



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 04:01 PM BST

PDB ID : 1M9L
Title : Relaxation-based Refined Structure Of Chlamydomonas Outer Arm Dynein Light Chain 1
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Deposited on : 2002-07-29

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
<http://wwpdb.org/validation/2016/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:

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : rb-20027457
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

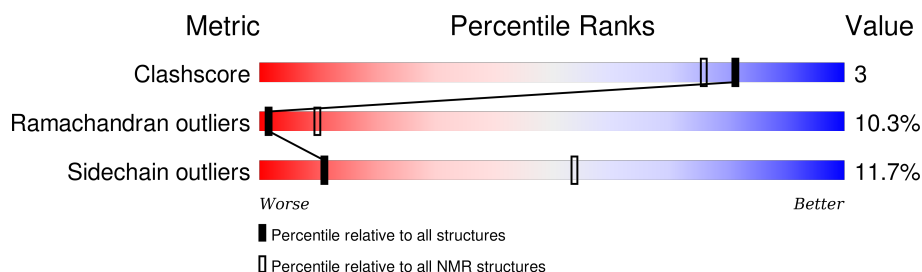
1 Overall quality at a glance

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	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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	199	

2 Ensemble composition and analysis ⓘ

This entry contains 15 models. Model 9 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:1-A:198 (198)	0.37	9

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 2 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 3, 5, 7, 8, 9, 14, 15
2	2, 4, 6, 10, 11, 12, 13

3 Entry composition

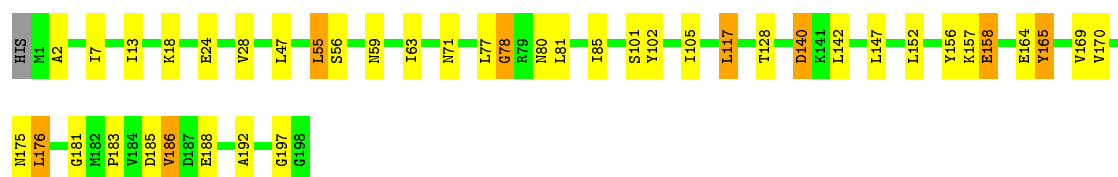
There is only 1 type of molecule in this entry. The entry contains 3161 atoms, of which 1610 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Outer Arm Dynein Light Chain 1.

Mol	Chain	Residues	Atoms						Trace
1	A	198	Total	C	H	N	O	S	0
			3161	975	1610	267	302	7	

There is a discrepancy between the modelled and reference sequences:

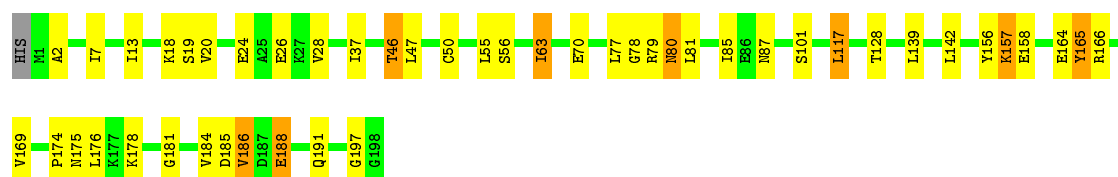
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	HIS	-	EXPRESSION TAG	UNP Q9XHH2



4.2.3 Score per residue for model 3

- Molecule 1: Outer Arm Dynein Light Chain 1

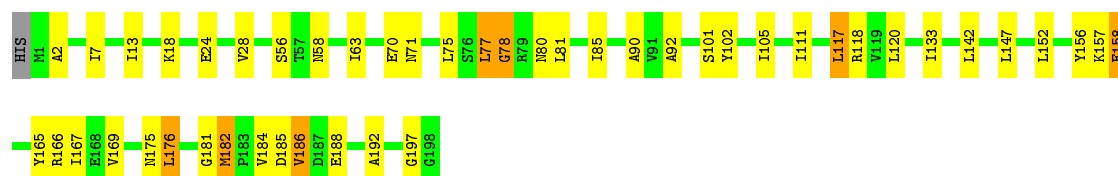
Chain A: 76% 20%



4.2.4 Score per residue for model 4

- Molecule 1: Outer Arm Dynein Light Chain 1

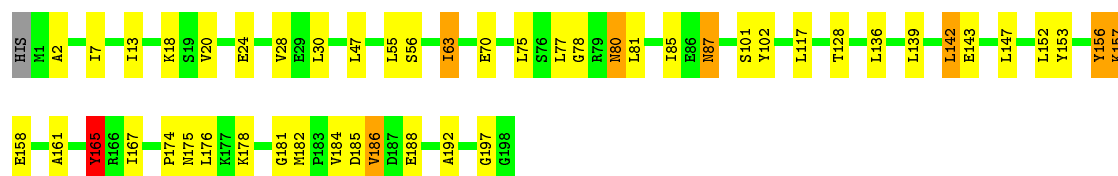
Chain A: 76% 20%



4.2.5 Score per residue for model 5

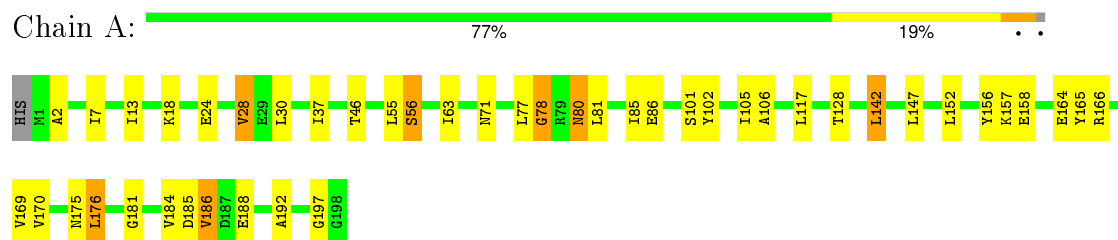
- Molecule 1: Outer Arm Dynein Light Chain 1

Chain A: 75% 21%



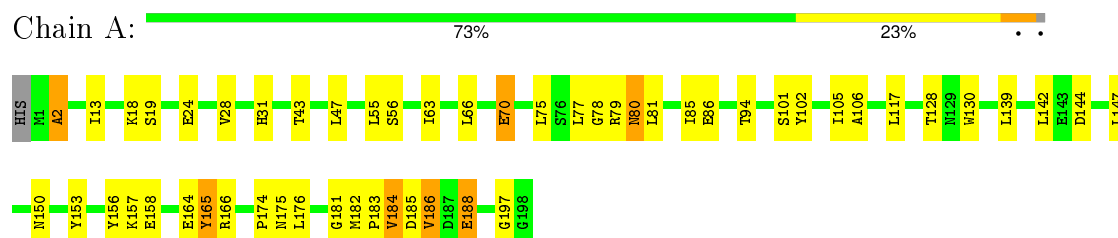
4.2.6 Score per residue for model 6

- Molecule 1: Outer Arm Dynein Light Chain 1



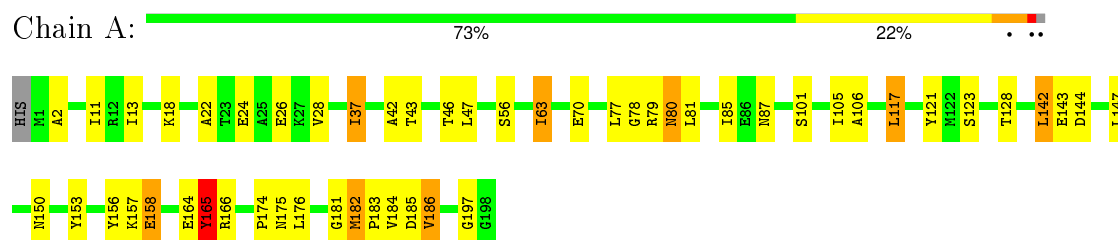
4.2.7 Score per residue for model 7

- Molecule 1: Outer Arm Dynein Light Chain 1



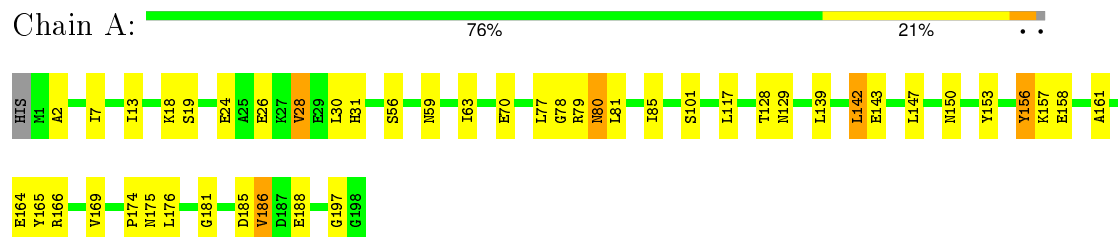
4.2.8 Score per residue for model 8

- Molecule 1: Outer Arm Dynein Light Chain 1



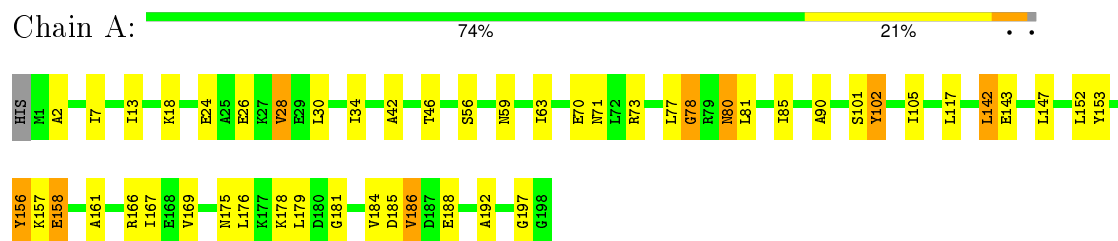
4.2.9 Score per residue for model 9 (medoid)

- Molecule 1: Outer Arm Dynein Light Chain 1



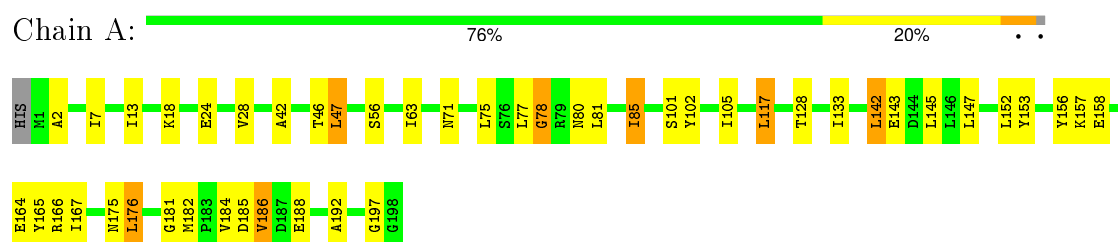
4.2.10 Score per residue for model 10

- Molecule 1: Outer Arm Dynein Light Chain 1



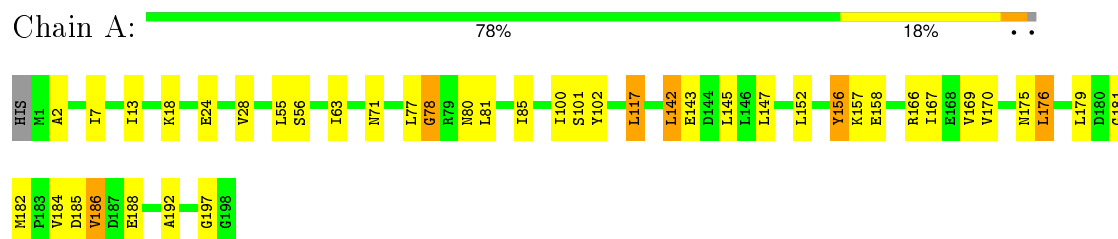
4.2.11 Score per residue for model 11

- Molecule 1: Outer Arm Dynein Light Chain 1



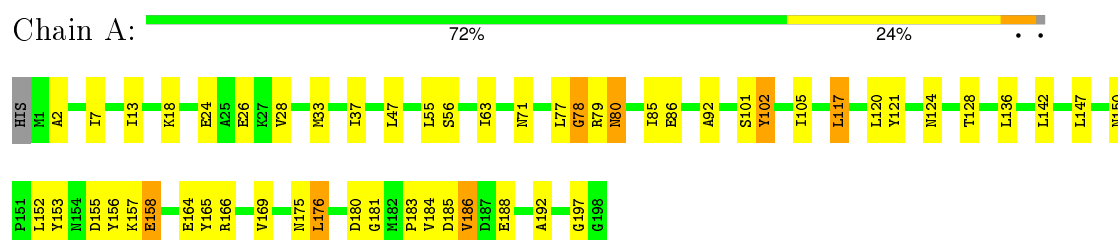
4.2.12 Score per residue for model 12

- Molecule 1: Outer Arm Dynein Light Chain 1



4.2.13 Score per residue for model 13

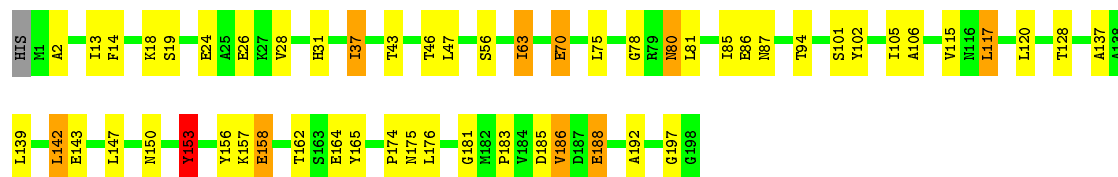
- Molecule 1: Outer Arm Dynein Light Chain 1



4.2.14 Score per residue for model 14

- Molecule 1: Outer Arm Dynein Light Chain 1

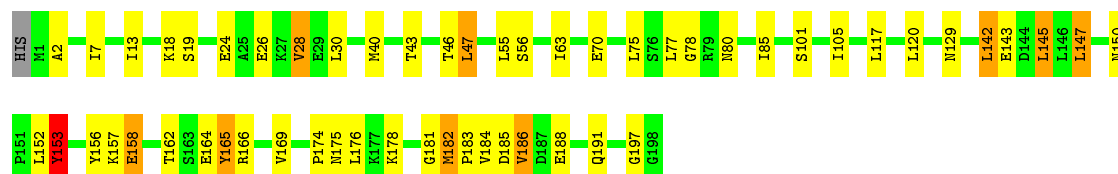
Chain A:  72% 23% 5% ..



4.2.15 Score per residue for model 15

- Molecule 1: Outer Arm Dynein Light Chain 1

Chain A:  72% 23% 5% ..



5 Refinement protocol and experimental data overview

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

Of the 15 calculated structures, 15 were deposited, based on the following criterion: *all calculated structures submitted*.

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

Software name	Classification	Version
DISCOVER	refinement	2.98

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality i

6.1 Standard geometry i

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.56±0.00	0±0/1567 (0.0±0.0%)	1.08±0.02	1±1/2113 (0.0±0.0%)
All	All	0.56	0/23505 (0.0%)	1.08	13/31695 (0.0%)

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	1.9±0.6
All	All	0	28

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	156	TYR	CB-CG-CD2	-7.43	116.54	121.00	12	1
1	A	153	TYR	CB-CG-CD2	-6.67	117.00	121.00	15	1
1	A	165	TYR	CB-CG-CD2	-6.26	117.24	121.00	8	6
1	A	102	TYR	CB-CG-CD2	-5.83	117.50	121.00	11	3
1	A	121	TYR	CB-CG-CD2	-5.23	117.86	121.00	8	1
1	A	77	LEU	CB-CA-C	5.21	120.10	110.20	4	1

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	156	TYR	Sidechain	15
1	A	153	TYR	Sidechain	7

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	165	TYR	Sidechain	4
1	A	121	TYR	Sidechain	1
1	A	102	TYR	Sidechain	1

6.2 Too-close contacts

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	1551	1610	1612	10±3
All	All	23265	24150	24180	154

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 3.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:77:LEU:HD21	1:A:80:ASN:CG	0.69	2.08	11	4
1:A:77:LEU:HD11	1:A:80:ASN:HB3	0.68	1.64	2	7
1:A:77:LEU:HD12	1:A:78:GLY:H	0.68	1.48	4	7
1:A:188:GLU:O	1:A:192:ALA:HB3	0.66	1.90	10	10
1:A:2:ALA:HB3	1:A:13:ILE:HG22	0.66	1.67	14	11
1:A:11:ILE:HG23	1:A:22:ALA:HB1	0.65	1.67	8	1
1:A:167:ILE:HG12	1:A:192:ALA:HB2	0.64	1.69	4	5
1:A:77:LEU:HD21	1:A:80:ASN:ND2	0.61	2.11	6	4
1:A:184:VAL:HG12	1:A:188:GLU:HG3	0.59	1.74	13	1
1:A:80:ASN:C	1:A:81:LEU:HD12	0.59	2.18	3	10
1:A:2:ALA:CB	1:A:13:ILE:CG2	0.54	2.85	3	4
1:A:181:GLY:O	1:A:184:VAL:HG13	0.53	2.03	13	1
1:A:63:ILE:HG23	1:A:87:ASN:CB	0.53	2.33	14	3
1:A:77:LEU:CD1	1:A:78:GLY:H	0.53	2.17	11	5
1:A:63:ILE:HG23	1:A:87:ASN:HB3	0.52	1.81	5	1
1:A:81:LEU:HD12	1:A:81:LEU:N	0.50	2.22	2	6
1:A:2:ALA:CB	1:A:13:ILE:HG22	0.50	2.36	6	8
1:A:162:THR:HG22	1:A:183:PRO:HB3	0.49	1.85	14	2
1:A:70:GLU:C	1:A:94:THR:HG21	0.49	2.28	7	3
1:A:142:LEU:HD23	1:A:143:GLU:N	0.48	2.23	11	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:170:VAL:CG1	1:A:192:ALA:HB1	0.48	2.37	2	3
1:A:156:TYR:CD2	1:A:161:ALA:HB1	0.48	2.43	10	3
1:A:70:GLU:HB2	1:A:90:ALA:HB1	0.48	1.85	4	2
1:A:42:ALA:O	1:A:46:THR:HG22	0.48	2.07	1	4
1:A:77:LEU:HD21	1:A:80:ASN:CB	0.48	2.39	4	1
1:A:59:ASN:ND2	1:A:81:LEU:HD13	0.47	2.24	9	1
1:A:33:MET:SD	1:A:37:ILE:HD13	0.47	2.50	13	1
1:A:34:ILE:O	1:A:34:ILE:HD12	0.47	2.10	10	1
1:A:55:LEU:HD22	1:A:55:LEU:N	0.46	2.26	2	1
1:A:81:LEU:N	1:A:81:LEU:HD12	0.46	2.26	14	4
1:A:170:VAL:HG11	1:A:192:ALA:HB1	0.45	1.88	2	1
1:A:28:VAL:HG12	1:A:30:LEU:HD21	0.45	1.87	5	5
1:A:145:LEU:HD12	1:A:147:LEU:HD11	0.45	1.88	15	1
1:A:181:GLY:C	1:A:183:PRO:HD2	0.45	2.32	1	1
1:A:59:ASN:OD1	1:A:81:LEU:HD13	0.44	2.13	2	2
1:A:185:ASP:O	1:A:186:VAL:HG12	0.43	2.13	1	1
1:A:47:LEU:HD23	1:A:47:LEU:C	0.43	2.35	1	3
1:A:153:TYR:CE1	1:A:162:THR:HG23	0.43	2.49	14	1
1:A:92:ALA:HA	1:A:117:LEU:HD13	0.42	1.90	4	2
1:A:77:LEU:HD23	1:A:100:ILE:HG22	0.42	1.92	12	1
1:A:166:ARG:HB2	1:A:183:PRO:CB	0.42	2.44	1	1
1:A:180:ASP:O	1:A:183:PRO:HD2	0.42	2.14	13	1
1:A:46:THR:HG23	1:A:50:CYS:SG	0.42	2.55	3	1
1:A:77:LEU:HD11	1:A:80:ASN:CB	0.42	2.43	6	1
1:A:20:VAL:HG21	1:A:30:LEU:HD23	0.41	1.92	5	1
1:A:184:VAL:HA	1:A:188:GLU:CG	0.41	2.45	3	2
1:A:47:LEU:C	1:A:47:LEU:HD23	0.41	2.36	5	2
1:A:111:ILE:HD13	1:A:133:ILE:HG23	0.41	1.91	4	1
1:A:142:LEU:HD23	1:A:143:GLU:H	0.41	1.74	11	1
1:A:115:VAL:O	1:A:142:LEU:HD11	0.41	2.15	14	1
1:A:102:TYR:HA	1:A:124:ASN:O	0.41	2.15	13	1
1:A:18:LYS:HB3	1:A:20:VAL:HG22	0.41	1.91	1	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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	196/199 (98%)	125±4 (64±2%)	51±5 (26±3%)	20±2 (10±1%)	1	10
All	All	2940/2985 (98%)	1871 (64%)	765 (26%)	304 (10%)	1	10

All 37 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	157	LYS	15
1	A	186	VAL	15
1	A	176	LEU	15
1	A	175	ASN	15
1	A	158	GLU	15
1	A	142	LEU	15
1	A	101	SER	15
1	A	185	ASP	15
1	A	78	GLY	15
1	A	197	GLY	15
1	A	117	LEU	15
1	A	24	GLU	15
1	A	181	GLY	14
1	A	56	SER	14
1	A	184	VAL	10
1	A	169	VAL	9
1	A	174	PRO	8
1	A	70	GLU	8
1	A	150	ASN	7
1	A	71	ASN	7
1	A	19	SER	6
1	A	105	ILE	6
1	A	182	MET	6
1	A	106	ALA	5
1	A	86	GLU	4
1	A	31	HIS	3
1	A	183	PRO	3
1	A	37	ILE	3
1	A	152	LEU	2
1	A	136	LEU	2
1	A	85	ILE	1
1	A	2	ALA	1
1	A	133	ILE	1
1	A	87	ASN	1
1	A	137	ALA	1
1	A	20	VAL	1

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Mol	Chain	Res	Type	Models (Total)
1	A	140	ASP	1

6.3.2 Protein sidechains ⓘ

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	172/173 (99%)	152±4 (88±2%)	20±4 (12±2%)	11	54
All	All	2580/2595 (99%)	2277 (88%)	303 (12%)	11	54

All 51 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	85	ILE	15
1	A	186	VAL	15
1	A	18	LYS	15
1	A	63	ILE	15
1	A	28	VAL	14
1	A	147	LEU	14
1	A	166	ARG	12
1	A	80	ASN	11
1	A	7	ILE	11
1	A	164	GLU	11
1	A	128	THR	11
1	A	165	TYR	11
1	A	26	GLU	8
1	A	55	LEU	8
1	A	47	LEU	7
1	A	152	LEU	7
1	A	75	LEU	7
1	A	102	TYR	7
1	A	158	GLU	7
1	A	77	LEU	7
1	A	139	LEU	6
1	A	176	LEU	6
1	A	79	ARG	6
1	A	117	LEU	6

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Mol	Chain	Res	Type	Models (Total)
1	A	188	GLU	5
1	A	153	TYR	5
1	A	105	ILE	5
1	A	46	THR	4
1	A	43	THR	4
1	A	37	ILE	4
1	A	178	LYS	4
1	A	182	MET	4
1	A	120	LEU	4
1	A	145	LEU	3
1	A	130	TRP	2
1	A	157	LYS	2
1	A	56	SER	2
1	A	144	ASP	2
1	A	191	GLN	2
1	A	179	LEU	2
1	A	129	ASN	2
1	A	14	PHE	1
1	A	58	ASN	1
1	A	155	ASP	1
1	A	66	LEU	1
1	A	123	SER	1
1	A	40	MET	1
1	A	73	ARG	1
1	A	142	LEU	1
1	A	140	ASP	1
1	A	118	ARG	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided