



Full wwPDB NMR Structure Validation Report ⓘ

Mar 3, 2022 – 07:17 AM EST

PDB ID : 2HFH
Title : THE NMR STRUCTURES OF A WINGED HELIX PROTEIN: GENESIS,
20 STRUCTURES
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Deposited on : 1998-01-27

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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

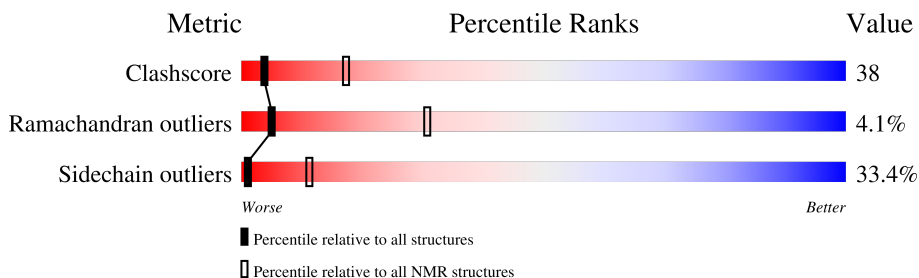
1 Overall quality at a glance

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	109	

2 Ensemble composition and analysis i

This entry contains 20 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:7-A:67, A:74-A:80 (68)	0.50	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 5 clusters and 2 single-model clusters were found.

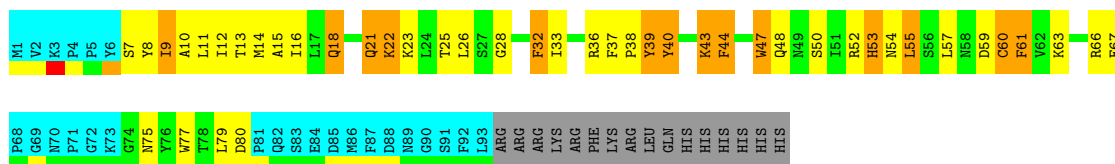
Cluster number	Models
1	1, 4, 6, 8, 10, 13, 18
2	3, 5, 20
3	2, 11, 12
4	7, 16, 17
5	15, 19
Single-model clusters	9; 14

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1503 atoms, of which 744 are hydrogens and 0 are deuteriums.

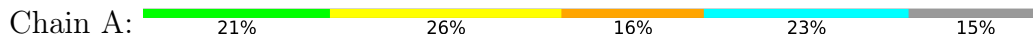
- Molecule 1 is a protein called GENESIS.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	93	1503	492	744	126	136	5	0



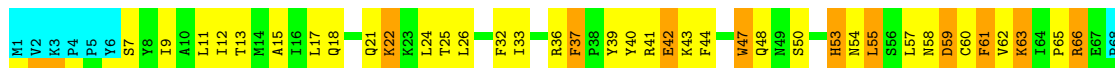
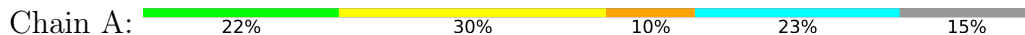
4.2.11 Score per residue for model 11

- Molecule 1: GENESIS



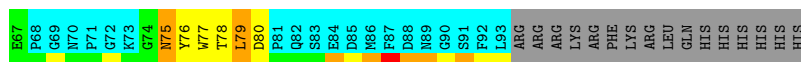
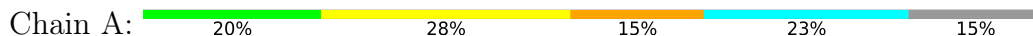
4.2.12 Score per residue for model 12

- Molecule 1: GENESIS



4.2.13 Score per residue for model 13

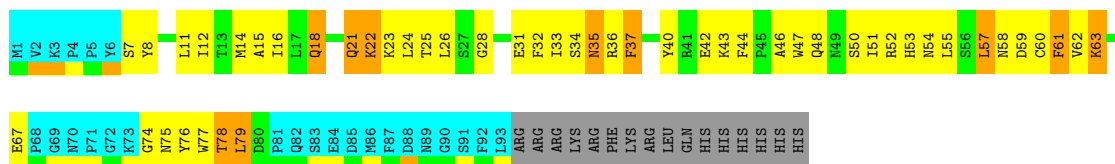
- Molecule 1: GENESIS



4.2.14 Score per residue for model 14

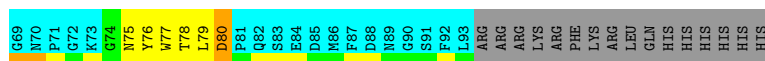
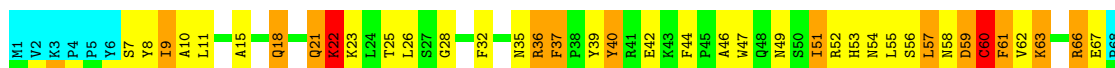
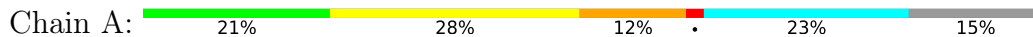
- Molecule 1: GENESIS





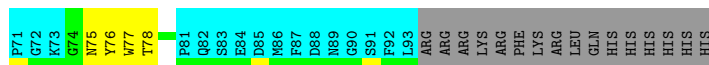
4.2.15 Score per residue for model 15

- Molecule 1: GENESIS



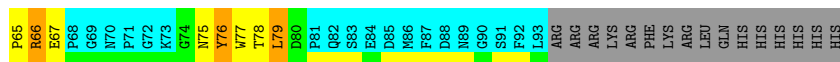
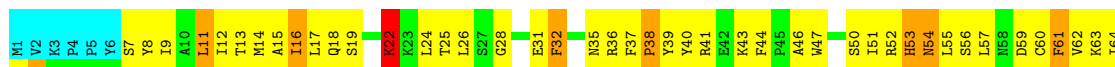
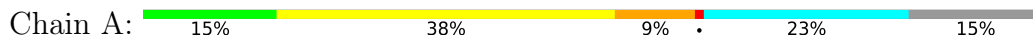
4.2.16 Score per residue for model 16

- Molecule 1: GENESIS



4.2.17 Score per residue for model 17

- Molecule 1: GENESIS



4.2.18 Score per residue for model 18

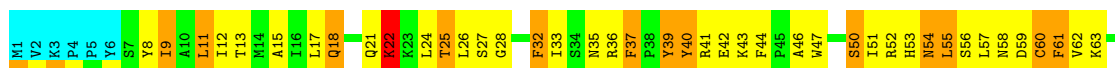
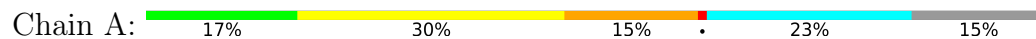
- Molecule 1: GENESIS





4.2.19 Score per residue for model 19

- Molecule 1: GENESIS



4.2.20 Score per residue for model 20

- Molecule 1: GENESIS



5 Refinement protocol and experimental data overview

The models were refined using the following method: *DIANA*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *LOWEST TARGET FUNCTION*.

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

Software name	Classification	Version
DIANA	refinement	
TRIAD	structure solution	

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	567	565	565	43±6
All	All	11340	11300	11300	865

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 38.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:25:THR:HG22	1:A:75:ASN:O	0.87	1.69	13	16
1:A:25:THR:HG23	1:A:75:ASN:O	0.87	1.67	15	2
1:A:44:PHE:O	1:A:47:TRP:CD1	0.86	2.29	18	20
1:A:9:ILE:O	1:A:13:THR:HG23	0.84	1.72	19	7
1:A:33:ILE:O	1:A:37:PHE:HB2	0.74	1.82	4	2
1:A:40:TYR:CE1	1:A:47:TRP:CZ3	0.74	2.75	9	7
1:A:51:ILE:O	1:A:55:LEU:N	0.73	2.20	3	9
1:A:8:TYR:CZ	1:A:47:TRP:CZ3	0.72	2.78	20	3
1:A:40:TYR:CZ	1:A:47:TRP:CZ3	0.71	2.78	1	3
1:A:15:ALA:O	1:A:18:GLN:HB2	0.70	1.85	5	6
1:A:55:LEU:O	1:A:61:PHE:CZ	0.70	2.45	14	15
1:A:40:TYR:CD1	1:A:47:TRP:CH2	0.70	2.80	9	7
1:A:22:LYS:O	1:A:78:THR:HG22	0.70	1.87	3	6
1:A:40:TYR:CE1	1:A:47:TRP:CH2	0.69	2.80	1	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:59:ASP:O	1:A:60:CYS:CB	0.69	2.40	11	10
1:A:59:ASP:HB2	1:A:61:PHE:CE2	0.68	2.23	8	13
1:A:64:ILE:CG1	1:A:64:ILE:O	0.68	2.41	20	3
1:A:11:LEU:CD2	1:A:37:PHE:CZ	0.68	2.77	6	2
1:A:59:ASP:O	1:A:60:CYS:HB2	0.67	1.88	19	10
1:A:59:ASP:CB	1:A:61:PHE:CE2	0.67	2.77	8	7
1:A:61:PHE:CD1	1:A:61:PHE:N	0.67	2.63	20	4
1:A:32:PHE:CE2	1:A:33:ILE:CD1	0.66	2.78	3	4
1:A:8:TYR:CE2	1:A:47:TRP:CZ3	0.66	2.84	20	2
1:A:40:TYR:CZ	1:A:47:TRP:CH2	0.65	2.84	1	3
1:A:18:GLN:OE1	1:A:32:PHE:CD2	0.65	2.49	5	1
1:A:29:ILE:O	1:A:33:ILE:N	0.65	2.27	3	1
1:A:37:PHE:N	1:A:38:PRO:HD3	0.64	2.06	10	4
1:A:11:LEU:CD1	1:A:37:PHE:CZ	0.64	2.80	13	2
1:A:63:LYS:CB	1:A:77:TRP:CE2	0.64	2.81	14	8
1:A:40:TYR:CD1	1:A:47:TRP:CZ3	0.64	2.86	9	2
1:A:36:ARG:CG	1:A:37:PHE:CE1	0.63	2.81	7	2
1:A:40:TYR:CG	1:A:47:TRP:CH2	0.62	2.87	8	3
1:A:59:ASP:O	1:A:60:CYS:HB3	0.62	1.95	11	2
1:A:16:ILE:CD1	1:A:61:PHE:CZ	0.62	2.82	20	1
1:A:55:LEU:O	1:A:61:PHE:CE1	0.61	2.53	19	13
1:A:75:ASN:O	1:A:76:TYR:CD1	0.61	2.52	15	6
1:A:61:PHE:CB	1:A:78:THR:O	0.61	2.48	15	18
1:A:64:ILE:O	1:A:64:ILE:HG12	0.61	1.94	20	2
1:A:44:PHE:CE1	1:A:46:ALA:CB	0.60	2.84	15	3
1:A:8:TYR:HA	1:A:11:LEU:HB2	0.60	1.73	9	1
1:A:8:TYR:CG	1:A:54:ASN:ND2	0.60	2.69	14	1
1:A:15:ALA:HA	1:A:32:PHE:CE2	0.60	2.32	4	7
1:A:55:LEU:CD2	1:A:77:TRP:CZ3	0.60	2.84	1	1
1:A:18:GLN:OE1	1:A:32:PHE:CG	0.60	2.55	5	1
1:A:59:ASP:O	1:A:60:CYS:SG	0.59	2.60	11	6
1:A:40:TYR:CE1	1:A:47:TRP:CE3	0.59	2.91	9	3
1:A:32:PHE:HA	1:A:35:ASN:OD1	0.59	1.98	4	3
1:A:62:VAL:O	1:A:77:TRP:HA	0.59	1.98	15	7
1:A:62:VAL:O	1:A:62:VAL:CG2	0.58	2.51	16	2
1:A:11:LEU:CD1	1:A:37:PHE:CE1	0.58	2.86	13	1
1:A:33:ILE:O	1:A:37:PHE:N	0.58	2.37	4	6
1:A:67:GLU:OE1	1:A:76:TYR:CE2	0.58	2.57	19	1
1:A:15:ALA:O	1:A:18:GLN:CG	0.58	2.51	10	10
1:A:32:PHE:CD2	1:A:33:ILE:HD13	0.58	2.34	16	3
1:A:63:LYS:NZ	1:A:77:TRP:CZ3	0.58	2.71	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:12:ILE:O	1:A:15:ALA:N	0.58	2.37	5	11
1:A:18:GLN:NE2	1:A:32:PHE:CE1	0.58	2.72	5	1
1:A:60:CYS:SG	1:A:60:CYS:O	0.58	2.62	16	2
1:A:64:ILE:CD1	1:A:76:TYR:CE2	0.58	2.87	9	1
1:A:64:ILE:CD1	1:A:76:TYR:CD2	0.57	2.87	13	2
1:A:67:GLU:CD	1:A:76:TYR:CE2	0.57	2.77	19	1
1:A:16:ILE:HD11	1:A:79:LEU:CD1	0.57	2.29	1	7
1:A:32:PHE:CE2	1:A:33:ILE:HG13	0.57	2.35	4	3
1:A:59:ASP:HB2	1:A:61:PHE:CD2	0.57	2.33	12	9
1:A:8:TYR:O	1:A:11:LEU:N	0.57	2.38	1	7
1:A:51:ILE:O	1:A:55:LEU:CB	0.57	2.53	14	5
1:A:33:ILE:CG2	1:A:37:PHE:CG	0.57	2.88	4	1
1:A:19:SER:OG	1:A:24:LEU:CD1	0.57	2.53	18	2
1:A:26:LEU:HD11	1:A:52:ARG:CG	0.56	2.29	10	1
1:A:77:TRP:CD1	1:A:77:TRP:N	0.56	2.71	20	14
1:A:37:PHE:CD2	1:A:40:TYR:CD2	0.56	2.93	20	2
1:A:63:LYS:HB2	1:A:77:TRP:CE2	0.56	2.35	15	8
1:A:23:LYS:CG	1:A:23:LYS:O	0.56	2.53	7	1
1:A:67:GLU:OE1	1:A:76:TYR:CZ	0.55	2.59	19	1
1:A:40:TYR:CD1	1:A:47:TRP:CZ2	0.55	2.94	11	6
1:A:32:PHE:CE2	1:A:33:ILE:HD11	0.55	2.36	3	2
1:A:32:PHE:O	1:A:35:ASN:ND2	0.55	2.39	4	3
1:A:64:ILE:HD11	1:A:76:TYR:CD1	0.55	2.35	17	2
1:A:55:LEU:CD1	1:A:77:TRP:CZ3	0.55	2.90	10	1
1:A:26:LEU:CD1	1:A:48:GLN:CD	0.55	2.75	3	1
1:A:62:VAL:CG2	1:A:78:THR:OG1	0.55	2.54	17	1
1:A:26:LEU:CD2	1:A:52:ARG:CZ	0.55	2.85	8	1
1:A:25:THR:HA	1:A:75:ASN:O	0.55	2.01	19	1
1:A:56:SER:O	1:A:60:CYS:N	0.55	2.39	15	1
1:A:37:PHE:N	1:A:38:PRO:CD	0.55	2.69	10	1
1:A:38:PRO:O	1:A:42:GLU:CB	0.54	2.56	1	2
1:A:47:TRP:O	1:A:51:ILE:CG1	0.54	2.55	17	2
1:A:11:LEU:C	1:A:11:LEU:HD13	0.54	2.22	6	1
1:A:50:SER:O	1:A:53:HIS:CD2	0.54	2.61	6	2
1:A:32:PHE:O	1:A:35:ASN:OD1	0.54	2.25	4	1
1:A:33:ILE:HG23	1:A:37:PHE:CG	0.54	2.38	4	1
1:A:44:PHE:CE1	1:A:46:ALA:HB3	0.54	2.38	15	4
1:A:59:ASP:CG	1:A:61:PHE:CE2	0.54	2.82	4	4
1:A:21:GLN:O	1:A:22:LYS:CB	0.54	2.56	2	6
1:A:63:LYS:HB3	1:A:77:TRP:CE2	0.54	2.37	14	4
1:A:28:GLY:O	1:A:32:PHE:N	0.53	2.38	6	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:32:PHE:CE2	1:A:33:ILE:HD13	0.53	2.39	3	3
1:A:59:ASP:HB3	1:A:61:PHE:CD2	0.53	2.37	9	2
1:A:32:PHE:O	1:A:35:ASN:CG	0.53	2.46	4	1
1:A:47:TRP:O	1:A:51:ILE:N	0.53	2.42	14	4
1:A:37:PHE:CD1	1:A:37:PHE:N	0.53	2.76	11	5
1:A:53:HIS:CG	1:A:54:ASN:N	0.53	2.76	17	4
1:A:15:ALA:O	1:A:18:GLN:CB	0.53	2.57	3	1
1:A:39:TYR:O	1:A:43:LYS:CB	0.53	2.57	4	4
1:A:63:LYS:HB3	1:A:77:TRP:CD2	0.52	2.39	7	7
1:A:11:LEU:HD23	1:A:37:PHE:CZ	0.52	2.39	6	1
1:A:11:LEU:O	1:A:14:MET:CG	0.52	2.58	10	2
1:A:32:PHE:CD2	1:A:33:ILE:CD1	0.52	2.93	16	1
1:A:32:PHE:CA	1:A:35:ASN:OD1	0.52	2.57	4	1
1:A:55:LEU:HD22	1:A:77:TRP:CZ3	0.52	2.40	1	1
1:A:61:PHE:CD2	1:A:78:THR:O	0.52	2.63	9	1
1:A:11:LEU:CD1	1:A:36:ARG:NH2	0.52	2.73	17	1
1:A:53:HIS:O	1:A:57:LEU:HB2	0.52	2.04	19	4
1:A:64:ILE:CD1	1:A:76:TYR:CE1	0.52	2.92	3	1
1:A:64:ILE:O	1:A:64:ILE:CD1	0.52	2.58	20	2
1:A:62:VAL:CG1	1:A:80:ASP:OD1	0.51	2.58	15	1
1:A:16:ILE:CD1	1:A:79:LEU:CD1	0.51	2.88	4	3
1:A:44:PHE:CD2	1:A:47:TRP:HB3	0.51	2.41	11	6
1:A:16:ILE:CD1	1:A:61:PHE:CE2	0.51	2.94	18	3
1:A:39:TYR:O	1:A:43:LYS:CG	0.51	2.58	12	2
1:A:25:THR:O	1:A:28:GLY:N	0.51	2.44	17	8
1:A:15:ALA:CA	1:A:32:PHE:CE2	0.51	2.94	16	1
1:A:11:LEU:HD21	1:A:37:PHE:CE1	0.51	2.40	6	2
1:A:64:ILE:HD13	1:A:76:TYR:CE2	0.51	2.41	9	1
1:A:64:ILE:N	1:A:65:PRO:HD3	0.51	2.20	3	2
1:A:15:ALA:O	1:A:24:LEU:CD2	0.51	2.58	12	1
1:A:12:ILE:CG2	1:A:58:ASN:ND2	0.50	2.74	7	2
1:A:64:ILE:CD1	1:A:76:TYR:O	0.50	2.60	4	1
1:A:8:TYR:CE2	1:A:47:TRP:CE3	0.50	2.99	20	1
1:A:40:TYR:O	1:A:44:PHE:CB	0.50	2.59	2	1
1:A:44:PHE:CZ	1:A:46:ALA:HB3	0.50	2.42	16	2
1:A:36:ARG:CG	1:A:37:PHE:CZ	0.50	2.95	7	2
1:A:36:ARG:HG2	1:A:37:PHE:CZ	0.50	2.42	13	2
1:A:59:ASP:CB	1:A:61:PHE:CD2	0.50	2.95	9	2
1:A:8:TYR:OH	1:A:50:SER:CB	0.50	2.59	20	2
1:A:64:ILE:O	1:A:64:ILE:HD13	0.50	2.05	7	2
1:A:62:VAL:N	1:A:78:THR:O	0.50	2.40	16	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:56:SER:HA	1:A:61:PHE:CE1	0.50	2.42	15	4
1:A:14:MET:HE2	1:A:36:ARG:NH2	0.50	2.22	17	1
1:A:15:ALA:HA	1:A:32:PHE:CZ	0.50	2.41	14	2
1:A:57:LEU:HD12	1:A:57:LEU:O	0.50	2.07	14	1
1:A:21:GLN:O	1:A:22:LYS:CE	0.50	2.59	19	1
1:A:53:HIS:O	1:A:57:LEU:N	0.49	2.43	17	3
1:A:11:LEU:HD13	1:A:37:PHE:CZ	0.49	2.41	13	1
1:A:63:LYS:HD3	1:A:77:TRP:CZ2	0.49	2.43	17	4
1:A:11:LEU:HD11	1:A:37:PHE:CE2	0.49	2.42	5	2
1:A:15:ALA:O	1:A:18:GLN:N	0.49	2.43	3	1
1:A:24:LEU:O	1:A:77:TRP:CD1	0.49	2.64	5	1
1:A:75:ASN:C	1:A:76:TYR:CD1	0.49	2.86	9	3
1:A:8:TYR:CB	1:A:51:ILE:CD1	0.49	2.90	9	1
1:A:36:ARG:HG3	1:A:37:PHE:CE1	0.49	2.43	7	2
1:A:54:ASN:HA	1:A:57:LEU:CD2	0.49	2.37	15	1
1:A:53:HIS:O	1:A:57:LEU:CB	0.49	2.60	19	1
1:A:13:THR:O	1:A:16:ILE:CG2	0.49	2.60	5	2
1:A:7:SER:O	1:A:11:LEU:CB	0.49	2.60	2	1
1:A:40:TYR:CG	1:A:47:TRP:CZ2	0.49	3.00	11	3
1:A:57:LEU:O	1:A:57:LEU:CG	0.49	2.60	16	2
1:A:7:SER:CB	1:A:9:ILE:CD1	0.49	2.90	18	1
1:A:12:ILE:O	1:A:16:ILE:N	0.49	2.40	6	2
1:A:8:TYR:CE2	1:A:9:ILE:HD11	0.49	2.43	9	1
1:A:21:GLN:O	1:A:22:LYS:HB2	0.49	2.07	2	2
1:A:15:ALA:HA	1:A:32:PHE:CE1	0.49	2.43	8	1
1:A:32:PHE:CE2	1:A:36:ARG:NE	0.49	2.81	18	1
1:A:26:LEU:O	1:A:26:LEU:CD2	0.49	2.60	20	1
1:A:56:SER:O	1:A:60:CYS:HA	0.49	2.06	17	4
1:A:67:GLU:OE1	1:A:74:GLY:O	0.49	2.31	7	1
1:A:64:ILE:HD11	1:A:76:TYR:CE1	0.49	2.42	3	1
1:A:36:ARG:HG3	1:A:37:PHE:CD2	0.48	2.43	18	3
1:A:7:SER:O	1:A:11:LEU:CD2	0.48	2.61	14	2
1:A:14:MET:CE	1:A:36:ARG:NH2	0.48	2.76	17	1
1:A:37:PHE:CE2	1:A:40:TYR:CD2	0.48	3.02	1	2
1:A:36:ARG:HB2	1:A:37:PHE:CE1	0.48	2.43	19	2
1:A:76:TYR:CD1	1:A:76:TYR:N	0.48	2.81	17	1
1:A:8:TYR:CZ	1:A:47:TRP:CE3	0.48	3.01	20	1
1:A:48:GLN:O	1:A:52:ARG:CG	0.48	2.62	7	1
1:A:8:TYR:O	1:A:12:ILE:CD1	0.48	2.61	9	2
1:A:16:ILE:HD11	1:A:61:PHE:CE1	0.48	2.43	20	1
1:A:15:ALA:O	1:A:24:LEU:CD1	0.48	2.61	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:33:ILE:HG23	1:A:37:PHE:CD1	0.48	2.44	4	3
1:A:61:PHE:CA	1:A:78:THR:O	0.48	2.61	16	1
1:A:16:ILE:HD11	1:A:61:PHE:CE2	0.48	2.44	9	4
1:A:48:GLN:O	1:A:52:ARG:CB	0.48	2.61	14	3
1:A:19:SER:OG	1:A:24:LEU:CD2	0.48	2.62	1	2
1:A:53:HIS:CE1	1:A:57:LEU:HD22	0.48	2.44	15	1
1:A:40:TYR:O	1:A:44:PHE:N	0.47	2.47	2	5
1:A:55:LEU:HD23	1:A:77:TRP:CZ3	0.47	2.44	17	7
1:A:55:LEU:HG	1:A:61:PHE:CE2	0.47	2.44	20	1
1:A:8:TYR:CE2	1:A:9:ILE:CD1	0.47	2.98	9	1
1:A:40:TYR:CD2	1:A:47:TRP:CH2	0.47	3.02	8	2
1:A:61:PHE:HB3	1:A:79:LEU:HA	0.47	1.86	9	3
1:A:63:LYS:HB2	1:A:77:TRP:NE1	0.47	2.25	7	2
1:A:36:ARG:HB3	1:A:37:PHE:CE1	0.47	2.45	11	1
1:A:11:LEU:HD11	1:A:37:PHE:CZ	0.47	2.44	13	2
1:A:53:HIS:NE2	1:A:54:ASN:OD1	0.47	2.48	6	1
1:A:33:ILE:O	1:A:36:ARG:N	0.47	2.48	11	3
1:A:36:ARG:HG3	1:A:37:PHE:CE2	0.47	2.44	18	1
1:A:44:PHE:CE2	1:A:47:TRP:HB3	0.47	2.45	5	1
1:A:8:TYR:CD2	1:A:54:ASN:ND2	0.47	2.83	14	1
1:A:7:SER:HB2	1:A:9:ILE:CD1	0.47	2.39	18	1
1:A:55:LEU:HD13	1:A:61:PHE:CE1	0.47	2.45	19	1
1:A:53:HIS:CE1	1:A:54:ASN:OD1	0.46	2.68	6	1
1:A:26:LEU:HD12	1:A:77:TRP:CZ2	0.46	2.45	10	2
1:A:23:LYS:HD2	1:A:76:TYR:CD1	0.46	2.46	11	1
1:A:15:ALA:O	1:A:29:ILE:CD1	0.46	2.63	13	1
1:A:19:SER:CB	1:A:24:LEU:HG	0.46	2.41	17	1
1:A:26:LEU:HA	1:A:29:ILE:CG1	0.46	2.40	3	1
1:A:54:ASN:ND2	1:A:58:ASN:OD1	0.46	2.48	3	1
1:A:11:LEU:HD11	1:A:37:PHE:CE1	0.46	2.45	11	1
1:A:49:ASN:O	1:A:52:ARG:N	0.46	2.49	16	1
1:A:39:TYR:CD1	1:A:39:TYR:O	0.46	2.68	20	1
1:A:7:SER:OG	1:A:10:ALA:HB3	0.46	2.11	2	1
1:A:64:ILE:O	1:A:75:ASN:CG	0.46	2.53	9	2
1:A:66:ARG:CG	1:A:66:ARG:O	0.46	2.59	1	2
1:A:24:LEU:CD2	1:A:77:TRP:O	0.46	2.63	6	1
1:A:63:LYS:CG	1:A:64:ILE:N	0.46	2.79	8	1
1:A:11:LEU:O	1:A:14:MET:N	0.46	2.45	9	1
1:A:36:ARG:CZ	1:A:36:ARG:HB3	0.46	2.41	18	1
1:A:58:ASN:OD1	1:A:59:ASP:OD2	0.46	2.34	13	2
1:A:58:ASN:ND2	1:A:59:ASP:OD2	0.46	2.49	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:61:PHE:HB3	1:A:78:THR:O	0.46	2.11	17	5
1:A:14:MET:CE	1:A:36:ARG:CZ	0.46	2.94	4	1
1:A:37:PHE:CD2	1:A:40:TYR:HB3	0.46	2.46	4	1
1:A:11:LEU:HD21	1:A:37:PHE:CZ	0.46	2.45	7	1
1:A:36:ARG:HG3	1:A:37:PHE:CZ	0.46	2.46	18	2
1:A:58:ASN:ND2	1:A:59:ASP:OD1	0.46	2.49	16	2
1:A:36:ARG:HG3	1:A:37:PHE:CG	0.46	2.46	18	2
1:A:67:GLU:OE2	1:A:74:GLY:O	0.46	2.34	2	1
1:A:31:GLU:O	1:A:35:ASN:OD1	0.46	2.33	7	4
1:A:65:PRO:O	1:A:66:ARG:HB2	0.46	2.10	17	2
1:A:57:LEU:O	1:A:57:LEU:HD23	0.46	2.11	16	1
1:A:54:ASN:OD1	1:A:58:ASN:ND2	0.45	2.49	2	1
1:A:33:ILE:HA	1:A:36:ARG:CG	0.45	2.40	4	1
1:A:28:GLY:O	1:A:32:PHE:CB	0.45	2.64	15	3
1:A:26:LEU:HD21	1:A:52:ARG:CZ	0.45	2.41	8	1
1:A:80:ASP:O	1:A:80:ASP:CG	0.45	2.53	13	4
1:A:55:LEU:HD12	1:A:77:TRP:CZ3	0.45	2.46	19	1
1:A:54:ASN:O	1:A:58:ASN:CB	0.45	2.65	2	1
1:A:25:THR:O	1:A:29:ILE:N	0.45	2.45	4	2
1:A:55:LEU:HG	1:A:61:PHE:CE1	0.45	2.47	14	2
1:A:39:TYR:O	1:A:43:LYS:N	0.45	2.49	8	1
1:A:9:ILE:HG12	1:A:10:ALA:N	0.45	2.27	15	1
1:A:24:LEU:O	1:A:77:TRP:N	0.45	2.49	5	1
1:A:11:LEU:HD12	1:A:37:PHE:CE2	0.45	2.47	18	2
1:A:9:ILE:O	1:A:13:THR:CB	0.45	2.65	10	1
1:A:53:HIS:NE2	1:A:57:LEU:CD2	0.45	2.80	15	1
1:A:9:ILE:N	1:A:9:ILE:HD13	0.45	2.27	1	2
1:A:57:LEU:O	1:A:57:LEU:HG	0.45	2.11	16	1
1:A:58:ASN:OD1	1:A:59:ASP:N	0.45	2.50	18	1
1:A:55:LEU:HD13	1:A:61:PHE:CZ	0.45	2.47	19	1
1:A:16:ILE:HD13	1:A:61:PHE:CE2	0.44	2.47	6	1
1:A:59:ASP:OD1	1:A:61:PHE:CE2	0.44	2.70	17	1
1:A:50:SER:O	1:A:53:HIS:N	0.44	2.50	14	1
1:A:55:LEU:HG	1:A:61:PHE:CZ	0.44	2.47	14	3
1:A:39:TYR:O	1:A:43:LYS:HB2	0.44	2.12	4	2
1:A:63:LYS:HB2	1:A:77:TRP:CD2	0.44	2.48	16	2
1:A:74:GLY:O	1:A:75:ASN:OD1	0.44	2.35	2	1
1:A:28:GLY:O	1:A:31:GLU:N	0.44	2.49	3	1
1:A:32:PHE:CD2	1:A:33:ILE:HG13	0.44	2.47	4	2
1:A:64:ILE:HG21	1:A:67:GLU:CG	0.44	2.42	4	1
1:A:15:ALA:HA	1:A:18:GLN:OE1	0.44	2.13	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:12:ILE:CD1	1:A:12:ILE:N	0.44	2.81	19	1
1:A:8:TYR:CZ	1:A:50:SER:HB3	0.44	2.48	20	1
1:A:54:ASN:O	1:A:58:ASN:CG	0.44	2.56	2	1
1:A:29:ILE:CD1	1:A:51:ILE:CD1	0.44	2.96	3	1
1:A:14:MET:CE	1:A:37:PHE:CZ	0.44	3.01	14	1
1:A:51:ILE:HA	1:A:54:ASN:OD1	0.44	2.13	19	1
1:A:8:TYR:CD2	1:A:51:ILE:HD12	0.44	2.47	20	1
1:A:47:TRP:CE2	1:A:51:ILE:HD11	0.44	2.48	1	2
1:A:64:ILE:O	1:A:75:ASN:CB	0.44	2.66	5	1
1:A:7:SER:O	1:A:11:LEU:N	0.44	2.50	9	1
1:A:53:HIS:O	1:A:57:LEU:HB3	0.44	2.12	16	1
1:A:16:ILE:HD11	1:A:61:PHE:CZ	0.44	2.47	20	1
1:A:40:TYR:O	1:A:44:PHE:HB3	0.43	2.14	9	1
1:A:11:LEU:CD1	1:A:12:ILE:HD12	0.43	2.42	10	1
1:A:12:ILE:N	1:A:12:ILE:HD12	0.43	2.28	19	1
1:A:12:ILE:CG2	1:A:55:LEU:HD23	0.43	2.43	4	1
1:A:26:LEU:HD22	1:A:52:ARG:CZ	0.43	2.44	8	1
1:A:53:HIS:CE1	1:A:57:LEU:CD2	0.43	3.00	15	1
1:A:54:ASN:O	1:A:58:ASN:HB2	0.43	2.13	15	1
1:A:16:ILE:CD1	1:A:79:LEU:HD11	0.43	2.43	5	1
1:A:63:LYS:HD2	1:A:77:TRP:CZ2	0.43	2.49	16	1
1:A:36:ARG:C	1:A:38:PRO:HD3	0.43	2.33	18	1
1:A:50:SER:O	1:A:54:ASN:OD1	0.43	2.36	19	1
1:A:63:LYS:C	1:A:65:PRO:HD3	0.43	2.33	3	2
1:A:15:ALA:O	1:A:18:GLN:HG3	0.43	2.14	19	2
1:A:16:ILE:HG21	1:A:79:LEU:CD1	0.43	2.44	7	1
1:A:19:SER:OG	1:A:24:LEU:CG	0.43	2.67	17	1
1:A:36:ARG:HG3	1:A:37:PHE:CD1	0.43	2.48	18	1
1:A:61:PHE:HB3	1:A:78:THR:C	0.43	2.33	16	3
1:A:51:ILE:CG1	1:A:52:ARG:N	0.43	2.82	3	1
1:A:26:LEU:HD12	1:A:77:TRP:CH2	0.43	2.49	14	2
1:A:44:PHE:CE1	1:A:46:ALA:HB2	0.43	2.47	15	1
1:A:44:PHE:CE2	1:A:46:ALA:HB3	0.43	2.49	19	2
1:A:80:ASP:OD1	1:A:80:ASP:O	0.43	2.37	6	1
1:A:11:LEU:HD22	1:A:37:PHE:CZ	0.43	2.48	9	2
1:A:32:PHE:CD2	1:A:36:ARG:NE	0.43	2.87	18	1
1:A:55:LEU:HD12	1:A:77:TRP:CE3	0.43	2.49	19	1
1:A:19:SER:OG	1:A:24:LEU:HD21	0.43	2.14	1	1
1:A:80:ASP:O	1:A:80:ASP:OD1	0.43	2.36	7	1
1:A:29:ILE:CD1	1:A:51:ILE:HD12	0.43	2.44	3	1
1:A:47:TRP:O	1:A:50:SER:N	0.43	2.51	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:51:ILE:C	1:A:53:HIS:N	0.42	2.71	19	1
1:A:7:SER:CB	1:A:10:ALA:HB3	0.42	2.45	2	2
1:A:64:ILE:HD11	1:A:76:TYR:CD2	0.42	2.50	9	1
1:A:36:ARG:C	1:A:37:PHE:CD1	0.42	2.92	15	1
1:A:47:TRP:HA	1:A:50:SER:HG	0.42	1.75	17	1
1:A:24:LEU:O	1:A:77:TRP:CG	0.42	2.72	19	1
1:A:48:GLN:O	1:A:52:ARG:HB2	0.42	2.15	7	3
1:A:11:LEU:CD1	1:A:33:ILE:CD1	0.42	2.98	16	1
1:A:14:MET:HE2	1:A:36:ARG:CZ	0.42	2.44	4	1
1:A:54:ASN:O	1:A:58:ASN:ND2	0.42	2.52	12	1
1:A:16:ILE:HG12	1:A:79:LEU:CD1	0.42	2.45	14	1
1:A:8:TYR:OH	1:A:50:SER:O	0.42	2.36	16	1
1:A:18:GLN:OE1	1:A:32:PHE:CE2	0.42	2.72	5	1
1:A:8:TYR:O	1:A:12:ILE:HD12	0.42	2.15	9	1
1:A:16:ILE:HD12	1:A:24:LEU:CD2	0.42	2.45	14	1
1:A:74:GLY:C	1:A:75:ASN:OD1	0.42	2.57	19	1
1:A:11:LEU:HD23	1:A:12:ILE:CD1	0.42	2.45	3	1
1:A:26:LEU:CD2	1:A:52:ARG:CG	0.42	2.98	5	1
1:A:60:CYS:O	1:A:80:ASP:OD2	0.42	2.38	7	1
1:A:8:TYR:HB2	1:A:51:ILE:CD1	0.42	2.45	9	1
1:A:11:LEU:HD22	1:A:37:PHE:CE2	0.42	2.50	9	2
1:A:21:GLN:O	1:A:22:LYS:CD	0.42	2.68	19	1
1:A:28:GLY:O	1:A:32:PHE:HB3	0.42	2.15	6	1
1:A:63:LYS:HD3	1:A:77:TRP:CH2	0.42	2.49	7	1
1:A:38:PRO:O	1:A:42:GLU:HB2	0.42	2.15	4	1
1:A:26:LEU:HB2	1:A:77:TRP:CZ2	0.42	2.50	5	1
1:A:11:LEU:CD2	1:A:37:PHE:CE1	0.42	3.02	6	1
1:A:40:TYR:CE2	1:A:47:TRP:CH2	0.42	3.08	6	1
1:A:24:LEU:N	1:A:77:TRP:O	0.41	2.49	19	1
1:A:14:MET:HA	1:A:17:LEU:CD2	0.41	2.45	2	1
1:A:34:SER:CB	1:A:41:ARG:NH1	0.41	2.83	8	1
1:A:10:ALA:O	1:A:13:THR:OG1	0.41	2.38	11	1
1:A:32:PHE:O	1:A:35:ASN:CB	0.41	2.68	17	1
1:A:59:ASP:C	1:A:60:CYS:SG	0.41	2.99	1	1
1:A:64:ILE:O	1:A:75:ASN:OD1	0.41	2.39	2	1
1:A:64:ILE:CD1	1:A:75:ASN:HB3	0.41	2.45	7	1
1:A:13:THR:O	1:A:17:LEU:HG	0.41	2.15	17	1
1:A:55:LEU:HD23	1:A:61:PHE:CE1	0.41	2.50	1	1
1:A:40:TYR:CE1	1:A:47:TRP:CZ2	0.41	3.08	1	1
1:A:18:GLN:CD	1:A:32:PHE:CD1	0.41	2.94	5	1
1:A:36:ARG:HG2	1:A:37:PHE:CE1	0.41	2.49	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:59:ASP:OD1	1:A:79:LEU:CD2	0.41	2.68	15	1
1:A:19:SER:OG	1:A:24:LEU:HG	0.41	2.15	17	1
1:A:46:ALA:O	1:A:50:SER:CB	0.41	2.67	17	1
1:A:8:TYR:OH	1:A:50:SER:OG	0.41	2.35	1	1
1:A:26:LEU:HD13	1:A:48:GLN:CG	0.41	2.46	3	1
1:A:29:ILE:HD12	1:A:51:ILE:CD1	0.41	2.46	3	1
1:A:12:ILE:HG23	1:A:55:LEU:CD2	0.41	2.46	4	1
1:A:26:LEU:HG	1:A:52:ARG:CD	0.41	2.46	4	1
1:A:60:CYS:O	1:A:80:ASP:OD1	0.41	2.38	7	1
1:A:8:TYR:CE2	1:A:50:SER:HB3	0.41	2.50	14	1
1:A:18:GLN:OE1	1:A:18:GLN:O	0.41	2.39	15	1
1:A:47:TRP:CZ2	1:A:51:ILE:HD11	0.41	2.50	1	1
1:A:16:ILE:CG2	1:A:17:LEU:N	0.41	2.83	18	2
1:A:32:PHE:C	1:A:35:ASN:OD1	0.41	2.59	4	1
1:A:26:LEU:CD2	1:A:52:ARG:HD3	0.41	2.46	6	1
1:A:63:LYS:HD2	1:A:77:TRP:CZ3	0.41	2.50	12	1
1:A:17:LEU:C	1:A:19:SER:N	0.41	2.74	17	1
1:A:32:PHE:CD1	1:A:32:PHE:C	0.41	2.93	17	1
1:A:9:ILE:O	1:A:13:THR:CG2	0.41	2.57	19	1
1:A:11:LEU:HD12	1:A:33:ILE:CG1	0.41	2.46	19	1
1:A:18:GLN:O	1:A:18:GLN:OE1	0.41	2.39	2	1
1:A:33:ILE:HG23	1:A:37:PHE:CD2	0.41	2.50	9	1
1:A:7:SER:HB3	1:A:10:ALA:CB	0.41	2.46	10	1
1:A:11:LEU:HD12	1:A:33:ILE:CD1	0.41	2.45	16	1
1:A:18:GLN:C	1:A:18:GLN:OE1	0.41	2.60	9	1
1:A:33:ILE:CD1	1:A:51:ILE:HG12	0.41	2.46	14	1
1:A:7:SER:HB2	1:A:10:ALA:HB3	0.41	1.92	15	1
1:A:7:SER:O	1:A:11:LEU:HB2	0.40	2.15	2	1
1:A:16:ILE:N	1:A:16:ILE:CD1	0.40	2.84	2	1
1:A:9:ILE:HG13	1:A:10:ALA:N	0.40	2.31	5	1
1:A:49:ASN:C	1:A:51:ILE:N	0.40	2.73	16	1
1:A:19:SER:HB3	1:A:24:LEU:CD2	0.40	2.45	17	1
1:A:20:PRO:O	1:A:21:GLN:OE1	0.40	2.39	6	1
1:A:63:LYS:HB2	1:A:77:TRP:CD1	0.40	2.51	8	1
1:A:30:CYS:SG	1:A:48:GLN:OE1	0.40	2.80	11	1
1:A:39:TYR:HA	1:A:42:GLU:CG	0.40	2.46	12	1
1:A:64:ILE:N	1:A:65:PRO:CD	0.40	2.83	3	1
1:A:23:LYS:O	1:A:23:LYS:HG2	0.40	2.17	7	1
1:A:47:TRP:CD1	1:A:47:TRP:C	0.40	2.95	13	1
1:A:55:LEU:O	1:A:58:ASN:HB3	0.40	2.15	14	1
1:A:15:ALA:HB2	1:A:32:PHE:CE2	0.40	2.51	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:54:ASN:O	1:A:58:ASN:N	0.40	2.54	11	1
1:A:15:ALA:O	1:A:29:ILE:HD11	0.40	2.17	13	1
1:A:14:MET:CE	1:A:36:ARG:HG3	0.40	2.46	14	1
1:A:26:LEU:CD1	1:A:48:GLN:NE2	0.40	2.84	3	1
1:A:32:PHE:CD1	1:A:36:ARG:HD3	0.40	2.52	11	1
1:A:36:ARG:CB	1:A:37:PHE:CE1	0.40	3.04	11	1
1:A:16:ILE:CD1	1:A:24:LEU:HD11	0.40	2.47	20	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	68/109 (62%)	55±3 (81±5%)	10±3 (15±5%)	3±1 (4±1%)	5	31
All	All	1360/2180 (62%)	1105 (81%)	199 (15%)	56 (4%)	5	31

All 6 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	22	LYS	20
1	A	66	ARG	17
1	A	60	CYS	13
1	A	38	PRO	4
1	A	44	PHE	1
1	A	61	PHE	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	63/101 (62%)	42±4 (67±6%)	21±4 (33±6%)	1	11
All	All	1260/2020 (62%)	839 (67%)	421 (33%)	1	11

All 56 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	61	PHE	20
1	A	43	LYS	16
1	A	63	LYS	16
1	A	79	LEU	16
1	A	40	TYR	15
1	A	22	LYS	14
1	A	32	PHE	14
1	A	18	GLN	12
1	A	21	GLN	12
1	A	47	TRP	12
1	A	53	HIS	12
1	A	66	ARG	12
1	A	37	PHE	11
1	A	11	LEU	10
1	A	39	TYR	10
1	A	41	ARG	10
1	A	7	SER	10
1	A	67	GLU	10
1	A	52	ARG	10
1	A	26	LEU	9
1	A	80	ASP	9
1	A	9	ILE	8
1	A	57	LEU	8
1	A	8	TYR	8
1	A	42	GLU	8
1	A	60	CYS	8
1	A	23	LYS	8
1	A	62	VAL	8
1	A	17	LEU	7
1	A	55	LEU	7
1	A	48	GLN	6
1	A	16	ILE	6
1	A	76	TYR	6
1	A	51	ILE	6
1	A	35	ASN	6
1	A	36	ARG	5

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Mol	Chain	Res	Type	Models (Total)
1	A	44	PHE	5
1	A	24	LEU	5
1	A	75	ASN	5
1	A	64	ILE	5
1	A	50	SER	4
1	A	54	ASN	4
1	A	59	ASP	4
1	A	34	SER	3
1	A	14	MET	3
1	A	56	SER	3
1	A	29	ILE	2
1	A	31	GLU	2
1	A	33	ILE	2
1	A	30	CYS	2
1	A	27	SER	2
1	A	58	ASN	1
1	A	78	THR	1
1	A	49	ASN	1
1	A	12	ILE	1
1	A	25	THR	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

No chemical shift data were provided