Full wwPDB NMR Structure Validation Report (i)

Apr 26, 2016 – 08:56 PM BST

PDB ID	:	2J48
Title	:	NMR STRUCTURE OF THE PSEUDO-RECEIVER DOMAIN OF THE CIKA PROTEIN.
Authors	:	Gao, T.; Zhang, X.; Golden, S.S.; Liwang, A.
Deposited on	:	2006-08-26

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 (i) symbol.

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

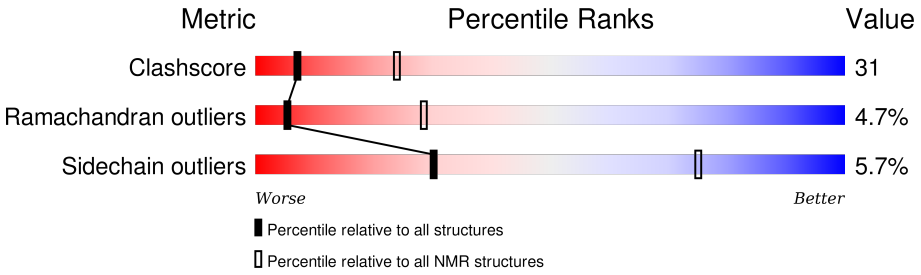
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal 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 (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 86%.

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	119	50% 41% 8%

2 Ensemble composition and analysis

This entry contains 20 models. Model 9 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:628-A:696, A:702-A:741 (109)	0.69	9

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 6 clusters. No single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1838 atoms, of which 933 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called TWO-COMPONENT SENSOR KINASE.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	119	1838	588	933	143	169	5	0

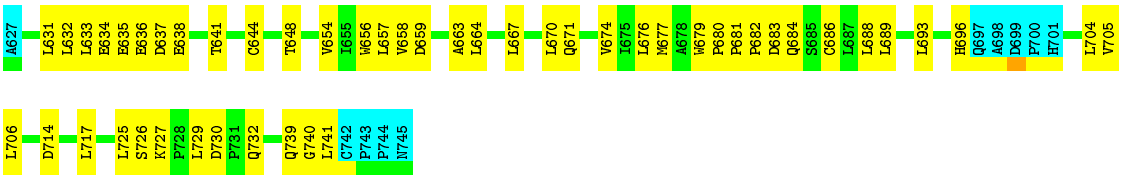
4 Residue-property plots

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: TWO-COMPONENT SENSOR KINASE

Chain A: 



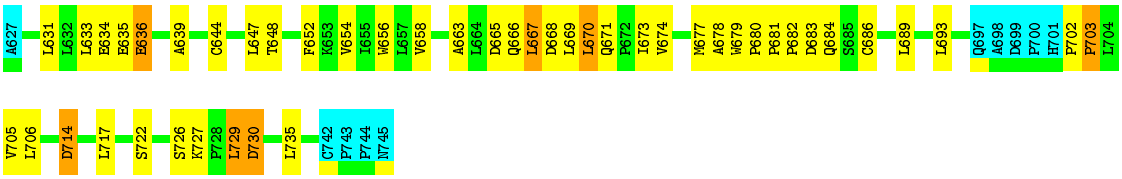
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: TWO-COMPONENT SENSOR KINASE

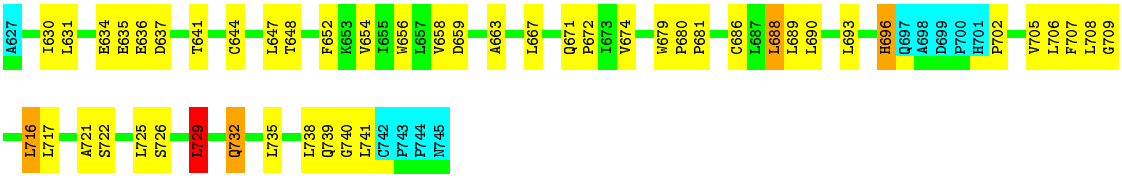
Chain A: 



4.2.2 Score per residue for model 2

• Molecule 1: TWO-COMPONENT SENSOR KINASE

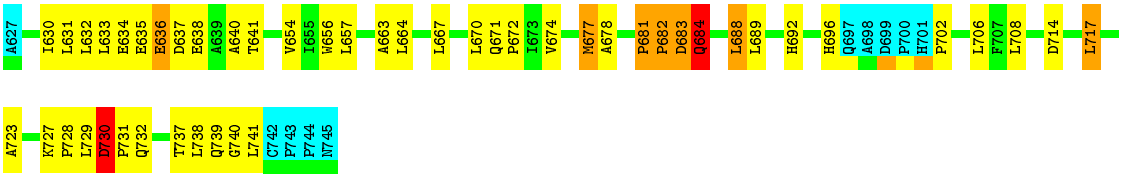
Chain A: 



4.2.3 Score per residue for model 3

- Molecule 1: TWO-COMPONENT SENSOR KINASE

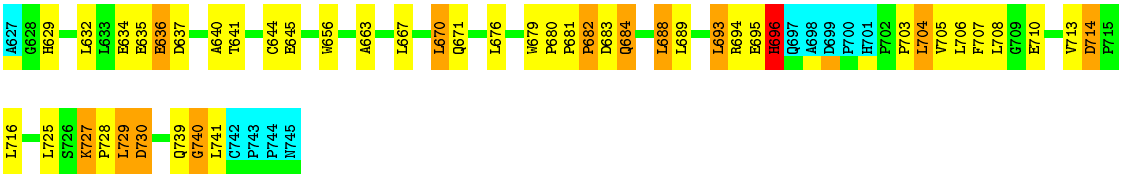
Chain A:



4.2.4 Score per residue for model 4

- Molecule 1: TWO-COMPONENT SENSOR KINASE

Chain A:



4.2.5 Score per residue for model 5

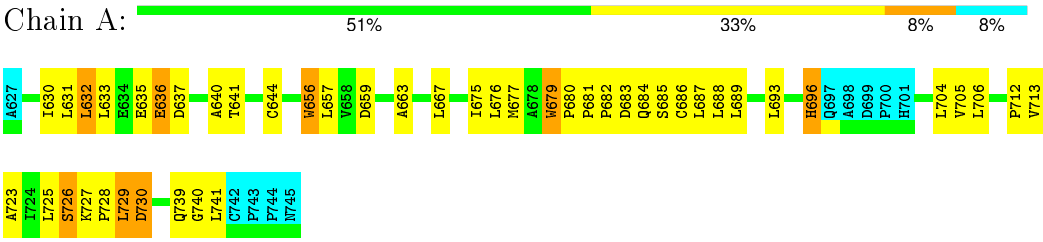
- Molecule 1: TWO-COMPONENT SENSOR KINASE

Chain A:

4.2.6 Score per residue for model 6

- Molecule 1: TWO-COMPONENT SENSOR KINASE

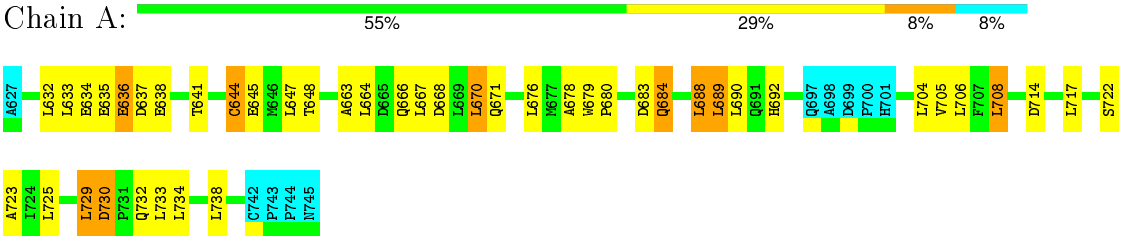
Chain A:



4.2.7 Score per residue for model 7

- Molecule 1: TWO-COMPONENT SENSOR KINASE

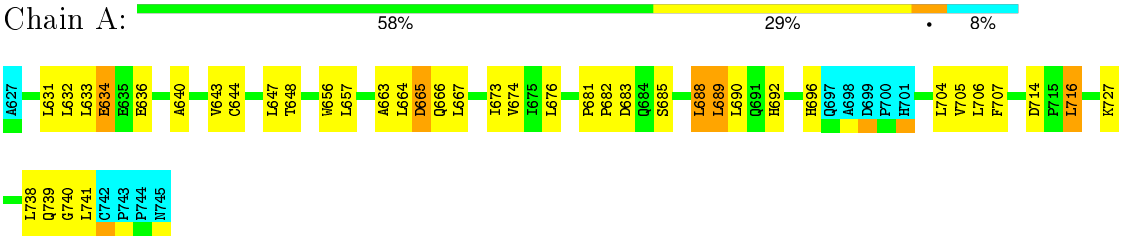
Chain A:



4.2.8 Score per residue for model 8

- Molecule 1: TWO-COMPONENT SENSOR KINASE

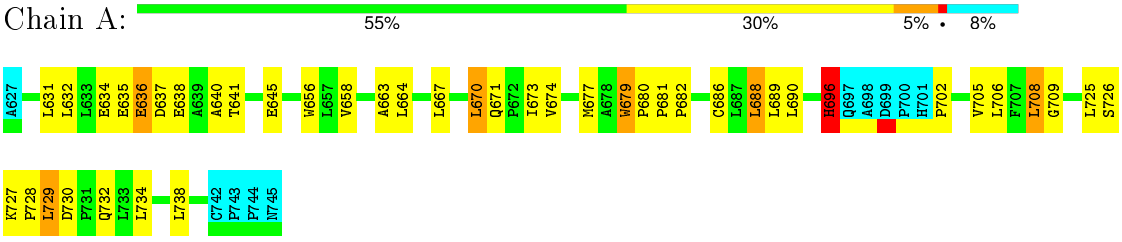
Chain A:



4.2.9 Score per residue for model 9 (medoid)

- Molecule 1: TWO-COMPONENT SENSOR KINASE

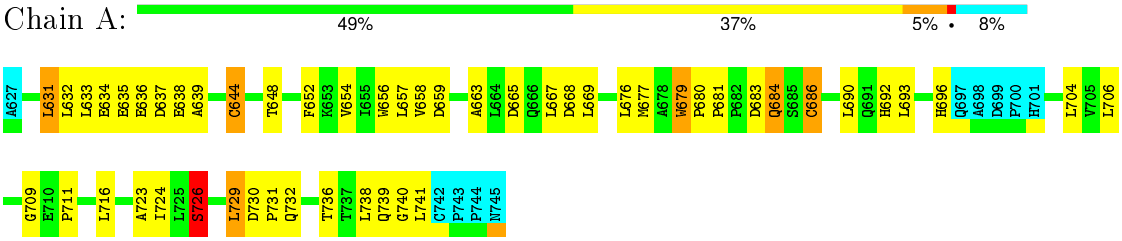
Chain A:



4.2.10 Score per residue for model 10

• Molecule 1: TWO-COMPONENT SENSOR KINASE

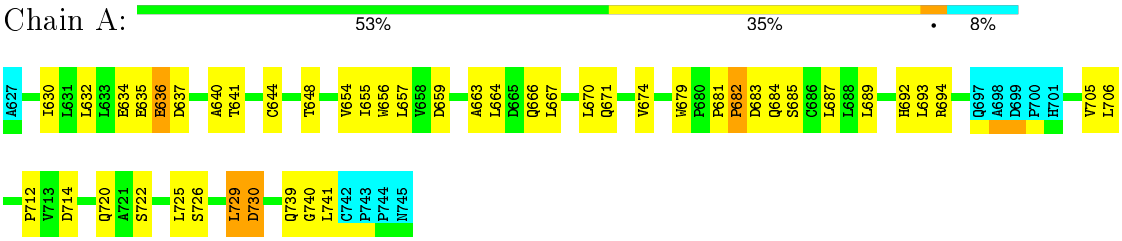
Chain A:



4.2.11 Score per residue for model 11

• Molecule 1: TWO-COMPONENT SENSOR KINASE

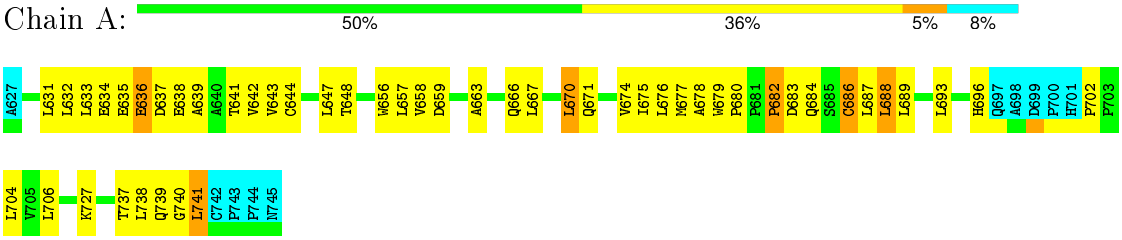
Chain A:



4.2.12 Score per residue for model 12

• Molecule 1: TWO-COMPONENT SENSOR KINASE

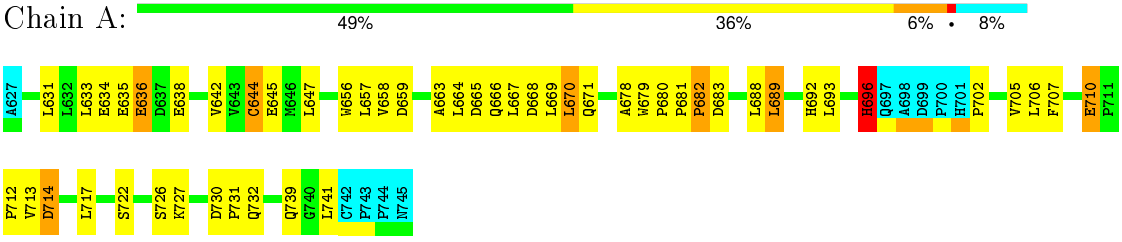
Chain A:



4.2.13 Score per residue for model 13

• Molecule 1: TWO-COMPONENT SENSOR KINASE

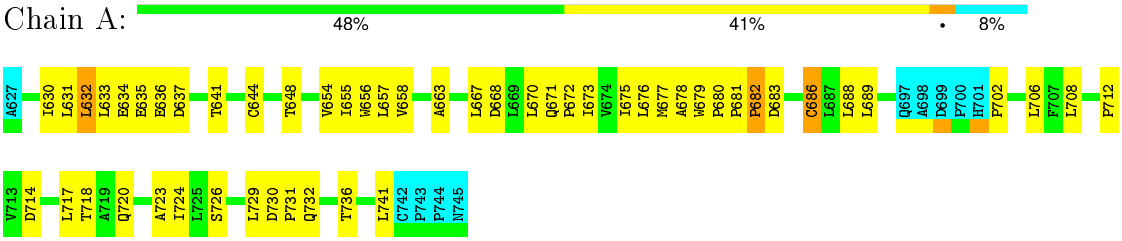
Chain A:



4.2.14 Score per residue for model 14

• Molecule 1: TWO-COMPONENT SENSOR KINASE

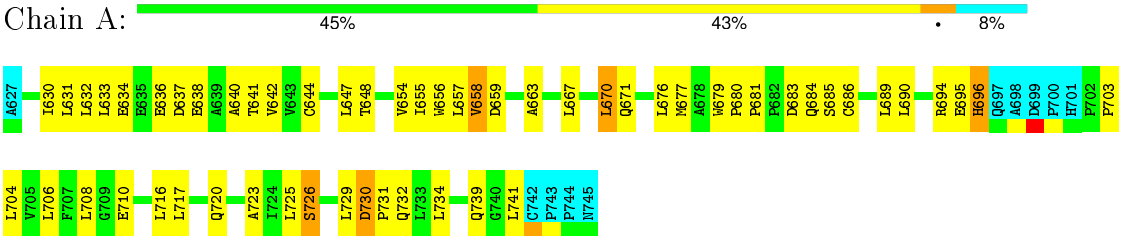
Chain A:



4.2.15 Score per residue for model 15

• Molecule 1: TWO-COMPONENT SENSOR KINASE

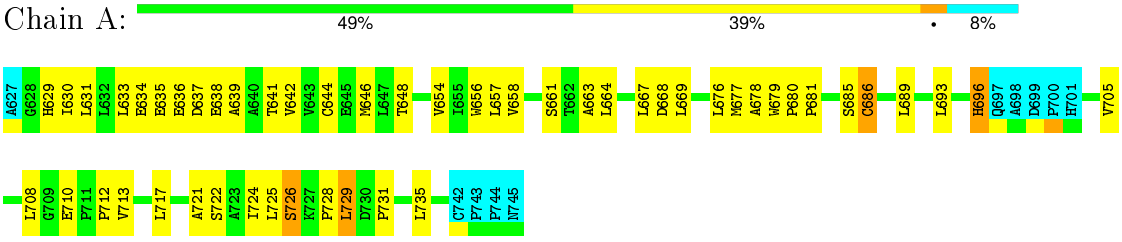
Chain A:



4.2.16 Score per residue for model 16

• Molecule 1: TWO-COMPONENT SENSOR KINASE

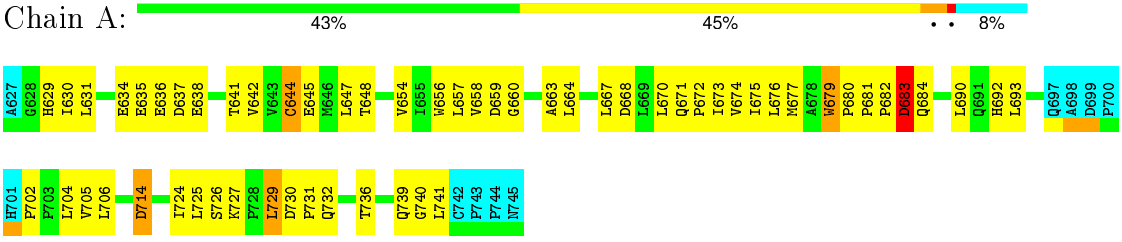
Chain A:



4.2.17 Score per residue for model 17

• Molecule 1: TWO-COMPONENT SENSOR KINASE

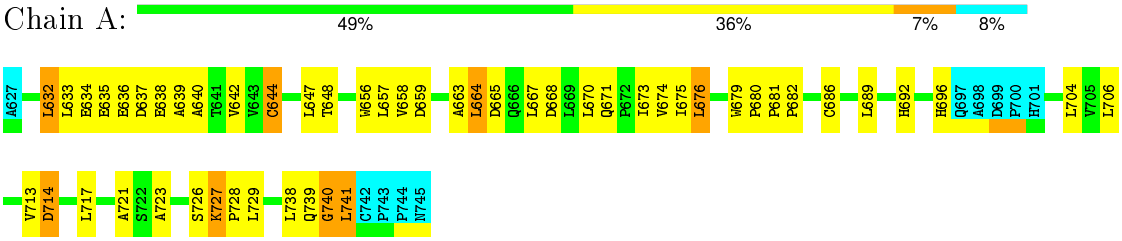
Chain A:



4.2.18 Score per residue for model 18

• Molecule 1: TWO-COMPONENT SENSOR KINASE

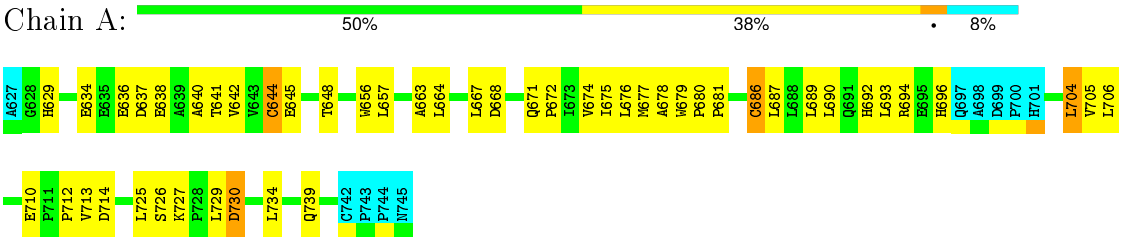
Chain A:



4.2.19 Score per residue for model 19

• Molecule 1: TWO-COMPONENT SENSOR KINASE

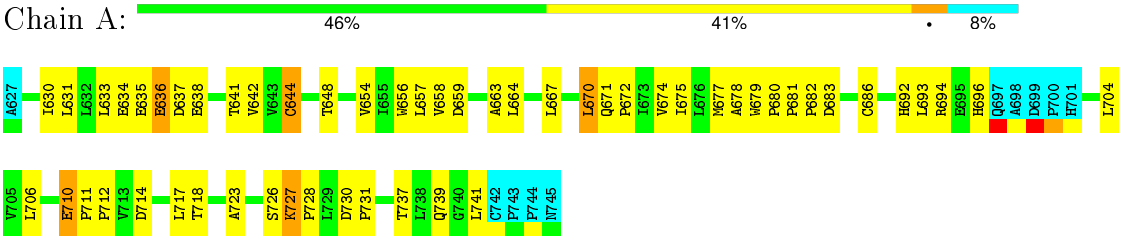
Chain A:



4.2.20 Score per residue for model 20

• Molecule 1: TWO-COMPONENT SENSOR KINASE

Chain A:



5 Refinement protocol and experimental data overview

The models were refined using the following method: *XPLOR-NIH*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *ENERGY*.

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

Software name	Classification	Version
XPLOR-NIH	refinement	
XPLOR-NIH	structure solution	
NMRPIPE	structure solution	
PIPP	structure solution	
NMRDRAW	structure solution	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	BMRB entry 6438
Number of chemical shift lists	1
Total number of shifts	1614
Number of shifts mapped to atoms	1442
Number of unparsed shifts	0
Number of shifts with mapping errors	172
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	86%

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	832	869	866	52±8
All	All	16640	17380	17320	1048

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 31.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:708:LEU:HD12	1:A:709:GLY:N	1.05	1.67	9	1
1:A:741:LEU:O	1:A:741:LEU:HD12	0.97	1.59	12	1
1:A:670:LEU:O	1:A:670:LEU:HD12	0.94	1.63	7	1
1:A:631:LEU:HD21	1:A:663:ALA:HB1	0.93	1.37	12	3
1:A:631:LEU:HD22	1:A:667:LEU:HD12	0.92	1.40	2	5
1:A:631:LEU:C	1:A:632:LEU:HD13	0.90	1.86	14	1
1:A:729:LEU:O	1:A:729:LEU:HD23	0.89	1.68	17	2
1:A:677:MET:SD	1:A:690:LEU:HD21	0.84	2.11	17	2
1:A:632:LEU:H	1:A:632:LEU:HD22	0.84	1.33	14	1
1:A:729:LEU:HD12	1:A:729:LEU:O	0.84	1.73	2	1
1:A:664:LEU:HD22	1:A:692:HIS:ND1	0.81	1.89	8	3
1:A:631:LEU:HD22	1:A:667:LEU:CD1	0.81	2.06	5	3
1:A:727:LYS:H	1:A:728:PRO:CD	0.80	1.90	18	2
1:A:689:LEU:HD13	1:A:689:LEU:C	0.80	1.96	11	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:631:LEU:HD13	1:A:631:LEU:C	0.79	1.97	15	3
1:A:632:LEU:HD13	1:A:632:LEU:N	0.79	1.93	14	1
1:A:706:LEU:HD12	1:A:706:LEU:N	0.79	1.92	8	6
1:A:633:LEU:HD12	1:A:657:LEU:O	0.78	1.78	5	3
1:A:631:LEU:HD12	1:A:670:LEU:HD12	0.78	1.55	14	1
1:A:679:TRP:N	1:A:680:PRO:CD	0.78	2.47	6	16
1:A:644:CYS:SG	1:A:656:TRP:CZ3	0.77	2.77	6	1
1:A:633:LEU:HD22	1:A:686:CYS:SG	0.76	2.21	10	2
1:A:638:GLU:O	1:A:642:VAL:HG23	0.76	1.80	20	9
1:A:690:LEU:C	1:A:690:LEU:HD13	0.76	2.01	9	2
1:A:634:GLU:OE1	1:A:678:ALA:HB2	0.76	1.81	7	2
1:A:632:LEU:C	1:A:632:LEU:HD12	0.76	2.01	18	1
1:A:675:ILE:HG22	1:A:677:MET:SD	0.75	2.20	6	2
1:A:708:LEU:N	1:A:708:LEU:HD12	0.75	1.97	16	2
1:A:688:LEU:C	1:A:688:LEU:HD12	0.75	2.02	3	5
1:A:707:PHE:CE2	1:A:721:ALA:HB2	0.74	2.17	2	1
1:A:676:LEU:N	1:A:676:LEU:HD12	0.74	1.96	19	5
1:A:631:LEU:HD13	1:A:667:LEU:HD12	0.74	1.58	14	1
1:A:632:LEU:HD23	1:A:632:LEU:C	0.74	2.01	8	4
1:A:677:MET:SD	1:A:678:ALA:N	0.74	2.61	3	1
1:A:706:LEU:HD22	1:A:723:ALA:HB3	0.74	1.60	10	3
1:A:647:LEU:HD21	1:A:734:LEU:HD21	0.73	1.60	7	1
1:A:681:PRO:O	1:A:683:ASP:N	0.73	2.22	11	6
1:A:676:LEU:HD12	1:A:676:LEU:N	0.73	1.98	6	3
1:A:706:LEU:N	1:A:706:LEU:HD12	0.73	1.99	17	5
1:A:693:LEU:HD12	1:A:693:LEU:C	0.72	2.04	4	1
1:A:688:LEU:HD12	1:A:688:LEU:C	0.72	2.05	2	5
1:A:664:LEU:HD22	1:A:692:HIS:HD1	0.72	1.42	8	1
1:A:725:LEU:HD12	1:A:725:LEU:N	0.72	1.98	17	6
1:A:677:MET:SD	1:A:689:LEU:HD13	0.72	2.24	16	2
1:A:679:TRP:CZ3	1:A:686:CYS:SG	0.72	2.82	6	1
1:A:664:LEU:O	1:A:664:LEU:HD12	0.72	1.85	18	1
1:A:664:LEU:C	1:A:664:LEU:HD12	0.72	2.04	18	1
1:A:679:TRP:H	1:A:680:PRO:CD	0.72	1.98	17	15
1:A:657:LEU:HD23	1:A:663:ALA:HB2	0.72	1.62	3	3
1:A:631:LEU:HD13	1:A:632:LEU:N	0.71	2.00	10	3
1:A:706:LEU:HD12	1:A:723:ALA:O	0.71	1.86	6	1
1:A:633:LEU:HD13	1:A:686:CYS:SG	0.71	2.25	10	1
1:A:632:LEU:N	1:A:632:LEU:HD22	0.71	1.99	14	1
1:A:704:LEU:CD2	1:A:704:LEU:N	0.71	2.54	19	1
1:A:637:ASP:OD1	1:A:638:GLU:N	0.71	2.24	20	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:704:LEU:N	1:A:704:LEU:CD2	0.71	2.54	4	2
1:A:634:GLU:CD	1:A:640:ALA:HB2	0.70	2.07	8	1
1:A:682:PRO:O	1:A:684:GLN:N	0.70	2.24	3	1
1:A:708:LEU:C	1:A:708:LEU:HD12	0.70	2.06	9	2
1:A:667:LEU:C	1:A:667:LEU:HD23	0.70	2.07	20	5
1:A:734:LEU:HD23	1:A:734:LEU:C	0.70	2.07	15	1
1:A:657:LEU:CD2	1:A:663:ALA:HB2	0.70	2.17	19	2
1:A:656:TRP:C	1:A:657:LEU:HD22	0.70	2.07	11	9
1:A:689:LEU:HD13	1:A:689:LEU:O	0.69	1.86	13	3
1:A:632:LEU:HD12	1:A:633:LEU:N	0.69	2.02	18	1
1:A:717:LEU:C	1:A:717:LEU:HD12	0.69	2.07	20	1
1:A:675:ILE:O	1:A:705:VAL:HG23	0.69	1.88	6	1
1:A:637:ASP:OD1	1:A:656:TRP:CH2	0.69	2.45	10	2
1:A:706:LEU:HD11	1:A:725:LEU:CD1	0.69	2.18	6	1
1:A:670:LEU:C	1:A:670:LEU:HD12	0.68	2.07	7	1
1:A:668:ASP:O	1:A:671:GLN:NE2	0.68	2.25	18	4
1:A:633:LEU:HD23	1:A:686:CYS:SG	0.68	2.29	16	1
1:A:667:LEU:HD23	1:A:667:LEU:O	0.68	1.89	3	4
1:A:739:GLN:O	1:A:741:LEU:N	0.67	2.27	8	10
1:A:689:LEU:O	1:A:689:LEU:HD23	0.67	1.88	15	4
1:A:694:ARG:NE	1:A:720:GLN:OE1	0.67	2.28	5	1
1:A:716:LEU:CD2	1:A:716:LEU:N	0.67	2.56	8	1
1:A:732:GLN:O	1:A:732:GLN:NE2	0.67	2.28	2	1
1:A:670:LEU:HD23	1:A:670:LEU:N	0.67	2.04	20	1
1:A:667:LEU:O	1:A:667:LEU:HD23	0.67	1.89	10	4
1:A:717:LEU:N	1:A:717:LEU:CD2	0.67	2.58	6	2
1:A:704:LEU:N	1:A:704:LEU:HD12	0.66	2.05	15	3
1:A:692:HIS:NE2	1:A:696:HIS:NE2	0.66	2.43	13	2
1:A:694:ARG:NH1	1:A:720:GLN:NE2	0.66	2.43	15	1
1:A:664:LEU:HD21	1:A:689:LEU:HD12	0.66	1.67	19	2
1:A:727:LYS:N	1:A:728:PRO:CD	0.66	2.58	20	2
1:A:695:GLU:O	1:A:696:HIS:CD2	0.66	2.48	15	1
1:A:663:ALA:O	1:A:667:LEU:N	0.66	2.28	6	19
1:A:683:ASP:O	1:A:684:GLN:CB	0.66	2.44	3	3
1:A:741:LEU:HD12	1:A:741:LEU:N	0.66	2.05	10	2
1:A:630:ILE:HG23	1:A:674:VAL:HG13	0.66	1.68	11	3
1:A:635:GLU:O	1:A:636:GLU:CB	0.66	2.43	6	8
1:A:728:PRO:O	1:A:729:LEU:CB	0.66	2.44	16	4
1:A:633:LEU:HD23	1:A:633:LEU:C	0.66	2.10	14	3
1:A:706:LEU:CD2	1:A:723:ALA:HB3	0.66	2.21	15	6
1:A:640:ALA:O	1:A:644:CYS:SG	0.66	2.54	8	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:633:LEU:HD13	1:A:659:ASP:O	0.66	1.90	18	1
1:A:634:GLU:CD	1:A:678:ALA:HB2	0.66	2.10	19	1
1:A:667:LEU:HD23	1:A:667:LEU:C	0.65	2.12	3	4
1:A:694:ARG:NH1	1:A:716:LEU:HD21	0.65	2.06	15	1
1:A:694:ARG:HH11	1:A:720:GLN:HE22	0.65	1.34	15	1
1:A:632:LEU:C	1:A:632:LEU:HD23	0.65	2.13	7	1
1:A:634:GLU:OE2	1:A:678:ALA:HB2	0.65	1.92	19	1
1:A:704:LEU:HD12	1:A:704:LEU:N	0.64	2.08	8	3
1:A:692:HIS:NE2	1:A:696:HIS:ND1	0.64	2.45	10	2
1:A:634:GLU:O	1:A:656:TRP:NE1	0.64	2.29	12	10
1:A:717:LEU:HD12	1:A:717:LEU:N	0.64	2.07	18	1
1:A:729:LEU:O	1:A:729:LEU:CD2	0.64	2.45	17	1
1:A:673:ILE:HG23	1:A:674:VAL:HG23	0.64	1.69	18	3
1:A:714:ASP:OD1	1:A:714:ASP:N	0.64	2.28	1	1
1:A:708:LEU:HD12	1:A:708:LEU:N	0.63	2.07	2	1
1:A:644:CYS:SG	1:A:654:VAL:HG13	0.63	2.32	10	2
1:A:706:LEU:HG	1:A:723:ALA:HB3	0.63	1.70	14	1
1:A:712:PRO:O	1:A:714:ASP:N	0.63	2.26	19	1
1:A:705:VAL:C	1:A:706:LEU:HD12	0.63	2.12	19	7
1:A:689:LEU:HD23	1:A:689:LEU:C	0.63	2.14	15	3
1:A:632:LEU:HD23	1:A:633:LEU:N	0.63	2.08	8	2
1:A:716:LEU:N	1:A:716:LEU:HD22	0.63	2.09	10	2
1:A:713:VAL:HG12	1:A:713:VAL:O	0.63	1.92	6	1
1:A:632:LEU:HD22	1:A:655:ILE:O	0.63	1.93	14	1
1:A:644:CYS:SG	1:A:656:TRP:CE3	0.63	2.91	6	1
1:A:708:LEU:CD2	1:A:725:LEU:HD12	0.63	2.24	15	1
1:A:688:LEU:HD12	1:A:688:LEU:O	0.62	1.94	2	2
1:A:696:HIS:C	1:A:696:HIS:ND1	0.62	2.51	2	1
1:A:663:ALA:O	1:A:667:LEU:CB	0.62	2.48	11	14
1:A:692:HIS:NE2	1:A:696:HIS:CD2	0.62	2.67	13	3
1:A:688:LEU:O	1:A:688:LEU:HD12	0.62	1.94	3	3
1:A:658:VAL:HG12	1:A:658:VAL:O	0.62	1.94	12	3
1:A:695:GLU:O	1:A:696:HIS:CG	0.62	2.53	15	1
1:A:704:LEU:N	1:A:704:LEU:HD22	0.62	2.09	18	1
1:A:696:HIS:O	1:A:696:HIS:ND1	0.62	2.32	2	1
1:A:668:ASP:OD1	1:A:669:LEU:N	0.62	2.32	16	4
1:A:704:LEU:H	1:A:704:LEU:HD22	0.62	1.54	18	1
1:A:705:VAL:O	1:A:722:SER:N	0.62	2.29	7	5
1:A:644:CYS:SG	1:A:656:TRP:CH2	0.62	2.93	6	1
1:A:717:LEU:N	1:A:717:LEU:HD22	0.62	2.10	6	2
1:A:696:HIS:CG	1:A:696:HIS:O	0.62	2.53	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:738:LEU:C	1:A:738:LEU:HD23	0.61	2.16	12	1
1:A:692:HIS:HE2	1:A:696:HIS:CE1	0.61	2.13	19	1
1:A:694:ARG:HH11	1:A:720:GLN:NE2	0.61	1.91	15	1
1:A:647:LEU:CD1	1:A:654:VAL:HG21	0.61	2.25	2	1
1:A:679:TRP:CZ3	1:A:717:LEU:CD2	0.61	2.83	7	1
1:A:658:VAL:O	1:A:659:ASP:OD1	0.61	2.18	20	7
1:A:692:HIS:NE2	1:A:696:HIS:CE1	0.61	2.68	10	2
1:A:630:ILE:HB	1:A:654:VAL:HG12	0.61	1.73	3	4
1:A:656:TRP:CZ2	1:A:658:VAL:CG2	0.61	2.84	10	1
1:A:631:LEU:C	1:A:631:LEU:CD1	0.60	2.70	15	1
1:A:710:GLU:CD	1:A:710:GLU:N	0.60	2.51	20	1
1:A:695:GLU:O	1:A:696:HIS:CB	0.60	2.48	15	2
1:A:682:PRO:O	1:A:683:ASP:OD1	0.60	2.20	8	2
1:A:679:TRP:CG	1:A:679:TRP:O	0.60	2.54	20	1
1:A:644:CYS:O	1:A:648:THR:OG1	0.60	2.18	19	14
1:A:711:PRO:HB3	1:A:724:ILE:HD13	0.60	1.74	10	1
1:A:716:LEU:HD22	1:A:716:LEU:N	0.60	2.12	8	1
1:A:676:LEU:HD23	1:A:676:LEU:N	0.60	2.12	18	1
1:A:730:ASP:N	1:A:730:ASP:OD1	0.59	2.35	4	2
1:A:690:LEU:O	1:A:690:LEU:HD13	0.59	1.96	7	2
1:A:647:LEU:N	1:A:647:LEU:CD2	0.59	2.65	15	1
1:A:631:LEU:HD23	1:A:667:LEU:HD12	0.59	1.73	3	2
1:A:683:ASP:OD1	1:A:687:LEU:CD1	0.59	2.50	11	1
1:A:647:LEU:HD12	1:A:654:VAL:HG21	0.59	1.74	2	1
1:A:678:ALA:O	1:A:683:ASP:OD2	0.59	2.20	1	1
1:A:673:ILE:HG13	1:A:674:VAL:HG23	0.59	1.73	9	3
1:A:678:ALA:O	1:A:686:CYS:SG	0.59	2.61	20	1
1:A:739:GLN:C	1:A:741:LEU:H	0.58	2.01	6	8
1:A:679:TRP:H	1:A:680:PRO:HD3	0.58	1.56	16	11
1:A:634:GLU:OE2	1:A:708:LEU:HD12	0.58	1.97	14	1
1:A:676:LEU:N	1:A:676:LEU:CD1	0.58	2.66	19	3
1:A:665:ASP:O	1:A:668:ASP:OD1	0.58	2.21	13	3
1:A:717:LEU:O	1:A:721:ALA:N	0.58	2.36	16	2
1:A:709:GLY:O	1:A:725:LEU:O	0.58	2.21	2	2
1:A:729:LEU:HD23	1:A:729:LEU:O	0.58	1.98	7	1
1:A:716:LEU:N	1:A:716:LEU:CD2	0.58	2.67	10	2
1:A:730:ASP:O	1:A:732:GLN:N	0.58	2.36	14	7
1:A:632:LEU:HD13	1:A:633:LEU:N	0.58	2.13	6	1
1:A:706:LEU:N	1:A:706:LEU:CD1	0.57	2.66	8	2
1:A:683:ASP:OD2	1:A:685:SER:OG	0.57	2.22	15	1
1:A:632:LEU:CD1	1:A:632:LEU:C	0.57	2.69	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:705:VAL:O	1:A:722:SER:OG	0.57	2.22	1	1
1:A:679:TRP:CD1	1:A:679:TRP:O	0.57	2.56	20	1
1:A:631:LEU:CD2	1:A:667:LEU:HD12	0.57	2.29	8	2
1:A:666:GLN:O	1:A:670:LEU:CD2	0.57	2.52	12	2
1:A:640:ALA:HB1	1:A:656:TRP:CD1	0.57	2.35	19	2
1:A:677:MET:C	1:A:677:MET:SD	0.57	2.83	3	1
1:A:633:LEU:HD22	1:A:689:LEU:HD22	0.57	1.77	3	1
1:A:706:LEU:CD1	1:A:723:ALA:HB3	0.57	2.30	6	1
1:A:696:HIS:C	1:A:696:HIS:HD1	0.56	2.03	2	1
1:A:633:LEU:HD23	1:A:634:GLU:N	0.56	2.15	14	1
1:A:664:LEU:CD1	1:A:664:LEU:C	0.56	2.72	18	1
1:A:637:ASP:OD1	1:A:641:THR:OG1	0.56	2.24	2	1
1:A:658:VAL:HG22	1:A:658:VAL:O	0.56	2.00	9	2
1:A:692:HIS:CD2	1:A:696:HIS:CD2	0.56	2.93	13	1
1:A:704:LEU:HD22	1:A:704:LEU:N	0.56	2.15	19	2
1:A:680:PRO:N	1:A:681:PRO:CD	0.56	2.69	19	10
1:A:635:GLU:OE2	1:A:682:PRO:O	0.56	2.22	14	1
1:A:708:LEU:N	1:A:708:LEU:CD1	0.56	2.69	16	2
1:A:730:ASP:C	1:A:732:GLN:H	0.56	2.04	14	8
1:A:710:GLU:CB	1:A:711:PRO:CD	0.56	2.84	20	1
1:A:637:ASP:O	1:A:641:THR:OG1	0.56	2.21	9	12
1:A:693:LEU:N	1:A:693:LEU:CD2	0.56	2.69	2	1
1:A:739:GLN:C	1:A:741:LEU:N	0.56	2.60	11	11
1:A:631:LEU:CD1	1:A:631:LEU:C	0.56	2.74	9	2
1:A:683:ASP:OD1	1:A:684:GLN:N	0.56	2.39	4	2
1:A:665:ASP:OD1	1:A:665:ASP:C	0.55	2.45	8	1
1:A:739:GLN:O	1:A:740:GLY:C	0.55	2.44	18	2
1:A:686:CYS:SG	1:A:687:LEU:N	0.55	2.79	19	2
1:A:632:LEU:CD2	1:A:632:LEU:C	0.55	2.74	8	1
1:A:681:PRO:C	1:A:683:ASP:H	0.55	2.04	4	6
1:A:657:LEU:HD11	1:A:666:GLN:OE1	0.55	2.01	11	1
1:A:712:PRO:HB3	1:A:717:LEU:HD23	0.55	1.77	14	2
1:A:681:PRO:N	1:A:682:PRO:CD	0.55	2.70	8	3
1:A:689:LEU:O	1:A:689:LEU:HD13	0.55	2.01	11	1
1:A:679:TRP:CH2	1:A:717:LEU:CD2	0.55	2.90	14	1
1:A:679:TRP:C	1:A:681:PRO:CD	0.55	2.75	16	3
1:A:681:PRO:C	1:A:683:ASP:N	0.55	2.61	11	6
1:A:656:TRP:CZ2	1:A:658:VAL:CG1	0.55	2.90	18	1
1:A:713:VAL:O	1:A:714:ASP:OD1	0.54	2.24	13	4
1:A:665:ASP:OD1	1:A:666:GLN:N	0.54	2.40	8	1
1:A:678:ALA:HB1	1:A:680:PRO:HD2	0.54	1.79	7	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:679:TRP:N	1:A:680:PRO:HD2	0.54	2.17	14	11
1:A:676:LEU:CD1	1:A:676:LEU:N	0.54	2.71	6	2
1:A:702:PRO:O	1:A:703:PRO:O	0.54	2.24	1	1
1:A:683:ASP:CG	1:A:685:SER:OG	0.54	2.46	15	1
1:A:679:TRP:C	1:A:683:ASP:OD2	0.54	2.45	14	2
1:A:725:LEU:CD1	1:A:725:LEU:N	0.54	2.70	17	4
1:A:647:LEU:CB	1:A:654:VAL:HG21	0.54	2.33	17	3
1:A:690:LEU:C	1:A:690:LEU:CD1	0.54	2.75	9	2
1:A:678:ALA:C	1:A:683:ASP:OD2	0.54	2.45	14	2
1:A:630:ILE:C	1:A:631:LEU:HD22	0.54	2.23	16	1
1:A:688:LEU:HD12	1:A:689:LEU:N	0.54	2.18	14	2
1:A:729:LEU:C	1:A:730:ASP:CG	0.54	2.66	3	1
1:A:631:LEU:HD21	1:A:670:LEU:HD12	0.53	1.79	20	1
1:A:633:LEU:HD12	1:A:633:LEU:N	0.53	2.19	3	2
1:A:657:LEU:N	1:A:657:LEU:HD22	0.53	2.18	8	3
1:A:677:MET:SD	1:A:689:LEU:HD22	0.53	2.44	15	2
1:A:688:LEU:C	1:A:688:LEU:CD1	0.53	2.70	3	2
1:A:677:MET:SD	1:A:686:CYS:SG	0.53	3.06	1	1
1:A:713:VAL:O	1:A:713:VAL:HG12	0.53	2.03	16	2
1:A:647:LEU:HD12	1:A:647:LEU:N	0.53	2.17	8	3
1:A:727:LYS:H	1:A:728:PRO:HD2	0.53	1.61	18	2
1:A:689:LEU:C	1:A:689:LEU:CD1	0.53	2.70	11	2
1:A:674:VAL:HG21	1:A:738:LEU:HD11	0.53	1.81	9	1
1:A:670:LEU:CD1	1:A:670:LEU:C	0.53	2.73	7	1
1:A:706:LEU:CD1	1:A:706:LEU:N	0.53	2.71	19	4
1:A:647:LEU:HB2	1:A:654:VAL:HG21	0.53	1.80	17	3
1:A:657:LEU:CD2	1:A:657:LEU:N	0.52	2.73	12	4
1:A:704:LEU:HD11	1:A:737:THR:HG22	0.52	1.80	20	1
1:A:690:LEU:HA	1:A:693:LEU:HD21	0.52	1.81	19	1
1:A:632:LEU:CD2	1:A:655:ILE:O	0.52	2.57	14	1
1:A:644:CYS:SG	1:A:654:VAL:CG1	0.52	2.98	10	2
1:A:673:ILE:CG2	1:A:741:LEU:HD12	0.52	2.34	14	1
1:A:633:LEU:C	1:A:633:LEU:HD23	0.52	2.25	6	1
1:A:710:GLU:N	1:A:710:GLU:CD	0.52	2.63	13	1
1:A:632:LEU:C	1:A:632:LEU:CD1	0.52	2.78	6	1
1:A:647:LEU:HD22	1:A:654:VAL:HG21	0.52	1.81	1	1
1:A:652:PHE:CE2	1:A:735:LEU:HD22	0.52	2.40	1	1
1:A:631:LEU:HG	1:A:667:LEU:HD12	0.52	1.80	10	1
1:A:729:LEU:O	1:A:730:ASP:O	0.52	2.28	1	4
1:A:676:LEU:N	1:A:676:LEU:CD2	0.52	2.73	18	1
1:A:637:ASP:O	1:A:641:THR:CB	0.52	2.58	16	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:706:LEU:HD12	1:A:723:ALA:C	0.52	2.25	6	1
1:A:729:LEU:HD23	1:A:729:LEU:C	0.51	2.25	7	1
1:A:631:LEU:N	1:A:631:LEU:CD2	0.51	2.73	16	1
1:A:634:GLU:OE2	1:A:639:ALA:HB1	0.51	2.05	16	4
1:A:658:VAL:O	1:A:658:VAL:HG22	0.51	2.05	17	1
1:A:679:TRP:CH2	1:A:717:LEU:CD1	0.51	2.93	1	1
1:A:632:LEU:CD2	1:A:632:LEU:N	0.51	2.67	14	1
1:A:729:LEU:C	1:A:729:LEU:HD12	0.51	2.25	2	1
1:A:682:PRO:O	1:A:683:ASP:O	0.51	2.29	17	1
1:A:679:TRP:H	1:A:680:PRO:HD2	0.51	1.65	9	3
1:A:686:CYS:O	1:A:690:LEU:CD1	0.51	2.58	2	2
1:A:688:LEU:CD1	1:A:688:LEU:C	0.51	2.76	7	4
1:A:696:HIS:CD2	1:A:696:HIS:O	0.51	2.64	9	1
1:A:730:ASP:OD1	1:A:730:ASP:N	0.51	2.40	6	1
1:A:630:ILE:HG23	1:A:674:VAL:CG1	0.51	2.33	11	1
1:A:738:LEU:O	1:A:738:LEU:HD23	0.51	2.06	12	1
1:A:657:LEU:N	1:A:657:LEU:CD2	0.51	2.73	13	3
1:A:630:ILE:HB	1:A:654:VAL:HG22	0.51	1.82	17	1
1:A:681:PRO:N	1:A:682:PRO:HD2	0.50	2.21	20	7
1:A:694:ARG:CZ	1:A:720:GLN:CD	0.50	2.79	11	1
1:A:666:GLN:O	1:A:670:LEU:HD23	0.50	2.06	1	1
1:A:631:LEU:HD12	1:A:675:ILE:HD12	0.50	1.82	20	1
1:A:712:PRO:C	1:A:714:ASP:H	0.50	2.06	19	1
1:A:688:LEU:HG	1:A:689:LEU:N	0.50	2.21	5	11
1:A:679:TRP:N	1:A:683:ASP:OD2	0.50	2.43	14	1
1:A:632:LEU:HD11	1:A:643:VAL:HG11	0.50	1.81	8	1
1:A:641:THR:O	1:A:645:GLU:N	0.50	2.38	19	5
1:A:664:LEU:HD13	1:A:692:HIS:CD2	0.50	2.41	18	1
1:A:741:LEU:CD1	1:A:741:LEU:O	0.50	2.48	12	1
1:A:732:GLN:O	1:A:736:THR:OG1	0.50	2.26	17	2
1:A:704:LEU:H	1:A:704:LEU:HD12	0.50	1.67	15	3
1:A:652:PHE:CG	1:A:738:LEU:HD13	0.50	2.42	10	1
1:A:634:GLU:OE2	1:A:640:ALA:HB2	0.50	2.06	8	1
1:A:679:TRP:N	1:A:680:PRO:HD3	0.50	2.21	12	4
1:A:683:ASP:OD1	1:A:687:LEU:HD13	0.50	2.07	11	1
1:A:693:LEU:HD13	1:A:696:HIS:CE1	0.50	2.42	2	1
1:A:664:LEU:CD2	1:A:689:LEU:HD12	0.50	2.36	19	1
1:A:632:LEU:N	1:A:632:LEU:HD12	0.49	2.22	11	1
1:A:680:PRO:N	1:A:681:PRO:HD3	0.49	2.22	15	3
1:A:704:LEU:CD1	1:A:737:THR:O	0.49	2.60	12	1
1:A:693:LEU:HD13	1:A:696:HIS:NE2	0.49	2.21	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:730:ASP:C	1:A:732:GLN:N	0.49	2.65	14	7
1:A:632:LEU:N	1:A:632:LEU:CD1	0.49	2.63	14	1
1:A:734:LEU:HD23	1:A:734:LEU:O	0.49	2.06	15	1
1:A:713:VAL:O	1:A:713:VAL:CG1	0.49	2.59	6	1
1:A:683:ASP:C	1:A:685:SER:H	0.49	2.11	15	2
1:A:666:GLN:CG	1:A:667:LEU:N	0.49	2.75	11	1
1:A:652:PHE:CZ	1:A:735:LEU:HD11	0.49	2.42	2	1
1:A:692:HIS:CD2	1:A:696:HIS:ND1	0.49	2.81	10	1
1:A:640:ALA:HB1	1:A:656:TRP:CE2	0.49	2.42	3	1
1:A:683:ASP:O	1:A:684:GLN:HB2	0.49	2.08	7	1
1:A:647:LEU:N	1:A:647:LEU:CD1	0.49	2.76	13	2
1:A:717:LEU:CD1	1:A:717:LEU:N	0.49	2.76	18	1
1:A:632:LEU:CD1	1:A:643:VAL:HG11	0.49	2.38	12	1
1:A:659:ASP:OD1	1:A:659:ASP:C	0.49	2.49	11	1
1:A:644:CYS:SG	1:A:645:GLU:N	0.49	2.85	13	2
1:A:690:LEU:HD23	1:A:693:LEU:HD21	0.49	1.83	19	1
1:A:647:LEU:HD22	1:A:647:LEU:N	0.48	2.23	15	1
1:A:706:LEU:C	1:A:706:LEU:HD23	0.48	2.29	5	1
1:A:692:HIS:CD2	1:A:696:HIS:NE2	0.48	2.81	13	1
1:A:717:LEU:C	1:A:717:LEU:CD1	0.48	2.77	20	1
1:A:727:LYS:H	1:A:728:PRO:HD3	0.48	1.67	18	2
1:A:677:MET:SD	1:A:690:LEU:CD2	0.48	2.95	17	1
1:A:689:LEU:C	1:A:689:LEU:HD23	0.48	2.29	1	3
1:A:695:GLU:C	1:A:696:HIS:CG	0.48	2.85	15	2
1:A:741:LEU:CD1	1:A:741:LEU:N	0.48	2.76	10	1
1:A:717:LEU:HD12	1:A:718:THR:N	0.48	2.22	20	1
1:A:684:GLN:CD	1:A:686:CYS:SG	0.48	2.92	6	1
1:A:684:GLN:CG	1:A:686:CYS:SG	0.48	3.01	6	1
1:A:644:CYS:SG	1:A:648:THR:OG1	0.48	2.72	7	1
1:A:634:GLU:HG2	1:A:635:GLU:N	0.48	2.24	5	13
1:A:667:LEU:O	1:A:671:GLN:N	0.48	2.42	1	2
1:A:640:ALA:CB	1:A:656:TRP:CD1	0.48	2.97	18	4
1:A:664:LEU:HD21	1:A:689:LEU:HD21	0.48	1.86	13	1
1:A:684:GLN:O	1:A:687:LEU:HD12	0.48	2.09	11	2
1:A:655:ILE:HG21	1:A:666:GLN:NE2	0.47	2.23	11	1
1:A:656:TRP:O	1:A:657:LEU:HD22	0.47	2.07	15	5
1:A:688:LEU:CG	1:A:689:LEU:N	0.47	2.77	14	3
1:A:647:LEU:N	1:A:647:LEU:HD12	0.47	2.24	13	2
1:A:680:PRO:N	1:A:683:ASP:OD2	0.47	2.48	14	1
1:A:704:LEU:N	1:A:704:LEU:CD1	0.47	2.76	6	2
1:A:656:TRP:CZ2	1:A:658:VAL:HG22	0.47	2.44	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:695:GLU:O	1:A:696:HIS:HB3	0.47	2.09	15	1
1:A:644:CYS:O	1:A:648:THR:N	0.47	2.39	19	4
1:A:633:LEU:O	1:A:634:GLU:CG	0.47	2.63	20	3
1:A:712:PRO:HB3	1:A:717:LEU:HD11	0.47	1.84	20	1
1:A:713:VAL:HG13	1:A:714:ASP:N	0.47	2.23	18	1
1:A:633:LEU:CD2	1:A:633:LEU:C	0.47	2.82	14	1
1:A:633:LEU:HD12	1:A:657:LEU:C	0.47	2.30	5	1
1:A:732:GLN:O	1:A:732:GLN:CD	0.47	2.53	2	1
1:A:714:ASP:N	1:A:714:ASP:OD1	0.47	2.46	17	1
1:A:640:ALA:CB	1:A:656:TRP:CZ2	0.47	2.97	3	1
1:A:738:LEU:N	1:A:738:LEU:HD12	0.47	2.25	7	1
1:A:708:LEU:CD1	1:A:708:LEU:N	0.47	2.78	3	1
1:A:671:GLN:N	1:A:672:PRO:HD3	0.46	2.25	19	5
1:A:640:ALA:HB1	1:A:656:TRP:CG	0.46	2.45	4	2
1:A:704:LEU:CD1	1:A:704:LEU:N	0.46	2.77	8	1
1:A:692:HIS:CE1	1:A:696:HIS:NE2	0.46	2.83	13	1
1:A:690:LEU:HD23	1:A:690:LEU:C	0.46	2.29	15	1
1:A:635:GLU:O	1:A:636:GLU:HB3	0.46	2.10	6	6
1:A:728:PRO:O	1:A:729:LEU:HB2	0.46	2.10	6	2
1:A:634:GLU:OE1	1:A:656:TRP:CD1	0.46	2.67	8	1
1:A:683:ASP:O	1:A:683:ASP:OD1	0.46	2.33	6	1
1:A:706:LEU:HD23	1:A:723:ALA:HB3	0.46	1.86	20	1
1:A:729:LEU:O	1:A:730:ASP:CG	0.46	2.54	3	1
1:A:640:ALA:CB	1:A:656:TRP:CE2	0.46	2.97	3	1
1:A:631:LEU:HD23	1:A:675:ILE:HG23	0.46	1.87	17	1
1:A:681:PRO:HG3	1:A:686:CYS:SG	0.46	2.51	15	1
1:A:692:HIS:C	1:A:692:HIS:CD2	0.46	2.88	13	1
1:A:631:LEU:HD13	1:A:670:LEU:CD1	0.46	2.40	3	1
1:A:708:LEU:C	1:A:708:LEU:CD1	0.46	2.83	7	1
1:A:667:LEU:C	1:A:667:LEU:CD2	0.46	2.84	10	2
1:A:736:THR:O	1:A:740:GLY:N	0.46	2.47	10	1
1:A:725:LEU:HD11	1:A:734:LEU:HD13	0.46	1.88	7	1
1:A:713:VAL:C	1:A:714:ASP:CG	0.46	2.74	4	1
1:A:677:MET:SD	1:A:677:MET:N	0.46	2.89	6	1
1:A:670:LEU:O	1:A:671:GLN:C	0.46	2.53	4	7
1:A:640:ALA:HB2	1:A:656:TRP:NE1	0.46	2.25	11	1
1:A:696:HIS:O	1:A:696:HIS:CG	0.46	2.68	9	1
1:A:734:LEU:C	1:A:734:LEU:CD2	0.46	2.79	15	1
1:A:712:PRO:C	1:A:714:ASP:N	0.46	2.68	19	1
1:A:741:LEU:C	1:A:741:LEU:HD12	0.45	2.31	12	1
1:A:664:LEU:HD21	1:A:689:LEU:HG	0.45	1.87	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:706:LEU:HD21	1:A:723:ALA:HB3	0.45	1.88	20	1
1:A:634:GLU:CD	1:A:634:GLU:C	0.45	2.73	8	1
1:A:681:PRO:O	1:A:682:PRO:C	0.45	2.54	3	1
1:A:683:ASP:OD1	1:A:683:ASP:C	0.45	2.54	6	1
1:A:695:GLU:CD	1:A:696:HIS:CE1	0.45	2.90	4	1
1:A:676:LEU:HD21	1:A:734:LEU:HD11	0.45	1.88	19	1
1:A:656:TRP:CZ2	1:A:658:VAL:HG12	0.45	2.46	16	1
1:A:658:VAL:O	1:A:658:VAL:CG1	0.45	2.63	12	1
1:A:706:LEU:HD21	1:A:725:LEU:HD13	0.45	1.87	6	1
1:A:655:ILE:HD12	1:A:670:LEU:HD22	0.45	1.89	15	1
1:A:638:GLU:O	1:A:642:VAL:CG2	0.45	2.61	13	2
1:A:693:LEU:HG	1:A:694:ARG:N	0.45	2.26	4	1
1:A:688:LEU:CD1	1:A:689:LEU:N	0.45	2.79	14	1
1:A:709:GLY:O	1:A:726:SER:OG	0.45	2.35	10	1
1:A:677:MET:SD	1:A:678:ALA:O	0.45	2.75	3	1
1:A:664:LEU:HD21	1:A:689:LEU:CD2	0.44	2.42	11	1
1:A:689:LEU:O	1:A:689:LEU:CD1	0.44	2.66	8	1
1:A:680:PRO:O	1:A:683:ASP:CB	0.44	2.66	4	1
1:A:664:LEU:HG	1:A:665:ASP:N	0.44	2.27	18	1
1:A:675:ILE:C	1:A:676:LEU:HD12	0.44	2.31	14	2
1:A:690:LEU:HD11	1:A:717:LEU:HD22	0.44	1.89	15	1
1:A:685:SER:C	1:A:687:LEU:N	0.44	2.71	11	2
1:A:657:LEU:CD1	1:A:663:ALA:HB2	0.44	2.43	6	1
1:A:680:PRO:N	1:A:681:PRO:HD2	0.44	2.27	18	1
1:A:655:ILE:HG22	1:A:657:LEU:CD2	0.44	2.42	14	2
1:A:725:LEU:O	1:A:726:SER:OG	0.44	2.33	15	1
1:A:683:ASP:OD2	1:A:686:CYS:CB	0.44	2.66	10	1
1:A:693:LEU:HD12	1:A:693:LEU:O	0.44	2.12	4	1
1:A:704:LEU:N	1:A:704:LEU:HD23	0.44	2.26	4	1
1:A:689:LEU:CD2	1:A:689:LEU:C	0.44	2.85	15	1
1:A:689:LEU:CD1	1:A:689:LEU:O	0.44	2.65	7	1
1:A:664:LEU:O	1:A:668:ASP:CG	0.44	2.56	19	1
1:A:657:LEU:HD12	1:A:657:LEU:N	0.44	2.27	17	1
1:A:631:LEU:HD21	1:A:657:LEU:HD11	0.44	1.89	10	1
1:A:694:ARG:NH1	1:A:720:GLN:OE1	0.44	2.51	11	1
1:A:724:ILE:C	1:A:725:LEU:HD12	0.44	2.33	17	1
1:A:693:LEU:HD12	1:A:694:ARG:N	0.44	2.27	19	1
1:A:716:LEU:HG	1:A:717:LEU:N	0.44	2.28	2	1
1:A:630:ILE:CG2	1:A:676:LEU:HD13	0.44	2.42	6	1
1:A:730:ASP:OD1	1:A:730:ASP:C	0.43	2.57	11	1
1:A:646:MET:SD	1:A:731:PRO:HB3	0.43	2.54	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:664:LEU:CD2	1:A:689:LEU:HD21	0.43	2.43	13	1
1:A:718:THR:HG23	1:A:724:ILE:HD12	0.43	1.89	14	1
1:A:707:PHE:CE2	1:A:717:LEU:HD21	0.43	2.48	13	1
1:A:667:LEU:CD2	1:A:667:LEU:C	0.43	2.83	19	2
1:A:647:LEU:CD1	1:A:647:LEU:N	0.43	2.82	18	1
1:A:684:GLN:O	1:A:687:LEU:CG	0.43	2.67	11	1
1:A:738:LEU:C	1:A:738:LEU:CD2	0.43	2.87	12	1
1:A:666:GLN:HG3	1:A:667:LEU:N	0.43	2.29	11	1
1:A:644:CYS:O	1:A:648:THR:CB	0.43	2.67	2	4
1:A:679:TRP:CA	1:A:683:ASP:OD2	0.43	2.67	14	1
1:A:729:LEU:C	1:A:729:LEU:HD23	0.43	2.34	10	1
1:A:681:PRO:CG	1:A:686:CYS:SG	0.43	3.07	15	1
1:A:693:LEU:HD22	1:A:693:LEU:N	0.43	2.28	2	1
1:A:689:LEU:CD1	1:A:689:LEU:C	0.43	2.87	13	2
1:A:632:LEU:HD11	1:A:654:VAL:HB	0.43	1.89	14	1
1:A:664:LEU:CD2	1:A:692:HIS:HD1	0.43	2.19	8	1
1:A:629:HIS:CE1	1:A:670:LEU:HB3	0.43	2.49	17	1
1:A:732:GLN:HG3	1:A:733:LEU:N	0.43	2.29	7	1
1:A:696:HIS:C	1:A:696:HIS:CD2	0.43	2.88	6	1
1:A:695:GLU:HG2	1:A:696:HIS:CE1	0.43	2.49	4	1
1:A:692:HIS:HE2	1:A:696:HIS:CD2	0.43	2.32	3	1
1:A:646:MET:SD	1:A:731:PRO:CB	0.42	3.07	16	1
1:A:634:GLU:HG3	1:A:635:GLU:N	0.42	2.29	7	1
1:A:635:GLU:HG2	1:A:636:GLU:N	0.42	2.30	7	2
1:A:632:LEU:HD13	1:A:632:LEU:C	0.42	2.34	6	1
1:A:655:ILE:CD1	1:A:670:LEU:HD22	0.42	2.44	15	1
1:A:674:VAL:HG21	1:A:738:LEU:HG	0.42	1.90	3	1
1:A:661:SER:N	1:A:685:SER:OG	0.42	2.52	16	1
1:A:633:LEU:CD1	1:A:657:LEU:O	0.42	2.61	5	1
1:A:706:LEU:HD23	1:A:707:PHE:N	0.42	2.29	5	1
1:A:635:GLU:O	1:A:636:GLU:O	0.42	2.38	20	1
1:A:693:LEU:CD1	1:A:693:LEU:C	0.42	2.73	4	1
1:A:706:LEU:HD21	1:A:737:THR:HG21	0.42	1.90	3	1
1:A:664:LEU:HD22	1:A:692:HIS:CE1	0.42	2.49	7	1
1:A:741:LEU:N	1:A:741:LEU:CD1	0.42	2.82	4	1
1:A:633:LEU:HD21	1:A:663:ALA:CB	0.42	2.45	3	1
1:A:674:VAL:CG1	1:A:706:LEU:CD1	0.42	2.98	12	1
1:A:712:PRO:CD	1:A:724:ILE:HD13	0.42	2.45	16	1
1:A:674:VAL:HG22	1:A:704:LEU:HB2	0.42	1.92	19	1
1:A:659:ASP:OD1	1:A:660:GLY:N	0.41	2.53	17	1
1:A:706:LEU:HD22	1:A:734:LEU:HD11	0.41	1.89	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:679:TRP:C	1:A:681:PRO:HD3	0.41	2.36	15	1
1:A:664:LEU:HD13	1:A:692:HIS:ND1	0.41	2.29	3	1
1:A:638:GLU:CG	1:A:639:ALA:N	0.41	2.83	10	1
1:A:692:HIS:CD2	1:A:692:HIS:C	0.41	2.94	11	1
1:A:717:LEU:CG	1:A:718:THR:N	0.41	2.83	20	1
1:A:695:GLU:HG3	1:A:696:HIS:CD2	0.41	2.50	15	1
1:A:632:LEU:C	1:A:633:LEU:HD12	0.41	2.35	3	1
1:A:630:ILE:CG2	1:A:676:LEU:CD1	0.41	2.98	15	2
1:A:730:ASP:N	1:A:731:PRO:HD3	0.41	2.29	20	1
1:A:679:TRP:N	1:A:708:LEU:O	0.41	2.49	4	1
1:A:629:HIS:C	1:A:629:HIS:ND1	0.41	2.73	19	1
1:A:679:TRP:C	1:A:681:PRO:HD2	0.41	2.36	16	2
1:A:725:LEU:N	1:A:725:LEU:HD12	0.41	2.30	4	1
1:A:671:GLN:N	1:A:672:PRO:CD	0.41	2.84	5	1
1:A:727:LYS:NZ	1:A:727:LYS:CB	0.41	2.83	4	1
1:A:631:LEU:HD13	1:A:667:LEU:CD1	0.41	2.38	14	1
1:A:640:ALA:HB1	1:A:656:TRP:NE1	0.41	2.31	6	1
1:A:679:TRP:CZ3	1:A:687:LEU:CD2	0.41	3.04	11	1
1:A:738:LEU:HD23	1:A:738:LEU:O	0.41	2.16	2	1
1:A:666:GLN:O	1:A:670:LEU:N	0.41	2.39	7	1
1:A:686:CYS:O	1:A:686:CYS:SG	0.41	2.79	1	1
1:A:647:LEU:O	1:A:650:ALA:HB3	0.41	2.15	5	1
1:A:690:LEU:HD21	1:A:707:PHE:CZ	0.41	2.51	8	1
1:A:690:LEU:N	1:A:690:LEU:CD2	0.41	2.83	8	1
1:A:690:LEU:HD11	1:A:707:PHE:CZ	0.41	2.50	8	1
1:A:659:ASP:C	1:A:659:ASP:OD1	0.41	2.59	6	1
1:A:705:VAL:HG12	1:A:707:PHE:CE1	0.41	2.50	4	1
1:A:727:LYS:N	1:A:728:PRO:HD3	0.41	2.30	3	1
1:A:677:MET:HE1	1:A:686:CYS:SG	0.41	2.56	9	1
1:A:683:ASP:OD1	1:A:685:SER:OG	0.41	2.39	15	1
1:A:684:GLN:C	1:A:684:GLN:CD	0.40	2.80	10	1
1:A:741:LEU:HD12	1:A:741:LEU:H	0.40	1.74	10	1
1:A:633:LEU:CD1	1:A:633:LEU:N	0.40	2.84	3	1
1:A:629:HIS:CE1	1:A:672:PRO:HB3	0.40	2.50	17	1
1:A:637:ASP:OD1	1:A:637:ASP:N	0.40	2.54	5	1
1:A:729:LEU:CG	1:A:730:ASP:H	0.40	2.29	4	1
1:A:693:LEU:CG	1:A:694:ARG:N	0.40	2.84	4	1
1:A:657:LEU:HD13	1:A:663:ALA:HB2	0.40	1.92	6	1
1:A:640:ALA:HA	1:A:656:TRP:CZ2	0.40	2.50	3	1
1:A:738:LEU:HD12	1:A:738:LEU:N	0.40	2.31	3	1
1:A:634:GLU:OE2	1:A:678:ALA:CB	0.40	2.68	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:735:LEU:CD2	1:A:735:LEU:N	0.40	2.84	16	1
1:A:728:PRO:O	1:A:729:LEU:HB3	0.40	2.15	9	1
1:A:710:GLU:CA	1:A:710:GLU:OE1	0.40	2.68	13	1
1:A:717:LEU:CD1	1:A:718:THR:N	0.40	2.85	20	1
1:A:674:VAL:HG21	1:A:738:LEU:CD2	0.40	2.46	18	1
1:A:675:ILE:C	1:A:676:LEU:HD23	0.40	2.37	18	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	109/119 (92%)	98±2 (90±2%)	6±3 (6±2%)	5±2 (5±1%)	5	28
All	All	2180/2380 (92%)	1953 (90%)	125 (6%)	102 (5%)	5	28

All 17 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	636	GLU	18
1	A	726	SER	15
1	A	740	GLY	10
1	A	682	PRO	9
1	A	729	LEU	9
1	A	684	GLN	9
1	A	731	PRO	7
1	A	730	ASP	5
1	A	679	TRP	4
1	A	696	HIS	4
1	A	703	PRO	3
1	A	712	PRO	2
1	A	683	ASP	2
1	A	727	LYS	2
1	A	681	PRO	1
1	A	713	VAL	1

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Mol	Chain	Res	Type	Models (Total)
1	A	628	GLY	1

6.3.2 Protein sidechains

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	95/103 (92%)	90±2 (94±2%)	5±2 (6±2%)	30	75
All	All	1900/2060 (92%)	1791 (94%)	109 (6%)	30	75

All 34 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	714	ASP	12
1	A	727	LYS	9
1	A	670	LEU	8
1	A	688	LEU	8
1	A	644	CYS	7
1	A	710	GLU	6
1	A	696	HIS	6
1	A	686	CYS	6
1	A	730	ASP	5
1	A	729	LEU	4
1	A	632	LEU	3
1	A	689	LEU	3
1	A	677	MET	3
1	A	726	SER	3
1	A	716	LEU	2
1	A	708	LEU	2
1	A	704	LEU	2
1	A	741	LEU	2
1	A	676	LEU	2
1	A	667	LEU	2
1	A	717	LEU	1
1	A	694	ARG	1
1	A	722	SER	1
1	A	631	LEU	1

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Mol	Chain	Res	Type	Models (Total)
1	A	665	ASP	1
1	A	664	LEU	1
1	A	656	TRP	1
1	A	658	VAL	1
1	A	732	GLN	1
1	A	693	LEU	1
1	A	684	GLN	1
1	A	683	ASP	1
1	A	679	TRP	1
1	A	634	GLU	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 carbohydrates 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

The completeness of assignment taking into account all chemical shift lists is 86% for the well-defined parts and 86% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 6438

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 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	1614
Number of shifts mapped to atoms	1442
Number of unparsed shifts	0
Number of shifts with mapping errors	172
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- Residue not found in structure. All 172 occurences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	136	SER	CB	64.03	0.5	1
A	130	SER	CB	63.93	0.5	1
A	130	SER	CA	58.41	0.5	1
A	5	ILE	HG13	1.14	0.05	2
A	131	GLU	HA	4.29	0.05	1
A	7	ASN	HB3	2.73	0.05	2
A	135	PRO	HG2	2.0	0.05	1
A	129	LEU	HB3	1.63	0.05	1
A	9	PRO	HA	4.42	0.05	1
A	134	ARG	CA	54.03	0.5	1
A	4	MET	H	8.3	0.05	1
A	137	SER	HB2	3.87	0.05	1
A	5	ILE	HD12	0.85	0.05	1
A	134	ARG	CG	26.69	0.5	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	8	LEU	HD23	0.86	0.05	1
A	129	LEU	CD1	25.08	0.5	1
A	9	PRO	HG2	2.22	0.05	2
A	133	ASP	CA	54.34	0.5	1
A	8	LEU	HB2	1.61	0.05	2
A	5	ILE	HG21	0.88	0.05	1
A	4	MET	CG	31.5	0.5	1
A	7	ASN	ND2	112.68	0.3	1
A	9	PRO	HD3	3.59	0.05	2
A	129	LEU	HD12	0.93	0.05	1
A	135	PRO	HA	4.51	0.05	1
A	129	LEU	CA	55.27	0.5	1
A	133	ASP	N	120.26	0.3	1
A	135	PRO	CG	27.37	0.5	1
A	132	GLY	N	109.28	0.3	1
A	131	GLU	HG3	2.28	0.05	1
A	131	GLU	CA	57.08	0.5	1
A	6	ASP	HB2	2.64	0.05	1
A	133	ASP	HB3	2.6	0.05	2
A	137	SER	CB	64.88	0.5	1
A	9	PRO	HB3	1.84	0.05	2
A	5	ILE	CB	38.78	0.5	1
A	4	MET	HE2	2.11	0.05	1
A	137	SER	H	7.98	0.05	1
A	136	SER	H	8.53	0.05	1
A	129	LEU	HA	4.4	0.05	1
A	5	ILE	HG22	0.88	0.05	1
A	135	PRO	CB	32.23	0.5	1
A	136	SER	N	116.83	0.3	1
A	6	ASP	N	123.68	0.3	1
A	8	LEU	CD1	23.47	0.5	1
A	132	GLY	CA	45.29	0.5	1
A	5	ILE	CD1	13.12	0.5	1
A	5	ILE	N	121.72	0.3	1
A	4	MET	CA	54.98	0.5	1
A	8	LEU	N	123.2	0.3	1
A	4	MET	HB3	1.99	0.05	2
A	9	PRO	CD	50.46	0.5	1
A	135	PRO	HB3	2.0	0.05	2
A	130	SER	HB3	3.88	0.05	2
A	5	ILE	HG12	1.43	0.05	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	4	MET	HA	4.43	0.05	1
A	8	LEU	H	8.12	0.05	1
A	6	ASP	CB	41.3	0.5	1
A	129	LEU	HB2	1.63	0.05	1
A	137	SER	HB3	3.87	0.05	1
A	8	LEU	HD13	0.86	0.05	1
A	8	LEU	HB3	1.48	0.05	2
A	5	ILE	HD13	0.85	0.05	1
A	8	LEU	CB	41.79	0.5	1
A	134	ARG	HE	7.22	0.05	1
A	8	LEU	CD2	23.47	0.5	1
A	134	ARG	HG3	1.68	0.05	1
A	132	GLY	HA2	3.96	0.05	1
A	129	LEU	CG	27.08	0.5	1
A	7	ASN	H	8.34	0.05	1
A	137	SER	CA	60.02	0.5	1
A	129	LEU	CD2	23.4	0.5	1
A	8	LEU	HA	4.58	0.05	1
A	9	PRO	HG3	2.02	0.05	2
A	133	ASP	CB	41.34	0.5	1
A	134	ARG	HA	4.65	0.05	1
A	9	PRO	HD2	3.77	0.05	2
A	129	LEU	HD11	0.93	0.05	1
A	134	ARG	CD	43.43	0.5	1
A	132	GLY	H	8.36	0.05	1
A	130	SER	H	8.38	0.05	1
A	131	GLU	HG2	2.28	0.05	1
A	131	GLU	HB2	2.09	0.05	2
A	135	PRO	HD3	3.65	0.05	2
A	3	HIS	CA	54.73	0.5	1
A	9	PRO	HB2	2.22	0.05	2
A	129	LEU	HG	1.09	0.05	1
A	135	PRO	CA	63.21	0.5	1
A	4	MET	HE3	2.11	0.05	1
A	137	SER	HA	4.28	0.05	1
A	4	MET	N	120.5	0.3	1
A	129	LEU	HD21	0.87	0.05	1
A	4	MET	HG2	2.1	0.05	2
A	3	HIS	N	121.66	0.3	1
A	4	MET	CB	32.98	0.5	1
A	5	ILE	HG23	0.88	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	134	ARG	HG2	1.68	0.05	1
A	134	ARG	NE	84.59	0.3	1
A	134	ARG	HB3	1.76	0.05	2
A	131	GLU	N	122.92	0.3	1
A	7	ASN	HD21	6.88	0.05	1
A	7	ASN	CA	53.3	0.5	1
A	4	MET	HB2	1.96	0.05	2
A	9	PRO	CG	27.3	0.5	1
A	136	SER	HB3	3.9	0.05	2
A	136	SER	HA	4.47	0.05	1
A	134	ARG	N	121.91	0.3	1
A	135	PRO	HB2	2.34	0.05	2
A	3	HIS	HB2	3.11	0.05	2
A	7	ASN	N	118.1	0.3	1
A	133	ASP	HA	4.62	0.05	1
A	3	HIS	CB	31.87	0.5	1
A	5	ILE	HA	4.17	0.05	1
A	130	SER	N	116.62	0.3	1
A	3	HIS	HD2	6.92	0.05	1
A	130	SER	HB2	4.06	0.05	2
A	6	ASP	CA	54.52	0.5	1
A	129	LEU	HD22	0.87	0.05	1
A	3	HIS	HA	4.14	0.05	1
A	7	ASN	HA	4.67	0.05	1
A	8	LEU	HG	0.86	0.05	1
A	134	ARG	HD3	3.22	0.05	1
A	131	GLU	H	8.45	0.05	1
A	8	LEU	HD12	0.86	0.05	1
A	8	LEU	CA	53.2	0.5	1
A	5	ILE	H	8.18	0.05	1
A	134	ARG	HD2	3.22	0.05	1
A	8	LEU	HD21	0.86	0.05	1
A	134	ARG	CB	30.32	0.5	1
A	132	GLY	HA3	3.96	0.05	1
A	5	ILE	HB	1.85	0.05	1
A	9	PRO	CB	32.11	0.5	1
A	4	MET	CE	17.07	0.5	1
A	130	SER	HA	4.46	0.05	1
A	135	PRO	CD	50.71	0.5	1
A	7	ASN	HB2	2.8	0.05	2
A	136	SER	CA	58.45	0.5	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	6	ASP	HA	4.58	0.05	1
A	131	GLU	HB3	1.97	0.05	2
A	129	LEU	N	123.24	0.3	1
A	135	PRO	HD2	3.81	0.05	2
A	5	ILE	HD11	0.85	0.05	1
A	9	PRO	N	136.48	0.3	1
A	7	ASN	HD22	7.55	0.05	1
A	8	LEU	HD22	0.86	0.05	1
A	4	MET	HG3	2.26	0.05	2
A	129	LEU	H	8.28	0.05	1
A	9	PRO	CA	63.01	0.5	1
A	131	GLU	CB	30.32	0.5	1
A	129	LEU	HD13	0.93	0.05	1
A	134	ARG	HB2	1.86	0.05	2
A	5	ILE	CG1	27.23	0.5	1
A	129	LEU	CB	42.37	0.5	1
A	7	ASN	CB	39.02	0.5	1
A	6	ASP	H	8.37	0.05	1
A	133	ASP	H	8.2	0.05	1
A	136	SER	HB2	3.94	0.05	2
A	3	HIS	CD2	117.53	0.5	1
A	6	ASP	HB3	2.64	0.05	1
A	133	ASP	HB2	2.68	0.05	2
A	3	HIS	HB3	2.85	0.05	2
A	134	ARG	H	8.19	0.05	1
A	5	ILE	CA	61.27	0.5	1
A	8	LEU	CG	26.29	0.5	1
A	4	MET	HE1	2.11	0.05	1
A	131	GLU	CG	36.34	0.5	1
A	129	LEU	HD23	0.87	0.05	1
A	135	PRO	N	137.93	0.3	1
A	8	LEU	HD11	0.86	0.05	1
A	137	SER	N	122.92	0.3	1
A	135	PRO	HG3	2.0	0.05	1
A	5	ILE	CG2	17.62	0.5	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	135	-0.12 ± 0.14	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	129	0.24 ± 0.08	None needed (< 0.5 ppm)
$^{13}C'$	0	—	—
^{15}N	135	0.28 ± 0.36	None needed (< 0.5 ppm)

7.1.3 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 86%, i.e. 1126 atoms were assigned a chemical shift out of a possible 1306. 34 out of 34 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	411/523 (79%)	204/207 (99%)	109/218 (50%)	98/98 (100%)
Sidechain	673/717 (94%)	403/415 (97%)	262/290 (90%)	8/12 (67%)
Aromatic	42/66 (64%)	21/34 (62%)	21/24 (88%)	0/8 (0%)
Overall	1126/1306 (86%)	628/656 (96%)	392/532 (74%)	106/118 (90%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 86%, i.e. 1217 atoms were assigned a chemical shift out of a possible 1416. 34 out of 34 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	445/567 (78%)	221/224 (99%)	119/238 (50%)	105/105 (100%)
Sidechain	728/775 (94%)	439/451 (97%)	279/310 (90%)	10/14 (71%)
Aromatic	44/74 (59%)	22/38 (58%)	22/26 (85%)	0/10 (0%)
Overall	1217/1416 (86%)	682/713 (96%)	420/574 (73%)	115/129 (89%)

7.1.4 Statistically unusual chemical shifts

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	640	ALA	HB1	0.01	2.61 – 0.11	-5.4
1	A	640	ALA	HB2	0.01	2.61 – 0.11	-5.4
1	A	640	ALA	HB3	0.01	2.61 – 0.11	-5.4

7.1.5 Random Coil Index (RCI) plots

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: