.42	1.91	1	2
1:F:24:ASP:HB3	1:F:27:SER:HB2	0.42	1.92	1	1
1:D:103:ILE:HG12	1:D:113:LEU:HG	0.42	1.89	8	2
1:E:131:ILE:CD1	1:E:156:VAL:HG12	0.42	2.45	4	1
1:C:84:ASN:HB3	1:C:102:GLN:HG2	0.42	1.91	5	1
1:C:99:VAL:HB	1:C:143:ALA:HB1	0.42	1.90	5	1
1:D:17:VAL:HG23	1:E:38:ARG:HA	0.42	1.92	7	1
1:C:86:LEU:HG	1:C:113:LEU:HD22	0.42	1.92	8	1
1:D:61:CYS:HB3	1:D:125:ASN:O	0.42	2.13	8	1
1:C:89:GLN:HG3	1:C:149:ASN:HB2	0.42	1.91	1	1
1:C:92:ALA:HB3	1:F:34:LEU:HB3	0.42	1.91	3	1
1:F:84:ASN:HB3	1:F:102:GLN:HG2	0.42	1.91	5	1
1:A:63:THR:HA	1:A:66:ALA:O	0.42	2.14	7	1
1:C:5:VAL:CB	1:D:17:VAL:HG12	0.42	2.45	8	1
1:C:6:ASN:CB	1:D:155:LYS:HE2	0.42	2.44	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:56:ILE:CG2	1:A:131:ILE:HD12	0.42	2.44	10	1
1:B:107:THR:HB	1:B:120:SER:HA	0.42	1.91	10	1
1:C:24:ASP:HB3	1:C:27:SER:HB2	0.42	1.92	1	1
1:D:89:GLN:HG3	1:D:149:ASN:HB2	0.42	1.91	1	1
1:A:77:ALA:HB2	1:A:83:THR:HG23	0.42	1.90	2	1
1:C:51:ALA:HA	1:C:136:ARG:HB3	0.42	1.90	3	1
1:D:73:PHE:HB2	1:D:103:ILE:HD13	0.42	1.92	3	1
1:D:73:PHE:HB3	1:D:113:LEU:HD23	0.42	1.92	4	1
1:A:62:ASP:HA	1:A:126:ASN:OD1	0.42	2.15	6	2
1:E:5:VAL:CB	1:F:17:VAL:HG12	0.42	2.45	8	1
1:A:4:THR:O	1:A:5:VAL:HG13	0.42	2.14	10	1
1:E:86:LEU:CD1	1:E:152:ALA:HB2	0.42	2.45	10	1
1:A:92:ALA:O	1:D:50:SER:HB3	0.42	2.14	1	1
1:A:73:PHE:HB2	1:A:103:ILE:HD13	0.42	1.92	3	2
1:B:124:LEU:HD12	1:B:129:ASN:CG	0.42	2.40	4	1
1:C:131:ILE:CD1	1:C:156:VAL:HG12	0.42	2.45	4	1
1:F:124:LEU:HD12	1:F:129:ASN:CG	0.42	2.40	4	1
1:B:5:VAL:CG1	1:D:146:GLY:HA2	0.42	2.44	6	1
1:D:62:ASP:HA	1:D:126:ASN:OD1	0.42	2.15	6	3
1:F:86:LEU:HG	1:F:113:LEU:HD22	0.42	1.92	8	1
1:E:4:THR:O	1:E:5:VAL:HG13	0.42	2.14	10	1
1:C:74:LEU:HD21	1:F:55:ASN:OD1	0.42	2.14	2	1
1:F:77:ALA:HB2	1:F:83:THR:HG23	0.42	1.90	2	1
1:B:17:VAL:HG21	1:C:36:GLN:HE21	0.42	1.75	3	1
1:C:73:PHE:HB2	1:C:103:ILE:HD13	0.42	1.92	3	1
1:E:17:VAL:HG21	1:F:36:GLN:HE21	0.42	1.75	3	1
1:F:73:PHE:HB3	1:F:113:LEU:HD23	0.42	1.92	4	1
1:B:116:ALA:HA	1:E:128:THR:O	0.42	2.15	5	1
1:E:84:ASN:HB3	1:E:102:GLN:HG2	0.42	1.91	5	1
1:F:99:VAL:HB	1:F:143:ALA:CB	0.42	2.45	5	1
1:A:15:GLU:HG3	1:B:147:ALA:HA	0.42	1.91	8	1
1:A:17:VAL:HG13	1:B:36:GLN:HG2	0.42	1.91	8	1
1:F:59:ASN:CA	1:F:128:THR:HG23	0.42	2.44	8	1
1:C:56:ILE:CG2	1:C:131:ILE:HD12	0.42	2.44	10	1
1:A:59:ASN:CA	1:A:128:THR:HG23	0.42	2.44	8	2
1:D:24:ASP:HB3	1:D:27:SER:HB2	0.42	1.92	1	1
1:E:39:THR:OG1	1:E:143:ALA:O	0.42	2.33	3	1
1:D:131:ILE:CD1	1:D:156:VAL:HG12	0.42	2.45	4	1
1:E:73:PHE:HB3	1:E:113:LEU:HD23	0.42	1.92	4	1
1:A:116:ALA:HA	1:D:128:THR:O	0.42	2.15	5	1
1:D:86:LEU:HG	1:D:113:LEU:HD22	0.42	1.92	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:E:98:ASN:HA	1:E:140:THR:OG1	0.42	2.13	9	1
1:C:107:THR:HB	1:C:120:SER:HA	0.42	1.91	10	1
1:A:92:ALA:HA	1:D:50:SER:HB3	0.41	1.91	5	1
1:C:56:ILE:CB	1:C:131:ILE:HD12	0.41	2.40	7	1
1:B:5:VAL:CB	1:C:17:VAL:HG12	0.41	2.45	8	1
1:E:17:VAL:HG13	1:F:36:GLN:HG2	0.41	1.91	8	1
1:B:56:ILE:CG2	1:B:131:ILE:HD12	0.41	2.44	10	1
1:E:56:ILE:CG2	1:E:131:ILE:HD12	0.41	2.44	10	1
1:A:90:SER:C	1:D:52:VAL:HG12	0.41	2.39	3	1
1:F:73:PHE:HB2	1:F:103:ILE:HD13	0.41	1.92	3	1
1:B:131:ILE:CD1	1:B:156:VAL:HG12	0.41	2.45	4	1
1:C:124:LEU:HD12	1:C:129:ASN:CG	0.41	2.40	4	1
1:A:84:ASN:HB3	1:A:102:GLN:HG2	0.41	1.91	5	1
1:C:17:VAL:HG13	1:D:36:GLN:HG2	0.41	1.91	8	1
1:B:89:GLN:OE1	1:B:91:SER:HB3	0.41	2.16	9	1
1:E:89:GLN:OE1	1:E:91:SER:HB3	0.41	2.16	9	1
1:F:4:THR:O	1:F:5:VAL:HG13	0.41	2.14	10	1
1:D:77:ALA:HB2	1:D:83:THR:HG23	0.41	1.90	2	1
1:E:73:PHE:HB2	1:E:103:ILE:HD13	0.41	1.92	2	2
1:A:73:PHE:HB3	1:A:113:LEU:HD23	0.41	1.92	4	1
1:A:22:ALA:HA	1:B:36:GLN:CB	0.41	2.46	5	1
1:D:84:ASN:HB3	1:D:102:GLN:HG2	0.41	1.91	5	1
1:E:4:THR:HG22	1:F:157:GLN:HB2	0.41	1.90	5	1
1:F:99:VAL:HB	1:F:143:ALA:HB1	0.41	1.90	5	1
1:D:63:THR:HA	1:D:66:ALA:O	0.41	2.14	7	1
1:A:5:VAL:CB	1:B:17:VAL:HG12	0.41	2.45	8	1
1:C:49:SER:HB2	1:C:137:TYR:HB2	0.41	1.93	8	1
1:C:86:LEU:CD1	1:C:152:ALA:HB2	0.41	2.45	10	1
1:E:86:LEU:HD23	1:E:87:ALA:H	0.41	1.75	10	1
1:C:92:ALA:O	1:F:50:SER:HB3	0.41	2.14	1	1
1:A:17:VAL:HG21	1:B:36:GLN:HE21	0.41	1.75	3	1
1:A:124:LEU:HD12	1:A:129:ASN:CG	0.41	2.40	4	1
1:E:124:LEU:HD12	1:E:129:ASN:CG	0.41	2.40	4	1
1:C:99:VAL:HB	1:C:143:ALA:CB	0.41	2.45	5	1
1:D:88:LEU:HD13	1:D:96:ALA:O	0.41	2.16	5	1
1:C:62:ASP:HA	1:C:126:ASN:OD1	0.41	2.15	6	2
1:A:86:LEU:HG	1:A:113:LEU:HD22	0.41	1.92	8	1
1:A:89:GLN:OE1	1:A:91:SER:HB3	0.41	2.16	9	1
1:C:86:LEU:HD23	1:C:87:ALA:H	0.41	1.75	10	1
1:D:4:THR:O	1:D:5:VAL:HG13	0.41	2.14	10	1
1:A:24:ASP:HB3	1:A:27:SER:HB2	0.41	1.92	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:24:ASP:HB3	1:B:27:SER:HB2	0.41	1.92	1	1
1:D:59:ASN:CA	1:D:128:THR:HG23	0.41	2.44	8	2
1:F:101:VAL:CG2	1:F:135:ALA:HB1	0.41	2.46	1	1
1:F:56:ILE:O	1:F:56:ILE:CG2	0.41	2.69	4	1
1:B:88:LEU:HD13	1:B:96:ALA:O	0.41	2.16	5	1
1:C:116:ALA:HA	1:F:128:THR:O	0.41	2.15	5	1
1:D:1:ALA:HA	1:E:159:GLN:HA	0.41	1.93	8	1
1:D:5:VAL:CB	1:E:17:VAL:HG12	0.41	2.45	8	1
1:E:49:SER:HB2	1:E:137:TYR:HB2	0.41	1.93	8	1
1:C:4:THR:O	1:C:5:VAL:HG13	0.41	2.14	10	1
1:D:86:LEU:CD1	1:D:152:ALA:HB2	0.41	2.45	10	1
1:F:86:LEU:HD23	1:F:87:ALA:H	0.41	1.75	10	1
1:F:86:LEU:CD1	1:F:152:ALA:HB2	0.41	2.45	10	1
1:B:101:VAL:CG2	1:B:135:ALA:HB1	0.41	2.46	1	1
1:D:17:VAL:HG21	1:E:36:GLN:HE21	0.41	1.75	3	1
1:C:73:PHE:HB3	1:C:113:LEU:HD23	0.41	1.92	4	1
1:A:99:VAL:HB	1:A:143:ALA:CB	0.41	2.45	5	1
1:B:99:VAL:HB	1:B:143:ALA:CB	0.41	2.45	5	1
1:D:22:ALA:HA	1:E:36:GLN:CB	0.41	2.46	5	1
1:D:58:LEU:HB2	1:D:129:ASN:O	0.41	2.15	5	1
1:E:88:LEU:HD13	1:E:96:ALA:O	0.41	2.16	5	1
1:F:88:LEU:HD13	1:F:96:ALA:O	0.41	2.15	5	1
1:E:62:ASP:HA	1:E:126:ASN:OD1	0.41	2.15	6	3
1:B:15:GLU:HG3	1:C:147:ALA:HA	0.41	1.91	8	2
1:A:86:LEU:CD1	1:A:152:ALA:HB2	0.41	2.45	10	1
1:E:58:LEU:O	1:E:61:CYS:SG	0.41	2.79	10	1
1:E:24:ASP:HB3	1:E:27:SER:HB2	0.41	1.92	1	1
1:A:17:VAL:HG11	1:B:36:GLN:HE21	0.41	1.74	2	1
1:A:45:GLU:HG3	1:A:140:THR:O	0.41	2.16	2	1
1:B:73:PHE:HB2	1:B:103:ILE:HD13	0.41	1.93	2	2
1:B:73:PHE:HB3	1:B:113:LEU:HD23	0.41	1.92	4	1
1:D:56:ILE:O	1:D:56:ILE:CG2	0.41	2.69	4	1
1:D:124:LEU:HD12	1:D:129:ASN:CG	0.41	2.40	4	1
1:B:22:ALA:HA	1:C:36:GLN:CB	0.41	2.46	5	1
1:C:58:LEU:HB2	1:C:129:ASN:O	0.41	2.15	5	1
1:C:88:LEU:HD13	1:C:96:ALA:O	0.41	2.15	5	1
1:F:84:ASN:HA	1:F:113:LEU:HB3	0.41	1.93	5	1
1:A:21:CYS:HB3	1:A:58:LEU:HD22	0.41	1.93	7	1
1:B:86:LEU:HD23	1:B:87:ALA:H	0.41	1.75	10	1
1:C:101:VAL:CG2	1:C:135:ALA:HB1	0.41	2.46	1	1
1:D:101:VAL:CG2	1:D:135:ALA:HB1	0.41	2.46	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:E:89:GLN:HG3	1:E:149:ASN:HB2	0.41	1.91	1	1
1:E:101:VAL:CG2	1:E:135:ALA:HB1	0.41	2.46	1	1
1:E:105:ASP:HB2	1:E:111:LEU:HB2	0.41	1.91	1	2
1:C:84:ASN:HA	1:C:113:LEU:HB3	0.41	1.93	5	1
1:E:58:LEU:HB2	1:E:129:ASN:O	0.41	2.15	5	1
1:B:89:GLN:O	1:E:52:VAL:HA	0.41	2.16	7	1
1:E:21:CYS:HB3	1:E:58:LEU:HD22	0.41	1.93	7	1
1:C:89:GLN:OE1	1:C:91:SER:HB3	0.41	2.16	9	1
1:A:101:VAL:CG2	1:A:135:ALA:HB1	0.41	2.46	1	1
1:C:79:ASP:HB2	1:C:140:THR:HG21	0.41	1.93	10	2
1:A:88:LEU:HD13	1:A:96:ALA:O	0.41	2.16	5	1
1:E:22:ALA:HA	1:F:36:GLN:CB	0.41	2.46	5	1
1:E:99:VAL:HB	1:E:143:ALA:CB	0.41	2.45	5	1
1:B:21:CYS:HB3	1:B:58:LEU:HD22	0.41	1.93	7	1
1:C:52:VAL:HG23	1:C:54:PHE:HD1	0.41	1.76	7	1
1:D:21:CYS:HB3	1:D:58:LEU:HD22	0.41	1.93	7	1
1:B:85:VAL:HG22	1:B:102:GLN:HG3	0.41	1.93	9	1
1:C:85:VAL:HG22	1:C:102:GLN:HG3	0.41	1.93	9	1
1:D:89:GLN:OE1	1:D:91:SER:HB3	0.41	2.16	9	1
1:F:89:GLN:OE1	1:F:91:SER:HB3	0.41	2.16	9	1
1:A:58:LEU:O	1:A:61:CYS:SG	0.41	2.79	10	1
1:B:58:LEU:O	1:B:61:CYS:SG	0.41	2.79	10	1
1:F:107:THR:HB	1:F:120:SER:HA	0.41	1.90	10	1
1:B:18:ASN:HA	1:C:39:THR:HG22	0.41	1.93	2	1
1:D:32:VAL:CG1	1:D:52:VAL:HG11	0.41	2.46	6	1
1:B:17:VAL:HG13	1:C:36:GLN:HG2	0.41	1.91	8	1
1:C:1:ALA:HA	1:D:159:GLN:HA	0.41	1.93	8	1
1:D:49:SER:HB2	1:D:137:TYR:HB2	0.41	1.93	8	1
1:C:84:ASN:O	1:C:103:ILE:HD12	0.41	2.16	9	1
1:F:79:ASP:HB2	1:F:140:THR:HG21	0.40	1.93	1	2
1:A:144:THR:HG22	1:A:145:PRO:N	0.40	2.31	2	1
1:E:18:ASN:HA	1:F:39:THR:HG22	0.40	1.93	2	1
1:F:42:LEU:HD23	1:F:99:VAL:CG1	0.40	2.46	2	1
1:A:58:LEU:HB2	1:A:129:ASN:O	0.40	2.15	5	1
1:C:111:LEU:HD11	1:C:117:THR:O	0.40	2.16	5	1
1:D:99:VAL:HB	1:D:143:ALA:CB	0.40	2.45	5	1
1:E:32:VAL:CG1	1:E:52:VAL:HG11	0.40	2.46	6	1
1:C:58:LEU:O	1:C:61:CYS:SG	0.40	2.79	10	1
1:B:42:LEU:HD23	1:B:99:VAL:CG1	0.40	2.46	2	1
1:E:45:GLU:HG3	1:E:140:THR:O	0.40	2.16	2	1
1:A:39:THR:OG1	1:A:143:ALA:O	0.40	2.33	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:17:VAL:HG21	1:D:36:GLN:HE21	0.40	1.75	3	1
1:F:58:LEU:HB2	1:F:129:ASN:O	0.40	2.15	5	1
1:F:97:THR:O	1:F:99:VAL:HG12	0.40	2.17	6	1
1:B:7:GLY:HA3	1:C:154:PHE:CZ	0.40	2.51	7	1
1:C:89:GLN:O	1:F:52:VAL:HA	0.40	2.16	7	1
1:D:85:VAL:HG22	1:D:102:GLN:HG3	0.40	1.93	9	1
1:F:84:ASN:O	1:F:103:ILE:HD12	0.40	2.17	9	1
1:A:86:LEU:HD23	1:A:87:ALA:H	0.40	1.75	10	1
1:B:21:CYS:HB3	1:B:158:TYR:OH	0.40	2.16	10	1
1:B:52:VAL:O	1:B:134:GLN:HA	0.40	2.16	10	1
1:C:12:PHE:CD1	1:D:34:LEU:HD11	0.40	2.52	10	1
1:D:58:LEU:O	1:D:61:CYS:SG	0.40	2.79	10	1
1:F:52:VAL:O	1:F:134:GLN:HA	0.40	2.16	10	1
1:C:144:THR:HG22	1:C:145:PRO:N	0.40	2.31	2	1
1:D:85:VAL:HG21	1:D:138:PHE:HB3	0.40	1.93	2	1
1:C:56:ILE:O	1:C:56:ILE:CG2	0.40	2.69	4	1
1:E:78:ILE:HG22	1:E:82:HIS:HB3	0.40	1.94	4	1
1:B:58:LEU:HB2	1:B:129:ASN:O	0.40	2.15	5	1
1:B:32:VAL:CG1	1:B:52:VAL:HG11	0.40	2.46	6	1
1:B:155:LYS:CE	1:E:128:THR:HG21	0.40	2.47	6	1
1:C:17:VAL:HG23	1:D:38:ARG:HA	0.40	1.92	7	1
1:E:7:GLY:HA3	1:F:154:PHE:CZ	0.40	2.51	7	1
1:D:27:SER:O	1:D:28:VAL:C	0.40	2.65	8	1
1:E:86:LEU:HG	1:E:113:LEU:HD22	0.40	1.92	8	1
1:B:116:ALA:HB3	1:E:125:ASN:HB3	0.40	1.94	9	1
1:E:85:VAL:HG22	1:E:102:GLN:HG3	0.40	1.93	9	1
1:D:12:PHE:CD1	1:E:34:LEU:HD11	0.40	2.52	10	1
1:E:97:THR:HB	1:E:144:THR:OG1	0.40	2.17	2	1
1:E:144:THR:HG22	1:E:145:PRO:N	0.40	2.32	2	1
1:F:97:THR:HB	1:F:144:THR:OG1	0.40	2.17	2	1
1:F:144:THR:HG22	1:F:145:PRO:N	0.40	2.31	2	1
1:C:10:VAL:HG13	1:D:32:VAL:HG23	0.40	1.94	3	1
1:C:39:THR:OG1	1:C:143:ALA:O	0.40	2.33	3	1
1:D:78:ILE:HG22	1:D:82:HIS:HB3	0.40	1.94	4	1
1:C:22:ALA:HA	1:D:36:GLN:CB	0.40	2.46	5	1
1:C:155:LYS:CE	1:F:128:THR:HG21	0.40	2.47	6	1
1:C:21:CYS:HB3	1:C:58:LEU:HD22	0.40	1.93	7	1
1:F:21:CYS:HB3	1:F:58:LEU:HD22	0.40	1.93	7	1
1:A:27:SER:O	1:A:28:VAL:C	0.40	2.65	8	1
1:A:12:PHE:CD1	1:B:34:LEU:HD11	0.40	2.51	10	1
1:E:52:VAL:O	1:E:134:GLN:HA	0.40	2.16	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:18:ASN:HA	1:D:39:THR:HG22	0.40	1.93	2	1
1:C:97:THR:HB	1:C:144:THR:OG1	0.40	2.17	2	1
1:A:56:ILE:O	1:A:56:ILE:CG2	0.40	2.69	4	1
1:C:78:ILE:HG22	1:C:82:HIS:HB3	0.40	1.94	4	1
1:D:131:ILE:HD13	1:D:156:VAL:HG11	0.40	1.94	5	1
1:F:131:ILE:HD13	1:F:156:VAL:HG11	0.40	1.93	5	1
1:C:97:THR:O	1:C:99:VAL:HG12	0.40	2.17	6	1
1:B:72:ALA:HA	1:B:117:THR:O	0.40	2.17	7	1
1:E:72:ALA:HA	1:E:117:THR:O	0.40	2.17	7	1
1:F:52:VAL:HG23	1:F:54:PHE:HD1	0.40	1.76	7	1
1:A:78:ILE:HG22	1:A:85:VAL:HB	0.40	1.93	9	1
1:B:84:ASN:O	1:B:103:ILE:HD12	0.40	2.17	9	1
1:D:52:VAL:O	1:D:134:GLN:HA	0.40	2.16	10	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	157/160 (98%)	135±4 (86±2%)	18±4 (12±3%)	4±2 (2±1%)	7	44
1	B	157/160 (98%)	135±4 (86±2%)	18±4 (12±3%)	4±2 (2±1%)	7	44
1	C	157/160 (98%)	135±4 (86±2%)	18±4 (12±3%)	4±2 (2±1%)	7	44
1	D	157/160 (98%)	135±4 (86±2%)	18±4 (12±3%)	4±2 (2±1%)	7	44
1	E	157/160 (98%)	135±4 (86±2%)	18±4 (12±3%)	4±2 (2±1%)	7	44
1	F	157/160 (98%)	135±4 (86±2%)	18±4 (12±3%)	4±2 (2±1%)	7	44
All	All	9420/9600 (98%)	8088 (86%)	1106 (12%)	226 (2%)	7	44

All 90 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	80	ALA	6
1	A	90	SER	6

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Mol	Chain	Res	Type	Models (Total)
1	B	80	ALA	6
1	B	90	SER	6
1	C	80	ALA	6
1	C	90	SER	6
1	D	80	ALA	6
1	D	90	SER	6
1	E	80	ALA	6
1	E	90	SER	6
1	F	80	ALA	6
1	F	90	SER	6
1	A	89	GLN	5
1	A	94	GLY	5
1	B	89	GLN	5
1	B	94	GLY	5
1	C	89	GLN	5
1	C	94	GLY	5
1	D	89	GLN	5
1	D	94	GLY	5
1	E	89	GLN	5
1	E	94	GLY	5
1	F	89	GLN	5
1	F	94	GLY	5
1	A	2	ALA	4
1	B	2	ALA	4
1	C	2	ALA	4
1	D	2	ALA	4
1	E	2	ALA	4
1	F	2	ALA	4
1	A	142	ALA	2
1	B	142	ALA	2
1	C	142	ALA	2
1	D	142	ALA	2
1	E	142	ALA	2
1	F	142	ALA	2
1	B	19	ALA	2
1	C	19	ALA	2
1	E	19	ALA	2
1	F	19	ALA	2
1	A	65	VAL	1
1	B	65	VAL	1
1	C	65	VAL	1
1	D	65	VAL	1

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Mol	Chain	Res	Type	Models (Total)
1	E	65	VAL	1
1	F	65	VAL	1
1	A	21	CYS	1
1	A	83	THR	1
1	B	21	CYS	1
1	B	83	THR	1
1	C	21	CYS	1
1	C	83	THR	1
1	D	21	CYS	1
1	D	83	THR	1
1	E	21	CYS	1
1	E	83	THR	1
1	F	21	CYS	1
1	F	83	THR	1
1	A	20	ALA	1
1	A	60	ASP	1
1	A	99	VAL	1
1	A	141	GLY	1
1	B	20	ALA	1
1	B	60	ASP	1
1	B	99	VAL	1
1	B	141	GLY	1
1	C	20	ALA	1
1	C	60	ASP	1
1	C	99	VAL	1
1	C	141	GLY	1
1	D	20	ALA	1
1	D	60	ASP	1
1	D	99	VAL	1
1	D	141	GLY	1
1	E	20	ALA	1
1	E	60	ASP	1
1	E	99	VAL	1
1	E	141	GLY	1
1	F	20	ALA	1
1	F	60	ASP	1
1	F	99	VAL	1
1	F	141	GLY	1
1	A	19	ALA	1
1	D	19	ALA	1
1	A	28	VAL	1
1	B	28	VAL	1

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Mol	Chain	Res	Type	Models (Total)
1	C	28	VAL	1
1	D	28	VAL	1
1	E	28	VAL	1
1	F	28	VAL	1

6.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	112/113 (99%)	70±4 (62±4%)	42±4 (38±4%)	0	7
1	B	112/113 (99%)	70±4 (63±4%)	42±4 (37±4%)	1	8
1	C	112/113 (99%)	70±4 (62±4%)	42±4 (38±4%)	0	7
1	D	112/113 (99%)	70±4 (63±4%)	42±4 (37±4%)	0	7
1	E	112/113 (99%)	70±4 (63±4%)	42±4 (37±4%)	0	7
1	F	112/113 (99%)	70±4 (63±4%)	42±4 (37±4%)	1	8
All	All	6720/6780 (99%)	4209 (63%)	2511 (37%)	0	7

All 591 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	76	THR	9
1	A	79	ASP	9
1	A	86	LEU	9
1	A	122	THR	9
1	B	76	THR	9
1	B	79	ASP	9
1	B	86	LEU	9
1	B	122	THR	9
1	C	76	THR	9
1	C	79	ASP	9
1	C	86	LEU	9
1	C	122	THR	9
1	D	76	THR	9
1	D	79	ASP	9

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Mol	Chain	Res	Type	Models (Total)
1	D	86	LEU	9
1	D	122	THR	9
1	E	76	THR	9
1	E	79	ASP	9
1	E	86	LEU	9
1	E	122	THR	9
1	F	76	THR	9
1	F	79	ASP	9
1	F	86	LEU	9
1	F	122	THR	9
1	A	13	LYS	8
1	A	21	CYS	8
1	A	68	LYS	8
1	A	88	LEU	8
1	A	103	ILE	8
1	A	130	THR	8
1	A	140	THR	8
1	B	13	LYS	8
1	B	21	CYS	8
1	B	68	LYS	8
1	B	88	LEU	8
1	B	103	ILE	8
1	B	130	THR	8
1	B	140	THR	8
1	C	13	LYS	8
1	C	21	CYS	8
1	C	68	LYS	8
1	C	88	LEU	8
1	C	103	ILE	8
1	C	130	THR	8
1	C	140	THR	8
1	D	13	LYS	8
1	D	21	CYS	8
1	D	68	LYS	8
1	D	88	LEU	8
1	D	103	ILE	8
1	D	130	THR	8
1	D	140	THR	8
1	E	13	LYS	8
1	E	21	CYS	8
1	E	68	LYS	8
1	E	88	LEU	8

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Mol	Chain	Res	Type	Models (Total)
1	E	103	ILE	8
1	E	130	THR	8
1	E	140	THR	8
1	F	13	LYS	8
1	F	21	CYS	8
1	F	68	LYS	8
1	F	88	LEU	8
1	F	103	ILE	8
1	F	130	THR	8
1	F	140	THR	8
1	A	31	THR	7
1	A	41	SER	7
1	A	58	LEU	7
1	A	63	THR	7
1	A	67	SER	7
1	A	73	PHE	7
1	A	83	THR	7
1	A	89	GLN	7
1	A	104	LEU	7
1	A	106	ARG	7
1	A	120	SER	7
1	A	153	THR	7
1	B	31	THR	7
1	B	41	SER	7
1	B	58	LEU	7
1	B	63	THR	7
1	B	67	SER	7
1	B	73	PHE	7
1	B	83	THR	7
1	B	89	GLN	7
1	B	104	LEU	7
1	B	106	ARG	7
1	B	120	SER	7
1	B	153	THR	7
1	C	31	THR	7
1	C	41	SER	7
1	C	58	LEU	7
1	C	63	THR	7
1	C	67	SER	7
1	C	73	PHE	7
1	C	83	THR	7
1	C	89	GLN	7

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Mol	Chain	Res	Type	Models (Total)
1	C	104	LEU	7
1	C	106	ARG	7
1	C	120	SER	7
1	C	153	THR	7
1	D	31	THR	7
1	D	41	SER	7
1	D	58	LEU	7
1	D	63	THR	7
1	D	67	SER	7
1	D	73	PHE	7
1	D	83	THR	7
1	D	89	GLN	7
1	D	104	LEU	7
1	D	106	ARG	7
1	D	120	SER	7
1	D	153	THR	7
1	E	31	THR	7
1	E	41	SER	7
1	E	58	LEU	7
1	E	63	THR	7
1	E	67	SER	7
1	E	73	PHE	7
1	E	83	THR	7
1	E	89	GLN	7
1	E	104	LEU	7
1	E	106	ARG	7
1	E	120	SER	7
1	E	153	THR	7
1	F	31	THR	7
1	F	41	SER	7
1	F	58	LEU	7
1	F	63	THR	7
1	F	67	SER	7
1	F	73	PHE	7
1	F	83	THR	7
1	F	89	GLN	7
1	F	104	LEU	7
1	F	106	ARG	7
1	F	120	SER	7
1	F	153	THR	7
1	A	57	GLN	7
1	B	57	GLN	7

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Mol	Chain	Res	Type	Models (Total)
1	C	57	GLN	7
1	D	57	GLN	7
1	E	57	GLN	7
1	F	57	GLN	7
1	A	42	LEU	6
1	A	62	ASP	6
1	A	114	ASP	6
1	A	117	THR	6
1	A	159	GLN	6
1	B	42	LEU	6
1	B	62	ASP	6
1	B	114	ASP	6
1	B	117	THR	6
1	B	159	GLN	6
1	C	42	LEU	6
1	C	62	ASP	6
1	C	114	ASP	6
1	C	117	THR	6
1	C	159	GLN	6
1	D	42	LEU	6
1	D	62	ASP	6
1	D	114	ASP	6
1	D	117	THR	6
1	D	159	GLN	6
1	E	42	LEU	6
1	E	62	ASP	6
1	E	114	ASP	6
1	E	117	THR	6
1	E	159	GLN	6
1	F	42	LEU	6
1	F	62	ASP	6
1	F	114	ASP	6
1	F	117	THR	6
1	F	159	GLN	6
1	A	36	GLN	6
1	A	74	LEU	6
1	A	102	GLN	6
1	B	74	LEU	6
1	B	102	GLN	6
1	C	36	GLN	6
1	C	74	LEU	6
1	C	102	GLN	6

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Mol	Chain	Res	Type	Models (Total)
1	D	36	GLN	6
1	D	74	LEU	6
1	D	102	GLN	6
1	E	36	GLN	6
1	E	74	LEU	6
1	E	102	GLN	6
1	F	74	LEU	6
1	F	102	GLN	6
1	A	133	PHE	6
1	B	133	PHE	6
1	C	133	PHE	6
1	D	133	PHE	6
1	E	133	PHE	6
1	F	133	PHE	6
1	A	97	THR	6
1	B	97	THR	6
1	C	97	THR	6
1	D	97	THR	6
1	E	97	THR	6
1	F	97	THR	6
1	A	56	ILE	5
1	A	71	VAL	5
1	A	154	PHE	5
1	B	56	ILE	5
1	B	71	VAL	5
1	B	154	PHE	5
1	C	56	ILE	5
1	C	71	VAL	5
1	C	154	PHE	5
1	D	56	ILE	5
1	D	71	VAL	5
1	D	154	PHE	5
1	E	56	ILE	5
1	E	71	VAL	5
1	E	154	PHE	5
1	F	56	ILE	5
1	F	71	VAL	5
1	F	154	PHE	5
1	A	18	ASN	5
1	A	34	LEU	5
1	B	18	ASN	5
1	B	34	LEU	5

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Mol	Chain	Res	Type	Models (Total)
1	C	18	ASN	5
1	C	34	LEU	5
1	D	18	ASN	5
1	D	34	LEU	5
1	E	18	ASN	5
1	E	34	LEU	5
1	F	18	ASN	5
1	F	34	LEU	5
1	A	78	ILE	5
1	A	112	THR	5
1	A	157	GLN	5
1	B	36	GLN	5
1	B	78	ILE	5
1	B	112	THR	5
1	B	157	GLN	5
1	C	78	ILE	5
1	C	112	THR	5
1	C	157	GLN	5
1	D	78	ILE	5
1	D	112	THR	5
1	D	157	GLN	5
1	E	78	ILE	5
1	E	112	THR	5
1	E	157	GLN	5
1	F	36	GLN	5
1	F	78	ILE	5
1	F	112	THR	5
1	F	157	GLN	5
1	A	33	GLN	5
1	B	33	GLN	5
1	C	33	GLN	5
1	D	33	GLN	5
1	E	33	GLN	5
1	F	33	GLN	5
1	A	124	LEU	5
1	B	124	LEU	5
1	C	124	LEU	5
1	D	124	LEU	5
1	E	124	LEU	5
1	F	124	LEU	5
1	A	39	THR	4
1	A	99	VAL	4

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Mol	Chain	Res	Type	Models (Total)
1	A	101	VAL	4
1	B	39	THR	4
1	B	99	VAL	4
1	B	101	VAL	4
1	C	39	THR	4
1	C	99	VAL	4
1	C	101	VAL	4
1	D	39	THR	4
1	D	99	VAL	4
1	D	101	VAL	4
1	E	39	THR	4
1	E	99	VAL	4
1	E	101	VAL	4
1	F	39	THR	4
1	F	99	VAL	4
1	F	101	VAL	4
1	A	23	VAL	4
1	B	23	VAL	4
1	C	23	VAL	4
1	D	23	VAL	4
1	E	23	VAL	4
1	F	23	VAL	4
1	A	125	ASN	4
1	B	125	ASN	4
1	C	125	ASN	4
1	D	125	ASN	4
1	E	125	ASN	4
1	F	125	ASN	4
1	A	5	VAL	4
1	A	59	ASN	4
1	A	137	TYR	4
1	B	5	VAL	4
1	B	59	ASN	4
1	B	137	TYR	4
1	C	5	VAL	4
1	C	59	ASN	4
1	C	137	TYR	4
1	D	5	VAL	4
1	D	59	ASN	4
1	D	137	TYR	4
1	E	5	VAL	4
1	E	59	ASN	4

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Mol	Chain	Res	Type	Models (Total)
1	E	137	TYR	4
1	F	5	VAL	4
1	F	59	ASN	4
1	F	137	TYR	4
1	A	16	VAL	3
1	A	38	ARG	3
1	A	60	ASP	3
1	A	129	ASN	3
1	B	16	VAL	3
1	B	38	ARG	3
1	B	60	ASP	3
1	B	129	ASN	3
1	C	16	VAL	3
1	C	38	ARG	3
1	C	60	ASP	3
1	C	129	ASN	3
1	D	16	VAL	3
1	D	38	ARG	3
1	D	60	ASP	3
1	D	129	ASN	3
1	E	16	VAL	3
1	E	38	ARG	3
1	E	60	ASP	3
1	E	129	ASN	3
1	F	16	VAL	3
1	F	38	ARG	3
1	F	60	ASP	3
1	F	129	ASN	3
1	A	91	SER	3
1	B	91	SER	3
1	C	91	SER	3
1	D	91	SER	3
1	E	91	SER	3
1	F	91	SER	3
1	A	32	VAL	3
1	A	95	SER	3
1	B	32	VAL	3
1	B	95	SER	3
1	C	32	VAL	3
1	C	95	SER	3
1	D	32	VAL	3
1	D	95	SER	3

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Mol	Chain	Res	Type	Models (Total)
1	E	32	VAL	3
1	E	95	SER	3
1	F	32	VAL	3
1	F	95	SER	3
1	A	15	GLU	3
1	A	29	ASP	3
1	A	44	GLN	3
1	A	64	ASN	3
1	A	119	SER	3
1	A	156	VAL	3
1	B	15	GLU	3
1	B	29	ASP	3
1	B	44	GLN	3
1	B	64	ASN	3
1	B	119	SER	3
1	B	156	VAL	3
1	C	15	GLU	3
1	C	29	ASP	3
1	C	44	GLN	3
1	C	64	ASN	3
1	C	119	SER	3
1	C	156	VAL	3
1	D	15	GLU	3
1	D	29	ASP	3
1	D	44	GLN	3
1	D	64	ASN	3
1	D	119	SER	3
1	D	156	VAL	3
1	E	15	GLU	3
1	E	29	ASP	3
1	E	44	GLN	3
1	E	64	ASN	3
1	E	119	SER	3
1	E	156	VAL	3
1	F	15	GLU	3
1	F	29	ASP	3
1	F	44	GLN	3
1	F	64	ASN	3
1	F	119	SER	3
1	F	156	VAL	3
1	A	4	THR	3
1	A	126	ASN	3

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Mol	Chain	Res	Type	Models (Total)
1	B	4	THR	3
1	B	126	ASN	3
1	C	4	THR	3
1	C	126	ASN	3
1	D	4	THR	3
1	D	126	ASN	3
1	E	4	THR	3
1	E	126	ASN	3
1	F	4	THR	3
1	F	126	ASN	3
1	A	27	SER	3
1	A	138	PHE	3
1	B	27	SER	3
1	B	138	PHE	3
1	C	27	SER	3
1	C	138	PHE	3
1	D	27	SER	3
1	D	138	PHE	3
1	E	27	SER	3
1	E	138	PHE	3
1	F	27	SER	3
1	F	138	PHE	3
1	A	3	THR	2
1	B	3	THR	2
1	C	3	THR	2
1	D	3	THR	2
1	E	3	THR	2
1	F	3	THR	2
1	A	90	SER	2
1	B	90	SER	2
1	C	90	SER	2
1	D	90	SER	2
1	E	90	SER	2
1	F	90	SER	2
1	A	82	HIS	2
1	B	82	HIS	2
1	C	82	HIS	2
1	D	82	HIS	2
1	E	82	HIS	2
1	F	82	HIS	2
1	A	10	VAL	2
1	A	85	VAL	2

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Mol	Chain	Res	Type	Models (Total)
1	A	123	THR	2
1	A	131	ILE	2
1	A	134	GLN	2
1	B	10	VAL	2
1	B	85	VAL	2
1	B	123	THR	2
1	B	131	ILE	2
1	B	134	GLN	2
1	C	10	VAL	2
1	C	85	VAL	2
1	C	123	THR	2
1	C	131	ILE	2
1	C	134	GLN	2
1	D	10	VAL	2
1	D	85	VAL	2
1	D	123	THR	2
1	D	131	ILE	2
1	D	134	GLN	2
1	E	10	VAL	2
1	E	85	VAL	2
1	E	123	THR	2
1	E	131	ILE	2
1	E	134	GLN	2
1	F	10	VAL	2
1	F	85	VAL	2
1	F	123	THR	2
1	F	131	ILE	2
1	F	134	GLN	2
1	A	17	VAL	2
1	A	111	LEU	2
1	A	136	ARG	2
1	A	155	LYS	2
1	B	17	VAL	2
1	B	111	LEU	2
1	B	136	ARG	2
1	B	155	LYS	2
1	C	17	VAL	2
1	C	111	LEU	2
1	C	136	ARG	2
1	C	155	LYS	2
1	D	17	VAL	2
1	D	111	LEU	2

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Mol	Chain	Res	Type	Models (Total)
1	D	136	ARG	2
1	D	155	LYS	2
1	E	17	VAL	2
1	E	111	LEU	2
1	E	136	ARG	2
1	E	155	LYS	2
1	F	17	VAL	2
1	F	111	LEU	2
1	F	136	ARG	2
1	F	155	LYS	2
1	A	9	THR	2
1	A	121	GLU	2
1	B	9	THR	2
1	C	9	THR	2
1	C	121	GLU	2
1	D	9	THR	2
1	E	9	THR	2
1	F	9	THR	2
1	A	24	ASP	1
1	A	30	GLN	1
1	A	50	SER	1
1	A	55	ASN	1
1	A	61	CYS	1
1	A	113	LEU	1
1	A	144	THR	1
1	B	24	ASP	1
1	B	30	GLN	1
1	B	50	SER	1
1	B	55	ASN	1
1	B	61	CYS	1
1	B	144	THR	1
1	C	24	ASP	1
1	C	30	GLN	1
1	C	50	SER	1
1	C	55	ASN	1
1	C	61	CYS	1
1	C	113	LEU	1
1	C	144	THR	1
1	D	24	ASP	1
1	D	30	GLN	1
1	D	50	SER	1
1	D	55	ASN	1

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Mol	Chain	Res	Type	Models (Total)
1	D	61	CYS	1
1	D	144	THR	1
1	E	24	ASP	1
1	E	30	GLN	1
1	E	50	SER	1
1	E	55	ASN	1
1	E	61	CYS	1
1	E	113	LEU	1
1	E	144	THR	1
1	F	24	ASP	1
1	F	30	GLN	1
1	F	50	SER	1
1	F	55	ASN	1
1	F	61	CYS	1
1	F	144	THR	1
1	A	49	SER	1
1	A	84	ASN	1
1	B	49	SER	1
1	B	84	ASN	1
1	C	49	SER	1
1	C	84	ASN	1
1	D	49	SER	1
1	D	84	ASN	1
1	E	49	SER	1
1	E	84	ASN	1
1	F	49	SER	1
1	F	84	ASN	1
1	A	107	THR	1
1	B	107	THR	1
1	C	107	THR	1
1	D	107	THR	1
1	E	107	THR	1
1	F	107	THR	1
1	A	149	ASN	1
1	B	121	GLU	1
1	B	149	ASN	1
1	C	149	ASN	1
1	D	121	GLU	1
1	D	149	ASN	1
1	E	121	GLU	1
1	E	149	ASN	1
1	F	121	GLU	1

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Mol	Chain	Res	Type	Models (Total)
1	F	149	ASN	1
1	A	11	HIS	1
1	A	12	PHE	1
1	A	37	VAL	1
1	A	65	VAL	1
1	A	105	ASP	1
1	B	11	HIS	1
1	B	12	PHE	1
1	B	37	VAL	1
1	B	65	VAL	1
1	B	105	ASP	1
1	C	11	HIS	1
1	C	12	PHE	1
1	C	37	VAL	1
1	C	65	VAL	1
1	C	105	ASP	1
1	D	11	HIS	1
1	D	12	PHE	1
1	D	37	VAL	1
1	D	65	VAL	1
1	D	105	ASP	1
1	E	11	HIS	1
1	E	12	PHE	1
1	E	37	VAL	1
1	E	65	VAL	1
1	E	105	ASP	1
1	F	11	HIS	1
1	F	12	PHE	1
1	F	37	VAL	1
1	F	65	VAL	1
1	F	105	ASP	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation [i](#)

The completeness of assignment taking into account all chemical shift lists is 7% for the well-defined parts and 7% 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	800
Number of shifts mapped to atoms	800
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
$^{13}\text{C}_\alpha$	159	0.24 ± 0.18	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	143	-0.41 ± 0.23	None needed (< 0.5 ppm)
$^{13}\text{C}'$	159	0.53 ± 0.11	Should be applied
^{15}N	159	0.45 ± 0.43	None needed (< 0.5 ppm)

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 7%, i.e. 783 atoms were assigned a chemical shift out of a possible 11361. 0 out of 150 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	472/4837 (10%)	0/1990 (0%)	316/1906 (17%)	156/941 (17%)
Sidechain	299/5912 (5%)	0/3903 (0%)	297/1811 (16%)	2/198 (1%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	12/612 (2%)	0/306 (0%)	12/294 (4%)	0/12 (0%)
Overall	783/11361 (7%)	0/6199 (0%)	625/4011 (16%)	158/1151 (14%)

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 7%, i.e. 787 atoms were assigned a chemical shift out of a possible 11370. 0 out of 150 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	475/4842 (10%)	0/1992 (0%)	318/1908 (17%)	157/942 (17%)
Sidechain	300/5916 (5%)	0/3906 (0%)	298/1812 (16%)	2/198 (1%)
Aromatic	12/612 (2%)	0/306 (0%)	12/294 (4%)	0/12 (0%)
Overall	787/11370 (7%)	0/6204 (0%)	628/4014 (16%)	159/1152 (14%)

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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:

