Full wwPDB NMR Structure Validation Report (i)

Apr 26, 2016 – 11:49 PM BST

PDB ID : 2KT6

Title : Structural homology between the C-terminal domain of the PapC usher and its plug

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Deposited on : 2010-01-19

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:

<table>
<tr><td>Cyrange</td><td>:</td><td>Kirchner and Güntert (2011)</td></tr>
<tr><td>NmrClust</td><td>:</td><td>Kelley et al. (1996)</td></tr>
<tr><td>MolProbity</td><td>:</td><td>4.02b-467</td></tr>
<tr><td>Mogul</td><td>:</td><td>unknown</td></tr>
<tr><td>Percentile statistics</td><td>:</td><td>20151230.v01 (using entries in the PDB archive December 30th 2015)</td></tr>
<tr><td>RCI</td><td>:</td><td>v_1n_11_5_13_A (Berjanski et al., 2005)</td></tr>
<tr><td>PANAV</td><td>:</td><td>Wang et al. (2010)</td></tr>
<tr><td>ShiftChecker</td><td>:</td><td>rb-20027457</td></tr>
<tr><td>Ideal geometry (proteins)</td><td>:</td><td>Engh & Huber (2001)</td></tr>
<tr><td>Ideal geometry (DNA, RNA)</td><td>:</td><td>Parkinson et al. (1996)</td></tr>
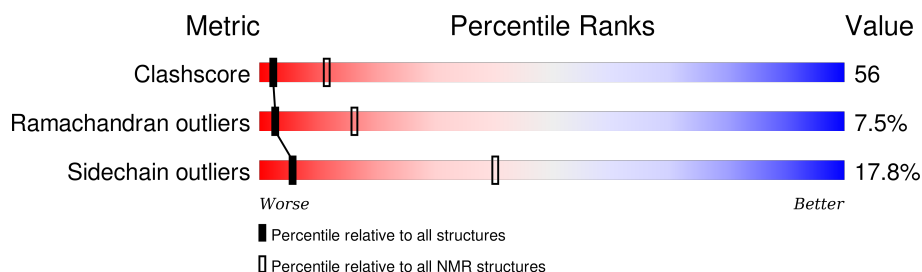<tr><td>Validation Pipeline (wwPDB-VP)</td><td>:</td><td>rb-20027457</td></tr>
</table>

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 81%.

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		56
Ramachandran outliers		7.5%
Sidechain outliers		17.8%

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	85	25% 58% 11% 7%

2 Ensemble composition and analysis (i)

This entry contains 10 models. Model 1 is the overall representative, medoid model (most similar to other models).

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:6-A:84 (79)	0.57	1

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 2 clusters and 3 single-model clusters were found.

Cluster number	Models
1	2, 4, 6, 7
2	1, 3, 5
Single-model clusters	8; 9; 10

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1283 atoms, of which 648 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Outer membrane usher protein papC.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	85	1283	401	648	109	122	3	0

4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• Molecule 1: Outer membrane usher protein papC
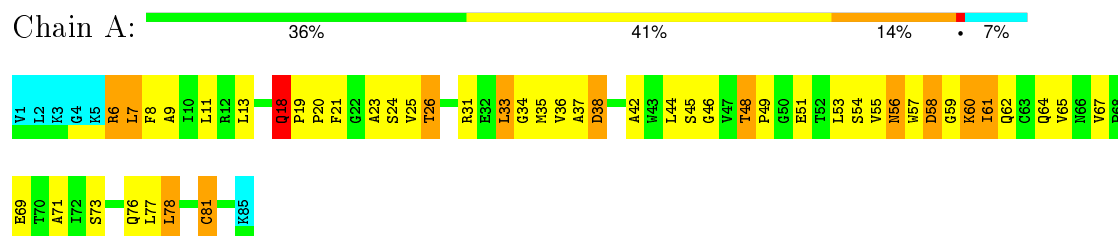
Chain A:
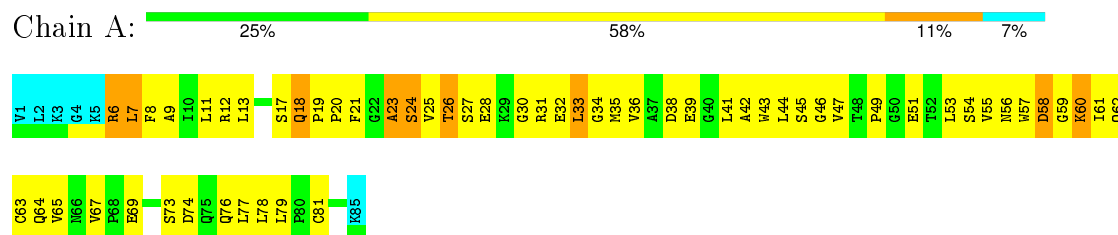
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

• Molecule 1: Outer membrane usher protein papC

Chain A:

4.2.2 Score per residue for model 2

• Molecule 1: Outer membrane usher protein papC

Chain A:

4.2.3 Score per residue for model 3

• Molecule 1: Outer membrane usher protein papC

4.2.4 Score per residue for model 4

• Molecule 1: Outer membrane usher protein papC

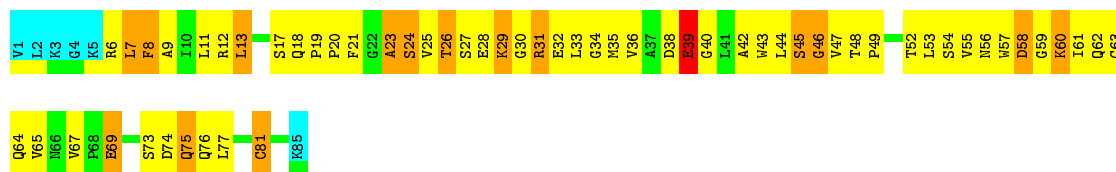### 4.2.5 Score per residue for model 5

• Molecule 1: Outer membrane usher protein papC

4.2.6 Score per residue for model 6

• Molecule 1: Outer membrane usher protein papC
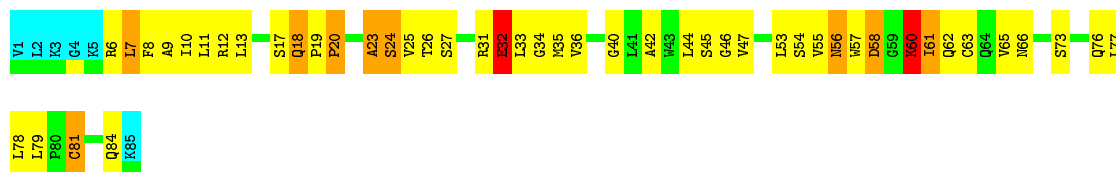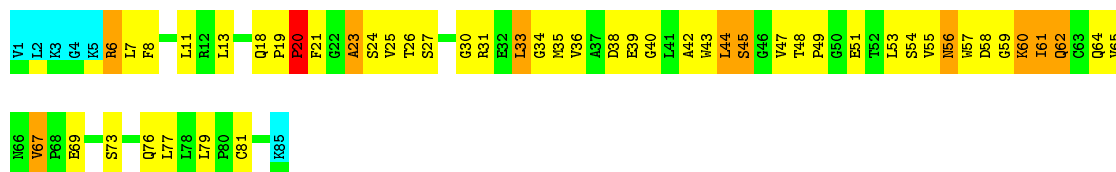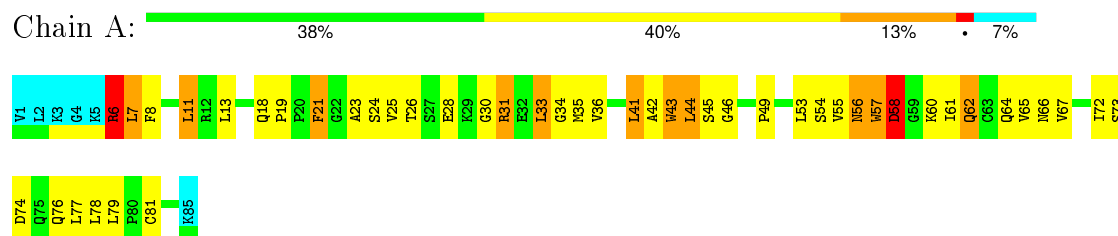
Chain A: 38% 40% 13% 7%

V1 L2 K3 G4 K5 R6 L7 F8 L11 R12 L13 Q18 P19 P20 F21 G22 A23 S24 V25 T26 S27 E28 K29 G30 R31 E32 L33 G34 M35 V36 L41 A42 W43 L44 S45 G46 P49 L53 S54 V55 N56 W57 D58 G59 K60 I61 Q62 C63 Q64 V65 N66 V67 I72 S73

D74 Q75 Q76 L77 L78 L79 P80 C81 K85

4.2.7 Score per residue for model 7

- Molecule 1: Outer membrane usher protein papC

Chain A: 34% 45% 13% 7%

V1 L2 K3 G4 K5 R6 L7 F8 A9 I10 L11 R12 L13 Q18 P19 P20 F21 G22 A23 S24 V25 T26 S27 E28 K29 G30 R31 E32 L33 G34 M35 V36 A37 D38 L41 L44 S45 G46 V47 T48 P49 G50 E51 T52 L53 S54 V55 N56 W57 D58 G59 K60 I61 Q62 C63 Q64 V65

N66 V67 P68 E69 I72 S73 Q76 L77 L78 L79 P80 C81 K85
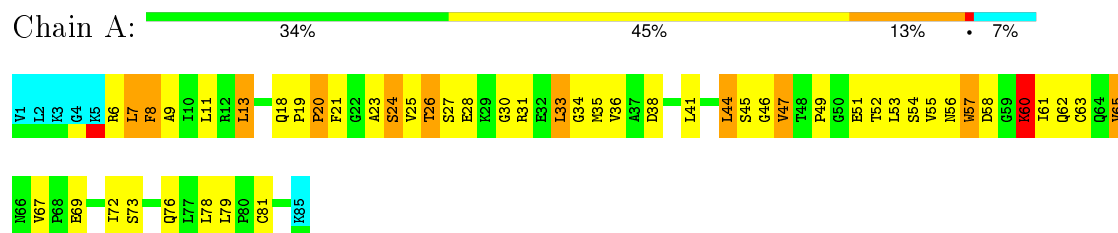
4.2.8 Score per residue for model 8

- Molecule 1: Outer membrane usher protein papC

Chain A: 33% 44% 14% 7%

V1 L2 K3 G4 K5 R6 L7 F8 A9 I10 L11 R12 L13 S17 Q18 P19 P20 F21 G22 A23 S24 V25 T26 S27 E28 R31 E32 L33 G34 M35 V36 L41 A42 W43 L44 S45 G46 V47 G50 E51 T52 L53 S54 V55 N56 W57 D58 G59 K60 I61 Q62 C63 Q64 V65 N66 V67

S73 Q76 L77 L78 C81 K85
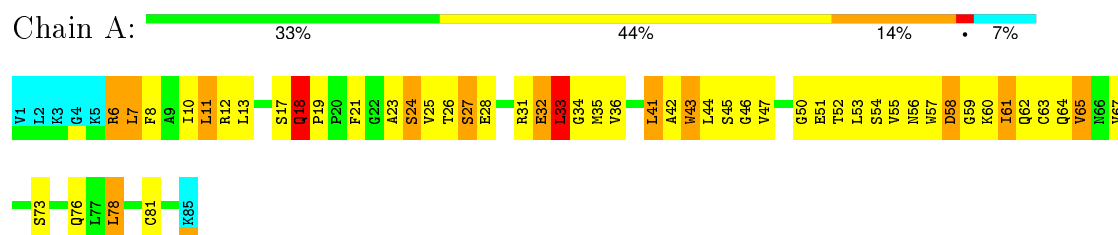
4.2.9 Score per residue for model 9

- Molecule 1: Outer membrane usher protein papC

Chain A: 34% 46% 12% 7%

V1 L2 K3 G4 K5 R6 L7 F8 A9 I10 L11 R12 L13 S17 Q18 P19 P20 F21 G22 A23 S24 V25 T26 S27 E28 K29 G30 R31 E32 L33 G34 M35 V36 A37 D38 E39 G40 L41 L44 S45 G46 P49 G50 E51 T52 L53 S54 V55 N56 W57 D58 G59 K60 I61 Q62 C63 Q64

V65 N66 V67 P68 E69 I72 S73 D74 L77 L78 K85
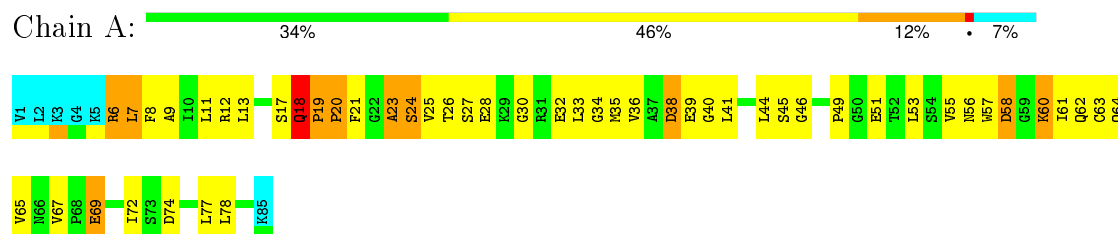
4.2.10 Score per residue for model 10

• Molecule 1: Outer membrane usher protein papC
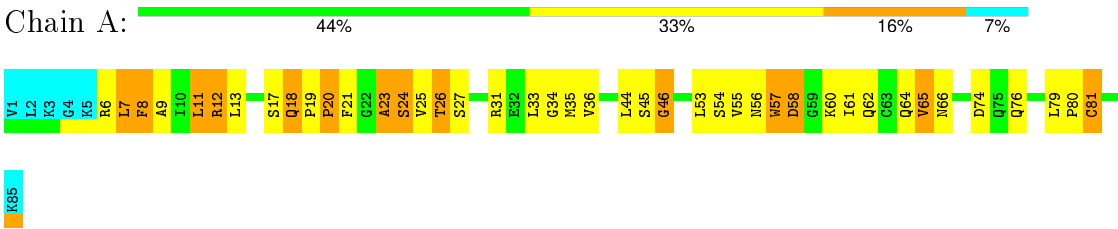
5 Refinement protocol and experimental data overview ⓘ

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

Of the 100 calculated structures, 10 were deposited, based on the following criterion: *Lowest Energy.*

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

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

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

Chemical shift file(s)	BMRB entry 16684
Number of chemical shift lists	1
Total number of shifts	895
Number of shifts mapped to atoms	868
Number of unparsed shifts	0
Number of shifts with mapping errors	27
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	81%

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

6 Model quality ⓘ

6.1 Standard geometry ⓘ

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	0.59±0.02	0±0/601 (0.0±0.0%)	0.73±0.02	0±0/821 (0.0±0.0%)
All	All	0.59	0/6010 (0.0%)	0.73	1/8210 (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	0.7±0.6
All	All	0	7

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	20	PRO	N-CA-CB	-5.00	97.10	102.60	5	1

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	18	GLN	Peptide	5
1	A	32	GLU	Peptide	1
1	A	6	ARG	Peptide	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	589	584	584	66±12
All	All	5890	5840	5840	661

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 56.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Models Total
1:A:25:VAL:HG22	1:A:34:GLY:HA3	1.04	1.22	5	4
1:A:34:GLY:HA2	1:A:44:LEU:HB2	1.02	1.27	8	3
1:A:34:GLY:HA2	1:A:44:LEU:HB3	0.98	1.35	5	1
1:A:6:ARG:HA	1:A:45:SER:HA	0.96	1.32	6	8
1:A:60:LYS:HG2	1:A:62:GLN:HG2	0.96	1.38	3	5
1:A:6:ARG:HB2	1:A:45:SER:HB2	0.96	1.35	2	1
1:A:8:PHE:HB3	1:A:76:GLN:HA	0.88	1.42	5	1
1:A:26:THR:HA	1:A:32:GLU:HB3	0.86	1.47	8	1
1:A:49:PRO:HB3	1:A:69:GLU:HA	0.86	1.47	5	1
1:A:7:LEU:HG	1:A:45:SER:HB3	0.85	1.48	5	1
1:A:7:LEU:HD22	1:A:73:SER:HA	0.85	1.47	3	1
1:A:6:ARG:HA	1:A:45:SER:CA	0.83	2.03	6	2
1:A:24:SER:O	1:A:55:VAL:HA	0.82	1.73	6	10
1:A:31:ARG:HE	1:A:31:ARG:HA	0.82	1.32	3	1
1:A:25:VAL:HG22	1:A:34:GLY:CA	0.81	2.05	5	4
1:A:25:VAL:HG23	1:A:34:GLY:C	0.80	1.97	2	1
1:A:11:LEU:HB2	1:A:19:PRO:HG2	0.79	1.53	8	1
1:A:49:PRO:HB2	1:A:69:GLU:HA	0.79	1.54	3	3
1:A:31:ARG:HG3	1:A:47:VAL:HG11	0.79	1.52	8	1
1:A:33:LEU:O	1:A:44:LEU:HB3	0.78	1.78	7	6
1:A:23:ALA:HB3	1:A:36:VAL:HG13	0.78	1.55	3	3
1:A:11:LEU:HB3	1:A:19:PRO:HG2	0.77	1.56	7	3
1:A:7:LEU:HD11	1:A:46:GLY:H	0.77	1.39	7	1
1:A:34:GLY:HA2	1:A:44:LEU:CB	0.76	2.11	8	5
1:A:7:LEU:HD11	1:A:46:GLY:N	0.76	1.96	7	3
1:A:34:GLY:N	1:A:44:LEU:HD12	0.76	1.95	7	4
1:A:51:GLU:H	1:A:67:VAL:HG22	0.76	1.41	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:7:LEU:HD12	1:A:46:GLY:H	0.75	1.40	9	1
1:A:7:LEU:HD13	1:A:46:GLY:HA3	0.75	1.56	6	1
1:A:36:VAL:HA	1:A:42:ALA:HB2	0.75	1.59	5	2
1:A:24:SER:OG	1:A:56:ASN:HB3	0.75	1.82	6	2
1:A:6:ARG:C	1:A:7:LEU:HD23	0.74	2.02	3	1
1:A:7:LEU:HD23	1:A:44:LEU:HB2	0.74	1.56	4	2
1:A:6:ARG:C	1:A:7:LEU:HD13	0.74	2.03	4	4
1:A:56:ASN:HA	1:A:61:ILE:HA	0.74	1.59	6	6
1:A:42:ALA:HB1	1:A:44:LEU:HD21	0.74	1.59	4	1
1:A:6:ARG:HB2	1:A:45:SER:CB	0.74	2.12	2	2
1:A:7:LEU:HG	1:A:44:LEU:O	0.74	1.82	3	1
1:A:23:ALA:HB3	1:A:36:VAL:HG12	0.73	1.59	6	2
1:A:23:ALA:HA	1:A:56:ASN:O	0.73	1.84	8	3
1:A:57:TRP:HD1	1:A:58:ASP:N	0.73	1.80	9	6
1:A:33:LEU:HD13	1:A:53:LEU:HD21	0.73	1.59	4	1
1:A:52:THR:HA	1:A:65:VAL:O	0.72	1.85	3	3
1:A:33:LEU:HD23	1:A:53:LEU:HD21	0.71	1.61	1	1
1:A:26:THR:HA	1:A:31:ARG:O	0.71	1.86	5	6
1:A:34:GLY:HA2	1:A:44:LEU:CG	0.71	2.14	7	2
1:A:60:LYS:HG2	1:A:62:GLN:CG	0.71	2.15	10	5
1:A:12:ARG:HD3	1:A:18:GLN:HG2	0.70	1.64	9	1
1:A:33:LEU:HB2	1:A:45:SER:HA	0.70	1.62	5	1
1:A:7:LEU:CD1	1:A:46:GLY:H	0.70	1.99	7	5
1:A:31:ARG:HA	1:A:31:ARG:NE	0.69	2.00	3	1
1:A:60:LYS:CG	1:A:62:GLN:HG2	0.69	2.16	3	5
1:A:23:ALA:O	1:A:35:MET:HA	0.69	1.88	3	10
1:A:34:GLY:HA2	1:A:44:LEU:HG	0.69	1.65	7	1
1:A:13:LEU:HD22	1:A:63:CYS:SG	0.68	2.28	8	1
1:A:12:ARG:HA	1:A:19:PRO:HD3	0.68	1.65	3	2
1:A:75:GLN:HE21	1:A:75:GLN:HA	0.68	1.48	2	1
1:A:8:PHE:HE1	1:A:41:LEU:HB2	0.68	1.48	9	1
1:A:57:TRP:CD1	1:A:58:ASP:N	0.68	2.62	2	10
1:A:6:ARG:CA	1:A:7:LEU:HD13	0.68	2.18	8	4
1:A:7:LEU:CD2	1:A:73:SER:HA	0.67	2.19	3	1
1:A:35:MET:N	1:A:44:LEU:HD12	0.67	2.03	5	1
1:A:7:LEU:HD12	1:A:73:SER:OG	0.67	1.89	8	1
1:A:13:LEU:HB3	1:A:81:CYS:SG	0.67	2.30	7	1
1:A:50:GLY:H	1:A:67:VAL:HG13	0.67	1.50	8	1
1:A:6:ARG:HB2	1:A:45:SER:HA	0.66	1.68	10	2
1:A:7:LEU:HD11	1:A:46:GLY:CA	0.66	2.21	8	4
1:A:13:LEU:HD22	1:A:18:GLN:HE21	0.66	1.50	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:LEU:HD12	1:A:65:VAL:HG21	0.66	1.65	9	2
1:A:18:GLN:CB	1:A:20:PRO:HD3	0.65	2.19	10	1
1:A:7:LEU:HD11	1:A:46:GLY:HA2	0.65	1.69	1	2
1:A:7:LEU:HD22	1:A:74:ASP:N	0.65	2.07	3	1
1:A:33:LEU:HD11	1:A:53:LEU:HD21	0.64	1.69	5	1
1:A:7:LEU:N	1:A:7:LEU:HD22	0.64	2.08	4	1
1:A:26:THR:HB	1:A:31:ARG:O	0.64	1.91	4	2
1:A:6:ARG:HG3	1:A:45:SER:H	0.64	1.52	5	1
1:A:25:VAL:HG22	1:A:34:GLY:O	0.64	1.93	8	1
1:A:8:PHE:HB2	1:A:76:GLN:HA	0.64	1.69	3	5
1:A:9:ALA:HB3	1:A:44:LEU:HD13	0.63	1.69	3	2
1:A:34:GLY:C	1:A:35:MET:HG3	0.63	2.14	4	5
1:A:33:LEU:HB3	1:A:44:LEU:HG	0.63	1.70	3	1
1:A:38:ASP:OD1	1:A:41:LEU:HG	0.63	1.92	9	1
1:A:7:LEU:HD22	1:A:74:ASP:H	0.63	1.52	3	1
1:A:55:VAL:HG21	1:A:81:CYS:SG	0.63	2.33	10	1
1:A:7:LEU:CG	1:A:45:SER:HB3	0.62	2.23	5	1
1:A:11:LEU:H	1:A:11:LEU:HD13	0.62	1.54	6	1
1:A:34:GLY:C	1:A:42:ALA:HB1	0.62	2.15	8	1
1:A:47:VAL:HG11	1:A:67:VAL:HG21	0.62	1.71	3	1
1:A:13:LEU:HB2	1:A:17:SER:O	0.62	1.95	10	1
1:A:7:LEU:HD22	1:A:46:GLY:N	0.62	2.10	6	1
1:A:7:LEU:HD22	1:A:73:SER:CA	0.62	2.24	3	1
1:A:57:TRP:HB3	1:A:62:GLN:HG3	0.61	1.72	9	3
1:A:23:ALA:H	1:A:36:VAL:HG22	0.61	1.54	3	1
1:A:33:LEU:HB2	1:A:45:SER:CA	0.61	2.25	5	1
1:A:53:LEU:O	1:A:64:GLN:HB3	0.61	1.95	1	5
1:A:48:THR:O	1:A:51:GLU:HG3	0.61	1.96	5	2
1:A:6:ARG:HG3	1:A:7:LEU:N	0.61	2.09	2	1
1:A:37:ALA:O	1:A:38:ASP:HB2	0.61	1.94	1	1
1:A:6:ARG:O	1:A:74:ASP:HA	0.61	1.95	9	2
1:A:7:LEU:CD2	1:A:44:LEU:HB2	0.61	2.26	4	3
1:A:33:LEU:C	1:A:44:LEU:HB3	0.61	2.15	8	2
1:A:8:PHE:HA	1:A:43:TRP:CE3	0.61	2.31	5	1
1:A:43:TRP:HA	1:A:43:TRP:CE3	0.61	2.29	6	1
1:A:23:ALA:HB3	1:A:36:VAL:CG1	0.60	2.26	3	5
1:A:12:ARG:HA	1:A:19:PRO:CD	0.60	2.25	3	1
1:A:42:ALA:CB	1:A:44:LEU:HD21	0.60	2.26	4	1
1:A:7:LEU:HD13	1:A:46:GLY:CA	0.60	2.25	6	1
1:A:8:PHE:O	1:A:76:GLN:HA	0.60	1.96	2	4
1:A:27:SER:OG	1:A:53:LEU:HD23	0.60	1.97	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:PRO:HA	1:A:39:GLU:O	0.60	1.97	3	1
1:A:78:LEU:H	1:A:78:LEU:HD23	0.60	1.57	7	3
1:A:7:LEU:CD1	1:A:44:LEU:HB2	0.60	2.26	9	1
1:A:8:PHE:HB3	1:A:76:GLN:CA	0.60	2.25	5	1
1:A:31:ARG:O	1:A:33:LEU:HD22	0.59	1.97	7	2
1:A:53:LEU:HB2	1:A:65:VAL:HG13	0.59	1.74	7	1
1:A:27:SER:OG	1:A:31:ARG:HB2	0.59	1.97	4	3
1:A:26:THR:HB	1:A:32:GLU:OE1	0.59	1.97	9	1
1:A:19:PRO:O	1:A:36:VAL:HG21	0.59	1.97	7	4
1:A:6:ARG:N	1:A:7:LEU:HD13	0.59	2.12	7	2
1:A:18:GLN:NE2	1:A:39:GLU:HB2	0.59	2.13	3	1
1:A:34:GLY:C	1:A:44:LEU:HD12	0.59	2.18	5	2
1:A:59:GLY:H	1:A:62:GLN:NE2	0.59	1.96	3	1
1:A:6:ARG:HA	1:A:44:LEU:O	0.59	1.97	7	1
1:A:13:LEU:HD13	1:A:81:CYS:SG	0.58	2.37	4	3
1:A:6:ARG:O	1:A:7:LEU:HD23	0.58	1.98	5	2
1:A:20:PRO:HB3	1:A:57:TRP:CD2	0.58	2.33	9	1
1:A:33:LEU:HB3	1:A:44:LEU:HD13	0.58	1.72	4	2
1:A:51:GLU:H	1:A:67:VAL:CG1	0.58	2.12	9	2
1:A:59:GLY:HA3	1:A:62:GLN:NE2	0.58	2.13	8	4
1:A:41:LEU:H	1:A:41:LEU:HD22	0.58	1.57	6	1
1:A:7:LEU:HD22	1:A:7:LEU:N	0.58	2.14	1	2
1:A:39:GLU:HG3	1:A:40:GLY:H	0.58	1.59	3	1
1:A:6:ARG:CA	1:A:45:SER:HA	0.58	2.29	3	4
1:A:6:ARG:HA	1:A:46:GLY:N	0.57	2.13	9	1
1:A:13:LEU:HG	1:A:17:SER:O	0.57	1.99	9	1
1:A:7:LEU:HD12	1:A:47:VAL:HG23	0.57	1.76	3	1
1:A:33:LEU:C	1:A:44:LEU:HD12	0.57	2.19	7	1
1:A:57:TRP:CD1	1:A:58:ASP:HB2	0.57	2.35	5	5
1:A:19:PRO:HG3	1:A:81:CYS:SG	0.57	2.39	3	1
1:A:55:VAL:HB	1:A:63:CYS:O	0.57	1.99	8	4
1:A:25:VAL:HB	1:A:53:LEU:HD22	0.56	1.77	5	2
1:A:53:LEU:HD22	1:A:53:LEU:N	0.56	2.15	3	1
1:A:55:VAL:O	1:A:61:ILE:HA	0.56	2.01	1	2
1:A:34:GLY:HA3	1:A:44:LEU:HD22	0.56	1.76	9	1
1:A:60:LYS:O	1:A:62:GLN:HG2	0.56	2.00	8	3
1:A:53:LEU:O	1:A:64:GLN:HA	0.56	2.01	3	2
1:A:13:LEU:HD23	1:A:18:GLN:C	0.56	2.21	5	5
1:A:26:THR:HB	1:A:32:GLU:HG2	0.56	1.76	2	1
1:A:13:LEU:CG	1:A:17:SER:HB2	0.56	2.30	8	1
1:A:7:LEU:HG	1:A:45:SER:CB	0.56	2.28	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Models Total
1:A:7:LEU:CD1	1:A:46:GLY:N	0.56	2.69	8	2
1:A:8:PHE:CE1	1:A:41:LEU:HB2	0.56	2.34	9	1
1:A:25:VAL:HB	1:A:53:LEU:HD13	0.56	1.76	6	4
1:A:20:PRO:HB2	1:A:23:ALA:HB2	0.56	1.78	9	1
1:A:19:PRO:HG3	1:A:63:CYS:SG	0.56	2.41	2	2
1:A:34:GLY:O	1:A:35:MET:HG3	0.55	2.02	2	1
1:A:56:ASN:HA	1:A:60:LYS:O	0.55	2.02	2	4
1:A:25:VAL:HG12	1:A:55:VAL:HG22	0.55	1.79	5	6
1:A:50:GLY:N	1:A:67:VAL:HG13	0.55	2.17	8	1
1:A:24:SER:HB2	1:A:56:ASN:HB2	0.55	1.79	2	6
1:A:26:THR:OG1	1:A:30:GLY:HA2	0.55	2.02	5	5
1:A:39:GLU:CG	1:A:40:GLY:H	0.55	2.14	3	1
1:A:7:LEU:HD22	1:A:7:LEU:H	0.55	1.61	7	3
1:A:44:LEU:O	1:A:45:SER:HB2	0.54	2.02	5	1
1:A:53:LEU:HB2	1:A:65:VAL:HG12	0.54	1.78	8	1
1:A:7:LEU:HD12	1:A:73:SER:CB	0.54	2.32	7	1
1:A:7:LEU:O	1:A:43:TRP:HA	0.54	2.03	5	2
1:A:49:PRO:HA	1:A:67:VAL:HG12	0.54	1.78	7	3
1:A:13:LEU:HG	1:A:17:SER:HB2	0.54	1.80	8	1
1:A:43:TRP:CE3	1:A:43:TRP:CA	0.54	2.90	6	2
1:A:20:PRO:HD2	1:A:57:TRP:CD2	0.54	2.38	5	1
1:A:8:PHE:HB2	1:A:76:GLN:HG2	0.54	1.80	1	1
1:A:6:ARG:HB2	1:A:46:GLY:N	0.54	2.18	10	1
1:A:32:GLU:C	1:A:46:GLY:HA2	0.54	2.23	8	1
1:A:24:SER:HA	1:A:34:GLY:O	0.54	2.03	5	1
1:A:26:THR:O	1:A:54:SER:HB2	0.54	2.02	4	2
1:A:36:VAL:HA	1:A:42:ALA:HA	0.53	1.79	2	4
1:A:13:LEU:HD22	1:A:81:CYS:SG	0.53	2.43	1	1
1:A:34:GLY:HA2	1:A:44:LEU:CD1	0.53	2.33	5	1
1:A:56:ASN:HA	1:A:60:LYS:C	0.53	2.24	1	4
1:A:47:VAL:HG21	1:A:67:VAL:HG11	0.53	1.80	5	1
1:A:53:LEU:HD12	1:A:65:VAL:HB	0.53	1.79	4	1
1:A:57:TRP:CD1	1:A:57:TRP:C	0.53	2.81	3	2
1:A:18:GLN:HB2	1:A:20:PRO:HD3	0.53	1.80	10	1
1:A:6:ARG:HA	1:A:45:SER:C	0.53	2.24	5	1
1:A:31:ARG:HD2	1:A:33:LEU:HD11	0.53	1.80	6	1
1:A:32:GLU:O	1:A:33:LEU:HB2	0.53	2.04	8	1
1:A:11:LEU:HA	1:A:79:LEU:O	0.52	2.03	10	1
1:A:25:VAL:HB	1:A:53:LEU:CD2	0.52	2.34	10	1
1:A:13:LEU:HG	1:A:18:GLN:N	0.52	2.19	8	1
1:A:25:VAL:HG22	1:A:34:GLY:N	0.52	2.19	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:10:ILE:O	1:A:78:LEU:HA	0.52	2.04	8	2
1:A:36:VAL:CA	1:A:42:ALA:HB2	0.52	2.31	5	1
1:A:33:LEU:HD22	1:A:46:GLY:O	0.52	2.05	9	1
1:A:33:LEU:HD23	1:A:44:LEU:HD23	0.52	1.80	3	1
1:A:23:ALA:CB	1:A:36:VAL:HG22	0.52	2.34	7	2
1:A:42:ALA:HB1	1:A:44:LEU:HB2	0.52	1.79	5	1
1:A:21:PHE:HA	1:A:36:VAL:O	0.52	2.04	6	1
1:A:6:ARG:HA	1:A:46:GLY:H	0.52	1.63	9	1
1:A:78:LEU:H	1:A:78:LEU:HD13	0.51	1.65	8	1
1:A:7:LEU:HD21	1:A:44:LEU:HD12	0.51	1.80	9	1
1:A:51:GLU:H	1:A:67:VAL:HG13	0.51	1.65	9	2
1:A:23:ALA:CB	1:A:36:VAL:HG12	0.51	2.35	6	1
1:A:25:VAL:HG12	1:A:55:VAL:CG2	0.51	2.36	8	1
1:A:7:LEU:HD13	1:A:33:LEU:O	0.51	2.06	2	1
1:A:25:VAL:HG23	1:A:32:GLU:HG3	0.51	1.81	8	1
1:A:6:ARG:HD3	1:A:7:LEU:N	0.51	2.21	9	1
1:A:71:ALA:HA	1:A:77:LEU:HD22	0.51	1.82	1	1
1:A:7:LEU:N	1:A:7:LEU:CD1	0.51	2.73	9	1
1:A:47:VAL:CG1	1:A:67:VAL:HG21	0.51	2.35	3	1
1:A:27:SER:CB	1:A:29:LYS:HE2	0.51	2.36	3	1
1:A:34:GLY:CA	1:A:44:LEU:HD12	0.51	2.36	6	3
1:A:25:VAL:HG23	1:A:32:GLU:CG	0.50	2.36	8	1
1:A:6:ARG:CB	1:A:45:SER:HA	0.50	2.36	1	1
1:A:34:GLY:HA3	1:A:44:LEU:CD2	0.50	2.36	9	1
1:A:11:LEU:H	1:A:11:LEU:HD23	0.50	1.66	10	1
1:A:33:LEU:CD2	1:A:47:VAL:HG13	0.50	2.36	7	1
1:A:7:LEU:HD13	1:A:77:LEU:HD23	0.50	1.84	5	1
1:A:43:TRP:HA	1:A:43:TRP:HE3	0.50	1.67	6	1
1:A:53:LEU:HB3	1:A:65:VAL:HB	0.50	1.84	10	1
1:A:53:LEU:HB2	1:A:65:VAL:HB	0.50	1.82	6	6
1:A:57:TRP:H	1:A:60:LYS:CA	0.50	2.20	8	2
1:A:7:LEU:HD11	1:A:46:GLY:HA3	0.50	1.84	7	1
1:A:33:LEU:CB	1:A:44:LEU:HD13	0.50	2.36	4	1
1:A:33:LEU:HD21	1:A:47:VAL:HA	0.50	1.83	3	1
1:A:61:ILE:O	1:A:61:ILE:HG23	0.50	2.07	10	4
1:A:54:SER:HB3	1:A:61:ILE:HD11	0.50	1.83	4	4
1:A:53:LEU:CD1	1:A:65:VAL:HB	0.50	2.37	4	1
1:A:53:LEU:O	1:A:55:VAL:HG23	0.50	2.07	8	1
1:A:6:ARG:C	1:A:6:ARG:HD2	0.50	2.27	7	1
1:A:13:LEU:HD23	1:A:19:PRO:HD3	0.49	1.84	7	2
1:A:34:GLY:CA	1:A:44:LEU:HD22	0.49	2.38	4	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Models Total
1:A:43:TRP:O	1:A:44:LEU:HD23	0.49	2.06	2	3
1:A:43:TRP:CE3	1:A:43:TRP:HA	0.49	2.42	5	2
1:A:57:TRP:HD1	1:A:58:ASP:H	0.49	1.50	2	3
1:A:33:LEU:HD21	1:A:47:VAL:HG12	0.49	1.84	4	1
1:A:57:TRP:CE2	1:A:62:GLN:NE2	0.49	2.80	2	1
1:A:7:LEU:HD13	1:A:7:LEU:N	0.49	2.22	7	1
1:A:36:VAL:HA	1:A:41:LEU:O	0.49	2.08	8	2
1:A:18:GLN:HB2	1:A:19:PRO:CD	0.48	2.38	9	1
1:A:33:LEU:HG	1:A:46:GLY:O	0.48	2.07	4	1
1:A:25:VAL:HG21	1:A:44:LEU:HG	0.48	1.84	10	1
1:A:25:VAL:HB	1:A:53:LEU:HD21	0.48	1.85	10	1
1:A:7:LEU:HD21	1:A:9:ALA:HB2	0.48	1.84	2	1
1:A:21:PHE:HA	1:A:36:VAL:HG12	0.48	1.84	2	1
1:A:31:ARG:O	1:A:32:GLU:HB2	0.48	2.08	4	1
1:A:59:GLY:N	1:A:62:GLN:NE2	0.48	2.60	3	1
1:A:7:LEU:HD22	1:A:44:LEU:O	0.48	2.09	7	1
1:A:7:LEU:CD2	1:A:74:ASP:H	0.47	2.20	3	1
1:A:56:ASN:CA	1:A:61:ILE:HG13	0.47	2.38	6	2
1:A:49:PRO:CB	1:A:69:GLU:HA	0.47	2.32	5	2
1:A:51:GLU:C	1:A:67:VAL:HG13	0.47	2.29	5	1
1:A:11:LEU:HD12	1:A:36:VAL:HG23	0.47	1.86	4	1
1:A:6:ARG:HB2	1:A:46:GLY:H	0.47	1.68	10	1
1:A:78:LEU:O	1:A:78:LEU:HD22	0.47	2.10	8	1
1:A:33:LEU:HD21	1:A:47:VAL:HG13	0.47	1.86	3	1
1:A:33:LEU:HD13	1:A:46:GLY:HA3	0.47	1.87	2	1
1:A:51:GLU:H	1:A:67:VAL:HB	0.47	1.69	7	2
1:A:7:LEU:N	1:A:7:LEU:HD13	0.47	2.25	8	2
1:A:8:PHE:HA	1:A:43:TRP:HE3	0.47	1.69	5	1
1:A:27:SER:HB3	1:A:29:LYS:HE2	0.47	1.87	3	1
1:A:6:ARG:O	1:A:7:LEU:HG	0.46	2.10	10	1
1:A:7:LEU:HD12	1:A:74:ASP:HA	0.46	1.87	10	1
1:A:12:ARG:HA	1:A:18:GLN:HG3	0.46	1.87	10	1
1:A:55:VAL:HB	1:A:63:CYS:HB3	0.46	1.85	7	1
1:A:20:PRO:O	1:A:36:VAL:HB	0.46	2.10	10	2
1:A:8:PHE:HD2	1:A:76:GLN:HB3	0.46	1.71	7	1
1:A:56:ASN:HB2	1:A:61:ILE:HG13	0.46	1.86	5	2
1:A:33:LEU:CB	1:A:44:LEU:HG	0.46	2.40	3	1
1:A:18:GLN:HB3	1:A:20:PRO:HD3	0.46	1.86	10	1
1:A:18:GLN:OE1	1:A:40:GLY:HA3	0.46	2.10	5	1
1:A:6:ARG:HG2	1:A:44:LEU:HD22	0.46	1.86	5	1
1:A:51:GLU:N	1:A:67:VAL:HG22	0.46	2.17	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:39:GLU:HG3	1:A:40:GLY:N	0.46	2.25	3	1
1:A:27:SER:HA	1:A:53:LEU:HA	0.46	1.86	10	1
1:A:19:PRO:HA	1:A:39:GLU:O	0.46	2.11	9	1
1:A:34:GLY:CA	1:A:44:LEU:CD1	0.45	2.94	5	1
1:A:41:LEU:HD21	1:A:43:TRP:NE1	0.45	2.26	2	1
1:A:54:SER:HA	1:A:64:GLN:HG2	0.45	1.87	5	3
1:A:9:ALA:O	1:A:41:LEU:HA	0.45	2.12	7	2
1:A:23:ALA:HB3	1:A:36:VAL:HG22	0.45	1.88	5	2
1:A:8:PHE:N	1:A:8:PHE:CD1	0.45	2.84	7	1
1:A:26:THR:HA	1:A:32:GLU:CB	0.45	2.33	8	1
1:A:27:SER:HB3	1:A:31:ARG:HB3	0.45	1.89	8	1
1:A:7:LEU:HD13	1:A:44:LEU:C	0.45	2.32	9	1
1:A:41:LEU:O	1:A:41:LEU:HD13	0.45	2.12	2	1
1:A:53:LEU:HD12	1:A:65:VAL:HG21	0.45	1.88	7	1
1:A:42:ALA:HB3	1:A:44:LEU:CD1	0.45	2.42	3	1
1:A:41:LEU:HD11	1:A:43:TRP:HE1	0.45	1.72	2	1
1:A:25:VAL:HG23	1:A:33:LEU:HG	0.45	1.87	5	1
1:A:7:LEU:HB2	1:A:45:SER:CB	0.45	2.42	5	1
1:A:20:PRO:HD2	1:A:57:TRP:CG	0.45	2.47	5	1
1:A:65:VAL:HA	1:A:81:CYS:HA	0.45	1.86	7	1
1:A:25:VAL:CG2	1:A:34:GLY:CA	0.45	2.95	8	1
1:A:11:LEU:HD22	1:A:11:LEU:O	0.44	2.12	6	1
1:A:31:ARG:HH11	1:A:33:LEU:HD12	0.44	1.73	2	1
1:A:78:LEU:CD1	1:A:78:LEU:H	0.44	2.26	1	2
1:A:60:LYS:HG2	1:A:62:GLN:CD	0.44	2.33	7	1
1:A:13:LEU:HD21	1:A:18:GLN:C	0.44	2.33	3	1
1:A:12:ARG:HD3	1:A:17:SER:O	0.44	2.13	4	1
1:A:13:LEU:HD23	1:A:18:GLN:CA	0.44	2.43	5	1
1:A:7:LEU:HD12	1:A:46:GLY:N	0.44	2.19	9	1
1:A:11:LEU:HD12	1:A:36:VAL:CG2	0.44	2.43	4	1
1:A:6:ARG:CA	1:A:46:GLY:H	0.44	2.25	6	1
1:A:49:PRO:HA	1:A:67:VAL:CG1	0.44	2.42	6	1
1:A:24:SER:HB2	1:A:56:ASN:HD22	0.44	1.72	1	1
1:A:59:GLY:CA	1:A:62:GLN:NE2	0.44	2.81	2	3
1:A:78:LEU:HD13	1:A:78:LEU:H	0.44	1.71	1	1
1:A:23:ALA:HB3	1:A:36:VAL:CG2	0.44	2.42	10	2
1:A:6:ARG:H	1:A:7:LEU:HD23	0.44	1.71	3	1
1:A:7:LEU:HD11	1:A:44:LEU:HB2	0.44	1.88	9	1
1:A:6:ARG:HA	1:A:45:SER:N	0.44	2.28	5	1
1:A:60:LYS:HE2	1:A:62:GLN:OE1	0.44	2.13	6	1
1:A:53:LEU:N	1:A:53:LEU:CD2	0.43	2.81	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:43:TRP:CA	1:A:43:TRP:CE3	0.43	3.01	5	1
1:A:41:LEU:HB3	1:A:43:TRP:CH2	0.43	2.48	6	1
1:A:13:LEU:HD23	1:A:19:PRO:N	0.43	2.28	6	1
1:A:25:VAL:CG2	1:A:34:GLY:HA3	0.43	2.44	8	1
1:A:32:GLU:H	1:A:47:VAL:HG13	0.43	1.74	8	1
1:A:25:VAL:HA	1:A:55:VAL:HG22	0.43	1.90	6	2
1:A:56:ASN:CB	1:A:61:ILE:HG13	0.43	2.43	6	2
1:A:57:TRP:O	1:A:60:LYS:HG2	0.43	2.13	5	3
1:A:11:LEU:O	1:A:19:PRO:HD2	0.43	2.14	2	2
1:A:35:MET:N	1:A:44:LEU:HG	0.43	2.29	6	1
1:A:72:ILE:H	1:A:77:LEU:HG	0.43	1.73	6	1
1:A:28:GLU:OE1	1:A:28:GLU:N	0.43	2.52	3	1
1:A:33:LEU:CD2	1:A:47:VAL:HG12	0.43	2.44	4	1
1:A:56:ASN:OD1	1:A:61:ILE:HB	0.43	2.13	10	1
1:A:35:MET:N	1:A:42:ALA:HB1	0.43	2.29	2	1
1:A:13:LEU:HA	1:A:81:CYS:O	0.43	2.13	7	1
1:A:13:LEU:HA	1:A:81:CYS:HB3	0.43	1.91	8	1
1:A:33:LEU:HD23	1:A:47:VAL:HG22	0.43	1.90	3	1
1:A:27:SER:CA	1:A:53:LEU:HD12	0.42	2.45	10	1
1:A:39:GLU:CG	1:A:40:GLY:N	0.42	2.82	3	1
1:A:17:SER:O	1:A:18:GLN:HG3	0.42	2.13	9	1
1:A:6:ARG:CG	1:A:44:LEU:HD22	0.42	2.44	5	1
1:A:32:GLU:O	1:A:46:GLY:HA2	0.42	2.14	8	1
1:A:58:ASP:OD1	1:A:59:GLY:N	0.42	2.52	3	1
1:A:23:ALA:HB1	1:A:55:VAL:CG1	0.42	2.45	9	1
1:A:7:LEU:CD2	1:A:7:LEU:N	0.42	2.77	4	1
1:A:20:PRO:CD	1:A:57:TRP:CD2	0.42	3.02	5	1
1:A:7:LEU:H	1:A:44:LEU:C	0.42	2.18	5	1
1:A:11:LEU:HD23	1:A:79:LEU:HB2	0.42	1.91	5	1
1:A:34:GLY:CA	1:A:44:LEU:HG	0.42	2.41	7	1
1:A:25:VAL:HG22	1:A:34:GLY:C	0.42	2.35	8	1
1:A:11:LEU:HG	1:A:18:GLN:OE1	0.42	2.15	10	1
1:A:41:LEU:N	1:A:41:LEU:HD13	0.42	2.30	6	1
1:A:31:ARG:HG3	1:A:47:VAL:CG1	0.42	2.35	8	1
1:A:32:GLU:OE2	1:A:46:GLY:HA3	0.42	2.15	8	1
1:A:57:TRP:N	1:A:60:LYS:HA	0.42	2.30	1	1
1:A:33:LEU:HB3	1:A:44:LEU:HB3	0.42	1.91	4	1
1:A:33:LEU:CD2	1:A:53:LEU:HD21	0.42	2.38	1	1
1:A:9:ALA:HA	1:A:77:LEU:O	0.42	2.15	9	2
1:A:10:ILE:HB	1:A:78:LEU:HG	0.42	1.91	4	1
1:A:7:LEU:HB2	1:A:45:SER:HA	0.42	1.92	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:25:VAL:CG2	1:A:34:GLY:N	0.42	2.83	7	1
1:A:23:ALA:HB3	1:A:36:VAL:HG23	0.41	1.91	1	2
1:A:35:MET:HG3	1:A:44:LEU:CD1	0.41	2.45	8	1
1:A:56:ASN:HA	1:A:61:ILE:HG13	0.41	1.91	9	1
1:A:7:LEU:HD21	1:A:46:GLY:N	0.41	2.30	7	1
1:A:7:LEU:HD23	1:A:7:LEU:O	0.41	2.14	6	1
1:A:13:LEU:CD2	1:A:18:GLN:HE21	0.41	2.24	10	1
1:A:7:LEU:HD12	1:A:73:SER:HA	0.41	1.92	4	1
1:A:6:ARG:O	1:A:7:LEU:CB	0.41	2.69	10	1
1:A:66:ASN:HB2	1:A:80:PRO:HG2	0.41	1.92	10	1
1:A:7:LEU:HD11	1:A:47:VAL:HB	0.41	1.92	2	1
1:A:8:PHE:HB2	1:A:75:GLN:O	0.41	2.15	3	1
1:A:7:LEU:HB2	1:A:45:SER:HB2	0.41	1.91	5	1
1:A:11:LEU:H	1:A:11:LEU:CD1	0.41	2.24	6	1
1:A:53:LEU:CB	1:A:65:VAL:HB	0.41	2.44	10	1
1:A:53:LEU:HD12	1:A:65:VAL:CG2	0.41	2.45	7	1
1:A:33:LEU:CD2	1:A:47:VAL:HG22	0.41	2.46	3	1
1:A:11:LEU:CB	1:A:19:PRO:HG2	0.41	2.45	5	2
1:A:7:LEU:CB	1:A:45:SER:HB3	0.41	2.46	5	1
1:A:6:ARG:O	1:A:74:ASP:CA	0.41	2.68	9	1
1:A:55:VAL:HG21	1:A:65:VAL:HG23	0.41	1.93	4	1
1:A:69:GLU:CD	1:A:69:GLU:H	0.41	2.19	7	1
1:A:57:TRP:H	1:A:60:LYS:HA	0.41	1.74	8	1
1:A:57:TRP:CD1	1:A:58:ASP:HB3	0.41	2.51	4	1
1:A:18:GLN:HB2	1:A:19:PRO:HD3	0.41	1.93	9	1
1:A:26:THR:HA	1:A:32:GLU:HB2	0.41	1.93	4	1
1:A:11:LEU:HD13	1:A:79:LEU:HB2	0.41	1.92	7	1
1:A:25:VAL:HG23	1:A:25:VAL:O	0.40	2.16	9	1
1:A:65:VAL:HG11	1:A:79:LEU:HB3	0.40	1.92	4	1
1:A:56:ASN:OD1	1:A:60:LYS:HA	0.40	2.16	5	1
1:A:34:GLY:CA	1:A:44:LEU:CB	0.40	2.93	8	1
1:A:33:LEU:CD2	1:A:44:LEU:HD23	0.40	2.47	10	1
1:A:9:ALA:HB3	1:A:44:LEU:HG	0.40	1.93	1	1
1:A:13:LEU:HD22	1:A:18:GLN:NE2	0.40	2.27	10	1
1:A:33:LEU:CD1	1:A:45:SER:HA	0.40	2.47	5	1
1:A:36:VAL:HA	1:A:42:ALA:CA	0.40	2.46	6	1
1:A:11:LEU:HB3	1:A:79:LEU:HB2	0.40	1.93	6	1
1:A:49:PRO:HB3	1:A:69:GLU:CA	0.40	2.33	5	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	79/85 (93%)	60±3 (76±4%)	13±3 (16±4%)	6±2 (7±2%)	3	16
All	All	790/850 (93%)	602 (76%)	129 (16%)	59 (7%)	3	16

All 20 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	23	ALA	6
1	A	60	LYS	6
1	A	20	PRO	6
1	A	38	ASP	6
1	A	58	ASP	5
1	A	21	PHE	5
1	A	28	GLU	4
1	A	39	GLU	3
1	A	46	GLY	3
1	A	45	SER	2
1	A	19	PRO	2
1	A	40	GLY	2
1	A	32	GLU	2
1	A	7	LEU	1
1	A	18	GLN	1
1	A	24	SER	1
1	A	57	TRP	1
1	A	33	LEU	1
1	A	75	GLN	1
1	A	6	ARG	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	65/70 (93%)	53±3 (82±4%)	12±3 (18±4%)	6	40
All	All	650/700 (93%)	534 (82%)	116 (18%)	6	40

All 42 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	7	LEU	7
1	A	6	ARG	6
1	A	81	CYS	6
1	A	24	SER	6
1	A	26	THR	5
1	A	18	GLN	5
1	A	11	LEU	5
1	A	61	ILE	5
1	A	33	LEU	5
1	A	56	ASN	4
1	A	78	LEU	3
1	A	65	VAL	3
1	A	58	ASP	3
1	A	20	PRO	3
1	A	57	TRP	3
1	A	44	LEU	3
1	A	8	PHE	3
1	A	41	LEU	3
1	A	21	PHE	3
1	A	27	SER	2
1	A	66	ASN	2
1	A	17	SER	2
1	A	69	GLU	2
1	A	31	ARG	2
1	A	48	THR	2
1	A	43	TRP	2
1	A	13	LEU	2
1	A	60	LYS	2
1	A	32	GLU	2
1	A	25	VAL	2
1	A	62	GLN	2
1	A	29	LYS	1
1	A	75	GLN	1
1	A	39	GLU	1
1	A	84	GLN	1
1	A	77	LEU	1

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Mol	Chain	Res	Type	Models (Total)
1	A	12	ARG	1
1	A	47	VAL	1
1	A	54	SER	1
1	A	63	CYS	1
1	A	67	VAL	1
1	A	72	ILE	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 (i)

The completeness of assignment taking into account all chemical shift lists is 81% for the well-defined parts and 78% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 16684

Chemical shift list name: *assigned_ chem_ shift_ list_ 1*

7.1.1 Bookkeeping (i)

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	895
Number of shifts mapped to atoms	868
Number of unparsed shifts	0
Number of shifts with mapping errors	27
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 27 occurences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	87	ALA	HB1	1.23894107914	0.0319588635374	1
A	88	TRP	HB2	3.1507094519	0.0141390992766	2
A	87	ALA	HB3	1.23894107914	0.0319588635374	1
A	86	SER	HB3	3.69579178848	0.00604192919501	2
A	86	SER	CA	58.3323304395	0.0607447065904	1
A	86	SER	C	173.017120204	0.171623154952	1
A	88	TRP	HA	4.48380102553	0.0107699775789	1
A	87	ALA	C	177.287119818	0.00228120172299	1
A	87	ALA	HB2	1.23894107914	0.0319588635374	1
A	88	TRP	NE1	129.317757293	0.027710333661	1
A	86	SER	N	117.378753701	0.0566921758566	1
A	88	TRP	C	172.499331906	-1.0	1
A	88	TRP	HE1	10.043188525	0.00601681967417	1
A	87	ALA	CB	19.6363795498	0.0779973621113	1

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Chain	Res	Type	Atom	Shift Data		Ambiguity
				Value	Uncertainty	
A	87	ALA	H	7.9650985451	0.00746665778482	1
A	87	ALA	HA	4.25566834272	0.0142761691386	1
A	86	SER	H	8.17564976126	0.00641173366315	1
A	88	TRP	HB3	3.3343058852	0.0237122918385	2
A	86	SER	HA	4.32833028589	0.0100519455797	1
A	88	TRP	H	7.46331209826	0.00577099796883	1
A	86	SER	CB	64.0876211387	0.0480954709273	1
A	87	ALA	N	126.112286886	0.0386978562146	1
A	88	TRP	N	124.713664104	0.0830203667322	1
A	88	TRP	CB	30.4369310124	0.102871700371	1
A	86	SER	HB2	3.70564292383	0.0175172176785	2
A	88	TRP	CA	58.7271831712	0.132441167295	1
A	87	ALA	CA	52.6470026929	0.0755238787884	1

7.1.2   Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	87	-0.23 ± 0.13	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	76	0.08 ± 0.14	None needed (< 0.5 ppm)
$^{13}C'$	87	-0.51 ± 0.29	None needed (imprecise)
^{15}N	80	-0.34 ± 0.37	None needed (< 0.5 ppm)

7.1.3   Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 81%, i.e. 737 atoms were assigned a chemical shift out of a possible 913. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	378/383 (99%)	149/152 (98%)	157/158 (99%)	72/73 (99%)
Sidechain	336/488 (69%)	212/285 (74%)	116/184 (63%)	8/19 (42%)
Aromatic	23/42 (55%)	11/22 (50%)	10/18 (56%)	2/2 (100%)
Overall	737/913 (81%)	372/459 (81%)	283/360 (79%)	82/94 (87%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 78%, i.e. 777 atoms were assigned a chemical shift out of a possible 997. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	404/413 (98%)	159/164 (97%)	168/170 (99%)	77/79 (97%)
Sidechain	350/542 (65%)	223/317 (70%)	119/203 (59%)	8/22 (36%)
Aromatic	23/42 (55%)	11/22 (50%)	10/18 (56%)	2/2 (100%)
Overall	777/997 (78%)	393/503 (78%)	297/391 (76%)	87/103 (84%)

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	62	GLN	HG2	0.22	3.67 − 0.97	-7.8
1	A	20	PRO	HD2	1.31	5.45 − 1.85	-6.5
1	A	62	GLN	HB3	0.50	3.37 − 0.67	-5.6

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: