Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	2DN7
Title	:	Solution structures of the 6th fn3 domain of human receptor-type tyrosine-protein phosphatase F
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Deposited on	:	2006-04-25

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:

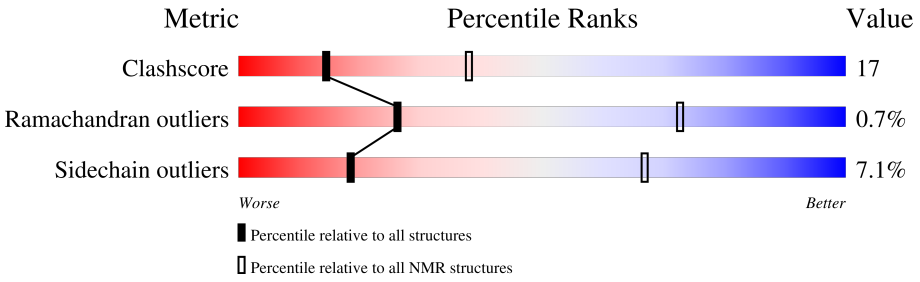
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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	107	59% 17% • 21%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 3 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:7-A:45, A:53-A:97 (84)	0.13	3

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 4 clusters and 1 single-model cluster was found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1617 atoms, of which 798 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Receptor-type tyrosine-protein phosphatase F.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	107	1617	509	798	146	160	4	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	cloning artifact	UNP P10586
A	2	SER	-	cloning artifact	UNP P10586
A	3	SER	-	cloning artifact	UNP P10586
A	4	GLY	-	cloning artifact	UNP P10586
A	5	SER	-	cloning artifact	UNP P10586
A	6	SER	-	cloning artifact	UNP P10586
A	7	GLY	-	cloning artifact	UNP P10586
A	102	SER	-	cloning artifact	UNP P10586
A	103	GLY	-	cloning artifact	UNP P10586
A	104	PRO	-	cloning artifact	UNP P10586
A	105	SER	-	cloning artifact	UNP P10586
A	106	SER	-	cloning artifact	UNP P10586
A	107	GLY	-	cloning artifact	UNP P10586

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: Receptor-type tyrosine-protein phosphatase F

Chain A: 59% 17% • 21%

G1 S2 S3 G4 S5 S6 I15 A19 T22 L25 L33 Y40 R41 L42 Q43 Y44 C45 R46 A47 D48 E49 A50 R51 P52 N53 T54 G58 K59 D60 D61 Q62 H63 F64 Y75 I76 F77 R78 L79 K93 E94 I95 P98 E99 D100 L101 S102 G103 P104 S105 S106

G107

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: Receptor-type tyrosine-protein phosphatase F

Chain A: 50% 24% • 21%

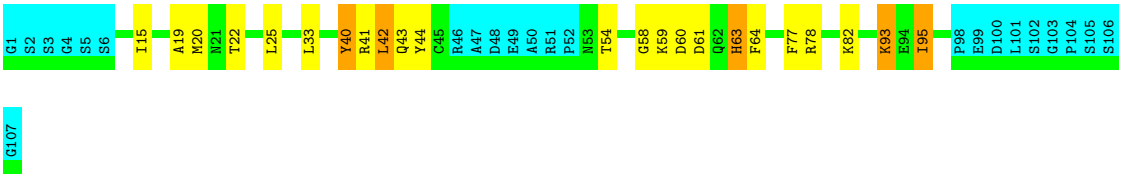
G1 S2 S3 G4 S5 S6 R10 I15 A19 T22 L25 Q26 W27 L33 Y40 R41 L42 Q43 Y44 C45 R46 A47 D48 E49 A50 R51 P52 N53 T54 G58 K59 D60 D61 Q62 H63 F64 Y75 I76 F77 R78 L79 A80 A81 K82 E90 F91 E92 K93 E94 I95

P98 E99 D100 L101 S102 G103 P104 S105 S106 G107

4.2.2 Score per residue for model 2

• Molecule 1: Receptor-type tyrosine-protein phosphatase F

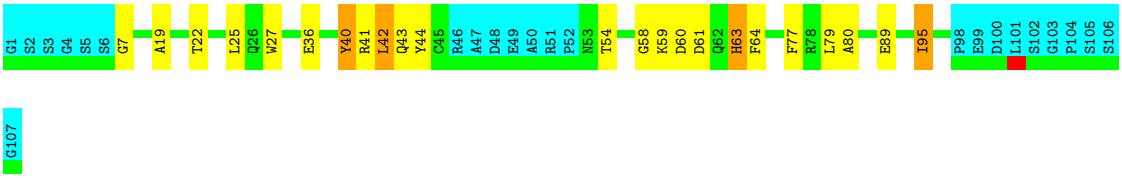
Chain A: 57% 17% 5% 21%



4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: Receptor-type tyrosine-protein phosphatase F

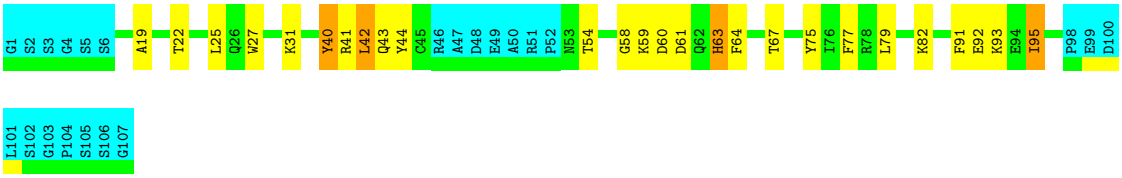
Chain A:



4.2.4 Score per residue for model 4

- Molecule 1: Receptor-type tyrosine-protein phosphatase F

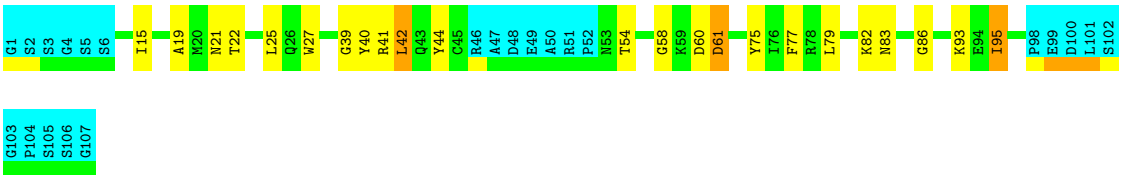
Chain A:



4.2.5 Score per residue for model 5

- Molecule 1: Receptor-type tyrosine-protein phosphatase F

Chain A:



4.2.6 Score per residue for model 6

- Molecule 1: Receptor-type tyrosine-protein phosphatase F

Chain A: 60% 14% 5% 21%

G1 S2 S3 G4 S5 S6 A19 T22 A23 L24 L25 Q26 Y40 R41 L42 Q43 Y44 C45 R46 A47 D48 E49 A50 R51 P52 N53 T54 H63 T67 Y75 I76 F77 R84 F91 E92 K93 E94 I95 P98 E99 D100 L101 S102 G103 P104 S105 S106 G107

4.2.7 Score per residue for model 7

- Molecule 1: Receptor-type tyrosine-protein phosphatase F

Chain A: 54% 21% • 21%

G1 S2 S3 G4 S5 S6 A19 M20 N21 T22 A23 L24 L25 Q26 W27 Y40 R41 L42 Q43 Y44 C45 R46 A47 D48 E49 A50 R51 P52 N53 T54 G58 K59 D60 D61 Q62 H63 T74 Y75 I76 F77 R78 L79 K82 F91 E92 K93 E94 I95 P98 E99 D100 L101 S102

G103 P104 S105 S106 G107

4.2.8 Score per residue for model 8

- Molecule 1: Receptor-type tyrosine-protein phosphatase F

Chain A: 59% 19% • 21%

G1 S2 S3 G4 S5 S6 T18 A19 T22 L25 Q26 W27 L33 Y40 R41 L42 Q43 Y44 C45 R46 A47 D48 E49 A50 R51 P52 N53 T54 G58 D61 Q62 H63 F64 T74 L79 N83 G86 E89 I95 P98 E99 D100 L101 S102 G103 P104

S105 S106 G107

4.2.9 Score per residue for model 9

- Molecule 1: Receptor-type tyrosine-protein phosphatase F

Chain A: 56% 20% • 21%

G1 S2 S3 G4 S5 S6 T18 A19 M20 N21 T22 L25 Q26 W27 K31 E32 L33 Y40 R41 L42 Q43 Y44 C45 R46 A47 D48 E49 A50 R51 P52 N53 T54 G58 D61 Q62 H63 F64 T74 Y75 L79 A80 K93 E94 I95 P98 E99 D100 L101 S102 G103

P104 S105 S106 G107

4.2.10 Score per residue for model 10

- Molecule 1: Receptor-type tyrosine-protein phosphatase F

Chain A: 51% 22% 5% 21%

G1 S2 S3 G4 S5 S6 I15 T18 A19 T22 A23 L24 L25 Q26 W27 L33 Y40 R41 L42 Q43 R46 A47 D48 E49 A50 R51 P52 N53 T54 G58 K59 D60 D61 Q62 H63 F64 T67 K71 Y75 I76 F77 R78 L79 A80 A81 K82 K93 E94 I95

P98 E99 D100 L101 S102 G103 P104 S105 S106 G107

4.2.11 Score per residue for model 11

- Molecule 1: Receptor-type tyrosine-protein phosphatase F

Chain A: 58% 18% • 21%

G1 S2 S3 G4 S5 S6 I15 A19 T22 L25 L33 E36 L37 Y40 R41 L42 Q43 Y44 C45 R46 A47 D48 E49 A50 R51 P52 N53 T54 I55 D56 K59 H63 F77 R78 L79 A80 E89 K93 E94 I95 P98 E99 D100 L101 S102 G103 P104

S105 S106 G107

4.2.12 Score per residue for model 12

- Molecule 1: Receptor-type tyrosine-protein phosphatase F

Chain A: 60% 16% • 21%

G1 S2 S3 G4 S5 S6 T12 I15 A19 M20 N21 T22 L25 H28 Y40 R41 L42 Q43 Y44 C45 R46 A47 D48 E49 A50 R51 P52 N53 T54 G58 D61 Q62 H63 F64 F77 R78 I95 P98 E99 D100 L101 S102 G103 P104 S105 S106 G107

4.2.13 Score per residue for model 13

- Molecule 1: Receptor-type tyrosine-protein phosphatase F

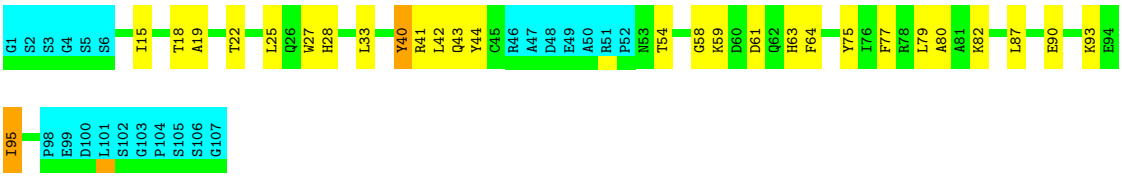
Chain A: 59% 18% • 21%

G1 S2 S3 G4 S5 S6 A19 M20 N21 T22 A23 L24 L25 Q26 W27 H28 L33 G39 Y40 R41 L42 Q43 Y44 C45 R46 A47 D48 E49 A50 R51 P52 N53 T54 D61 Y75 L79 K82 N83 L87 I95 P98 E99 D100 L101 S102 G103 P104 S105 S106 G107

4.2.14 Score per residue for model 14

- Molecule 1: Receptor-type tyrosine-protein phosphatase F

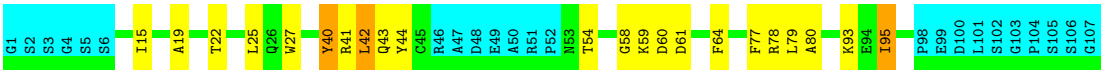
Chain A: 52% 24% • 21%



4.2.15 Score per residue for model 15

- Molecule 1: Receptor-type tyrosine-protein phosphatase F

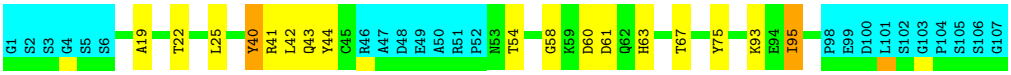
Chain A: 58% 18% • 21%



4.2.16 Score per residue for model 16

- Molecule 1: Receptor-type tyrosine-protein phosphatase F

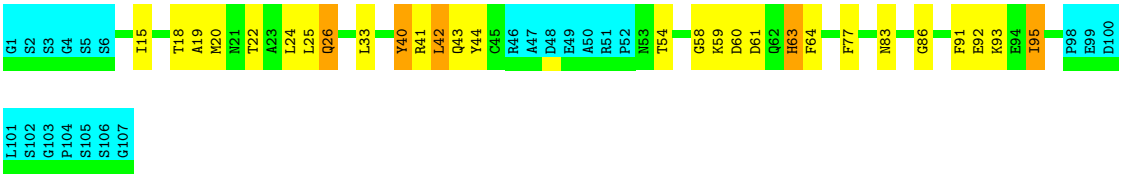
Chain A: 63% 14% • 21%



4.2.17 Score per residue for model 17

- Molecule 1: Receptor-type tyrosine-protein phosphatase F

Chain A: 52% 21% 5% 21%



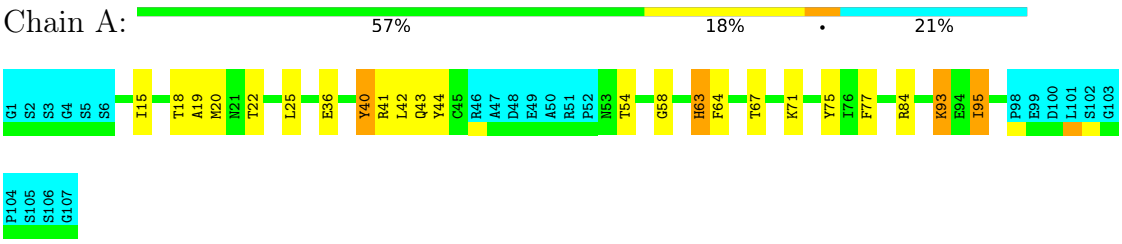
4.2.18 Score per residue for model 18

- Molecule 1: Receptor-type tyrosine-protein phosphatase F

Chain A: 50% 25% • 21%

4.2.19 Score per residue for model 19

- Molecule 1: Receptor-type tyrosine-protein phosphatase F



4.2.20 Score per residue for model 20

- Molecule 1: Receptor-type tyrosine-protein phosphatase F

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 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	666	663	660	23±4
All	All	13320	13260	13200	457

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 17.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:15:ILE:HD12	1:A:93:LYS:HG2	0.82	1.52	2	7
1:A:19:ALA:HB3	1:A:22:THR:OG1	0.79	1.77	6	20
1:A:24:LEU:HD21	1:A:26:GLN:NE2	0.73	1.98	20	4
1:A:41:ARG:HD3	1:A:54:THR:HG23	0.72	1.60	12	11
1:A:25:LEU:HD13	1:A:42:LEU:HD11	0.71	1.61	7	13
1:A:25:LEU:HD12	1:A:64:PHE:HB3	0.69	1.63	8	13
1:A:41:ARG:HD2	1:A:54:THR:HG23	0.68	1.65	20	6
1:A:44:TYR:CD2	1:A:77:PHE:CE1	0.68	2.82	18	1
1:A:15:ILE:HD12	1:A:93:LYS:CG	0.68	2.18	5	7
1:A:95:ILE:HD13	1:A:95:ILE:H	0.67	1.50	2	16
1:A:41:ARG:CD	1:A:54:THR:HG23	0.67	2.20	12	14
1:A:93:LYS:NZ	1:A:95:ILE:HG22	0.67	2.04	11	1
1:A:24:LEU:HD13	1:A:25:LEU:N	0.66	2.05	10	2
1:A:20:MET:O	1:A:22:THR:HG23	0.65	1.92	19	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:93:LYS:HE3	1:A:95:ILE:HG22	0.63	1.69	9	5
1:A:77:PHE:CE1	1:A:95:ILE:HD11	0.62	2.29	15	4
1:A:33:LEU:O	1:A:33:LEU:HD23	0.61	1.95	8	9
1:A:75:TYR:HB2	1:A:95:ILE:HD11	0.61	1.71	9	10
1:A:44:TYR:CD1	1:A:44:TYR:O	0.60	2.54	1	16
1:A:41:ARG:O	1:A:79:LEU:HD12	0.60	1.96	7	9
1:A:42:LEU:HD23	1:A:43:GLN:N	0.60	2.11	9	16
1:A:41:ARG:NE	1:A:54:THR:CG2	0.60	2.65	6	12
1:A:91:PHE:CE1	1:A:92:GLU:O	0.60	2.55	1	6
1:A:91:PHE:CD1	1:A:92:GLU:N	0.59	2.70	7	6
1:A:24:LEU:HD21	1:A:26:GLN:HE21	0.59	1.58	13	1
1:A:74:THR:HG23	1:A:95:ILE:O	0.58	1.97	18	5
1:A:44:TYR:CB	1:A:77:PHE:CD2	0.58	2.86	15	8
1:A:27:TRP:CG	1:A:79:LEU:CD2	0.57	2.88	10	10
1:A:95:ILE:HD13	1:A:95:ILE:N	0.55	2.16	11	14
1:A:44:TYR:CG	1:A:77:PHE:CE1	0.54	2.95	18	1
1:A:82:LYS:HD2	1:A:87:LEU:HD21	0.54	1.78	14	1
1:A:28:HIS:ND1	1:A:28:HIS:C	0.53	2.61	12	1
1:A:22:THR:CG2	1:A:67:THR:HG22	0.53	2.34	20	5
1:A:24:LEU:HD12	1:A:26:GLN:HG3	0.53	1.80	10	1
1:A:77:PHE:HE1	1:A:95:ILE:HD11	0.52	1.61	15	4
1:A:44:TYR:HB3	1:A:77:PHE:CD2	0.52	2.39	11	6
1:A:22:THR:HG22	1:A:67:THR:HG22	0.50	1.83	20	2
1:A:15:ILE:HD12	1:A:93:LYS:HE2	0.50	1.83	19	1
1:A:41:ARG:CZ	1:A:43:GLN:OE1	0.50	2.60	17	1
1:A:44:TYR:O	1:A:53:ASN:ND2	0.50	2.44	18	1
1:A:25:LEU:O	1:A:63:HIS:CB	0.50	2.60	1	14
1:A:25:LEU:HD13	1:A:42:LEU:CD1	0.49	2.36	6	1
1:A:58:GLY:O	1:A:61:ASP:N	0.49	2.46	1	15
1:A:95:ILE:N	1:A:95:ILE:CD1	0.49	2.75	11	14
1:A:24:LEU:HD12	1:A:26:GLN:CG	0.49	2.37	10	2
1:A:40:TYR:CD1	1:A:40:TYR:N	0.49	2.78	2	13
1:A:44:TYR:HB3	1:A:77:PHE:CD1	0.48	2.43	4	2
1:A:15:ILE:HD12	1:A:93:LYS:HD2	0.48	1.85	1	1
1:A:33:LEU:HD23	1:A:33:LEU:C	0.47	2.30	8	2
1:A:41:ARG:CD	1:A:54:THR:CG2	0.47	2.92	12	2
1:A:44:TYR:CB	1:A:77:PHE:CD1	0.47	2.98	18	3
1:A:44:TYR:O	1:A:44:TYR:CD1	0.47	2.68	16	1
1:A:27:TRP:CD1	1:A:79:LEU:HD21	0.46	2.45	3	4
1:A:44:TYR:CD1	1:A:44:TYR:C	0.46	2.89	20	7
1:A:44:TYR:CG	1:A:77:PHE:CD1	0.46	3.03	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:24:LEU:HD13	1:A:25:LEU:H	0.46	1.71	10	2
1:A:24:LEU:C	1:A:26:GLN:NE2	0.46	2.68	17	1
1:A:58:GLY:O	1:A:60:ASP:N	0.46	2.48	3	10
1:A:40:TYR:N	1:A:40:TYR:CD1	0.46	2.82	16	1
1:A:15:ILE:HD11	1:A:77:PHE:HB2	0.45	1.87	19	5
1:A:75:TYR:O	1:A:95:ILE:HD13	0.44	2.12	16	4
1:A:15:ILE:HD12	1:A:93:LYS:CE	0.44	2.42	19	1
1:A:40:TYR:CB	1:A:80:ALA:O	0.44	2.65	10	6
1:A:12:THR:HB	1:A:28:HIS:CD2	0.44	2.48	12	1
1:A:80:ALA:HB2	1:A:90:GLU:HG2	0.44	1.87	14	2
1:A:18:THR:OG1	1:A:19:ALA:N	0.44	2.51	14	3
1:A:36:GLU:OE1	1:A:37:LEU:N	0.44	2.51	11	1
1:A:24:LEU:CD1	1:A:25:LEU:N	0.44	2.81	6	1
1:A:58:GLY:C	1:A:60:ASP:N	0.43	2.72	3	11
1:A:42:LEU:HD22	1:A:44:TYR:HD2	0.43	1.71	8	1
1:A:42:LEU:O	1:A:55:ILE:N	0.43	2.51	18	1
1:A:78:ARG:NH2	1:A:92:GLU:OE1	0.43	2.51	18	1
1:A:25:LEU:HD21	1:A:77:PHE:CE2	0.43	2.47	17	4
1:A:41:ARG:NE	1:A:54:THR:HG23	0.43	2.28	8	2
1:A:91:PHE:CD1	1:A:91:PHE:C	0.43	2.92	1	1
1:A:43:GLN:O	1:A:78:ARG:N	0.42	2.53	15	5
1:A:39:GLY:O	1:A:82:LYS:CB	0.42	2.67	13	2
1:A:43:GLN:OE1	1:A:53:ASN:C	0.42	2.57	10	1
1:A:84:ARG:O	1:A:84:ARG:NH1	0.42	2.51	19	1
1:A:83:ASN:O	1:A:86:GLY:N	0.42	2.53	5	3
1:A:75:TYR:CB	1:A:95:ILE:HD11	0.42	2.45	7	2
1:A:93:LYS:CE	1:A:95:ILE:HG22	0.42	2.45	11	1
1:A:42:LEU:HD23	1:A:43:GLN:H	0.42	1.75	16	3
1:A:25:LEU:HD21	1:A:77:PHE:CE1	0.42	2.50	6	1
1:A:27:TRP:CG	1:A:79:LEU:HD22	0.42	2.50	10	1
1:A:41:ARG:HG2	1:A:42:LEU:N	0.42	2.30	3	6
1:A:44:TYR:CG	1:A:77:PHE:CE2	0.42	3.08	11	1
1:A:82:LYS:HD3	1:A:87:LEU:HD21	0.42	1.91	13	1
1:A:93:LYS:HE2	1:A:95:ILE:HG22	0.42	1.90	1	1
1:A:93:LYS:CE	1:A:95:ILE:CG2	0.41	2.98	11	1
1:A:43:GLN:OE1	1:A:54:THR:N	0.41	2.53	10	1
1:A:33:LEU:HD11	1:A:83:ASN:HB3	0.41	1.93	13	1
1:A:77:PHE:CE1	1:A:95:ILE:CD1	0.41	3.04	3	1
1:A:82:LYS:HD2	1:A:87:LEU:CD2	0.41	2.46	14	1
1:A:40:TYR:CE1	1:A:58:GLY:O	0.41	2.73	19	1
1:A:77:PHE:CD1	1:A:95:ILE:CD1	0.41	3.04	3	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:GLU:OE1	1:A:36:GLU:N	0.40	2.54	3	1
1:A:15:ILE:HG12	1:A:25:LEU:HD23	0.40	1.94	18	1
1:A:33:LEU:HD23	1:A:33:LEU:O	0.40	2.16	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	84/107 (79%)	78±1 (93±1%)	5±1 (6±1%)	1±1 (1±1%)	26	73
All	All	1680/2140 (79%)	1560 (93%)	109 (6%)	11 (1%)	26	73

All 4 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	LYS	7
1	A	89	GLU	2
1	A	7	GLY	1
1	A	61	ASP	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	70/87 (80%)	65±1 (93±2%)	5±1 (7±2%)	18	67
All	All	1400/1740 (80%)	1301 (93%)	99 (7%)	18	67

All 20 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	40	TYR	20
1	A	95	ILE	20
1	A	42	LEU	12
1	A	63	HIS	8
1	A	61	ASP	5
1	A	82	LYS	5
1	A	18	THR	5
1	A	93	LYS	3
1	A	28	HIS	3
1	A	89	GLU	2
1	A	31	LYS	2
1	A	21	ASN	2
1	A	24	LEU	2
1	A	56	ASP	2
1	A	59	LYS	2
1	A	36	GLU	2
1	A	10	ARG	1
1	A	84	ARG	1
1	A	20	MET	1
1	A	26	GLN	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