



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 02:38 PM BST

PDB ID : 1FHQ
Title : REFINED SOLUTION STRUCTURE OF THE FHA2 DOMAIN OF RAD53
Authors : Byeon, I.-J.L.; Liao, H.; Tsai, M.-D.
Deposited on : 2000-08-02

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
<http://wwpdb.org/validation/2016/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
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : rb-20027457
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

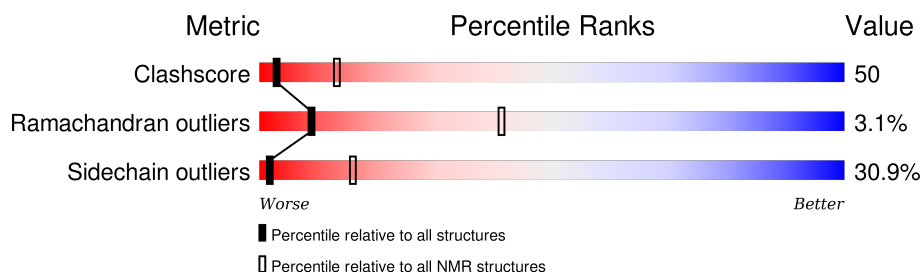
1 Overall quality at a glance

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	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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	158	<div> <div>21%</div> <div>49%</div> <div>11%</div> <div>20%</div> </div>

2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 20 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:576-A:631, A:644-A:700, A:715-A:728 (127)	0.23	20

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, 6, 7, 8, 9, 10, 11, 12, 13, 15, 16, 17, 19, 20
2	14, 18

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 2551 atoms, of which 1277 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called PROTEIN KINASE SPK1.

Mol	Chain	Residues	Atoms						Trace
1	A	158	Total	C	H	N	O	S	0
			2551	806	1277	222	239	7	

4 Residue-property plots [i](#)

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 KINASE SPK1

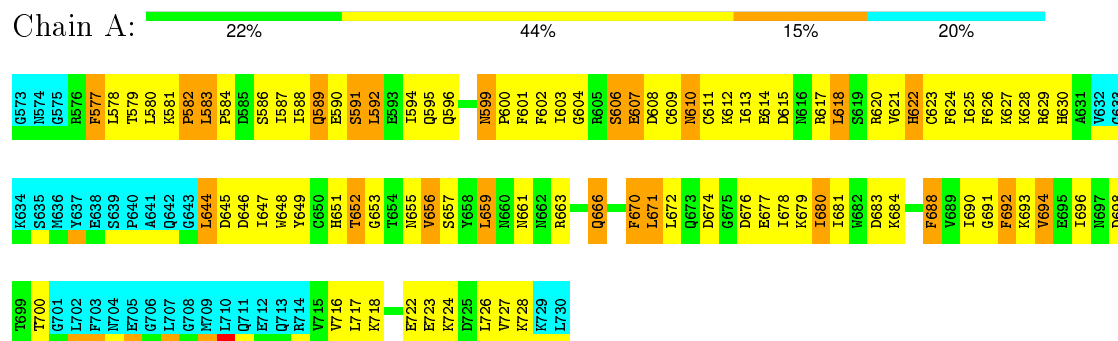


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

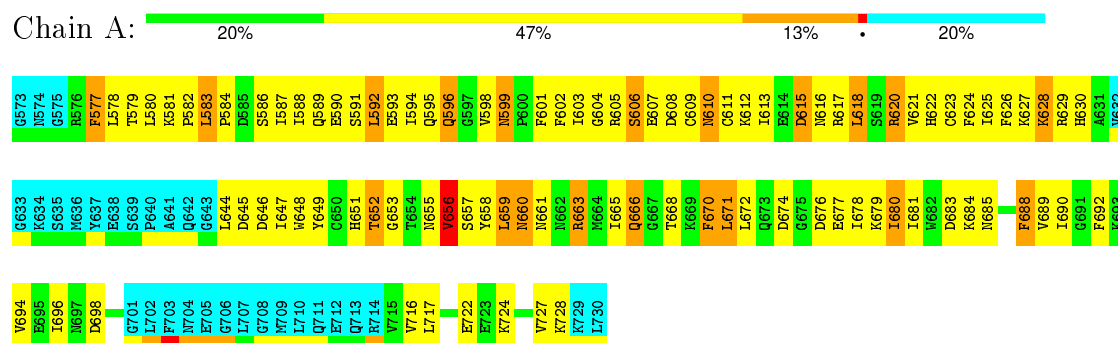
4.2.1 Score per residue for model 1

- Molecule 1: PROTEIN KINASE SPK1



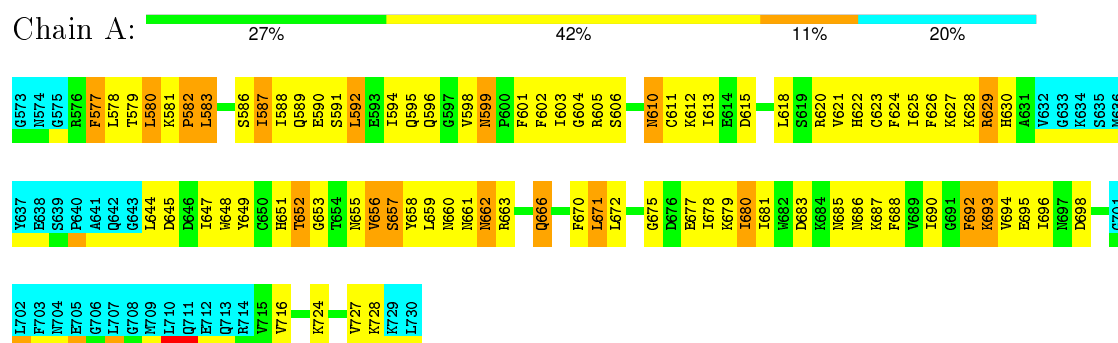
4.2.2 Score per residue for model 2

- Molecule 1: PROTEIN KINASE SPK1



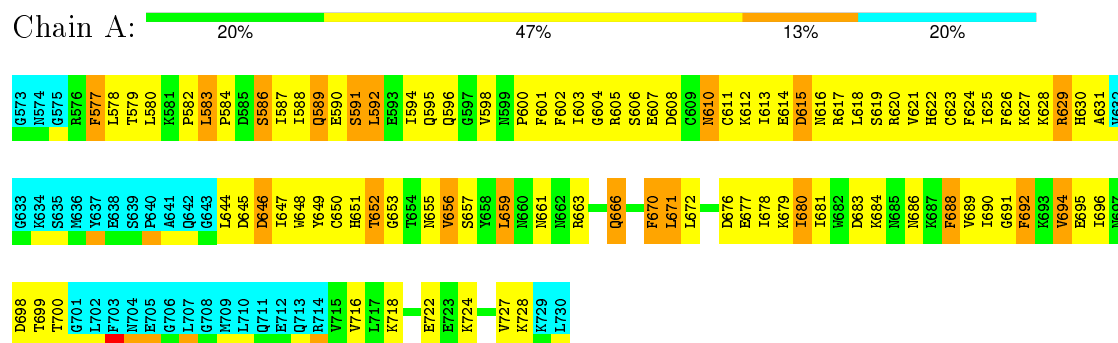
4.2.3 Score per residue for model 3

- Molecule 1: PROTEIN KINASE SPK1



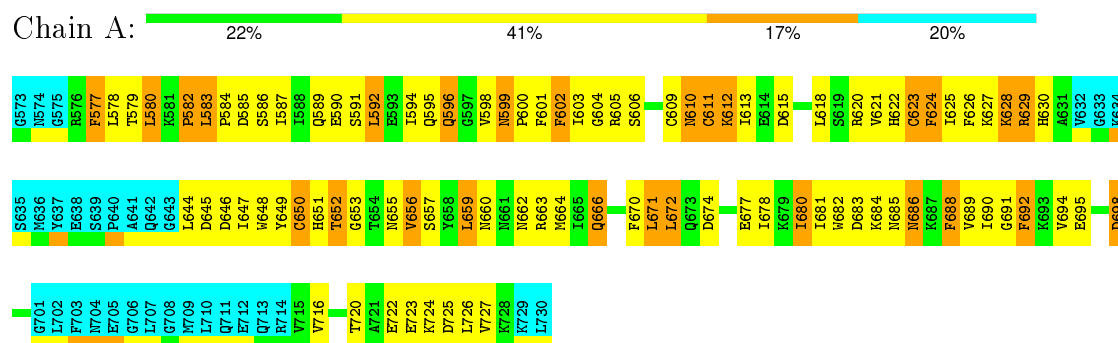
4.2.4 Score per residue for model 4

- Molecule 1: PROTEIN KINASE SPK1



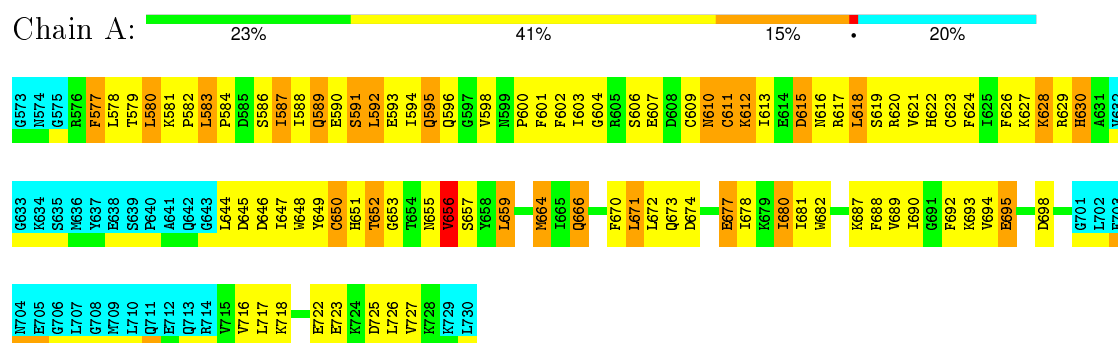
4.2.5 Score per residue for model 5

- Molecule 1: PROTEIN KINASE SPK1



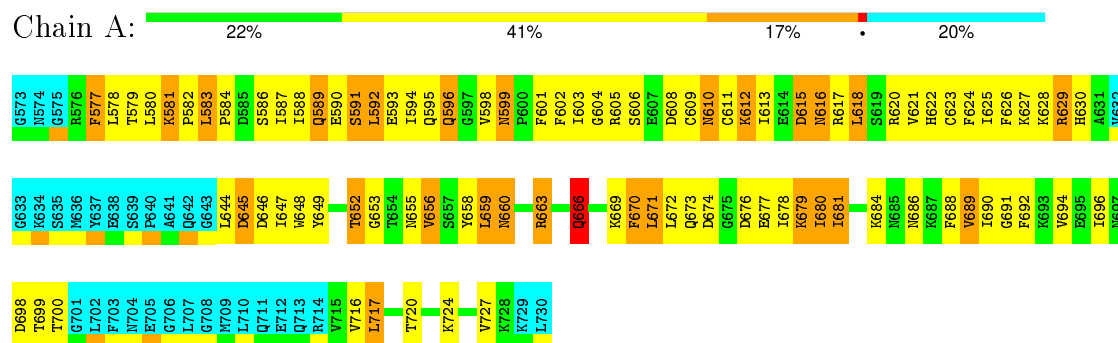
4.2.6 Score per residue for model 6

- Molecule 1: PROTEIN KINASE SPK1



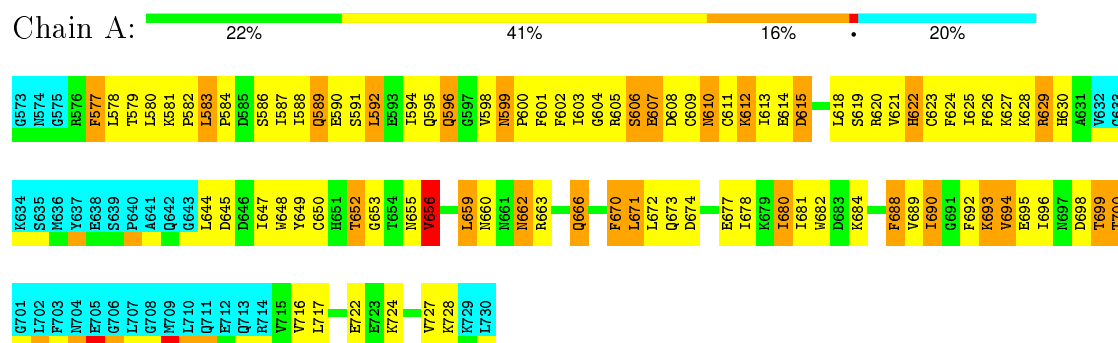
4.2.7 Score per residue for model 7

- Molecule 1: PROTEIN KINASE SPK1



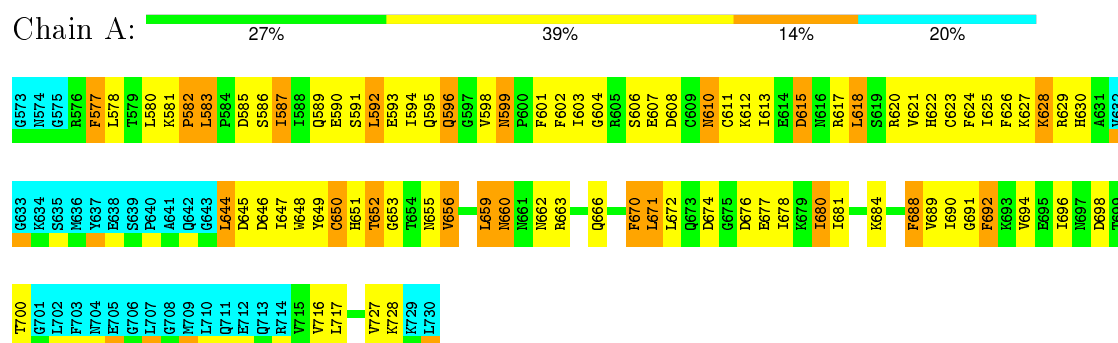
4.2.8 Score per residue for model 8

- Molecule 1: PROTEIN KINASE SPK1



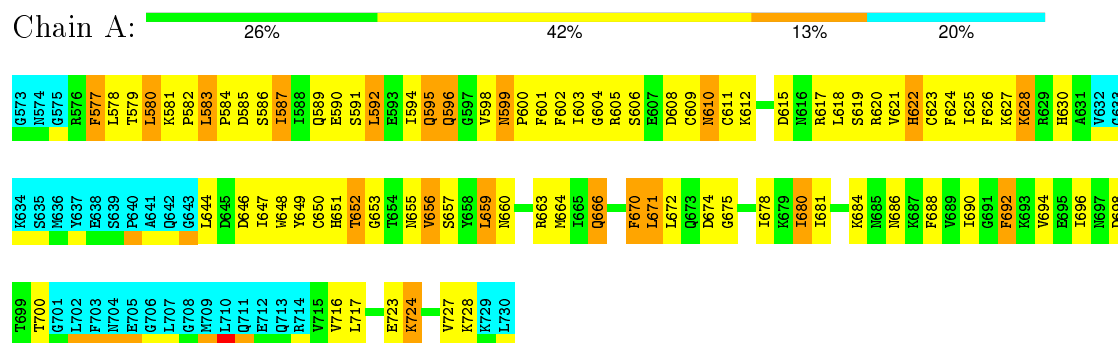
4.2.9 Score per residue for model 9

- Molecule 1: PROTEIN KINASE SPK1



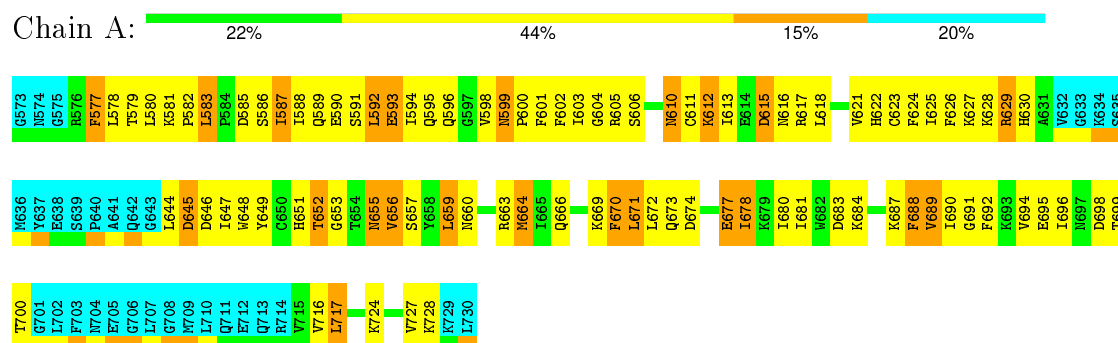
4.2.10 Score per residue for model 10

- Molecule 1: PROTEIN KINASE SPK1



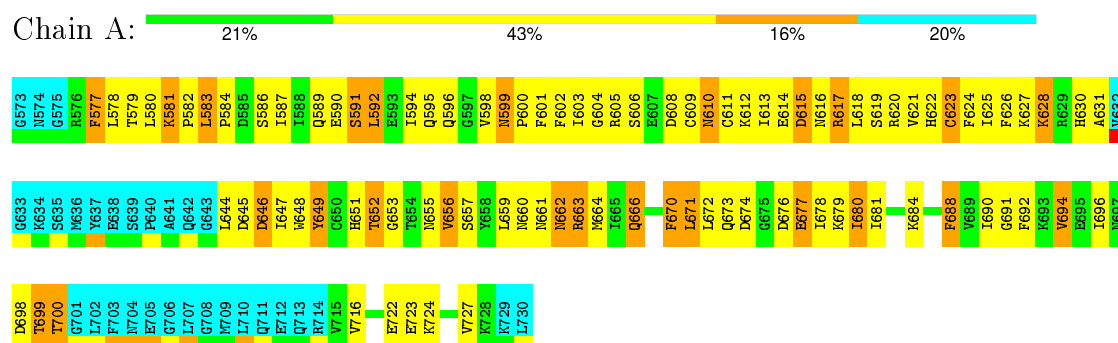
4.2.11 Score per residue for model 11

- Molecule 1: PROTEIN KINASE SPK1



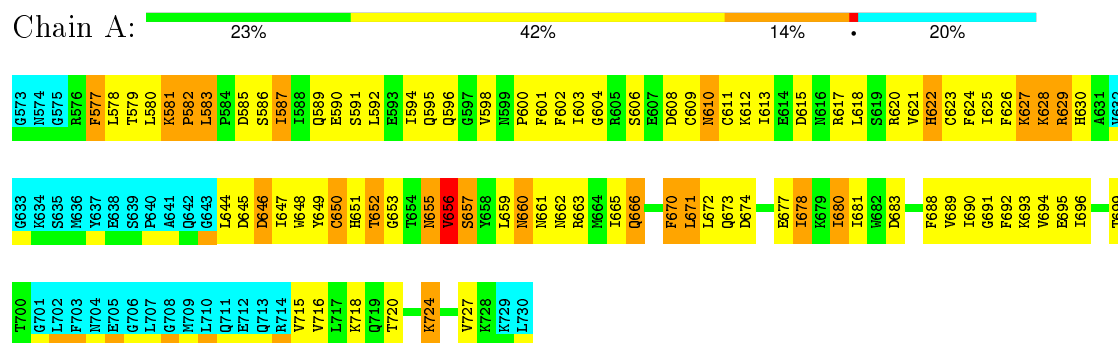
4.2.12 Score per residue for model 12

- Molecule 1: PROTEIN KINASE SPK1



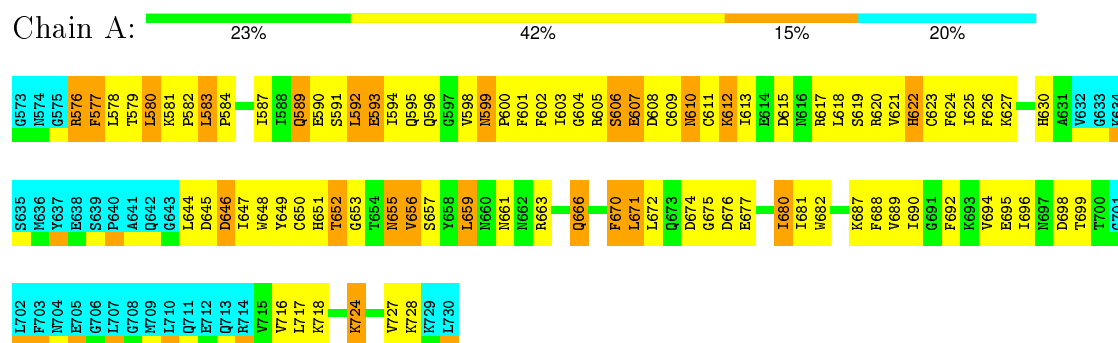
4.2.13 Score per residue for model 13

- Molecule 1: PROTEIN KINASE SPK1



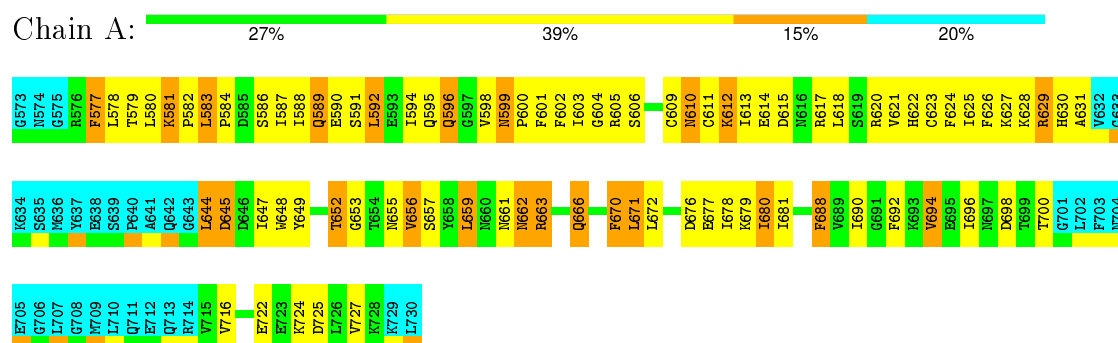
4.2.14 Score per residue for model 14

- Molecule 1: PROTEIN KINASE SPK1



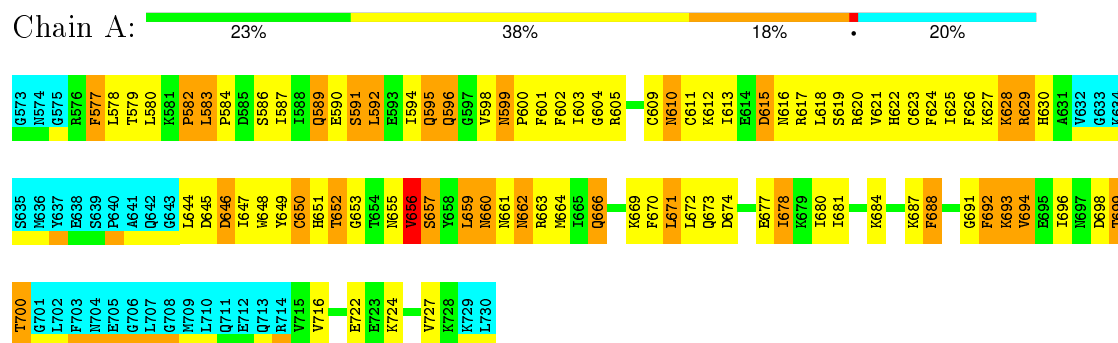
4.2.15 Score per residue for model 15

- Molecule 1: PROTEIN KINASE SPK1



4.2.16 Score per residue for model 16

- Molecule 1: PROTEIN KINASE SPK1



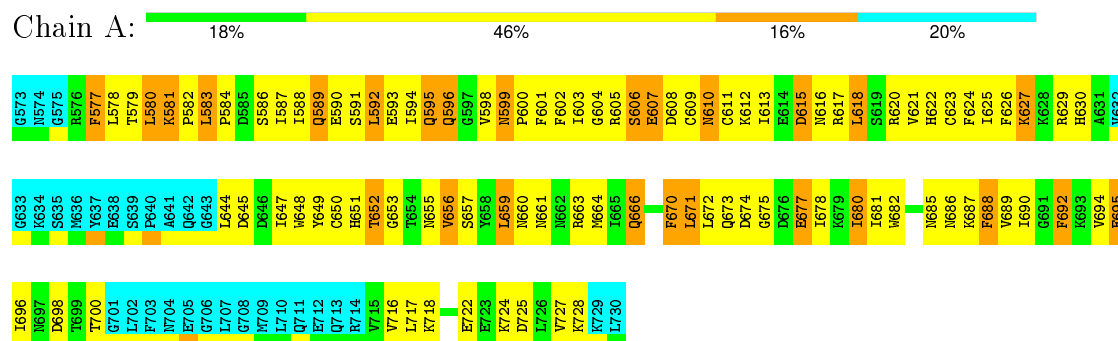
4.2.17 Score per residue for model 17

- Molecule 1: PROTEIN KINASE SPK1



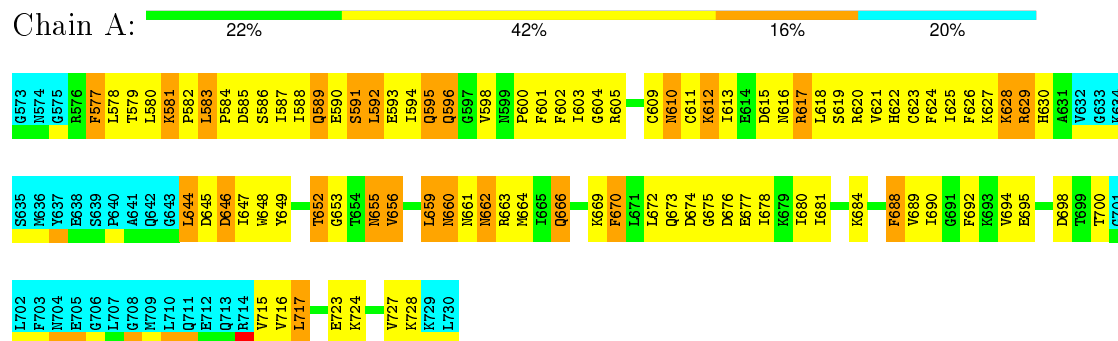
4.2.18 Score per residue for model 18

- Molecule 1: PROTEIN KINASE SPK1



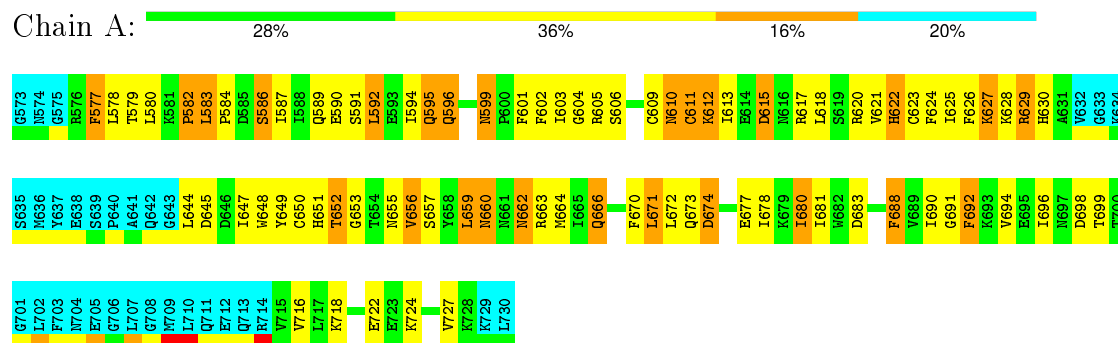
4.2.19 Score per residue for model 19

- Molecule 1: PROTEIN KINASE SPK1



4.2.20 Score per residue for model 20 (medoid)

• Molecule 1: PROTEIN KINASE SPK1



5 Refinement protocol and experimental data overview ⓘ

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

Of the 60 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	structure solution	3.851
X-PLOR	refinement	3.851

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality ⓘ

6.1 Standard geometry ⓘ

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1044	1052	1049	105±5
All	All	20880	21040	20980	2105

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 50.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:578:LEU:HD22	1:A:594:ILE:HD12	1.13	1.19	13	18
1:A:582:PRO:HD2	1:A:590:GLU:O	1.10	1.47	14	20
1:A:621:VAL:HG11	1:A:727:VAL:HG23	1.00	1.31	18	16
1:A:659:LEU:HD13	1:A:678:ILE:HG22	0.99	1.28	12	3
1:A:578:LEU:HD12	1:A:647:ILE:HD13	0.96	1.34	8	18
1:A:648:TRP:CH2	1:A:671:LEU:HD22	0.92	2.00	10	14
1:A:603:ILE:HG23	1:A:611:CYS:HB3	0.90	1.42	11	20
1:A:648:TRP:CZ3	1:A:671:LEU:HD22	0.89	2.02	20	14
1:A:618:LEU:HD11	1:A:680:ILE:CG2	0.86	2.01	14	5
1:A:592:LEU:HD11	1:A:613:ILE:HD11	0.86	1.48	5	2
1:A:578:LEU:HD23	1:A:594:ILE:HD12	0.86	1.47	9	2
1:A:659:LEU:HD21	1:A:678:ILE:HG22	0.84	1.48	17	5
1:A:618:LEU:HD22	1:A:622:HIS:NE2	0.84	1.86	11	9
1:A:578:LEU:HD22	1:A:594:ILE:CD1	0.84	2.02	16	13

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:659:LEU:HD23	1:A:670:PHE:CD2	0.84	2.08	12	4
1:A:592:LEU:HD21	1:A:613:ILE:HD11	0.83	1.46	6	3
1:A:577:PHE:CZ	1:A:647:ILE:HG21	0.83	2.09	13	17
1:A:663:ARG:O	1:A:716:VAL:HG21	0.82	1.74	4	19
1:A:680:ILE:HD11	1:A:692:PHE:CE2	0.82	2.09	1	7
1:A:613:ILE:HD12	1:A:692:PHE:CZ	0.82	2.09	11	6
1:A:659:LEU:HD12	1:A:670:PHE:CE1	0.82	2.10	16	1
1:A:582:PRO:CD	1:A:590:GLU:O	0.82	2.28	18	20
1:A:615:ASP:CB	1:A:618:LEU:HD13	0.81	2.05	13	7
1:A:592:LEU:HD13	1:A:611:CYS:SG	0.81	2.16	11	14
1:A:594:ILE:HG23	1:A:601:PHE:CD1	0.80	2.11	5	18
1:A:659:LEU:CD2	1:A:678:ILE:HG22	0.80	2.07	17	5
1:A:681:ILE:HG22	1:A:690:ILE:HG22	0.79	1.54	18	2
1:A:578:LEU:HD12	1:A:579:THR:N	0.79	1.93	5	1
1:A:612:LYS:O	1:A:613:ILE:HD13	0.79	1.78	14	9
1:A:615:ASP:OD2	1:A:690:ILE:HD11	0.78	1.79	1	2
1:A:649:TYR:CE2	1:A:678:ILE:HG21	0.78	2.12	5	10
1:A:580:LEU:CD2	1:A:694:VAL:HG23	0.78	2.07	20	14
1:A:580:LEU:HD21	1:A:694:VAL:HG23	0.78	1.52	20	13
1:A:681:ILE:HG22	1:A:690:ILE:CG2	0.78	2.09	3	2
1:A:629:ARG:NH1	1:A:631:ALA:HB2	0.78	1.94	15	2
1:A:578:LEU:HD21	1:A:694:VAL:HG22	0.77	1.56	4	17
1:A:680:ILE:HD13	1:A:692:PHE:CE2	0.76	2.15	9	1
1:A:672:LEU:HD13	1:A:694:VAL:HG21	0.76	1.57	13	8
1:A:580:LEU:HD11	1:A:625:ILE:HD12	0.76	1.54	1	5
1:A:659:LEU:HD13	1:A:678:ILE:CG2	0.76	2.07	12	2
1:A:603:ILE:HD12	1:A:624:PHE:HA	0.75	1.58	20	9
1:A:659:LEU:HD22	1:A:678:ILE:CG2	0.75	2.11	10	1
1:A:621:VAL:HG11	1:A:727:VAL:CG2	0.75	2.11	8	20
1:A:582:PRO:HD3	1:A:592:LEU:HD22	0.74	1.58	6	4
1:A:615:ASP:HB3	1:A:618:LEU:HD13	0.74	1.60	15	8
1:A:621:VAL:HG21	1:A:727:VAL:CG2	0.74	2.13	19	9
1:A:618:LEU:HD22	1:A:622:HIS:CD2	0.73	2.18	18	9
1:A:618:LEU:HD11	1:A:680:ILE:HG21	0.73	1.60	15	4
1:A:680:ILE:HD12	1:A:692:PHE:CE2	0.73	2.19	7	4
1:A:613:ILE:HD12	1:A:692:PHE:CE2	0.72	2.19	11	1
1:A:578:LEU:CD2	1:A:594:ILE:HD12	0.72	2.14	5	15
1:A:587:ILE:HG22	1:A:690:ILE:HD11	0.72	1.60	13	4
1:A:581:LYS:O	1:A:583:LEU:HD23	0.71	1.84	7	10
1:A:582:PRO:HD2	1:A:590:GLU:C	0.71	2.06	18	11
1:A:578:LEU:HD23	1:A:579:THR:N	0.71	2.01	8	17

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:587:ILE:HD13	1:A:688:PHE:CE1	0.71	2.20	20	1
1:A:649:TYR:CB	1:A:672:LEU:HD21	0.70	2.16	19	13
1:A:595:GLN:HB2	1:A:598:VAL:HG23	0.70	1.63	15	17
1:A:580:LEU:CD1	1:A:594:ILE:HD11	0.70	2.16	3	5
1:A:588:ILE:HG22	1:A:690:ILE:HD11	0.70	1.62	18	2
1:A:659:LEU:HD11	1:A:672:LEU:CD2	0.70	2.16	9	11
1:A:578:LEU:CD1	1:A:647:ILE:HD13	0.70	2.15	8	17
1:A:603:ILE:HG23	1:A:611:CYS:SG	0.69	2.27	3	13
1:A:618:LEU:HG	1:A:622:HIS:CD2	0.69	2.22	5	11
1:A:659:LEU:CD1	1:A:678:ILE:HG22	0.69	2.15	12	1
1:A:579:THR:HG23	1:A:593:GLU:HG3	0.69	1.64	2	1
1:A:583:LEU:N	1:A:583:LEU:HD23	0.69	2.03	14	5
1:A:580:LEU:O	1:A:592:LEU:HD12	0.69	1.88	18	2
1:A:591:SER:C	1:A:592:LEU:HD13	0.69	2.08	7	4
1:A:583:LEU:HD23	1:A:583:LEU:N	0.69	2.03	6	5
1:A:603:ILE:HD11	1:A:625:ILE:CD1	0.69	2.18	18	2
1:A:615:ASP:CG	1:A:618:LEU:HD13	0.69	2.08	17	3
1:A:659:LEU:HD21	1:A:672:LEU:CD2	0.69	2.18	19	5
1:A:646:ASP:OD1	1:A:671:LEU:HD21	0.68	1.89	9	1
1:A:613:ILE:HD11	1:A:692:PHE:CZ	0.68	2.23	13	1
1:A:615:ASP:OD2	1:A:681:ILE:HG21	0.68	1.89	11	1
1:A:592:LEU:HD22	1:A:611:CYS:SG	0.68	2.29	16	9
1:A:580:LEU:HB3	1:A:592:LEU:HD12	0.68	1.66	4	9
1:A:586:SER:O	1:A:589:GLN:NE2	0.67	2.27	8	18
1:A:580:LEU:HD11	1:A:625:ILE:CD1	0.67	2.20	1	15
1:A:615:ASP:HB2	1:A:618:LEU:HD13	0.67	1.64	13	1
1:A:613:ILE:O	1:A:618:LEU:HD12	0.67	1.90	4	9
1:A:603:ILE:HG23	1:A:611:CYS:CB	0.66	2.19	19	18
1:A:596:GLN:CB	1:A:700:THR:HG21	0.66	2.20	18	1
1:A:648:TRP:CH2	1:A:671:LEU:HD12	0.66	2.24	9	1
1:A:600:PRO:HG3	1:A:726:LEU:HD13	0.66	1.66	5	1
1:A:586:SER:HB2	1:A:690:ILE:HD13	0.66	1.67	2	2
1:A:659:LEU:HD21	1:A:672:LEU:HD22	0.66	1.65	19	3
1:A:578:LEU:HD12	1:A:647:ILE:CD1	0.66	2.21	14	11
1:A:649:TYR:O	1:A:664:MET:HE3	0.66	1.91	12	1
1:A:689:VAL:C	1:A:690:ILE:HD12	0.65	2.12	4	1
1:A:659:LEU:HD11	1:A:672:LEU:HD21	0.65	1.67	2	4
1:A:577:PHE:HZ	1:A:647:ILE:HG21	0.65	1.52	20	16
1:A:588:ILE:HG21	1:A:613:ILE:HG23	0.65	1.68	17	4
1:A:623:CYS:SG	1:A:680:ILE:HD11	0.65	2.31	4	3
1:A:622:HIS:CD2	1:A:680:ILE:HD12	0.65	2.27	17	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:621:VAL:HG11	1:A:727:VAL:HG21	0.64	1.69	9	9
1:A:580:LEU:HD12	1:A:594:ILE:HD11	0.64	1.67	18	3
1:A:659:LEU:HD13	1:A:678:ILE:CG1	0.64	2.22	13	2
1:A:623:CYS:SG	1:A:680:ILE:HD13	0.64	2.33	16	3
1:A:578:LEU:HD13	1:A:696:ILE:HG12	0.64	1.69	9	1
1:A:583:LEU:HD12	1:A:693:LYS:HB2	0.63	1.70	16	4
1:A:662:ASN:ND2	1:A:716:VAL:HG23	0.63	2.08	15	2
1:A:592:LEU:N	1:A:592:LEU:HD13	0.63	2.08	7	3
1:A:649:TYR:CE1	1:A:678:ILE:HD12	0.63	2.29	16	1
1:A:587:ILE:HG22	1:A:690:ILE:CD1	0.63	2.24	13	5
1:A:662:ASN:OD1	1:A:716:VAL:HG23	0.63	1.93	20	4
1:A:577:PHE:O	1:A:696:ILE:HG23	0.63	1.94	8	4
1:A:602:PHE:N	1:A:602:PHE:CD1	0.62	2.64	5	1
1:A:659:LEU:HD13	1:A:678:ILE:HG12	0.62	1.69	3	4
1:A:659:LEU:HG	1:A:678:ILE:HG23	0.62	1.71	1	4
1:A:681:ILE:HG21	1:A:688:PHE:CZ	0.62	2.30	5	3
1:A:644:LEU:N	1:A:644:LEU:CD2	0.61	2.63	17	2
1:A:602:PHE:CE1	1:A:624:PHE:CZ	0.61	2.88	5	1
1:A:669:LYS:O	1:A:717:LEU:HD12	0.61	1.95	7	2
1:A:621:VAL:HG21	1:A:727:VAL:HG23	0.61	1.72	8	8
1:A:602:PHE:CD1	1:A:624:PHE:CZ	0.61	2.89	5	1
1:A:579:THR:HG23	1:A:593:GLU:CG	0.60	2.26	11	1
1:A:659:LEU:HG	1:A:678:ILE:HG22	0.60	1.72	7	2
1:A:644:LEU:CD2	1:A:644:LEU:N	0.60	2.64	9	1
1:A:682:TRP:CD1	1:A:689:VAL:HG12	0.60	2.31	8	4
1:A:578:LEU:HD23	1:A:594:ILE:CD1	0.60	2.26	9	1
1:A:652:THR:O	1:A:666:GLN:NE2	0.60	2.35	6	20
1:A:592:LEU:N	1:A:592:LEU:HD22	0.60	2.12	13	1
1:A:579:THR:HG23	1:A:593:GLU:HG2	0.60	1.73	11	1
1:A:689:VAL:O	1:A:690:ILE:HD13	0.60	1.95	19	1
1:A:600:PRO:HG3	1:A:726:LEU:HD23	0.60	1.74	17	3
1:A:600:PRO:HG2	1:A:602:PHE:CZ	0.59	2.32	6	14
1:A:681:ILE:HG22	1:A:690:ILE:CG1	0.59	2.27	20	6
1:A:648:TRP:CH2	1:A:671:LEU:CD1	0.59	2.85	9	1
1:A:615:ASP:HB2	1:A:618:LEU:HD22	0.59	1.73	20	4
1:A:622:HIS:O	1:A:653:GLY:N	0.59	2.36	15	20
1:A:655:ASN:O	1:A:656:VAL:O	0.59	2.21	7	16
1:A:659:LEU:HD22	1:A:678:ILE:HG22	0.59	1.73	10	1
1:A:580:LEU:N	1:A:592:LEU:O	0.59	2.35	5	20
1:A:578:LEU:HD22	1:A:647:ILE:HD13	0.59	1.73	5	2
1:A:580:LEU:HD11	1:A:625:ILE:HD11	0.59	1.75	4	11

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:596:GLN:HB2	1:A:700:THR:HG21	0.59	1.74	18	3
1:A:603:ILE:O	1:A:623:CYS:N	0.58	2.36	5	1
1:A:580:LEU:HD22	1:A:692:PHE:HB2	0.58	1.75	9	3
1:A:622:HIS:NE2	1:A:680:ILE:HG23	0.58	2.13	14	1
1:A:622:HIS:CD2	1:A:680:ILE:HG21	0.58	2.32	1	8
1:A:662:ASN:HB3	1:A:716:VAL:HG23	0.58	1.75	16	1
1:A:630:HIS:N	1:A:644:LEU:O	0.58	2.35	14	20
1:A:648:TRP:CZ3	1:A:671:LEU:HG	0.58	2.34	13	5
1:A:613:ILE:HG22	1:A:618:LEU:HD11	0.58	1.74	4	5
1:A:603:ILE:CG2	1:A:611:CYS:HB3	0.57	2.27	7	11
1:A:621:VAL:CG1	1:A:727:VAL:HG23	0.57	2.20	18	3
1:A:603:ILE:N	1:A:623:CYS:O	0.57	2.38	9	19
1:A:602:PHE:HA	1:A:624:PHE:HB3	0.57	1.76	19	19
1:A:586:SER:OG	1:A:690:ILE:HG23	0.57	2.00	19	1
1:A:681:ILE:HB	1:A:690:ILE:HD13	0.57	1.74	4	1
1:A:624:PHE:O	1:A:650:CYS:N	0.57	2.36	5	5
1:A:594:ILE:HD11	1:A:625:ILE:HD12	0.57	1.77	20	4
1:A:615:ASP:OD2	1:A:618:LEU:HD13	0.57	2.00	15	1
1:A:578:LEU:HD12	1:A:579:THR:H	0.56	1.58	5	1
1:A:606:SER:O	1:A:609:CYS:SG	0.56	2.62	8	2
1:A:587:ILE:HD12	1:A:688:PHE:CE1	0.56	2.35	10	1
1:A:613:ILE:HD12	1:A:692:PHE:CE1	0.56	2.35	2	1
1:A:588:ILE:CG2	1:A:690:ILE:HD11	0.56	2.30	18	1
1:A:587:ILE:HD11	1:A:615:ASP:OD1	0.56	2.00	4	3
1:A:689:VAL:C	1:A:690:ILE:HD13	0.56	2.20	19	1
1:A:587:ILE:HD11	1:A:615:ASP:OD2	0.56	2.00	18	2
1:A:659:LEU:HD22	1:A:678:ILE:HG21	0.56	1.76	10	1
1:A:592:LEU:CD1	1:A:613:ILE:HD11	0.56	2.29	5	1
1:A:690:ILE:HD12	1:A:690:ILE:N	0.56	2.16	4	1
1:A:578:LEU:C	1:A:578:LEU:HD23	0.55	2.22	8	13
1:A:583:LEU:H	1:A:583:LEU:HD13	0.55	1.60	1	4
1:A:603:ILE:CA	1:A:609:CYS:HB2	0.55	2.31	8	4
1:A:578:LEU:HD13	1:A:696:ILE:CG1	0.55	2.30	9	1
1:A:592:LEU:HD22	1:A:612:LYS:H	0.55	1.59	5	3
1:A:618:LEU:HD23	1:A:681:ILE:HD11	0.55	1.77	4	1
1:A:615:ASP:CG	1:A:690:ILE:HD11	0.55	2.22	1	1
1:A:617:ARG:HB2	1:A:681:ILE:HD13	0.55	1.77	20	1
1:A:659:LEU:HD12	1:A:670:PHE:HE1	0.55	1.59	16	1
1:A:580:LEU:CB	1:A:592:LEU:HD12	0.54	2.32	1	2
1:A:649:TYR:HB3	1:A:672:LEU:HD21	0.54	1.76	19	1
1:A:592:LEU:HD23	1:A:611:CYS:SG	0.54	2.43	6	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:587:ILE:HD11	1:A:615:ASP:CG	0.54	2.22	18	1
1:A:586:SER:OG	1:A:588:ILE:O	0.54	2.26	7	7
1:A:648:TRP:CH2	1:A:671:LEU:CD2	0.54	2.89	17	12
1:A:583:LEU:HD13	1:A:583:LEU:H	0.54	1.61	13	5
1:A:677:GLU:HA	1:A:692:PHE:O	0.54	2.02	19	6
1:A:672:LEU:CD1	1:A:694:VAL:HG21	0.54	2.32	13	1
1:A:659:LEU:HD22	1:A:678:ILE:HG12	0.54	1.79	18	3
1:A:582:PRO:HB3	1:A:692:PHE:CE2	0.54	2.38	11	1
1:A:602:PHE:CD1	1:A:624:PHE:CE1	0.54	2.96	5	1
1:A:681:ILE:HG22	1:A:690:ILE:HB	0.54	1.79	2	3
1:A:649:TYR:CD2	1:A:678:ILE:HG21	0.54	2.38	13	2
1:A:604:GLY:HA2	1:A:622:HIS:CB	0.53	2.33	8	20
1:A:628:LYS:O	1:A:646:ASP:N	0.53	2.41	2	9
1:A:618:LEU:HG	1:A:622:HIS:CG	0.53	2.38	13	9
1:A:659:LEU:CG	1:A:678:ILE:HG22	0.53	2.33	9	5
1:A:580:LEU:HD11	1:A:692:PHE:HB2	0.53	1.80	6	1
1:A:613:ILE:CD1	1:A:692:PHE:CZ	0.53	2.91	13	6
1:A:592:LEU:HD21	1:A:613:ILE:CD1	0.53	2.27	6	1
1:A:584:PRO:HA	1:A:589:GLN:CD	0.53	2.24	19	8
1:A:613:ILE:HD11	1:A:692:PHE:CE1	0.53	2.38	13	1
1:A:621:VAL:O	1:A:621:VAL:HG13	0.53	2.04	8	1
1:A:615:ASP:OD2	1:A:690:ILE:HD13	0.53	2.03	18	2
1:A:615:ASP:CB	1:A:618:LEU:HG	0.53	2.33	11	8
1:A:626:PHE:O	1:A:648:TRP:N	0.52	2.40	19	15
1:A:618:LEU:CD1	1:A:622:HIS:NE2	0.52	2.72	1	5
1:A:649:TYR:N	1:A:670:PHE:O	0.52	2.39	10	13
1:A:581:LYS:O	1:A:583:LEU:CD2	0.52	2.57	17	8
1:A:649:TYR:HB2	1:A:672:LEU:HD11	0.52	1.79	10	4
1:A:615:ASP:O	1:A:618:LEU:N	0.52	2.42	5	18
1:A:663:ARG:NH2	1:A:665:ILE:HG22	0.52	2.20	17	1
1:A:617:ARG:HB2	1:A:681:ILE:HD12	0.52	1.81	9	1
1:A:670:PHE:CE1	1:A:716:VAL:HG22	0.52	2.40	6	1
1:A:613:ILE:CD1	1:A:692:PHE:CE1	0.52	2.93	2	2
1:A:581:LYS:O	1:A:583:LEU:HD13	0.52	2.05	11	2
1:A:680:ILE:CG2	1:A:690:ILE:HG21	0.52	2.34	12	3
1:A:578:LEU:HD23	1:A:578:LEU:C	0.52	2.25	14	5
1:A:655:ASN:O	1:A:656:VAL:CG1	0.52	2.58	14	13
1:A:649:TYR:HB2	1:A:672:LEU:HD21	0.52	1.82	19	5
1:A:659:LEU:HD21	1:A:678:ILE:CG2	0.51	2.35	16	1
1:A:583:LEU:HD21	1:A:693:LYS:N	0.51	2.21	6	2
1:A:724:LYS:O	1:A:727:VAL:HG12	0.51	2.06	5	15

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:587:ILE:HG12	1:A:690:ILE:HD12	0.51	1.82	19	1
1:A:592:LEU:HD13	1:A:592:LEU:N	0.51	2.21	19	1
1:A:680:ILE:HG22	1:A:690:ILE:HG21	0.51	1.83	12	1
1:A:692:PHE:N	1:A:692:PHE:CD1	0.51	2.79	3	5
1:A:681:ILE:HG21	1:A:688:PHE:CE1	0.51	2.40	2	1
1:A:648:TRP:CZ3	1:A:671:LEU:CG	0.51	2.94	9	1
1:A:595:GLN:HB3	1:A:598:VAL:HG23	0.51	1.83	6	1
1:A:618:LEU:HD12	1:A:622:HIS:NE2	0.51	2.21	5	4
1:A:577:PHE:CE2	1:A:647:ILE:HG21	0.51	2.40	13	3
1:A:681:ILE:HG22	1:A:690:ILE:HG13	0.51	1.81	9	1
1:A:586:SER:HA	1:A:689:VAL:O	0.51	2.06	8	3
1:A:669:LYS:HE2	1:A:717:LEU:HD11	0.50	1.83	11	1
1:A:583:LEU:HD11	1:A:677:GLU:CG	0.50	2.36	18	2
1:A:577:PHE:CZ	1:A:578:LEU:HB2	0.50	2.41	16	12
1:A:602:PHE:CG	1:A:624:PHE:CE1	0.50	2.99	5	1
1:A:577:PHE:CE2	1:A:578:LEU:HB2	0.50	2.41	8	9
1:A:586:SER:OG	1:A:691:GLY:N	0.50	2.44	4	1
1:A:587:ILE:CG2	1:A:690:ILE:HD11	0.50	2.37	6	3
1:A:655:ASN:C	1:A:656:VAL:HG23	0.50	2.26	13	1
1:A:592:LEU:CD2	1:A:613:ILE:HD11	0.50	2.29	6	1
1:A:651:HIS:NE2	1:A:653:GLY:O	0.50	2.44	16	14
1:A:680:ILE:HG22	1:A:690:ILE:CG2	0.50	2.36	4	3
1:A:580:LEU:HD11	1:A:692:PHE:CB	0.50	2.37	6	1
1:A:621:VAL:HG12	1:A:621:VAL:O	0.50	2.06	3	10
1:A:700:THR:O	1:A:700:THR:HG23	0.50	2.07	12	4
1:A:680:ILE:HD12	1:A:692:PHE:CZ	0.50	2.41	20	2
1:A:627:LYS:NZ	1:A:700:THR:HG21	0.50	2.21	1	1
1:A:583:LEU:CD2	1:A:691:GLY:O	0.50	2.60	20	1
1:A:577:PHE:CG	1:A:578:LEU:N	0.50	2.80	1	14
1:A:681:ILE:HD13	1:A:682:TRP:N	0.50	2.22	17	1
1:A:655:ASN:O	1:A:656:VAL:HG13	0.49	2.07	8	6
1:A:663:ARG:C	1:A:716:VAL:HG21	0.49	2.28	16	1
1:A:659:LEU:HB2	1:A:678:ILE:HG23	0.49	1.84	13	1
1:A:580:LEU:O	1:A:592:LEU:N	0.49	2.38	15	11
1:A:584:PRO:HA	1:A:589:GLN:CG	0.49	2.37	10	3
1:A:588:ILE:HD12	1:A:690:ILE:HD12	0.49	1.84	11	1
1:A:588:ILE:O	1:A:588:ILE:HG23	0.49	2.07	15	3
1:A:655:ASN:C	1:A:656:VAL:HG13	0.49	2.27	3	3
1:A:615:ASP:O	1:A:617:ARG:N	0.49	2.45	7	9
1:A:604:GLY:HA2	1:A:622:HIS:HB3	0.49	1.83	5	11
1:A:644:LEU:HD23	1:A:644:LEU:N	0.49	2.22	19	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:618:LEU:HD12	1:A:622:HIS:CE1	0.49	2.42	9	2
1:A:688:PHE:O	1:A:688:PHE:CG	0.49	2.66	5	4
1:A:587:ILE:HD13	1:A:587:ILE:N	0.49	2.23	10	1
1:A:615:ASP:OD2	1:A:681:ILE:HD12	0.49	2.07	19	1
1:A:646:ASP:CG	1:A:671:LEU:HD21	0.49	2.28	9	1
1:A:580:LEU:HD12	1:A:594:ILE:CD1	0.49	2.38	14	3
1:A:682:TRP:CD1	1:A:689:VAL:CG1	0.48	2.96	18	2
1:A:651:HIS:ND1	1:A:657:SER:CB	0.48	2.77	13	8
1:A:587:ILE:HG12	1:A:690:ILE:HD11	0.48	1.84	2	2
1:A:577:PHE:HB3	1:A:596:GLN:HB3	0.48	1.85	2	5
1:A:613:ILE:CD1	1:A:692:PHE:CE2	0.48	2.95	11	1
1:A:622:HIS:CD2	1:A:680:ILE:CG2	0.48	2.96	13	4
1:A:666:GLN:O	1:A:666:GLN:CG	0.48	2.62	10	4
1:A:618:LEU:HD11	1:A:680:ILE:HG23	0.48	1.82	14	2
1:A:662:ASN:CB	1:A:670:PHE:CE2	0.48	2.97	5	1
1:A:675:GLY:N	1:A:694:VAL:O	0.48	2.46	3	5
1:A:577:PHE:HB3	1:A:596:GLN:HG3	0.48	1.84	1	1
1:A:617:ARG:CB	1:A:681:ILE:HD13	0.48	2.38	7	1
1:A:691:GLY:C	1:A:692:PHE:CD1	0.48	2.87	20	1
1:A:595:GLN:CB	1:A:598:VAL:HG23	0.48	2.38	16	1
1:A:648:TRP:CH2	1:A:671:LEU:HG	0.48	2.44	9	5
1:A:656:VAL:HG23	1:A:657:SER:N	0.48	2.23	3	3
1:A:587:ILE:CG1	1:A:690:ILE:HD11	0.48	2.39	2	1
1:A:601:PHE:CE1	1:A:610:ASN:ND2	0.48	2.81	9	5
1:A:629:ARG:HA	1:A:644:LEU:O	0.47	2.09	5	11
1:A:599:ASN:OD1	1:A:599:ASN:O	0.47	2.32	2	9
1:A:648:TRP:CE3	1:A:671:LEU:HG	0.47	2.44	9	1
1:A:659:LEU:O	1:A:661:ASN:N	0.47	2.47	16	8
1:A:584:PRO:HA	1:A:589:GLN:HB3	0.47	1.86	18	3
1:A:577:PHE:CB	1:A:596:GLN:HG3	0.47	2.39	1	1
1:A:602:PHE:HB2	1:A:609:CYS:HA	0.47	1.86	19	2
1:A:599:ASN:O	1:A:599:ASN:OD1	0.47	2.33	7	7
1:A:586:SER:HB2	1:A:690:ILE:HA	0.47	1.85	7	2
1:A:601:PHE:CE1	1:A:610:ASN:HB3	0.47	2.44	16	16
1:A:659:LEU:CD2	1:A:678:ILE:CG2	0.47	2.93	16	1
1:A:583:LEU:HD11	1:A:677:GLU:OE2	0.47	2.09	12	1
1:A:587:ILE:CD1	1:A:688:PHE:CZ	0.47	2.97	10	3
1:A:583:LEU:N	1:A:583:LEU:CD2	0.47	2.78	20	5
1:A:681:ILE:CG2	1:A:690:ILE:CG1	0.47	2.93	13	4
1:A:587:ILE:HD12	1:A:688:PHE:CZ	0.47	2.45	4	1
1:A:582:PRO:HB3	1:A:692:PHE:CZ	0.47	2.44	13	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:578:LEU:CD1	1:A:647:ILE:CD1	0.47	2.92	11	16
1:A:592:LEU:HD21	1:A:612:LYS:O	0.47	2.10	5	1
1:A:656:VAL:CG2	1:A:658:TYR:CZ	0.47	2.98	3	1
1:A:609:CYS:SG	1:A:611:CYS:O	0.47	2.72	18	3
1:A:580:LEU:HG	1:A:694:VAL:HG22	0.47	1.87	10	1
1:A:680:ILE:CD1	1:A:692:PHE:CE2	0.47	2.98	10	1
1:A:603:ILE:HA	1:A:609:CYS:HB2	0.47	1.86	8	4
1:A:659:LEU:HG	1:A:670:PHE:CD1	0.47	2.45	16	1
1:A:587:ILE:HD13	1:A:688:PHE:HB2	0.47	1.87	5	1
1:A:629:ARG:O	1:A:629:ARG:HG3	0.47	2.10	4	2
1:A:603:ILE:CG1	1:A:611:CYS:HB3	0.46	2.40	16	6
1:A:700:THR:HG22	1:A:700:THR:O	0.46	2.09	8	1
1:A:670:PHE:CD1	1:A:716:VAL:HG22	0.46	2.45	6	1
1:A:666:GLN:CG	1:A:666:GLN:O	0.46	2.63	18	3
1:A:580:LEU:HD11	1:A:594:ILE:HD11	0.46	1.87	10	1
1:A:580:LEU:HG	1:A:694:VAL:HG23	0.46	1.88	4	2
1:A:587:ILE:CD1	1:A:688:PHE:CE1	0.46	2.98	14	3
1:A:583:LEU:N	1:A:583:LEU:HD13	0.46	2.25	4	1
1:A:603:ILE:HG13	1:A:611:CYS:HB2	0.46	1.88	5	1
1:A:626:PHE:N	1:A:648:TRP:O	0.46	2.46	8	14
1:A:603:ILE:HG12	1:A:611:CYS:CB	0.46	2.41	7	6
1:A:606:SER:O	1:A:608:ASP:N	0.46	2.48	8	4
1:A:618:LEU:HD21	1:A:680:ILE:HD11	0.46	1.86	17	1
1:A:587:ILE:HD11	1:A:690:ILE:HD11	0.46	1.86	15	1
1:A:629:ARG:C	1:A:629:ARG:CD	0.46	2.84	19	1
1:A:622:HIS:NE2	1:A:680:ILE:CG2	0.46	2.79	5	7
1:A:622:HIS:HD2	1:A:680:ILE:HD12	0.46	1.69	17	1
1:A:662:ASN:CB	1:A:670:PHE:CZ	0.46	2.98	19	1
1:A:690:ILE:CG2	1:A:692:PHE:CE1	0.46	2.98	17	2
1:A:595:GLN:O	1:A:598:VAL:N	0.46	2.49	14	9
1:A:649:TYR:CD2	1:A:664:MET:CE	0.46	2.99	5	6
1:A:618:LEU:CD1	1:A:622:HIS:CD2	0.46	2.99	3	3
1:A:626:PHE:CE1	1:A:627:LYS:O	0.46	2.69	10	20
1:A:622:HIS:CD2	1:A:680:ILE:HG12	0.46	2.46	9	1
1:A:583:LEU:H	1:A:583:LEU:HD22	0.46	1.71	4	1
1:A:583:LEU:N	1:A:583:LEU:HD22	0.46	2.26	4	1
1:A:577:PHE:CE1	1:A:578:LEU:CB	0.45	3.00	6	1
1:A:722:GLU:O	1:A:726:LEU:HD13	0.45	2.11	6	2
1:A:624:PHE:N	1:A:650:CYS:O	0.45	2.50	5	1
1:A:651:HIS:CG	1:A:657:SER:HG	0.45	2.29	12	2
1:A:694:VAL:O	1:A:694:VAL:HG12	0.45	2.11	20	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:583:LEU:CD2	1:A:583:LEU:H	0.45	2.24	20	1
1:A:649:TYR:CE1	1:A:678:ILE:CD1	0.45	2.99	16	1
1:A:583:LEU:HD22	1:A:583:LEU:N	0.45	2.26	19	1
1:A:649:TYR:CE2	1:A:678:ILE:CG2	0.45	2.98	1	4
1:A:680:ILE:HD11	1:A:692:PHE:CZ	0.45	2.46	3	1
1:A:659:LEU:HD11	1:A:672:LEU:HD22	0.45	1.87	17	3
1:A:615:ASP:HB3	1:A:618:LEU:CD1	0.45	2.37	15	3
1:A:681:ILE:CG2	1:A:690:ILE:HD12	0.45	2.42	15	1
1:A:580:LEU:O	1:A:592:LEU:O	0.45	2.35	6	1
1:A:601:PHE:N	1:A:625:ILE:O	0.45	2.46	11	12
1:A:681:ILE:HG22	1:A:690:ILE:CB	0.45	2.41	3	2
1:A:588:ILE:CG2	1:A:588:ILE:O	0.45	2.65	18	1
1:A:659:LEU:C	1:A:659:LEU:HD12	0.45	2.31	10	2
1:A:604:GLY:HA2	1:A:622:HIS:HB2	0.45	1.87	13	1
1:A:587:ILE:HD13	1:A:688:PHE:CZ	0.45	2.46	20	2
1:A:648:TRP:CZ3	1:A:671:LEU:CB	0.45	2.99	9	1
1:A:624:PHE:N	1:A:624:PHE:CD1	0.45	2.83	10	2
1:A:577:PHE:CD1	1:A:696:ILE:HG23	0.45	2.46	7	2
1:A:587:ILE:HD13	1:A:688:PHE:CD1	0.45	2.47	8	1
1:A:699:THR:O	1:A:699:THR:OG1	0.45	2.34	8	4
1:A:603:ILE:CG1	1:A:611:CYS:CB	0.45	2.95	5	9
1:A:588:ILE:HD12	1:A:613:ILE:CG2	0.45	2.42	8	1
1:A:615:ASP:HB3	1:A:618:LEU:HD22	0.45	1.89	14	3
1:A:618:LEU:HB3	1:A:622:HIS:CG	0.45	2.47	11	8
1:A:583:LEU:HD22	1:A:691:GLY:O	0.45	2.11	5	4
1:A:656:VAL:HG22	1:A:657:SER:N	0.45	2.27	11	4
1:A:659:LEU:CD2	1:A:672:LEU:CD2	0.45	2.95	19	1
1:A:601:PHE:CE1	1:A:610:ASN:OD1	0.45	2.69	2	11
1:A:670:PHE:CE2	1:A:716:VAL:HG22	0.45	2.47	5	1
1:A:659:LEU:HD13	1:A:670:PHE:CD2	0.45	2.47	6	1
1:A:588:ILE:HD13	1:A:613:ILE:HG23	0.45	1.89	11	1
1:A:615:ASP:HB3	1:A:618:LEU:HG	0.45	1.89	11	3
1:A:659:LEU:HB3	1:A:670:PHE:CE1	0.45	2.47	16	1
1:A:589:GLN:OE1	1:A:589:GLN:N	0.44	2.50	4	1
1:A:594:ILE:HG12	1:A:601:PHE:CG	0.44	2.47	5	9
1:A:692:PHE:CD1	1:A:692:PHE:N	0.44	2.85	1	5
1:A:583:LEU:CD2	1:A:583:LEU:N	0.44	2.74	15	2
1:A:658:TYR:CD1	1:A:658:TYR:N	0.44	2.85	17	1
1:A:630:HIS:CE1	1:A:646:ASP:OD2	0.44	2.71	5	4
1:A:655:ASN:O	1:A:656:VAL:HG12	0.44	2.12	14	2
1:A:608:ASP:OD1	1:A:609:CYS:N	0.44	2.51	2	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:678:ILE:O	1:A:691:GLY:HA2	0.44	2.12	16	2
1:A:665:ILE:HG13	1:A:668:THR:HG23	0.44	1.88	2	1
1:A:595:GLN:HB3	1:A:598:VAL:CG2	0.44	2.42	6	1
1:A:681:ILE:CG2	1:A:688:PHE:CE1	0.44	3.00	2	1
1:A:688:PHE:CD1	1:A:688:PHE:C	0.44	2.89	14	1
1:A:586:SER:OG	1:A:690:ILE:CG2	0.44	2.66	19	1
1:A:587:ILE:CD1	1:A:688:PHE:CE2	0.44	3.01	4	2
1:A:592:LEU:CD1	1:A:592:LEU:N	0.44	2.80	6	2
1:A:601:PHE:CD1	1:A:610:ASN:HB3	0.44	2.48	5	7
1:A:596:GLN:CB	1:A:700:THR:OG1	0.44	2.66	8	2
1:A:582:PRO:HG3	1:A:692:PHE:CE2	0.44	2.48	13	1
1:A:583:LEU:HD22	1:A:583:LEU:H	0.44	1.73	20	3
1:A:607:GLU:CB	1:A:612:LYS:HD2	0.44	2.43	14	1
1:A:678:ILE:O	1:A:678:ILE:CG1	0.44	2.66	9	2
1:A:613:ILE:CG2	1:A:618:LEU:HD22	0.44	2.43	13	1
1:A:602:PHE:HA	1:A:624:PHE:CB	0.44	2.43	19	6
1:A:587:ILE:HD13	1:A:688:PHE:CE2	0.44	2.47	19	2
1:A:659:LEU:CG	1:A:670:PHE:CD1	0.44	3.01	16	1
1:A:648:TRP:CH2	1:A:671:LEU:CG	0.44	3.00	9	1
1:A:655:ASN:C	1:A:656:VAL:CG1	0.43	2.86	16	5
1:A:671:LEU:O	1:A:672:LEU:HD23	0.43	2.13	10	2
1:A:615:ASP:OD2	1:A:688:PHE:CE1	0.43	2.71	11	3
1:A:621:VAL:O	1:A:621:VAL:HG12	0.43	2.13	11	2
1:A:624:PHE:CD1	1:A:624:PHE:N	0.43	2.85	11	1
1:A:582:PRO:CG	1:A:590:GLU:O	0.43	2.66	13	4
1:A:577:PHE:CE1	1:A:647:ILE:HG21	0.43	2.48	1	1
1:A:578:LEU:HD11	1:A:694:VAL:HG22	0.43	1.89	5	1
1:A:583:LEU:HB2	1:A:584:PRO:HD2	0.43	1.91	16	4
1:A:583:LEU:HD11	1:A:677:GLU:CD	0.43	2.34	8	2
1:A:656:VAL:CG2	1:A:657:SER:N	0.43	2.81	12	9
1:A:587:ILE:HG21	1:A:688:PHE:CE1	0.43	2.48	17	1
1:A:580:LEU:CG	1:A:694:VAL:HG23	0.43	2.43	9	2
1:A:644:LEU:N	1:A:644:LEU:HD12	0.43	2.29	18	1
1:A:607:GLU:O	1:A:608:ASP:C	0.43	2.57	1	4
1:A:656:VAL:HG23	1:A:664:MET:O	0.43	2.12	10	1
1:A:588:ILE:HG23	1:A:588:ILE:O	0.43	2.13	4	2
1:A:658:TYR:N	1:A:658:TYR:CD1	0.43	2.86	2	1
1:A:615:ASP:OD2	1:A:688:PHE:CE2	0.43	2.72	17	2
1:A:579:THR:O	1:A:695:GLU:N	0.43	2.42	6	2
1:A:690:ILE:CG2	1:A:691:GLY:N	0.43	2.82	13	4
1:A:651:HIS:ND1	1:A:657:SER:OG	0.43	2.52	12	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:649:TYR:CD2	1:A:664:MET:HE1	0.42	2.49	6	2
1:A:582:PRO:HB2	1:A:588:ILE:O	0.42	2.14	7	1
1:A:613:ILE:CG2	1:A:690:ILE:HD11	0.42	2.44	14	1
1:A:618:LEU:CD2	1:A:622:HIS:NE2	0.42	2.79	19	3
1:A:603:ILE:HD11	1:A:625:ILE:HD13	0.42	1.90	18	1
1:A:613:ILE:CG2	1:A:618:LEU:HD11	0.42	2.44	4	3
1:A:694:VAL:HG12	1:A:694:VAL:O	0.42	2.14	15	2
1:A:576:ARG:CG	1:A:593:GLU:HB3	0.42	2.45	14	1
1:A:662:ASN:HB2	1:A:670:PHE:CZ	0.42	2.49	19	1
1:A:613:ILE:HG13	1:A:692:PHE:CZ	0.42	2.49	9	5
1:A:629:ARG:HG3	1:A:629:ARG:O	0.42	2.14	16	1
1:A:618:LEU:HD23	1:A:681:ILE:CD1	0.42	2.45	4	1
1:A:580:LEU:CD1	1:A:692:PHE:CB	0.42	2.97	6	1
1:A:602:PHE:O	1:A:609:CYS:HB3	0.42	2.14	5	6
1:A:582:PRO:HD2	1:A:591:SER:HA	0.42	1.92	16	4
1:A:604:GLY:N	1:A:609:CYS:SG	0.42	2.93	1	1
1:A:680:ILE:HD13	1:A:692:PHE:CZ	0.42	2.47	9	1
1:A:578:LEU:O	1:A:594:ILE:N	0.42	2.53	6	4
1:A:659:LEU:HD13	1:A:670:PHE:HD2	0.42	1.75	6	1
1:A:589:GLN:CA	1:A:589:GLN:OE1	0.42	2.67	6	1
1:A:606:SER:HB2	1:A:620:ARG:HA	0.42	1.92	2	1
1:A:583:LEU:HD23	1:A:583:LEU:O	0.42	2.15	20	1
1:A:603:ILE:CB	1:A:623:CYS:O	0.42	2.68	11	7
1:A:615:ASP:OD1	1:A:688:PHE:CZ	0.42	2.72	16	2
1:A:681:ILE:HB	1:A:690:ILE:HG22	0.42	1.91	14	1
1:A:681:ILE:HG22	1:A:690:ILE:HD12	0.42	1.90	15	2
1:A:617:ARG:CB	1:A:681:ILE:CD1	0.42	2.98	4	3
1:A:680:ILE:CG2	1:A:690:ILE:CG2	0.42	2.98	2	1
1:A:659:LEU:CG	1:A:678:ILE:HG23	0.42	2.43	4	1
1:A:584:PRO:HA	1:A:589:GLN:HG3	0.41	1.93	12	1
1:A:602:PHE:O	1:A:610:ASN:N	0.41	2.53	8	1
1:A:601:PHE:O	1:A:624:PHE:HA	0.41	2.15	8	1
1:A:622:HIS:CD2	1:A:680:ILE:CG1	0.41	3.03	9	1
1:A:680:ILE:HG23	1:A:681:ILE:HG13	0.41	1.92	4	1
1:A:623:CYS:HA	1:A:652:THR:OG1	0.41	2.16	9	2
1:A:603:ILE:HA	1:A:609:CYS:HB3	0.41	1.92	7	9
1:A:598:VAL:HG11	1:A:610:ASN:ND2	0.41	2.31	16	1
1:A:579:THR:HG22	1:A:581:LYS:HG2	0.41	1.91	13	1
1:A:673:GLN:O	1:A:674:ASP:C	0.41	2.58	6	1
1:A:615:ASP:O	1:A:618:LEU:HB2	0.41	2.15	9	2
1:A:615:ASP:OD1	1:A:688:PHE:CE1	0.41	2.72	16	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:578:LEU:HD11	1:A:694:VAL:HG13	0.41	1.91	9	1
1:A:685:ASN:ND2	1:A:686:ASN:N	0.41	2.69	5	2
1:A:582:PRO:HB2	1:A:590:GLU:H	0.41	1.76	2	1
1:A:584:PRO:O	1:A:589:GLN:NE2	0.41	2.54	7	1
1:A:699:THR:OG1	1:A:699:THR:O	0.41	2.39	7	1
1:A:618:LEU:HD21	1:A:680:ILE:CD1	0.41	2.45	17	1
1:A:615:ASP:O	1:A:616:ASN:C	0.41	2.58	7	1
1:A:681:ILE:HB	1:A:690:ILE:HD12	0.41	1.92	1	1
1:A:601:PHE:O	1:A:625:ILE:N	0.41	2.52	5	1
1:A:658:TYR:O	1:A:679:LYS:N	0.41	2.53	7	1
1:A:689:VAL:CG1	1:A:689:VAL:O	0.41	2.69	7	1
1:A:589:GLN:OE1	1:A:589:GLN:CA	0.41	2.68	1	2
1:A:649:TYR:CD2	1:A:659:LEU:HD12	0.41	2.51	1	1
1:A:648:TRP:CZ3	1:A:671:LEU:HB2	0.41	2.51	9	1
1:A:592:LEU:N	1:A:592:LEU:CD2	0.41	2.82	13	1
1:A:585:ASP:O	1:A:689:VAL:CG1	0.41	2.69	11	1
1:A:586:SER:O	1:A:589:GLN:OE1	0.41	2.39	8	1
1:A:583:LEU:O	1:A:589:GLN:OE1	0.41	2.39	7	2
1:A:649:TYR:O	1:A:664:MET:CE	0.41	2.69	19	1
1:A:630:HIS:ND1	1:A:646:ASP:OD1	0.41	2.54	19	1
1:A:651:HIS:ND1	1:A:657:SER:HB2	0.41	2.31	16	1
1:A:649:TYR:O	1:A:670:PHE:N	0.41	2.45	13	1
1:A:648:TRP:HB3	1:A:669:LYS:CG	0.41	2.46	16	1
1:A:659:LEU:CD1	1:A:672:LEU:CD2	0.41	2.99	4	1
1:A:603:ILE:C	1:A:609:CYS:SG	0.40	3.00	15	2
1:A:630:HIS:CD2	1:A:630:HIS:C	0.40	2.93	13	1
1:A:577:PHE:CD1	1:A:578:LEU:N	0.40	2.89	6	1
1:A:698:ASP:OD1	1:A:698:ASP:N	0.40	2.54	5	1
1:A:649:TYR:C	1:A:649:TYR:CD1	0.40	2.94	12	1
1:A:582:PRO:HB3	1:A:692:PHE:CE1	0.40	2.51	7	2
1:A:577:PHE:CE1	1:A:578:LEU:HB2	0.40	2.50	6	1
1:A:615:ASP:OD2	1:A:688:PHE:CZ	0.40	2.73	6	1
1:A:627:LYS:CE	1:A:647:ILE:HG23	0.40	2.45	18	1
1:A:630:HIS:ND1	1:A:646:ASP:OD2	0.40	2.55	10	2
1:A:613:ILE:HD11	1:A:692:PHE:HE2	0.40	1.76	19	1
1:A:587:ILE:H	1:A:587:ILE:HD13	0.40	1.75	10	1
1:A:621:VAL:O	1:A:623:CYS:N	0.40	2.55	8	1
1:A:726:LEU:CD1	1:A:726:LEU:N	0.40	2.84	17	1
1:A:601:PHE:CE2	1:A:611:CYS:HB2	0.40	2.52	4	1
1:A:663:ARG:NH2	1:A:665:ILE:CG2	0.40	2.85	13	1
1:A:607:GLU:C	1:A:609:CYS:N	0.40	2.74	8	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:603:ILE:CG1	1:A:611:CYS:HB2	0.40	2.46	20	1
1:A:690:ILE:HG22	1:A:691:GLY:N	0.40	2.32	20	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	127/158 (80%)	111±1 (87±1%)	13±2 (10±1%)	4±1 (3±1%)	9	41
All	All	2540/3160 (80%)	2210 (87%)	250 (10%)	80 (3%)	9	41

All 10 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	656	VAL	20
1	A	660	ASN	14
1	A	666	GLN	11
1	A	616	ASN	9
1	A	622	HIS	7
1	A	582	PRO	7
1	A	700	THR	5
1	A	607	GLU	4
1	A	644	LEU	2
1	A	631	ALA	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	119/142 (84%)	82±2 (69±2%)	37±2 (31±2%)	2	16
All	All	2380/2840 (84%)	1644 (69%)	736 (31%)	2	16

All 85 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	583	LEU	20
1	A	652	THR	20
1	A	612	LYS	20
1	A	577	PHE	20
1	A	610	ASN	20
1	A	591	SER	20
1	A	592	LEU	19
1	A	698	ASP	19
1	A	671	LEU	19
1	A	620	ARG	19
1	A	596	GLN	19
1	A	680	ILE	18
1	A	606	SER	18
1	A	628	LYS	18
1	A	659	LEU	17
1	A	688	PHE	16
1	A	670	PHE	16
1	A	599	ASN	16
1	A	605	ARG	16
1	A	629	ARG	15
1	A	677	GLU	14
1	A	684	LYS	13
1	A	650	CYS	12
1	A	728	LYS	12
1	A	615	ASP	11
1	A	717	LEU	11
1	A	589	GLN	11
1	A	722	GLU	10
1	A	581	LYS	10
1	A	662	ASN	10
1	A	676	ASP	10
1	A	695	GLU	10
1	A	587	ILE	9
1	A	692	PHE	9
1	A	619	SER	9
1	A	683	ASP	9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	646	ASP	8
1	A	660	ASN	8
1	A	593	GLU	8
1	A	666	GLN	8
1	A	718	LYS	8
1	A	679	LYS	7
1	A	595	GLN	7
1	A	617	ARG	7
1	A	580	LEU	6
1	A	618	LEU	6
1	A	724	LYS	6
1	A	694	VAL	6
1	A	608	ASP	6
1	A	723	GLU	6
1	A	687	LYS	6
1	A	656	VAL	5
1	A	614	GLU	5
1	A	585	ASP	5
1	A	645	ASP	5
1	A	686	ASN	5
1	A	663	ARG	4
1	A	661	ASN	4
1	A	725	ASP	4
1	A	689	VAL	4
1	A	655	ASN	4
1	A	607	GLU	4
1	A	720	THR	3
1	A	693	LYS	3
1	A	657	SER	3
1	A	681	ILE	3
1	A	699	THR	3
1	A	678	ILE	3
1	A	644	LEU	3
1	A	627	LYS	3
1	A	611	CYS	3
1	A	674	ASP	3
1	A	664	MET	3
1	A	586	SER	2
1	A	623	CYS	2
1	A	685	ASN	2
1	A	690	ILE	2
1	A	715	VAL	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	576	ARG	1
1	A	602	PHE	1
1	A	624	PHE	1
1	A	669	LYS	1
1	A	672	LEU	1
1	A	649	TYR	1
1	A	630	HIS	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no carbohydrates 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