Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	2YU0
Title	:	Solution structures of the PAAD_DAPIN domain of mus musculus interferon -activatable protein 205
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Deposited on	:	2007-04-05

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:

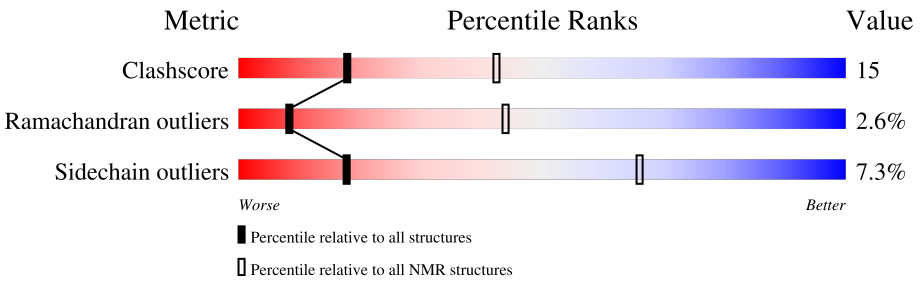
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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	94	57% 21% • 20%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 14 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:11-A:85 (75)	0.29	14

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 3 clusters and 2 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1473 atoms, of which 740 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Interferon-activable protein 205.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	94	1473	457	740	128	144	4	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP Q08619
A	2	SER	-	expression tag	UNP Q08619
A	3	SER	-	expression tag	UNP Q08619
A	4	GLY	-	expression tag	UNP Q08619
A	5	SER	-	expression tag	UNP Q08619
A	6	SER	-	expression tag	UNP Q08619
A	7	GLY	-	expression tag	UNP Q08619
A	89	SER	-	expression tag	UNP Q08619
A	90	GLY	-	expression tag	UNP Q08619
A	91	PRO	-	expression tag	UNP Q08619
A	92	SER	-	expression tag	UNP Q08619
A	93	SER	-	expression tag	UNP Q08619
A	94	GLY	-	expression tag	UNP Q08619

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: Interferon-activable protein 205

Chain A: 57% 21% • 20%

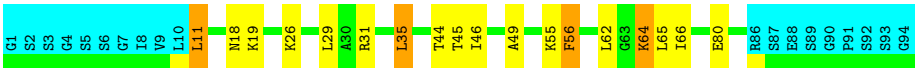
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Interferon-activable protein 205

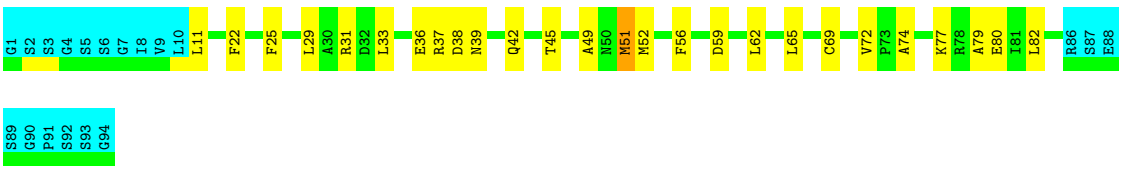
Chain A: 61% 15% • 20%



4.2.2 Score per residue for model 2

• Molecule 1: Interferon-activable protein 205

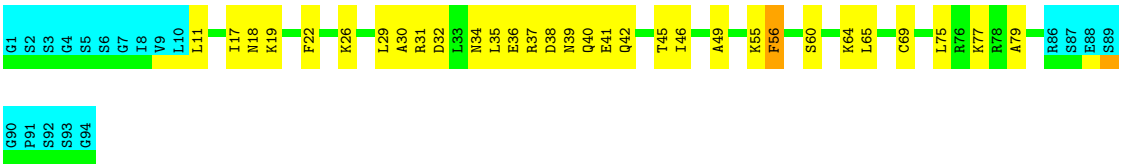
Chain A: 52% 27% • 20%



4.2.3 Score per residue for model 3

- Molecule 1: Interferon-activable protein 205

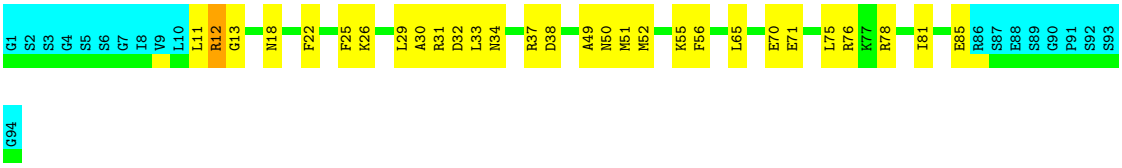
Chain A: 47% 32% • 20%



4.2.4 Score per residue for model 4

- Molecule 1: Interferon-activable protein 205

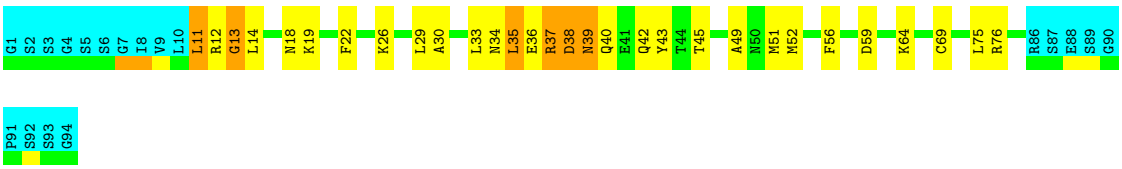
Chain A: 49% 30% • 20%



4.2.5 Score per residue for model 5

- Molecule 1: Interferon-activable protein 205

Chain A: 48% 26% 6% 20%



4.2.6 Score per residue for model 6

- Molecule 1: Interferon-activable protein 205

Chain A: 51% 28% • 20%

4.2.7 Score per residue for model 7

- Molecule 1: Interferon-activable protein 205

Chain A: 52% 21% 6% 20%

G1 S2 S3 G4 S5 S6 G7 I8 V9 L10 L11 R12 N18 K19 H20 Y21 F25 K26 L29 A30 R31 D32 L33 N34 L35 E36 R37 D38 N39 Q42 M51 K55 F56 L62 L65 I66 C69 V72 A79 R86 S87 E88 S89 G90 P91 S92 S93 G94

4.2.8 Score per residue for model 8

- Molecule 1: Interferon-activable protein 205

Chain A: 55% 23% • 20%

G1 S2 S3 G4 S5 S6 G7 I8 V9 L10 L11 R12 G13 L14 F22 S23 L24 R31 E36 R37 D38 N39 Q42 Y43 T44 T45 I46 A49 E54 K55 L62 L65 V72 P73 A74 E85 R86 S87 E88 S89 G90 P91 S92 S93 G94

4.2.9 Score per residue for model 9

- Molecule 1: Interferon-activable protein 205

Chain A: 47% 31% • 20%

G1 S2 S3 G4 S5 S6 G7 I8 V9 L10 L11 R12 G13 L14 I17 F22 F25 K26 S27 L28 L29 A30 R31 N34 L35 E36 R37 D38 N39 Q40 E41 Q42 Y43 T44 T45 N50 M51 K55 F56 D59 L65 K77 E80 I81 R86 S87 E88 S89 G90

P91 S92 S93 G94

4.2.10 Score per residue for model 10

- Molecule 1: Interferon-activable protein 205

Chain A: 50% 26% • 20%

G1 S2 S3 G4 S5 S6 G7 I8 V9 L10 L11 N18 K19 H20 Y21 F22 K26 L29 A30 R31 E36 N39 Q40 T45 I46 Q47 I48 A49 N50 E53 E54 K55 F56 D59 L62 G63 K64 L65 C69 E70 A79 R86 S87 E88 S89 G90 P91 S92

S93 G94

4.2.11 Score per residue for model 11

- Molecule 1: Interferon-activable protein 205

Chain A: 48% 24% 7% 20%

G1 S2 S3 G4 S5 S6 G7 I8 V9 L10 L11 R12 G13 L14 N18 K19 H20 Y21 L29 A30 R31 D32 L33 E36 R37 D38 N39 Q40 E41 Q42 Y43 A49 N50 M51 K55 L62 G63 K64 L65 I66 V72 P73 A74 E80 E85 R86 S87 E88 S89 G90 P91

S92 S93 G94

4.2.12 Score per residue for model 12

- Molecule 1: Interferon-activable protein 205

Chain A: 57% 19% • 20%

G1 S2 S3 G4 S5 S6 G7 I8 V9 L10 L11 R12 G13 A30 R31 E36 R37 D38 N39 Q40 E41 Q42 A49 K55 F56 L62 L65 L75 R78 L82 K83 K84 E85 R86 S87 E88 S89 G90 P91 S92 S93 G94

4.2.13 Score per residue for model 13

- Molecule 1: Interferon-activable protein 205

Chain A: 50% 26% • • 20%

G1 S2 S3 G4 S5 S6 G7 I8 V9 L10 L11 R12 G13 N18 K19 H20 Y21 F22 K26 A30 R31 D32 L33 N34 L35 E36 R37 D38 N39 A49 N50 M51 K55 F56 L62 L65 I66 L75 R76 K77 R78 I81 R86 S87 E88 S89 G90 P91 S92 S93

G94

4.2.14 Score per residue for model 14 (medoid)

- Molecule 1: Interferon-activable protein 205

Chain A: 48% 26% 5% • 20%

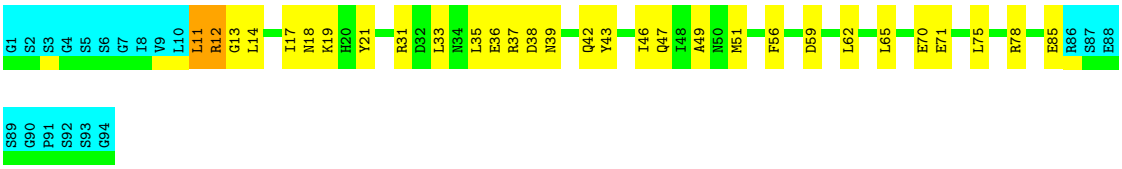
G1 S2 S3 G4 S5 S6 G7 I8 V9 L10 L11 R12 G13 L14 N18 K19 H20 F25 L28 L29 A30 N34 L35 E36 R37 D38 E41 Q42 Y43 T44 T45 I46 A49 N50 F56 L62 L65 C69 E70 E71 V72 A79 R86 S87 E88 S89 G90 P91

S92 S93 G94

4.2.15 Score per residue for model 15

- Molecule 1: Interferon-activable protein 205

Chain A: 48% 30% • 20%



4.2.16 Score per residue for model 16

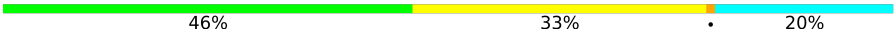
- Molecule 1: Interferon-activable protein 205

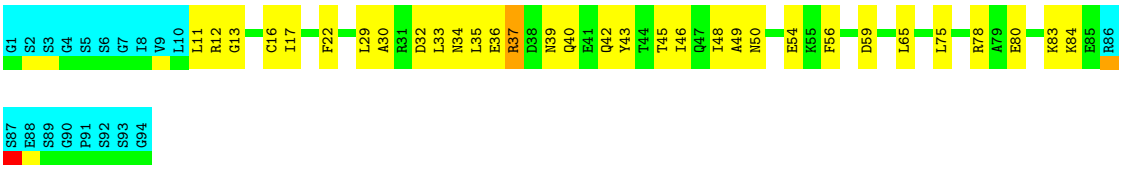
Chain A:

4.2.17 Score per residue for model 17

- Molecule 1: Interferon-activable protein 205

Chain A:





4.2.18 Score per residue for model 18

- Molecule 1: Interferon-activable protein 205

Chain A:

4.2.19 Score per residue for model 19

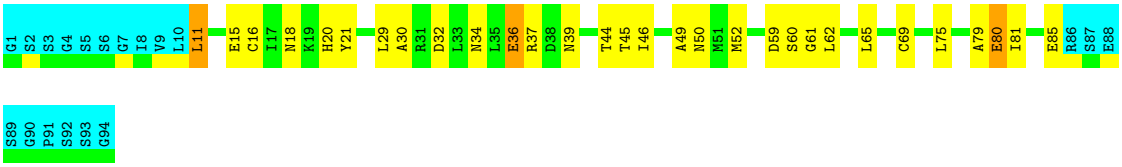
- Molecule 1: Interferon-activable protein 205

Chain A:

4.2.20 Score per residue for model 20

- Molecule 1: Interferon-activable protein 205

Chain A:



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: *structures with the least restraint violations, target function*.

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	615	628	627	18±5
All	All	12300	12560	12540	369

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 15.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:LEU:HD11	1:A:49:ALA:HB1	0.96	1.38	4	6
1:A:11:LEU:HD21	1:A:49:ALA:HB1	0.86	1.44	13	8
1:A:39:ASN:ND2	1:A:43:TYR:CE1	0.68	2.60	5	1
1:A:65:LEU:HD13	1:A:65:LEU:O	0.68	1.89	9	4
1:A:39:ASN:ND2	1:A:43:TYR:CZ	0.62	2.68	5	1
1:A:29:LEU:HD21	1:A:64:LYS:HG2	0.62	1.71	5	4
1:A:11:LEU:HD11	1:A:49:ALA:CB	0.62	2.25	20	2
1:A:35:LEU:HD22	1:A:43:TYR:CD2	0.61	2.31	15	2
1:A:39:ASN:O	1:A:43:TYR:CD2	0.60	2.54	9	3
1:A:39:ASN:OD1	1:A:43:TYR:CE2	0.60	2.55	9	2
1:A:21:TYR:CZ	1:A:72:VAL:HG11	0.59	2.32	7	2
1:A:39:ASN:ND2	1:A:42:GLN:NE2	0.58	2.51	19	3
1:A:69:CYS:HB2	1:A:79:ALA:HB2	0.58	1.74	7	6
1:A:33:LEU:HD23	1:A:55:LYS:HG3	0.58	1.75	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:39:ASN:ND2	1:A:42:GLN:CG	0.57	2.67	5	1
1:A:33:LEU:HD22	1:A:51:MET:HB3	0.57	1.76	11	8
1:A:33:LEU:HD21	1:A:52:MET:HG2	0.57	1.76	2	2
1:A:65:LEU:C	1:A:65:LEU:HD13	0.56	2.21	18	12
1:A:30:ALA:HB2	1:A:40:GLN:NE2	0.56	2.15	3	3
1:A:39:ASN:ND2	1:A:42:GLN:CD	0.55	2.60	19	8
1:A:65:LEU:HD13	1:A:65:LEU:C	0.54	2.23	9	2
1:A:21:TYR:CD2	1:A:75:LEU:HD21	0.53	2.39	20	1
1:A:78:ARG:HA	1:A:81:ILE:HD12	0.53	1.81	4	2
1:A:39:ASN:O	1:A:43:TYR:CE2	0.53	2.61	18	1
1:A:46:ILE:H	1:A:46:ILE:HD12	0.52	1.65	14	3
1:A:30:ALA:HA	1:A:35:LEU:HD12	0.52	1.81	14	2
1:A:29:LEU:HD21	1:A:64:LYS:CG	0.52	2.35	5	3
1:A:55:LYS:HG2	1:A:56:PHE:CZ	0.51	2.41	7	10
1:A:25:PHE:CE1	1:A:29:LEU:CD2	0.51	2.93	7	1
1:A:36:GLU:O	1:A:38:ASP:N	0.51	2.44	14	11
1:A:65:LEU:HD12	1:A:82:LEU:HD13	0.51	1.83	12	2
1:A:36:GLU:O	1:A:40:GLN:N	0.51	2.44	9	3
1:A:46:ILE:HG22	1:A:50:ASN:ND2	0.51	2.21	20	3
1:A:39:ASN:ND2	1:A:42:GLN:OE1	0.51	2.44	9	2
1:A:39:ASN:OD1	1:A:43:TYR:CZ	0.51	2.64	9	1
1:A:29:LEU:HD11	1:A:64:LYS:HG2	0.51	1.82	16	3
1:A:39:ASN:CG	1:A:42:GLN:CD	0.51	2.70	5	1
1:A:30:ALA:O	1:A:34:ASN:N	0.50	2.44	16	10
1:A:36:GLU:O	1:A:39:ASN:N	0.50	2.45	9	7
1:A:29:LEU:HD11	1:A:64:LYS:HE2	0.50	1.83	10	2
1:A:17:ILE:HG22	1:A:75:LEU:HD22	0.50	1.82	15	3
1:A:80:GLU:CG	1:A:81:ILE:N	0.50	2.75	9	2
1:A:16:CYS:SG	1:A:78:ARG:NE	0.50	2.85	17	1
1:A:22:PHE:CZ	1:A:45:THR:HA	0.49	2.42	8	10
1:A:83:LYS:O	1:A:85:GLU:N	0.49	2.45	18	1
1:A:25:PHE:CE1	1:A:29:LEU:HD21	0.49	2.41	7	2
1:A:46:ILE:O	1:A:49:ALA:N	0.49	2.45	15	6
1:A:12:ARG:O	1:A:14:LEU:N	0.49	2.46	5	8
1:A:69:CYS:O	1:A:76:ARG:N	0.49	2.45	5	1
1:A:80:GLU:OE1	1:A:81:ILE:N	0.49	2.45	20	1
1:A:59:ASP:OD1	1:A:61:GLY:N	0.49	2.45	20	1
1:A:50:ASN:O	1:A:53:GLU:N	0.48	2.45	10	1
1:A:11:LEU:O	1:A:13:GLY:N	0.48	2.47	11	7
1:A:25:PHE:CE1	1:A:65:LEU:HA	0.48	2.44	4	2
1:A:25:PHE:HA	1:A:28:LEU:HD12	0.48	1.86	14	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:39:ASN:OD1	1:A:43:TYR:CD2	0.48	2.67	9	1
1:A:35:LEU:HD22	1:A:43:TYR:CE2	0.48	2.42	15	1
1:A:59:ASP:O	1:A:62:LEU:N	0.48	2.46	20	1
1:A:26:LYS:O	1:A:30:ALA:N	0.48	2.47	5	6
1:A:32:ASP:O	1:A:34:ASN:ND2	0.48	2.47	17	1
1:A:77:LYS:O	1:A:80:GLU:CG	0.47	2.62	2	1
1:A:36:GLU:O	1:A:40:GLN:NE2	0.47	2.47	11	2
1:A:36:GLU:O	1:A:37:ARG:C	0.47	2.53	20	8
1:A:11:LEU:HD11	1:A:49:ALA:HB2	0.47	1.87	20	1
1:A:72:VAL:HG12	1:A:74:ALA:H	0.47	1.68	16	5
1:A:26:LYS:O	1:A:35:LEU:HD12	0.47	2.10	5	2
1:A:22:PHE:CD2	1:A:26:LYS:HE2	0.47	2.45	13	1
1:A:39:ASN:OD1	1:A:42:GLN:NE2	0.46	2.49	3	3
1:A:70:GLU:O	1:A:72:VAL:N	0.46	2.48	6	1
1:A:37:ARG:N	1:A:40:GLN:OE1	0.46	2.49	17	1
1:A:46:ILE:O	1:A:47:GLN:C	0.46	2.54	16	4
1:A:41:GLU:CD	1:A:42:GLN:N	0.46	2.69	12	2
1:A:22:PHE:CE2	1:A:26:LYS:HE2	0.45	2.46	10	4
1:A:18:ASN:O	1:A:19:LYS:C	0.45	2.55	15	10
1:A:39:ASN:OD1	1:A:42:GLN:CD	0.45	2.55	15	4
1:A:17:ILE:HG22	1:A:75:LEU:CD2	0.45	2.41	17	1
1:A:29:LEU:O	1:A:30:ALA:C	0.45	2.55	20	11
1:A:65:LEU:O	1:A:68:PHE:N	0.45	2.50	6	1
1:A:50:ASN:O	1:A:54:GLU:CD	0.45	2.55	10	1
1:A:75:LEU:O	1:A:76:ARG:C	0.45	2.55	4	2
1:A:11:LEU:O	1:A:11:LEU:HD13	0.45	2.12	10	2
1:A:30:ALA:O	1:A:34:ASN:CA	0.45	2.64	13	4
1:A:33:LEU:O	1:A:34:ASN:CG	0.45	2.55	6	1
1:A:52:MET:O	1:A:54:GLU:N	0.45	2.50	18	1
1:A:65:LEU:HD12	1:A:82:LEU:CD1	0.45	2.42	12	2
1:A:30:ALA:CB	1:A:40:GLN:NE2	0.45	2.80	12	2
1:A:32:ASP:OD2	1:A:64:LYS:NZ	0.45	2.50	11	1
1:A:11:LEU:O	1:A:12:ARG:C	0.45	2.56	4	2
1:A:49:ALA:O	1:A:52:MET:N	0.45	2.49	4	1
1:A:54:GLU:CD	1:A:55:LYS:N	0.45	2.70	6	1
1:A:11:LEU:HD13	1:A:11:LEU:O	0.45	2.11	20	1
1:A:18:ASN:O	1:A:20:HIS:N	0.44	2.50	10	4
1:A:42:GLN:O	1:A:43:TYR:C	0.44	2.56	11	1
1:A:65:LEU:O	1:A:66:ILE:C	0.44	2.55	11	6
1:A:36:GLU:C	1:A:38:ASP:N	0.44	2.71	8	9
1:A:75:LEU:O	1:A:78:ARG:N	0.43	2.51	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:39:ASN:O	1:A:42:GLN:CG	0.43	2.66	17	1
1:A:83:LYS:C	1:A:85:GLU:N	0.43	2.72	18	1
1:A:29:LEU:CD1	1:A:52:MET:HE3	0.43	2.43	20	1
1:A:80:GLU:OE1	1:A:80:GLU:C	0.43	2.55	11	1
1:A:80:GLU:HG3	1:A:81:ILE:N	0.43	2.28	9	1
1:A:44:THR:O	1:A:45:THR:C	0.43	2.57	14	2
1:A:11:LEU:CD1	1:A:49:ALA:HB1	0.43	2.26	4	1
1:A:71:GLU:HG3	1:A:72:VAL:HG23	0.43	1.90	14	1
1:A:83:LYS:O	1:A:84:LYS:C	0.43	2.56	17	2
1:A:49:ALA:O	1:A:50:ASN:C	0.43	2.57	4	1
1:A:43:TYR:HB3	1:A:48:ILE:HD11	0.43	1.91	17	1
1:A:59:ASP:OD1	1:A:59:ASP:N	0.43	2.52	19	1
1:A:59:ASP:OD1	1:A:59:ASP:C	0.42	2.57	20	1
1:A:50:ASN:O	1:A:51:MET:C	0.42	2.58	18	2
1:A:12:ARG:O	1:A:13:GLY:C	0.42	2.57	11	2
1:A:39:ASN:OD1	1:A:39:ASN:O	0.42	2.38	11	1
1:A:11:LEU:C	1:A:13:GLY:N	0.42	2.72	17	6
1:A:44:THR:O	1:A:46:ILE:N	0.42	2.53	1	4
1:A:12:ARG:C	1:A:14:LEU:N	0.42	2.73	6	4
1:A:65:LEU:C	1:A:65:LEU:CD1	0.42	2.87	9	1
1:A:70:GLU:C	1:A:72:VAL:N	0.42	2.72	6	1
1:A:69:CYS:O	1:A:70:GLU:C	0.42	2.58	10	1
1:A:78:ARG:O	1:A:79:ALA:C	0.42	2.58	18	1
1:A:14:LEU:O	1:A:17:ILE:CG1	0.41	2.68	9	1
1:A:18:ASN:O	1:A:21:TYR:N	0.41	2.53	15	1
1:A:30:ALA:CA	1:A:35:LEU:HD12	0.41	2.45	14	1
1:A:54:GLU:O	1:A:55:LYS:C	0.41	2.58	8	1
1:A:21:TYR:CE1	1:A:72:VAL:HG11	0.41	2.50	11	1
1:A:29:LEU:HB3	1:A:33:LEU:HD12	0.41	1.90	17	1
1:A:15:GLU:O	1:A:16:CYS:C	0.41	2.58	20	1
1:A:70:GLU:O	1:A:71:GLU:C	0.41	2.59	4	2
1:A:33:LEU:HD21	1:A:52:MET:CG	0.41	2.46	5	1
1:A:24:LEU:H	1:A:24:LEU:HD12	0.41	1.75	8	1
1:A:69:CYS:HA	1:A:75:LEU:CB	0.41	2.46	5	1
1:A:52:MET:C	1:A:54:GLU:N	0.41	2.74	18	1
1:A:22:PHE:CE1	1:A:45:THR:HG22	0.40	2.51	3	1
1:A:42:GLN:O	1:A:43:TYR:O	0.40	2.40	11	2
1:A:79:ALA:HA	1:A:82:LEU:HD12	0.40	1.94	16	1
1:A:41:GLU:CG	1:A:42:GLN:N	0.40	2.85	9	1
1:A:41:GLU:C	1:A:43:TYR:N	0.40	2.74	14	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	75/94 (80%)	59±3 (79±4%)	14±3 (18±5%)	2±1 (3±1%)	8 44
All	All	1500/1880 (80%)	1187 (79%)	274 (18%)	39 (3%)	8 44

All 13 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	37	ARG	11
1	A	12	ARG	6
1	A	13	GLY	6
1	A	35	LEU	4
1	A	45	THR	2
1	A	43	TYR	2
1	A	19	LYS	2
1	A	71	GLU	1
1	A	66	ILE	1
1	A	20	HIS	1
1	A	53	GLU	1
1	A	84	LYS	1
1	A	60	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	67/81 (83%)	62±1 (93±2%)	5±1 (7±2%)	18 66
All	All	1340/1620 (83%)	1242 (93%)	98 (7%)	18 66

All 21 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	56	PHE	16
1	A	31	ARG	14
1	A	11	LEU	13
1	A	59	ASP	8
1	A	38	ASP	7
1	A	32	ASP	6
1	A	37	ARG	6
1	A	80	GLU	5
1	A	39	ASN	5
1	A	64	LYS	3
1	A	36	GLU	3
1	A	77	LYS	2
1	A	84	LYS	2
1	A	51	MET	1
1	A	60	SER	1
1	A	18	ASN	1
1	A	19	LYS	1
1	A	55	LYS	1
1	A	71	GLU	1
1	A	78	ARG	1
1	A	54	GLU	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