Full wwPDB NMR Structure Validation Report (i)

Feb 23, 2022 – 08:44 AM EST

PDB ID	:	1X0O
Title	:	human ARNT C-terminal PAS domain
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Deposited on	:	2005-03-25

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:

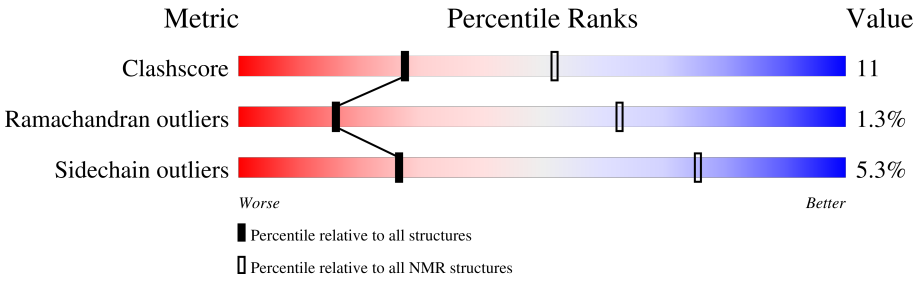
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

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	119	59% 24% • 17%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 5 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:9-A:96, A:103-A:113 (99)	0.26	5

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 7 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1925 atoms, of which 945 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Aryl hydrocarbon receptor nuclear translocator.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	119	1925	618	945	169	186	7	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	cloning artifact	UNP P27540
A	2	ALA	-	cloning artifact	UNP P27540
A	3	MET	-	cloning artifact	UNP P27540
A	4	ASP	-	cloning artifact	UNP P27540

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: Aryl hydrocarbon receptor nuclear translocator

Chain A: 59% 24% • 17%

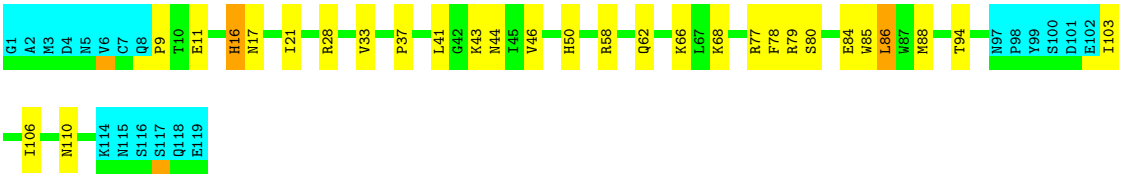
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Aryl hydrocarbon receptor nuclear translocator

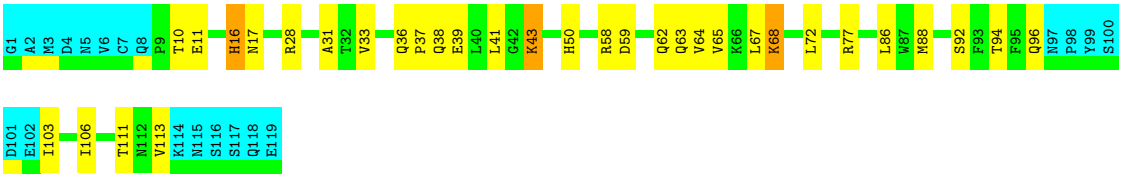
Chain A: 59% 23% • 17%



4.2.2 Score per residue for model 2

• Molecule 1: Aryl hydrocarbon receptor nuclear translocator

Chain A: 55% 25% • 17%



4.2.3 Score per residue for model 3

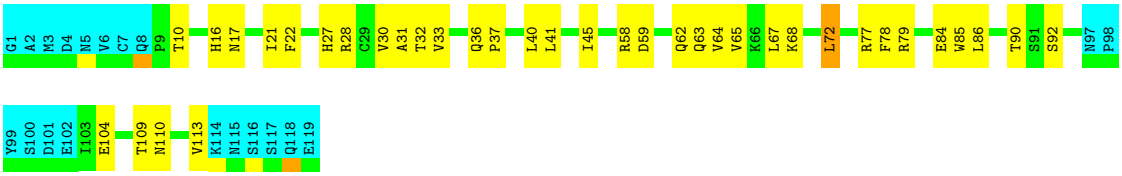
- Molecule 1: Aryl hydrocarbon receptor nuclear translocator

Chain A:

4.2.4 Score per residue for model 4

- Molecule 1: Aryl hydrocarbon receptor nuclear translocator

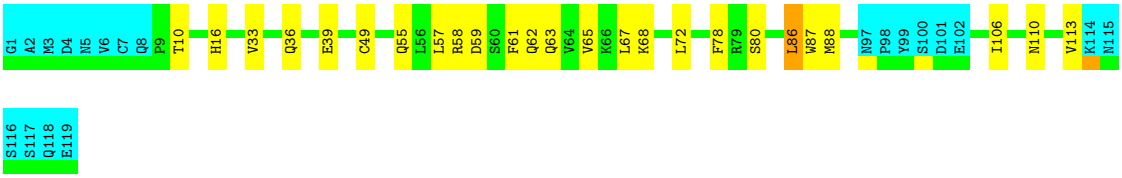
Chain A:



4.2.5 Score per residue for model 5 (medoid)

- Molecule 1: Aryl hydrocarbon receptor nuclear translocator

Chain A:



4.2.6 Score per residue for model 6

- Molecule 1: Aryl hydrocarbon receptor nuclear translocator

Chain A: 59% 22% • 17%

G1 A2 M3 D4 N5 V6 C7 Q8 P9 T10 E11 H16 N17 R28 P37 Q38 K43 H50 Q54 Q55 R58 D59 S60 F61 Q62 Q63 V64 V65 K66 L67 K68 L72 R77 E84 W87 M88 T94 F95 Q96 N97 P98 Y99 S100 D101 E102 I103 I106

N110 K114 N115 S116 S117 Q118 E119

4.2.7 Score per residue for model 7

• Molecule 1: Aryl hydrocarbon receptor nuclear translocator

Chain A: 53% 29% • 17%

G1 A2 M3 D4 N5 V6 C7 Q8 H16 V25 R28 C29 V30 A31 T32 V33 G34 Y35 Q36 P37 Q38 E39 L40 L41 G42 K43 H50 D59 S60 F61 Q62 Q63 V64 V65 K68 V71 L72 R77 F78 R79 S80 K81 E84 W85 L86 S91 S92 F93 T94

N97 P98 Y99 S100 D101 E102 I103 T109 N110 T111 N112 V113 K114 N115 S116 S117 Q118 E119

4.2.8 Score per residue for model 8

• Molecule 1: Aryl hydrocarbon receptor nuclear translocator

Chain A: 50% 33% 17%

G1 A2 M3 D4 N5 V6 C7 Q8 P9 T10 E11 H16 V30 V33 G34 Y35 Q36 P37 L41 G42 K43 D53 L56 L57 R58 D59 S60 F61 Q62 Q63 V64 V65 K66 L67 K68 G69 Q70 F78 R79 S80 K81 W85 L86 T90 S91 S92 F93 T94 F95 Q96 N97

P98 Y99 S100 D101 E102 I103 C108 T109 N110 V113 K114 N115 S116 S117 Q118 E119

4.2.9 Score per residue for model 9

• Molecule 1: Aryl hydrocarbon receptor nuclear translocator

Chain A: 63% 18% • 17%

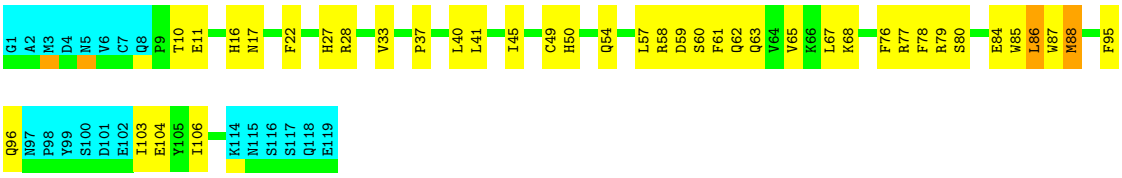
G1 A2 M3 D4 N5 V6 C7 Q8 E11 H16 R28 C29 V30 V33 Q36 P37 L41 G42 K43 N44 E47 F48 C49 L57 R58 D59 Q63 L67 K68 R77 F78 L86 S91 N97 P98 Y99 S100 D101 E102 C108 T111 N112 V113 K114

N115 S116 S117 Q118 E119

4.2.10 Score per residue for model 10

• Molecule 1: Aryl hydrocarbon receptor nuclear translocator

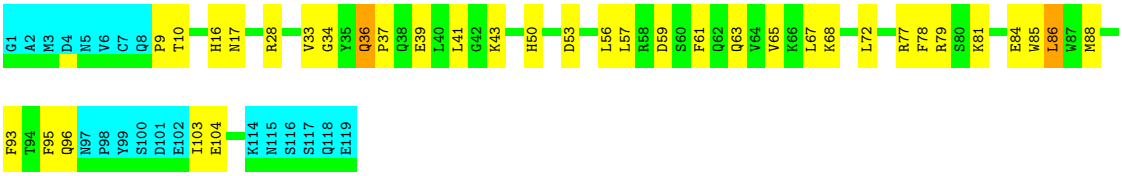
Chain A: 50% 32% • 17%



4.2.11 Score per residue for model 11

• Molecule 1: Aryl hydrocarbon receptor nuclear translocator

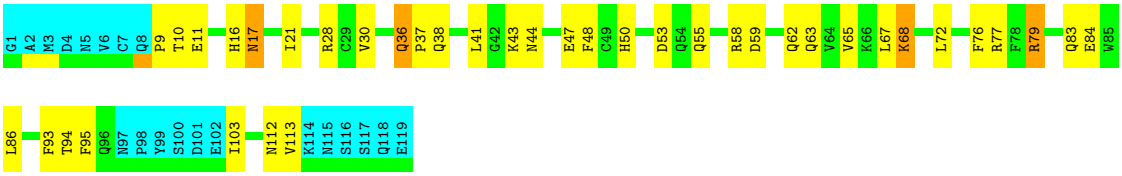
Chain A: 53% 29% • 17%



4.2.12 Score per residue for model 12

• Molecule 1: Aryl hydrocarbon receptor nuclear translocator

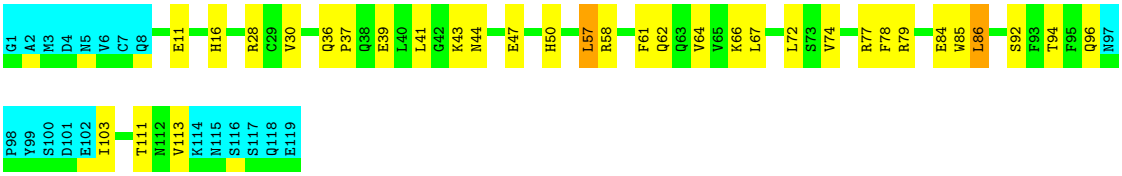
Chain A: 50% 29% • 17%



4.2.13 Score per residue for model 13

• Molecule 1: Aryl hydrocarbon receptor nuclear translocator

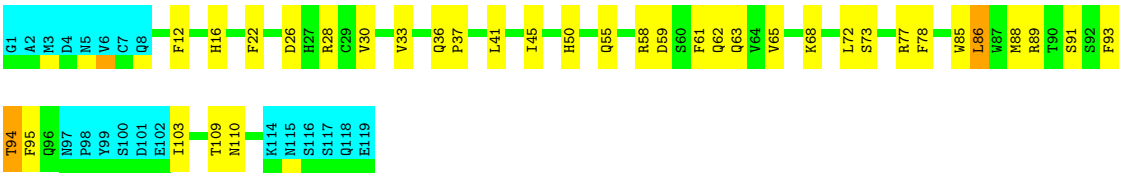
Chain A: 55% 26% • 17%



4.2.14 Score per residue for model 14

• Molecule 1: Aryl hydrocarbon receptor nuclear translocator

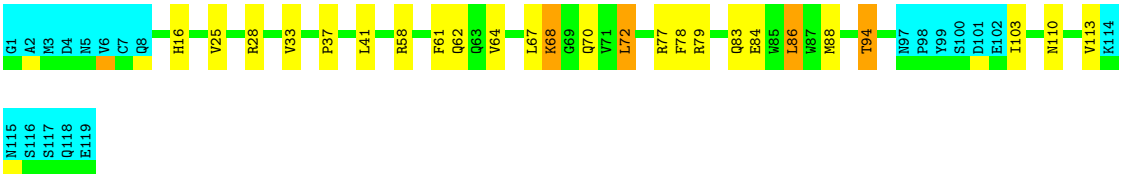
Chain A: 54% 28% • 17%



4.2.15 Score per residue for model 15

• Molecule 1: Aryl hydrocarbon receptor nuclear translocator

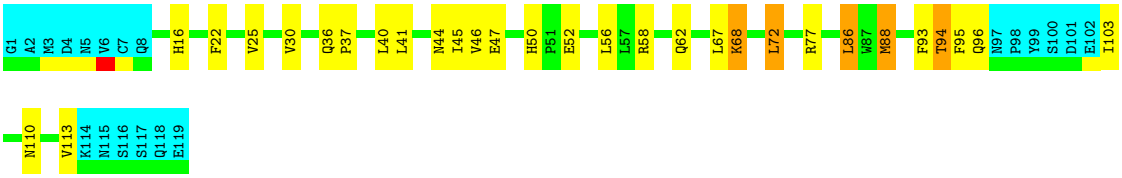
Chain A: 62% 18% • 17%



4.2.16 Score per residue for model 16

• Molecule 1: Aryl hydrocarbon receptor nuclear translocator

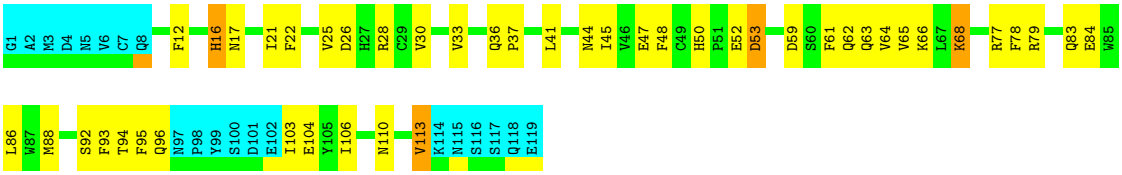
Chain A: 58% 21% • 17%



4.2.17 Score per residue for model 17

• Molecule 1: Aryl hydrocarbon receptor nuclear translocator

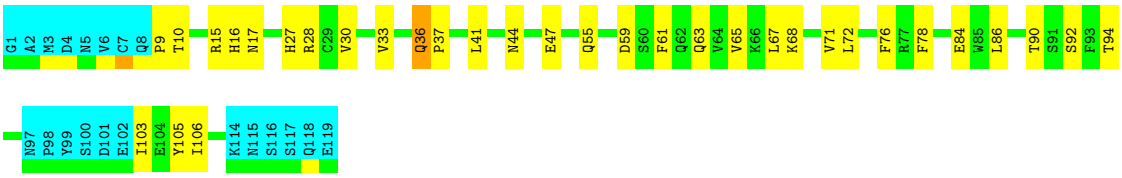
Chain A: 45% 34% • 17%



4.2.18 Score per residue for model 18

- Molecule 1: Aryl hydrocarbon receptor nuclear translocator

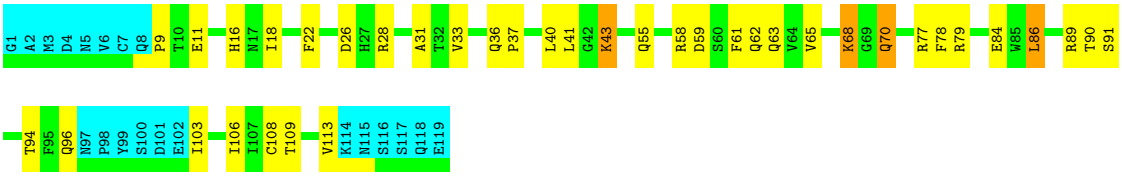
Chain A: 55% 27% • 17%



4.2.19 Score per residue for model 19

- Molecule 1: Aryl hydrocarbon receptor nuclear translocator

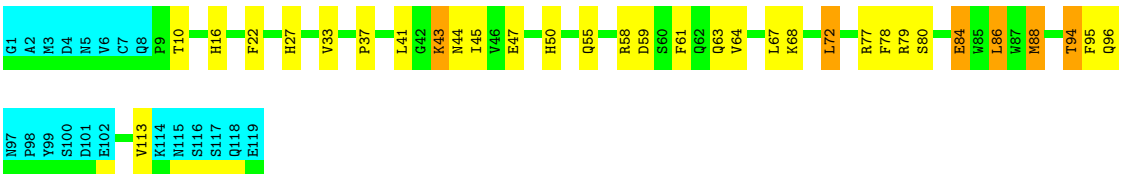
Chain A: 51% 29% • 17%



4.2.20 Score per residue for model 20

- Molecule 1: Aryl hydrocarbon receptor nuclear translocator

Chain A: 56% 22% 5% 17%



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *simulated annealing*.

Of the 1000 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
ARIA	structure solution	1.2
CNS	structure solution	1.1
CNS	refinement	1.1

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.

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

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	79	ARG	Sidechain	1

6.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	827	814	811	18±3
All	All	16540	16280	16220	355

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:96:GLN:HG2	1:A:103:ILE:HG12	0.84	1.47	10	2
1:A:80:SER:HB3	1:A:86:LEU:HD11	0.75	1.57	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:43:LYS:HA	1:A:43:LYS:HE2	0.70	1.63	1	4
1:A:50:HIS:HB2	1:A:77:ARG:HB2	0.69	1.63	1	7
1:A:67:LEU:HB3	1:A:70:GLN:HB2	0.69	1.65	15	2
1:A:62:GLN:HE21	1:A:62:GLN:HA	0.67	1.48	3	1
1:A:11:GLU:HG2	1:A:111:THR:HA	0.65	1.66	9	3
1:A:67:LEU:HD12	1:A:72:LEU:HD23	0.65	1.68	13	4
1:A:30:VAL:HG12	1:A:36:GLN:HA	0.65	1.69	17	8
1:A:9:PRO:HD2	1:A:28:ARG:HG2	0.65	1.68	12	7
1:A:43:LYS:HA	1:A:43:LYS:HE3	0.64	1.69	20	2
1:A:68:LYS:HG2	1:A:103:ILE:HD11	0.64	1.69	17	7
1:A:67:LEU:HD11	1:A:72:LEU:HD13	0.64	1.69	12	1
1:A:37:PRO:O	1:A:41:LEU:HG	0.64	1.92	19	18
1:A:59:ASP:O	1:A:63:GLN:HG2	0.64	1.92	4	13
1:A:79:ARG:HA	1:A:84:GLU:O	0.63	1.94	10	11
1:A:43:LYS:HE2	1:A:43:LYS:HA	0.62	1.72	11	2
1:A:73:SER:HB2	1:A:89:ARG:HE	0.61	1.56	14	1
1:A:65:VAL:HA	1:A:94:THR:HG21	0.61	1.73	7	4
1:A:94:THR:HB	1:A:103:ILE:HD12	0.61	1.72	13	8
1:A:17:ASN:HB3	1:A:21:ILE:HB	0.61	1.71	1	3
1:A:33:VAL:HG11	1:A:78:PHE:CD1	0.60	2.31	9	11
1:A:50:HIS:HB3	1:A:53:ASP:OD1	0.60	1.96	17	1
1:A:43:LYS:HE3	1:A:43:LYS:HA	0.59	1.75	19	2
1:A:78:PHE:HB2	1:A:88:MET:SD	0.58	2.38	20	2
1:A:63:GLN:O	1:A:67:LEU:HG	0.58	1.99	9	5
1:A:77:ARG:HA	1:A:86:LEU:O	0.57	1.99	4	15
1:A:33:VAL:O	1:A:80:SER:HA	0.57	1.99	20	2
1:A:79:ARG:HG2	1:A:83:GLN:HA	0.56	1.78	17	2
1:A:17:ASN:OD1	1:A:21:ILE:HB	0.56	2.01	4	1
1:A:58:ARG:O	1:A:62:GLN:HG3	0.56	2.01	16	2
1:A:58:ARG:O	1:A:62:GLN:HG2	0.56	2.00	10	11
1:A:53:ASP:OD2	1:A:76:PHE:HB2	0.56	2.00	12	1
1:A:96:GLN:HG2	1:A:103:ILE:HD13	0.55	1.79	19	2
1:A:61:PHE:O	1:A:64:VAL:HG12	0.55	2.01	7	4
1:A:16:HIS:CD2	1:A:106:ILE:HB	0.55	2.36	1	8
1:A:59:ASP:HA	1:A:62:GLN:HE21	0.55	1.62	7	1
1:A:11:GLU:O	1:A:28:ARG:HD3	0.55	2.01	19	2
1:A:80:SER:HB3	1:A:84:GLU:HG2	0.54	1.80	1	1
1:A:11:GLU:O	1:A:28:ARG:HD2	0.54	2.03	13	4
1:A:33:VAL:HG12	1:A:88:MET:HE1	0.54	1.77	2	1
1:A:67:LEU:HD11	1:A:72:LEU:HD23	0.54	1.79	4	2
1:A:88:MET:SD	1:A:110:ASN:HB3	0.53	2.44	5	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:64:VAL:HG11	1:A:92:SER:OG	0.53	2.04	2	4
1:A:36:GLN:HB2	1:A:39:GLU:HG3	0.53	1.81	5	3
1:A:50:HIS:NE2	1:A:52:GLU:HB2	0.53	2.19	16	1
1:A:22:PHE:CE2	1:A:45:ILE:HB	0.52	2.40	17	3
1:A:86:LEU:HD13	1:A:88:MET:HE1	0.52	1.81	10	1
1:A:12:PHE:HB3	1:A:28:ARG:HB2	0.51	1.82	17	2
1:A:30:VAL:HG22	1:A:36:GLN:HA	0.51	1.80	7	1
1:A:22:PHE:CE1	1:A:45:ILE:HB	0.51	2.40	4	3
1:A:93:PHE:CE2	1:A:95:PHE:HA	0.51	2.41	14	7
1:A:22:PHE:CZ	1:A:45:ILE:HB	0.51	2.40	3	2
1:A:32:THR:HG21	1:A:110:ASN:HD21	0.51	1.64	4	1
1:A:33:VAL:HG11	1:A:78:PHE:CD2	0.51	2.41	18	1
1:A:68:LYS:HA	1:A:94:THR:OG1	0.50	2.06	3	7
1:A:50:HIS:HB3	1:A:53:ASP:CB	0.50	2.36	12	1
1:A:65:VAL:O	1:A:68:LYS:HG3	0.50	2.05	5	5
1:A:34:GLY:HA3	1:A:81:LYS:HB2	0.50	1.83	11	3
1:A:26:ASP:OD1	1:A:28:ARG:HG3	0.50	2.06	19	3
1:A:61:PHE:O	1:A:65:VAL:HG23	0.50	2.07	5	11
1:A:91:SER:O	1:A:108:CYS:HA	0.50	2.06	19	3
1:A:27:HIS:HA	1:A:37:PRO:CG	0.50	2.37	20	1
1:A:48:PHE:HB3	1:A:79:ARG:HB3	0.49	1.85	17	1
1:A:49:CYS:SG	1:A:57:LEU:HD12	0.49	2.47	3	3
1:A:77:ARG:HB3	1:A:85:TRP:HB3	0.49	1.84	3	3
1:A:79:ARG:NH2	1:A:83:GLN:HG3	0.49	2.21	12	1
1:A:57:LEU:HA	1:A:74:VAL:HG21	0.49	1.85	13	1
1:A:25:VAL:HG21	1:A:40:LEU:HB3	0.49	1.84	16	1
1:A:94:THR:HB	1:A:103:ILE:HD13	0.49	1.83	2	5
1:A:22:PHE:CD2	1:A:40:LEU:HG	0.49	2.43	19	1
1:A:70:GLN:HE21	1:A:70:GLN:HA	0.49	1.68	19	1
1:A:88:MET:HE1	1:A:110:ASN:HB3	0.48	1.85	6	2
1:A:78:PHE:O	1:A:85:TRP:HA	0.48	2.08	8	2
1:A:22:PHE:CD1	1:A:40:LEU:HG	0.48	2.43	3	2
1:A:91:SER:OG	1:A:109:THR:HB	0.48	2.08	7	2
1:A:45:ILE:HG12	1:A:49:CYS:SG	0.48	2.49	10	1
1:A:50:HIS:CD2	1:A:77:ARG:HB2	0.48	2.44	2	1
1:A:53:ASP:O	1:A:56:LEU:HB3	0.48	2.08	8	1
1:A:11:GLU:HA	1:A:110:ASN:O	0.47	2.09	8	2
1:A:22:PHE:CD2	1:A:40:LEU:HB3	0.47	2.44	10	1
1:A:53:ASP:O	1:A:56:LEU:HG	0.47	2.09	11	1
1:A:50:HIS:HA	1:A:85:TRP:CE3	0.47	2.45	14	1
1:A:33:VAL:HB	1:A:80:SER:HA	0.46	1.85	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:50:HIS:O	1:A:54:GLN:HG3	0.46	2.09	10	1
1:A:44:ASN:HB2	1:A:47:GLU:HG2	0.46	1.87	16	3
1:A:67:LEU:CD1	1:A:72:LEU:HD23	0.46	2.41	6	5
1:A:80:SER:HB3	1:A:84:GLU:HB2	0.46	1.87	7	2
1:A:68:LYS:HD3	1:A:96:GLN:NE2	0.46	2.26	2	1
1:A:36:GLN:HB2	1:A:39:GLU:HG2	0.46	1.87	13	2
1:A:43:LYS:HE2	1:A:48:PHE:CZ	0.46	2.46	12	1
1:A:30:VAL:CG1	1:A:36:GLN:HA	0.45	2.40	16	1
1:A:44:ASN:HB3	1:A:46:VAL:HG12	0.45	1.88	1	2
1:A:67:LEU:HD12	1:A:72:LEU:HD13	0.45	1.88	18	1
1:A:62:GLN:O	1:A:66:LYS:HG3	0.45	2.12	1	3
1:A:71:VAL:HA	1:A:92:SER:O	0.45	2.12	7	2
1:A:79:ARG:HB2	1:A:85:TRP:CZ3	0.44	2.47	13	1
1:A:59:ASP:HA	1:A:62:GLN:HG2	0.44	1.89	19	1
1:A:57:LEU:HD11	1:A:76:PHE:CD2	0.44	2.47	10	1
1:A:16:HIS:HB3	1:A:22:PHE:HA	0.44	1.88	3	1
1:A:56:LEU:HD12	1:A:57:LEU:N	0.44	2.28	11	1
1:A:44:ASN:CB	1:A:46:VAL:HG12	0.43	2.43	1	1
1:A:78:PHE:O	1:A:86:LEU:HD12	0.43	2.13	3	1
1:A:32:THR:HG23	1:A:112:ASN:HB2	0.43	1.91	7	1
1:A:59:ASP:O	1:A:63:GLN:HG3	0.43	2.13	18	2
1:A:18:ILE:HA	1:A:106:ILE:CD1	0.43	2.43	3	2
1:A:95:PHE:O	1:A:104:GLU:HG2	0.43	2.13	11	2
1:A:25:VAL:HB	1:A:37:PRO:HA	0.43	1.91	15	1
1:A:27:HIS:O	1:A:30:VAL:HG22	0.43	2.14	18	1
1:A:80:SER:HB3	1:A:84:GLU:CG	0.43	2.44	1	1
1:A:79:ARG:HD3	1:A:85:TRP:CH2	0.42	2.49	1	1
1:A:67:LEU:CD1	1:A:72:LEU:HD13	0.42	2.43	12	1
1:A:90:THR:HA	1:A:109:THR:O	0.42	2.14	19	3
1:A:55:GLN:O	1:A:58:ARG:HB2	0.42	2.13	20	1
1:A:44:ASN:HB3	1:A:47:GLU:HG3	0.42	1.90	12	2
1:A:15:ARG:HD2	1:A:105:TYR:CE1	0.42	2.50	18	1
1:A:50:HIS:HA	1:A:85:TRP:CZ3	0.42	2.49	10	1
1:A:94:THR:HB	1:A:103:ILE:CD1	0.41	2.45	18	1
1:A:86:LEU:HD13	1:A:88:MET:CE	0.41	2.46	10	1
1:A:50:HIS:ND1	1:A:52:GLU:HG2	0.41	2.30	17	1
1:A:80:SER:HB3	1:A:86:LEU:CD1	0.41	2.46	5	1
1:A:37:PRO:HB2	1:A:38:GLN:OE1	0.41	2.16	6	1
1:A:53:ASP:O	1:A:57:LEU:HD23	0.41	2.16	8	1
1:A:57:LEU:HA	1:A:60:SER:OG	0.41	2.16	10	1
1:A:44:ASN:HB3	1:A:47:GLU:HG2	0.41	1.91	17	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:76:PHE:HE1	1:A:90:THR:HG1	0.40	1.58	18	1
1:A:9:PRO:HD2	1:A:28:ARG:CG	0.40	2.46	6	1
1:A:72:LEU:HB3	1:A:92:SER:HB2	0.40	1.92	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	99/119 (83%)	94±1 (95±1%)	4±2 (4±2%)	1±1 (1±1%)	16	63
All	All	1980/2380 (83%)	1872 (95%)	82 (4%)	26 (1%)	16	63

All 2 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	68	LYS	13
1	A	113	VAL	13

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	94/112 (84%)	89±2 (95±2%)	5±2 (5±2%)	26	75
All	All	1880/2240 (84%)	1780 (95%)	100 (5%)	26	75

All 27 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	16	HIS	15
1	A	86	LEU	14
1	A	10	THR	9
1	A	72	LEU	8
1	A	17	ASN	7
1	A	88	MET	6
1	A	55	GLN	6
1	A	94	THR	5
1	A	43	LYS	4
1	A	36	GLN	4
1	A	113	VAL	3
1	A	104	GLU	2
1	A	84	GLU	2
1	A	25	VAL	2
1	A	62	GLN	1
1	A	54	GLN	1
1	A	110	ASN	1
1	A	80	SER	1
1	A	68	LYS	1
1	A	11	GLU	1
1	A	112	ASN	1
1	A	57	LEU	1
1	A	56	LEU	1
1	A	53	ASP	1
1	A	70	GLN	1
1	A	89	ARG	1
1	A	95	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