Full wwPDB NMR Structure Validation Report (i)

Apr 26, 2016 – 07:33 PM BST

PDB ID	:	2AYX
Title	:	Solution structure of the E.coli RcsC C-terminus (residues 700-949) containing linker region and phosphoreceiver domain
Authors	:	Rogov, V.V.; Rogova, N.Y.; Bernhard, F.; Koglin, A.; Lohr, F.; Dotsch, V.
Deposited on	:	2005-09-09

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:

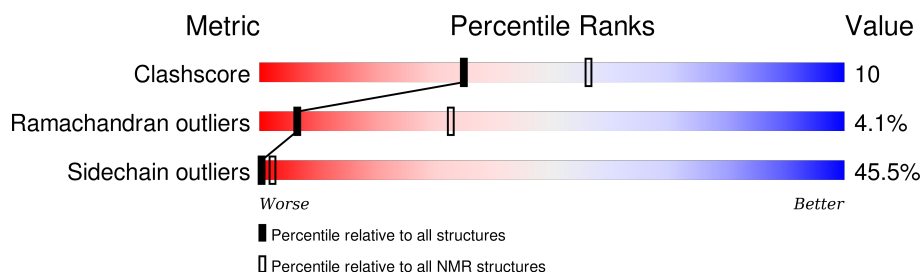|		
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457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

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

The overall completeness of chemical shifts assignment is 88%.

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	Percentile Ranks	Value
Clashscore		10
Ramachandran outliers		4.1%
Sidechain outliers		45.5%

Worse | | *Better*

▮ Percentile relative to all structures
▯ Percentile relative to all NMR structures

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	254	33% 50% • 15%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 2 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy and fewest violation*.

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:705-A:800 (96)	0.53	12
2	A:824-A:878,　A:883-A:948 (121)	0.68	2

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 5 clusters. No single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 3930 atoms, of which 1978 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Sensor kinase protein rcsC.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	254	3930	1213	1978	346	380	13	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	696	MET	-	CLONING ARTIFACT	UNP P14376
A	697	GLY	-	CLONING ARTIFACT	UNP P14376
A	698	GLY	-	CLONING ARTIFACT	UNP P14376
A	699	SER	-	CLONING ARTIFACT	UNP P14376

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.

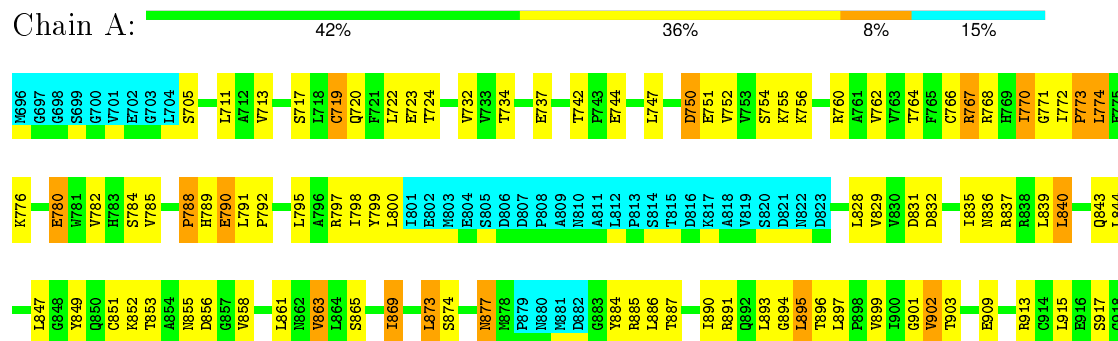- Molecule 1: Sensor kinase protein rcsC
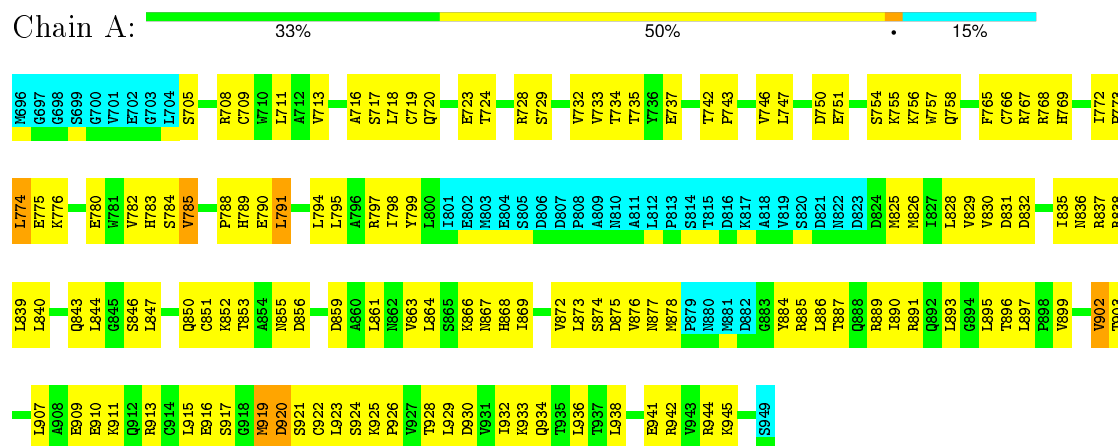
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Sensor kinase protein rcsC

4.2.2 Score per residue for model 2 (medoid)

• Molecule 1: Sensor kinase protein rcsC

4.2.3 Score per residue for model 3
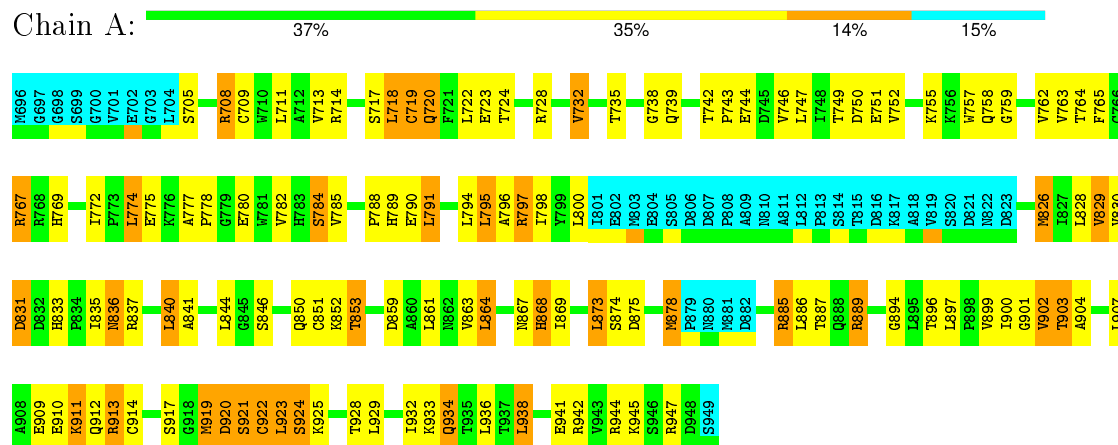
• Molecule 1: Sensor kinase protein rcsC

4.2.4 Score per residue for model 4

• Molecule 1: Sensor kinase protein rcsC

4.2.5 Score per residue for model 5

• Molecule 1: Sensor kinase protein rcsC

Chain A: 37% 36% 12% 15%

4.2.6 Score per residue for model 6

• Molecule 1: Sensor kinase protein rcsC

Chain A: 35% 38% 12% 15%

4.2.7 Score per residue for model 7

• Molecule 1: Sensor kinase protein rcsC

Chain A:

4.2.8 Score per residue for model 8

• Molecule 1: Sensor kinase protein rcsC

Chain A:
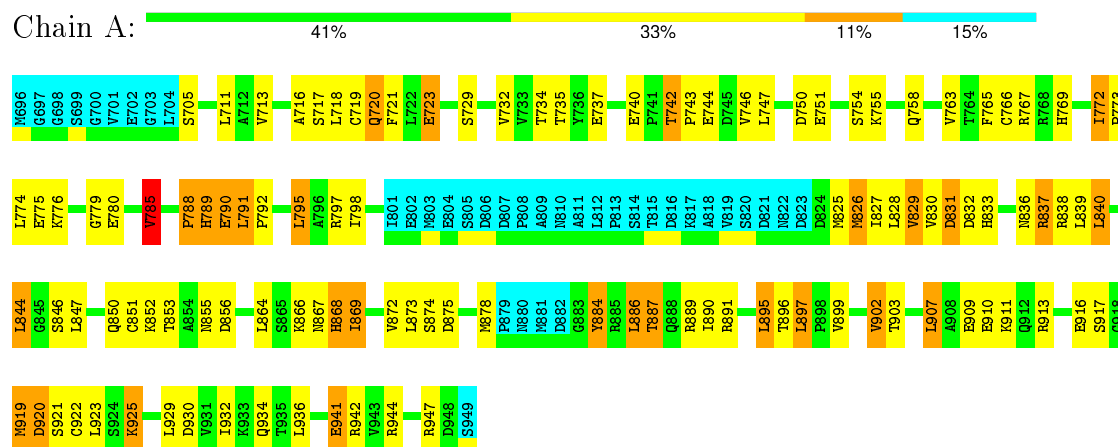

4.2.9 Score per residue for model 9

• Molecule 1: Sensor kinase protein rcsC

Chain A:
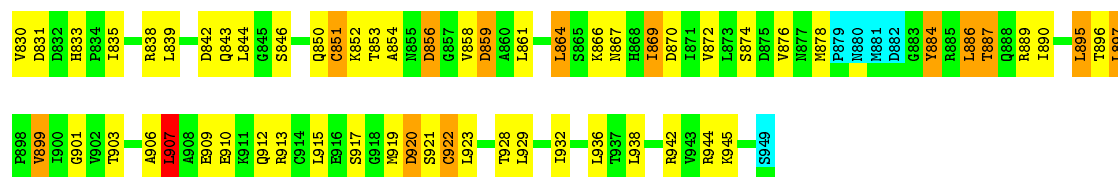
4.2.10 Score per residue for model 10

• Molecule 1: Sensor kinase protein rcsC

Chain A: 34% | 38% | 13% | 15%
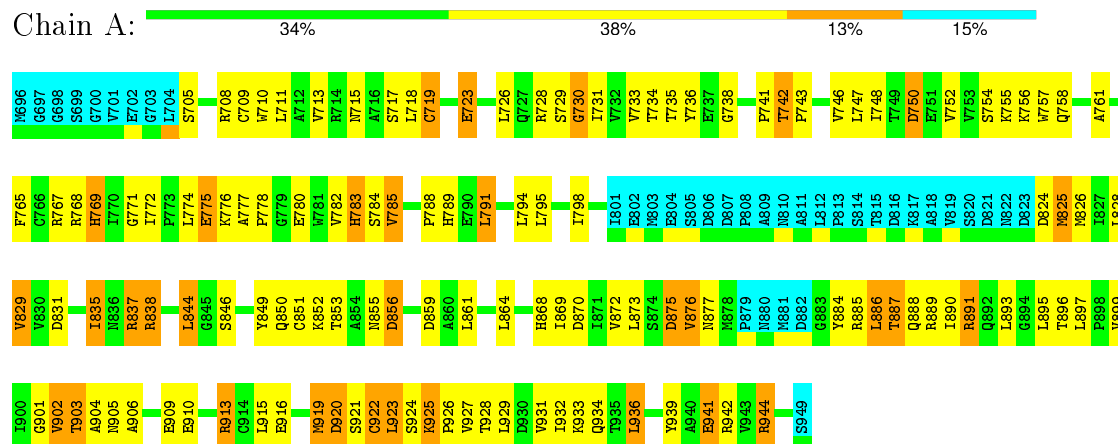
4.2.11 Score per residue for model 11

• Molecule 1: Sensor kinase protein rcsC

Chain A: 37% | 37% | 11% | 15%
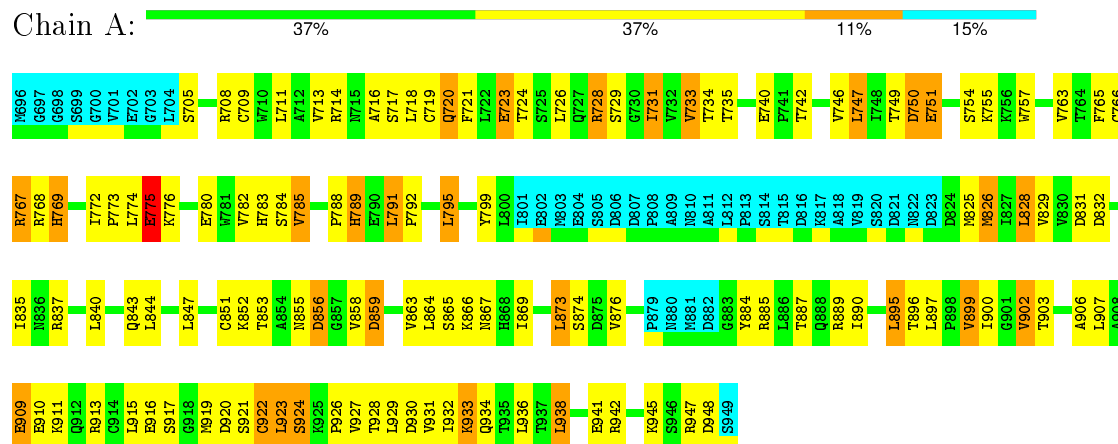
4.2.12 Score per residue for model 12

• Molecule 1: Sensor kinase protein rcsC

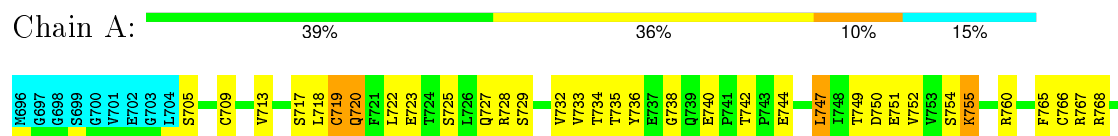Chain A: 37% | 37% | 11% | 15%
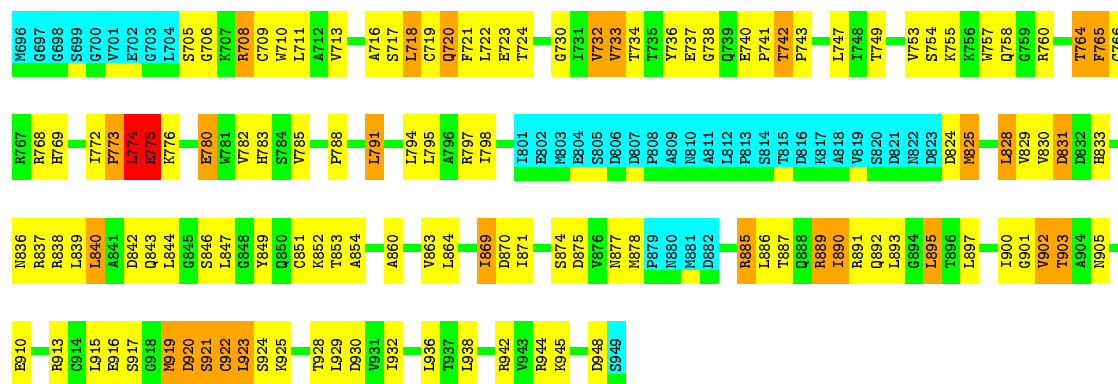
4.2.13 Score per residue for model 13
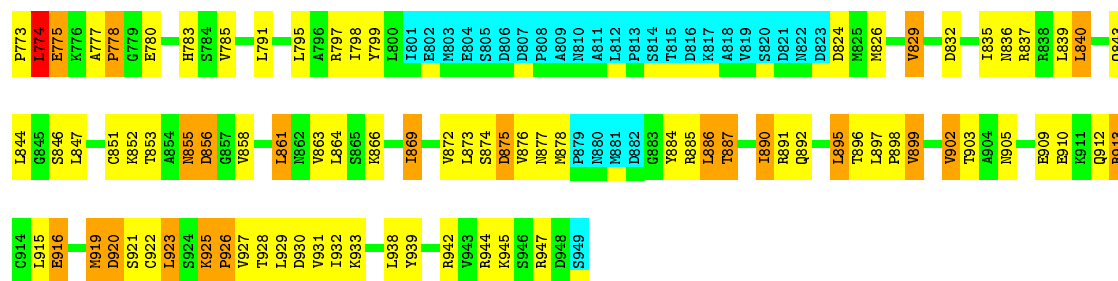
• Molecule 1: Sensor kinase protein rcsC
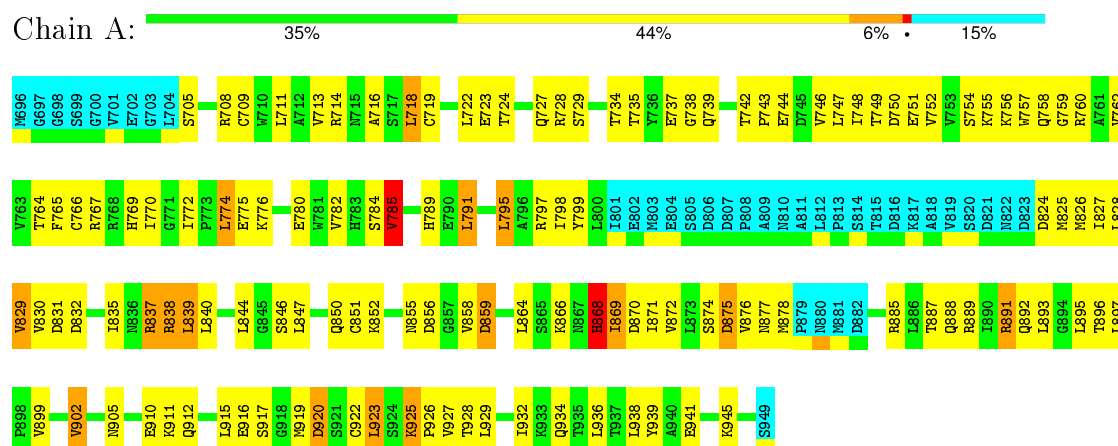
4.2.14 Score per residue for model 14

• Molecule 1: Sensor kinase protein rcsC
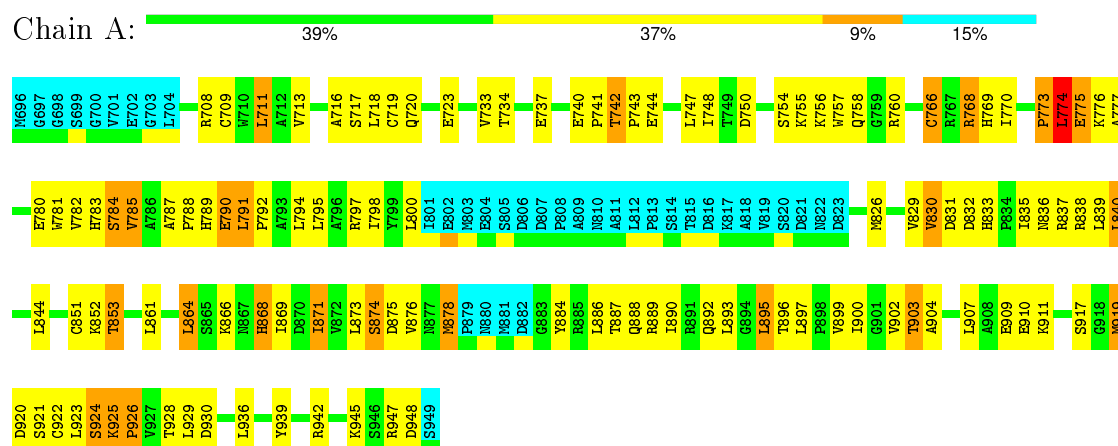
4.2.15 Score per residue for model 15

• Molecule 1: Sensor kinase protein rcsC

Chain A:
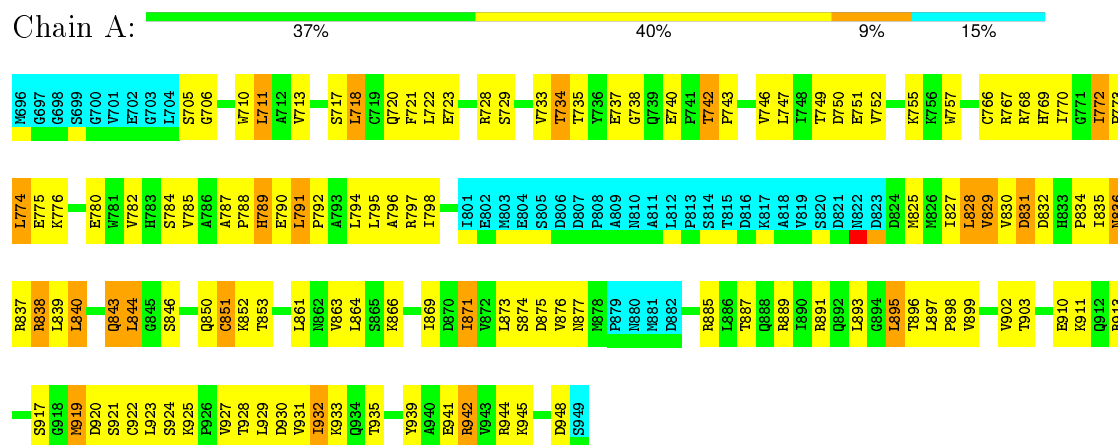
4.2.16 Score per residue for model 16

• Molecule 1: Sensor kinase protein rcsC

Chain A:
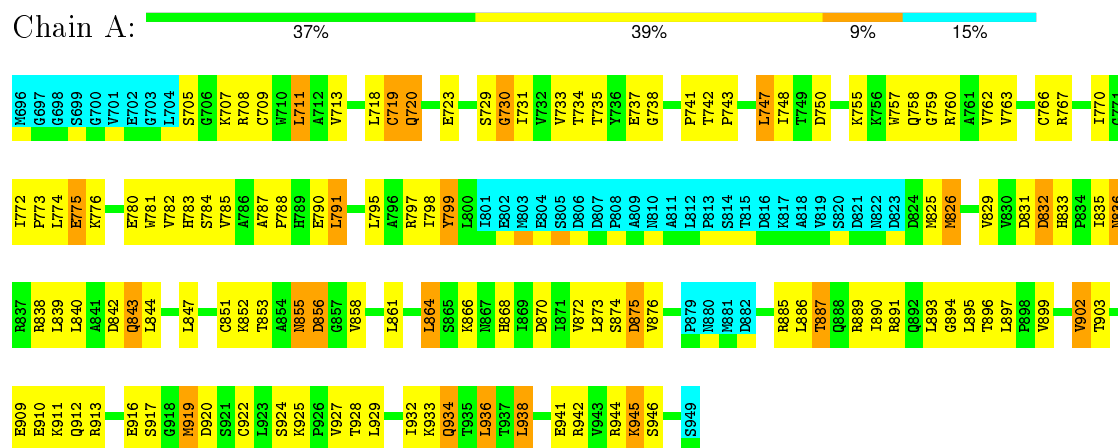
4.2.17 Score per residue for model 17

• Molecule 1: Sensor kinase protein rcsC

Chain A:
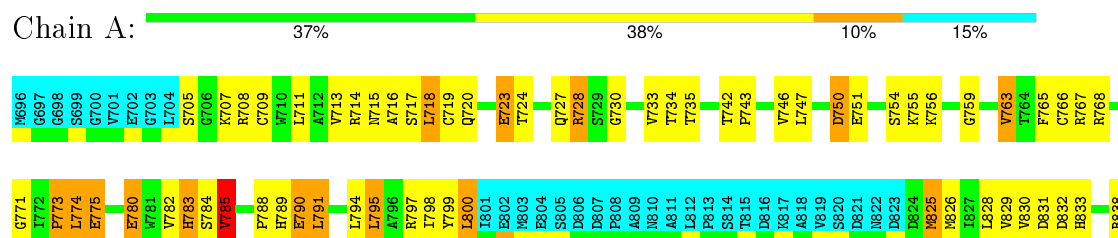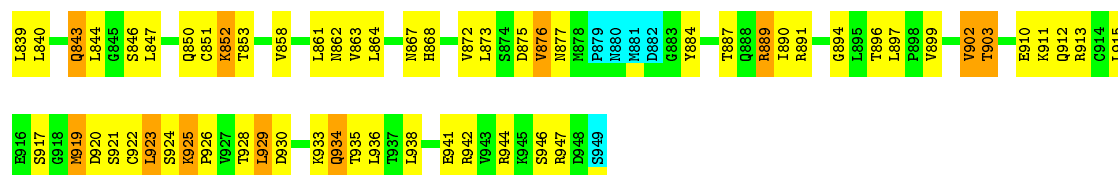
4.2.18 Score per residue for model 18
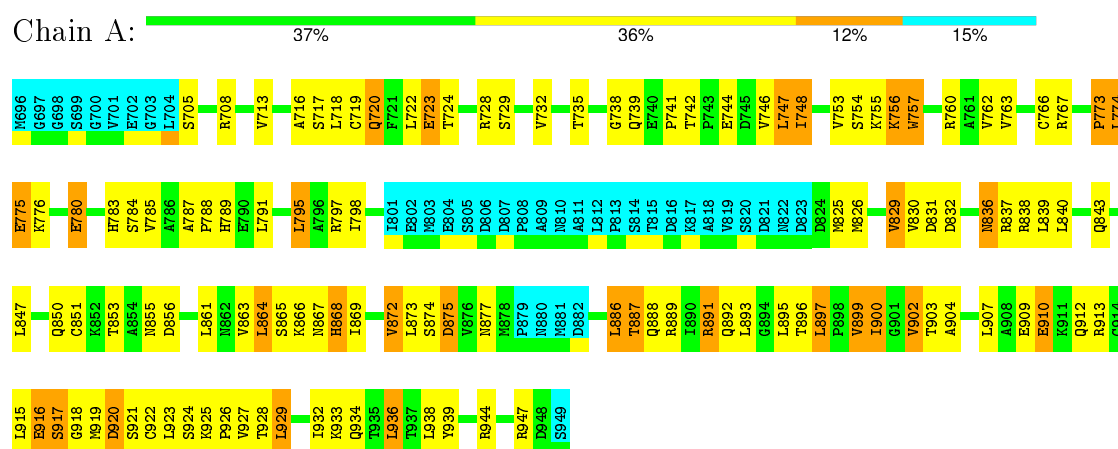
• Molecule 1: Sensor kinase protein rcsC
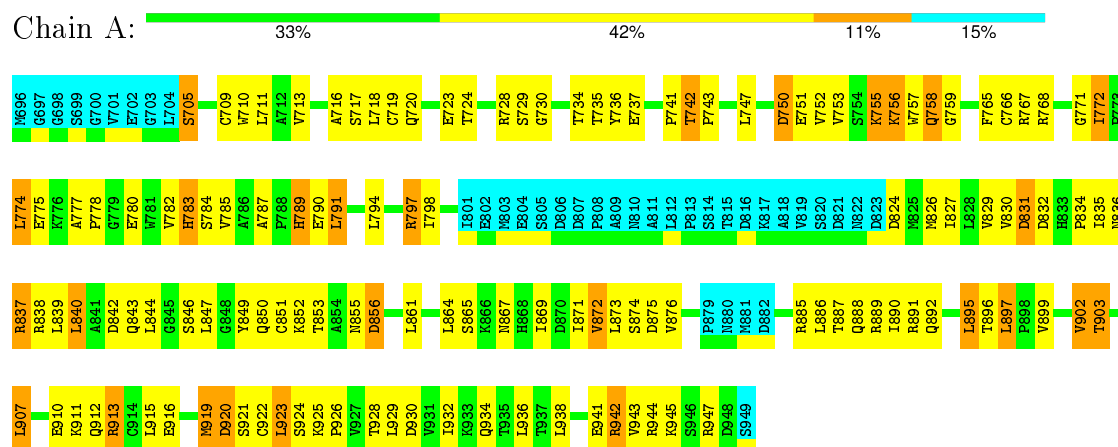
4.2.19 Score per residue for model 19
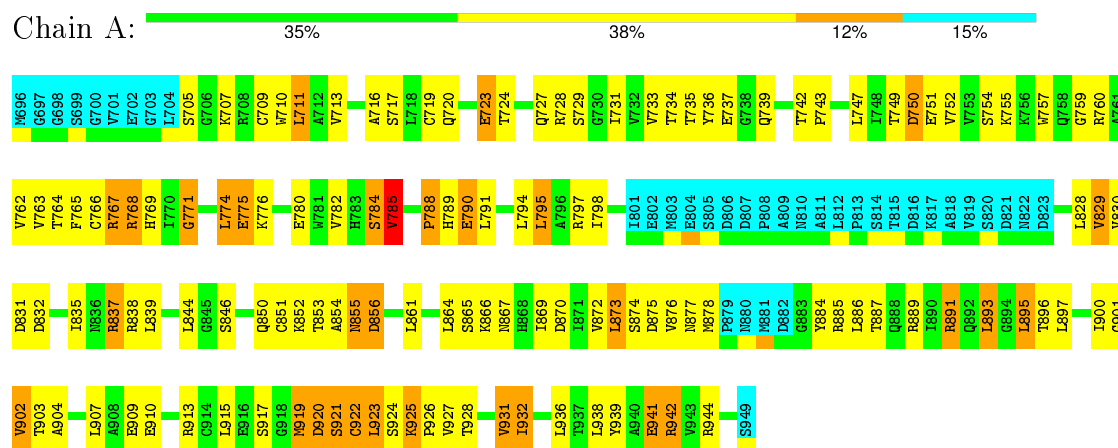
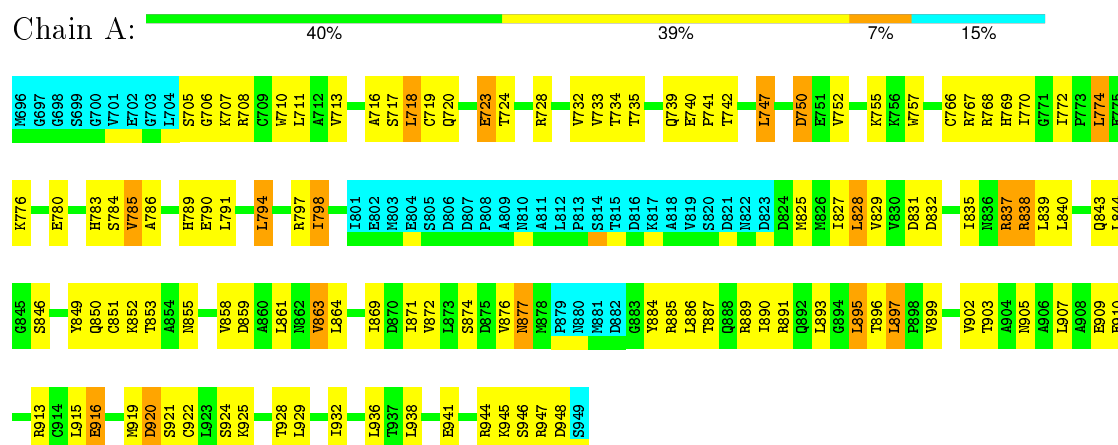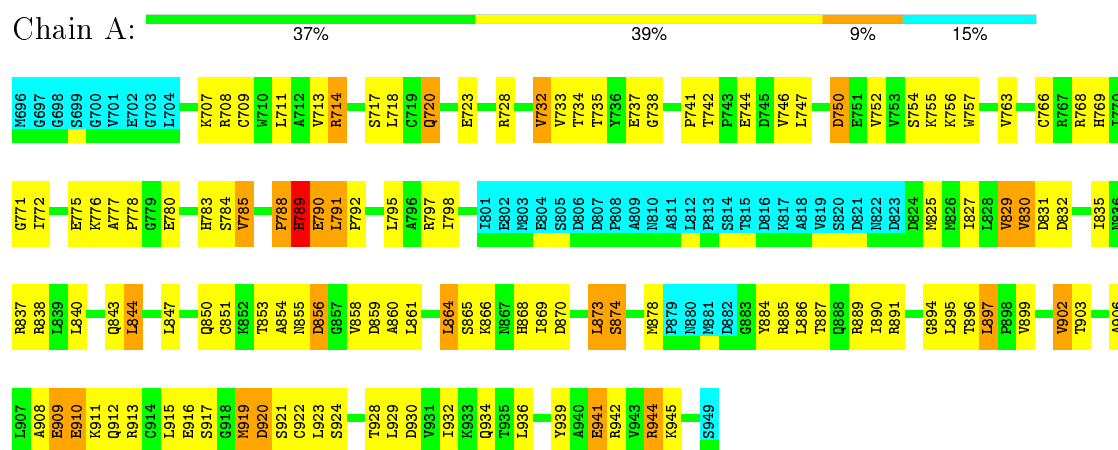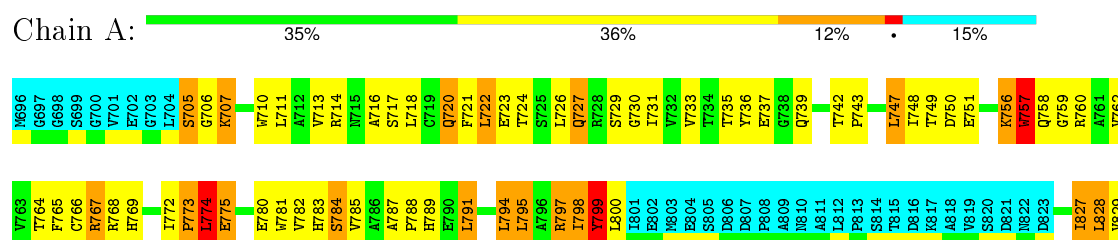• Molecule 1: Sensor kinase protein rcsC
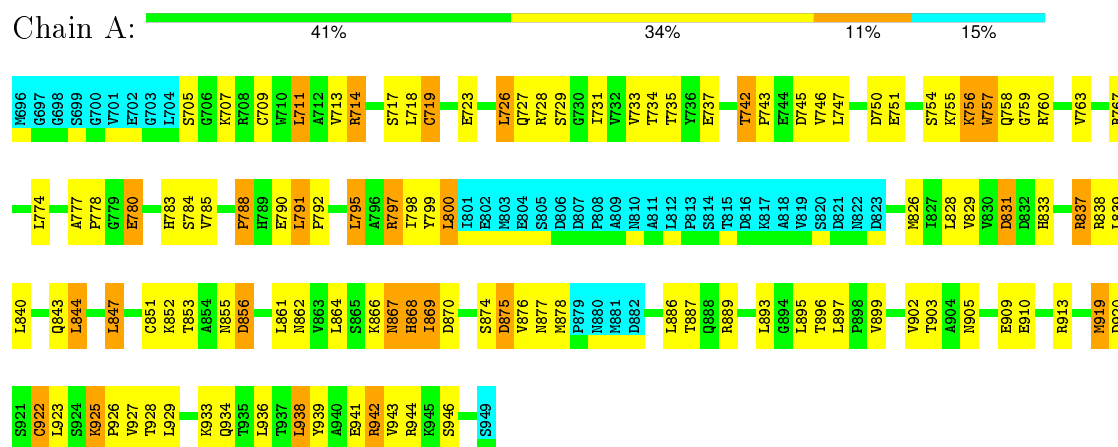
4.2.20 Score per residue for model 20

• Molecule 1: Sensor kinase protein rcsC
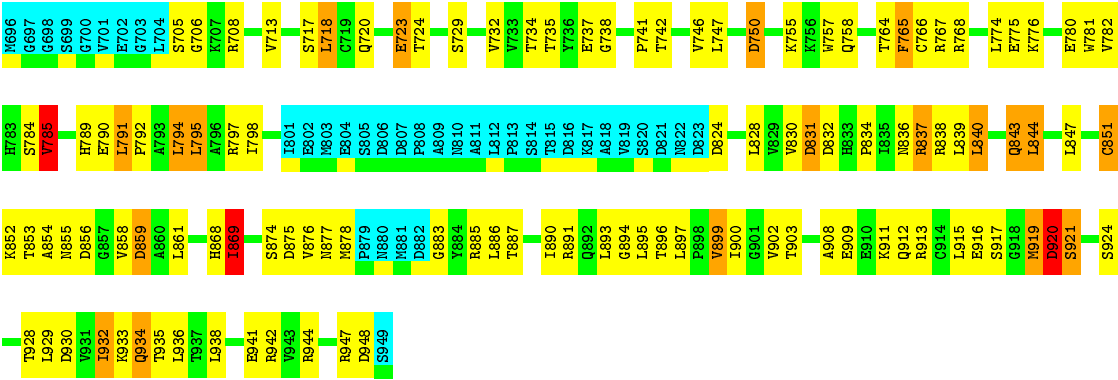
5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *Energy minimization*.

Of the 30 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
DYANA	structure solution	1.5
CNS	refinement	1.1

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 6810
Number of chemical shift lists	1
Total number of shifts	3026
Number of shifts mapped to atoms	3026
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	88%

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

6 Model quality (i)

6.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.29±0.02	0±0/1719 (0.0±0.0%)	0.40±0.01	0±0/2335 (0.0±0.0%)
All	All	0.29	1/34380 (0.0%)	0.40	0/46700 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.1±0.2
All	All	0	1

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	799	TYR	CE2-CZ	6.80	1.47	1.38	9	1

There are no bond-angle outliers.

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	799	TYR	Sidechain	1

6.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1692	1745	1740	36±7
All	All	33840	34900	34800	721

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 11.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:831:ASP:HB3	1:A:837:ARG:HB2	0.88	1.46	20	8
1:A:772:ILE:HG13	1:A:773:PRO:HD2	0.88	1.44	1	2
1:A:832:ASP:HB3	1:A:876:VAL:HB	0.85	1.45	16	1
1:A:743:PRO:HA	1:A:759:GLY:HA2	0.84	1.49	9	8
1:A:843:GLN:HG2	1:A:929:LEU:HD23	0.81	1.53	12	3
1:A:751:GLU:HG2	1:A:752:VAL:H	0.80	1.37	6	1
1:A:902:VAL:HB	1:A:923:LEU:HB2	0.80	1.53	8	3
1:A:827:ILE:HB	1:A:844:LEU:HD21	0.78	1.55	8	3
1:A:713:VAL:HA	1:A:750:ASP:HB2	0.78	1.54	19	6
1:A:711:LEU:HD21	1:A:733:VAL:HG13	0.76	1.57	19	1
1:A:843:GLN:HG2	1:A:929:LEU:HD12	0.76	1.56	8	1
1:A:751:GLU:HG2	1:A:767:ARG:HH21	0.75	1.41	9	2
1:A:891:ARG:HA	1:A:895:LEU:HB2	0.74	1.59	1	2
1:A:902:VAL:HB	1:A:923:LEU:HB3	0.74	1.57	18	1
1:A:752:VAL:HG21	1:A:770:ILE:HB	0.74	1.60	13	1
1:A:764:THR:HB	1:A:782:VAL:HG12	0.72	1.59	20	5
1:A:899:VAL:HB	1:A:919:MET:HA	0.71	1.59	1	12
1:A:829:VAL:HB	1:A:837:ARG:HD2	0.71	1.60	6	2
1:A:723:GLU:HA	1:A:733:VAL:HG21	0.70	1.60	6	1
1:A:828:LEU:HD23	1:A:869:ILE:HG12	0.70	1.62	7	1
1:A:877:ASN:HB2	1:A:925:LYS:HE3	0.70	1.62	12	1
1:A:887:THR:HG21	1:A:919:MET:HG2	0.70	1.63	3	1
1:A:713:VAL:HB	1:A:719:CYS:SG	0.69	2.27	19	3
1:A:752:VAL:HG22	1:A:772:ILE:HB	0.69	1.64	10	1
1:A:765:PHE:HZ	1:A:791:LEU:HG	0.69	1.47	9	3
1:A:765:PHE:CZ	1:A:791:LEU:HG	0.69	2.22	9	5
1:A:723:GLU:HB2	1:A:733:VAL:HG11	0.68	1.64	8	2
1:A:774:LEU:HA	1:A:782:VAL:HG13	0.68	1.65	14	5
1:A:899:VAL:HG13	1:A:919:MET:HA	0.68	1.65	4	5
1:A:777:ALA:HB1	1:A:778:PRO:HD2	0.67	1.66	10	6
1:A:861:LEU:HG	1:A:890:ILE:HA	0.67	1.65	7	1
1:A:726:LEU:HD23	1:A:731:ILE:HD12	0.67	1.65	19	1
1:A:902:VAL:HB	1:A:923:LEU:HD12	0.67	1.66	4	7
1:A:872:VAL:HB	1:A:899:VAL:HB	0.67	1.66	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:746:VAL:HG21	1:A:795:LEU:HD11	0.67	1.66	2	8
1:A:765:PHE:HE1	1:A:785:VAL:HG23	0.66	1.51	20	4
1:A:723:GLU:HA	1:A:733:VAL:HG11	0.66	1.66	11	2
1:A:843:GLN:HG3	1:A:929:LEU:HD23	0.66	1.67	15	4
1:A:788:PRO:HD2	1:A:790:GLU:OE1	0.66	1.91	8	6
1:A:861:LEU:HD23	1:A:890:ILE:HG13	0.65	1.69	7	1
1:A:713:VAL:HG13	1:A:750:ASP:HB3	0.65	1.68	1	9
1:A:713:VAL:HA	1:A:750:ASP:CB	0.65	2.21	13	5
1:A:767:ARG:HA	1:A:784:SER:HB3	0.64	1.69	2	1
1:A:742:THR:HG22	1:A:743:PRO:HD2	0.64	1.68	12	6
1:A:831:ASP:HB2	1:A:837:ARG:NE	0.64	2.08	6	2
1:A:919:MET:O	1:A:920:ASP:HB2	0.64	1.92	18	13
1:A:913:ARG:HD2	1:A:922:CYS:HB2	0.64	1.70	11	1
1:A:913:ARG:HA	1:A:919:MET:HE1	0.64	1.67	4	1
1:A:705:SER:HA	1:A:730:GLY:O	0.64	1.93	18	3
1:A:720:GLN:HA	1:A:723:GLU:HG2	0.63	1.69	16	8
1:A:785:VAL:HG13	1:A:787:ALA:H	0.63	1.54	14	4
1:A:752:VAL:HG13	1:A:772:ILE:HG13	0.63	1.70	18	2
1:A:904:ALA:HA	1:A:925:LYS:HB2	0.63	1.71	14	2
1:A:716:ALA:HA	1:A:719:CYS:SG	0.63	2.34	13	9
1:A:861:LEU:HD21	1:A:890:ILE:HA	0.63	1.70	18	2
1:A:861:LEU:HD13	1:A:890:ILE:HA	0.62	1.69	1	1
1:A:762:VAL:HG13	1:A:780:GLU:HG2	0.62	1.69	1	1
1:A:885:ARG:O	1:A:889:ARG:HB2	0.62	1.94	12	2
1:A:751:GLU:HG2	1:A:752:VAL:N	0.62	2.09	6	1
1:A:788:PRO:HG2	1:A:790:GLU:HG2	0.62	1.69	2	1
1:A:902:VAL:HG12	1:A:925:LYS:HA	0.62	1.71	19	1
1:A:831:ASP:HB2	1:A:875:ASP:HB3	0.61	1.72	12	4
1:A:873:LEU:HD11	1:A:936:LEU:HD11	0.61	1.71	16	1
1:A:899:VAL:HG22	1:A:919:MET:HB3	0.61	1.73	4	1
1:A:710:TRP:HB3	1:A:736:TYR:HB2	0.61	1.73	6	5
1:A:902:VAL:HG22	1:A:925:LYS:HE2	0.61	1.73	17	1
1:A:713:VAL:HB	1:A:719:CYS:HB3	0.61	1.73	5	3
1:A:773:PRO:O	1:A:774:LEU:HB3	0.60	1.97	12	5
1:A:831:ASP:HA	1:A:875:ASP:HB2	0.60	1.72	16	2
1:A:841:ALA:HB2	1:A:853:THR:HG21	0.60	1.72	2	1
1:A:764:THR:HG21	1:A:772:ILE:HG13	0.60	1.72	9	2
1:A:901:GLY:HA3	1:A:919:MET:SD	0.60	2.37	10	1
1:A:830:VAL:HG23	1:A:874:SER:HA	0.60	1.73	14	1
1:A:748:ILE:HG23	1:A:763:VAL:HB	0.59	1.73	5	1
1:A:861:LEU:HD21	1:A:893:LEU:HD12	0.59	1.73	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:713:VAL:HG13	1:A:750:ASP:HB2	0.59	1.75	4	3
1:A:872:VAL:HG23	1:A:897:LEU:HD11	0.58	1.73	16	4
1:A:828:LEU:HB3	1:A:872:VAL:HG22	0.58	1.75	13	2
1:A:924:SER:HB2	1:A:926:PRO:HD2	0.58	1.75	14	2
1:A:837:ARG:NH2	1:A:840:LEU:HD11	0.58	2.13	13	1
1:A:831:ASP:HA	1:A:875:ASP:O	0.58	1.97	3	7
1:A:888:GLN:HA	1:A:891:ARG:HD3	0.58	1.74	13	2
1:A:726:LEU:HB3	1:A:731:ILE:HB	0.58	1.75	10	1
1:A:855:ASN:O	1:A:856:ASP:HB2	0.57	1.99	19	8
1:A:910:GLU:HA	1:A:913:ARG:NH1	0.57	2.14	11	1
1:A:829:VAL:HG12	1:A:873:LEU:HD12	0.57	1.75	17	1
1:A:901:GLY:O	1:A:922:CYS:HA	0.57	1.98	10	6
1:A:708:ARG:HA	1:A:732:VAL:HG23	0.57	1.76	20	2
1:A:829:VAL:HG23	1:A:840:LEU:HD12	0.57	1.77	15	1
1:A:875:ASP:CG	1:A:925:LYS:HZ3	0.57	2.02	3	1
1:A:830:VAL:HG22	1:A:854:ALA:HB3	0.57	1.76	20	3
1:A:742:THR:HB	1:A:745:ASP:HB2	0.57	1.76	19	1
1:A:843:GLN:HB3	1:A:932:ILE:HG21	0.57	1.75	15	1
1:A:765:PHE:CE1	1:A:785:VAL:HG23	0.57	2.35	20	5
1:A:831:ASP:HB2	1:A:837:ARG:NH1	0.57	2.14	13	1
1:A:707:LYS:NZ	1:A:745:ASP:HA	0.56	2.15	19	1
1:A:886:LEU:HG	1:A:887:THR:N	0.56	2.16	10	4
1:A:899:VAL:HG22	1:A:919:MET:HG2	0.56	1.76	11	1
1:A:856:ASP:HB3	1:A:859:ASP:HB2	0.56	1.78	20	6
1:A:875:ASP:OD1	1:A:925:LYS:HG2	0.56	2.01	10	2
1:A:913:ARG:HB2	1:A:922:CYS:SG	0.56	2.41	12	2
1:A:837:ARG:HH21	1:A:840:LEU:HD11	0.56	1.59	13	1
1:A:826:MET:HG3	1:A:869:ILE:HA	0.56	1.77	4	2
1:A:906:ALA:HB3	1:A:909:GLU:HB3	0.56	1.76	11	1
1:A:828:LEU:HB2	1:A:869:ILE:HG12	0.55	1.77	13	2
1:A:864:LEU:HD21	1:A:897:LEU:HD11	0.55	1.78	9	3
1:A:877:ASN:HB2	1:A:925:LYS:HE2	0.55	1.78	1	1
1:A:831:ASP:OD1	1:A:837:ARG:HB2	0.55	2.00	19	2
1:A:831:ASP:HA	1:A:875:ASP:HB3	0.55	1.78	14	1
1:A:756:LYS:O	1:A:757:TRP:HB2	0.55	2.02	19	3
1:A:941:GLU:O	1:A:945:LYS:HG2	0.55	2.02	7	1
1:A:752:VAL:HG22	1:A:772:ILE:HG12	0.55	1.77	13	2
1:A:775:GLU:HA	1:A:780:GLU:O	0.54	2.02	14	9
1:A:895:LEU:O	1:A:895:LEU:HG	0.54	2.02	18	5
1:A:867:ASN:O	1:A:868:HIS:HB2	0.54	2.02	19	1
1:A:864:LEU:HD23	1:A:869:ILE:HD12	0.54	1.77	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Models Total
1:A:836:ASN:O	1:A:840:LEU:HG	0.54	2.03	2	9
1:A:716:ALA:O	1:A:720:GLN:HB2	0.54	2.02	12	5
1:A:831:ASP:HB2	1:A:837:ARG:HE	0.54	1.60	10	1
1:A:757:TRP:HB2	1:A:762:VAL:HB	0.54	1.79	5	1
1:A:775:GLU:HG3	1:A:781:TRP:HA	0.54	1.79	16	2
1:A:831:ASP:HB3	1:A:837:ARG:CB	0.54	2.29	20	1
1:A:942:ARG:HG3	1:A:943:VAL:N	0.54	2.17	19	2
1:A:713:VAL:HA	1:A:750:ASP:HB3	0.54	1.79	15	3
1:A:743:PRO:HA	1:A:759:GLY:CA	0.54	2.30	9	1
1:A:833:HIS:HB2	1:A:836:ASN:ND2	0.54	2.18	16	1
1:A:938:LEU:O	1:A:941:GLU:HG2	0.54	2.03	20	1
1:A:900:ILE:HG23	1:A:921:SER:HB2	0.54	1.80	20	5
1:A:788:PRO:HB2	1:A:790:GLU:OE2	0.53	2.03	19	1
1:A:844:LEU:HD13	1:A:851:CYS:HB3	0.53	1.80	20	1
1:A:909:GLU:HB3	1:A:922:CYS:HB2	0.53	1.80	10	1
1:A:912:GLN:O	1:A:916:GLU:HG2	0.53	2.03	13	1
1:A:864:LEU:HD13	1:A:897:LEU:HD21	0.53	1.81	7	1
1:A:898:PRO:HB2	1:A:939:TYR:HE2	0.53	1.64	4	1
1:A:932:ILE:O	1:A:936:LEU:HB2	0.53	2.03	6	2
1:A:724:THR:O	1:A:728:ARG:HG3	0.53	2.04	13	2
1:A:873:LEU:HD11	1:A:936:LEU:HD12	0.53	1.80	10	1
1:A:708:ARG:HG3	1:A:732:VAL:HB	0.53	1.81	8	1
1:A:832:ASP:CB	1:A:876:VAL:HB	0.52	2.28	16	1
1:A:723:GLU:HG3	1:A:724:THR:N	0.52	2.17	18	7
1:A:763:VAL:HG11	1:A:791:LEU:HD21	0.52	1.80	8	6
1:A:904:ALA:HB2	1:A:925:LYS:HB2	0.52	1.79	2	2
1:A:837:ARG:NE	1:A:837:ARG:HA	0.52	2.19	6	2
1:A:709:CYS:SG	1:A:726:LEU:HD22	0.52	2.45	19	1
1:A:724:THR:HA	1:A:727:GLN:HG2	0.52	1.80	9	1
1:A:767:ARG:HB3	1:A:784:SER:HB3	0.52	1.82	9	1
1:A:927:VAL:HG13	1:A:931:VAL:HB	0.52	1.81	10	2
1:A:828:LEU:HD22	1:A:869:ILE:HD13	0.52	1.81	9	1
1:A:797:ARG:HA	1:A:800:LEU:HD23	0.52	1.82	17	1
1:A:775:GLU:HG3	1:A:780:GLU:O	0.52	2.05	16	7
1:A:895:LEU:HG	1:A:895:LEU:O	0.51	2.05	4	2
1:A:705:SER:O	1:A:846:SER:HA	0.51	2.05	9	1
1:A:723:GLU:HB2	1:A:733:VAL:HG21	0.51	1.82	10	1
1:A:890:ILE:HG12	1:A:895:LEU:HG	0.51	1.82	1	1
1:A:708:ARG:HG2	1:A:732:VAL:HG13	0.51	1.80	2	1
1:A:875:ASP:HA	1:A:902:VAL:O	0.51	2.06	15	2
1:A:939:TYR:HA	1:A:942:ARG:HB2	0.51	1.81	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:910:GLU:HG2	1:A:911:LYS:N	0.51	2.20	2	2
1:A:868:HIS:O	1:A:869:ILE:HB	0.51	2.05	19	2
1:A:713:VAL:HB	1:A:719:CYS:HB2	0.51	1.81	1	4
1:A:741:PRO:HA	1:A:757:TRP:CH2	0.51	2.41	20	5
1:A:827:ILE:HD12	1:A:871:ILE:HB	0.51	1.83	18	2
1:A:785:VAL:HG12	1:A:787:ALA:H	0.51	1.66	9	1
1:A:723:GLU:HG2	1:A:724:THR:N	0.50	2.21	17	1
1:A:831:ASP:CB	1:A:837:ARG:HG2	0.50	2.36	13	1
1:A:890:ILE:HG23	1:A:895:LEU:HD13	0.50	1.83	14	1
1:A:886:LEU:O	1:A:890:ILE:HG13	0.50	2.06	10	1
1:A:714:ARG:HH12	1:A:751:GLU:HG3	0.50	1.66	19	1
1:A:860:ALA:O	1:A:864:LEU:HG	0.50	2.07	12	1
1:A:765:PHE:HE2	1:A:791:LEU:HD22	0.50	1.66	13	1
1:A:830:VAL:HA	1:A:854:ALA:O	0.50	2.06	12	2
1:A:833:HIS:HB2	1:A:836:ASN:HD21	0.50	1.66	16	1
1:A:829:VAL:HG13	1:A:873:LEU:HD12	0.50	1.82	2	1
1:A:752:VAL:HG23	1:A:771:GLY:HA3	0.50	1.82	6	1
1:A:765:PHE:HA	1:A:783:HIS:O	0.50	2.05	10	4
1:A:767:ARG:NE	1:A:767:ARG:HA	0.50	2.22	1	1
1:A:828:LEU:HB3	1:A:869:ILE:HD13	0.50	1.84	12	1
1:A:752:VAL:HG13	1:A:772:ILE:HG12	0.50	1.83	10	1
1:A:829:VAL:HB	1:A:837:ARG:CZ	0.50	2.37	13	1
1:A:707:LYS:NZ	1:A:799:TYR:OH	0.50	2.44	9	1
1:A:875:ASP:HA	1:A:902:VAL:HG13	0.50	1.82	12	1
1:A:941:GLU:O	1:A:945:LYS:HB3	0.50	2.07	16	1
1:A:830:VAL:HG13	1:A:854:ALA:HB3	0.50	1.83	8	1
1:A:934:GLN:O	1:A:938:LEU:HB2	0.50	2.06	20	5
1:A:828:LEU:HD12	1:A:852:LYS:HB3	0.50	1.84	17	1
1:A:831:ASP:OD2	1:A:836:ASN:HB3	0.49	2.07	5	1
1:A:777:ALA:HB3	1:A:780:GLU:HB2	0.49	1.84	19	3
1:A:906:ALA:HB3	1:A:909:GLU:HG3	0.49	1.84	8	1
1:A:774:LEU:O	1:A:780:GLU:HB3	0.49	2.08	4	3
1:A:906:ALA:O	1:A:907:LEU:HB2	0.49	2.06	9	1
1:A:791:LEU:N	1:A:792:PRO:HD2	0.49	2.22	1	8
1:A:829:VAL:HG12	1:A:873:LEU:HD11	0.49	1.84	6	3
1:A:774:LEU:HA	1:A:782:VAL:HB	0.49	1.85	9	1
1:A:832:ASP:HB3	1:A:877:ASN:HB3	0.49	1.83	7	1
1:A:938:LEU:O	1:A:942:ARG:HG2	0.49	2.07	20	1
1:A:875:ASP:HB2	1:A:925:LYS:HE2	0.49	1.85	5	1
1:A:751:GLU:HG2	1:A:752:VAL:HG12	0.49	1.84	6	1
1:A:899:VAL:HB	1:A:919:MET:CA	0.49	2.38	3	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:781:TRP:HZ3	1:A:794:LEU:HD13	0.49	1.67	20	1
1:A:925:LYS:N	1:A:926:PRO:HD2	0.48	2.23	4	5
1:A:751:GLU:HG3	1:A:752:VAL:H	0.48	1.68	1	2
1:A:826:MET:HB2	1:A:869:ILE:HA	0.48	1.85	3	1
1:A:742:THR:CG2	1:A:743:PRO:HD2	0.48	2.38	12	1
1:A:843:GLN:HG2	1:A:932:ILE:HG21	0.48	1.86	20	1
1:A:770:ILE:HG22	1:A:771:GLY:H	0.48	1.68	1	1
1:A:726:LEU:HD22	1:A:731:ILE:HD12	0.48	1.85	11	1
1:A:741:PRO:HA	1:A:757:TRP:CZ3	0.48	2.44	16	2
1:A:908:ALA:O	1:A:912:GLN:HB2	0.48	2.08	8	1
1:A:741:PRO:HB3	1:A:757:TRP:CH2	0.48	2.43	12	1
1:A:875:ASP:HA	1:A:902:VAL:HG22	0.48	1.84	16	1
1:A:912:GLN:O	1:A:916:GLU:HG3	0.48	2.09	18	1
1:A:927:VAL:HG13	1:A:931:VAL:HG12	0.48	1.86	6	1
1:A:766:CYS:O	1:A:784:SER:HA	0.48	2.09	14	2
1:A:941:GLU:HG3	1:A:942:ARG:N	0.48	2.24	6	3
1:A:772:ILE:HG12	1:A:773:PRO:HD2	0.48	1.84	3	1
1:A:747:LEU:HB2	1:A:757:TRP:CD2	0.47	2.44	5	3
1:A:720:GLN:O	1:A:723:GLU:HG3	0.47	2.09	5	1
1:A:864:LEU:HG	1:A:895:LEU:HD11	0.47	1.87	14	1
1:A:913:ARG:HA	1:A:916:GLU:OE2	0.47	2.10	18	1
1:A:903:THR:HG21	1:A:909:GLU:HG2	0.47	1.85	14	1
1:A:749:THR:HG21	1:A:753:VAL:HB	0.47	1.87	12	1
1:A:765:PHE:CE2	1:A:791:LEU:HD22	0.47	2.44	13	3
1:A:863:VAL:HG13	1:A:869:ILE:HD13	0.47	1.86	1	2
1:A:855:ASN:O	1:A:856:ASP:HB3	0.47	2.09	16	1
1:A:873:LEU:HD22	1:A:900:ILE:HD12	0.47	1.87	11	1
1:A:746:VAL:HG21	1:A:795:LEU:HD21	0.47	1.86	11	1
1:A:941:GLU:O	1:A:944:ARG:HG3	0.47	2.10	10	1
1:A:828:LEU:HD11	1:A:863:VAL:HG13	0.47	1.87	15	1
1:A:726:LEU:HD11	1:A:795:LEU:HD12	0.47	1.87	9	1
1:A:724:THR:O	1:A:728:ARG:HB2	0.47	2.10	17	1
1:A:757:TRP:HB3	1:A:762:VAL:HB	0.47	1.86	2	1
1:A:904:ALA:HB2	1:A:925:LYS:HG3	0.47	1.84	10	1
1:A:741:PRO:HG2	1:A:758:GLN:HB2	0.47	1.87	12	1
1:A:707:LYS:HB2	1:A:731:ILE:HG12	0.47	1.87	16	1
1:A:906:ALA:HB3	1:A:909:GLU:CG	0.47	2.40	8	1
1:A:903:THR:HB	1:A:906:ALA:HB2	0.47	1.86	10	1
1:A:886:LEU:HD13	1:A:887:THR:N	0.47	2.24	9	1
1:A:829:VAL:HB	1:A:837:ARG:CD	0.46	2.40	10	2
1:A:708:ARG:HG2	1:A:732:VAL:HG23	0.46	1.87	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:863:VAL:HA	1:A:866:LYS:HB2	0.46	1.87	15	1
1:A:765:PHE:CZ	1:A:791:LEU:HD13	0.46	2.46	13	1
1:A:877:ASN:ND2	1:A:904:ALA:HB3	0.46	2.24	5	1
1:A:829:VAL:HB	1:A:873:LEU:HD12	0.46	1.87	1	1
1:A:752:VAL:CG2	1:A:769:HIS:HA	0.46	2.40	10	1
1:A:844:LEU:HA	1:A:847:LEU:HD23	0.46	1.87	19	1
1:A:887:THR:HB	1:A:916:GLU:OE1	0.46	2.10	4	1
1:A:887:THR:O	1:A:890:ILE:HG22	0.46	2.10	3	1
1:A:826:MET:HG2	1:A:868:HIS:O	0.46	2.11	2	1
1:A:718:LEU:HD21	1:A:765:PHE:CD2	0.46	2.45	20	1
1:A:741:PRO:HB2	1:A:758:GLN:O	0.46	2.10	18	1
1:A:757:TRP:CB	1:A:762:VAL:HB	0.46	2.40	5	1
1:A:899:VAL:HB	1:A:919:MET:HB3	0.46	1.87	7	1
1:A:711:LEU:HD11	1:A:719:CYS:SG	0.46	2.51	16	1
1:A:747:LEU:HB3	1:A:762:VAL:HG23	0.46	1.87	9	2
1:A:891:ARG:HA	1:A:895:LEU:HD23	0.46	1.86	6	2
1:A:930:ASP:O	1:A:934:GLN:HG2	0.46	2.11	8	1
1:A:707:LYS:CE	1:A:799:TYR:OH	0.46	2.64	9	1
1:A:831:ASP:OD2	1:A:837:ARG:HB2	0.46	2.11	12	2
1:A:887:THR:HB	1:A:916:GLU:HB3	0.46	1.88	16	1
1:A:714:ARG:HD2	1:A:750:ASP:OD2	0.46	2.11	8	1
1:A:757:TRP:CE3	1:A:757:TRP:HA	0.46	2.45	9	1
1:A:752:VAL:HG11	1:A:771:GLY:H	0.46	1.71	10	1
1:A:705:SER:HA	1:A:730:GLY:HA3	0.46	1.87	10	1
1:A:864:LEU:HG	1:A:890:ILE:HD11	0.46	1.87	16	1
1:A:837:ARG:NH2	1:A:853:THR:HB	0.46	2.26	2	1
1:A:781:TRP:CZ3	1:A:794:LEU:HD11	0.46	2.46	9	1
1:A:831:ASP:HB2	1:A:875:ASP:HB2	0.45	1.88	19	1
1:A:747:LEU:HD22	1:A:749:THR:HG23	0.45	1.86	4	1
1:A:724:THR:HA	1:A:727:GLN:CG	0.45	2.40	6	1
1:A:886:LEU:HD13	1:A:887:THR:H	0.45	1.71	9	1
1:A:765:PHE:CE1	1:A:785:VAL:HB	0.45	2.46	9	1
1:A:934:GLN:HG3	1:A:935:THR:N	0.45	2.26	17	1
1:A:887:THR:HG21	1:A:916:GLU:HB2	0.45	1.88	7	1
1:A:828:LEU:HB2	1:A:869:ILE:HG21	0.45	1.87	6	3
1:A:888:GLN:O	1:A:891:ARG:HG2	0.45	2.11	10	1
1:A:837:ARG:HG3	1:A:853:THR:HG22	0.45	1.88	14	1
1:A:876:VAL:HB	1:A:903:THR:HG23	0.45	1.88	17	1
1:A:837:ARG:HA	1:A:837:ARG:NE	0.45	2.26	10	1
1:A:825:MET:O	1:A:850:GLN:HB2	0.45	2.12	17	2
1:A:787:ALA:N	1:A:788:PRO:HD3	0.45	2.26	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:774:LEU:HB2	1:A:782:VAL:HG22	0.45	1.88	16	1
1:A:718:LEU:HD11	1:A:786:ALA:HA	0.45	1.88	7	1
1:A:774:LEU:HB3	1:A:782:VAL:HG22	0.45	1.89	15	2
1:A:829:VAL:HB	1:A:853:THR:HG23	0.45	1.88	2	1
1:A:923:LEU:HD11	1:A:935:THR:HG21	0.45	1.87	15	1
1:A:831:ASP:HB3	1:A:837:ARG:HG3	0.45	1.88	18	1
1:A:711:LEU:O	1:A:711:LEU:HG	0.44	2.12	15	2
1:A:897:LEU:HD22	1:A:897:LEU:N	0.44	2.26	7	1
1:A:752:VAL:HG22	1:A:771:GLY:H	0.44	1.73	8	1
1:A:891:ARG:HB3	1:A:918:GLY:HA2	0.44	1.88	5	1
1:A:747:LEU:HD12	1:A:757:TRP:CE3	0.44	2.48	9	1
1:A:869:ILE:O	1:A:897:LEU:HD12	0.44	2.12	7	1
1:A:843:GLN:HG3	1:A:929:LEU:CD2	0.44	2.43	16	1
1:A:902:VAL:HA	1:A:923:LEU:O	0.44	2.13	17	2
1:A:829:VAL:HG21	1:A:840:LEU:HD11	0.43	1.90	5	1
1:A:710:TRP:CZ3	1:A:739:GLN:HG3	0.43	2.48	7	1
1:A:713:VAL:HG11	1:A:718:LEU:HB3	0.43	1.88	13	2
1:A:890:ILE:HG12	1:A:895:LEU:HD13	0.43	1.88	12	1
1:A:789:HIS:HA	1:A:792:PRO:HG2	0.43	1.90	15	1
1:A:871:ILE:HG12	1:A:939:TYR:HD2	0.43	1.73	14	1
1:A:788:PRO:O	1:A:789:HIS:HB3	0.43	2.14	8	1
1:A:753:VAL:HG13	1:A:755:LYS:HB2	0.43	1.91	18	1
1:A:772:ILE:HG13	1:A:773:PRO:CD	0.43	2.32	1	1
1:A:718:LEU:HD21	1:A:765:PHE:HD2	0.43	1.74	12	1
1:A:872:VAL:HG22	1:A:897:LEU:HD12	0.43	1.91	18	1
1:A:711:LEU:HD21	1:A:719:CYS:HB2	0.43	1.89	6	1
1:A:919:MET:HB3	1:A:920:ASP:H	0.43	1.45	13	1
1:A:875:ASP:HB3	1:A:902:VAL:HG22	0.43	1.90	5	1
1:A:867:ASN:O	1:A:868:HIS:CB	0.43	2.67	19	1
1:A:722:LEU:HD13	1:A:748:ILE:HG21	0.43	1.91	13	1
1:A:871:ILE:HG13	1:A:898:PRO:HG2	0.43	1.89	15	1
1:A:794:LEU:HA	1:A:797:ARG:HD3	0.43	1.90	18	1
1:A:736:TYR:HE2	1:A:755:LYS:HD3	0.43	1.74	4	1
1:A:751:GLU:HG2	1:A:767:ARG:NH2	0.43	2.20	9	1
1:A:909:GLU:O	1:A:922:CYS:HB2	0.43	2.14	7	1
1:A:928:THR:OG1	1:A:931:VAL:HB	0.43	2.14	6	1
1:A:794:LEU:O	1:A:798:ILE:HB	0.42	2.14	7	1
1:A:903:THR:O	1:A:924:SER:HA	0.42	2.14	2	3
1:A:719:CYS:O	1:A:723:GLU:HB3	0.42	2.14	3	1
1:A:718:LEU:O	1:A:722:LEU:HG	0.42	2.14	9	1
1:A:877:ASN:CB	1:A:925:LYS:HE3	0.42	2.40	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:756:LYS:O	1:A:756:LYS:HD2	0.42	2.13	18	1
1:A:934:GLN:HG2	1:A:935:THR:N	0.42	2.29	20	1
1:A:715:ASN:HB3	1:A:718:LEU:HB2	0.42	1.90	17	1
1:A:774:LEU:HG	1:A:776:LYS:HG2	0.42	1.91	7	1
1:A:795:LEU:HD22	1:A:795:LEU:HA	0.42	1.75	17	1
1:A:797:ARG:HA	1:A:800:LEU:HD13	0.42	1.89	2	1
1:A:875:ASP:N	1:A:875:ASP:OD1	0.42	2.52	5	1
1:A:872:VAL:HB	1:A:899:VAL:HG13	0.42	1.91	7	1
1:A:705:SER:CB	1:A:730:GLY:HA3	0.42	2.45	10	1
1:A:829:VAL:HG21	1:A:840:LEU:HD12	0.42	1.90	3	1
1:A:718:LEU:HD11	1:A:765:PHE:HD2	0.42	1.73	2	1
1:A:847:LEU:HD21	1:A:933:LYS:HG2	0.42	1.90	11	1
1:A:711:LEU:HD12	1:A:719:CYS:SG	0.42	2.54	10	1
1:A:900:ILE:CG2	1:A:923:LEU:HG	0.42	2.45	5	1
1:A:797:ARG:HG3	1:A:798:ILE:N	0.42	2.29	9	1
1:A:861:LEU:HD11	1:A:889:ARG:HB3	0.42	1.92	17	1
1:A:830:VAL:HG11	1:A:860:ALA:HB2	0.42	1.92	8	1
1:A:835:ILE:O	1:A:838:ARG:HG3	0.42	2.15	15	3
1:A:889:ARG:HD3	1:A:892:GLN:OE1	0.42	2.15	5	1
1:A:844:LEU:HD22	1:A:851:CYS:HB3	0.42	1.90	15	1
1:A:945:LYS:HE2	1:A:945:LYS:HB2	0.42	1.37	16	1
1:A:710:TRP:C	1:A:711:LEU:HD23	0.42	2.35	18	1
1:A:750:ASP:O	1:A:751:GLU:HB2	0.41	2.15	18	1
1:A:830:VAL:O	1:A:874:SER:HA	0.41	2.15	8	1
1:A:757:TRP:CD1	1:A:762:VAL:HB	0.41	2.49	13	2
1:A:830:VAL:HG13	1:A:874:SER:HA	0.41	1.92	13	1
1:A:828:LEU:HD23	1:A:872:VAL:HG13	0.41	1.91	10	1
1:A:825:MET:O	1:A:849:TYR:HB3	0.41	2.14	12	1
1:A:772:ILE:CG1	1:A:773:PRO:HD2	0.41	2.37	15	1
1:A:707:LYS:HB3	1:A:799:TYR:CE2	0.41	2.50	16	1
1:A:840:LEU:HA	1:A:843:GLN:NE2	0.41	2.29	18	1
1:A:774:LEU:CB	1:A:782:VAL:HG22	0.41	2.45	2	1
1:A:902:VAL:CG2	1:A:925:LYS:HA	0.41	2.46	13	1
1:A:724:THR:O	1:A:728:ARG:HB3	0.41	2.16	11	1
1:A:768:ARG:HA	1:A:768:ARG:HD2	0.41	1.73	7	1
1:A:707:LYS:HE2	1:A:799:TYR:CE2	0.41	2.50	9	1
1:A:844:LEU:HD13	1:A:849:TYR:HB2	0.41	1.93	10	1
1:A:944:ARG:HG3	1:A:945:LYS:N	0.41	2.29	8	1
1:A:875:ASP:HB3	1:A:925:LYS:HE3	0.41	1.93	13	1
1:A:887:THR:O	1:A:891:ARG:HG2	0.41	2.15	5	1
1:A:751:GLU:CD	1:A:769:HIS:HB2	0.41	2.36	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Models Total
1:A:869:ILE:O	1:A:897:LEU:HD22	0.41	2.16	18	1
1:A:719:CYS:SG	1:A:720:GLN:N	0.41	2.94	14	1
1:A:931:VAL:O	1:A:934:GLN:HG2	0.41	2.16	11	1
1:A:751:GLU:OE1	1:A:767:ARG:HB2	0.41	2.15	15	1
1:A:711:LEU:HD22	1:A:733:VAL:CG1	0.41	2.46	16	1
1:A:826:MET:HG3	1:A:868:HIS:O	0.41	2.16	16	1
1:A:720:GLN:O	1:A:723:GLU:HG2	0.41	2.16	4	1
1:A:838:ARG:HG3	1:A:839:LEU:N	0.41	2.30	13	1
1:A:764:THR:HB	1:A:782:VAL:HG22	0.41	1.91	9	1
1:A:746:VAL:HA	1:A:761:ALA:O	0.41	2.16	10	1
1:A:834:PRO:HA	1:A:837:ARG:HD3	0.41	1.92	18	1
1:A:913:ARG:HG3	1:A:914:CYS:N	0.41	2.30	2	1
1:A:923:LEU:HA	1:A:923:LEU:HD12	0.40	1.77	18	1
1:A:910:GLU:H	1:A:910:GLU:HG3	0.40	1.52	5	2
1:A:916:GLU:HG2	1:A:917:SER:N	0.40	2.31	5	1
1:A:861:LEU:HD21	1:A:893:LEU:HG	0.40	1.93	6	1
1:A:876:VAL:HG22	1:A:878:MET:H	0.40	1.76	13	1
1:A:726:LEU:HD23	1:A:731:ILE:HG21	0.40	1.93	9	1
1:A:710:TRP:CZ3	1:A:734:THR:HB	0.40	2.52	15	1
1:A:718:LEU:HG	1:A:787:ALA:HB2	0.40	1.92	15	1
1:A:913:ARG:NH1	1:A:921:SER:HA	0.40	2.31	4	1
1:A:795:LEU:HA	1:A:795:LEU:HD22	0.40	1.78	6	1
1:A:773:PRO:HB2	1:A:774:LEU:H	0.40	1.59	14	1
1:A:827:ILE:O	1:A:851:CYS:HA	0.40	2.17	9	1
1:A:913:ARG:HD2	1:A:913:ARG:O	0.40	2.16	10	1
1:A:756:LYS:O	1:A:757:TRP:HB3	0.40	2.16	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	217/254 (85%)	185±3 (85±1%)	23±3 (11±1%)	9±2 (4±1%)	6	33
All	All	4340/5080 (85%)	3705 (85%)	459 (11%)	176 (4%)	6	33

All 36 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	920	ASP	20
1	A	775	GLU	15
1	A	856	ASP	11
1	A	788	PRO	10
1	A	738	GLY	10
1	A	785	VAL	10
1	A	773	PRO	9
1	A	789	HIS	8
1	A	869	ILE	8
1	A	774	LEU	7
1	A	868	HIS	6
1	A	894	GLY	6
1	A	919	MET	6
1	A	926	PRO	5
1	A	706	GLY	5
1	A	757	TRP	4
1	A	884	TYR	3
1	A	730	GLY	3
1	A	824	ASP	3
1	A	771	GLY	3
1	A	907	LEU	3
1	A	770	ILE	3
1	A	867	ASN	2
1	A	769	HIS	2
1	A	768	ARG	2
1	A	834	PRO	2
1	A	908	ALA	1
1	A	767	ARG	1
1	A	778	PRO	1
1	A	800	LEU	1
1	A	878	MET	1
1	A	883	GLY	1
1	A	948	ASP	1
1	A	905	ASN	1
1	A	705	SER	1
1	A	779	GLY	1

6.3.2　Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR

entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	189/219 (86%)	103±4 (54±2%)	86±4 (46±2%)	0	2
All	All	3780/4380 (86%)	2059 (54%)	1721 (46%)	0	2

All 168 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	747	LEU	20
1	A	742	THR	20
1	A	851	CYS	20
1	A	896	THR	19
1	A	755	LYS	19
1	A	903	THR	19
1	A	844	LEU	19
1	A	853	THR	19
1	A	887	THR	19
1	A	798	ILE	19
1	A	895	LEU	18
1	A	922	CYS	18
1	A	791	LEU	18
1	A	852	LYS	18
1	A	717	SER	18
1	A	928	THR	18
1	A	874	SER	17
1	A	797	ARG	17
1	A	784	SER	17
1	A	902	VAL	17
1	A	936	LEU	17
1	A	735	THR	17
1	A	718	LEU	17
1	A	734	THR	17
1	A	795	LEU	17
1	A	944	ARG	17
1	A	829	VAL	17
1	A	897	LEU	17
1	A	932	ILE	16
1	A	889	ARG	16
1	A	766	CYS	16
1	A	864	LEU	16
1	A	838	ARG	16

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Mol	Chain	Res	Type	Models (Total)
1	A	774	LEU	16
1	A	767	ARG	16
1	A	839	LEU	16
1	A	886	LEU	16
1	A	711	LEU	15
1	A	913	ARG	15
1	A	917	SER	15
1	A	840	LEU	15
1	A	785	VAL	15
1	A	910	GLU	15
1	A	915	LEU	14
1	A	832	ASP	14
1	A	705	SER	14
1	A	942	ARG	14
1	A	938	LEU	14
1	A	923	LEU	14
1	A	921	SER	14
1	A	885	ARG	14
1	A	776	LYS	13
1	A	737	GLU	13
1	A	924	SER	13
1	A	720	GLN	13
1	A	754	SER	13
1	A	768	ARG	13
1	A	891	ARG	12
1	A	941	GLU	12
1	A	929	LEU	12
1	A	847	LEU	12
1	A	783	HIS	12
1	A	876	VAL	12
1	A	909	GLU	12
1	A	729	SER	12
1	A	723	GLU	12
1	A	789	HIS	12
1	A	709	CYS	12
1	A	835	ILE	12
1	A	826	MET	11
1	A	925	LYS	11
1	A	825	MET	11
1	A	728	ARG	11
1	A	893	LEU	11
1	A	933	LYS	11

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Mol	Chain	Res	Type	Models (Total)
1	A	790	GLU	11
1	A	846	SER	11
1	A	861	LEU	11
1	A	866	LYS	11
1	A	708	ARG	10
1	A	911	LYS	10
1	A	930	ASP	10
1	A	858	VAL	10
1	A	884	TYR	10
1	A	794	LEU	10
1	A	934	GLN	10
1	A	877	ASN	10
1	A	780	GLU	10
1	A	945	LYS	10
1	A	758	GLN	10
1	A	947	ARG	10
1	A	850	GLN	10
1	A	837	ARG	10
1	A	873	LEU	10
1	A	756	LYS	10
1	A	769	HIS	10
1	A	878	MET	9
1	A	916	GLU	9
1	A	760	ARG	9
1	A	750	ASP	9
1	A	919	MET	9
1	A	828	LEU	9
1	A	907	LEU	9
1	A	831	ASP	8
1	A	863	VAL	8
1	A	870	ASP	8
1	A	744	GLU	8
1	A	732	VAL	8
1	A	830	VAL	8
1	A	855	ASN	8
1	A	799	TYR	8
1	A	868	HIS	8
1	A	843	GLN	8
1	A	722	LEU	7
1	A	714	ARG	7
1	A	890	ILE	7
1	A	875	ASP	7

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Mol	Chain	Res	Type	Models (Total)
1	A	939	TYR	7
1	A	867	ASN	7
1	A	833	HIS	7
1	A	733	VAL	7
1	A	912	GLN	7
1	A	740	GLU	7
1	A	719	CYS	6
1	A	865	SER	6
1	A	749	THR	6
1	A	859	ASP	6
1	A	927	VAL	6
1	A	772	ILE	6
1	A	946	SER	5
1	A	727	GLN	5
1	A	899	VAL	5
1	A	748	ILE	5
1	A	739	GLN	5
1	A	905	ASN	5
1	A	707	LYS	5
1	A	892	GLN	5
1	A	721	PHE	5
1	A	751	GLU	5
1	A	948	ASP	5
1	A	869	ILE	5
1	A	836	ASN	4
1	A	871	ILE	4
1	A	842	ASP	4
1	A	800	LEU	4
1	A	872	VAL	3
1	A	849	TYR	3
1	A	763	VAL	3
1	A	775	GLU	3
1	A	824	ASP	3
1	A	888	GLN	3
1	A	731	ILE	2
1	A	900	ILE	2
1	A	827	ILE	2
1	A	770	ILE	2
1	A	765	PHE	2
1	A	931	VAL	2
1	A	862	ASN	2
1	A	782	VAL	2

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Mol	Chain	Res	Type	Models (Total)
1	A	725	SER	1
1	A	746	VAL	1
1	A	752	VAL	1
1	A	715	ASN	1
1	A	753	VAL	1
1	A	726	LEU	1
1	A	920	ASP	1
1	A	764	THR	1
1	A	757	TRP	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 ⓘ

The completeness of assignment taking into account all chemical shift lists is 88% for the well-defined parts and 87% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 6810

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	3026
Number of shifts mapped to atoms	3026
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	4

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_\alpha$	250	-0.11 ± 0.14	None needed (< 0.5 ppm)
$^{13}C_\beta$	234	0.40 ± 0.13	None needed (< 0.5 ppm)
$^{13}C'$	244	-0.00 ± 0.11	None needed (< 0.5 ppm)
^{15}N	230	-0.48 ± 0.27	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 88%, i.e. 2371 atoms were assigned a chemical shift out of a possible 2687. 47 out of 49 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	1052/1067 (99%)	421/425 (99%)	429/434 (99%)	202/208 (97%)
Sidechain	1217/1486 (82%)	750/864 (87%)	461/547 (84%)	6/75 (8%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	102/134 (76%)	52/68 (76%)	46/53 (87%)	4/13 (31%)
Overall	2371/2687 (88%)	1223/1357 (90%)	936/1034 (91%)	212/296 (72%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 87%, i.e. 2660 atoms were assigned a chemical shift out of a possible 3060. 50 out of 53 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	1203/1246 (97%)	479/496 (97%)	494/508 (97%)	230/242 (95%)
Sidechain	1355/1680 (81%)	835/977 (85%)	513/624 (82%)	7/79 (9%)
Aromatic	102/134 (76%)	52/68 (76%)	46/53 (87%)	4/13 (31%)
Overall	2660/3060 (87%)	1366/1541 (89%)	1053/1185 (89%)	241/334 (72%)

7.1.4 Statistically unusual chemical shifts (i)

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	775	GLU	HB3	-0.57	$3.10 - 0.90$	-11.7
1	A	775	GLU	HG3	0.28	$3.31 - 1.21$	-9.4
1	A	747	LEU	HB3	-1.22	$3.34 - -0.26$	-7.7
1	A	741	PRO	HG3	-0.20	$3.56 - 0.26$	-6.4

7.1.5 Random Coil Index (RCI) plots (i)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A: