



Full wwPDB NMR Structure Validation Report ⓘ

May 28, 2020 – 11:00 pm BST

PDB ID : 2L8B
Title : TraI (381-569)
Authors : Wright, N.T.; Raththagala, M.U.; Edwards, S.; Krueger, S.; Schildbach, J.F.
Deposited on : 2011-01-07

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : 2.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

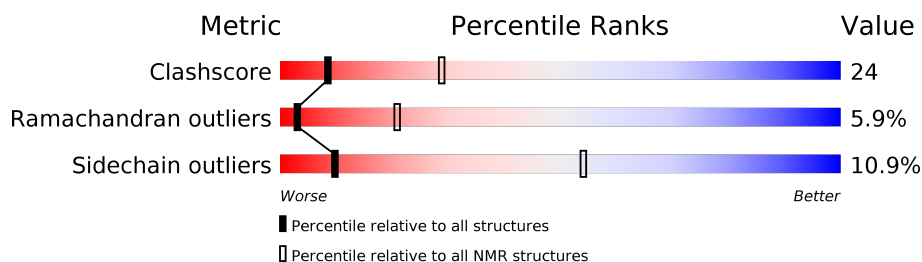
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 80%.

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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	189	

2 Ensemble composition and analysis

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:389-A:555 (167)	0.65	1

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. No single-model clusters were found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 2884 atoms, of which 1454 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Protein traI.

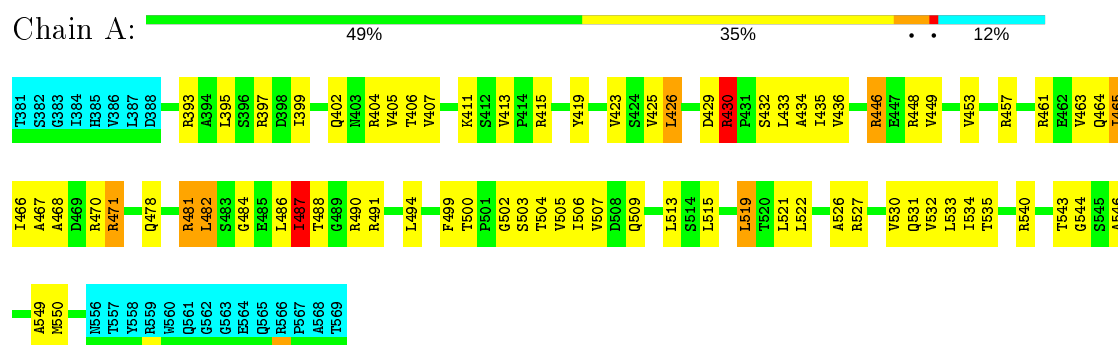
Mol	Chain	Residues	Atoms						Trace
1	A	189	Total	C	H	N	O	S	0
			2884	867	1454	274	281	8	

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA 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: Protein traI

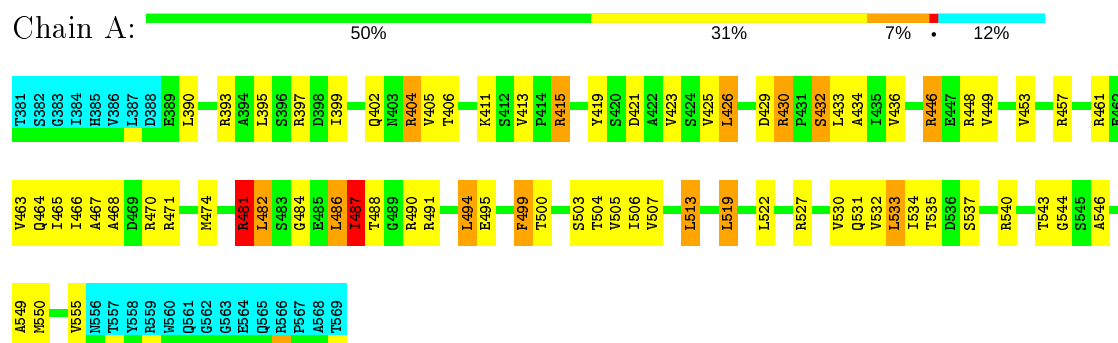


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

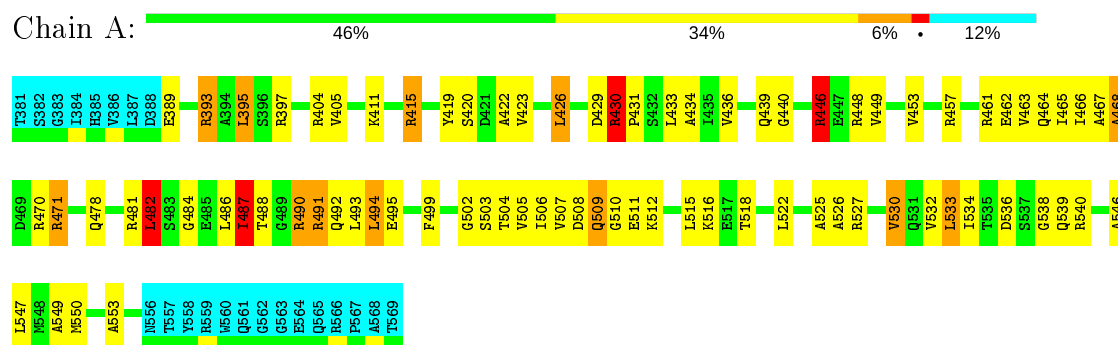
4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Protein traI



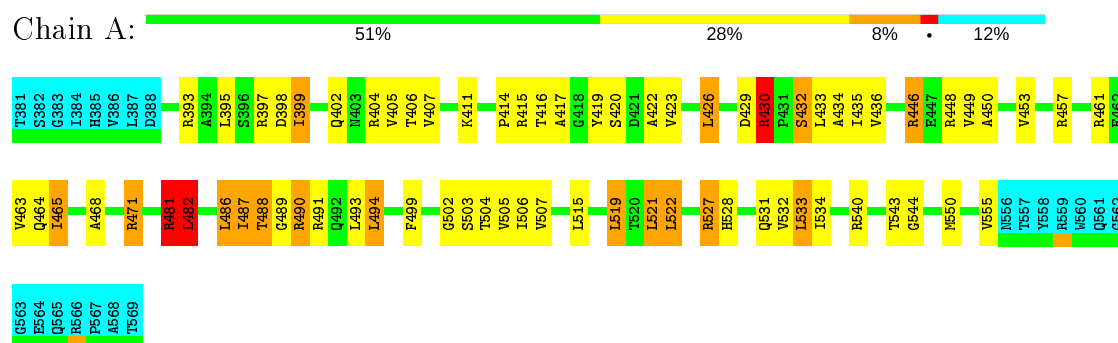
4.2.2 Score per residue for model 2

- Molecule 1: Protein traI



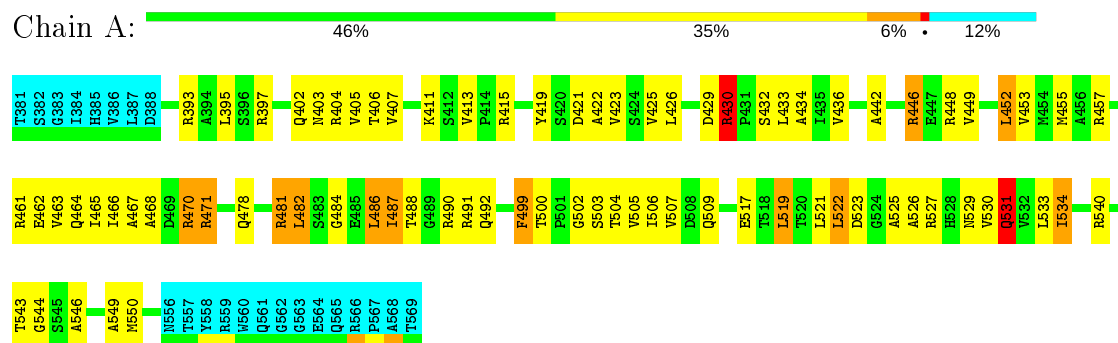
4.2.3 Score per residue for model 3

- Molecule 1: Protein traI



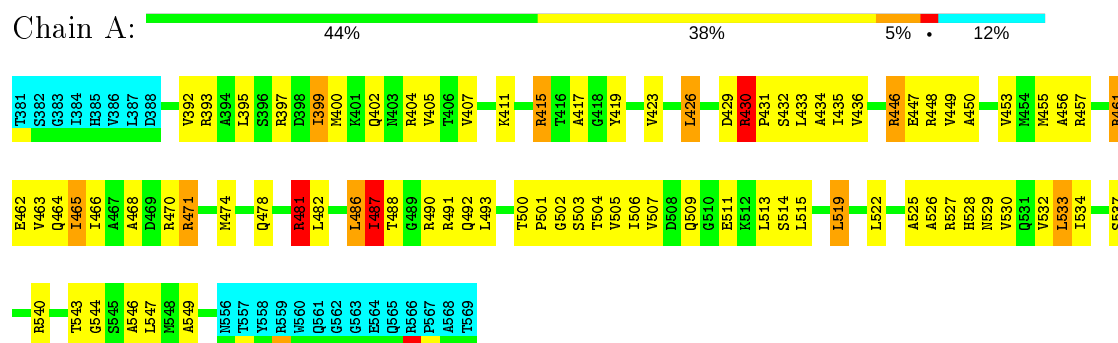
4.2.4 Score per residue for model 4

- Molecule 1: Protein traI



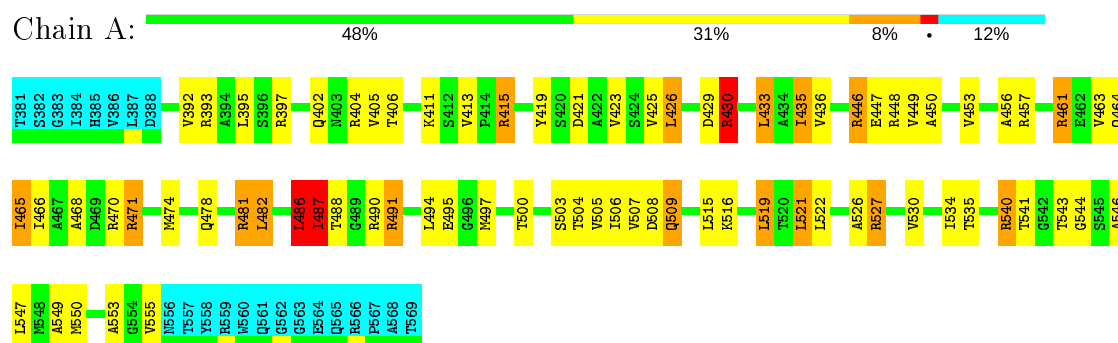
4.2.5 Score per residue for model 5

- Molecule 1: Protein traI



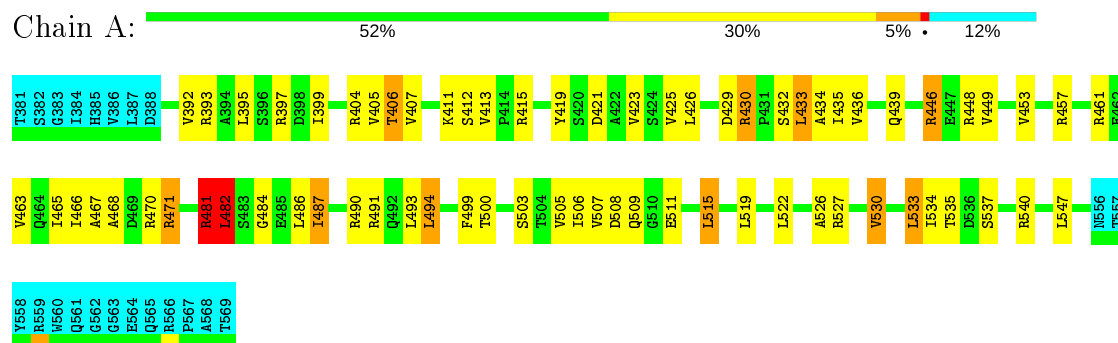
4.2.6 Score per residue for model 6

- Molecule 1: Protein traI



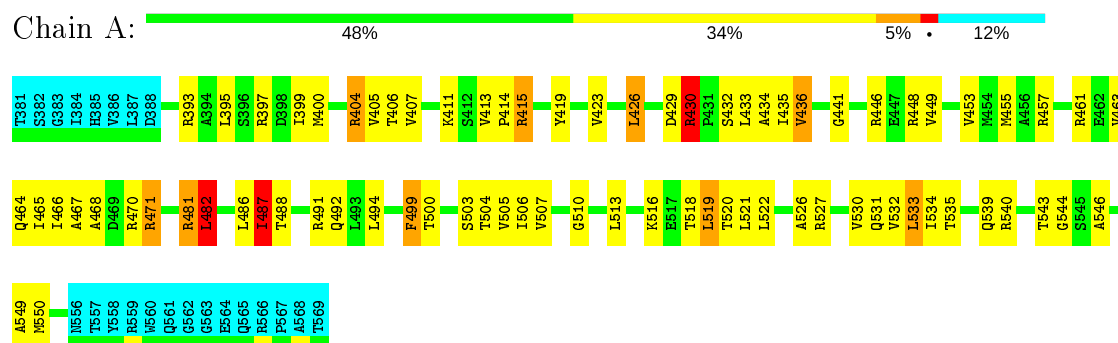
4.2.7 Score per residue for model 7

- Molecule 1: Protein traI



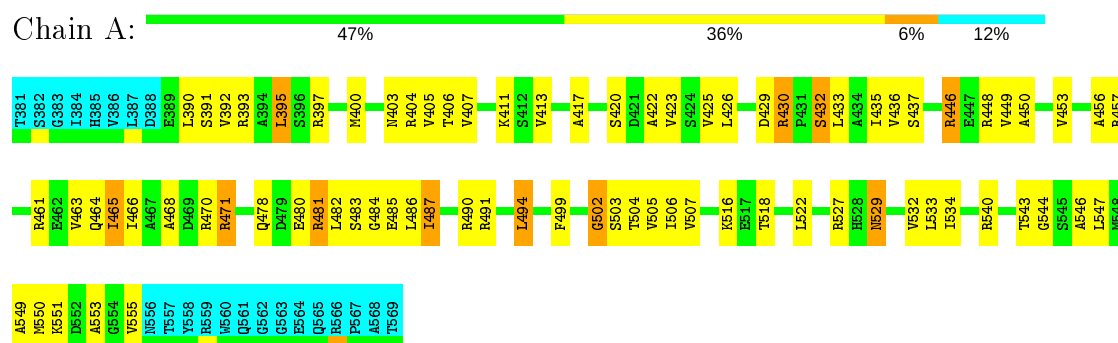
4.2.8 Score per residue for model 8

- Molecule 1: Protein traI



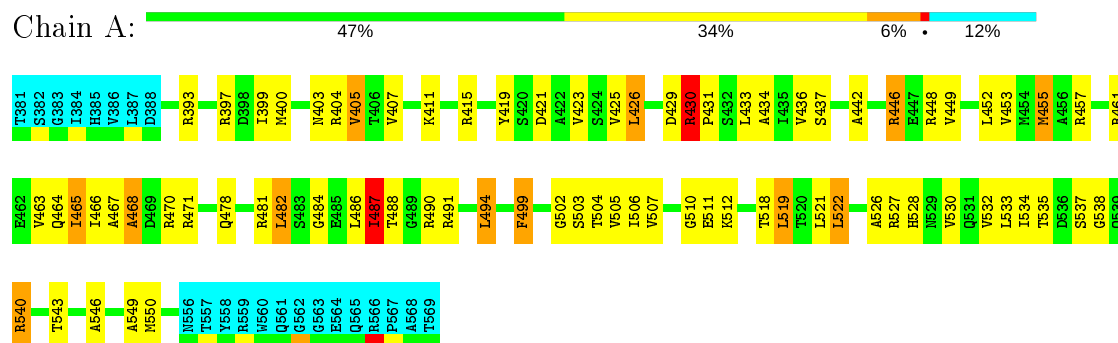
4.2.9 Score per residue for model 9

- Molecule 1: Protein traI



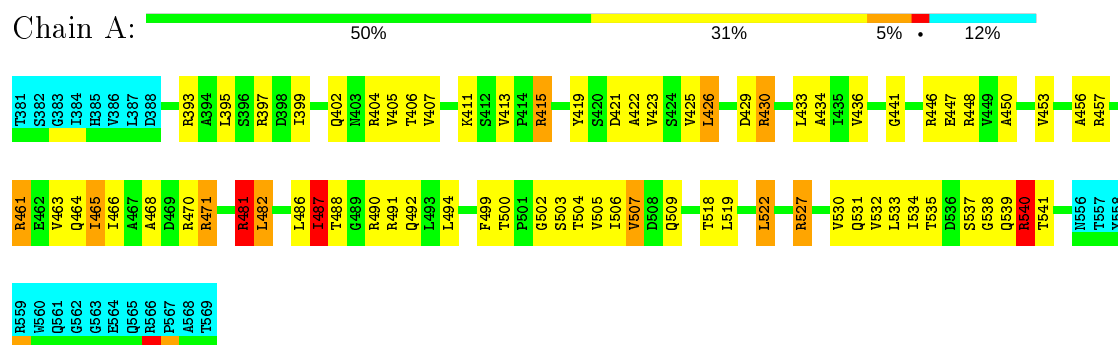
4.2.10 Score per residue for model 10

- Molecule 1: Protein traI



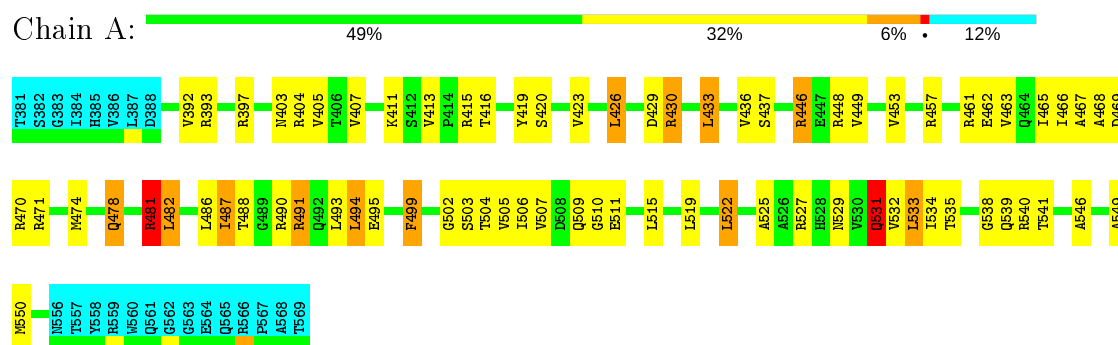
4.2.11 Score per residue for model 11

- Molecule 1: Protein traI



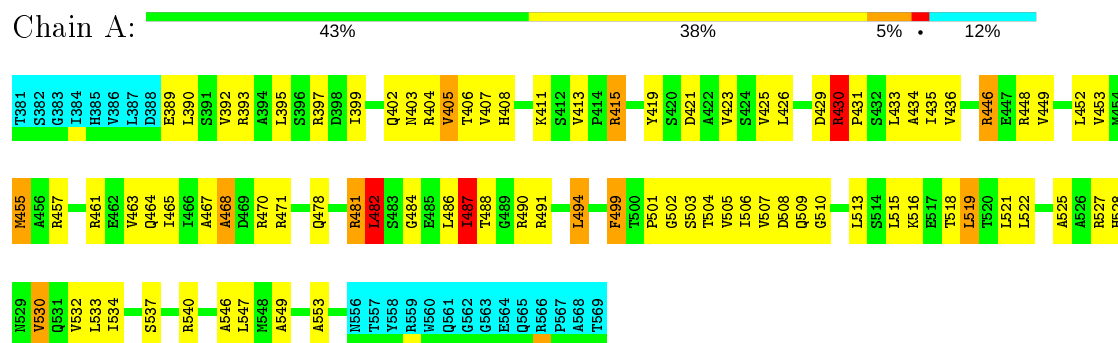
4.2.12 Score per residue for model 12

- Molecule 1: Protein traI



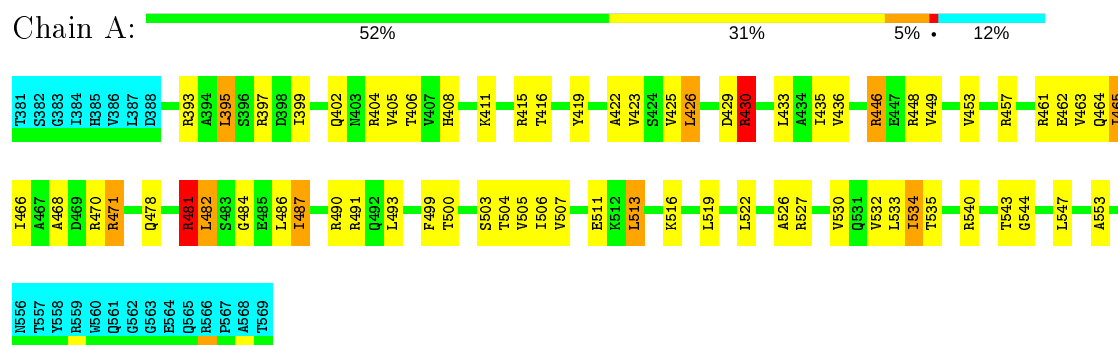
4.2.13 Score per residue for model 13

- Molecule 1: Protein traI



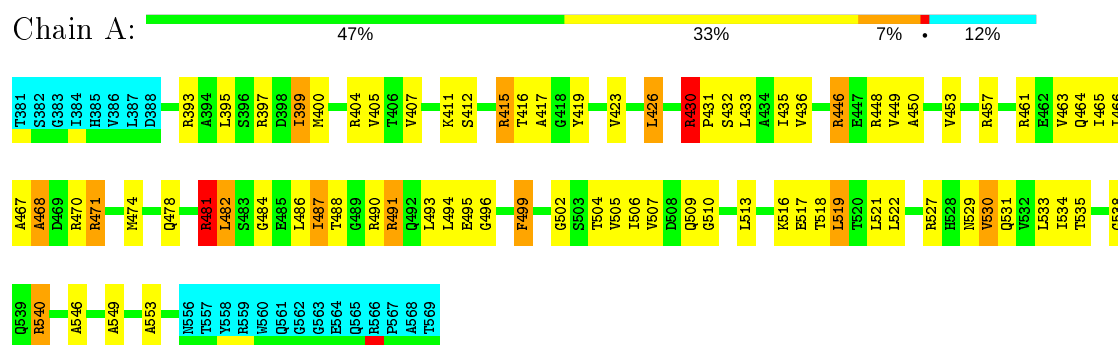
4.2.14 Score per residue for model 14

- Molecule 1: Protein traI



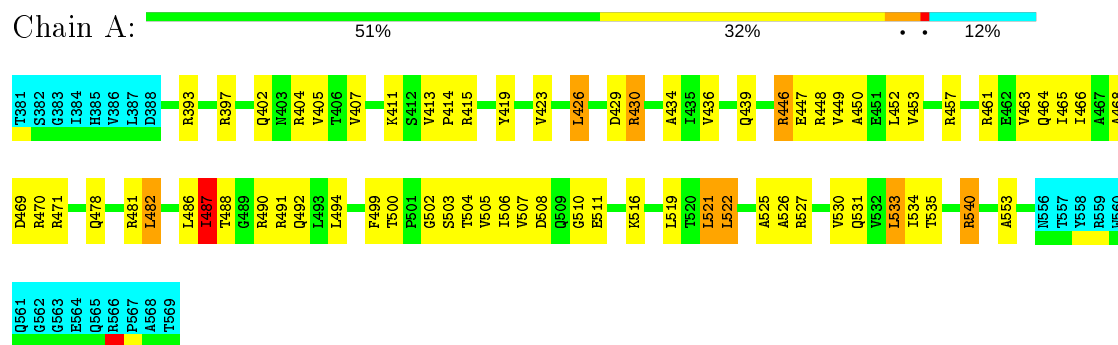
4.2.15 Score per residue for model 15

- Molecule 1: Protein traI



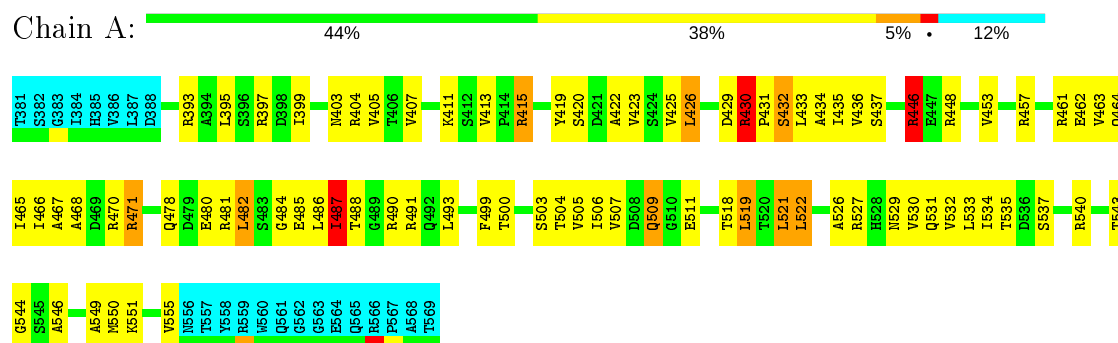
4.2.16 Score per residue for model 16

- Molecule 1: Protein traI



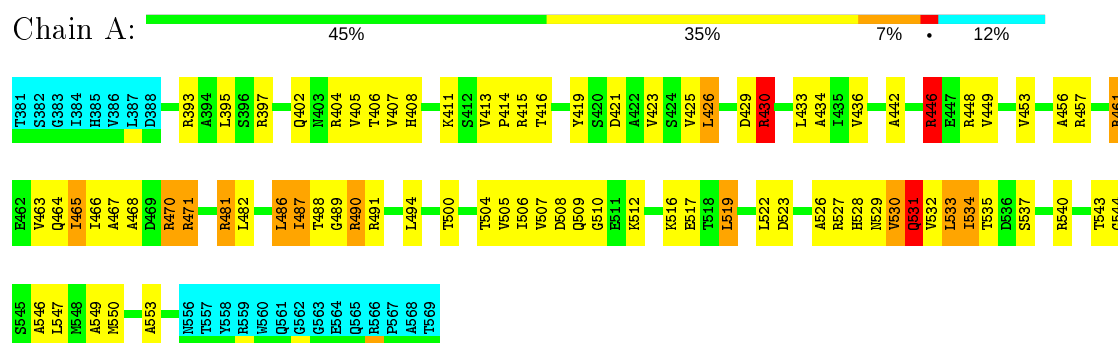
4.2.17 Score per residue for model 17

- Molecule 1: Protein traI



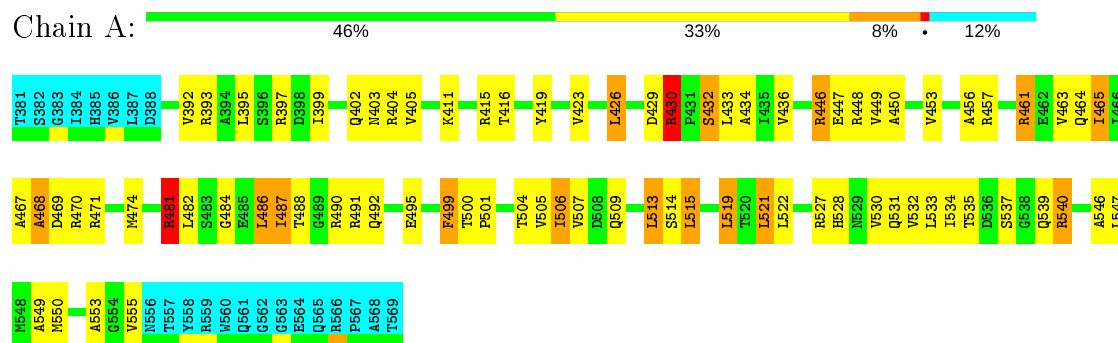
4.2.18 Score per residue for model 18

- Molecule 1: Protein traI



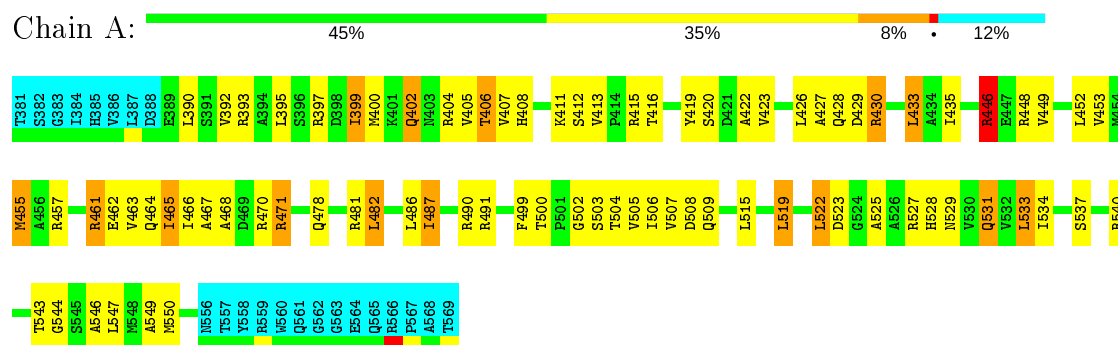
4.2.19 Score per residue for model 19

- Molecule 1: Protein traI



4.2.20 Score per residue for model 20

● Molecule 1: Protein traI



5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
X-PLOR NIH	structure solution	
X-PLOR NIH	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 6 of this report.

Chemical shift file(s)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	1999
Number of shifts mapped to atoms	1999
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	80%

No validations of the models with respect to experimental NMR restraints is performed at this time.

COVALENT-GEOMETRY INFOmissingINFO

5.1 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1254	1290	1290	61±8
All	All	25080	25800	25800	1223

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 24.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:505:VAL:HG11	1:A:522:LEU:HD21	0.90	1.41	20	9
1:A:487:ILE:HG22	1:A:488:THR:HG23	0.88	1.44	19	8
1:A:487:ILE:HD13	1:A:503:SER:CB	0.86	2.01	17	12
1:A:507:VAL:HG12	1:A:534:ILE:HG22	0.85	1.49	6	20
1:A:453:VAL:HG13	1:A:463:VAL:CG2	0.84	2.01	9	19
1:A:449:VAL:HG22	1:A:506:ILE:HD12	0.83	1.49	14	5
1:A:423:VAL:HG21	1:A:436:VAL:CG2	0.82	2.05	11	15
1:A:505:VAL:HG21	1:A:522:LEU:HD21	0.82	1.52	14	1
1:A:515:LEU:O	1:A:519:LEU:HD22	0.81	1.75	5	1
1:A:465:ILE:HD11	1:A:482:LEU:HD13	0.81	1.51	6	1
1:A:453:VAL:HG13	1:A:463:VAL:HG22	0.80	1.54	19	15
1:A:426:LEU:CD2	1:A:434:ALA:HB2	0.79	2.07	7	11
1:A:407:VAL:HG21	1:A:415:ARG:CZ	0.79	2.07	13	1
1:A:487:ILE:HG21	1:A:503:SER:OG	0.79	1.78	3	2
1:A:423:VAL:HA	1:A:426:LEU:HD23	0.78	1.55	15	17
1:A:405:VAL:O	1:A:407:VAL:HG23	0.78	1.77	11	6
1:A:423:VAL:HG21	1:A:436:VAL:HG22	0.78	1.54	16	5
1:A:416:THR:HG22	1:A:419:TYR:OH	0.77	1.79	14	4
1:A:488:THR:HG22	1:A:499:PHE:HB3	0.77	1.57	4	2
1:A:463:VAL:HG12	1:A:504:THR:HB	0.76	1.56	15	18
1:A:505:VAL:CG1	1:A:522:LEU:HD21	0.76	2.11	13	7
1:A:433:LEU:HA	1:A:532:VAL:O	0.76	1.81	9	13
1:A:423:VAL:HG13	1:A:533:LEU:HD21	0.75	1.56	8	2
1:A:505:VAL:HG11	1:A:522:LEU:CD1	0.75	2.11	9	6
1:A:426:LEU:HD21	1:A:434:ALA:HB2	0.74	1.58	7	3
1:A:465:ILE:HD11	1:A:482:LEU:HD22	0.74	1.59	8	3
1:A:464:GLN:HA	1:A:486:LEU:HD22	0.74	1.60	16	9
1:A:453:VAL:CG2	1:A:465:ILE:HG21	0.74	2.13	5	10
1:A:505:VAL:CB	1:A:522:LEU:HD21	0.73	2.12	8	5
1:A:507:VAL:HG22	1:A:509:GLN:HG2	0.73	1.59	19	4
1:A:519:LEU:HD11	1:A:550:MET:CE	0.73	2.13	20	2
1:A:399:ILE:HG21	1:A:435:ILE:O	0.73	1.83	7	5
1:A:453:VAL:HG22	1:A:463:VAL:HG21	0.73	1.60	12	4
1:A:423:VAL:CG2	1:A:436:VAL:HG21	0.73	2.14	9	2
1:A:453:VAL:HG13	1:A:463:VAL:HG21	0.72	1.58	6	8
1:A:407:VAL:HG21	1:A:413:VAL:HG22	0.72	1.61	12	1
1:A:504:THR:HG23	1:A:531:GLN:CB	0.72	2.15	18	1
1:A:487:ILE:HD13	1:A:503:SER:HB2	0.71	1.62	17	5
1:A:449:VAL:HG11	1:A:508:ASP:OD2	0.71	1.86	16	5
1:A:487:ILE:HD12	1:A:503:SER:OG	0.71	1.86	4	1
1:A:487:ILE:CG2	1:A:488:THR:HG23	0.70	2.15	6	2
1:A:419:TYR:CG	1:A:436:VAL:HG13	0.70	2.20	14	7

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:546:ALA:O	1:A:549:ALA:HB3	0.70	1.87	2	15
1:A:421:ASP:O	1:A:425:VAL:HG23	0.69	1.87	4	6
1:A:432:SER:O	1:A:433:LEU:HD22	0.69	1.86	7	1
1:A:515:LEU:HD21	1:A:550:MET:HG3	0.69	1.61	12	1
1:A:464:GLN:HB3	1:A:505:VAL:HG22	0.69	1.64	14	11
1:A:446:ARG:O	1:A:449:VAL:HG12	0.69	1.87	3	12
1:A:506:ILE:HG23	1:A:533:LEU:HD22	0.68	1.64	9	2
1:A:540:ARG:HG3	1:A:541:THR:HG23	0.68	1.63	6	2
1:A:507:VAL:CG1	1:A:534:ILE:HG22	0.68	2.18	8	14
1:A:395:LEU:HD11	1:A:422:ALA:O	0.68	1.87	9	7
1:A:518:THR:O	1:A:522:LEU:HD12	0.68	1.89	17	2
1:A:522:LEU:HD11	1:A:530:VAL:CG2	0.68	2.19	6	1
1:A:494:LEU:O	1:A:494:LEU:HD13	0.68	1.87	1	5
1:A:419:TYR:CB	1:A:436:VAL:HG13	0.68	2.19	17	6
1:A:456:ALA:HB1	1:A:461:ARG:O	0.68	1.89	11	5
1:A:402:GLN:O	1:A:405:VAL:HG12	0.68	1.90	16	9
1:A:505:VAL:HG11	1:A:522:LEU:HD11	0.68	1.65	11	5
1:A:453:VAL:HG21	1:A:465:ILE:HD13	0.67	1.64	1	1
1:A:463:VAL:CA	1:A:487:ILE:HD11	0.67	2.19	12	3
1:A:432:SER:OG	1:A:533:LEU:HD12	0.67	1.89	9	2
1:A:505:VAL:HG11	1:A:522:LEU:HD12	0.67	1.66	1	1
1:A:446:ARG:HG2	1:A:467:ALA:HB1	0.67	1.64	20	2
1:A:446:ARG:HD3	1:A:467:ALA:HB1	0.67	1.66	18	1
1:A:505:VAL:HG21	1:A:522:LEU:CD1	0.67	2.19	9	5
1:A:422:ALA:O	1:A:425:VAL:HG12	0.67	1.90	9	2
1:A:464:GLN:HG3	1:A:486:LEU:HD13	0.66	1.66	13	5
1:A:506:ILE:HG22	1:A:533:LEU:HB2	0.66	1.67	1	4
1:A:407:VAL:HG13	1:A:413:VAL:HG12	0.66	1.67	13	1
1:A:509:GLN:CD	1:A:515:LEU:HD23	0.66	2.11	7	1
1:A:487:ILE:HG21	1:A:503:SER:HB2	0.66	1.66	14	3
1:A:506:ILE:HG22	1:A:533:LEU:CB	0.66	2.21	1	3
1:A:487:ILE:HD13	1:A:503:SER:HB3	0.65	1.66	5	5
1:A:481:ARG:HG2	1:A:482:LEU:HD22	0.65	1.66	1	1
1:A:482:LEU:O	1:A:482:LEU:HD12	0.65	1.92	14	2
1:A:519:LEU:HD11	1:A:550:MET:CG	0.65	2.22	8	4
1:A:462:GLU:C	1:A:487:ILE:HD11	0.65	2.12	4	6
1:A:423:VAL:CG1	1:A:533:LEU:HD21	0.65	2.22	20	6
1:A:518:THR:HG22	1:A:522:LEU:HD12	0.65	1.67	13	2
1:A:407:VAL:CG2	1:A:413:VAL:HG22	0.65	2.21	12	1
1:A:434:ALA:HB3	1:A:533:LEU:CD1	0.65	2.22	19	2
1:A:423:VAL:HG21	1:A:436:VAL:HG21	0.64	1.68	4	12

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:493:LEU:N	1:A:493:LEU:HD23	0.64	2.07	7	4
1:A:525:ALA:HB1	1:A:530:VAL:HG21	0.64	1.69	5	3
1:A:449:VAL:HG22	1:A:506:ILE:CD1	0.64	2.22	2	7
1:A:395:LEU:CD2	1:A:399:ILE:HD11	0.64	2.22	5	4
1:A:494:LEU:HD13	1:A:494:LEU:O	0.64	1.93	12	3
1:A:395:LEU:CD2	1:A:426:LEU:HD22	0.64	2.22	19	1
1:A:463:VAL:HG13	1:A:504:THR:O	0.63	1.92	20	1
1:A:503:SER:O	1:A:530:VAL:HG22	0.63	1.93	10	2
1:A:463:VAL:N	1:A:487:ILE:HD11	0.63	2.08	12	3
1:A:505:VAL:HB	1:A:522:LEU:HD21	0.63	1.68	11	5
1:A:466:ILE:HG23	1:A:471:ARG:HD3	0.63	1.69	9	6
1:A:433:LEU:HD23	1:A:532:VAL:O	0.63	1.94	19	1
1:A:482:LEU:N	1:A:482:LEU:HD22	0.63	2.09	9	1
1:A:506:ILE:HG22	1:A:533:LEU:HB3	0.62	1.69	18	6
1:A:446:ARG:CD	1:A:467:ALA:HB1	0.62	2.24	10	2
1:A:407:VAL:HG13	1:A:412:SER:HA	0.62	1.71	15	1
1:A:519:LEU:HD11	1:A:550:MET:HG3	0.62	1.71	17	6
1:A:464:GLN:HB2	1:A:486:LEU:HD11	0.62	1.72	6	1
1:A:522:LEU:HD11	1:A:530:VAL:HG21	0.62	1.72	6	1
1:A:402:GLN:NE2	1:A:405:VAL:HG11	0.62	2.10	18	1
1:A:486:LEU:HD11	1:A:489:GLY:HA3	0.61	1.71	3	1
1:A:506:ILE:HG23	1:A:533:LEU:HB3	0.61	1.71	9	2
1:A:465:ILE:CD1	1:A:482:LEU:HD13	0.61	2.22	6	1
1:A:522:LEU:HD23	1:A:530:VAL:CG1	0.61	2.25	8	1
1:A:526:ALA:CB	1:A:530:VAL:HG11	0.61	2.25	16	1
1:A:464:GLN:OE1	1:A:486:LEU:HD13	0.61	1.95	18	1
1:A:453:VAL:HG13	1:A:463:VAL:HB	0.61	1.72	20	1
1:A:466:ILE:HD12	1:A:466:ILE:N	0.61	2.11	16	3
1:A:507:VAL:HG22	1:A:509:GLN:CG	0.61	2.26	19	2
1:A:516:LYS:HG3	1:A:553:ALA:HB2	0.61	1.70	9	3
1:A:427:ALA:HB2	1:A:533:LEU:CD1	0.61	2.25	20	1
1:A:522:LEU:O	1:A:526:ALA:HB3	0.61	1.96	10	1
1:A:442:ALA:HB3	1:A:470:ARG:NH2	0.61	2.11	18	1
1:A:467:ALA:HB3	1:A:471:ARG:HB2	0.61	1.72	8	4
1:A:505:VAL:HG11	1:A:522:LEU:CD2	0.61	2.21	20	5
1:A:481:ARG:HG2	1:A:482:LEU:HD23	0.61	1.71	11	2
1:A:405:VAL:HG13	1:A:407:VAL:HG23	0.61	1.72	10	2
1:A:453:VAL:HG22	1:A:465:ILE:HG21	0.61	1.73	5	7
1:A:395:LEU:HD23	1:A:399:ILE:HD11	0.61	1.72	5	2
1:A:526:ALA:HB1	1:A:530:VAL:HG11	0.60	1.73	16	1
1:A:513:LEU:HD12	1:A:514:SER:N	0.60	2.10	5	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:405:VAL:HG11	1:A:415:ARG:CZ	0.60	2.26	6	1
1:A:481:ARG:CG	1:A:482:LEU:HD23	0.60	2.27	15	3
1:A:505:VAL:CG2	1:A:522:LEU:HD21	0.60	2.25	14	2
1:A:446:ARG:HD2	1:A:467:ALA:HB1	0.60	1.73	10	2
1:A:395:LEU:HD12	1:A:399:ILE:HD11	0.59	1.72	15	1
1:A:435:ILE:O	1:A:435:ILE:HD12	0.59	1.97	9	2
1:A:465:ILE:HD13	1:A:465:ILE:H	0.59	1.57	9	2
1:A:519:LEU:HD12	1:A:555:VAL:HG21	0.59	1.73	6	1
1:A:466:ILE:HG23	1:A:471:ARG:CD	0.58	2.28	9	5
1:A:419:TYR:HB3	1:A:436:VAL:HG13	0.58	1.74	1	1
1:A:505:VAL:CG1	1:A:522:LEU:HD11	0.58	2.28	8	1
1:A:481:ARG:C	1:A:482:LEU:HD12	0.58	2.18	5	1
1:A:400:MET:HG3	1:A:435:ILE:HD11	0.58	1.75	15	3
1:A:449:VAL:CG2	1:A:506:ILE:HD13	0.58	2.28	16	2
1:A:513:LEU:O	1:A:513:LEU:HD13	0.58	1.98	14	3
1:A:487:ILE:HG21	1:A:503:SER:HB3	0.58	1.75	11	5
1:A:487:ILE:HG22	1:A:488:THR:N	0.58	2.13	6	5
1:A:413:VAL:HG23	1:A:413:VAL:O	0.58	1.99	12	1
1:A:426:LEU:HD22	1:A:434:ALA:HB2	0.57	1.76	11	10
1:A:395:LEU:HD13	1:A:426:LEU:HB3	0.57	1.76	9	4
1:A:505:VAL:HG21	1:A:522:LEU:HD12	0.57	1.75	9	2
1:A:466:ILE:HB	1:A:507:VAL:HG23	0.57	1.77	18	9
1:A:488:THR:CG2	1:A:500:THR:HG22	0.57	2.29	18	1
1:A:507:VAL:CG2	1:A:518:THR:HG21	0.57	2.30	2	2
1:A:484:GLY:O	1:A:486:LEU:HD23	0.57	1.99	4	1
1:A:436:VAL:HB	1:A:535:THR:HG22	0.57	1.76	15	10
1:A:519:LEU:HD11	1:A:550:MET:HE3	0.57	1.76	20	2
1:A:474:MET:CE	1:A:482:LEU:HD21	0.57	2.30	15	1
1:A:449:VAL:CG2	1:A:506:ILE:HD12	0.57	2.30	7	8
1:A:518:THR:HG22	1:A:522:LEU:CD1	0.57	2.30	13	3
1:A:465:ILE:HD13	1:A:465:ILE:N	0.56	2.16	9	2
1:A:399:ILE:HG23	1:A:419:TYR:CD1	0.56	2.35	10	3
1:A:516:LYS:O	1:A:520:THR:HG23	0.56	2.00	8	1
1:A:442:ALA:HB3	1:A:470:ARG:NH1	0.56	2.15	4	1
1:A:407:VAL:HG23	1:A:413:VAL:HG12	0.56	1.76	20	4
1:A:465:ILE:HG22	1:A:506:ILE:CG1	0.56	2.30	8	1
1:A:466:ILE:HD13	1:A:518:THR:CG2	0.56	2.29	10	1
1:A:507:VAL:HG12	1:A:534:ILE:CG2	0.56	2.30	11	2
1:A:449:VAL:HG22	1:A:506:ILE:HD13	0.56	1.76	16	1
1:A:435:ILE:HD13	1:A:435:ILE:H	0.56	1.60	6	1
1:A:399:ILE:HG23	1:A:419:TYR:HD1	0.56	1.61	11	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:399:ILE:HG23	1:A:419:TYR:HB3	0.56	1.76	3	1
1:A:500:THR:HG23	1:A:500:THR:O	0.55	2.01	7	8
1:A:507:VAL:CB	1:A:518:THR:HG21	0.55	2.31	2	2
1:A:481:ARG:HB2	1:A:482:LEU:HD23	0.55	1.78	8	2
1:A:406:THR:HG23	1:A:406:THR:O	0.55	2.02	1	3
1:A:515:LEU:O	1:A:519:LEU:HD23	0.55	2.02	13	2
1:A:392:VAL:HG11	1:A:433:LEU:HB3	0.55	1.78	7	3
1:A:505:VAL:HG11	1:A:522:LEU:HD13	0.55	1.79	2	3
1:A:492:GLN:HG2	1:A:493:LEU:HD23	0.55	1.77	5	1
1:A:442:ALA:HB1	1:A:446:ARG:HH22	0.55	1.60	10	1
1:A:507:VAL:O	1:A:507:VAL:HG13	0.55	2.02	7	6
1:A:478:GLN:CG	1:A:482:LEU:HD21	0.54	2.31	14	1
1:A:486:LEU:C	1:A:487:ILE:HD12	0.54	2.22	15	3
1:A:407:VAL:HG21	1:A:415:ARG:NH1	0.54	2.17	13	1
1:A:466:ILE:CB	1:A:507:VAL:HG23	0.54	2.32	18	1
1:A:507:VAL:HB	1:A:518:THR:HG21	0.54	1.78	2	3
1:A:507:VAL:HG13	1:A:507:VAL:O	0.54	2.02	14	5
1:A:423:VAL:HG13	1:A:533:LEU:HD11	0.54	1.78	19	1
1:A:413:VAL:O	1:A:413:VAL:HG13	0.54	2.02	9	2
1:A:400:MET:CG	1:A:435:ILE:HD11	0.54	2.32	20	4
1:A:427:ALA:HB2	1:A:533:LEU:HD11	0.54	1.79	20	1
1:A:539:GLN:NE2	1:A:546:ALA:HB2	0.54	2.18	12	1
1:A:392:VAL:HG11	1:A:433:LEU:CB	0.54	2.33	19	2
1:A:481:ARG:C	1:A:482:LEU:HD23	0.54	2.22	13	3
1:A:465:ILE:H	1:A:465:ILE:HD13	0.54	1.63	11	4
1:A:434:ALA:HB3	1:A:533:LEU:HD13	0.54	1.78	7	1
1:A:395:LEU:CD2	1:A:399:ILE:HD12	0.54	2.33	11	1
1:A:453:VAL:HG22	1:A:463:VAL:CG2	0.54	2.33	4	2
1:A:436:VAL:HG22	1:A:535:THR:CB	0.54	2.33	8	1
1:A:505:VAL:HG21	1:A:522:LEU:CD2	0.54	2.29	14	1
1:A:465:ILE:HG22	1:A:506:ILE:HG13	0.53	1.80	8	2
1:A:525:ALA:HB1	1:A:529:ASN:HB2	0.53	1.78	20	1
1:A:419:TYR:O	1:A:423:VAL:HG23	0.53	2.03	13	4
1:A:413:VAL:HG13	1:A:413:VAL:O	0.53	2.03	6	5
1:A:488:THR:HG22	1:A:499:PHE:CB	0.53	2.33	4	1
1:A:465:ILE:HD11	1:A:482:LEU:CD1	0.53	2.29	6	1
1:A:487:ILE:HG22	1:A:488:THR:CG2	0.53	2.27	19	5
1:A:480:GLU:CB	1:A:482:LEU:HD23	0.53	2.34	17	1
1:A:504:THR:HG23	1:A:531:GLN:HB3	0.53	1.78	18	1
1:A:515:LEU:HD21	1:A:550:MET:HB2	0.53	1.80	3	2
1:A:533:LEU:C	1:A:533:LEU:HD12	0.53	2.23	18	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:449:VAL:HG11	1:A:508:ASP:CG	0.53	2.23	2	1
1:A:466:ILE:N	1:A:466:ILE:HD12	0.53	2.19	2	4
1:A:465:ILE:HG22	1:A:506:ILE:HG12	0.53	1.81	6	5
1:A:419:TYR:HB2	1:A:436:VAL:HG22	0.53	1.81	14	1
1:A:446:ARG:NH2	1:A:468:ALA:HB3	0.53	2.19	15	1
1:A:405:VAL:O	1:A:405:VAL:HG13	0.52	2.04	8	8
1:A:521:LEU:O	1:A:521:LEU:HD13	0.52	2.03	6	3
1:A:505:VAL:HG11	1:A:522:LEU:CG	0.52	2.34	8	2
1:A:423:VAL:HG22	1:A:436:VAL:HG21	0.52	1.80	9	1
1:A:551:LYS:HA	1:A:555:VAL:HG23	0.52	1.82	9	1
1:A:529:ASN:C	1:A:530:VAL:HG22	0.52	2.24	15	2
1:A:539:GLN:CD	1:A:546:ALA:HB2	0.52	2.25	12	1
1:A:467:ALA:HB3	1:A:471:ARG:CB	0.52	2.35	15	5
1:A:522:LEU:HD23	1:A:530:VAL:HG11	0.52	1.81	8	1
1:A:533:LEU:HD12	1:A:533:LEU:C	0.52	2.25	16	2
1:A:487:ILE:HG21	1:A:503:SER:CB	0.52	2.33	20	1
1:A:482:LEU:N	1:A:482:LEU:HD23	0.52	2.20	13	2
1:A:405:VAL:HG13	1:A:405:VAL:O	0.51	2.05	9	3
1:A:480:GLU:HB2	1:A:482:LEU:HD23	0.51	1.82	17	1
1:A:449:VAL:HG21	1:A:508:ASP:OD1	0.51	2.05	2	1
1:A:505:VAL:HG21	1:A:522:LEU:HD11	0.51	1.81	16	2
1:A:405:VAL:HG13	1:A:407:VAL:CG2	0.51	2.35	15	1
1:A:466:ILE:HD12	1:A:518:THR:CG2	0.51	2.35	11	1
1:A:466:ILE:CD1	1:A:507:VAL:HG23	0.51	2.35	12	1
1:A:500:THR:O	1:A:500:THR:HG23	0.51	2.06	17	2
1:A:526:ALA:HA	1:A:530:VAL:HB	0.51	1.81	5	4
1:A:395:LEU:C	1:A:395:LEU:HD13	0.51	2.25	8	1
1:A:505:VAL:O	1:A:531:GLN:O	0.51	2.29	4	4
1:A:466:ILE:HD12	1:A:507:VAL:HG23	0.51	1.82	12	1
1:A:453:VAL:HA	1:A:463:VAL:HG21	0.51	1.83	20	1
1:A:532:VAL:HG12	1:A:534:ILE:CG2	0.51	2.36	2	1
1:A:400:MET:SD	1:A:435:ILE:HD12	0.51	2.45	8	1
1:A:447:GLU:O	1:A:450:ALA:HB3	0.50	2.06	5	5
1:A:442:ALA:HB1	1:A:446:ARG:NH2	0.50	2.21	10	1
1:A:426:LEU:HD12	1:A:426:LEU:C	0.50	2.27	6	3
1:A:395:LEU:HD12	1:A:399:ILE:CD1	0.50	2.35	1	1
1:A:509:GLN:CD	1:A:515:LEU:HD13	0.50	2.26	6	1
1:A:555:VAL:O	1:A:555:VAL:HG23	0.50	2.07	19	1
1:A:426:LEU:C	1:A:426:LEU:HD12	0.50	2.28	12	6
1:A:555:VAL:HG23	1:A:555:VAL:O	0.50	2.07	9	2
1:A:423:VAL:HG12	1:A:533:LEU:HD21	0.50	1.84	20	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:511:GLU:OE1	1:A:513:LEU:HD21	0.50	2.07	5	1
1:A:506:ILE:CG2	1:A:533:LEU:HD22	0.50	2.37	9	1
1:A:399:ILE:HG22	1:A:403:ASN:ND2	0.49	2.22	13	1
1:A:466:ILE:HD12	1:A:518:THR:OG1	0.49	2.07	15	1
1:A:494:LEU:C	1:A:494:LEU:HD23	0.49	2.28	15	1
1:A:506:ILE:HA	1:A:533:LEU:O	0.49	2.07	11	7
1:A:555:VAL:O	1:A:555:VAL:HG13	0.49	2.06	17	2
1:A:466:ILE:HG23	1:A:471:ARG:HD2	0.49	1.83	14	3
1:A:533:LEU:HD12	1:A:534:ILE:N	0.49	2.22	16	1
1:A:516:LYS:HG2	1:A:553:ALA:HB2	0.49	1.84	14	3
1:A:464:GLN:CD	1:A:521:LEU:HD23	0.49	2.27	15	1
1:A:493:LEU:HD23	1:A:493:LEU:H	0.49	1.68	2	1
1:A:493:LEU:N	1:A:493:LEU:CD2	0.49	2.76	7	1
1:A:390:LEU:HD12	1:A:391:SER:N	0.49	2.23	9	1
1:A:515:LEU:HD11	1:A:550:MET:SD	0.49	2.47	6	1
1:A:522:LEU:O	1:A:526:ALA:HB2	0.49	2.07	7	3
1:A:505:VAL:HB	1:A:522:LEU:HD11	0.49	1.84	5	1
1:A:402:GLN:NE2	1:A:405:VAL:HG21	0.49	2.23	19	1
1:A:446:ARG:HD3	1:A:467:ALA:HB2	0.49	1.83	19	1
1:A:509:GLN:O	1:A:536:ASP:HA	0.48	2.08	2	1
1:A:432:SER:CB	1:A:533:LEU:HD12	0.48	2.38	1	2
1:A:499:PHE:N	1:A:499:PHE:CD1	0.48	2.80	2	2
1:A:493:LEU:HD21	1:A:521:LEU:HD21	0.48	1.84	3	1
1:A:506:ILE:HD12	1:A:506:ILE:O	0.48	2.08	16	1
1:A:516:LYS:HA	1:A:553:ALA:HB2	0.48	1.86	13	2
1:A:464:GLN:OE1	1:A:488:THR:HG21	0.48	2.08	11	1
1:A:494:LEU:O	1:A:494:LEU:HD23	0.48	2.08	3	2
1:A:465:ILE:HD13	1:A:506:ILE:HG13	0.48	1.84	3	2
1:A:525:ALA:HB1	1:A:529:ASN:OD1	0.48	2.08	12	1
1:A:467:ALA:HB3	1:A:471:ARG:CA	0.48	2.39	15	2
1:A:423:VAL:CG1	1:A:533:LEU:HD23	0.48	2.39	14	1
1:A:414:PRO:HB2	1:A:417:ALA:HB2	0.48	1.86	3	1
1:A:525:ALA:HB1	1:A:529:ASN:HB3	0.48	1.85	4	1
1:A:526:ALA:HA	1:A:530:VAL:HG13	0.48	1.86	18	1
1:A:452:LEU:HD13	1:A:452:LEU:O	0.47	2.10	4	1
1:A:395:LEU:HD21	1:A:426:LEU:HD22	0.47	1.84	19	1
1:A:449:VAL:HG21	1:A:506:ILE:HD13	0.47	1.86	8	1
1:A:453:VAL:HG11	1:A:482:LEU:HG	0.47	1.86	9	1
1:A:481:ARG:O	1:A:482:LEU:HD12	0.47	2.10	19	1
1:A:486:LEU:O	1:A:487:ILE:HG13	0.47	2.10	15	2
1:A:508:ASP:OD1	1:A:535:THR:HG23	0.47	2.09	7	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:482:LEU:N	1:A:482:LEU:CD2	0.47	2.76	9	1
1:A:505:VAL:HB	1:A:531:GLN:O	0.47	2.09	20	2
1:A:521:LEU:HD13	1:A:521:LEU:O	0.47	2.10	19	2
1:A:488:THR:HG21	1:A:500:THR:HG22	0.47	1.84	18	1
1:A:395:LEU:HD22	1:A:426:LEU:CB	0.47	2.40	15	2
1:A:547:LEU:N	1:A:547:LEU:HD12	0.47	2.25	6	6
1:A:466:ILE:HG22	1:A:467:ALA:N	0.47	2.24	18	3
1:A:506:ILE:O	1:A:506:ILE:HG13	0.47	2.09	14	1
1:A:450:ALA:HB1	1:A:481:ARG:HE	0.47	1.69	15	1
1:A:413:VAL:HG13	1:A:414:PRO:HD2	0.47	1.86	16	1
1:A:395:LEU:HD22	1:A:426:LEU:HD22	0.47	1.84	19	1
1:A:523:ASP:O	1:A:526:ALA:HB3	0.47	2.09	18	2
1:A:466:ILE:HG22	1:A:509:GLN:NE2	0.47	2.26	5	1
1:A:433:LEU:C	1:A:433:LEU:HD12	0.47	2.30	6	1
1:A:463:VAL:HG23	1:A:465:ILE:HG23	0.47	1.86	8	1
1:A:522:LEU:HD23	1:A:526:ALA:CB	0.47	2.40	10	1
1:A:446:ARG:NE	1:A:467:ALA:HB2	0.47	2.25	13	1
1:A:464:GLN:OE1	1:A:521:LEU:HD23	0.47	2.09	15	1
1:A:402:GLN:HE22	1:A:405:VAL:HG21	0.47	1.70	19	1
1:A:450:ALA:HB1	1:A:481:ARG:HA	0.46	1.86	9	1
1:A:466:ILE:HD12	1:A:518:THR:HG21	0.46	1.87	11	2
1:A:464:GLN:NE2	1:A:521:LEU:HD23	0.46	2.24	10	1
1:A:407:VAL:CG1	1:A:413:VAL:HG12	0.46	2.39	13	1
1:A:487:ILE:O	1:A:499:PHE:CD2	0.46	2.68	10	3
1:A:430:ARG:HB3	1:A:431:PRO:HD3	0.46	1.88	15	5
1:A:519:LEU:CD2	1:A:519:LEU:N	0.46	2.78	15	1
1:A:526:ALA:CA	1:A:530:VAL:HG11	0.46	2.40	16	1
1:A:492:GLN:NE2	1:A:499:PHE:CD1	0.46	2.83	19	1
1:A:395:LEU:O	1:A:399:ILE:CG1	0.46	2.64	15	1
1:A:493:LEU:CD2	1:A:521:LEU:HD21	0.46	2.40	3	1
1:A:462:GLU:O	1:A:487:ILE:HD11	0.46	2.10	14	3
1:A:415:ARG:O	1:A:419:TYR:CE2	0.46	2.68	17	2
1:A:481:ARG:HG3	1:A:482:LEU:HD23	0.46	1.88	15	2
1:A:464:GLN:HG2	1:A:466:ILE:HD11	0.46	1.87	4	1
1:A:515:LEU:HD21	1:A:550:MET:HG2	0.46	1.86	6	1
1:A:466:ILE:HD13	1:A:518:THR:OG1	0.46	2.11	10	1
1:A:487:ILE:O	1:A:499:PHE:CD1	0.46	2.69	13	1
1:A:449:VAL:HG22	1:A:506:ILE:HD11	0.46	1.88	10	1
1:A:491:ARG:O	1:A:495:GLU:N	0.46	2.48	15	3
1:A:547:LEU:HD12	1:A:547:LEU:N	0.46	2.26	20	2
1:A:464:GLN:CB	1:A:486:LEU:HD11	0.46	2.39	6	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:406:THR:O	1:A:406:THR:HG23	0.45	2.11	14	1
1:A:532:VAL:C	1:A:533:LEU:HD12	0.45	2.32	14	1
1:A:488:THR:HG21	1:A:525:ALA:CB	0.45	2.40	2	2
1:A:529:ASN:C	1:A:530:VAL:HG13	0.45	2.31	4	1
1:A:395:LEU:CD1	1:A:426:LEU:HB3	0.45	2.42	6	2
1:A:415:ARG:O	1:A:417:ALA:N	0.45	2.49	15	1
1:A:464:GLN:HA	1:A:486:LEU:CD1	0.45	2.41	19	1
1:A:395:LEU:HD13	1:A:399:ILE:HD12	0.45	1.87	13	1
1:A:423:VAL:HG21	1:A:436:VAL:HG11	0.45	1.86	8	1
1:A:435:ILE:HD13	1:A:435:ILE:N	0.45	2.27	6	1
1:A:464:GLN:O	1:A:505:VAL:HG23	0.45	2.11	10	1
1:A:551:LYS:HA	1:A:555:VAL:HG13	0.45	1.88	17	1
1:A:487:ILE:HG23	1:A:503:SER:OG	0.45	2.12	4	1
1:A:513:LEU:HD22	1:A:513:LEU:N	0.45	2.26	13	3
1:A:465:ILE:CG2	1:A:482:LEU:HD22	0.45	2.41	12	1
1:A:432:SER:CB	1:A:531:GLN:HB3	0.45	2.42	3	1
1:A:543:THR:HG23	1:A:544:GLY:N	0.45	2.27	9	11
1:A:486:LEU:O	1:A:487:ILE:HD13	0.45	2.12	4	1
1:A:436:VAL:HG22	1:A:535:THR:CA	0.45	2.42	8	1
1:A:478:GLN:NE2	1:A:482:LEU:HD21	0.45	2.27	12	1
1:A:446:ARG:CG	1:A:467:ALA:HB1	0.44	2.42	1	1
1:A:506:ILE:HG13	1:A:506:ILE:O	0.44	2.11	1	1
1:A:494:LEU:C	1:A:494:LEU:HD13	0.44	2.32	11	4
1:A:486:LEU:O	1:A:487:ILE:HD12	0.44	2.12	5	3
1:A:421:ASP:O	1:A:425:VAL:HG12	0.44	2.13	11	1
1:A:426:LEU:CD1	1:A:432:SER:HA	0.44	2.43	19	2
1:A:392:VAL:CG1	1:A:433:LEU:O	0.44	2.66	9	4
1:A:506:ILE:O	1:A:506:ILE:CG1	0.44	2.65	13	3
1:A:502:GLY:HA2	1:A:529:ASN:CB	0.44	2.42	9	1
1:A:433:LEU:HD12	1:A:433:LEU:C	0.44	2.32	12	1
1:A:509:GLN:NE2	1:A:515:LEU:HD22	0.44	2.26	2	1
1:A:487:ILE:HD13	1:A:503:SER:OG	0.44	2.12	6	1
1:A:507:VAL:HG21	1:A:518:THR:HG21	0.44	1.89	2	1
1:A:419:TYR:N	1:A:419:TYR:CD1	0.44	2.85	5	2
1:A:488:THR:HA	1:A:499:PHE:CG	0.44	2.48	12	1
1:A:395:LEU:HD21	1:A:426:LEU:CD2	0.44	2.42	19	1
1:A:501:PRO:CG	1:A:528:HIS:CB	0.44	2.96	19	1
1:A:465:ILE:C	1:A:465:ILE:HD13	0.44	2.32	20	1
1:A:465:ILE:HG23	1:A:482:LEU:HD22	0.44	1.89	12	1
1:A:419:TYR:N	1:A:419:TYR:CD2	0.44	2.86	13	1
1:A:436:VAL:CB	1:A:535:THR:HG22	0.44	2.43	14	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:487:ILE:CG2	1:A:488:THR:N	0.44	2.80	6	1
1:A:422:ALA:O	1:A:425:VAL:HG22	0.44	2.12	14	1
1:A:507:VAL:CG1	1:A:534:ILE:CG2	0.44	2.96	11	5
1:A:436:VAL:HG22	1:A:535:THR:HA	0.44	1.89	8	1
1:A:513:LEU:CD2	1:A:513:LEU:N	0.44	2.80	13	3
1:A:465:ILE:N	1:A:465:ILE:CD1	0.44	2.79	9	1
1:A:532:VAL:CG1	1:A:534:ILE:CG2	0.43	2.96	2	1
1:A:550:MET:O	1:A:555:VAL:HG22	0.43	2.13	19	2
1:A:492:GLN:HB2	1:A:499:PHE:CE2	0.43	2.48	11	1
1:A:423:VAL:HG13	1:A:533:LEU:CD1	0.43	2.43	19	1
1:A:465:ILE:HD13	1:A:466:ILE:N	0.43	2.28	20	1
1:A:488:THR:HA	1:A:499:PHE:CD2	0.43	2.47	11	2
1:A:464:GLN:HG3	1:A:486:LEU:HD12	0.43	1.90	5	1
1:A:407:VAL:HG13	1:A:412:SER:CA	0.43	2.41	15	1
1:A:504:THR:HG23	1:A:531:GLN:HB2	0.43	1.87	18	1
1:A:432:SER:CB	1:A:531:GLN:CB	0.43	2.97	19	1
1:A:446:ARG:CD	1:A:467:ALA:HB2	0.43	2.43	19	1
1:A:522:LEU:HD12	1:A:522:LEU:C	0.43	2.33	19	1
1:A:395:LEU:HD22	1:A:426:LEU:HB3	0.43	1.90	1	2
1:A:490:ARG:N	1:A:493:LEU:CD2	0.43	2.80	2	1
1:A:519:LEU:HD23	1:A:519:LEU:N	0.43	2.28	15	1
1:A:488:THR:HG21	1:A:500:THR:H	0.43	1.73	6	1
1:A:403:ASN:ND2	1:A:437:SER:CB	0.43	2.82	12	3
1:A:486:LEU:O	1:A:487:ILE:CB	0.43	2.67	2	1
1:A:532:VAL:HG12	1:A:534:ILE:HG23	0.43	1.91	2	1
1:A:486:LEU:O	1:A:487:ILE:CG1	0.43	2.67	11	5
1:A:399:ILE:HG22	1:A:403:ASN:OD1	0.43	2.13	19	1
1:A:419:TYR:CD1	1:A:436:VAL:HG11	0.43	2.49	4	1
1:A:526:ALA:HA	1:A:530:VAL:CG2	0.43	2.43	7	1
1:A:481:ARG:CB	1:A:482:LEU:HD23	0.43	2.43	8	1
1:A:529:ASN:O	1:A:530:VAL:HG22	0.43	2.13	15	1
1:A:487:ILE:O	1:A:499:PHE:CE2	0.43	2.71	19	1
1:A:400:MET:HG2	1:A:435:ILE:HD11	0.43	1.89	20	1
1:A:480:GLU:O	1:A:482:LEU:HD22	0.43	2.14	9	1
1:A:405:VAL:O	1:A:407:VAL:N	0.43	2.52	4	1
1:A:501:PRO:HG2	1:A:528:HIS:CG	0.43	2.49	13	1
1:A:463:VAL:HG22	1:A:504:THR:HB	0.43	1.90	20	1
1:A:521:LEU:HD23	1:A:521:LEU:C	0.43	2.34	8	1
1:A:432:SER:HB3	1:A:533:LEU:HD12	0.43	1.90	8	1
1:A:487:ILE:HG23	1:A:500:THR:O	0.43	2.13	11	1
1:A:522:LEU:O	1:A:526:ALA:CB	0.43	2.67	17	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:491:ARG:O	1:A:495:GLU:CG	0.43	2.67	6	1
1:A:526:ALA:CA	1:A:530:VAL:HG21	0.43	2.44	7	1
1:A:494:LEU:HD13	1:A:494:LEU:C	0.43	2.34	9	1
1:A:505:VAL:HG21	1:A:522:LEU:HD13	0.43	1.91	18	1
1:A:398:ASP:O	1:A:419:TYR:CE1	0.42	2.72	3	1
1:A:474:MET:HE1	1:A:482:LEU:HD21	0.42	1.90	15	1
1:A:486:LEU:HB2	1:A:487:ILE:HD12	0.42	1.91	18	1
1:A:402:GLN:CG	1:A:415:ARG:NH1	0.42	2.82	1	1
1:A:488:THR:HG21	1:A:525:ALA:HB2	0.42	1.90	2	1
1:A:547:LEU:CD1	1:A:547:LEU:N	0.42	2.83	20	2
1:A:449:VAL:CG2	1:A:506:ILE:HD11	0.42	2.43	19	1
1:A:416:THR:O	1:A:420:SER:CB	0.42	2.66	3	3
1:A:426:LEU:HD11	1:A:432:SER:HA	0.42	1.90	15	2
1:A:456:ALA:CB	1:A:463:VAL:HG11	0.42	2.45	9	1
1:A:488:THR:CB	1:A:499:PHE:CD2	0.42	3.03	3	1
1:A:414:PRO:O	1:A:415:ARG:HG3	0.42	2.15	8	1
1:A:446:ARG:NH1	1:A:468:ALA:HB3	0.42	2.30	10	1
1:A:478:GLN:HG3	1:A:482:LEU:HD21	0.42	1.91	14	1
1:A:423:VAL:HG12	1:A:533:LEU:HD23	0.42	1.90	14	1
1:A:513:LEU:HD12	1:A:513:LEU:C	0.42	2.35	5	1
1:A:402:GLN:HG2	1:A:419:TYR:CD2	0.42	2.49	16	1
1:A:395:LEU:HD11	1:A:426:LEU:HB3	0.42	1.91	18	1
1:A:488:THR:HA	1:A:499:PHE:CB	0.42	2.45	15	2
1:A:504:THR:C	1:A:505:VAL:HG23	0.42	2.35	6	1
1:A:543:THR:O	1:A:546:ALA:HB3	0.42	2.14	10	1
1:A:413:VAL:CG2	1:A:413:VAL:O	0.42	2.67	12	1
1:A:452:LEU:CD2	1:A:452:LEU:N	0.42	2.83	16	1
1:A:449:VAL:HG21	1:A:506:ILE:HD12	0.42	1.91	5	1
1:A:519:LEU:HD11	1:A:550:MET:HG2	0.42	1.91	8	1
1:A:436:VAL:HB	1:A:535:THR:HA	0.42	1.91	18	2
1:A:452:LEU:O	1:A:455:MET:CG	0.42	2.68	10	4
1:A:526:ALA:HA	1:A:530:VAL:CB	0.42	2.45	6	1
1:A:481:ARG:CD	1:A:481:ARG:N	0.42	2.83	14	1
1:A:522:LEU:O	1:A:526:ALA:N	0.42	2.52	4	1
1:A:506:ILE:HG23	1:A:533:LEU:CD2	0.42	2.40	9	1
1:A:426:LEU:HD12	1:A:426:LEU:O	0.42	2.15	11	1
1:A:529:ASN:C	1:A:530:VAL:CG2	0.42	2.88	18	2
1:A:446:ARG:CD	1:A:467:ALA:CB	0.42	2.98	17	1
1:A:505:VAL:CG2	1:A:522:LEU:HD13	0.42	2.45	18	1
1:A:464:GLN:HA	1:A:486:LEU:HD11	0.42	1.92	19	1
1:A:505:VAL:CG1	1:A:522:LEU:CD1	0.41	2.98	1	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:547:LEU:N	1:A:547:LEU:CD1	0.41	2.83	13	4
1:A:463:VAL:HG23	1:A:465:ILE:CG2	0.41	2.45	8	1
1:A:464:GLN:HE22	1:A:521:LEU:HD23	0.41	1.74	10	1
1:A:417:ALA:HA	1:A:420:SER:HB3	0.41	1.92	9	1
1:A:453:VAL:HG21	1:A:465:ILE:HG21	0.41	1.92	19	2
1:A:419:TYR:CG	1:A:436:VAL:CG1	0.41	3.02	12	2
1:A:466:ILE:CG2	1:A:467:ALA:N	0.41	2.84	18	2
1:A:446:ARG:NE	1:A:467:ALA:CB	0.41	2.83	13	1
1:A:467:ALA:HB3	1:A:471:ARG:HA	0.41	1.91	18	1
1:A:395:LEU:O	1:A:399:ILE:HG13	0.41	2.15	20	1
1:A:515:LEU:O	1:A:515:LEU:HD13	0.41	2.15	7	1
1:A:464:GLN:O	1:A:505:VAL:HA	0.41	2.16	9	1
1:A:413:VAL:HG23	1:A:414:PRO:HD2	0.41	1.92	18	1
1:A:421:ASP:O	1:A:425:VAL:HG13	0.41	2.14	18	1
1:A:446:ARG:HG3	1:A:467:ALA:HB1	0.41	1.91	1	1
1:A:450:ALA:O	1:A:453:VAL:HB	0.41	2.15	3	1
1:A:433:LEU:CD1	1:A:532:VAL:O	0.41	2.69	8	1
1:A:480:GLU:O	1:A:482:LEU:CD2	0.41	2.68	9	1
1:A:453:VAL:CG1	1:A:463:VAL:CG2	0.41	2.91	4	1
1:A:464:GLN:HE22	1:A:521:LEU:HD22	0.41	1.75	8	1
1:A:506:ILE:CG1	1:A:506:ILE:O	0.41	2.68	10	3
1:A:487:ILE:CG2	1:A:503:SER:CB	0.41	2.98	12	1
1:A:423:VAL:CG1	1:A:533:LEU:HD11	0.41	2.44	19	1
1:A:501:PRO:O	1:A:528:HIS:CD2	0.41	2.74	5	1
1:A:430:ARG:HB3	1:A:431:PRO:CD	0.41	2.45	13	1
1:A:467:ALA:O	1:A:468:ALA:O	0.41	2.38	19	1
1:A:488:THR:OG1	1:A:499:PHE:CD2	0.41	2.70	3	1
1:A:402:GLN:OE1	1:A:415:ARG:O	0.41	2.39	5	1
1:A:465:ILE:N	1:A:465:ILE:HD13	0.41	2.31	6	1
1:A:509:GLN:NE2	1:A:515:LEU:HD13	0.41	2.31	6	1
1:A:465:ILE:HG22	1:A:506:ILE:HB	0.41	1.93	9	1
1:A:466:ILE:CD1	1:A:518:THR:CG2	0.41	2.99	11	1
1:A:491:ARG:O	1:A:496:GLY:N	0.41	2.54	15	1
1:A:526:ALA:HA	1:A:530:VAL:CG1	0.41	2.46	4	2
1:A:463:VAL:HA	1:A:487:ILE:HD11	0.41	1.93	15	1
1:A:403:ASN:OD1	1:A:437:SER:CB	0.41	2.69	17	1
1:A:468:ALA:N	1:A:508:ASP:O	0.40	2.54	2	2
1:A:530:VAL:CG1	1:A:531:GLN:N	0.40	2.84	11	1
1:A:493:LEU:HD23	1:A:493:LEU:N	0.40	2.31	17	1
1:A:529:ASN:C	1:A:530:VAL:HG23	0.40	2.36	17	1
1:A:432:SER:N	1:A:531:GLN:HG2	0.40	2.31	17	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:519:LEU:HB3	1:A:553:ALA:HB1	0.40	1.92	19	1
1:A:449:VAL:CG2	1:A:506:ILE:CD1	0.40	2.99	5	1
1:A:465:ILE:HB	1:A:506:ILE:HD11	0.40	1.93	5	1
1:A:466:ILE:HG22	1:A:509:GLN:HE22	0.40	1.76	5	1
1:A:436:VAL:HG22	1:A:535:THR:HB	0.40	1.93	8	1
1:A:522:LEU:CD2	1:A:530:VAL:CG1	0.40	2.99	8	1
1:A:430:ARG:CB	1:A:431:PRO:CD	0.40	3.00	10	1
1:A:402:GLN:O	1:A:405:VAL:CG1	0.40	2.69	13	1
1:A:407:VAL:CG1	1:A:412:SER:CB	0.40	2.99	15	1
1:A:469:ASP:OD1	1:A:469:ASP:N	0.40	2.54	16	1
1:A:509:GLN:HG3	1:A:511:GLU:O	0.40	2.16	17	1
1:A:515:LEU:HD21	1:A:550:MET:SD	0.40	2.56	19	1
1:A:481:ARG:C	1:A:482:LEU:HD13	0.40	2.37	1	1
1:A:505:VAL:HG11	1:A:522:LEU:HD22	0.40	1.94	19	1
1:A:392:VAL:HG13	1:A:433:LEU:O	0.40	2.16	5	1
1:A:510:GLY:HA2	1:A:537:SER:N	0.40	2.31	18	1

5.2 Torsion angles ⓘ

5.2.1 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	167/189 (88%)	139±4 (83±2%)	18±3 (11±2%)	10±3 (6±2%)	3	21
All	All	3340/3780 (88%)	2775 (83%)	368 (11%)	197 (6%)	3	21

All 32 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	468	ALA	20
1	A	487	ILE	20
1	A	430	ARG	20
1	A	429	ASP	19
1	A	502	GLY	12
1	A	406	THR	10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	482	LEU	10
1	A	478	GLN	10
1	A	484	GLY	10
1	A	510	GLY	7
1	A	486	LEU	6
1	A	405	VAL	6
1	A	511	GLU	6
1	A	538	GLY	5
1	A	531	GLN	4
1	A	481	ARG	4
1	A	540	ARG	4
1	A	527	ARG	3
1	A	389	GLU	2
1	A	485	GLU	2
1	A	441	GLY	2
1	A	412	SER	2
1	A	512	LYS	2
1	A	439	GLN	2
1	A	469	ASP	2
1	A	417	ALA	1
1	A	507	VAL	1
1	A	416	THR	1
1	A	440	GLY	1
1	A	489	GLY	1
1	A	541	THR	1
1	A	539	GLN	1

5.2.2 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	134/152 (88%)	119±3 (89±2%)	15±3 (11±2%)	10	54
All	All	2680/3040 (88%)	2387 (89%)	293 (11%)	10	54

All 61 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	411	LYS	20
1	A	519	LEU	18
1	A	426	LEU	15
1	A	482	LEU	15
1	A	499	PHE	14
1	A	465	ILE	13
1	A	430	ARG	12
1	A	481	ARG	11
1	A	494	LEU	11
1	A	533	LEU	10
1	A	487	ILE	10
1	A	537	SER	9
1	A	530	VAL	8
1	A	522	LEU	8
1	A	521	LEU	7
1	A	433	LEU	7
1	A	432	SER	6
1	A	531	GLN	6
1	A	395	LEU	5
1	A	455	MET	5
1	A	474	MET	5
1	A	486	LEU	4
1	A	446	ARG	4
1	A	399	ILE	4
1	A	492	GLN	4
1	A	408	HIS	4
1	A	528	HIS	4
1	A	509	GLN	3
1	A	513	LEU	3
1	A	534	ILE	3
1	A	517	GLU	3
1	A	539	GLN	3
1	A	515	LEU	2
1	A	529	ASN	2
1	A	435	ILE	2
1	A	404	ARG	2
1	A	420	SER	2
1	A	402	GLN	2
1	A	495	GLU	2
1	A	490	ARG	2
1	A	478	GLN	2
1	A	390	LEU	2
1	A	393	ARG	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	400	MET	1
1	A	439	GLN	1
1	A	436	VAL	1
1	A	483	SER	1
1	A	415	ARG	1
1	A	428	GLN	1
1	A	512	LYS	1
1	A	461	ARG	1
1	A	506	ILE	1
1	A	497	MET	1
1	A	452	LEU	1
1	A	462	GLU	1
1	A	540	ARG	1
1	A	471	ARG	1
1	A	488	THR	1
1	A	403	ASN	1
1	A	523	ASP	1
1	A	514	SER	1

5.2.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.4 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.5 Ligand geometry [i](#)

There are no ligands in this entry.

5.6 Other polymers [i](#)

There are no such molecules in this entry.

5.7 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 80% for the well-defined parts and 77% for the entire structure.

6.1 Chemical shift list 1

File name: input_cs.cif

Chemical shift list name: *f20chem.txt*

6.1.1 Bookkeeping

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

Total number of shifts	1999
Number of shifts mapped to atoms	1999
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

6.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	175	-0.34 ± 0.11	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	161	0.12 ± 0.06	None needed (< 0.5 ppm)
$^{13}\text{C}'$	171	-0.15 ± 0.12	None needed (< 0.5 ppm)
^{15}N	162	0.05 ± 0.19	None needed (< 0.5 ppm)

6.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 80%, i.e. 1591 atoms were assigned a chemical shift out of a possible 2000. 24 out of 31 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	774/827 (94%)	313/330 (95%)	314/334 (94%)	147/163 (90%)
Sidechain	817/1142 (72%)	523/665 (79%)	281/408 (69%)	13/69 (19%)

Continued on next page...

Continued from previous page...

	Total	^1H	^{13}C	^{15}N
Aromatic	0/31 (0%)	0/17 (0%)	0/12 (0%)	0/2 (0%)
Overall	1591/2000 (80%)	836/1012 (83%)	595/754 (79%)	160/234 (68%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 77%, i.e. 1749 atoms were assigned a chemical shift out of a possible 2268. 25 out of 33 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	855/935 (91%)	347/373 (93%)	346/378 (92%)	162/184 (88%)
Sidechain	893/1275 (70%)	575/743 (77%)	302/454 (67%)	16/78 (21%)
Aromatic	1/58 (2%)	0/31 (0%)	0/23 (0%)	1/4 (25%)
Overall	1749/2268 (77%)	922/1147 (80%)	648/855 (76%)	179/266 (67%)

6.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

6.1.5 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.

Random coil index (RCI) for chain A:

