



Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2026 – 09:19 PM UTC

PDB ID : 1UTA / pdb_00001uta
Title : Solution structure of the C-terminal RNP domain from the divisome protein FtsN
Authors : Yang, J.-C.; van den Ent, F.; Neuhaus, D.; Brevier, J.; Lowe, J.
Deposited on : 2003-12-04

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

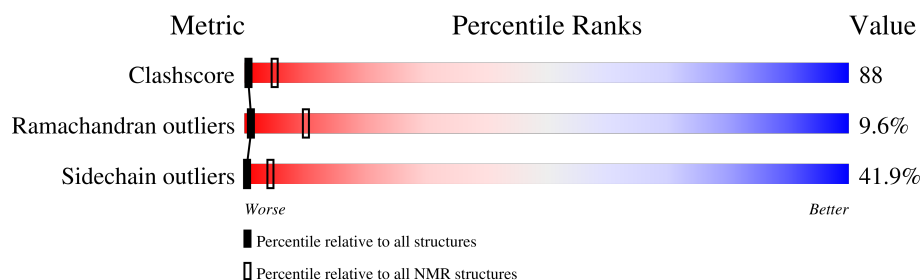
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	81	17% 47% 23% 7% 5%

2 Ensemble composition and analysis

This entry contains 45 models. Model 5 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative.

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:247-A:317 (71)	0.73	5

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 8 clusters and 7 single-model clusters were found.

Cluster number	Models
1	9, 10, 16, 19, 21, 29, 30, 36, 37
2	5, 6, 14, 15, 18, 20, 25
3	1, 2, 3, 4, 12, 13, 17
4	11, 27, 28, 32, 33, 34
5	23, 38, 40
6	44, 45
7	24, 35
8	31, 42
Single-model clusters	7; 8; 22; 26; 39; 41; 43

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1181 atoms, of which 588 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called CELL DIVISION PROTEIN FTSN.

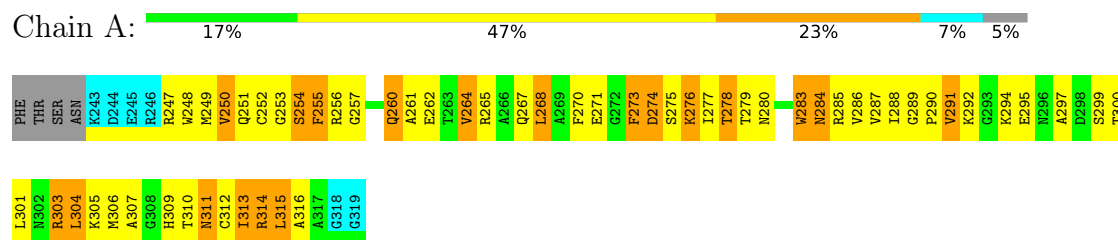
Mol	Chain	Residues	Atoms						Trace
1	A	77	Total	C	H	N	O	S	0
			1181	362	588	116	111	4	

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: CELL DIVISION PROTEIN FTSN

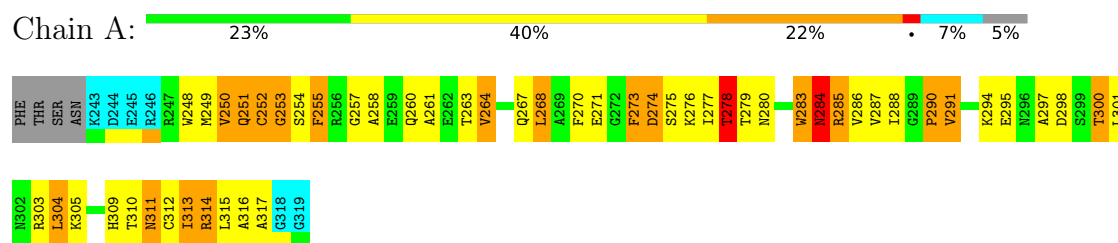


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

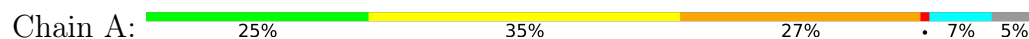
4.2.1 Score per residue for model 1

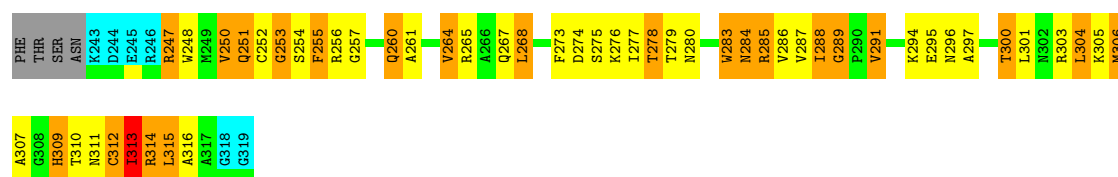
- Molecule 1: CELL DIVISION PROTEIN FTSN



4.2.2 Score per residue for model 2

- Molecule 1: CELL DIVISION PROTEIN FTSN

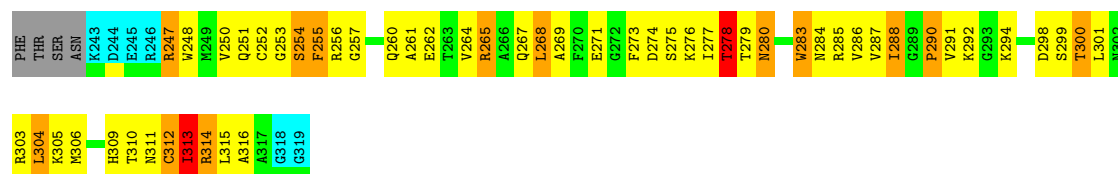




4.2.3 Score per residue for model 3

- Molecule 1: CELL DIVISION PROTEIN FTSN

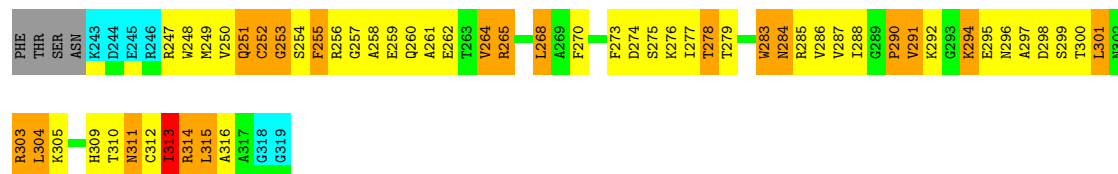
Chain A: 22% 47% 16% 7% 5%



4.2.4 Score per residue for model 4

- Molecule 1: CELL DIVISION PROTEIN FTSN

Chain A: 20% 43% 23% 7% 5%



4.2.5 Score per residue for model 5 (medoid)

- Molecule 1: CELL DIVISION PROTEIN FTSN

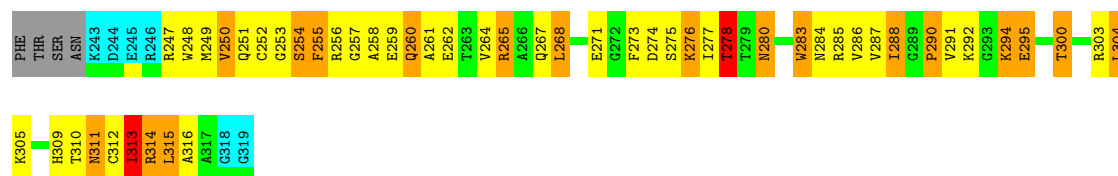
Chain A: 20% 44% 20% 7% 5%



4.2.6 Score per residue for model 6

- Molecule 1: CELL DIVISION PROTEIN FTSN

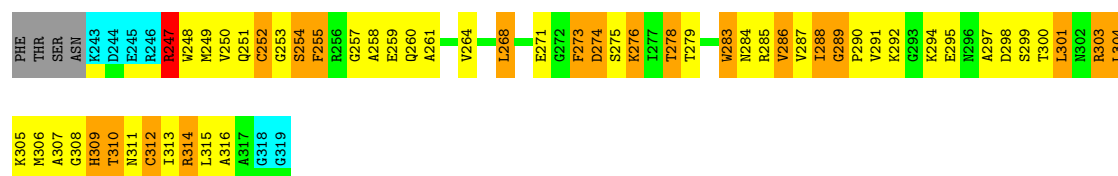
Chain A: 25% 38% 22% 7% 5%



4.2.7 Score per residue for model 7

- Molecule 1: CELL DIVISION PROTEIN FTSN

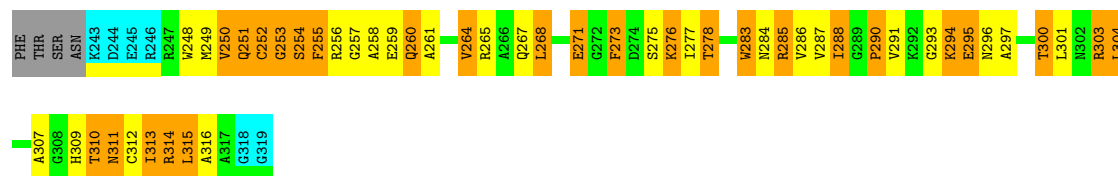
Chain A: 21% 42% 23% 7% 5%



4.2.8 Score per residue for model 8

- Molecule 1: CELL DIVISION PROTEIN FTSN

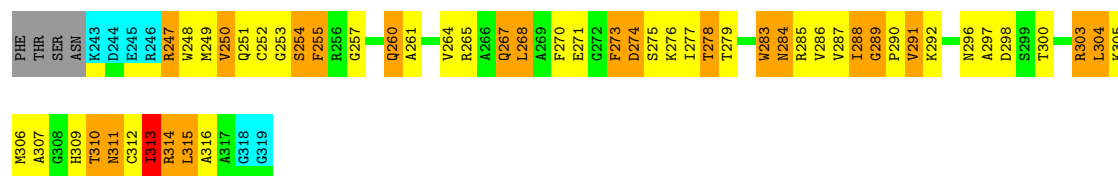
Chain A: 26% 28% 33% 7% 5%



4.2.9 Score per residue for model 9

- Molecule 1: CELL DIVISION PROTEIN FTSN

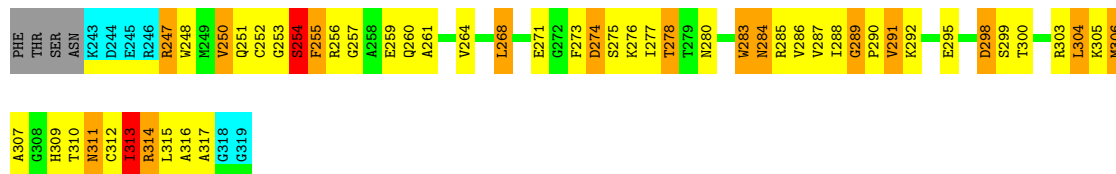
Chain A: 23% 37% 26% 7% 5%



4.2.10 Score per residue for model 10

- Molecule 1: CELL DIVISION PROTEIN FTSN

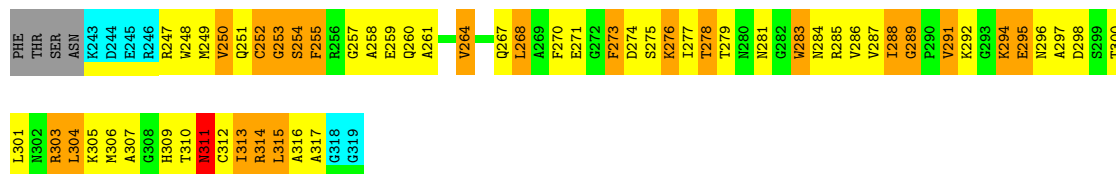
Chain A: 25% 42% 19% 7% 5%



4.2.11 Score per residue for model 11

- Molecule 1: CELL DIVISION PROTEIN FTSN

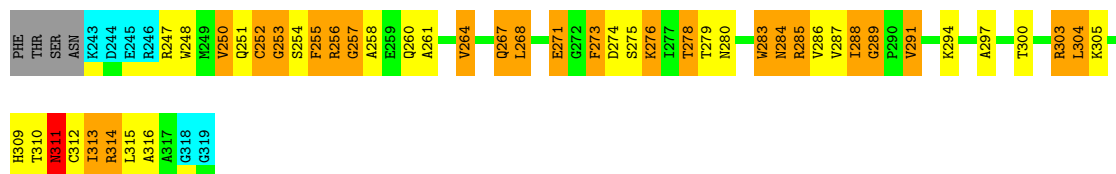
Chain A: 17% 43% 26% 7% 5%



4.2.12 Score per residue for model 12

- Molecule 1: CELL DIVISION PROTEIN FTSN

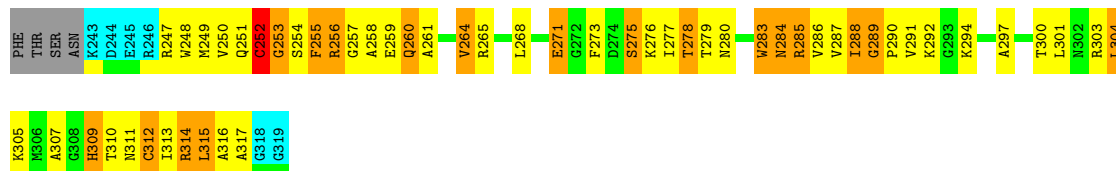
Chain A: 31% 27% 28% 7% 5%



4.2.13 Score per residue for model 13

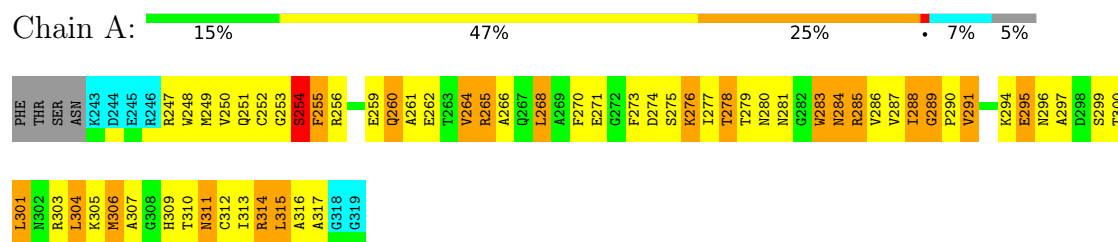
- Molecule 1: CELL DIVISION PROTEIN FTSN

Chain A: 22% 42% 22% 7% 5%



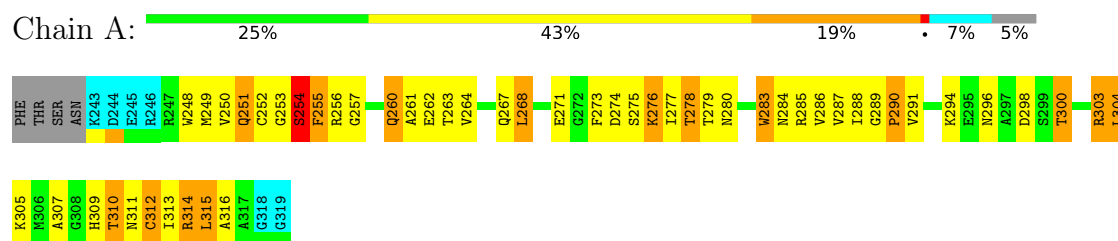
4.2.14 Score per residue for model 14

- Molecule 1: CELL DIVISION PROTEIN FTSN



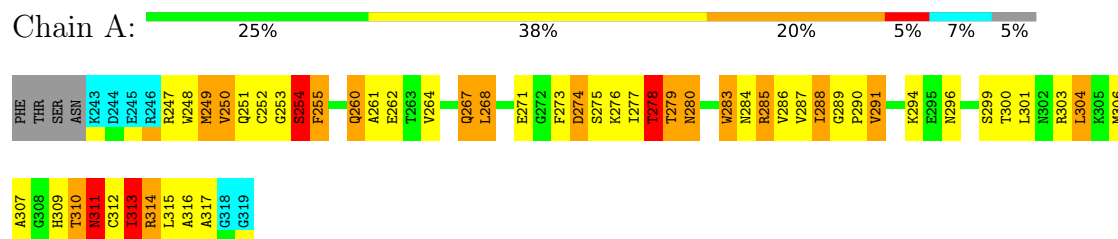
4.2.15 Score per residue for model 15

- Molecule 1: CELL DIVISION PROTEIN FTSN



4.2.16 Score per residue for model 16

- Molecule 1: CELL DIVISION PROTEIN FTSN

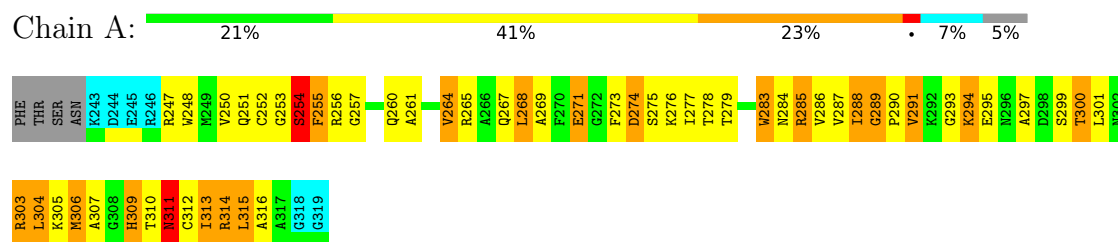


4.2.17 Score per residue for model 17

- Molecule 1: CELL DIVISION PROTEIN FTSN

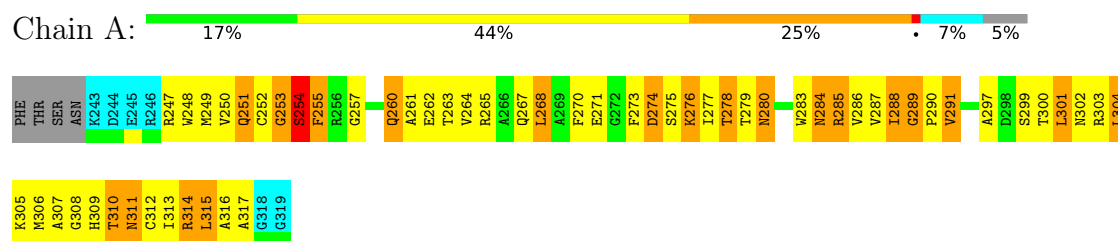
4.2.18 Score per residue for model 18

- Molecule 1: CELL DIVISION PROTEIN FTSN



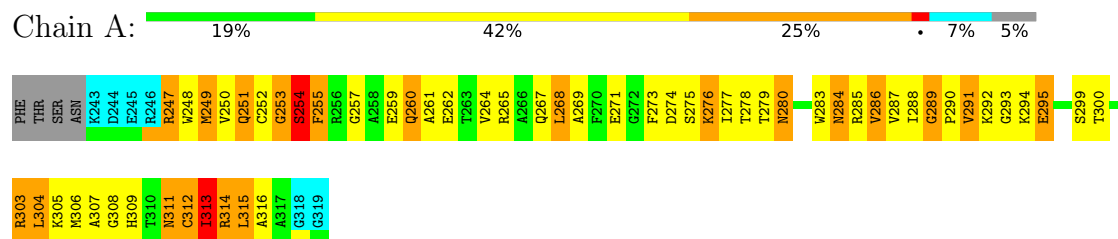
4.2.19 Score per residue for model 19

- Molecule 1: CELL DIVISION PROTEIN FTSN



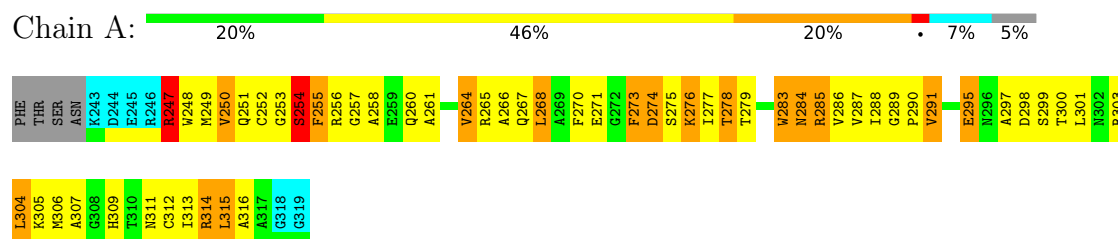
4.2.20 Score per residue for model 20

- Molecule 1: CELL DIVISION PROTEIN FTSN



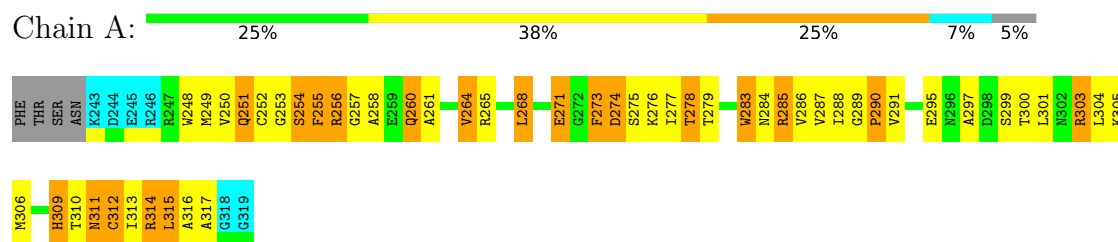
4.2.21 Score per residue for model 21

- Molecule 1: CELL DIVISION PROTEIN FTSN



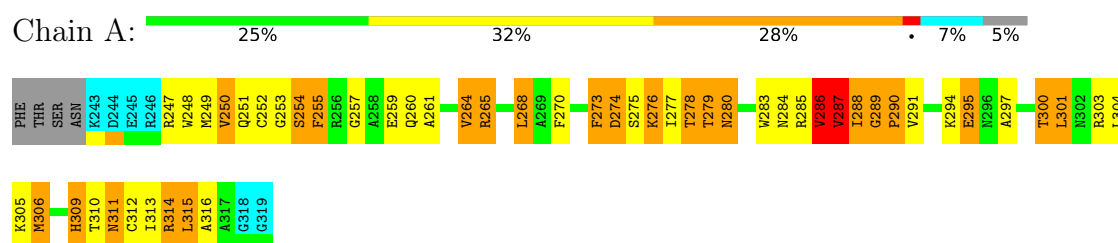
4.2.22 Score per residue for model 22

- Molecule 1: CELL DIVISION PROTEIN FTSN



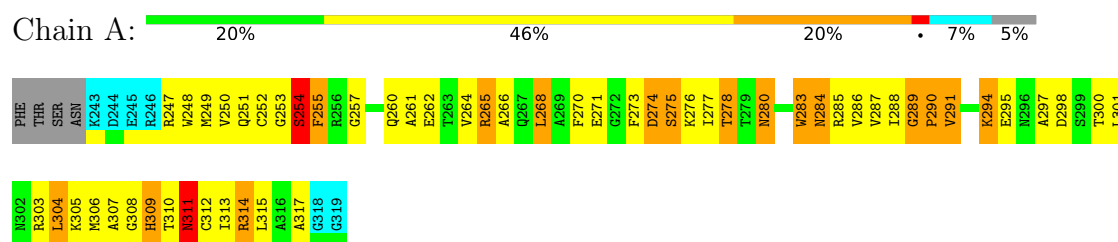
4.2.23 Score per residue for model 23

- Molecule 1: CELL DIVISION PROTEIN FTSN



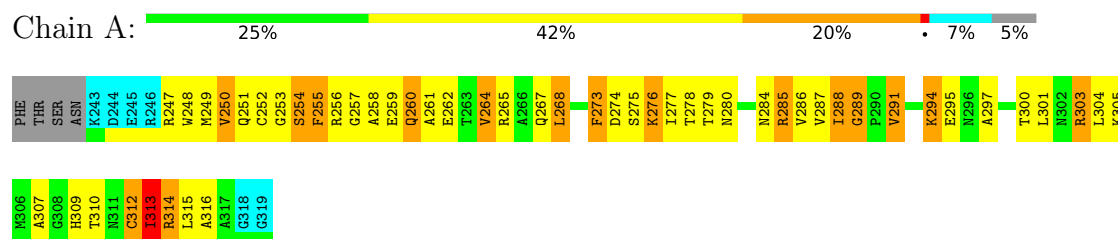
4.2.24 Score per residue for model 24

- Molecule 1: CELL DIVISION PROTEIN FTSN



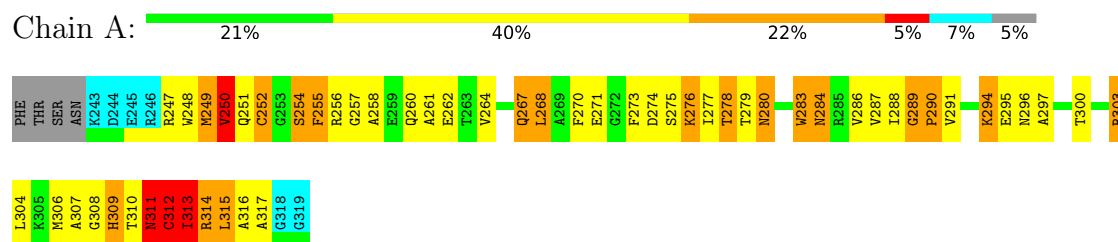
4.2.25 Score per residue for model 25

- Molecule 1: CELL DIVISION PROTEIN FTSN



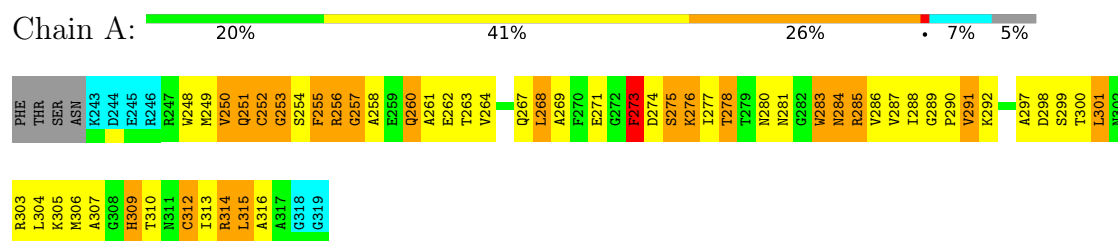
4.2.26 Score per residue for model 26

- Molecule 1: CELL DIVISION PROTEIN FTSN



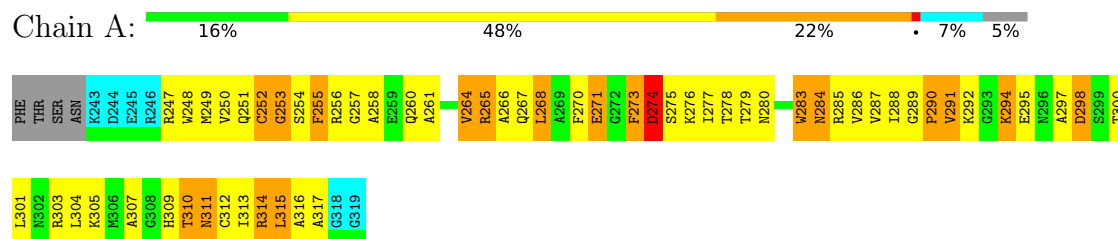
4.2.27 Score per residue for model 27

- Molecule 1: CELL DIVISION PROTEIN FTSN



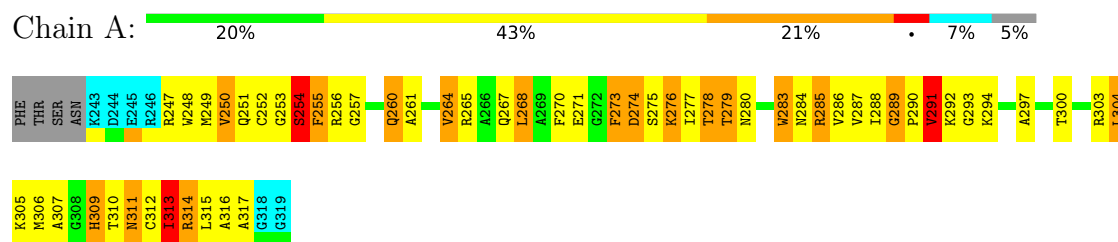
4.2.28 Score per residue for model 28

- Molecule 1: CELL DIVISION PROTEIN FTSN



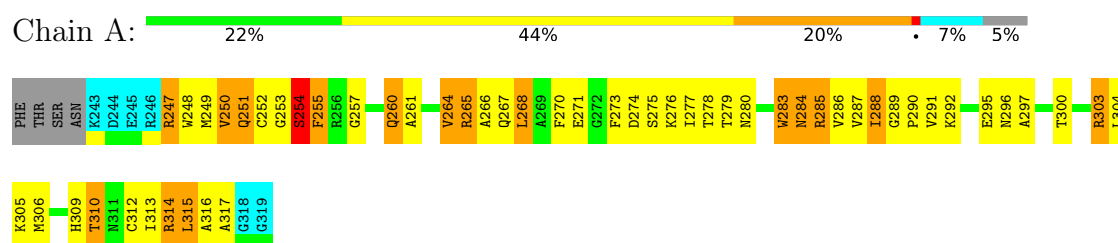
4.2.30 Score per residue for model 30

- Molecule 1: CELL DIVISION PROTEIN FTSN



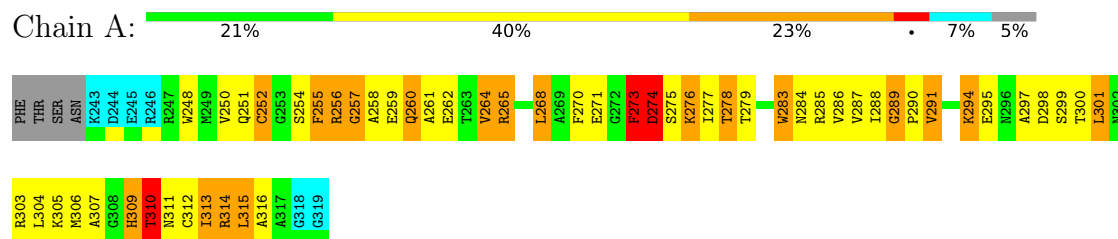
4.2.31 Score per residue for model 31

- Molecule 1: CELL DIVISION PROTEIN FTSN



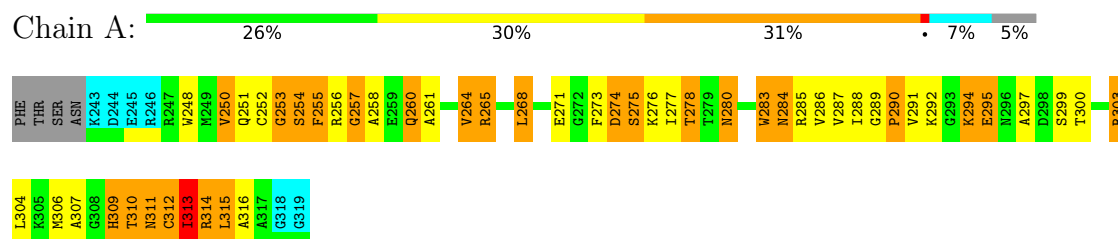
4.2.32 Score per residue for model 32

- Molecule 1: CELL DIVISION PROTEIN FTSN



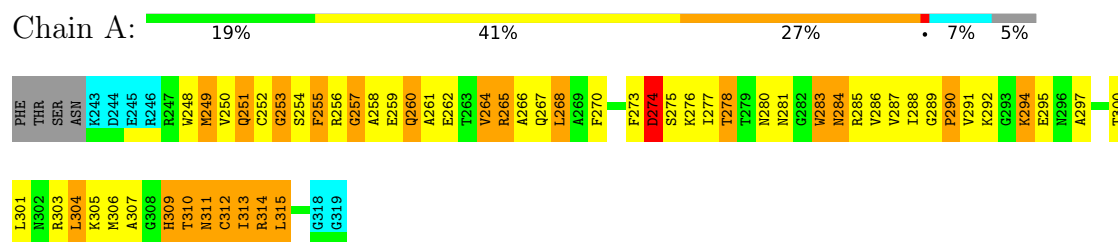
4.2.33 Score per residue for model 33

- Molecule 1: CELL DIVISION PROTEIN FTSN



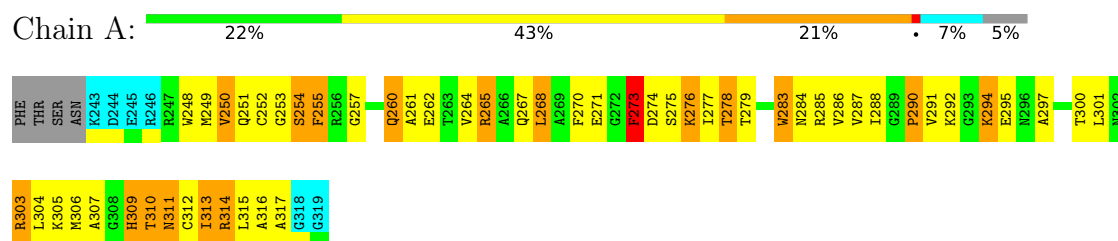
4.2.34 Score per residue for model 34

- Molecule 1: CELL DIVISION PROTEIN FTSN



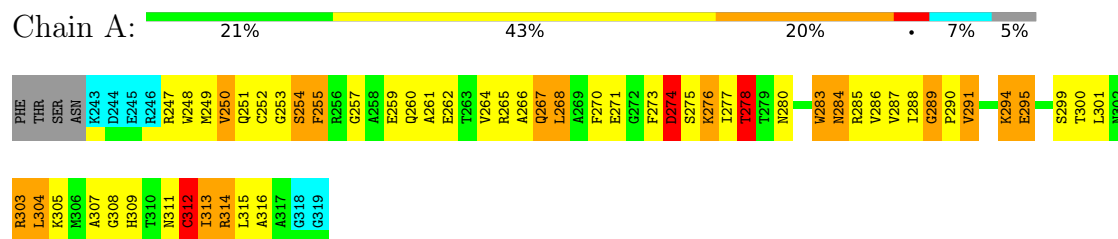
4.2.35 Score per residue for model 35

- Molecule 1: CELL DIVISION PROTEIN FTSN



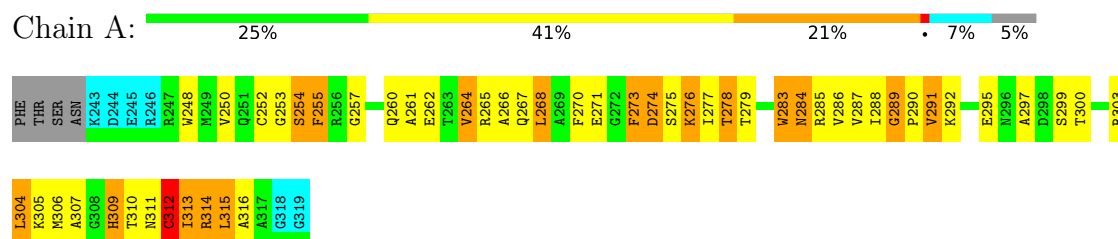
4.2.36 Score per residue for model 36

- Molecule 1: CELL DIVISION PROTEIN FTSN



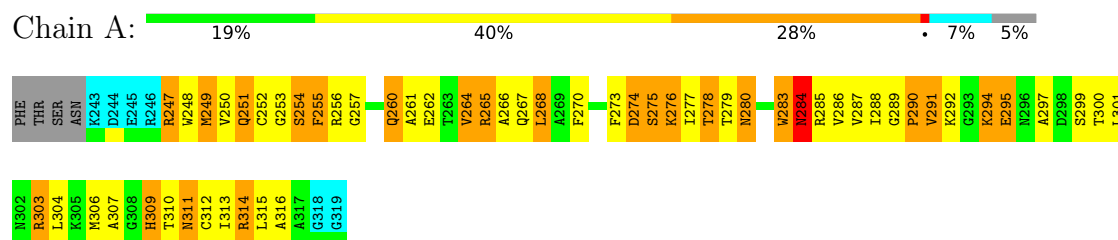
4.2.37 Score per residue for model 37

- Molecule 1: CELL DIVISION PROTEIN FTSN



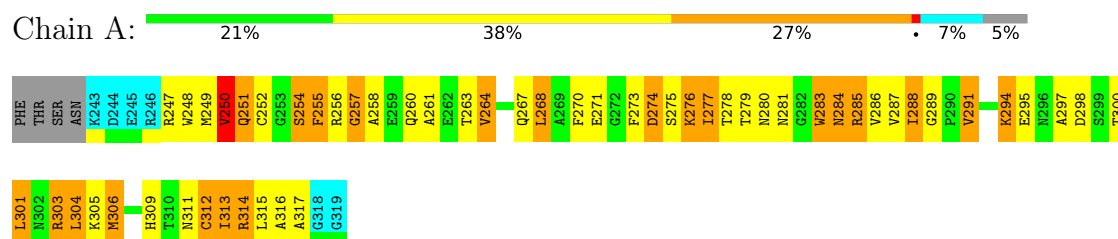
4.2.38 Score per residue for model 38

- Molecule 1: CELL DIVISION PROTEIN FTSN



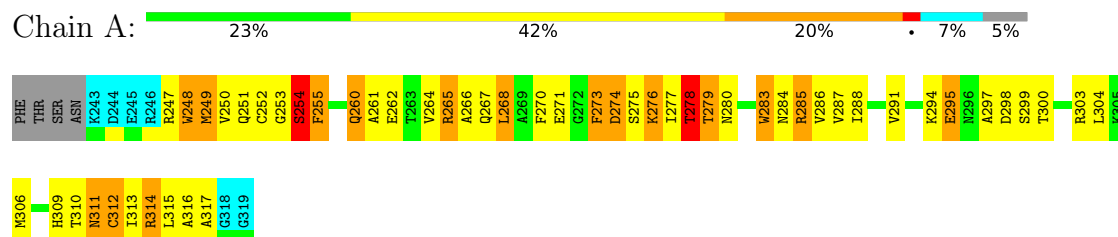
4.2.39 Score per residue for model 39

- Molecule 1: CELL DIVISION PROTEIN FTSN



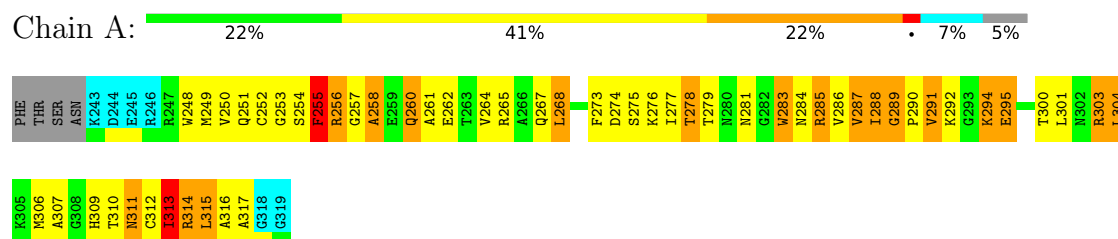
4.2.40 Score per residue for model 40

- Molecule 1: CELL DIVISION PROTEIN FTSN



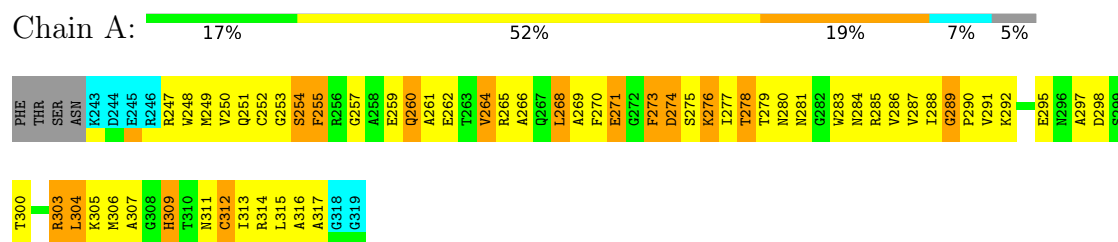
4.2.41 Score per residue for model 41

- Molecule 1: CELL DIVISION PROTEIN FTSN



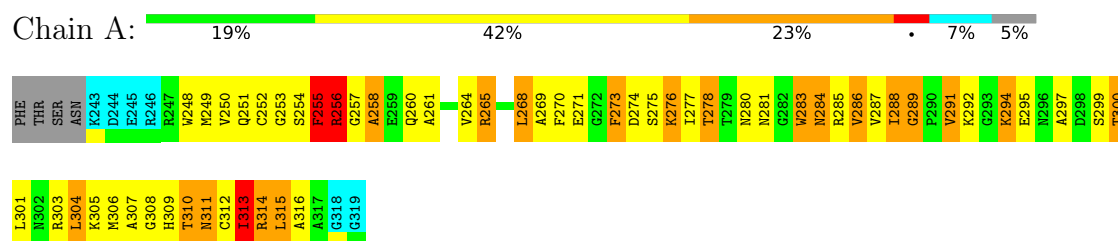
4.2.42 Score per residue for model 42

- Molecule 1: CELL DIVISION PROTEIN FTSN



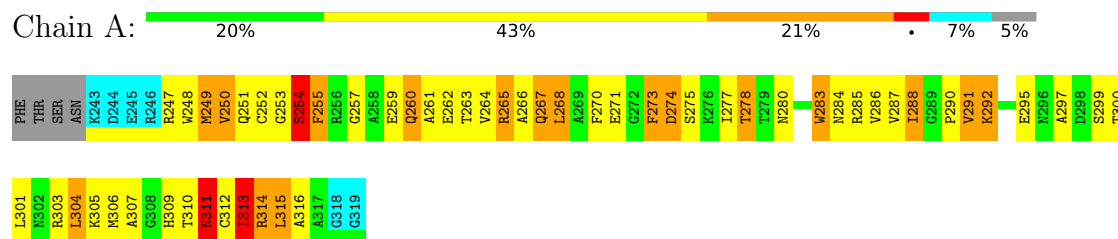
4.2.43 Score per residue for model 43

- Molecule 1: CELL DIVISION PROTEIN FTSN



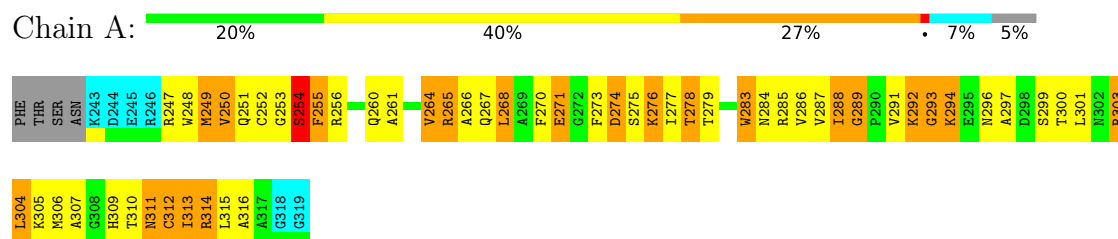
4.2.44 Score per residue for model 44

- Molecule 1: CELL DIVISION PROTEIN FTSN



4.2.45 Score per residue for model 45

- Molecule 1: CELL DIVISION PROTEIN FTSN



5 Refinement protocol and experimental data overview

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

Of the 50 calculated structures, 45 were deposited, based on the following criterion: *LOW NOE ENERGY*.

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

Software name	Classification	Version
CNS	refinement	
CNS	structure solution	

No chemical shift data was provided.

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	0.40±0.02	0±0/556 (0.0± 0.0%)	0.76±0.03	0±0/749 (0.0± 0.0%)
All	All	0.40	0/25020 (0.0%)	0.76	7/33705 (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	A	255	PHE	N-CA-C	5.50	115.83	108.23	41	2
1	A	312	CYS	N-CA-C	5.47	117.11	108.96	39	1
1	A	248	TRP	N-CA-C	5.15	115.85	108.74	40	1
1	A	273	PHE	CA-CB-CG	5.11	118.91	113.80	32	3

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	547	545	544	96±11
All	All	24615	24525	24480	4310

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 88.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:250:VAL:HG11	1:A:288:ILE:HD12	1.13	1.18	16	29
1:A:277:ILE:HG22	1:A:286:VAL:HG22	1.09	1.13	36	4
1:A:291:VAL:HG21	1:A:297:ALA:HB2	1.03	1.29	44	6
1:A:250:VAL:HG21	1:A:288:ILE:HD12	1.02	1.25	4	7
1:A:248:TRP:NE1	1:A:297:ALA:HB3	1.02	1.70	44	2
1:A:268:LEU:HD12	1:A:273:PHE:CD2	1.00	1.91	32	12
1:A:268:LEU:HD13	1:A:304:LEU:HD21	0.99	1.33	21	10
1:A:268:LEU:HD13	1:A:286:VAL:HG11	0.96	1.37	19	2
1:A:268:LEU:HD22	1:A:273:PHE:CZ	0.96	1.95	18	2
1:A:275:SER:HA	1:A:288:ILE:HG23	0.96	1.34	41	28
1:A:264:VAL:HG23	1:A:309:HIS:CE1	0.94	1.97	19	1
1:A:268:LEU:HD13	1:A:273:PHE:CE2	0.93	1.99	26	5
1:A:304:LEU:HD23	1:A:309:HIS:CE1	0.92	1.99	34	7
1:A:253:GLY:CA	1:A:286:VAL:HG12	0.92	1.94	38	8
1:A:250:VAL:HG23	1:A:291:VAL:HG21	0.92	1.41	5	8
1:A:288:ILE:HD11	1:A:300:THR:HG21	0.91	1.40	19	21
1:A:268:LEU:HD11	1:A:309:HIS:CE1	0.91	2.00	23	2
1:A:268:LEU:HD12	1:A:273:PHE:CE2	0.91	2.00	34	4
1:A:248:TRP:HB2	1:A:291:VAL:HG23	0.90	1.41	35	28
1:A:248:TRP:CB	1:A:291:VAL:HG23	0.90	1.97	28	40
1:A:268:LEU:HD22	1:A:304:LEU:CD2	0.90	1.97	26	2
1:A:251:GLN:HA	1:A:287:VAL:HG12	0.89	1.44	11	24
1:A:301:LEU:HD13	1:A:314:ARG:NH2	0.89	1.83	38	8
1:A:264:VAL:HG22	1:A:309:HIS:ND1	0.89	1.83	7	7
1:A:268:LEU:HD23	1:A:273:PHE:CD2	0.88	2.03	39	23
1:A:268:LEU:HD21	1:A:275:SER:CB	0.87	1.98	33	8
1:A:268:LEU:HD13	1:A:273:PHE:CD2	0.87	2.05	30	7
1:A:300:THR:HG22	1:A:304:LEU:HD12	0.87	1.47	21	13
1:A:253:GLY:HA2	1:A:255:PHE:CZ	0.87	2.05	20	11
1:A:268:LEU:O	1:A:273:PHE:O	0.87	1.91	36	16
1:A:268:LEU:HD22	1:A:275:SER:CB	0.86	1.99	3	23
1:A:276:LYS:N	1:A:287:VAL:O	0.86	2.08	20	42
1:A:268:LEU:HD22	1:A:275:SER:HB3	0.85	1.45	11	13
1:A:274:ASP:O	1:A:288:ILE:HG23	0.85	1.70	29	30
1:A:268:LEU:HD22	1:A:275:SER:HB2	0.85	1.49	39	11
1:A:255:PHE:CE1	1:A:309:HIS:HB3	0.84	2.07	30	12
1:A:250:VAL:HG11	1:A:288:ILE:CD1	0.84	2.02	9	28
1:A:253:GLY:HA2	1:A:255:PHE:CE1	0.84	2.08	37	23
1:A:273:PHE:CE1	1:A:303:ARG:HB3	0.83	2.09	16	22
1:A:260:GLN:O	1:A:264:VAL:HG23	0.83	1.73	7	32
1:A:288:ILE:CD1	1:A:300:THR:HG21	0.82	2.03	19	38
1:A:261:ALA:O	1:A:264:VAL:HG12	0.82	1.74	19	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:253:GLY:HA3	1:A:286:VAL:HG12	0.82	1.50	10	8
1:A:304:LEU:HD23	1:A:309:HIS:CD2	0.82	2.09	16	21
1:A:304:LEU:HD23	1:A:309:HIS:NE2	0.82	1.87	34	8
1:A:300:THR:HG22	1:A:304:LEU:CD1	0.82	2.04	21	11
1:A:261:ALA:HB3	1:A:284:ASN:HB2	0.82	1.49	43	4
1:A:301:LEU:HD13	1:A:314:ARG:NH1	0.82	1.88	18	3
1:A:257:GLY:O	1:A:261:ALA:N	0.82	2.13	34	30
1:A:301:LEU:HD22	1:A:314:ARG:NH2	0.81	1.90	1	9
1:A:248:TRP:HB3	1:A:291:VAL:HG23	0.81	1.53	43	31
1:A:255:PHE:CZ	1:A:309:HIS:HB3	0.81	2.09	37	12
1:A:268:LEU:HD11	1:A:275:SER:HB3	0.81	1.53	34	3
1:A:277:ILE:HD11	1:A:284:ASN:HB3	0.81	1.53	43	3
1:A:277:ILE:HD11	1:A:284:ASN:OD1	0.81	1.76	32	11
1:A:268:LEU:HD21	1:A:304:LEU:HD11	0.80	1.50	19	5
1:A:268:LEU:HD12	1:A:275:SER:CB	0.80	2.05	30	5
1:A:277:ILE:HG22	1:A:286:VAL:CG2	0.80	2.05	36	1
1:A:268:LEU:HD13	1:A:304:LEU:CD2	0.80	2.06	32	9
1:A:268:LEU:HD21	1:A:275:SER:HB3	0.79	1.52	32	4
1:A:265:ARG:HA	1:A:268:LEU:HD23	0.79	1.53	28	4
1:A:301:LEU:CA	1:A:313:ILE:HD11	0.79	2.06	39	1
1:A:268:LEU:HD23	1:A:273:PHE:HD2	0.79	1.37	39	6
1:A:288:ILE:HD13	1:A:300:THR:HG21	0.79	1.54	29	10
1:A:250:VAL:CG2	1:A:288:ILE:HD12	0.79	2.06	4	1
1:A:250:VAL:HG13	1:A:288:ILE:H	0.79	1.37	12	23
1:A:268:LEU:HD12	1:A:275:SER:HB3	0.79	1.55	18	3
1:A:268:LEU:CD1	1:A:286:VAL:HG11	0.79	2.07	19	1
1:A:264:VAL:HG23	1:A:309:HIS:NE2	0.78	1.91	19	1
1:A:250:VAL:HG22	1:A:314:ARG:HD3	0.78	1.56	25	3
1:A:250:VAL:HG21	1:A:288:ILE:HD11	0.78	1.55	13	1
1:A:268:LEU:HD21	1:A:275:SER:OG	0.78	1.79	28	3
1:A:254:SER:HG	1:A:283:TRP:CD1	0.77	1.97	45	8
1:A:268:LEU:HD13	1:A:275:SER:CB	0.77	2.09	13	1
1:A:264:VAL:HG13	1:A:309:HIS:CE1	0.77	2.15	16	17
1:A:255:PHE:CZ	1:A:264:VAL:HG11	0.77	2.14	10	13
1:A:250:VAL:HG22	1:A:314:ARG:HG3	0.77	1.55	19	12
1:A:264:VAL:O	1:A:268:LEU:HD12	0.77	1.77	11	16
1:A:286:VAL:O	1:A:287:VAL:HG13	0.77	1.79	42	28
1:A:264:VAL:HG12	1:A:268:LEU:HD12	0.77	1.55	10	1
1:A:301:LEU:HD12	1:A:314:ARG:NH2	0.77	1.94	14	1
1:A:304:LEU:CD1	1:A:313:ILE:HD13	0.77	2.10	39	1
1:A:273:PHE:CD2	1:A:300:THR:HG23	0.76	2.15	31	31

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:255:PHE:CD1	1:A:255:PHE:N	0.76	2.54	25	20
1:A:250:VAL:HG22	1:A:314:ARG:CD	0.76	2.09	25	3
1:A:268:LEU:HA	1:A:273:PHE:CE2	0.76	2.15	40	14
1:A:275:SER:CA	1:A:288:ILE:HG23	0.76	2.10	8	10
1:A:255:PHE:CE2	1:A:264:VAL:HG11	0.76	2.15	21	29
1:A:301:LEU:HD13	1:A:302:ASN:N	0.76	1.96	19	1
1:A:268:LEU:HD21	1:A:309:HIS:CE1	0.76	2.16	22	2
1:A:255:PHE:CE1	1:A:286:VAL:HG23	0.76	2.16	25	2
1:A:255:PHE:CE2	1:A:261:ALA:HA	0.75	2.17	25	6
1:A:268:LEU:HB2	1:A:273:PHE:CE2	0.75	2.16	28	5
1:A:250:VAL:CG1	1:A:288:ILE:HD12	0.75	2.09	20	12
1:A:277:ILE:CG2	1:A:286:VAL:HG22	0.75	2.10	25	3
1:A:268:LEU:HD13	1:A:304:LEU:HD11	0.75	1.55	36	1
1:A:268:LEU:HD23	1:A:273:PHE:CE2	0.75	2.17	13	17
1:A:264:VAL:O	1:A:307:ALA:HB1	0.75	1.82	24	3
1:A:307:ALA:HB3	1:A:309:HIS:NE2	0.74	1.97	24	21
1:A:300:THR:O	1:A:304:LEU:HD23	0.74	1.82	45	3
1:A:255:PHE:CE2	1:A:264:VAL:HG21	0.74	2.18	19	6
1:A:250:VAL:HG22	1:A:314:ARG:CG	0.74	2.12	43	5
1:A:254:SER:N	1:A:285:ARG:HA	0.74	1.97	43	23
1:A:250:VAL:HB	1:A:314:ARG:NH1	0.74	1.97	44	4
1:A:248:TRP:CZ3	1:A:316:ALA:HB2	0.74	2.18	40	39
1:A:304:LEU:HB3	1:A:309:HIS:CD2	0.74	2.18	39	29
1:A:277:ILE:HD11	1:A:284:ASN:CG	0.74	2.08	15	4
1:A:268:LEU:HD12	1:A:275:SER:HB2	0.74	1.57	14	2
1:A:263:THR:HG22	1:A:267:GLN:HG3	0.73	1.59	19	3
1:A:268:LEU:HA	1:A:273:PHE:CE1	0.73	2.17	27	29
1:A:301:LEU:HA	1:A:313:ILE:HD11	0.73	1.60	39	1
1:A:253:GLY:N	1:A:286:VAL:HG12	0.73	1.98	16	3
1:A:268:LEU:HD12	1:A:268:LEU:O	0.73	1.83	26	2
1:A:247:ARG:HA	1:A:292:LYS:HA	0.73	1.61	44	5
1:A:300:THR:O	1:A:304:LEU:HD12	0.73	1.84	7	15
1:A:252:CYS:SG	1:A:304:LEU:HD21	0.73	2.24	13	5
1:A:250:VAL:HG12	1:A:291:VAL:CG2	0.72	2.13	39	4
1:A:291:VAL:CG2	1:A:297:ALA:HB2	0.72	2.12	44	6
1:A:297:ALA:HB1	1:A:314:ARG:HG3	0.72	1.61	4	10
1:A:273:PHE:HD2	1:A:300:THR:HG23	0.72	1.45	32	21
1:A:301:LEU:HD13	1:A:314:ARG:CZ	0.72	2.14	1	7
1:A:312:CYS:O	1:A:313:ILE:HG23	0.72	1.85	43	40
1:A:297:ALA:HB1	1:A:314:ARG:CG	0.72	2.15	26	12
1:A:301:LEU:HA	1:A:304:LEU:HD12	0.71	1.59	23	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:256:ARG:CG	1:A:264:VAL:HG21	0.71	2.15	41	2
1:A:252:CYS:SG	1:A:286:VAL:HG13	0.71	2.25	8	5
1:A:253:GLY:HA2	1:A:255:PHE:CE2	0.71	2.19	41	2
1:A:268:LEU:HD12	1:A:273:PHE:O	0.71	1.85	27	2
1:A:304:LEU:HD23	1:A:309:HIS:CG	0.71	2.20	13	4
1:A:261:ALA:HB1	1:A:284:ASN:HB3	0.70	1.63	22	33
1:A:313:ILE:CD1	1:A:315:LEU:HD12	0.70	2.15	27	2
1:A:268:LEU:HD13	1:A:273:PHE:HD2	0.70	1.46	22	2
1:A:268:LEU:HD12	1:A:273:PHE:HD2	0.70	1.46	36	6
1:A:250:VAL:HG23	1:A:291:VAL:CG2	0.70	2.15	29	7
1:A:309:HIS:CG	1:A:312:CYS:SG	0.70	2.84	39	1
1:A:256:ARG:HB3	1:A:260:GLN:HB3	0.70	1.64	43	2
1:A:277:ILE:O	1:A:278:THR:HG23	0.69	1.87	38	41
1:A:268:LEU:HD21	1:A:309:HIS:NE2	0.69	2.01	18	2
1:A:268:LEU:HD11	1:A:275:SER:HB2	0.69	1.63	38	6
1:A:265:ARG:HB2	1:A:277:ILE:HD13	0.69	1.65	43	2
1:A:248:TRP:CD1	1:A:297:ALA:HB3	0.69	2.21	45	2
1:A:310:THR:HG22	1:A:311:ASN:OD1	0.69	1.88	1	1
1:A:251:GLN:HB3	1:A:315:LEU:HD13	0.69	1.65	22	6
1:A:314:ARG:N	1:A:314:ARG:HD2	0.69	2.01	39	1
1:A:304:LEU:HD13	1:A:309:HIS:NE2	0.69	2.02	42	1
1:A:276:LYS:O	1:A:286:VAL:HG23	0.69	1.88	43	1
1:A:304:LEU:HD13	1:A:312:CYS:SG	0.69	2.28	7	4
1:A:277:ILE:HG22	1:A:286:VAL:HB	0.69	1.63	17	5
1:A:268:LEU:HD21	1:A:275:SER:HB2	0.69	1.64	33	3
1:A:252:CYS:SG	1:A:304:LEU:HD11	0.68	2.28	35	7
1:A:264:VAL:HG21	1:A:309:HIS:HB3	0.68	1.64	23	9
1:A:268:LEU:HD21	1:A:304:LEU:CD1	0.68	2.18	19	7
1:A:291:VAL:HG11	1:A:314:ARG:NH2	0.68	2.02	39	1
1:A:268:LEU:HD13	1:A:275:SER:OG	0.68	1.89	2	3
1:A:252:CYS:HB3	1:A:304:LEU:HD22	0.68	1.65	16	9
1:A:264:VAL:HA	1:A:307:ALA:HB1	0.68	1.66	28	9
1:A:264:VAL:HG22	1:A:309:HIS:HD1	0.68	1.47	36	4
1:A:260:GLN:O	1:A:264:VAL:N	0.68	2.26	27	36
1:A:264:VAL:HG13	1:A:307:ALA:HB1	0.68	1.64	25	2
1:A:250:VAL:HB	1:A:314:ARG:HD3	0.68	1.64	33	2
1:A:268:LEU:HD23	1:A:273:PHE:O	0.68	1.88	4	2
1:A:250:VAL:HG13	1:A:314:ARG:CD	0.68	2.19	4	2
1:A:250:VAL:HG13	1:A:314:ARG:NE	0.68	2.03	4	1
1:A:250:VAL:HB	1:A:314:ARG:CZ	0.68	2.19	31	5
1:A:276:LYS:O	1:A:287:VAL:HG23	0.68	1.89	37	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:279:THR:HG23	1:A:283:TRP:C	0.67	2.14	29	8
1:A:261:ALA:HB1	1:A:284:ASN:CB	0.67	2.19	40	42
1:A:300:THR:CG2	1:A:304:LEU:HD12	0.67	2.19	4	3
1:A:288:ILE:HD12	1:A:300:THR:HG21	0.67	1.65	13	3
1:A:268:LEU:HD21	1:A:304:LEU:CG	0.67	2.19	9	4
1:A:251:GLN:HG2	1:A:315:LEU:HD13	0.67	1.65	15	1
1:A:288:ILE:HD11	1:A:300:THR:CG2	0.67	2.20	43	5
1:A:252:CYS:HA	1:A:312:CYS:HA	0.67	1.66	13	28
1:A:253:GLY:HA2	1:A:286:VAL:N	0.66	2.04	23	1
1:A:248:TRP:HB2	1:A:316:ALA:HA	0.66	1.65	44	2
1:A:286:VAL:HG13	1:A:287:VAL:N	0.66	2.03	23	1
1:A:265:ARG:HB2	1:A:277:ILE:HD12	0.66	1.68	35	5
1:A:255:PHE:CE1	1:A:309:HIS:HB2	0.66	2.25	14	3
1:A:297:ALA:HB1	1:A:314:ARG:HG2	0.66	1.67	12	13
1:A:252:CYS:SG	1:A:304:LEU:HD13	0.66	2.30	22	7
1:A:297:ALA:HA	1:A:314:ARG:NH2	0.66	2.05	31	6
1:A:313:ILE:N	1:A:313:ILE:HD13	0.66	2.06	20	2
1:A:304:LEU:HB3	1:A:309:HIS:NE2	0.66	2.06	39	19
1:A:255:PHE:HE1	1:A:286:VAL:HG23	0.66	1.51	25	1
1:A:255:PHE:CD1	1:A:309:HIS:HB2	0.66	2.26	41	1
1:A:268:LEU:HD13	1:A:304:LEU:CD1	0.66	2.21	36	1
1:A:250:VAL:HG21	1:A:288:ILE:CD1	0.66	2.14	4	3
1:A:268:LEU:O	1:A:273:PHE:CD2	0.65	2.50	37	6
1:A:253:GLY:HA3	1:A:286:VAL:N	0.65	2.06	40	13
1:A:264:VAL:HG13	1:A:309:HIS:CD2	0.65	2.26	7	3
1:A:268:LEU:HD22	1:A:273:PHE:CE2	0.65	2.26	22	2
1:A:264:VAL:HG22	1:A:309:HIS:CE1	0.65	2.26	44	8
1:A:250:VAL:HB	1:A:288:ILE:HB	0.65	1.69	3	1
1:A:301:LEU:HD22	1:A:314:ARG:HH22	0.65	1.52	18	8
1:A:304:LEU:HD13	1:A:312:CYS:HB3	0.65	1.68	25	1
1:A:250:VAL:HG12	1:A:291:VAL:HG21	0.65	1.67	39	1
1:A:268:LEU:HA	1:A:273:PHE:CZ	0.65	2.26	38	6
1:A:297:ALA:HA	1:A:314:ARG:CZ	0.65	2.21	40	6
1:A:268:LEU:HD11	1:A:304:LEU:CD2	0.65	2.22	22	2
1:A:268:LEU:HD11	1:A:275:SER:CB	0.65	2.22	24	7
1:A:297:ALA:HB1	1:A:314:ARG:NH1	0.64	2.06	31	3
1:A:313:ILE:HD12	1:A:315:LEU:HD12	0.64	1.67	18	4
1:A:263:THR:HG22	1:A:267:GLN:CG	0.64	2.22	19	3
1:A:271:GLU:OE2	1:A:306:MET:HE2	0.64	1.93	3	1
1:A:255:PHE:HB3	1:A:310:THR:HG22	0.64	1.68	22	2
1:A:313:ILE:HD12	1:A:314:ARG:HH11	0.64	1.53	39	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:268:LEU:CD1	1:A:273:PHE:CD2	0.64	2.81	28	5
1:A:261:ALA:CB	1:A:284:ASN:HB2	0.64	2.23	24	34
1:A:268:LEU:HG	1:A:273:PHE:CZ	0.64	2.28	3	14
1:A:268:LEU:O	1:A:273:PHE:CD1	0.64	2.51	27	22
1:A:268:LEU:HD21	1:A:304:LEU:HD21	0.64	1.68	10	2
1:A:313:ILE:HD12	1:A:313:ILE:O	0.64	1.93	27	2
1:A:273:PHE:CG	1:A:300:THR:HG23	0.63	2.28	22	7
1:A:250:VAL:HG22	1:A:288:ILE:H	0.63	1.53	26	1
1:A:275:SER:CB	1:A:288:ILE:HG22	0.63	2.23	27	1
1:A:269:ALA:HB2	1:A:274:ASP:OD1	0.63	1.91	3	1
1:A:312:CYS:C	1:A:313:ILE:HD13	0.63	2.18	29	3
1:A:268:LEU:CD1	1:A:304:LEU:HD21	0.63	2.22	40	1
1:A:250:VAL:HB	1:A:314:ARG:NE	0.63	2.09	42	3
1:A:265:ARG:HG3	1:A:277:ILE:HG23	0.63	1.71	5	6
1:A:250:VAL:O	1:A:287:VAL:HG12	0.63	1.94	39	10
1:A:268:LEU:HD22	1:A:275:SER:OG	0.63	1.94	8	6
1:A:268:LEU:HD13	1:A:275:SER:HB3	0.63	1.71	13	1
1:A:256:ARG:O	1:A:258:ALA:N	0.63	2.31	34	13
1:A:301:LEU:HD12	1:A:304:LEU:HD12	0.62	1.69	22	1
1:A:268:LEU:HD22	1:A:304:LEU:HD21	0.62	1.70	27	1
1:A:273:PHE:CE2	1:A:304:LEU:HD22	0.62	2.29	31	2
1:A:275:SER:CB	1:A:288:ILE:HG12	0.62	2.24	22	32
1:A:255:PHE:CE1	1:A:309:HIS:ND1	0.62	2.68	38	10
1:A:251:GLN:CB	1:A:315:LEU:HD12	0.62	2.24	19	2
1:A:304:LEU:HD13	1:A:309:HIS:CE1	0.62	2.29	42	1
1:A:253:GLY:O	1:A:255:PHE:N	0.62	2.32	20	2
1:A:250:VAL:HA	1:A:315:LEU:H	0.62	1.54	27	10
1:A:304:LEU:HD23	1:A:309:HIS:HD2	0.62	1.54	21	3
1:A:248:TRP:HB2	1:A:291:VAL:CG2	0.62	2.24	34	4
1:A:300:THR:HG22	1:A:314:ARG:NH1	0.62	2.10	12	1
1:A:255:PHE:CZ	1:A:286:VAL:HG21	0.61	2.30	1	7
1:A:255:PHE:CE1	1:A:309:HIS:CG	0.61	2.88	38	7
1:A:273:PHE:HE2	1:A:304:LEU:HD22	0.61	1.55	31	1
1:A:268:LEU:HB3	1:A:273:PHE:O	0.61	1.95	31	16
1:A:250:VAL:HG11	1:A:288:ILE:HD11	0.61	1.71	27	1
1:A:255:PHE:CZ	1:A:264:VAL:HG21	0.61	2.30	19	1
1:A:268:LEU:O	1:A:273:PHE:CG	0.61	2.53	35	4
1:A:304:LEU:HD12	1:A:313:ILE:HD13	0.61	1.71	39	1
1:A:255:PHE:O	1:A:261:ALA:HB2	0.61	1.94	41	2
1:A:249:MET:HG3	1:A:317:ALA:HB2	0.61	1.73	39	8
1:A:269:ALA:HB1	1:A:274:ASP:OD2	0.61	1.96	17	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:268:LEU:HB2	1:A:273:PHE:CZ	0.61	2.30	24	5
1:A:251:GLN:HB3	1:A:315:LEU:HD12	0.61	1.73	11	2
1:A:251:GLN:CG	1:A:287:VAL:HG12	0.61	2.26	32	1
1:A:252:CYS:O	1:A:304:LEU:HD22	0.61	1.96	10	5
1:A:273:PHE:CB	1:A:300:THR:HG23	0.61	2.26	29	6
1:A:313:ILE:HD13	1:A:313:ILE:N	0.61	2.11	29	1
1:A:253:GLY:CA	1:A:286:VAL:HG13	0.61	2.26	43	1
1:A:248:TRP:CE2	1:A:297:ALA:HB3	0.61	2.31	44	2
1:A:301:LEU:C	1:A:301:LEU:HD22	0.60	2.21	19	1
1:A:255:PHE:N	1:A:255:PHE:HD1	0.60	1.92	25	1
1:A:291:VAL:HG11	1:A:314:ARG:HH22	0.60	1.56	39	3
1:A:263:THR:HG22	1:A:267:GLN:OE1	0.60	1.97	15	2
1:A:301:LEU:HD13	1:A:314:ARG:HH22	0.60	1.55	38	1
1:A:268:LEU:HD21	1:A:286:VAL:CG1	0.60	2.27	29	2
1:A:254:SER:HA	1:A:284:ASN:O	0.60	1.95	7	5
1:A:275:SER:HB3	1:A:288:ILE:HG22	0.60	1.74	27	1
1:A:310:THR:O	1:A:311:ASN:CB	0.60	2.50	19	24
1:A:275:SER:OG	1:A:286:VAL:HG12	0.60	1.96	19	3
1:A:268:LEU:HD12	1:A:275:SER:OG	0.60	1.96	30	2
1:A:264:VAL:HG23	1:A:309:HIS:CD2	0.60	2.32	19	1
1:A:253:GLY:CA	1:A:255:PHE:CZ	0.60	2.85	20	1
1:A:253:GLY:O	1:A:254:SER:CB	0.60	2.50	23	9
1:A:268:LEU:CD2	1:A:273:PHE:CE2	0.59	2.85	8	17
1:A:250:VAL:CG2	1:A:288:ILE:HD11	0.59	2.26	13	1
1:A:268:LEU:HG	1:A:273:PHE:CE2	0.59	2.33	31	13
1:A:300:THR:O	1:A:304:LEU:N	0.59	2.32	23	22
1:A:250:VAL:HG13	1:A:314:ARG:HD3	0.59	1.73	29	7
1:A:301:LEU:HD22	1:A:301:LEU:O	0.59	1.97	19	1
1:A:311:ASN:O	1:A:312:CYS:CB	0.59	2.50	7	3
1:A:248:TRP:N	1:A:291:VAL:O	0.59	2.35	42	6
1:A:250:VAL:CG2	1:A:313:ILE:HG22	0.59	2.28	39	1
1:A:301:LEU:N	1:A:313:ILE:HD11	0.59	2.13	39	1
1:A:268:LEU:CD1	1:A:304:LEU:HD11	0.59	2.28	36	2
1:A:310:THR:HG22	1:A:311:ASN:ND2	0.59	2.13	7	1
1:A:249:MET:HE2	1:A:317:ALA:HA	0.59	1.74	11	4
1:A:309:HIS:CE1	1:A:311:ASN:O	0.59	2.56	15	2
1:A:254:SER:HB2	1:A:283:TRP:CD1	0.58	2.33	36	17
1:A:255:PHE:HE2	1:A:261:ALA:HA	0.58	1.58	24	5
1:A:253:GLY:HA2	1:A:286:VAL:HG13	0.58	1.75	43	1
1:A:261:ALA:CB	1:A:284:ASN:CB	0.58	2.81	36	32
1:A:251:GLN:CB	1:A:315:LEU:HD13	0.58	2.28	17	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:276:LYS:HB2	1:A:287:VAL:HG23	0.58	1.75	41	2
1:A:255:PHE:CE2	1:A:309:HIS:HB2	0.58	2.33	27	11
1:A:253:GLY:HA3	1:A:286:VAL:H	0.58	1.59	37	6
1:A:264:VAL:CG1	1:A:309:HIS:CE1	0.58	2.87	25	5
1:A:273:PHE:O	1:A:275:SER:N	0.58	2.36	40	8
1:A:274:ASP:C	1:A:288:ILE:HG23	0.58	2.22	34	9
1:A:253:GLY:HA3	1:A:286:VAL:HG23	0.58	1.74	19	6
1:A:250:VAL:CG2	1:A:314:ARG:NH1	0.58	2.67	40	1
1:A:250:VAL:HG23	1:A:251:GLN:N	0.57	2.13	26	3
1:A:301:LEU:HD12	1:A:314:ARG:HH21	0.57	1.57	32	2
1:A:250:VAL:HG12	1:A:288:ILE:H	0.57	1.58	7	1
1:A:250:VAL:HG13	1:A:314:ARG:HD2	0.57	1.75	40	1
1:A:255:PHE:CD2	1:A:309:HIS:CG	0.57	2.93	41	1
1:A:250:VAL:HB	1:A:314:ARG:HG3	0.57	1.76	32	6
1:A:252:CYS:C	1:A:286:VAL:HG12	0.57	2.25	23	2
1:A:260:GLN:O	1:A:264:VAL:HB	0.57	1.99	42	11
1:A:254:SER:OG	1:A:254:SER:O	0.57	2.22	5	3
1:A:248:TRP:CB	1:A:291:VAL:HG22	0.57	2.29	40	1
1:A:268:LEU:HD23	1:A:273:PHE:CZ	0.57	2.35	13	1
1:A:276:LYS:O	1:A:286:VAL:HG13	0.57	2.00	24	1
1:A:277:ILE:HA	1:A:286:VAL:HA	0.57	1.76	17	6
1:A:268:LEU:CD2	1:A:275:SER:OG	0.57	2.53	16	4
1:A:249:MET:HE3	1:A:317:ALA:HB2	0.57	1.77	40	1
1:A:304:LEU:O	1:A:309:HIS:CD2	0.57	2.57	43	20
1:A:248:TRP:O	1:A:291:VAL:HG22	0.57	1.98	45	2
1:A:273:PHE:CZ	1:A:303:ARG:HB3	0.56	2.34	15	18
1:A:250:VAL:HG21	1:A:300:THR:HG21	0.56	1.77	3	1
1:A:307:ALA:HB3	1:A:309:HIS:HE2	0.56	1.60	30	5
1:A:250:VAL:HB	1:A:314:ARG:HD2	0.56	1.77	34	2
1:A:255:PHE:CG	1:A:309:HIS:HB3	0.56	2.35	43	1
1:A:248:TRP:O	1:A:290:PRO:HA	0.56	2.01	6	34
1:A:264:VAL:HG12	1:A:265:ARG:N	0.56	2.16	29	12
1:A:278:THR:O	1:A:285:ARG:N	0.56	2.37	30	10
1:A:275:SER:HA	1:A:288:ILE:HG22	0.56	1.78	27	2
1:A:268:LEU:HD11	1:A:304:LEU:HD21	0.56	1.77	44	2
1:A:252:CYS:SG	1:A:252:CYS:O	0.56	2.63	23	1
1:A:261:ALA:HB3	1:A:284:ASN:CB	0.56	2.29	43	1
1:A:253:GLY:HA3	1:A:286:VAL:CB	0.56	2.31	41	12
1:A:268:LEU:HD13	1:A:275:SER:HB2	0.56	1.78	13	1
1:A:255:PHE:CZ	1:A:309:HIS:HB2	0.56	2.35	28	12
1:A:250:VAL:CG2	1:A:251:GLN:N	0.56	2.69	44	23

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:268:LEU:HD22	1:A:273:PHE:HE2	0.56	1.61	22	1
1:A:275:SER:HB2	1:A:288:ILE:HG12	0.56	1.77	23	5
1:A:312:CYS:C	1:A:313:ILE:HD12	0.56	2.25	7	1
1:A:253:GLY:HA3	1:A:286:VAL:CG2	0.56	2.30	19	4
1:A:253:GLY:C	1:A:284:ASN:O	0.56	2.48	20	2
1:A:267:GLN:O	1:A:307:ALA:HB2	0.55	2.01	29	1
1:A:251:GLN:OE1	1:A:315:LEU:HD22	0.55	2.02	32	1
1:A:301:LEU:HD22	1:A:314:ARG:CZ	0.55	2.31	1	2
1:A:252:CYS:SG	1:A:255:PHE:CZ	0.55	2.99	7	2
1:A:275:SER:OG	1:A:288:ILE:HG13	0.55	2.01	19	1
1:A:252:CYS:CB	1:A:304:LEU:HG	0.55	2.31	31	2
1:A:261:ALA:HB1	1:A:284:ASN:HB2	0.55	1.77	19	9
1:A:255:PHE:CE2	1:A:264:VAL:CG1	0.55	2.88	21	1
1:A:268:LEU:HG	1:A:275:SER:OG	0.55	2.00	27	3
1:A:255:PHE:C	1:A:257:GLY:N	0.55	2.64	43	7
1:A:268:LEU:CD2	1:A:286:VAL:HG11	0.55	2.32	36	4
1:A:253:GLY:O	1:A:255:PHE:CE1	0.55	2.60	11	7
1:A:278:THR:O	1:A:285:ARG:CB	0.55	2.54	9	14
1:A:252:CYS:CB	1:A:304:LEU:HD13	0.55	2.32	10	12
1:A:273:PHE:CE1	1:A:303:ARG:CG	0.55	2.90	42	9
1:A:255:PHE:CZ	1:A:309:HIS:CE1	0.55	2.94	43	1
1:A:250:VAL:HB	1:A:288:ILE:H	0.55	1.61	40	3
1:A:260:GLN:C	1:A:264:VAL:HG23	0.55	2.26	7	2
1:A:264:VAL:HG12	1:A:268:LEU:CD1	0.55	2.32	10	2
1:A:271:GLU:HG3	1:A:306:MET:HE2	0.55	1.79	18	1
1:A:255:PHE:CD2	1:A:309:HIS:HB3	0.55	2.36	43	1
1:A:252:CYS:CB	1:A:304:LEU:HD22	0.55	2.32	9	4
1:A:297:ALA:O	1:A:300:THR:HB	0.54	2.01	4	3
1:A:301:LEU:HB2	1:A:314:ARG:CZ	0.54	2.32	13	5
1:A:300:THR:HG22	1:A:304:LEU:CD2	0.54	2.33	42	2
1:A:250:VAL:HB	1:A:288:ILE:HG13	0.54	1.80	41	5
1:A:254:SER:CB	1:A:283:TRP:CD1	0.54	2.91	37	26
1:A:254:SER:HB3	1:A:283:TRP:CD1	0.54	2.37	31	11
1:A:275:SER:CB	1:A:288:ILE:HG23	0.54	2.32	13	1
1:A:250:VAL:CG2	1:A:291:VAL:HG21	0.54	2.28	29	3
1:A:250:VAL:HG22	1:A:314:ARG:HD2	0.54	1.79	40	1
1:A:255:PHE:CZ	1:A:286:VAL:CG2	0.54	2.90	4	11
1:A:250:VAL:CG1	1:A:288:ILE:HB	0.54	2.33	30	12
1:A:310:THR:HG22	1:A:311:ASN:N	0.54	2.16	15	1
1:A:255:PHE:CZ	1:A:309:HIS:CB	0.54	2.91	20	4
1:A:297:ALA:HB1	1:A:314:ARG:HE	0.54	1.63	22	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:264:VAL:CG2	1:A:309:HIS:ND1	0.54	2.70	42	11
1:A:313:ILE:N	1:A:314:ARG:NH2	0.54	2.55	27	3
1:A:275:SER:CA	1:A:288:ILE:HG22	0.54	2.33	27	1
1:A:304:LEU:CD2	1:A:309:HIS:CD2	0.54	2.90	1	9
1:A:311:ASN:O	1:A:312:CYS:O	0.54	2.26	22	4
1:A:268:LEU:CD2	1:A:275:SER:HB3	0.54	2.33	7	3
1:A:267:GLN:O	1:A:271:GLU:N	0.54	2.41	39	10
1:A:291:VAL:HG21	1:A:314:ARG:HH22	0.54	1.60	11	1
1:A:304:LEU:HD22	1:A:309:HIS:NE2	0.54	2.18	40	3
1:A:250:VAL:HG22	1:A:288:ILE:N	0.54	2.18	26	1
1:A:268:LEU:HD21	1:A:304:LEU:HG	0.54	1.78	3	4
1:A:265:ARG:CG	1:A:277:ILE:HG23	0.54	2.33	37	4
1:A:275:SER:HA	1:A:288:ILE:CG2	0.53	2.26	8	5
1:A:250:VAL:HB	1:A:288:ILE:HG12	0.53	1.80	13	1
1:A:252:CYS:CA	1:A:312:CYS:HA	0.53	2.33	13	13
1:A:250:VAL:HG23	1:A:313:ILE:CB	0.53	2.33	39	1
1:A:255:PHE:CZ	1:A:312:CYS:SG	0.53	2.94	39	1
1:A:250:VAL:HG11	1:A:288:ILE:HG13	0.53	1.79	40	1
1:A:286:VAL:C	1:A:287:VAL:HG22	0.53	2.28	23	1
1:A:265:ARG:CG	1:A:277:ILE:HB	0.53	2.33	14	5
1:A:314:ARG:NE	1:A:314:ARG:CA	0.53	2.71	4	2
1:A:271:GLU:CG	1:A:306:MET:HE2	0.53	2.32	18	1
1:A:264:VAL:HG22	1:A:268:LEU:CD1	0.53	2.33	19	1
1:A:264:VAL:CG2	1:A:309:HIS:HB3	0.53	2.32	27	1
1:A:273:PHE:CD1	1:A:273:PHE:N	0.53	2.76	40	5
1:A:274:ASP:O	1:A:288:ILE:HG12	0.53	2.03	24	2
1:A:253:GLY:HA2	1:A:286:VAL:HG12	0.53	1.78	5	4
1:A:301:LEU:HD22	1:A:314:ARG:HH21	0.53	1.63	28	2
1:A:252:CYS:C	1:A:286:VAL:HB	0.53	2.29	36	1
1:A:297:ALA:HB1	1:A:314:ARG:NE	0.53	2.18	39	1
1:A:303:ARG:O	1:A:306:MET:HB2	0.53	2.04	39	8
1:A:252:CYS:HB3	1:A:314:ARG:NH1	0.53	2.19	36	2
1:A:306:MET:HA	1:A:306:MET:HE3	0.53	1.79	42	1
1:A:250:VAL:HG12	1:A:251:GLN:N	0.53	2.19	24	13
1:A:265:ARG:CB	1:A:277:ILE:HD12	0.53	2.34	35	3
1:A:252:CYS:HB3	1:A:304:LEU:HD13	0.53	1.80	40	3
1:A:266:ALA:O	1:A:270:PHE:CB	0.53	2.57	42	13
1:A:310:THR:O	1:A:311:ASN:HB2	0.53	2.03	35	8
1:A:248:TRP:CB	1:A:291:VAL:CG2	0.53	2.86	26	7
1:A:264:VAL:HG12	1:A:309:HIS:CE1	0.53	2.38	35	1
1:A:275:SER:OG	1:A:288:ILE:HG12	0.52	2.05	16	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:268:LEU:HD12	1:A:268:LEU:C	0.52	2.29	26	2
1:A:264:VAL:HG13	1:A:309:HIS:NE2	0.52	2.19	36	2
1:A:251:GLN:CA	1:A:287:VAL:HG12	0.52	2.33	15	6
1:A:286:VAL:HG11	1:A:309:HIS:CE1	0.52	2.39	22	1
1:A:257:GLY:O	1:A:260:GLN:N	0.52	2.42	13	26
1:A:273:PHE:O	1:A:273:PHE:CG	0.52	2.62	4	7
1:A:265:ARG:HG2	1:A:277:ILE:HG23	0.52	1.82	4	1
1:A:248:TRP:CZ3	1:A:314:ARG:HB3	0.52	2.39	40	31
1:A:286:VAL:HG22	1:A:287:VAL:N	0.52	2.20	15	8
1:A:251:GLN:HA	1:A:286:VAL:O	0.52	2.04	39	5
1:A:255:PHE:HE2	1:A:264:VAL:HG11	0.52	1.63	7	7
1:A:253:GLY:O	1:A:255:PHE:CG	0.52	2.63	20	2
1:A:297:ALA:O	1:A:314:ARG:HD2	0.52	2.04	12	6
1:A:268:LEU:HD13	1:A:304:LEU:CG	0.52	2.34	36	3
1:A:255:PHE:HA	1:A:310:THR:HG22	0.52	1.80	25	1
1:A:252:CYS:HB2	1:A:304:LEU:HD22	0.52	1.81	36	3
1:A:264:VAL:HG13	1:A:309:HIS:ND1	0.52	2.19	21	1
1:A:250:VAL:HG22	1:A:314:ARG:NH1	0.52	2.20	40	1
1:A:288:ILE:O	1:A:289:GLY:C	0.52	2.52	26	27
1:A:254:SER:OG	1:A:283:TRP:CD1	0.52	2.63	4	5
1:A:268:LEU:HD13	1:A:286:VAL:CG1	0.52	2.26	19	1
1:A:248:TRP:O	1:A:291:VAL:CG2	0.52	2.58	45	2
1:A:276:LYS:HG3	1:A:287:VAL:HG23	0.52	1.82	36	2
1:A:273:PHE:CZ	1:A:303:ARG:C	0.51	2.88	43	26
1:A:309:HIS:CE1	1:A:312:CYS:HB3	0.51	2.39	9	9
1:A:249:MET:O	1:A:315:LEU:O	0.51	2.28	44	10
1:A:304:LEU:CD2	1:A:309:HIS:CE1	0.51	2.94	23	4
1:A:264:VAL:HG21	1:A:309:HIS:CB	0.51	2.34	27	1
1:A:268:LEU:HD21	1:A:286:VAL:HG11	0.51	1.83	36	2
1:A:300:THR:HA	1:A:303:ARG:HB2	0.51	1.82	42	7
1:A:252:CYS:HB2	1:A:286:VAL:HB	0.51	1.82	34	3
1:A:251:GLN:CB	1:A:287:VAL:HG12	0.51	2.36	22	2
1:A:310:THR:O	1:A:310:THR:HG23	0.51	2.05	22	1
1:A:268:LEU:O	1:A:268:LEU:HG	0.51	2.06	21	4
1:A:300:THR:HB	1:A:314:ARG:NH1	0.51	2.21	39	1
1:A:275:SER:CB	1:A:288:ILE:CG1	0.51	2.89	10	11
1:A:250:VAL:HG13	1:A:288:ILE:N	0.51	2.20	34	12
1:A:253:GLY:O	1:A:255:PHE:CD2	0.51	2.63	19	1
1:A:255:PHE:CD1	1:A:255:PHE:C	0.51	2.89	41	1
1:A:254:SER:O	1:A:254:SER:OG	0.51	2.28	29	3
1:A:304:LEU:HD22	1:A:309:HIS:CE1	0.51	2.40	26	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:264:VAL:HG21	1:A:308:GLY:O	0.51	2.06	24	2
1:A:253:GLY:CA	1:A:255:PHE:CE1	0.51	2.94	20	6
1:A:286:VAL:CG1	1:A:287:VAL:N	0.51	2.70	23	12
1:A:252:CYS:SG	1:A:312:CYS:HB3	0.51	2.46	23	1
1:A:268:LEU:HD11	1:A:309:HIS:NE2	0.51	2.20	25	2
1:A:288:ILE:HD12	1:A:314:ARG:NH2	0.51	2.20	22	6
1:A:268:LEU:CD1	1:A:273:PHE:CE2	0.51	2.90	24	4
1:A:291:VAL:HG21	1:A:314:ARG:HH21	0.51	1.66	39	1
1:A:304:LEU:CD1	1:A:313:ILE:HG21	0.50	2.36	39	1
1:A:288:ILE:HD12	1:A:314:ARG:CZ	0.50	2.36	40	1
1:A:255:PHE:CG	1:A:309:HIS:HB2	0.50	2.41	41	1
1:A:286:VAL:O	1:A:287:VAL:CG1	0.50	2.59	6	22
1:A:253:GLY:O	1:A:254:SER:O	0.50	2.30	7	1
1:A:254:SER:N	1:A:284:ASN:O	0.50	2.44	44	10
1:A:250:VAL:CG2	1:A:314:ARG:HD3	0.50	2.33	4	3
1:A:254:SER:HG	1:A:283:TRP:HD1	0.50	1.44	35	3
1:A:297:ALA:O	1:A:314:ARG:HG2	0.50	2.07	45	2
1:A:304:LEU:CD2	1:A:309:HIS:NE2	0.50	2.74	23	3
1:A:252:CYS:O	1:A:286:VAL:O	0.50	2.30	38	1
1:A:255:PHE:C	1:A:257:GLY:H	0.50	2.14	43	2
1:A:250:VAL:CG1	1:A:251:GLN:N	0.50	2.75	13	11
1:A:253:GLY:CA	1:A:286:VAL:HG23	0.50	2.37	41	2
1:A:275:SER:N	1:A:288:ILE:HG23	0.50	2.21	34	2
1:A:253:GLY:CA	1:A:286:VAL:HB	0.50	2.37	41	8
1:A:250:VAL:CB	1:A:288:ILE:HD12	0.50	2.37	24	3
1:A:250:VAL:HG23	1:A:314:ARG:NE	0.50	2.22	12	1
1:A:268:LEU:CG	1:A:273:PHE:CE2	0.50	2.95	31	2
1:A:304:LEU:CD1	1:A:314:ARG:NH1	0.50	2.75	23	3
1:A:250:VAL:HB	1:A:288:ILE:CB	0.50	2.35	3	1
1:A:251:GLN:HG3	1:A:287:VAL:HG12	0.50	1.84	32	1
1:A:248:TRP:HB2	1:A:291:VAL:HG22	0.50	1.82	40	1
1:A:264:VAL:HG13	1:A:309:HIS:CG	0.49	2.42	7	2
1:A:264:VAL:CG1	1:A:265:ARG:N	0.49	2.74	32	6
1:A:268:LEU:HD13	1:A:304:LEU:HD23	0.49	1.81	32	1
1:A:268:LEU:O	1:A:273:PHE:N	0.49	2.42	11	11
1:A:271:GLU:CB	1:A:273:PHE:CE1	0.49	2.94	10	9
1:A:256:ARG:CB	1:A:264:VAL:HG21	0.49	2.37	43	2
1:A:253:GLY:CA	1:A:286:VAL:CG1	0.49	2.90	43	4
1:A:250:VAL:HG23	1:A:314:ARG:HD2	0.49	1.83	22	1
1:A:252:CYS:HB2	1:A:286:VAL:HG12	0.49	1.84	33	1
1:A:255:PHE:CE2	1:A:309:HIS:HB3	0.49	2.41	42	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:255:PHE:CD2	1:A:309:HIS:ND1	0.49	2.81	41	1
1:A:314:ARG:NE	1:A:314:ARG:N	0.49	2.60	13	9
1:A:248:TRP:CH2	1:A:316:ALA:HB2	0.49	2.43	40	1
1:A:275:SER:HB3	1:A:288:ILE:HG12	0.49	1.83	17	9
1:A:252:CYS:O	1:A:304:LEU:CD2	0.49	2.60	20	5
1:A:252:CYS:HB2	1:A:286:VAL:CG1	0.49	2.38	32	2
1:A:304:LEU:HD11	1:A:313:ILE:HG21	0.49	1.83	39	1
1:A:264:VAL:CG1	1:A:286:VAL:HG21	0.49	2.38	19	1
1:A:275:SER:HB3	1:A:288:ILE:CG1	0.49	2.38	15	3
1:A:251:GLN:CD	1:A:315:LEU:HD12	0.49	2.33	5	1
1:A:273:PHE:CE2	1:A:304:LEU:HD23	0.49	2.43	26	1
1:A:283:TRP:CD1	1:A:283:TRP:N	0.49	2.80	43	12
1:A:275:SER:CA	1:A:288:ILE:HG12	0.49	2.37	16	12
1:A:250:VAL:CB	1:A:314:ARG:NH1	0.49	2.74	45	3
1:A:265:ARG:HG3	1:A:277:ILE:CG2	0.49	2.38	38	4
1:A:250:VAL:HG11	1:A:288:ILE:CG1	0.49	2.38	23	4
1:A:250:VAL:HG21	1:A:314:ARG:NH1	0.49	2.23	37	1
1:A:248:TRP:CZ3	1:A:316:ALA:N	0.48	2.81	12	21
1:A:297:ALA:HB1	1:A:314:ARG:CZ	0.48	2.38	31	4
1:A:250:VAL:HG22	1:A:251:GLN:N	0.48	2.23	38	8
1:A:249:MET:SD	1:A:317:ALA:HB2	0.48	2.48	16	3
1:A:261:ALA:C	1:A:264:VAL:HG12	0.48	2.33	19	1
1:A:301:LEU:HD13	1:A:301:LEU:C	0.48	2.32	19	1
1:A:252:CYS:SG	1:A:288:ILE:HD11	0.48	2.48	24	2
1:A:250:VAL:HB	1:A:314:ARG:HH11	0.48	1.66	44	2
1:A:251:GLN:NE2	1:A:313:ILE:HD11	0.48	2.23	4	1
1:A:286:VAL:HG12	1:A:287:VAL:N	0.48	2.23	29	16
1:A:273:PHE:CE2	1:A:304:LEU:HG	0.48	2.43	34	1
1:A:301:LEU:CD2	1:A:314:ARG:NH2	0.48	2.76	41	2
1:A:311:ASN:O	1:A:312:CYS:HB3	0.48	2.09	8	2
1:A:255:PHE:CE2	1:A:309:HIS:CB	0.48	2.96	20	1
1:A:250:VAL:CG2	1:A:288:ILE:HG13	0.48	2.38	8	2
1:A:304:LEU:HD23	1:A:309:HIS:ND1	0.48	2.23	13	1
1:A:249:MET:HE2	1:A:317:ALA:CA	0.48	2.39	11	1
1:A:253:GLY:O	1:A:284:ASN:O	0.48	2.31	20	1
1:A:252:CYS:CB	1:A:312:CYS:HA	0.48	2.38	22	2
1:A:250:VAL:HG22	1:A:288:ILE:HG13	0.48	1.85	8	1
1:A:275:SER:OG	1:A:286:VAL:HG21	0.48	2.08	15	2
1:A:309:HIS:CE1	1:A:312:CYS:N	0.48	2.81	31	1
1:A:250:VAL:HB	1:A:288:ILE:HD12	0.48	1.86	24	1
1:A:268:LEU:HG	1:A:273:PHE:O	0.48	2.08	33	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:253:GLY:HA2	1:A:286:VAL:CG1	0.48	2.38	43	1
1:A:303:ARG:O	1:A:306:MET:N	0.48	2.44	30	19
1:A:307:ALA:HB3	1:A:309:HIS:CE1	0.48	2.44	7	4
1:A:247:ARG:HD2	1:A:317:ALA:HB3	0.48	1.85	31	1
1:A:253:GLY:HA2	1:A:255:PHE:CD2	0.48	2.43	41	1
1:A:268:LEU:HD13	1:A:286:VAL:HG21	0.48	1.86	10	1
1:A:301:LEU:HD12	1:A:312:CYS:SG	0.48	2.49	13	1
1:A:264:VAL:HG12	1:A:277:ILE:HD11	0.48	1.85	18	1
1:A:268:LEU:CD1	1:A:273:PHE:O	0.48	2.60	27	1
1:A:271:GLU:HB3	1:A:273:PHE:CE1	0.48	2.44	42	12
1:A:254:SER:H	1:A:285:ARG:HA	0.48	1.68	25	1
1:A:255:PHE:CG	1:A:309:HIS:CG	0.48	3.02	41	1
1:A:301:LEU:HD13	1:A:314:ARG:HH21	0.47	1.65	2	2
1:A:254:SER:C	1:A:283:TRP:HB2	0.47	2.34	11	6
1:A:304:LEU:CD1	1:A:309:HIS:CE1	0.47	2.96	42	1
1:A:248:TRP:O	1:A:249:MET:HG2	0.47	2.09	8	1
1:A:271:GLU:HB2	1:A:273:PHE:CE1	0.47	2.43	39	4
1:A:265:ARG:HA	1:A:268:LEU:HD22	0.47	1.86	33	1
1:A:255:PHE:C	1:A:255:PHE:CD1	0.47	2.92	43	1
1:A:255:PHE:CZ	1:A:286:VAL:HG11	0.47	2.44	43	1
1:A:255:PHE:HE2	1:A:264:VAL:HG21	0.47	1.69	1	2
1:A:250:VAL:HG23	1:A:314:ARG:CD	0.47	2.39	7	1
1:A:250:VAL:HG12	1:A:291:VAL:HG22	0.47	1.85	10	2
1:A:299:SER:O	1:A:303:ARG:N	0.47	2.45	37	13
1:A:255:PHE:CZ	1:A:286:VAL:HB	0.47	2.45	23	1
1:A:255:PHE:HZ	1:A:286:VAL:HG21	0.47	1.68	28	1
1:A:297:ALA:CB	1:A:314:ARG:NH2	0.47	2.77	39	1
1:A:252:CYS:O	1:A:253:GLY:C	0.47	2.56	13	5
1:A:252:CYS:SG	1:A:286:VAL:HG23	0.47	2.49	39	2
1:A:270:PHE:CD1	1:A:270:PHE:C	0.47	2.92	1	11
1:A:264:VAL:HG22	1:A:307:ALA:O	0.47	2.10	25	2
1:A:250:VAL:HG11	1:A:288:ILE:HB	0.47	1.85	39	2
1:A:254:SER:CA	1:A:283:TRP:CD1	0.47	2.97	5	8
1:A:255:PHE:O	1:A:283:TRP:HB2	0.47	2.10	19	12
1:A:255:PHE:C	1:A:283:TRP:CB	0.47	2.87	12	7
1:A:314:ARG:NE	1:A:314:ARG:HA	0.47	2.24	4	2
1:A:301:LEU:HB2	1:A:314:ARG:NE	0.47	2.25	7	2
1:A:271:GLU:HG3	1:A:307:ALA:HB2	0.47	1.85	10	2
1:A:286:VAL:HG21	1:A:309:HIS:CE1	0.47	2.45	25	1
1:A:268:LEU:CG	1:A:275:SER:HB3	0.47	2.40	35	1
1:A:267:GLN:HG2	1:A:307:ALA:HB1	0.47	1.86	36	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:255:PHE:CE2	1:A:286:VAL:CG1	0.47	2.97	43	1
1:A:256:ARG:HG2	1:A:308:GLY:O	0.47	2.10	43	1
1:A:253:GLY:HA3	1:A:286:VAL:HB	0.47	1.86	20	7
1:A:298:ASP:HA	1:A:314:ARG:NH2	0.47	2.24	32	2
1:A:255:PHE:CE2	1:A:286:VAL:HG21	0.47	2.45	3	2
1:A:255:PHE:CE1	1:A:261:ALA:HA	0.47	2.45	43	1
1:A:253:GLY:CA	1:A:286:VAL:N	0.47	2.78	23	1
1:A:300:THR:O	1:A:304:LEU:CD2	0.47	2.63	31	1
1:A:268:LEU:CD1	1:A:275:SER:HB3	0.47	2.35	34	1
1:A:268:LEU:CD2	1:A:304:LEU:HD11	0.46	2.32	19	2
1:A:268:LEU:HD22	1:A:286:VAL:HG11	0.46	1.86	42	1
1:A:288:ILE:CD1	1:A:314:ARG:NH2	0.46	2.78	44	3
1:A:255:PHE:C	1:A:283:TRP:HB2	0.46	2.35	4	4
1:A:273:PHE:CE1	1:A:303:ARG:CB	0.46	2.98	36	5
1:A:253:GLY:CA	1:A:286:VAL:CG2	0.46	2.92	41	1
1:A:256:ARG:HG2	1:A:264:VAL:HG21	0.46	1.86	41	1
1:A:251:GLN:O	1:A:253:GLY:N	0.46	2.47	13	1
1:A:275:SER:OG	1:A:287:VAL:C	0.46	2.58	13	1
1:A:264:VAL:HG13	1:A:309:HIS:HE1	0.46	1.70	45	2
1:A:252:CYS:HB3	1:A:312:CYS:CB	0.46	2.41	31	1
1:A:255:PHE:CD2	1:A:309:HIS:HB2	0.46	2.44	40	3
1:A:253:GLY:O	1:A:285:ARG:CB	0.46	2.64	22	1
1:A:261:ALA:CB	1:A:284:ASN:HB3	0.46	2.41	27	1
1:A:264:VAL:O	1:A:268:LEU:N	0.46	2.48	37	4
1:A:252:CYS:CB	1:A:286:VAL:HG13	0.46	2.40	32	1
1:A:260:GLN:O	1:A:264:VAL:CG2	0.46	2.64	39	17
1:A:265:ARG:O	1:A:268:LEU:HD23	0.46	2.11	24	1
1:A:278:THR:O	1:A:285:ARG:CG	0.46	2.64	15	4
1:A:268:LEU:HD21	1:A:304:LEU:HD23	0.46	1.86	23	1
1:A:255:PHE:CD1	1:A:284:ASN:O	0.46	2.69	25	1
1:A:297:ALA:O	1:A:314:ARG:NE	0.46	2.49	11	5
1:A:252:CYS:HB3	1:A:312:CYS:HA	0.46	1.86	33	2
1:A:264:VAL:HG11	1:A:286:VAL:HG21	0.46	1.87	4	1
1:A:248:TRP:O	1:A:249:MET:CG	0.46	2.64	34	2
1:A:252:CYS:SG	1:A:301:LEU:HD13	0.46	2.51	44	1
1:A:268:LEU:O	1:A:273:PHE:C	0.45	2.59	18	8
1:A:254:SER:CB	1:A:283:TRP:NE1	0.45	2.79	19	10
1:A:268:LEU:CD2	1:A:273:PHE:CD2	0.45	2.96	23	2
1:A:263:THR:O	1:A:267:GLN:N	0.45	2.45	19	1
1:A:253:GLY:O	1:A:285:ARG:HA	0.45	2.11	22	1
1:A:264:VAL:HG12	1:A:309:HIS:ND1	0.45	2.26	24	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:252:CYS:O	1:A:253:GLY:O	0.45	2.34	12	3
1:A:278:THR:N	1:A:285:ARG:O	0.45	2.49	16	5
1:A:252:CYS:HB2	1:A:304:LEU:HD13	0.45	1.88	43	2
1:A:275:SER:HA	1:A:288:ILE:CB	0.45	2.41	27	1
1:A:268:LEU:CA	1:A:273:PHE:CE2	0.45	2.97	42	3
1:A:274:ASP:O	1:A:288:ILE:CG2	0.45	2.64	40	11
1:A:268:LEU:HD21	1:A:304:LEU:CD2	0.45	2.42	25	2
1:A:250:VAL:HG23	1:A:313:ILE:HG22	0.45	1.88	39	1
1:A:253:GLY:N	1:A:311:ASN:O	0.45	2.50	11	2
1:A:278:THR:O	1:A:285:ARG:HB3	0.45	2.12	21	6
1:A:252:CYS:HA	1:A:313:ILE:H	0.45	1.71	18	2
1:A:264:VAL:CG1	1:A:309:HIS:ND1	0.45	2.79	21	1
1:A:300:THR:O	1:A:304:LEU:HG	0.45	2.11	27	3
1:A:256:ARG:O	1:A:260:GLN:CB	0.45	2.64	41	2
1:A:253:GLY:C	1:A:254:SER:OG	0.45	2.59	3	4
1:A:273:PHE:CE2	1:A:300:THR:HG23	0.45	2.46	4	2
1:A:255:PHE:CE1	1:A:309:HIS:CB	0.45	3.00	44	3
1:A:303:ARG:O	1:A:306:MET:CB	0.45	2.65	43	14
1:A:252:CYS:HB2	1:A:304:LEU:CD1	0.45	2.41	43	2
1:A:249:MET:O	1:A:315:LEU:HB3	0.45	2.12	27	1
1:A:255:PHE:CD1	1:A:310:THR:O	0.45	2.70	27	1
1:A:269:ALA:HA	1:A:273:PHE:O	0.45	2.10	42	1
1:A:309:HIS:O	1:A:310:THR:C	0.45	2.59	31	3
1:A:309:HIS:ND1	1:A:309:HIS:C	0.45	2.75	41	6
1:A:273:PHE:CD2	1:A:300:THR:CG2	0.45	3.00	22	1
1:A:304:LEU:CD1	1:A:309:HIS:NE2	0.45	2.77	42	1
1:A:268:LEU:CD2	1:A:275:SER:HB2	0.45	2.35	1	3
1:A:273:PHE:O	1:A:274:ASP:O	0.45	2.34	28	3
1:A:253:GLY:C	1:A:255:PHE:CD1	0.45	2.94	25	1
1:A:250:VAL:CG2	1:A:313:ILE:CG2	0.45	2.94	39	1
1:A:300:THR:HG22	1:A:304:LEU:HD21	0.45	1.88	31	1
1:A:301:LEU:HD13	1:A:314:ARG:NE	0.45	2.27	1	1
1:A:314:ARG:CZ	1:A:314:ARG:HB2	0.45	2.42	16	5
1:A:308:GLY:C	1:A:309:HIS:ND1	0.45	2.75	7	2
1:A:313:ILE:HD12	1:A:313:ILE:N	0.45	2.27	7	1
1:A:253:GLY:HA2	1:A:255:PHE:HE1	0.45	1.68	29	3
1:A:268:LEU:HB3	1:A:275:SER:HB3	0.45	1.89	7	1
1:A:250:VAL:CG1	1:A:288:ILE:HG13	0.45	2.42	23	2
1:A:275:SER:OG	1:A:288:ILE:HG23	0.45	2.11	13	1
1:A:267:GLN:HB3	1:A:307:ALA:HB1	0.45	1.87	21	1
1:A:264:VAL:O	1:A:268:LEU:HB3	0.45	2.11	40	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:252:CYS:SG	1:A:286:VAL:N	0.45	2.90	39	1
1:A:257:GLY:O	1:A:258:ALA:HB2	0.45	2.12	41	1
1:A:260:GLN:O	1:A:264:VAL:CB	0.44	2.66	33	14
1:A:275:SER:OG	1:A:286:VAL:CG1	0.44	2.63	19	2
1:A:275:SER:HB3	1:A:286:VAL:CG1	0.44	2.42	13	1
1:A:254:SER:OG	1:A:285:ARG:CB	0.44	2.65	27	1
1:A:275:SER:OG	1:A:286:VAL:CG2	0.44	2.65	43	1
1:A:265:ARG:HB2	1:A:277:ILE:CG2	0.44	2.42	44	1
1:A:293:GLY:O	1:A:294:LYS:CB	0.44	2.65	30	3
1:A:297:ALA:O	1:A:314:ARG:CZ	0.44	2.65	22	3
1:A:249:MET:C	1:A:315:LEU:O	0.44	2.60	34	6
1:A:252:CYS:CB	1:A:286:VAL:HB	0.44	2.43	13	2
1:A:273:PHE:HE2	1:A:304:LEU:HD12	0.44	1.73	13	1
1:A:253:GLY:HA3	1:A:286:VAL:O	0.44	2.13	23	1
1:A:268:LEU:CD1	1:A:275:SER:HB2	0.44	2.39	38	3
1:A:288:ILE:O	1:A:288:ILE:HG22	0.44	2.12	29	2
1:A:304:LEU:HD13	1:A:313:ILE:HD13	0.44	1.88	39	1
1:A:268:LEU:CB	1:A:273:PHE:O	0.44	2.65	4	1
1:A:254:SER:O	1:A:283:TRP:CG	0.44	2.71	11	1
1:A:279:THR:HG23	1:A:283:TRP:O	0.44	2.10	29	1
1:A:304:LEU:CD1	1:A:313:ILE:CG2	0.44	2.95	39	1
1:A:249:MET:O	1:A:315:LEU:CB	0.44	2.65	23	5
1:A:314:ARG:CA	1:A:314:ARG:NE	0.44	2.81	23	2
1:A:249:MET:O	1:A:315:LEU:N	0.44	2.50	40	2
1:A:286:VAL:CG2	1:A:287:VAL:N	0.44	2.80	44	7
1:A:299:SER:O	1:A:303:ARG:HB2	0.44	2.13	16	4
1:A:264:VAL:CG1	1:A:268:LEU:HD12	0.44	2.43	16	1
1:A:268:LEU:CD2	1:A:273:PHE:CZ	0.44	2.87	18	1
1:A:266:ALA:O	1:A:270:PHE:N	0.44	2.49	31	1
1:A:297:ALA:CB	1:A:314:ARG:CZ	0.44	2.96	34	2
1:A:301:LEU:HG	1:A:313:ILE:HG13	0.44	1.89	39	1
1:A:252:CYS:HB3	1:A:286:VAL:HB	0.44	1.88	2	1
1:A:307:ALA:CB	1:A:309:HIS:CE1	0.44	2.99	7	2
1:A:273:PHE:CE2	1:A:303:ARG:CB	0.44	3.01	13	1
1:A:268:LEU:HD11	1:A:275:SER:OG	0.44	2.13	33	1
1:A:248:TRP:CZ3	1:A:314:ARG:O	0.44	2.71	41	12
1:A:298:ASP:HA	1:A:314:ARG:NH1	0.44	2.28	10	1
1:A:303:ARG:O	1:A:306:MET:HB3	0.44	2.13	10	3
1:A:252:CYS:O	1:A:309:HIS:CE1	0.44	2.70	15	1
1:A:268:LEU:HG	1:A:286:VAL:HG21	0.44	1.89	22	1
1:A:304:LEU:HD11	1:A:314:ARG:NH1	0.44	2.27	27	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:268:LEU:CD2	1:A:286:VAL:CG1	0.44	2.96	42	2
1:A:309:HIS:ND1	1:A:312:CYS:SG	0.44	2.91	39	1
1:A:273:PHE:CE2	1:A:303:ARG:HB3	0.44	2.48	2	1
1:A:314:ARG:CZ	1:A:314:ARG:N	0.44	2.81	33	2
1:A:254:SER:OG	1:A:283:TRP:C	0.44	2.61	39	2
1:A:252:CYS:HB2	1:A:312:CYS:CB	0.44	2.43	35	1
1:A:258:ALA:HA	1:A:283:TRP:HA	0.44	1.89	43	2
1:A:276:LYS:CG	1:A:287:VAL:O	0.43	2.66	15	4
1:A:250:VAL:CG2	1:A:314:ARG:NE	0.43	2.80	12	1
1:A:249:MET:HA	1:A:289:GLY:O	0.43	2.14	19	2
1:A:304:LEU:C	1:A:309:HIS:CD2	0.43	2.96	39	2
1:A:301:LEU:HD13	1:A:314:ARG:HE	0.43	1.72	28	1
1:A:281:ASN:ND2	1:A:283:TRP:CZ2	0.43	2.85	42	1
1:A:273:PHE:CE1	1:A:303:ARG:HG3	0.43	2.48	5	1
1:A:273:PHE:CE1	1:A:303:ARG:HG2	0.43	2.48	22	5
1:A:250:VAL:CB	1:A:288:ILE:HD11	0.43	2.43	13	1
1:A:252:CYS:O	1:A:286:VAL:HB	0.43	2.13	35	1
1:A:250:VAL:CG2	1:A:288:ILE:HB	0.43	2.42	40	1
1:A:255:PHE:O	1:A:257:GLY:N	0.43	2.51	43	1
1:A:294:LYS:O	1:A:298:ASP:CB	0.43	2.67	7	1
1:A:304:LEU:HD22	1:A:312:CYS:HB3	0.43	1.88	2	1
1:A:268:LEU:CD2	1:A:309:HIS:CE1	0.43	3.00	18	2
1:A:269:ALA:HB2	1:A:275:SER:OG	0.43	2.12	27	1
1:A:256:ARG:CB	1:A:260:GLN:HB3	0.43	2.43	41	1
1:A:283:TRP:CD1	1:A:283:TRP:H	0.43	2.31	33	6
1:A:273:PHE:HB2	1:A:300:THR:HG23	0.43	1.90	10	1
1:A:291:VAL:HG21	1:A:314:ARG:NH2	0.43	2.28	39	2
1:A:252:CYS:O	1:A:286:VAL:CG1	0.43	2.67	18	1
1:A:289:GLY:O	1:A:291:VAL:HG13	0.43	2.14	34	2
1:A:264:VAL:CA	1:A:307:ALA:HB1	0.43	2.40	28	1
1:A:255:PHE:HB3	1:A:310:THR:HG23	0.43	1.89	31	1
1:A:270:PHE:CD1	1:A:270:PHE:O	0.43	2.72	30	16
1:A:255:PHE:CE2	1:A:261:ALA:CA	0.43	2.97	25	2
1:A:275:SER:HA	1:A:288:ILE:CG1	0.43	2.43	24	2
1:A:250:VAL:CG2	1:A:314:ARG:HD2	0.43	2.43	44	1
1:A:276:LYS:O	1:A:287:VAL:HG22	0.43	2.13	4	1
1:A:285:ARG:O	1:A:285:ARG:HG3	0.43	2.13	17	3
1:A:289:GLY:O	1:A:290:PRO:C	0.43	2.62	26	4
1:A:273:PHE:CD1	1:A:303:ARG:HG2	0.43	2.48	41	3
1:A:250:VAL:HG21	1:A:288:ILE:HB	0.43	1.91	40	1
1:A:269:ALA:HB2	1:A:274:ASP:CG	0.43	2.39	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:255:PHE:HZ	1:A:286:VAL:HG12	0.43	1.73	22	1
1:A:314:ARG:HH11	1:A:314:ARG:HG3	0.43	1.73	44	1
1:A:288:ILE:O	1:A:289:GLY:O	0.43	2.37	30	8
1:A:251:GLN:O	1:A:252:CYS:O	0.43	2.37	7	1
1:A:301:LEU:CB	1:A:314:ARG:CZ	0.43	2.97	7	1
1:A:313:ILE:HG22	1:A:314:ARG:N	0.43	2.29	7	1
1:A:267:GLN:CB	1:A:307:ALA:HB1	0.43	2.44	9	1
1:A:253:GLY:C	1:A:255:PHE:CE1	0.43	2.97	20	1
1:A:275:SER:HA	1:A:288:ILE:HA	0.43	1.90	28	4
1:A:309:HIS:O	1:A:311:ASN:N	0.43	2.51	26	1
1:A:255:PHE:CZ	1:A:309:HIS:ND1	0.43	2.87	43	2
1:A:264:VAL:O	1:A:267:GLN:N	0.43	2.51	29	1
1:A:273:PHE:HZ	1:A:303:ARG:C	0.43	2.22	30	1
1:A:274:ASP:O	1:A:275:SER:HB2	0.43	2.13	36	1
1:A:277:ILE:HG22	1:A:286:VAL:HG13	0.43	1.91	1	1
1:A:288:ILE:HD12	1:A:300:THR:CG2	0.43	2.44	3	1
1:A:250:VAL:CB	1:A:288:ILE:CD1	0.43	2.97	13	1
1:A:288:ILE:CD1	1:A:300:THR:CG2	0.43	2.97	34	4
1:A:300:THR:HB	1:A:314:ARG:CZ	0.43	2.44	22	1
1:A:250:VAL:CG1	1:A:288:ILE:CG1	0.43	2.97	23	1
1:A:301:LEU:HG	1:A:314:ARG:NH1	0.43	2.28	23	1
1:A:301:LEU:HD12	1:A:301:LEU:O	0.43	2.14	27	1
1:A:267:GLN:O	1:A:271:GLU:CG	0.43	2.67	40	3
1:A:300:THR:HG22	1:A:313:ILE:HD13	0.43	1.90	39	1
1:A:253:GLY:CA	1:A:255:PHE:HE1	0.42	2.27	18	1
1:A:268:LEU:CD2	1:A:273:PHE:O	0.42	2.67	2	3
1:A:248:TRP:CE3	1:A:316:ALA:CA	0.42	3.03	40	5
1:A:248:TRP:CE3	1:A:316:ALA:HA	0.42	2.49	26	1
1:A:268:LEU:CD2	1:A:275:SER:CB	0.42	2.95	28	2
1:A:250:VAL:CB	1:A:314:ARG:HD2	0.42	2.44	34	1
1:A:300:THR:O	1:A:304:LEU:CD1	0.42	2.67	37	1
1:A:268:LEU:CD1	1:A:275:SER:OG	0.42	2.67	40	1
1:A:250:VAL:HG13	1:A:252:CYS:SG	0.42	2.55	5	1
1:A:250:VAL:HG21	1:A:314:ARG:CZ	0.42	2.44	9	1
1:A:278:THR:O	1:A:285:ARG:HG3	0.42	2.14	17	1
1:A:252:CYS:HB3	1:A:312:CYS:HB3	0.42	1.91	18	1
1:A:253:GLY:O	1:A:254:SER:HB2	0.42	2.14	30	2
1:A:297:ALA:O	1:A:314:ARG:CD	0.42	2.67	34	1
1:A:266:ALA:O	1:A:270:PHE:HB3	0.42	2.14	38	1
1:A:273:PHE:O	1:A:274:ASP:C	0.42	2.62	28	2
1:A:264:VAL:CG1	1:A:309:HIS:CG	0.42	3.02	26	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:297:ALA:CB	1:A:314:ARG:NH1	0.42	2.81	45	2
1:A:248:TRP:CZ3	1:A:316:ALA:CB	0.42	2.97	40	1
1:A:253:GLY:N	1:A:312:CYS:HA	0.42	2.29	7	1
1:A:277:ILE:CG2	1:A:286:VAL:HG23	0.42	2.45	38	1
1:A:255:PHE:C	1:A:283:TRP:HB3	0.42	2.40	7	3
1:A:250:VAL:CG1	1:A:314:ARG:HD3	0.42	2.44	27	2
1:A:276:LYS:O	1:A:287:VAL:CG2	0.42	2.65	25	1
1:A:267:GLN:O	1:A:271:GLU:CB	0.42	2.67	26	3
1:A:250:VAL:CG1	1:A:314:ARG:NH1	0.42	2.83	34	1
1:A:248:TRP:CE3	1:A:316:ALA:N	0.42	2.87	39	1
1:A:265:ARG:HG3	1:A:277:ILE:HB	0.42	1.90	42	3
1:A:255:PHE:CD1	1:A:309:HIS:HB3	0.42	2.50	45	2
1:A:288:ILE:O	1:A:288:ILE:HG13	0.42	2.14	27	1
1:A:247:ARG:HG2	1:A:248:TRP:N	0.42	2.29	38	1
1:A:297:ALA:CA	1:A:314:ARG:CZ	0.42	2.98	39	1
1:A:286:VAL:C	1:A:287:VAL:HG13	0.42	2.39	6	4
1:A:268:LEU:HD21	1:A:286:VAL:HG13	0.42	1.91	29	2
1:A:251:GLN:CG	1:A:287:VAL:CG1	0.42	2.98	22	1
1:A:253:GLY:CA	1:A:311:ASN:O	0.42	2.68	24	1
1:A:254:SER:OG	1:A:283:TRP:O	0.42	2.37	34	1
1:A:261:ALA:HA	1:A:264:VAL:HB	0.42	1.90	42	2
1:A:265:ARG:HB2	1:A:277:ILE:CD1	0.42	2.45	40	1
1:A:275:SER:OG	1:A:286:VAL:HG22	0.42	2.15	43	1
1:A:275:SER:OG	1:A:286:VAL:HG13	0.42	2.14	2	1
1:A:275:SER:HA	1:A:288:ILE:HG12	0.42	1.91	9	1
1:A:251:GLN:OE1	1:A:313:ILE:HD11	0.42	2.15	10	1
1:A:286:VAL:HG22	1:A:287:VAL:H	0.42	1.74	10	2
1:A:296:ASN:O	1:A:300:THR:N	0.42	2.52	11	1
1:A:277:ILE:HG21	1:A:286:VAL:HG22	0.42	1.89	25	1
1:A:250:VAL:CB	1:A:288:ILE:HG13	0.42	2.45	41	1
1:A:255:PHE:O	1:A:283:TRP:CB	0.42	2.68	42	1
1:A:314:ARG:HB2	1:A:314:ARG:NH1	0.42	2.30	14	1
1:A:264:VAL:HG22	1:A:307:ALA:C	0.42	2.40	20	1
1:A:252:CYS:SG	1:A:286:VAL:CG1	0.42	3.08	22	3
1:A:252:CYS:HA	1:A:312:CYS:CA	0.42	2.45	24	1
1:A:300:THR:HG22	1:A:304:LEU:HD11	0.42	1.85	37	1
1:A:257:GLY:O	1:A:258:ALA:C	0.41	2.63	8	7
1:A:301:LEU:CD1	1:A:314:ARG:NH2	0.41	2.81	3	3
1:A:248:TRP:O	1:A:291:VAL:N	0.41	2.53	7	2
1:A:309:HIS:CE1	1:A:312:CYS:SG	0.41	3.13	14	2
1:A:308:GLY:C	1:A:309:HIS:CG	0.41	2.98	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:268:LEU:CD1	1:A:304:LEU:CD2	0.41	2.98	33	1
1:A:271:GLU:HB3	1:A:273:PHE:CD1	0.41	2.50	13	1
1:A:264:VAL:O	1:A:268:LEU:HD23	0.41	2.15	14	1
1:A:309:HIS:CE1	1:A:311:ASN:C	0.41	2.98	15	1
1:A:249:MET:N	1:A:315:LEU:O	0.41	2.53	19	3
1:A:313:ILE:N	1:A:313:ILE:CD1	0.41	2.77	20	1
1:A:270:PHE:O	1:A:270:PHE:CD1	0.41	2.73	21	1
1:A:255:PHE:CE1	1:A:284:ASN:O	0.41	2.74	25	1
1:A:249:MET:HE3	1:A:290:PRO:HG3	0.41	1.92	34	1
1:A:251:GLN:H	1:A:313:ILE:HA	0.41	1.75	39	1
1:A:265:ARG:CB	1:A:277:ILE:HD13	0.41	2.40	43	1
1:A:254:SER:C	1:A:283:TRP:CD1	0.41	2.98	37	2
1:A:255:PHE:HB3	1:A:310:THR:OG1	0.41	2.14	26	1
1:A:268:LEU:CG	1:A:275:SER:CB	0.41	2.98	40	1
1:A:297:ALA:HB1	1:A:314:ARG:HH11	0.41	1.74	43	1
1:A:248:TRP:CD1	1:A:297:ALA:CB	0.41	3.02	44	1
1:A:273:PHE:CE2	1:A:303:ARG:HB2	0.41	2.50	13	1
1:A:253:GLY:O	1:A:255:PHE:CD1	0.41	2.73	20	1
1:A:252:CYS:SG	1:A:304:LEU:CD2	0.41	3.09	32	2
1:A:250:VAL:HG23	1:A:313:ILE:CG2	0.41	2.45	39	1
1:A:312:CYS:O	1:A:313:ILE:CG2	0.41	2.68	37	4
1:A:277:ILE:HG22	1:A:278:THR:N	0.41	2.30	18	1
1:A:252:CYS:O	1:A:304:LEU:HD21	0.41	2.16	19	1
1:A:289:GLY:O	1:A:291:VAL:N	0.41	2.53	24	1
1:A:257:GLY:O	1:A:261:ALA:HB2	0.41	2.15	25	1
1:A:311:ASN:C	1:A:312:CYS:SG	0.41	3.03	40	2
1:A:267:GLN:O	1:A:271:GLU:HB2	0.41	2.15	28	2
1:A:312:CYS:O	1:A:313:ILE:O	0.41	2.38	39	1
1:A:314:ARG:N	1:A:314:ARG:CD	0.41	2.80	39	1
1:A:311:ASN:O	1:A:312:CYS:HB2	0.41	2.16	7	1
1:A:254:SER:HB2	1:A:283:TRP:C	0.41	2.40	8	2
1:A:308:GLY:O	1:A:309:HIS:ND1	0.41	2.53	19	1
1:A:249:MET:CB	1:A:315:LEU:O	0.41	2.68	40	1
1:A:268:LEU:HG	1:A:275:SER:CB	0.41	2.46	42	1
1:A:256:ARG:HG3	1:A:264:VAL:HG11	0.41	1.91	43	1
1:A:250:VAL:CG1	1:A:291:VAL:HG21	0.41	2.46	27	1
1:A:300:THR:O	1:A:303:ARG:N	0.41	2.54	31	1
1:A:268:LEU:HD22	1:A:309:HIS:HE1	0.41	1.75	35	1
1:A:250:VAL:HG13	1:A:288:ILE:HG13	0.41	1.92	8	1
1:A:268:LEU:CD2	1:A:304:LEU:HG	0.41	2.46	9	1
1:A:278:THR:C	1:A:279:THR:HG1	0.41	2.22	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:311:ASN:O	1:A:312:CYS:SG	0.41	2.78	20	2
1:A:273:PHE:N	1:A:273:PHE:CD1	0.41	2.89	22	1
1:A:250:VAL:CG1	1:A:288:ILE:CB	0.41	2.98	34	1
1:A:256:ARG:HB3	1:A:260:GLN:CB	0.41	2.40	43	1
1:A:248:TRP:CE3	1:A:315:LEU:O	0.41	2.73	44	2
1:A:265:ARG:HB2	1:A:277:ILE:HG21	0.41	1.91	44	1
1:A:248:TRP:O	1:A:249:MET:O	0.41	2.39	45	1
1:A:250:VAL:CG1	1:A:288:ILE:H	0.41	2.26	45	1
1:A:254:SER:HB3	1:A:285:ARG:HA	0.41	1.92	4	1
1:A:248:TRP:HB3	1:A:291:VAL:CG2	0.41	2.44	12	1
1:A:251:GLN:CG	1:A:285:ARG:NH1	0.41	2.84	13	1
1:A:285:ARG:O	1:A:285:ARG:CG	0.41	2.68	17	1
1:A:254:SER:CA	1:A:285:ARG:HB3	0.41	2.46	22	1
1:A:288:ILE:CD1	1:A:300:THR:OG1	0.41	2.69	43	1
1:A:252:CYS:SG	1:A:304:LEU:CD1	0.41	3.07	14	2
1:A:264:VAL:CG1	1:A:286:VAL:CG2	0.41	2.99	19	1
1:A:298:ASP:O	1:A:301:LEU:HB2	0.40	2.15	4	1
1:A:313:ILE:HD12	1:A:314:ARG:H	0.40	1.76	8	1
1:A:268:LEU:HD23	1:A:307:ALA:HB2	0.40	1.93	14	1
1:A:250:VAL:HG23	1:A:314:ARG:HD3	0.40	1.93	16	1
1:A:277:ILE:HG12	1:A:286:VAL:HG23	0.40	1.93	18	1
1:A:279:THR:HG23	1:A:284:ASN:N	0.40	2.31	23	2
1:A:257:GLY:O	1:A:261:ALA:CB	0.40	2.69	25	1
1:A:250:VAL:CG1	1:A:288:ILE:HG12	0.40	2.47	27	1
1:A:310:THR:O	1:A:311:ASN:ND2	0.40	2.54	40	1
1:A:249:MET:HE3	1:A:315:LEU:HD22	0.40	1.93	44	1
1:A:310:THR:O	1:A:311:ASN:CG	0.40	2.64	9	1
1:A:273:PHE:HE2	1:A:304:LEU:HG	0.40	1.77	14	1
1:A:264:VAL:CG2	1:A:308:GLY:O	0.40	2.69	20	1
1:A:268:LEU:HD13	1:A:304:LEU:HG	0.40	1.92	24	1
1:A:254:SER:O	1:A:311:ASN:ND2	0.40	2.54	40	1
1:A:251:GLN:NE2	1:A:315:LEU:CD1	0.40	2.84	41	1
1:A:248:TRP:CD1	1:A:293:GLY:HA2	0.40	2.51	18	2
1:A:250:VAL:HG13	1:A:288:ILE:HG12	0.40	1.93	27	1
1:A:314:ARG:HD2	1:A:314:ARG:HA	0.40	1.73	31	1
1:A:255:PHE:CB	1:A:309:HIS:HB3	0.40	2.47	43	1
1:A:258:ALA:O	1:A:261:ALA:HB3	0.40	2.17	21	1
1:A:248:TRP:C	1:A:249:MET:CG	0.40	2.94	22	1
1:A:255:PHE:C	1:A:255:PHE:HD1	0.40	2.24	41	1
1:A:250:VAL:CG2	1:A:314:ARG:HG3	0.40	2.41	43	1
1:A:264:VAL:HG22	1:A:268:LEU:HD12	0.40	1.92	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:277:ILE:HB	1:A:285:ARG:O	0.40	2.16	31	1
1:A:267:GLN:CB	1:A:307:ALA:HA	0.40	2.47	34	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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	71/81 (88%)	49±2 (69±3%)	15±3 (22±4%)	7±2 (10±3%)	1	10
All	All	3195/3645 (88%)	2194 (69%)	695 (22%)	306 (10%)	1	10

All 27 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	311	ASN	36
1	A	289	GLY	31
1	A	274	ASP	25
1	A	294	LYS	25
1	A	295	GLU	24
1	A	280	ASN	23
1	A	313	ILE	23
1	A	254	SER	22
1	A	290	PRO	17
1	A	253	GLY	13
1	A	312	CYS	12
1	A	250	VAL	7
1	A	247	ARG	7
1	A	278	THR	6
1	A	257	GLY	6
1	A	249	MET	5
1	A	284	ASN	4
1	A	310	THR	4
1	A	286	VAL	3
1	A	317	ALA	3

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Mol	Chain	Res	Type	Models (Total)
1	A	252	CYS	2
1	A	291	VAL	2
1	A	258	ALA	2
1	A	287	VAL	1
1	A	275	SER	1
1	A	256	ARG	1
1	A	293	GLY	1

6.3.2 Protein sidechains [i](#)

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	56/64 (88%)	33±3 (58±5%)	23±3 (42±5%)	0	4
All	All	2520/2880 (88%)	1465 (58%)	1055 (42%)	0	4

All 51 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	255	PHE	45
1	A	268	LEU	44
1	A	314	ARG	44
1	A	278	THR	40
1	A	283	TRP	40
1	A	315	LEU	40
1	A	305	LYS	38
1	A	304	LEU	33
1	A	254	SER	31
1	A	279	THR	30
1	A	291	VAL	28
1	A	294	LYS	27
1	A	264	VAL	26
1	A	276	LYS	26
1	A	313	ILE	25
1	A	247	ARG	25
1	A	260	GLN	25
1	A	284	ASN	24

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Mol	Chain	Res	Type	Models (Total)
1	A	285	ARG	24
1	A	295	GLU	24
1	A	262	GLU	24
1	A	303	ARG	24
1	A	273	PHE	23
1	A	288	ILE	22
1	A	292	LYS	22
1	A	256	ARG	20
1	A	265	ARG	20
1	A	271	GLU	19
1	A	280	ASN	18
1	A	250	VAL	18
1	A	309	HIS	17
1	A	310	THR	17
1	A	259	GLU	17
1	A	298	ASP	15
1	A	267	GLN	15
1	A	251	GLN	14
1	A	301	LEU	14
1	A	296	ASN	12
1	A	300	THR	11
1	A	252	CYS	10
1	A	311	ASN	10
1	A	299	SER	9
1	A	312	CYS	8
1	A	306	MET	7
1	A	281	ASN	7
1	A	249	MET	7
1	A	274	ASP	6
1	A	275	SER	4
1	A	277	ILE	2
1	A	286	VAL	2
1	A	287	VAL	2

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided