Full wwPDB NMR Structure Validation Report (i)

Feb 27, 2022 – 10:04 PM EST

PDB ID	:	2DLW
Title	:	Solution structure of the IRS domain of human docking protein 2, isoform a
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Deposited on	:	2006-04-20

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

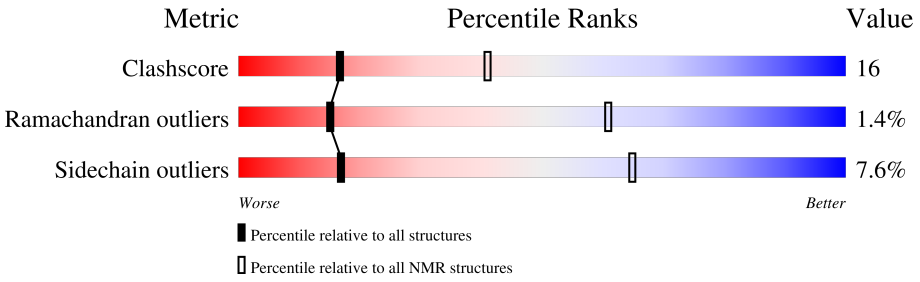
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment was not calculated.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	113	57% 25% 19%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 13 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*.

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:9-A:43, A:48-A:104 (92)	0.39	13

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	1, 2, 3, 4, 6, 7, 9, 10, 13, 14, 15, 16, 17, 18, 19
2	5, 20
Single-model clusters	8; 11; 12

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1708 atoms, of which 828 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Docking protein 2, isoform a.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	113	1708	545	828	161	171	3	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	cloning artifact	UNP Q8N5A4
A	2	SER	-	cloning artifact	UNP Q8N5A4
A	3	SER	-	cloning artifact	UNP Q8N5A4
A	4	GLY	-	cloning artifact	UNP Q8N5A4
A	5	SER	-	cloning artifact	UNP Q8N5A4
A	6	SER	-	cloning artifact	UNP Q8N5A4
A	7	GLY	-	cloning artifact	UNP Q8N5A4
A	108	SER	-	cloning artifact	UNP Q8N5A4
A	109	GLY	-	cloning artifact	UNP Q8N5A4
A	110	PRO	-	cloning artifact	UNP Q8N5A4
A	111	SER	-	cloning artifact	UNP Q8N5A4
A	112	SER	-	cloning artifact	UNP Q8N5A4
A	113	GLY	-	cloning artifact	UNP Q8N5A4

4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

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

• Molecule 1: Docking protein 2, isoform a

Chain A: 57% 25% 19%

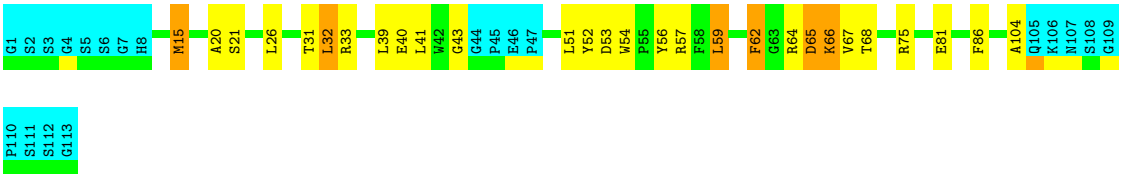
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Docking protein 2, isoform a

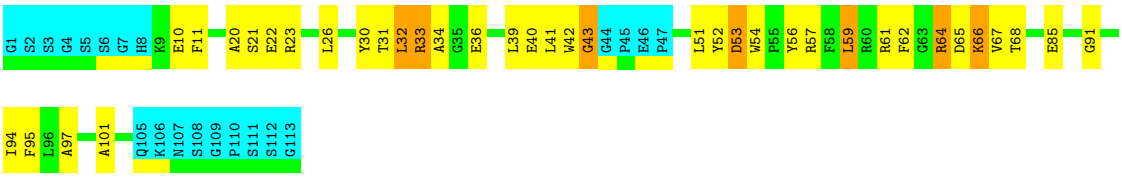
Chain A: 57% 19% 5% 19%



4.2.2 Score per residue for model 2

• Molecule 1: Docking protein 2, isoform a

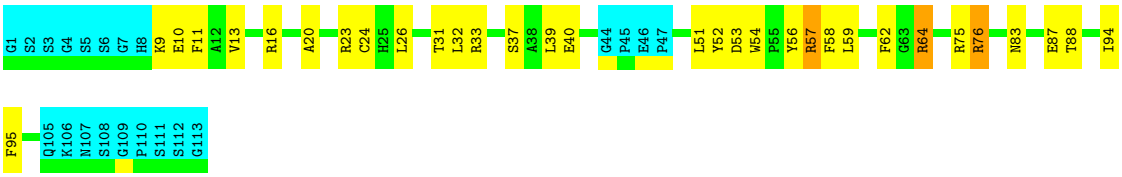
Chain A: 48% 27% 6% 19%



4.2.3 Score per residue for model 3

- Molecule 1: Docking protein 2, isoform a

Chain A: 53% 26% • 19%



4.2.4 Score per residue for model 4

- Molecule 1: Docking protein 2, isoform a

Chain A: 58% 22% • 19%

4.2.5 Score per residue for model 5

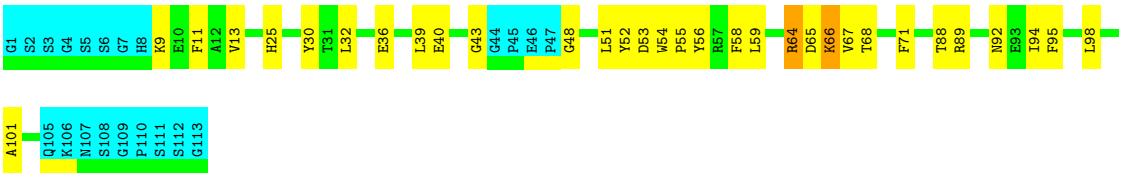
- Molecule 1: Docking protein 2, isoform a

Chain A: 60% 21% 19%

4.2.6 Score per residue for model 6

- Molecule 1: Docking protein 2, isoform a

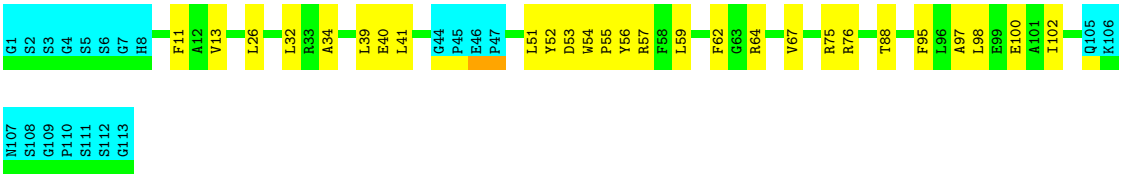
Chain A: 53% 27% • 19%



4.2.7 Score per residue for model 7

- Molecule 1: Docking protein 2, isoform a

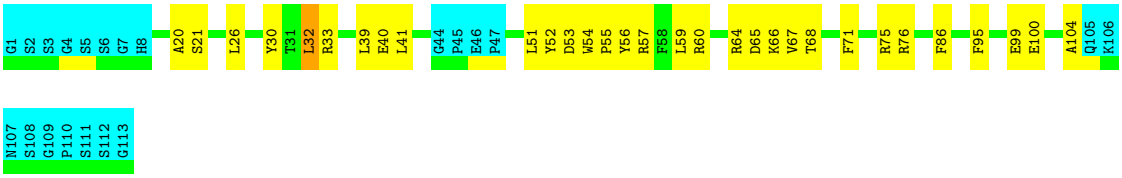
Chain A:



4.2.8 Score per residue for model 8

- Molecule 1: Docking protein 2, isoform a

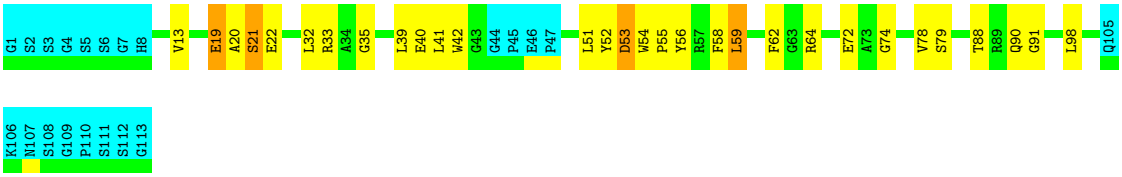
Chain A:



4.2.9 Score per residue for model 9

- Molecule 1: Docking protein 2, isoform a

Chain A:



4.2.10 Score per residue for model 10

- Molecule 1: Docking protein 2, isoform a

Chain A: 53% 26% • 19%

G1 S2 S3 G4 S5 S6 G7 H8 K9 E10 F11 A12 V13 T14 M15 T18 E19 A20 S21 E22 L26 Y30 T31 L32 G35 E36 S37 A38 L39 E40 L41 G44 P45 E46 P47 L51 Y52 D53 W54 P55 Y56 R57 F58 L59 R60 R64 A73 E87 T88 I94

F95 L98 I102 Q105 K106 N107 S108 G109 P110 S111 S112 G113

4.2.11 Score per residue for model 11

- Molecule 1: Docking protein 2, isoform a

Chain A: 60% 20% • 19%

G1 S2 S3 G4 S5 S6 G7 H8 F11 A12 V13 L26 Y30 T31 L32 E36 L39 E40 G43 G44 P45 E46 P47 L51 Y52 D53 W54 P55 Y56 F62 G63 R64 F71 T88 G91 N92 E93 I94 F95 L98 A101 Q105 K106 N107 S108 G109

P110 S111 S112 G113

4.2.12 Score per residue for model 12

- Molecule 1: Docking protein 2, isoform a

Chain A: 50% 29% • 19%

G1 S2 S3 G4 S5 S6 G7 H8 V13 R16 P17 E22 R23 T31 L32 R33 E36 L39 E40 L41 W42 G43 G44 P45 E46 P47 L51 Y52 D53 W54 P55 Y56 R57 F58 L59 R64 D65 K66 V67 E72 A73 G74 R75 V78 S79 G80 F86 E87 T88

R89 Q90 G91 N92 E93 L98 Q105 K106 N107 S108 G109 P110 S111 S112 G113

4.2.13 Score per residue for model 13 (medoid)

- Molecule 1: Docking protein 2, isoform a

Chain A: 52% 26% • 19%

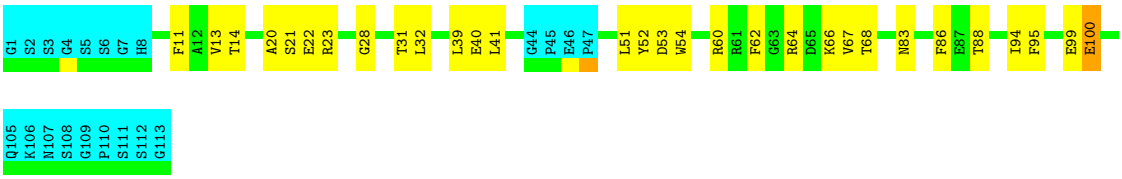
G1 S2 S3 G4 S5 S6 G7 H8 K9 E10 F11 A12 V13 R16 P17 T18 E19 A20 S21 T31 L32 R33 S37 A38 L39 E40 L41 W42 G43 G44 P45 E46 P47 G48 L51 Y52 D53 Y56 R57 F58 L59 R64 S70 F71 E72 F84 T88 R89 Q90 G91 N92

E93 I94 F95 L96 Q105 K106 N107 S108 G109 P110 S111 S112 G113

4.2.14 Score per residue for model 14

• Molecule 1: Docking protein 2, isoform a

Chain A: 55% 26% • 19%



4.2.15 Score per residue for model 15

• Molecule 1: Docking protein 2, isoform a

Chain A: 56% 24% • 19%

4.2.16 Score per residue for model 16

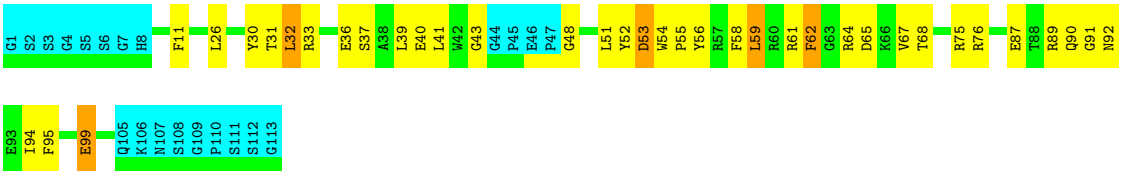
• Molecule 1: Docking protein 2, isoform a

Chain A: 56% 24% • 19%

4.2.17 Score per residue for model 17

• Molecule 1: Docking protein 2, isoform a

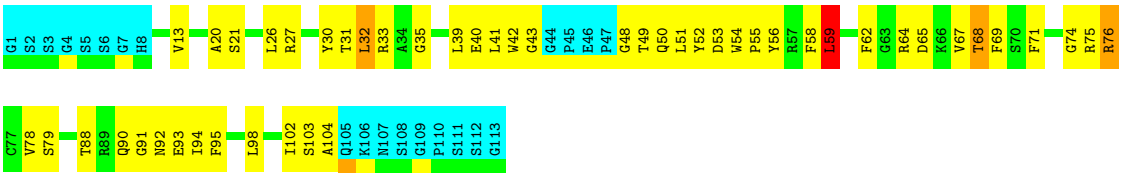
Chain A: 49% 28% • 19%



4.2.18 Score per residue for model 18

• Molecule 1: Docking protein 2, isoform a

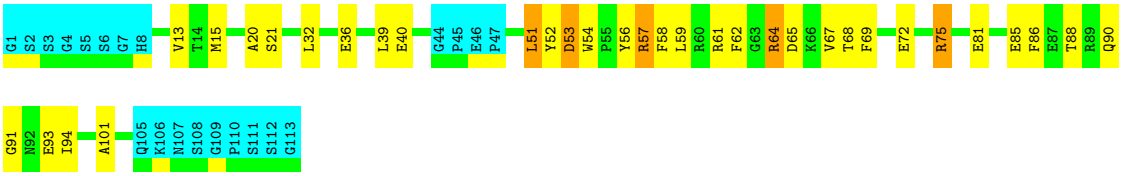
Chain A: 38% 40% • • 19%



4.2.19 Score per residue for model 19

• Molecule 1: Docking protein 2, isoform a

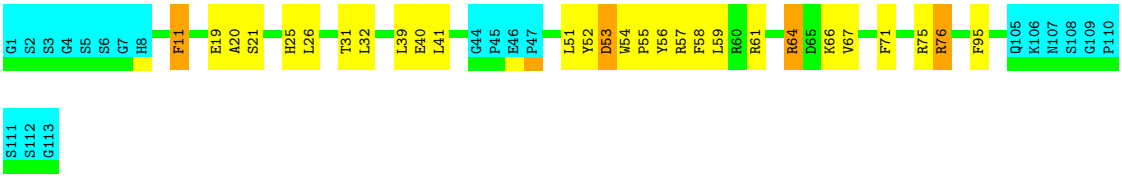
Chain A: 51% 26% • 19%



4.2.20 Score per residue for model 20

• Molecule 1: Docking protein 2, isoform a

Chain A: 57% 21% • 19%



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *torsion angle dynamics*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *target function, structures with the lowest energy, structures with the least restraint violations*.

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

Software name	Classification	Version
CYANA	structure solution	2.0.17
CYANA	refinement	2.0.17

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

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 (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	748	713	712	23±6
All	All	14960	14260	14240	455

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 16.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:13:VAL:HG11	1:A:32:LEU:HD12	1.08	1.19	9	5
1:A:32:LEU:HD23	1:A:94:ILE:CD1	0.94	1.92	3	4
1:A:32:LEU:HD23	1:A:94:ILE:HD13	0.88	1.45	3	4
1:A:13:VAL:HG12	1:A:88:THR:HB	0.78	1.54	10	11
1:A:36:GLU:O	1:A:101:ALA:HB1	0.76	1.81	19	4
1:A:31:THR:O	1:A:41:LEU:HD12	0.76	1.79	16	10
1:A:13:VAL:HG21	1:A:32:LEU:HD23	0.76	1.58	7	1
1:A:32:LEU:HD22	1:A:41:LEU:HD13	0.73	1.59	17	6
1:A:39:LEU:HD23	1:A:40:GLU:N	0.71	2.00	2	17
1:A:56:TYR:HA	1:A:59:LEU:HD23	0.68	1.65	18	2
1:A:56:TYR:HA	1:A:59:LEU:HD12	0.68	1.64	7	7
1:A:59:LEU:HD22	1:A:59:LEU:H	0.68	1.49	18	2
1:A:15:MET:SD	1:A:26:LEU:HD13	0.66	2.31	1	2
1:A:32:LEU:HD22	1:A:41:LEU:CD1	0.65	2.21	17	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:56:TYR:CE1	1:A:98:LEU:HD22	0.64	2.28	10	3
1:A:38:ALA:N	1:A:56:TYR:CE2	0.62	2.67	15	1
1:A:39:LEU:HD23	1:A:40:GLU:H	0.62	1.55	4	2
1:A:98:LEU:O	1:A:102:ILE:HD12	0.60	1.95	10	2
1:A:30:TYR:CE2	1:A:43:GLY:O	0.60	2.55	18	1
1:A:13:VAL:CG1	1:A:32:LEU:HD12	0.59	2.12	9	2
1:A:69:PHE:CE2	1:A:94:ILE:HG21	0.59	2.33	19	2
1:A:10:GLU:OE1	1:A:31:THR:HG23	0.59	1.97	3	1
1:A:52:TYR:O	1:A:54:TRP:CD2	0.57	2.58	18	18
1:A:59:LEU:HD23	1:A:72:GLU:O	0.57	2.00	5	2
1:A:13:VAL:HG12	1:A:88:THR:CB	0.57	2.30	7	3
1:A:26:LEU:O	1:A:26:LEU:HD12	0.57	1.99	11	1
1:A:33:ARG:NH1	1:A:42:TRP:CD1	0.56	2.73	2	1
1:A:91:GLY:HA2	1:A:94:ILE:HD12	0.56	1.75	2	3
1:A:55:PRO:O	1:A:59:LEU:HD22	0.56	2.01	9	2
1:A:42:TRP:CE3	1:A:48:GLY:O	0.55	2.59	18	1
1:A:32:LEU:HD13	1:A:33:ARG:N	0.55	2.16	4	9
1:A:68:THR:HG23	1:A:86:PHE:O	0.55	2.02	1	4
1:A:95:PHE:CE2	1:A:99:GLU:OE2	0.55	2.59	17	1
1:A:64:ARG:NH2	1:A:69:PHE:CE2	0.55	2.73	19	1
1:A:33:ARG:NH1	1:A:42:TRP:NE1	0.55	2.55	2	2
1:A:52:TYR:CD2	1:A:54:TRP:CZ2	0.55	2.95	15	2
1:A:56:TYR:CD1	1:A:98:LEU:HD23	0.55	2.37	12	1
1:A:69:PHE:CZ	1:A:94:ILE:HG21	0.54	2.37	19	1
1:A:26:LEU:HD21	1:A:52:TYR:OH	0.54	2.03	7	1
1:A:30:TYR:CE2	1:A:43:GLY:HA2	0.54	2.38	15	2
1:A:24:CYS:SG	1:A:26:LEU:HD12	0.54	2.43	3	1
1:A:14:THR:HG23	1:A:28:GLY:O	0.54	2.03	14	1
1:A:55:PRO:HG2	1:A:58:PHE:CD1	0.53	2.39	4	7
1:A:69:PHE:CE2	1:A:94:ILE:CG2	0.53	2.92	19	2
1:A:65:ASP:N	1:A:68:THR:O	0.53	2.42	19	2
1:A:39:LEU:O	1:A:53:ASP:CB	0.52	2.58	19	18
1:A:32:LEU:CD2	1:A:94:ILE:HD13	0.52	2.27	3	4
1:A:32:LEU:HD13	1:A:33:ARG:H	0.52	1.63	4	5
1:A:16:ARG:HG2	1:A:18:THR:HG23	0.52	1.80	13	1
1:A:9:LYS:O	1:A:11:PHE:CZ	0.52	2.63	16	1
1:A:75:ARG:O	1:A:76:ARG:CG	0.51	2.58	20	1
1:A:10:GLU:CG	1:A:33:ARG:NE	0.51	2.74	13	1
1:A:13:VAL:HG11	1:A:32:LEU:HD22	0.51	1.82	6	4
1:A:56:TYR:O	1:A:59:LEU:N	0.50	2.44	19	13
1:A:26:LEU:HD11	1:A:52:TYR:CE2	0.50	2.42	18	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:52:TYR:O	1:A:54:TRP:CE2	0.50	2.64	12	4
1:A:67:VAL:HG23	1:A:68:THR:N	0.50	2.21	6	4
1:A:11:PHE:CD1	1:A:94:ILE:HG12	0.50	2.42	6	5
1:A:65:ASP:O	1:A:67:VAL:N	0.50	2.45	8	4
1:A:26:LEU:HD11	1:A:52:TYR:HE2	0.50	1.66	2	2
1:A:69:PHE:CZ	1:A:94:ILE:HG22	0.50	2.42	18	1
1:A:42:TRP:CZ3	1:A:48:GLY:O	0.50	2.65	13	2
1:A:18:THR:O	1:A:21:SER:N	0.50	2.45	16	1
1:A:19:GLU:O	1:A:22:GLU:CG	0.49	2.60	9	1
1:A:51:LEU:HD12	1:A:52:TYR:N	0.49	2.23	19	3
1:A:13:VAL:CG2	1:A:32:LEU:HD23	0.49	2.35	7	1
1:A:74:GLY:O	1:A:75:ARG:CG	0.49	2.61	12	1
1:A:56:TYR:O	1:A:58:PHE:N	0.49	2.45	13	3
1:A:69:PHE:CD1	1:A:69:PHE:C	0.49	2.86	19	1
1:A:59:LEU:HD12	1:A:72:GLU:O	0.48	2.07	9	1
1:A:64:ARG:NE	1:A:92:ASN:N	0.48	2.61	6	1
1:A:62:PHE:CD2	1:A:95:PHE:CE2	0.48	3.02	11	1
1:A:37:SER:O	1:A:56:TYR:CD2	0.48	2.67	5	5
1:A:102:ILE:O	1:A:104:ALA:N	0.48	2.47	18	1
1:A:33:ARG:CZ	1:A:42:TRP:NE1	0.48	2.77	12	1
1:A:30:TYR:CD2	1:A:43:GLY:HA2	0.48	2.44	15	4
1:A:10:GLU:C	1:A:11:PHE:CD1	0.48	2.86	13	2
1:A:25:HIS:O	1:A:25:HIS:CG	0.47	2.67	6	1
1:A:71:PHE:C	1:A:71:PHE:CD1	0.47	2.87	8	4
1:A:33:ARG:CG	1:A:40:GLU:HB2	0.47	2.39	17	1
1:A:95:PHE:CE1	1:A:99:GLU:HG3	0.47	2.44	8	1
1:A:55:PRO:HG2	1:A:58:PHE:CG	0.47	2.44	18	2
1:A:30:TYR:CE2	1:A:43:GLY:CA	0.47	2.97	15	1
1:A:66:LYS:O	1:A:67:VAL:HG22	0.47	2.09	20	2
1:A:51:LEU:HD12	1:A:52:TYR:H	0.47	1.69	19	1
1:A:33:ARG:NH1	1:A:42:TRP:CE2	0.47	2.82	12	1
1:A:39:LEU:C	1:A:40:GLU:OE1	0.46	2.54	17	1
1:A:11:PHE:CE1	1:A:94:ILE:HG12	0.46	2.46	6	3
1:A:78:VAL:O	1:A:79:SER:C	0.46	2.54	12	3
1:A:38:ALA:C	1:A:56:TYR:CZ	0.46	2.89	15	1
1:A:20:ALA:O	1:A:22:GLU:N	0.46	2.49	10	2
1:A:56:TYR:O	1:A:57:ARG:C	0.46	2.54	8	12
1:A:65:ASP:O	1:A:68:THR:N	0.46	2.49	1	4
1:A:68:THR:CG2	1:A:85:GLU:OE1	0.46	2.64	2	1
1:A:64:ARG:HD2	1:A:95:PHE:CD2	0.46	2.46	11	1
1:A:63:GLY:HA2	1:A:95:PHE:CE1	0.46	2.46	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:56:TYR:CE1	1:A:98:LEU:HG	0.46	2.46	12	3
1:A:62:PHE:N	1:A:62:PHE:CD1	0.46	2.84	1	1
1:A:75:ARG:O	1:A:76:ARG:C	0.46	2.55	7	5
1:A:33:ARG:HG2	1:A:40:GLU:CB	0.46	2.41	17	1
1:A:67:VAL:C	1:A:88:THR:O	0.45	2.55	7	3
1:A:49:THR:HG22	1:A:50:GLN:N	0.45	2.26	18	1
1:A:21:SER:O	1:A:22:GLU:C	0.45	2.55	2	2
1:A:55:PRO:O	1:A:56:TYR:C	0.45	2.54	8	4
1:A:99:GLU:O	1:A:100:GLU:C	0.45	2.55	14	1
1:A:40:GLU:OE1	1:A:40:GLU:N	0.45	2.50	17	1
1:A:64:ARG:C	1:A:65:ASP:OD1	0.45	2.55	6	1
1:A:66:LYS:O	1:A:67:VAL:CG2	0.45	2.65	12	3
1:A:56:TYR:CD1	1:A:98:LEU:HG	0.45	2.46	9	2
1:A:16:ARG:NH1	1:A:87:GLU:OE1	0.45	2.50	3	1
1:A:90:GLN:O	1:A:91:GLY:C	0.45	2.54	19	8
1:A:18:THR:O	1:A:19:GLU:C	0.45	2.55	10	3
1:A:98:LEU:C	1:A:102:ILE:HD12	0.45	2.31	10	2
1:A:78:VAL:O	1:A:80:GLY:N	0.45	2.50	12	1
1:A:9:LYS:HG2	1:A:11:PHE:CE1	0.45	2.46	16	1
1:A:10:GLU:HG3	1:A:33:ARG:NE	0.45	2.27	13	1
1:A:61:ARG:O	1:A:72:GLU:CB	0.45	2.65	19	1
1:A:95:PHE:O	1:A:98:LEU:N	0.45	2.49	10	1
1:A:91:GLY:O	1:A:92:ASN:C	0.45	2.55	17	2
1:A:59:LEU:CD2	1:A:72:GLU:O	0.45	2.65	12	2
1:A:95:PHE:CD1	1:A:95:PHE:C	0.45	2.90	14	2
1:A:11:PHE:N	1:A:11:PHE:CD1	0.45	2.85	20	1
1:A:41:LEU:HD23	1:A:52:TYR:HB2	0.44	1.88	1	2
1:A:26:LEU:HD21	1:A:52:TYR:CE2	0.44	2.47	8	1
1:A:69:PHE:CE1	1:A:94:ILE:HG21	0.44	2.47	18	1
1:A:26:LEU:HD11	1:A:52:TYR:OH	0.44	2.12	15	1
1:A:64:ARG:NH2	1:A:92:ASN:OD1	0.44	2.50	15	1
1:A:41:LEU:HD22	1:A:54:TRP:CH2	0.44	2.48	9	2
1:A:26:LEU:HD22	1:A:30:TYR:CZ	0.44	2.48	15	2
1:A:64:ARG:HD3	1:A:95:PHE:CG	0.44	2.47	18	1
1:A:64:ARG:CZ	1:A:69:PHE:CE2	0.44	3.00	19	1
1:A:20:ALA:O	1:A:21:SER:C	0.44	2.56	15	13
1:A:93:GLU:O	1:A:94:ILE:C	0.44	2.56	15	2
1:A:65:ASP:CB	1:A:68:THR:O	0.44	2.66	18	1
1:A:62:PHE:CD1	1:A:62:PHE:N	0.44	2.86	17	3
1:A:11:PHE:CD1	1:A:11:PHE:N	0.44	2.86	3	4
1:A:95:PHE:C	1:A:95:PHE:CD1	0.44	2.91	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:35:GLY:N	1:A:56:TYR:OH	0.44	2.51	10	1
1:A:64:ARG:CD	1:A:95:PHE:CB	0.44	2.96	18	1
1:A:9:LYS:O	1:A:11:PHE:CE1	0.43	2.71	3	2
1:A:33:ARG:HD3	1:A:42:TRP:CD1	0.43	2.48	9	1
1:A:70:SER:CB	1:A:84:PHE:O	0.43	2.66	13	1
1:A:65:ASP:C	1:A:67:VAL:N	0.43	2.71	8	4
1:A:90:GLN:O	1:A:93:GLU:N	0.43	2.52	19	1
1:A:9:LYS:O	1:A:11:PHE:CE2	0.43	2.72	16	1
1:A:64:ARG:HD2	1:A:95:PHE:CG	0.43	2.48	2	1
1:A:32:LEU:HD23	1:A:41:LEU:CD1	0.42	2.43	15	1
1:A:62:PHE:CD2	1:A:95:PHE:CE1	0.42	3.07	17	1
1:A:33:ARG:CB	1:A:40:GLU:HB2	0.42	2.44	3	1
1:A:64:ARG:HG2	1:A:95:PHE:CB	0.42	2.45	6	1
1:A:102:ILE:C	1:A:104:ALA:N	0.42	2.71	18	1
1:A:69:PHE:O	1:A:86:PHE:N	0.42	2.52	19	1
1:A:20:ALA:O	1:A:23:ARG:N	0.42	2.53	3	1
1:A:9:LYS:O	1:A:33:ARG:CD	0.42	2.67	4	1
1:A:66:LYS:O	1:A:89:ARG:CD	0.42	2.68	6	1
1:A:15:MET:SD	1:A:86:PHE:CE2	0.42	3.13	19	1
1:A:74:GLY:O	1:A:81:GLU:CB	0.42	2.68	5	1
1:A:34:ALA:CB	1:A:97:ALA:CB	0.42	2.98	2	1
1:A:59:LEU:HD23	1:A:73:ALA:HA	0.42	1.91	10	1
1:A:33:ARG:HB2	1:A:40:GLU:CB	0.41	2.44	8	2
1:A:13:VAL:HG21	1:A:86:PHE:CD1	0.41	2.50	12	1
1:A:25:HIS:O	1:A:25:HIS:CD2	0.41	2.73	20	1
1:A:102:ILE:O	1:A:103:SER:C	0.41	2.58	4	1
1:A:62:PHE:HZ	1:A:102:ILE:HD13	0.41	1.75	7	1
1:A:64:ARG:CD	1:A:64:ARG:C	0.41	2.89	3	1
1:A:65:ASP:O	1:A:66:LYS:C	0.41	2.58	1	1
1:A:16:ARG:NE	1:A:17:PRO:HD2	0.41	2.30	12	1
1:A:41:LEU:HD22	1:A:52:TYR:HB2	0.41	1.91	7	1
1:A:92:ASN:HD21	1:A:96:LEU:HD11	0.41	1.75	13	1
1:A:35:GLY:N	1:A:40:GLU:OE1	0.41	2.52	18	1
1:A:95:PHE:O	1:A:96:LEU:C	0.41	2.59	4	1
1:A:34:ALA:CB	1:A:97:ALA:HB1	0.41	2.46	7	1
1:A:64:ARG:HD2	1:A:95:PHE:CB	0.41	2.46	18	1
1:A:68:THR:HG22	1:A:85:GLU:OE1	0.41	2.16	2	1
1:A:26:LEU:HA	1:A:30:TYR:CE1	0.41	2.50	8	1
1:A:22:GLU:HG3	1:A:23:ARG:N	0.41	2.30	12	1
1:A:32:LEU:CD2	1:A:41:LEU:CD1	0.41	2.99	15	1
1:A:60:ARG:CZ	1:A:60:ARG:HB3	0.40	2.46	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:75:ARG:CA	1:A:81:GLU:HG2	0.40	2.46	19	1
1:A:15:MET:CE	1:A:15:MET:HA	0.40	2.47	1	1
1:A:64:ARG:HG3	1:A:95:PHE:CD2	0.40	2.52	13	1
1:A:64:ARG:NH1	1:A:95:PHE:CD2	0.40	2.89	20	1
1:A:68:THR:HG22	1:A:69:PHE:N	0.40	2.31	15	1
1:A:30:TYR:CD2	1:A:43:GLY:O	0.40	2.75	18	1
1:A:67:VAL:O	1:A:88:THR:O	0.40	2.40	19	1
1:A:57:ARG:HG3	1:A:58:PHE:N	0.40	2.32	15	1
1:A:64:ARG:C	1:A:64:ARG:HD3	0.40	2.37	6	1
1:A:90:GLN:O	1:A:92:ASN:N	0.40	2.54	13	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	92/113 (81%)	81±3 (88±3%)	10±2 (10±3%)	1±1 (1±1%)	15	61
All	All	1840/2260 (81%)	1622 (88%)	192 (10%)	26 (1%)	15	61

All 11 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	59	LEU	5
1	A	43	GLY	4
1	A	66	LYS	4
1	A	57	ARG	3
1	A	48	GLY	2
1	A	21	SER	2
1	A	74	GLY	2
1	A	35	GLY	1
1	A	79	SER	1
1	A	91	GLY	1
1	A	103	SER	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	75/90 (83%)	69±2 (92±3%)	6±2 (8±3%)	17	65
All	All	1500/1800 (83%)	1386 (92%)	114 (8%)	17	65

All 32 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	51	LEU	20
1	A	64	ARG	17
1	A	32	LEU	10
1	A	62	PHE	8
1	A	53	ASP	8
1	A	75	ARG	4
1	A	66	LYS	4
1	A	100	GLU	4
1	A	61	ARG	3
1	A	76	ARG	3
1	A	15	MET	2
1	A	23	ARG	2
1	A	83	ASN	2
1	A	60	ARG	2
1	A	19	GLU	2
1	A	59	LEU	2
1	A	10	GLU	2
1	A	87	GLU	2
1	A	36	GLU	2
1	A	89	ARG	2
1	A	92	ASN	2
1	A	65	ASP	1
1	A	81	GLU	1
1	A	33	ARG	1
1	A	93	GLU	1
1	A	90	GLN	1
1	A	99	GLU	1
1	A	27	ARG	1
1	A	68	THR	1

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Mol	Chain	Res	Type	Models (Total)
1	A	71	PHE	1
1	A	85	GLU	1
1	A	11	PHE	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 monosaccharides 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 (i)

No chemical shift data were provided