Full wwPDB NMR Structure Validation Report (i)

Feb 12, 2022 – 04:06 PM EST

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
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

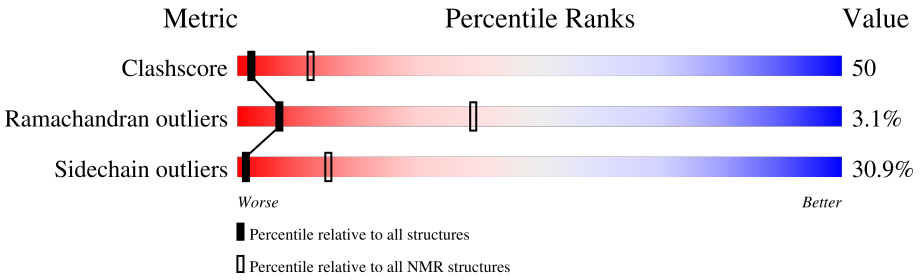
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

1 Overall quality at a glance (i)

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	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 <=5%

Mol	Chain	Length	Quality of chain
1	A	158	21% 49% 11% 20%

2 Ensemble composition and analysis (i)

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.

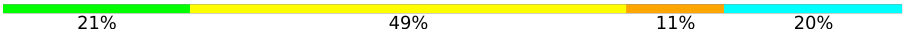
Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	158	2551	806	1277	222	239	7	0

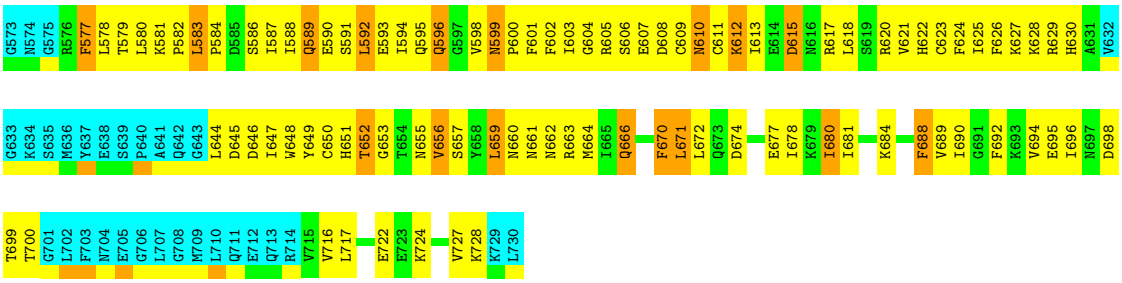
4 Residue-property plots (i)

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: PROTEIN KINASE SPK1

Chain A: 

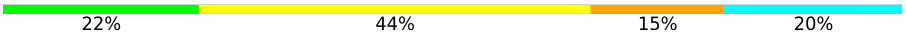


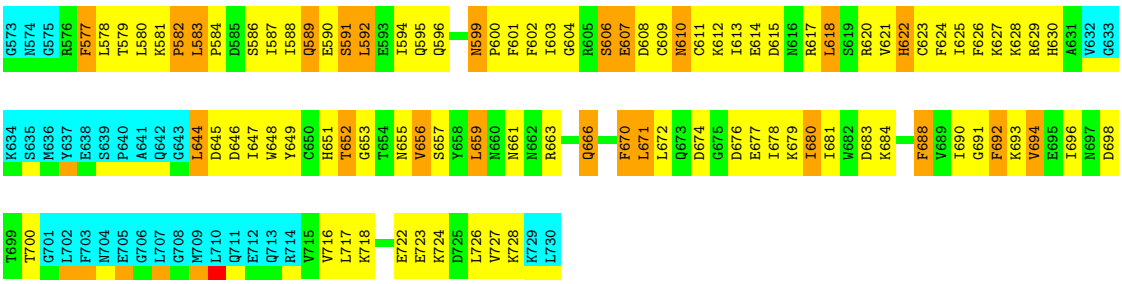
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: PROTEIN KINASE SPK1

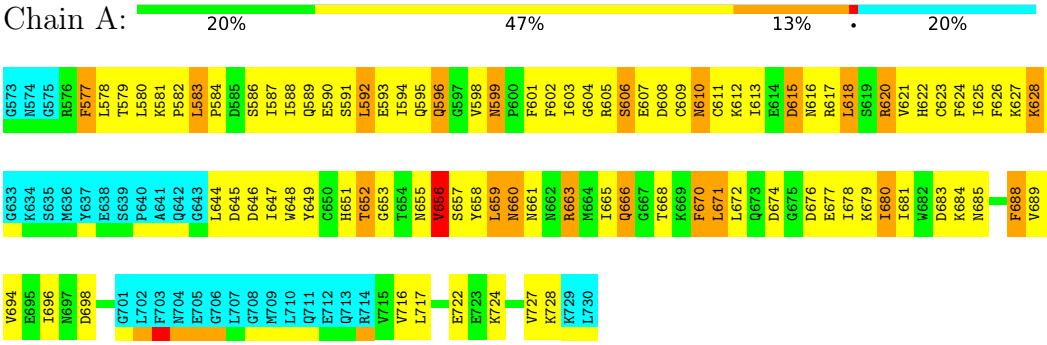
Chain A: 



4.2.2 Score per residue for model 2

• Molecule 1: PROTEIN KINASE SPK1

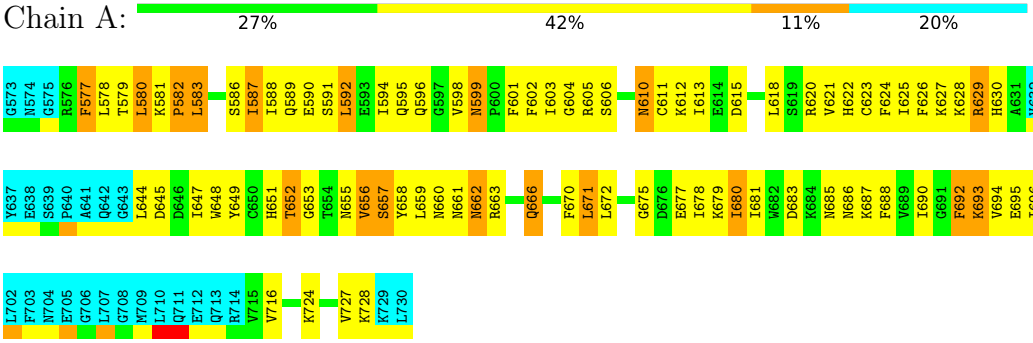
Chain A:



4.2.3 Score per residue for model 3

• Molecule 1: PROTEIN KINASE SPK1

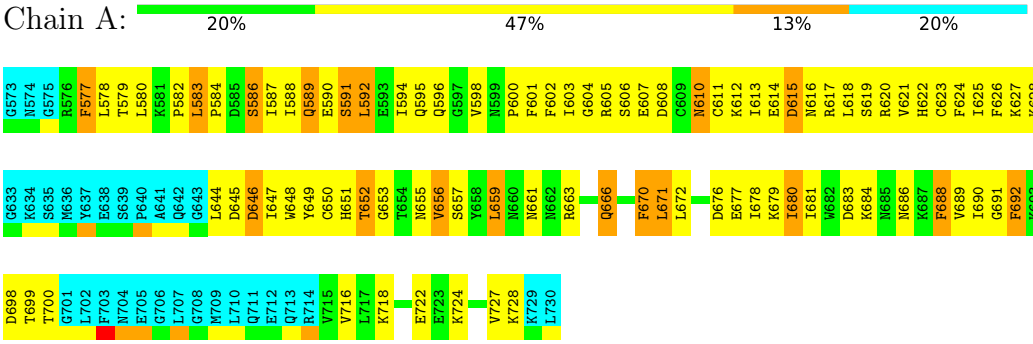
Chain A:



4.2.4 Score per residue for model 4

• Molecule 1: PROTEIN KINASE SPK1

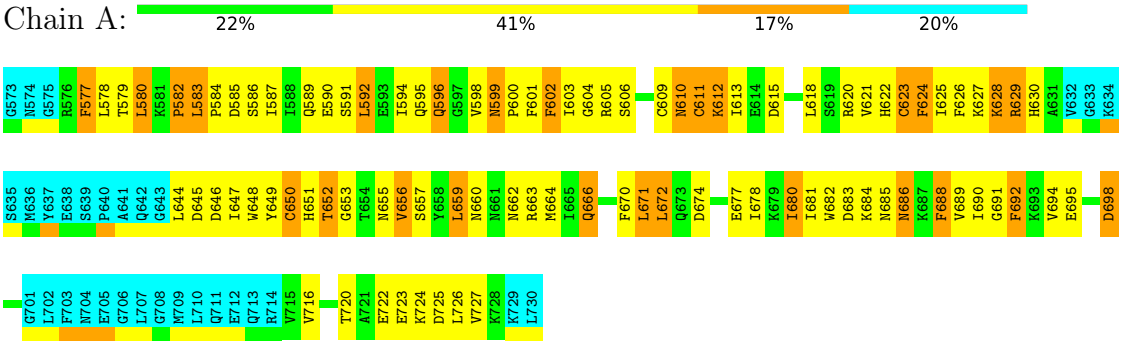
Chain A:



4.2.5 Score per residue for model 5

• Molecule 1: PROTEIN KINASE SPK1

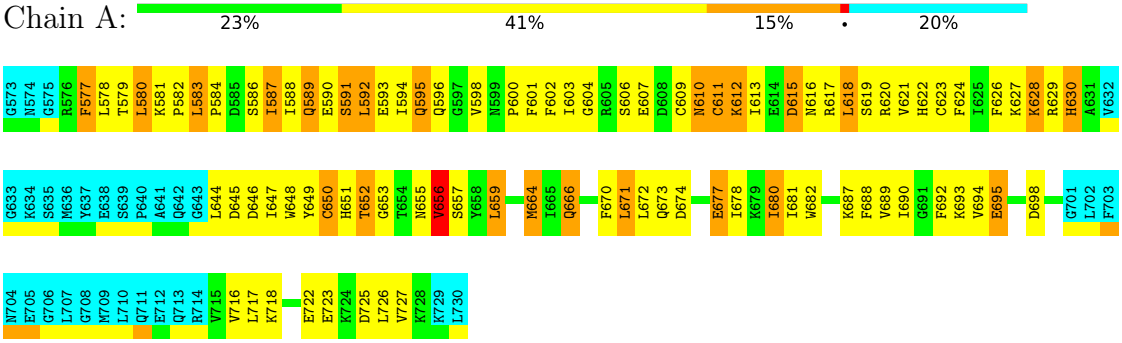
Chain A:



4.2.6 Score per residue for model 6

• Molecule 1: PROTEIN KINASE SPK1

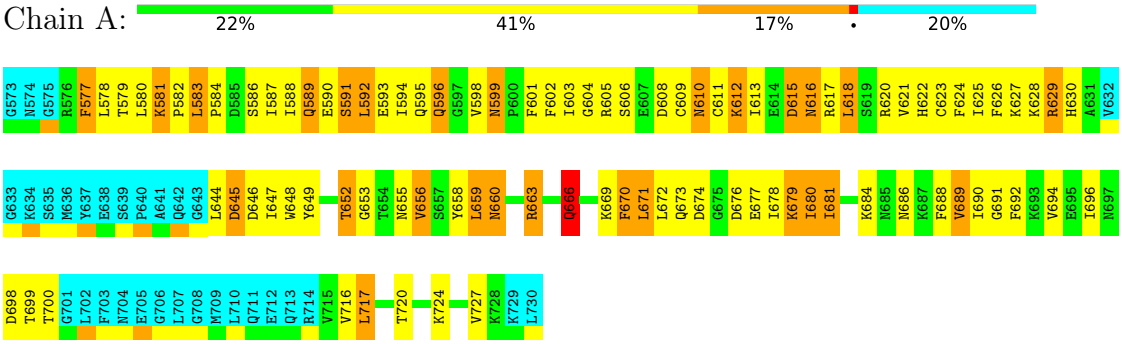
Chain A:



4.2.7 Score per residue for model 7

• Molecule 1: PROTEIN KINASE SPK1

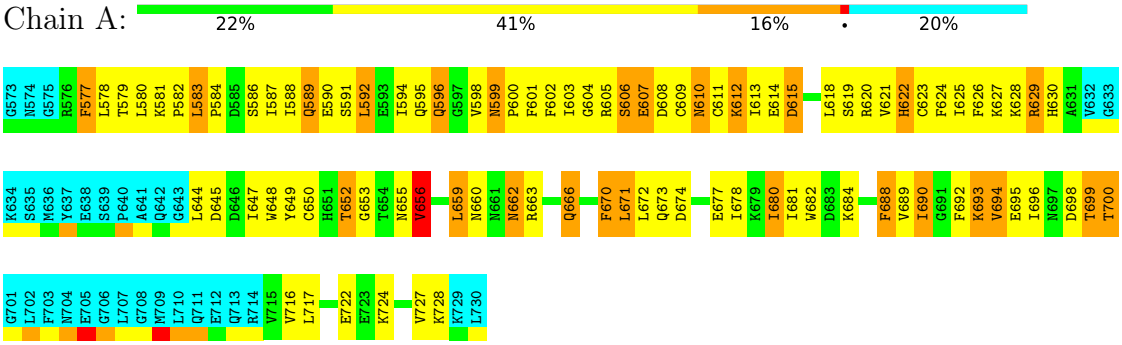
Chain A:



4.2.8 Score per residue for model 8

• Molecule 1: PROTEIN KINASE SPK1

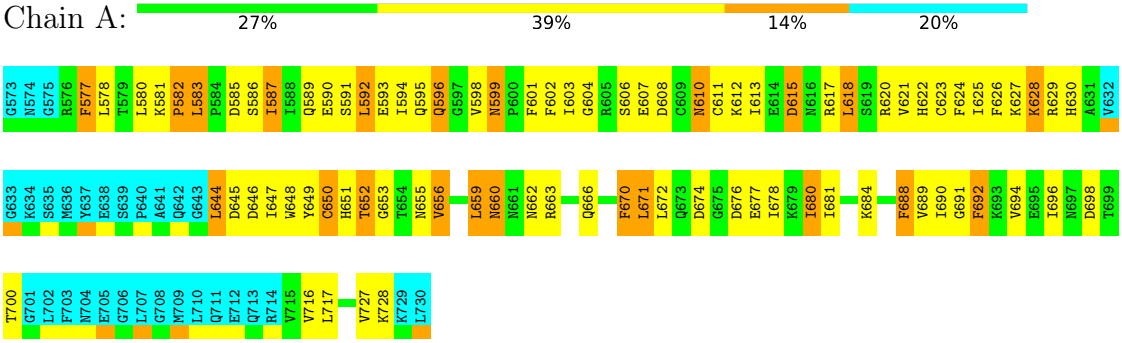
Chain A:



4.2.9 Score per residue for model 9

• Molecule 1: PROTEIN KINASE SPK1

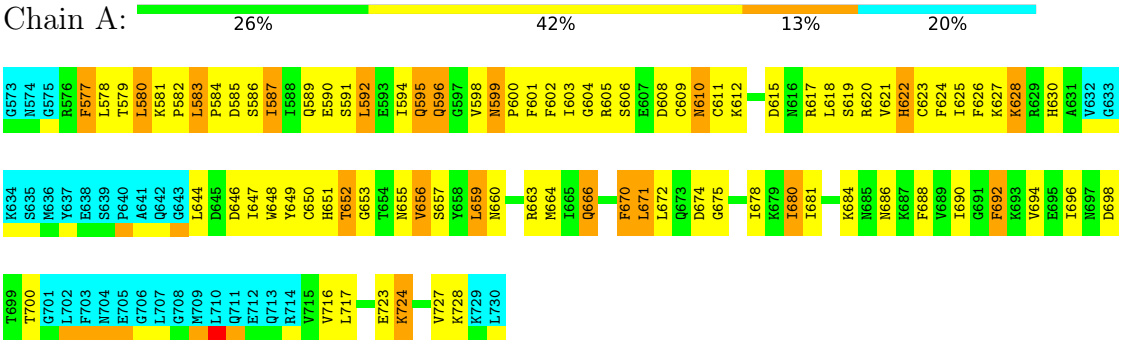
Chain A:



4.2.10 Score per residue for model 10

• Molecule 1: PROTEIN KINASE SPK1

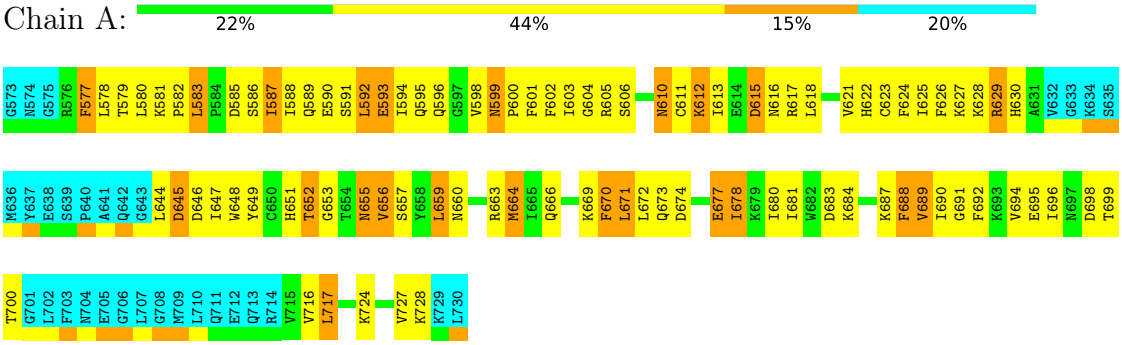
Chain A:



4.2.11 Score per residue for model 11

• Molecule 1: PROTEIN KINASE SPK1

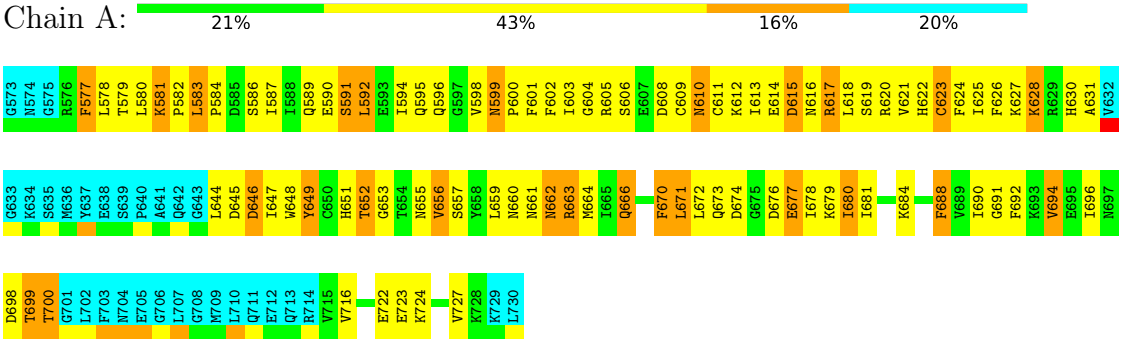
Chain A:



4.2.12 Score per residue for model 12

• Molecule 1: PROTEIN KINASE SPK1

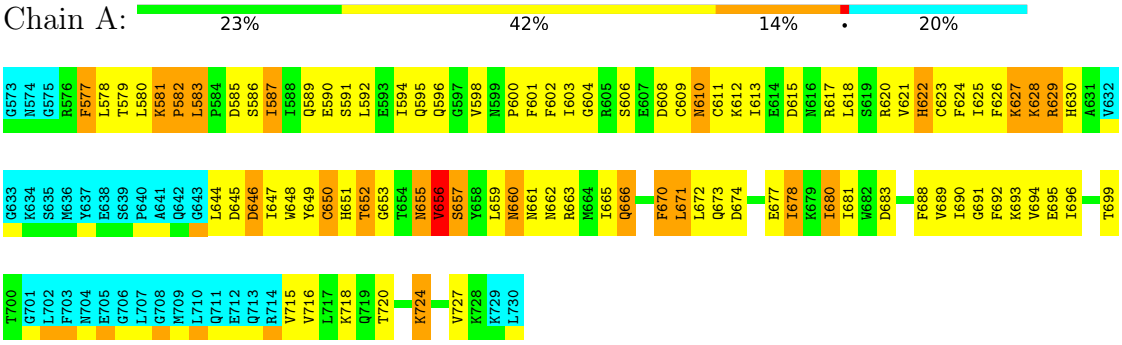
Chain A:



4.2.13 Score per residue for model 13

• Molecule 1: PROTEIN KINASE SPK1

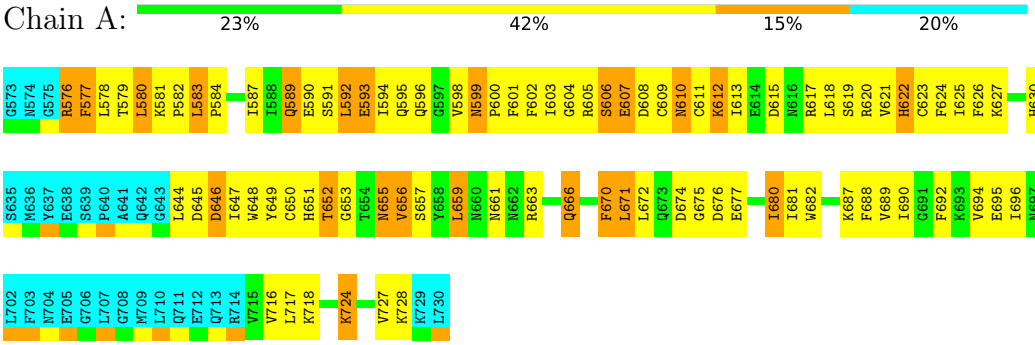
Chain A:



4.2.14 Score per residue for model 14

• Molecule 1: PROTEIN KINASE SPK1

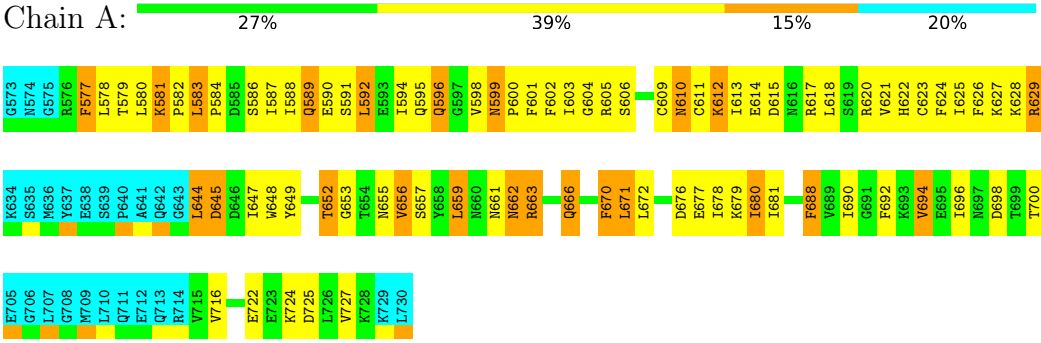
Chain A:



4.2.15 Score per residue for model 15

• Molecule 1: PROTEIN KINASE SPK1

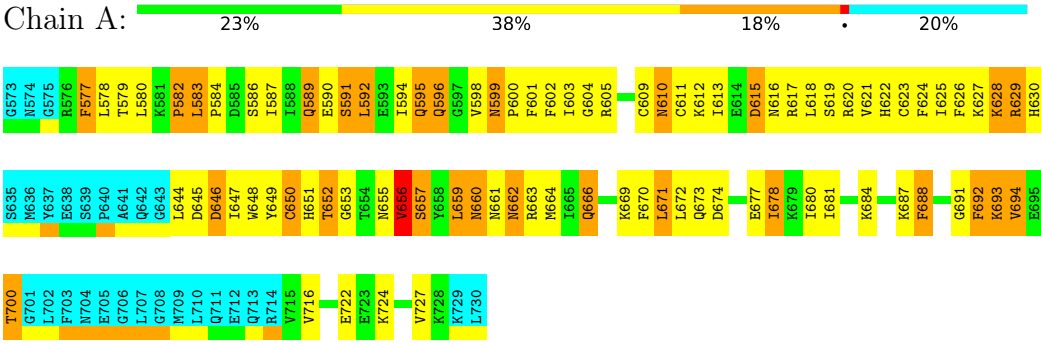
Chain A:



4.2.16 Score per residue for model 16

• Molecule 1: PROTEIN KINASE SPK1

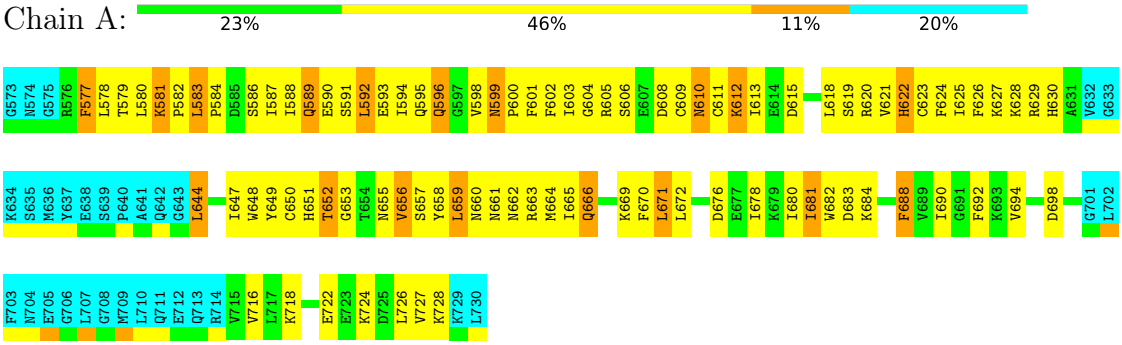
Chain A:



4.2.17 Score per residue for model 17

• Molecule 1: PROTEIN KINASE SPK1

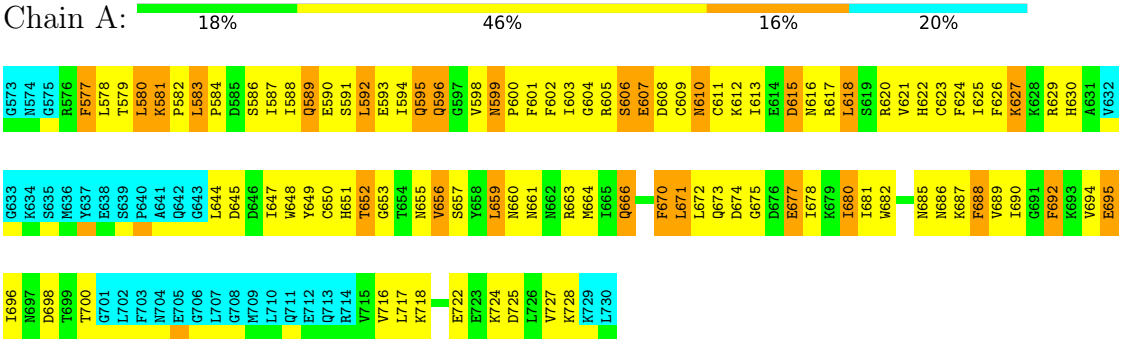
Chain A:



4.2.18 Score per residue for model 18

• Molecule 1: PROTEIN KINASE SPK1

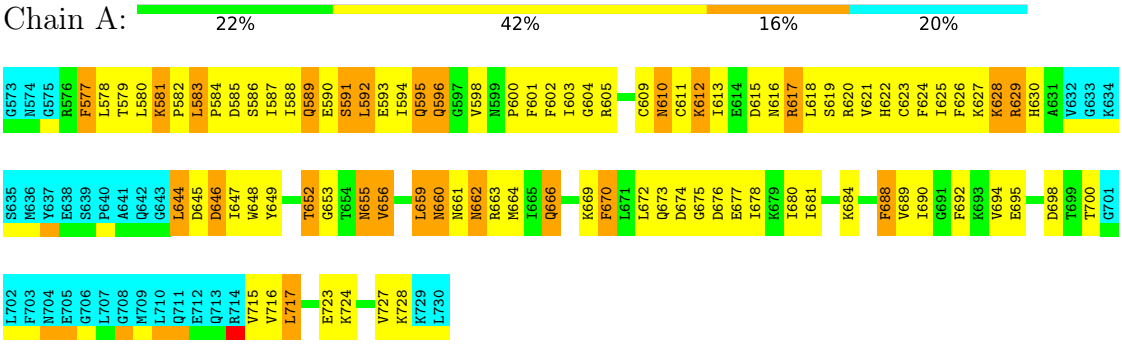
Chain A:



4.2.19 Score per residue for model 19

• Molecule 1: PROTEIN KINASE SPK1

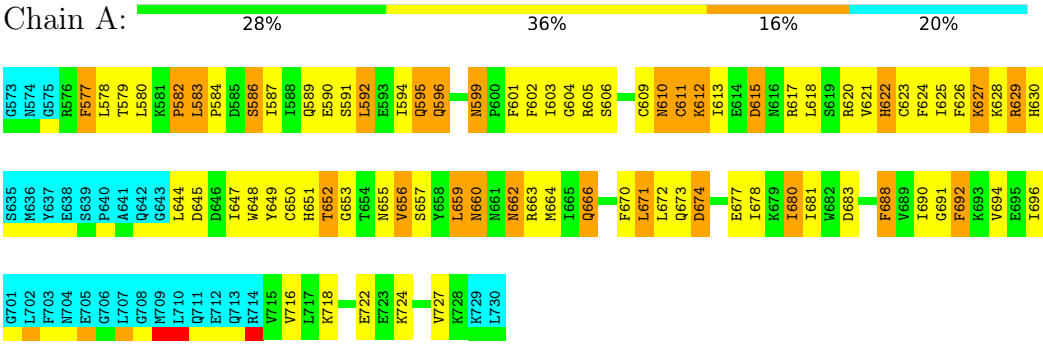
Chain A:



4.2.20 Score per residue for model 20 (medoid)

• Molecule 1: PROTEIN KINASE SPK1

Chain A:



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.

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

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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:580:LEU:HD11	1:A:625:ILE:HD12	0.76	1.54	1	5
1:A:672:LEU:HD13	1:A:694:VAL:HG21	0.76	1.57	13	8
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

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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	3
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: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:592:LEU:HD22	1:A:611:CYS:SG	0.68	2.29	16	9
1:A:615:ASP:OD2	1:A:681:ILE:HG21	0.68	1.89	11	1
1:A:580:LEU:HB3	1:A:592:LEU:HD12	0.68	1.66	4	9
1:A:580:LEU:HD11	1:A:625:ILE:CD1	0.67	2.20	1	15
1:A:586:SER:O	1:A:589:GLN:NE2	0.67	2.27	8	18
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:648:TRP:CH2	1:A:671:LEU:HD12	0.66	2.24	9	1
1:A:596:GLN:CB	1:A:700:THR:HG21	0.66	2.20	18	1
1:A:583:LEU:HD23	1:A:583:LEU:N	0.66	2.05	17	7
1:A:586:SER:HB2	1:A:690:ILE:HD13	0.66	1.67	2	2
1:A:600:PRO:HG3	1:A:726:LEU:HD13	0.66	1.66	5	1
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:580:LEU:HD12	1:A:594:ILE:HD11	0.64	1.67	18	3
1:A:621:VAL:HG11	1:A:727:VAL:HG21	0.64	1.69	9	9
1:A:659:LEU:HD13	1:A:678:ILE:CG1	0.64	2.22	13	2
1:A:578:LEU:HD13	1:A:696:ILE:HG12	0.64	1.69	9	1
1:A:623:CYS:SG	1:A:680:ILE:HD13	0.64	2.33	16	3
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:HD13	1:A:592:LEU:N	0.63	2.08	7	4
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:577:PHE:O	1:A:696:ILE:HG23	0.63	1.94	8	4
1:A:662:ASN:OD1	1:A:716:VAL:HG23	0.63	1.93	20	4
1:A:659:LEU:HD13	1:A:678:ILE:HG12	0.62	1.69	3	4
1:A:602:PHE:CD1	1:A:602:PHE:N	0.62	2.64	5	1
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:CD2	1:A:644:LEU:N	0.61	2.63	17	3
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:659:LEU:HG	1:A:678:ILE:HG22	0.60	1.72	7	2
1:A:579:THR:HG23	1:A:593:GLU:CG	0.60	2.26	11	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:HD22	1:A:592:LEU:N	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:648:TRP:CH2	1:A:671:LEU:CD1	0.59	2.85	9	1
1:A:681:ILE:HG22	1:A:690:ILE:CG1	0.59	2.27	20	6
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
1:A:596:GLN:HB2	1:A:700:THR:HG21	0.59	1.74	18	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:580:LEU:HD22	1:A:692:PHE:HB2	0.58	1.75	9	3
1:A:603:ILE:O	1:A:623:CYS:N	0.58	2.36	5	1
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:602:PHE:HA	1:A:624:PHE:HB3	0.57	1.76	19	19
1:A:603:ILE:N	1:A:623:CYS:O	0.57	2.38	9	19
1:A:681:ILE:HB	1:A:690:ILE:HD13	0.57	1.74	4	1
1:A:586:SER:OG	1:A:690:ILE:HG23	0.57	2.00	19	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:587:ILE:HD11	1:A:615:ASP:OD1	0.56	2.00	4	3
1:A:588:ILE:CG2	1:A:690:ILE:HD11	0.56	2.30	18	1
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:HD23	1:A:578:LEU:C	0.55	2.22	8	14
1:A:583:LEU:H	1:A:583:LEU:HD13	0.55	1.60	1	8
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:618:LEU:HD23	1:A:681:ILE:HD11	0.55	1.77	4	1
1:A:592:LEU:HD22	1:A:612:LYS:H	0.55	1.59	5	3
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
1:A:587:ILE:HD11	1:A:615:ASP:CG	0.54	2.22	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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: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:681:ILE:HG22	1:A:690:ILE:HB	0.54	1.79	2	3
1:A:602:PHE:CD1	1:A:624:PHE:CE1	0.54	2.96	5	1
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:659:LEU:CG	1:A:678:ILE:HG22	0.53	2.33	9	5
1:A:618:LEU:HG	1:A:622:HIS:CG	0.53	2.38	13	9
1:A:613:ILE:CD1	1:A:692:PHE:CZ	0.53	2.91	13	6
1:A:580:LEU:HD11	1:A:692:PHE:HB2	0.53	1.80	6	1
1:A:584:PRO:HA	1:A:589:GLN:CD	0.53	2.24	19	8
1:A:592:LEU:HD21	1:A:613:ILE:CD1	0.53	2.27	6	1
1:A:613:ILE:HD11	1:A:692:PHE:CE1	0.53	2.38	13	1
1:A:621:VAL:HG13	1:A:621:VAL:O	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:618:LEU:CD1	1:A:622:HIS:NE2	0.52	2.72	1	5
1:A:626:PHE:O	1:A:648:TRP:N	0.52	2.40	19	15
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:613:ILE:CD1	1:A:692:PHE:CE1	0.52	2.93	2	2
1:A:670:PHE:CE1	1:A:716:VAL:HG22	0.52	2.40	6	1
1:A:680:ILE:CG2	1:A:690:ILE:HG21	0.52	2.34	12	3
1:A:581:LYS:O	1:A:583:LEU:HD13	0.52	2.05	11	2
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:724:LYS:O	1:A:727:VAL:HG12	0.51	2.06	5	15
1:A:583:LEU:HD21	1:A:693:LYS:N	0.51	2.21	6	2
1:A:587:ILE:HG12	1:A:690:ILE:HD12	0.51	1.82	19	1
1:A:680:ILE:HG22	1:A:690:ILE:HG21	0.51	1.83	12	1
1:A:692:PHE:CD1	1:A:692:PHE:N	0.51	2.79	3	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:618:LEU:HD12	1:A:622:HIS:NE2	0.51	2.21	5	4
1:A:595:GLN:HB3	1:A:598:VAL:HG23	0.51	1.83	6	1
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:583:LEU:HD11	1:A:677:GLU:CG	0.50	2.36	18	2
1:A:669:LYS:HE2	1:A:717:LEU:HD11	0.50	1.83	11	1
1:A:577:PHE:CZ	1:A:578:LEU:HB2	0.50	2.41	16	12
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:602:PHE:CG	1:A:624:PHE:CE1	0.50	2.99	5	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: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:592:LEU:CD2	1:A:613:ILE:HD11	0.50	2.29	6	1
1:A:621:VAL:HG12	1:A:621:VAL:O	0.50	2.06	3	10
1:A:580:LEU:HD11	1:A:692:PHE:CB	0.50	2.37	6	1
1:A:627:LYS:NZ	1:A:700:THR:HG21	0.50	2.21	1	1
1:A:700:THR:HG23	1:A:700:THR:O	0.50	2.07	12	3
1:A:680:ILE:HD12	1:A:692:PHE:CZ	0.50	2.41	20	2
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:659:LEU:HB2	1:A:678:ILE:HG23	0.49	1.84	13	1
1:A:663:ARG:C	1:A:716:VAL:HG21	0.49	2.28	16	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:655:ASN:C	1:A:656:VAL:HG13	0.49	2.27	3	3
1:A:588:ILE:O	1:A:588:ILE:HG23	0.49	2.07	15	3
1:A:604:GLY:HA2	1:A:622:HIS:HB3	0.49	1.83	5	11
1:A:615:ASP:O	1:A:617:ARG:N	0.49	2.45	7	9
1:A:644:LEU:N	1:A:644:LEU:HD23	0.49	2.22	19	1
1:A:618:LEU:HD12	1:A:622:HIS:CE1	0.49	2.42	9	2
1:A:688:PHE:CG	1:A:688:PHE:O	0.49	2.66	5	2
1:A:646:ASP:CG	1:A:671:LEU:HD21	0.49	2.28	9	1
1:A:587:ILE:HD13	1:A:587:ILE:N	0.49	2.23	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:615:ASP:OD2	1:A:681:ILE:HD12	0.49	2.07	19	1
1:A:580:LEU:HD12	1:A:594:ILE:CD1	0.49	2.38	14	3
1:A:692:PHE:N	1:A:692:PHE:CD1	0.49	2.81	9	4
1:A:651:HIS:ND1	1:A:657:SER:CB	0.48	2.77	13	8
1:A:682:TRP:CD1	1:A:689:VAL:CG1	0.48	2.96	18	2
1:A:587:ILE:HG12	1:A:690:ILE:HD11	0.48	1.84	2	2
1:A:578:LEU:C	1:A:578:LEU:HD23	0.48	2.29	20	4
1:A:622:HIS:CD2	1:A:680:ILE:CG2	0.48	2.96	13	4
1:A:577:PHE:HB3	1:A:596:GLN:HB3	0.48	1.85	2	5
1:A:666:GLN:O	1:A:666:GLN:CG	0.48	2.62	10	7
1:A:613:ILE:CD1	1:A:692:PHE:CE2	0.48	2.95	11	1
1:A:618:LEU:HD11	1:A:680:ILE:HG23	0.48	1.82	14	2
1:A:577:PHE:HB3	1:A:596:GLN:HG3	0.48	1.84	1	1
1:A:675:GLY:N	1:A:694:VAL:O	0.48	2.46	3	5
1:A:662:ASN:CB	1:A:670:PHE:CE2	0.48	2.97	5	1
1:A:617:ARG:CB	1:A:681:ILE:HD13	0.48	2.38	7	1
1:A:595:GLN:CB	1:A:598:VAL:HG23	0.48	2.38	16	1
1:A:691:GLY:C	1:A:692:PHE:CD1	0.48	2.87	20	1
1:A:587:ILE:CG1	1:A:690:ILE:HD11	0.48	2.39	2	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:601:PHE:CE1	1:A:610:ASN:ND2	0.48	2.81	9	5
1:A:599:ASN:O	1:A:599:ASN:OD1	0.47	2.32	2	16
1:A:629:ARG:HA	1:A:644:LEU:O	0.47	2.09	5	11
1:A:648:TRP:CE3	1:A:671:LEU:HG	0.47	2.44	9	1
1:A:577:PHE:CB	1:A:596:GLN:HG3	0.47	2.39	1	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:602:PHE:HB2	1:A:609:CYS:HA	0.47	1.86	19	2
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:587:ILE:CD1	1:A:688:PHE:CZ	0.47	2.97	10	3
1:A:583:LEU:HD11	1:A:677:GLU:OE2	0.47	2.09	12	1
1:A:587:ILE:HD12	1:A:688:PHE:CZ	0.47	2.45	4	1
1:A:681:ILE:CG2	1:A:690:ILE:CG1	0.47	2.93	13	4
1:A:582:PRO:HB3	1:A:692:PHE:CZ	0.47	2.44	13	1
1:A:583:LEU:CD2	1:A:583:LEU:N	0.47	2.78	20	1
1:A:578:LEU:CD1	1:A:647:ILE:CD1	0.47	2.92	11	16
1:A:609:CYS:SG	1:A:611:CYS:O	0.47	2.72	1	3
1:A:656:VAL:CG2	1:A:658:TYR:CZ	0.47	2.98	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:592:LEU:HD21	1:A:612:LYS:O	0.47	2.10	5	1
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:629:ARG:O	1:A:629:ARG:HG3	0.47	2.10	4	3
1:A:587:ILE:HD13	1:A:688:PHE:HB2	0.47	1.87	5	1
1:A:603:ILE:CG1	1:A:611:CYS:HB3	0.46	2.40	16	6
1:A:700:THR:O	1:A:700:THR:HG22	0.46	2.09	8	1
1:A:670:PHE:CD1	1:A:716:VAL:HG22	0.46	2.45	6	1
1:A:580:LEU:HG	1:A:694:VAL:HG23	0.46	1.88	4	2
1:A:580:LEU:HD11	1:A:594:ILE:HD11	0.46	1.87	10	1
1:A:583:LEU:HD13	1:A:583:LEU:N	0.46	2.25	4	1
1:A:587:ILE:CD1	1:A:688:PHE:CE1	0.46	2.98	14	3
1:A:626:PHE:N	1:A:648:TRP:O	0.46	2.46	8	14
1:A:603:ILE:HG13	1:A:611:CYS:HB2	0.46	1.88	5	1
1:A:606:SER:O	1:A:608:ASP:N	0.46	2.48	8	4
1:A:603:ILE:HG12	1:A:611:CYS:CB	0.46	2.41	7	6
1:A:587:ILE:HD11	1:A:690:ILE:HD11	0.46	1.86	15	1
1:A:618:LEU:HD21	1:A:680:ILE:HD11	0.46	1.86	17	1
1:A:629:ARG:CD	1:A:629:ARG:C	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:595:GLN:O	1:A:598:VAL:N	0.46	2.49	14	9
1:A:690:ILE:CG2	1:A:692:PHE:CE1	0.46	2.98	17	2
1:A:618:LEU:CD1	1:A:622:HIS:CD2	0.46	2.99	3	3
1:A:649:TYR:CD2	1:A:664:MET:CE	0.46	2.99	5	6
1:A:626:PHE:CE1	1:A:627:LYS:O	0.46	2.69	10	20
1:A:583:LEU:H	1:A:583:LEU:HD22	0.46	1.71	4	4
1:A:583:LEU:N	1:A:583:LEU:HD22	0.46	2.26	4	1
1:A:622:HIS:CD2	1:A:680:ILE:HG12	0.46	2.46	9	1
1:A:694:VAL:O	1:A:694:VAL:HG12	0.45	2.11	20	4
1:A:722:GLU:O	1:A:726:LEU:HD13	0.45	2.11	6	2
1:A:651:HIS:CG	1:A:657:SER:HG	0.45	2.29	12	2
1:A:624:PHE:N	1:A:650:CYS:O	0.45	2.50	5	1
1:A:577:PHE:CE1	1:A:578:LEU:CB	0.45	3.00	6	1
1:A:649:TYR:CE1	1:A:678:ILE:CD1	0.45	2.99	16	1
1:A:583:LEU:CD2	1:A:583:LEU:H	0.45	2.24	20	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:583:LEU:N	1:A:583:LEU:CD2	0.45	2.73	6	6
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: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:580:LEU:O	1:A:592:LEU:O	0.45	2.35	6	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:588:ILE:CG2	1:A:588:ILE:O	0.45	2.65	18	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	3
1:A:577:PHE:CD1	1:A:696:ILE:HG23	0.45	2.46	7	2
1:A:699:THR:O	1:A:699:THR:OG1	0.45	2.34	8	5
1:A:587:ILE:HD13	1:A:688:PHE:CD1	0.45	2.47	8	1
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: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:618:LEU:HB3	1:A:622:HIS:CG	0.45	2.47	11	8
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:615:ASP:HB3	1:A:618:LEU:HG	0.45	1.89	11	3
1:A:588:ILE:HD13	1:A:613:ILE:HG23	0.45	1.89	11	1
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:658:TYR:N	1:A:658:TYR:CD1	0.44	2.85	17	1
1:A:630:HIS:CE1	1:A:646:ASP:OD2	0.44	2.71	5	4
1:A:678:ILE:O	1:A:691:GLY:HA2	0.44	2.12	16	2
1:A:608:ASP:OD1	1:A:609:CYS:N	0.44	2.51	2	2
1:A:655:ASN:O	1:A:656:VAL:HG12	0.44	2.12	14	2
1:A:665:ILE:HG13	1:A:668:THR:HG23	0.44	1.88	2	1
1:A:681:ILE:CG2	1:A:688:PHE:CE1	0.44	3.00	2	1
1:A:587:ILE:CD1	1:A:688:PHE:CE2	0.44	3.01	4	2
1:A:595:GLN:HB3	1:A:598:VAL:CG2	0.44	2.42	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:601:PHE:CD1	1:A:610:ASN:HB3	0.44	2.48	5	7
1:A:592:LEU:N	1:A:592:LEU:CD1	0.44	2.80	6	2
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:678:ILE:CG1	1:A:678:ILE:O	0.44	2.66	9	1
1:A:613:ILE:CG2	1:A:618:LEU:HD22	0.44	2.43	13	1
1:A:607:GLU:CB	1:A:612:LYS:HD2	0.44	2.43	14	1
1:A:602:PHE:HA	1:A:624:PHE:CB	0.44	2.43	19	6
1:A:648:TRP:CH2	1:A:671:LEU:CG	0.44	3.00	9	1
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: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:577:PHE:CE1	1:A:647:ILE:HG21	0.43	2.48	1	1
1:A:582:PRO:CG	1:A:590:GLU:O	0.43	2.66	13	4
1:A:583:LEU:HB2	1:A:584:PRO:HD2	0.43	1.91	16	4
1:A:578:LEU:HD11	1:A:694:VAL:HG22	0.43	1.89	5	1
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:580:LEU:CG	1:A:694:VAL:HG23	0.43	2.43	9	2
1:A:583:LEU:HD13	1:A:583:LEU:H	0.43	1.73	11	1
1:A:587:ILE:HG21	1:A:688:PHE:CE1	0.43	2.48	17	1
1:A:607:GLU:O	1:A:608:ASP:C	0.43	2.57	1	4
1:A:588:ILE:HG23	1:A:588:ILE:O	0.43	2.13	4	2
1:A:656:VAL:HG23	1:A:664:MET:O	0.43	2.12	10	1
1:A:644:LEU:HD12	1:A:644:LEU:N	0.43	2.29	18	1
1:A:658:TYR:CD1	1:A:658:TYR:N	0.43	2.86	2	1
1:A:651:HIS:ND1	1:A:657:SER:OG	0.43	2.52	12	3
1:A:579:THR:O	1:A:695:GLU:N	0.43	2.42	6	2
1:A:615:ASP:OD2	1:A:688:PHE:CE2	0.43	2.72	17	2
1:A:690:ILE:CG2	1:A:691:GLY:N	0.43	2.82	13	4
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:576:ARG:CG	1:A:593:GLU:HB3	0.42	2.45	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:618:LEU:HD23	1:A:681:ILE:CD1	0.42	2.45	4	1
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:602:PHE:O	1:A:609:CYS:HB3	0.42	2.14	5	6
1:A:580:LEU:CD1	1:A:692:PHE:CB	0.42	2.97	6	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:OE1	1:A:589:GLN:CA	0.42	2.67	6	2
1:A:606:SER:HB2	1:A:620:ARG:HA	0.42	1.92	2	1
1:A:583:LEU:O	1:A:583:LEU:HD23	0.42	2.15	20	1
1:A:603:ILE:CB	1:A:623:CYS:O	0.42	2.68	11	7
1:A:617:ARG:CB	1:A:681:ILE:CD1	0.42	2.98	4	3
1:A:681:ILE:HG22	1:A:690:ILE:HD12	0.42	1.90	15	2
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: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:680:ILE:HG23	1:A:681:ILE:HG13	0.41	1.92	4	1
1:A:601:PHE:O	1:A:624:PHE:HA	0.41	2.15	8	1
1:A:602:PHE:O	1:A:610:ASN:N	0.41	2.53	8	1
1:A:622:HIS:CD2	1:A:680:ILE:CG1	0.41	3.03	9	1
1:A:623:CYS:HA	1:A:652:THR:OG1	0.41	2.16	9	2
1:A:688:PHE:O	1:A:688:PHE:CG	0.41	2.74	2	2
1:A:603:ILE:HA	1:A:609:CYS:HB3	0.41	1.92	7	9
1:A:579:THR:HG22	1:A:581:LYS:HG2	0.41	1.91	13	1
1:A:598:VAL:HG11	1:A:610:ASN:ND2	0.41	2.31	16	1
1:A:615:ASP:O	1:A:618:LEU:HB2	0.41	2.15	9	2
1:A:673:GLN:O	1:A:674:ASP:C	0.41	2.58	6	1
1:A:678:ILE:O	1:A:678:ILE:CG1	0.41	2.68	7	1
1:A:578:LEU:HD11	1:A:694:VAL:HG13	0.41	1.91	9	1
1:A:615:ASP:OD1	1:A:688:PHE:CE1	0.41	2.72	16	1
1:A:582:PRO:HB2	1:A:590:GLU:H	0.41	1.76	2	1
1:A:685:ASN:ND2	1:A:686:ASN:N	0.41	2.69	5	2
1:A:584:PRO:O	1:A:589:GLN:NE2	0.41	2.54	7	1
1:A:681:ILE:HB	1:A:690:ILE:HD12	0.41	1.92	1	1
1:A:615:ASP:O	1:A:616:ASN:C	0.41	2.58	7	1
1:A:618:LEU:HD21	1:A:680:ILE:CD1	0.41	2.45	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:649:TYR:CD2	1:A:659:LEU:HD12	0.41	2.51	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:O	1:A:689:VAL:CG1	0.41	2.69	7	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:583:LEU:O	1:A:589:GLN:OE1	0.41	2.39	7	2
1:A:621:VAL:O	1:A:621:VAL:HG12	0.41	2.16	7	2
1:A:586:SER:O	1:A:589:GLN:OE1	0.41	2.39	8	1
1:A:585:ASP:O	1:A:689:VAL:CG1	0.41	2.69	11	1
1:A:649:TYR:O	1:A:670:PHE:N	0.41	2.45	13	1
1:A:651:HIS:ND1	1:A:657:SER:HB2	0.41	2.31	16	1
1:A:630:HIS:ND1	1:A:646:ASP:OD1	0.41	2.54	19	1
1:A:649:TYR:O	1:A:664:MET:CE	0.41	2.69	19	1
1:A:659:LEU:CD1	1:A:672:LEU:CD2	0.41	2.99	4	1
1:A:648:TRP:HB3	1:A:669:LYS:CG	0.41	2.46	16	1
1:A:630:HIS:CD2	1:A:630:HIS:C	0.40	2.93	13	1
1:A:603:ILE:C	1:A:609:CYS:SG	0.40	3.00	15	2
1:A:582:PRO:HB3	1:A:692:PHE:CE1	0.40	2.51	7	2
1:A:698:ASP:OD1	1:A:698:ASP:N	0.40	2.54	5	1
1:A:577:PHE:CD1	1:A:578:LEU:N	0.40	2.89	6	1
1:A:649:TYR:CD1	1:A:649:TYR:C	0.40	2.94	12	1
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:700:THR:O	1:A:700:THR:HG23	0.40	2.16	7	1
1:A:630:HIS:ND1	1:A:646:ASP:OD2	0.40	2.55	10	2
1:A:627:LYS:CE	1:A:647:ILE:HG23	0.40	2.45	18	1
1:A:613:ILE:HD11	1:A:692:PHE:HE2	0.40	1.76	19	1
1:A:601:PHE:CE2	1:A:611:CYS:HB2	0.40	2.52	4	1
1:A:621:VAL:O	1:A:623:CYS:N	0.40	2.55	8	1
1:A:587:ILE:HD13	1:A:587:ILE:H	0.40	1.75	10	1
1:A:663:ARG:NH2	1:A:665:ILE:CG2	0.40	2.85	13	1
1:A:726:LEU:CD1	1:A:726:LEU:N	0.40	2.84	17	1
1:A:607:GLU:C	1:A:609:CYS:N	0.40	2.74	8	1
1:A:589:GLN:CA	1:A:589:GLN:OE1	0.40	2.70	19	1
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%)	110±1 (87±1%)	12±2 (10±1%)	4±1 (3±1%)	7 39
All	All	2540/3160 (80%)	2210 (87%)	250 (10%)	80 (3%)	7 39

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	582	PRO	7
1	A	622	HIS	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%)	1 15
All	All	2380/2840 (84%)	1644 (69%)	736 (31%)	1 15

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	577	PHE	20
1	A	583	LEU	20
1	A	591	SER	20
1	A	610	ASN	20
1	A	612	LYS	20
1	A	652	THR	20
1	A	592	LEU	19
1	A	620	ARG	19
1	A	671	LEU	19
1	A	698	ASP	19
1	A	596	GLN	19
1	A	606	SER	18
1	A	628	LYS	18
1	A	680	ILE	18
1	A	659	LEU	17
1	A	599	ASN	16
1	A	670	PHE	16
1	A	688	PHE	16
1	A	605	ARG	16
1	A	629	ARG	15
1	A	677	GLU	14
1	A	684	LYS	13
1	A	728	LYS	12
1	A	650	CYS	12
1	A	589	GLN	11
1	A	717	LEU	11
1	A	615	ASP	11
1	A	581	LYS	10
1	A	676	ASP	10
1	A	722	GLU	10
1	A	662	ASN	10
1	A	695	GLU	10
1	A	683	ASP	9
1	A	692	PHE	9
1	A	587	ILE	9
1	A	619	SER	9
1	A	718	LYS	8
1	A	660	ASN	8
1	A	666	GLN	8
1	A	646	ASP	8
1	A	593	GLU	8
1	A	595	GLN	7
1	A	617	ARG	7

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Mol	Chain	Res	Type	Models (Total)
1	A	679	LYS	7
1	A	618	LEU	6
1	A	694	VAL	6
1	A	723	GLU	6
1	A	580	LEU	6
1	A	687	LYS	6
1	A	608	ASP	6
1	A	724	LYS	6
1	A	614	GLU	5
1	A	656	VAL	5
1	A	686	ASN	5
1	A	645	ASP	5
1	A	585	ASP	5
1	A	607	GLU	4
1	A	661	ASN	4
1	A	663	ARG	4
1	A	725	ASP	4
1	A	689	VAL	4
1	A	655	ASN	4
1	A	657	SER	3
1	A	693	LYS	3
1	A	611	CYS	3
1	A	720	THR	3
1	A	664	MET	3
1	A	681	ILE	3
1	A	674	ASP	3
1	A	699	THR	3
1	A	644	LEU	3
1	A	678	ILE	3
1	A	627	LYS	3
1	A	685	ASN	2
1	A	586	SER	2
1	A	623	CYS	2
1	A	690	ILE	2
1	A	602	PHE	1
1	A	624	PHE	1
1	A	672	LEU	1
1	A	630	HIS	1
1	A	649	TYR	1
1	A	576	ARG	1
1	A	669	LYS	1
1	A	715	VAL	1

6.3.3 RNA

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates

There are no monosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided