



Full wwPDB NMR Structure Validation Report ⓘ

Mar 19, 2026 – 08:41 PM UTC

PDB ID : 2KXJ / pdb_00002kxj
Title : Solution structure of UBX domain of human UBXD2 protein
Authors : Wu, Q.; Huang, H.; Zhang, J.; Hu, Q.; Wu, J.; Shi, Y.
Deposited on : 2010-05-06

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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

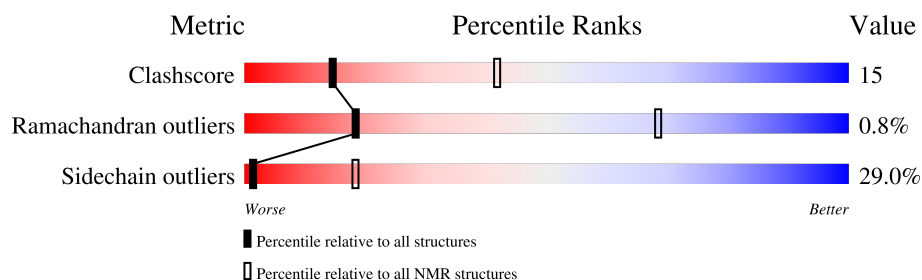
1 Overall quality at a glance

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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	90	52% 31% 6% 11%

2 Ensemble composition and analysis

This entry contains 20 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: *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:318-A:397 (80)	0.55	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 4 clusters and 3 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1409 atoms, of which 696 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called UBX domain-containing protein 4.

Mol	Chain	Residues	Atoms						Trace
1	A	90	Total	C	H	N	O	S	0
			1409	451	696	128	131	3	

There are 9 discrepancies between the modelled and reference sequences:

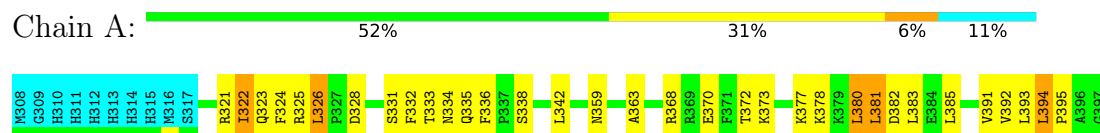
Chain	Residue	Modelled	Actual	Comment	Reference
A	308	MET	-	expression tag	UNP Q92575
A	309	GLY	-	expression tag	UNP Q92575
A	310	HIS	-	expression tag	UNP Q92575
A	311	HIS	-	expression tag	UNP Q92575
A	312	HIS	-	expression tag	UNP Q92575
A	313	HIS	-	expression tag	UNP Q92575
A	314	HIS	-	expression tag	UNP Q92575
A	315	HIS	-	expression tag	UNP Q92575
A	316	MET	-	expression tag	UNP Q92575

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: UBX domain-containing protein 4

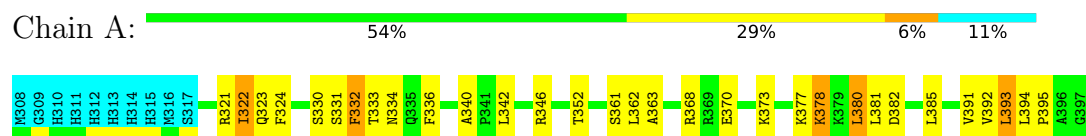


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

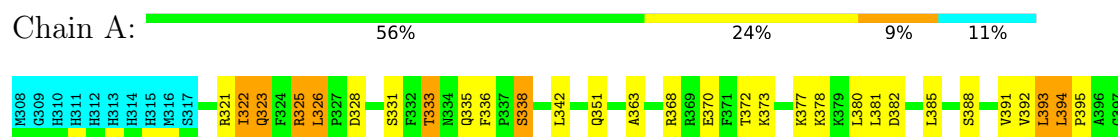
4.2.1 Score per residue for model 1

- Molecule 1: UBX domain-containing protein 4



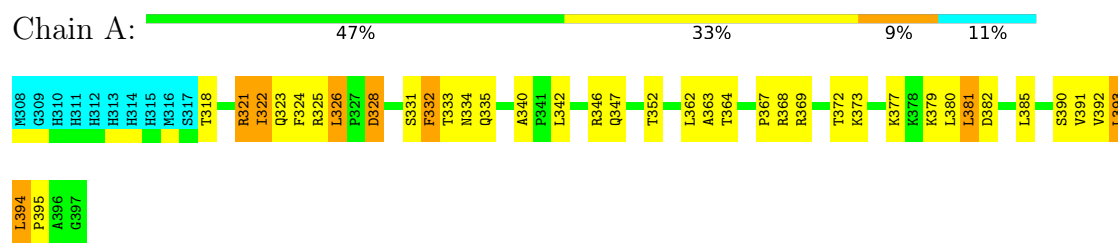
4.2.2 Score per residue for model 2

- Molecule 1: UBX domain-containing protein 4



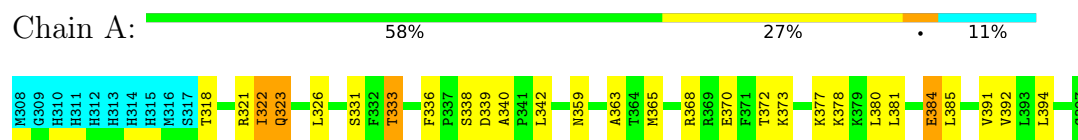
4.2.3 Score per residue for model 3

- Molecule 1: UBX domain-containing protein 4



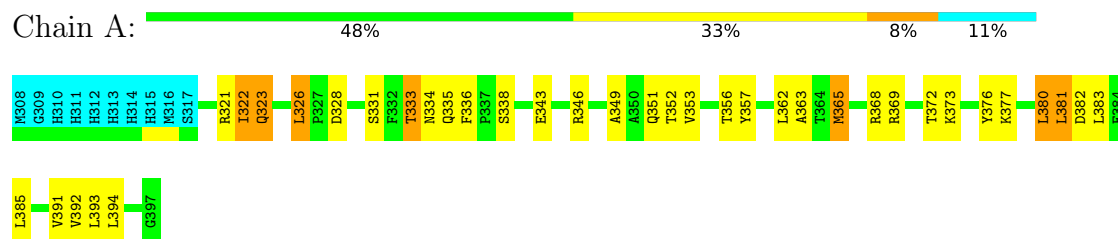
4.2.4 Score per residue for model 4

- Molecule 1: UBX domain-containing protein 4



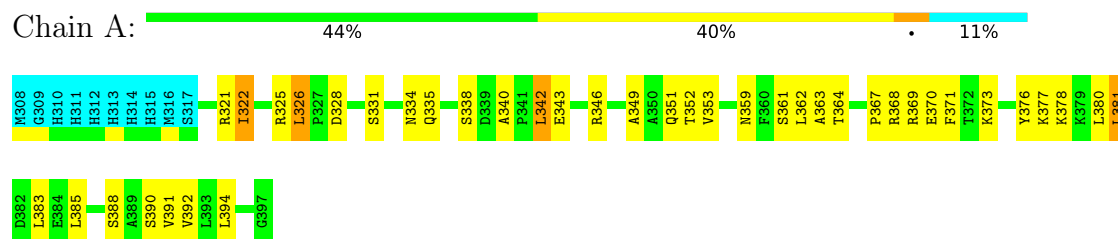
4.2.5 Score per residue for model 5

- Molecule 1: UBX domain-containing protein 4



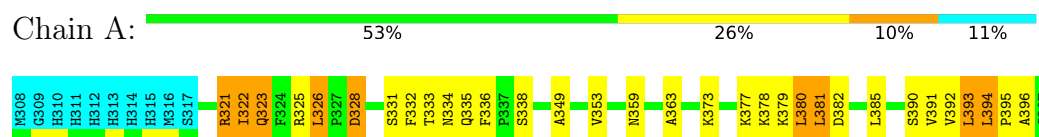
4.2.6 Score per residue for model 6

- Molecule 1: UBX domain-containing protein 4



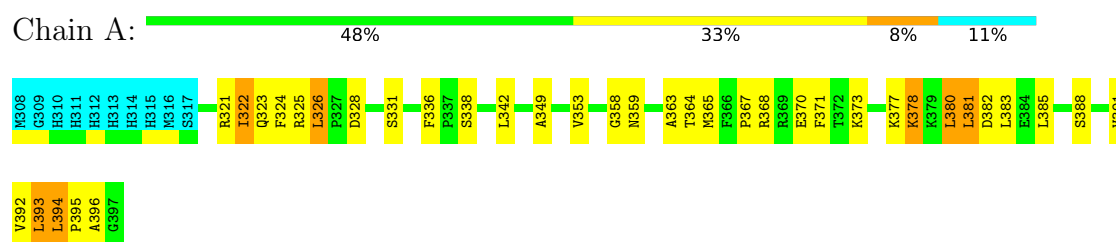
4.2.7 Score per residue for model 7

- Molecule 1: UBX domain-containing protein 4



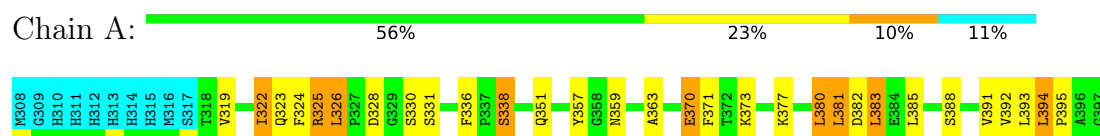
4.2.8 Score per residue for model 8

- Molecule 1: UBX domain-containing protein 4



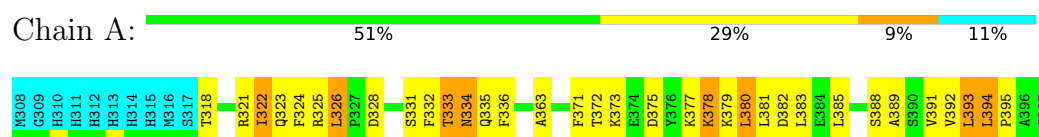
4.2.9 Score per residue for model 9 (medoid)

- Molecule 1: UBX domain-containing protein 4



4.2.10 Score per residue for model 10

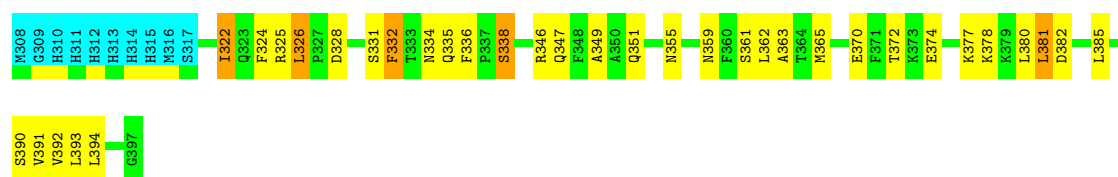
- Molecule 1: UBX domain-containing protein 4



4.2.11 Score per residue for model 11

- Molecule 1: UBX domain-containing protein 4





4.2.12 Score per residue for model 12

- Molecule 1: UBX domain-containing protein 4

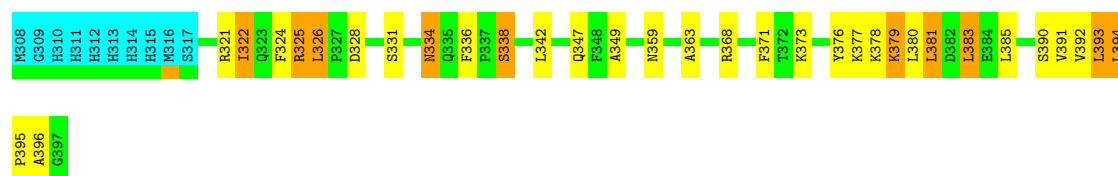
Chain A: 42% 38% 9% 11%



4.2.13 Score per residue for model 13

- Molecule 1: UBX domain-containing protein 4

Chain A: 52% 26% 11% 11%



4.2.14 Score per residue for model 14

- Molecule 1: UBX domain-containing protein 4

Chain A: 46% 37% 7% 11%



4.2.15 Score per residue for model 15

- Molecule 1: UBX domain-containing protein 4

Chain A:  59% 23% 7% 11%



4.2.16 Score per residue for model 16

- Molecule 1: UBX domain-containing protein 4

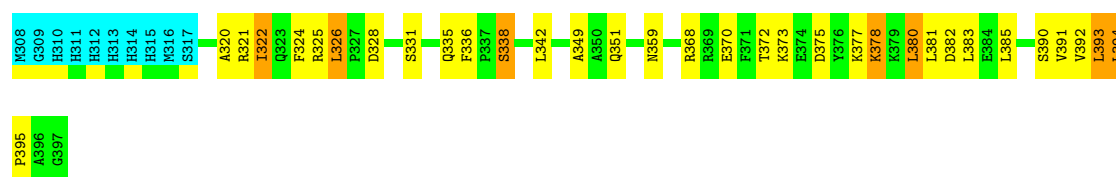
Chain A:  60% 21% 8% 11%



4.2.17 Score per residue for model 17

- Molecule 1: UBX domain-containing protein 4

Chain A:  52% 29% 8% 11%



4.2.18 Score per residue for model 18

- Molecule 1: UBX domain-containing protein 4

Chain A:  53% 30% 6% 11%



4.2.19 Score per residue for model 19

- Molecule 1: UBX domain-containing protein 4

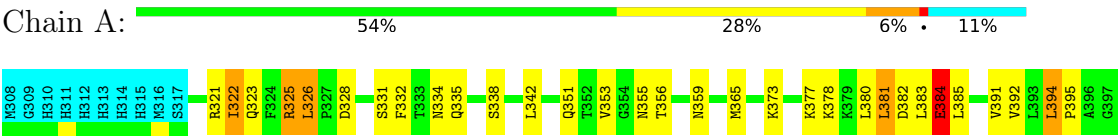
Chain A:  50% 33% 6% 11%





4.2.20 Score per residue for model 20

- Molecule 1: UBX domain-containing protein 4



5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics*.

Of the 200 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
CNS	structure solution	1.1
CNS	refinement	1.1

No chemical shift data was provided.

6 Model quality

6.1 Standard geometry

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

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	627	620	620	19±4
All	All	12540	12400	12400	382

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:322:ILE:HD12	1:A:385:LEU:HD12	1.02	1.32	16	6
1:A:322:ILE:HD11	1:A:380:LEU:HD23	0.83	1.50	8	14
1:A:380:LEU:HD23	1:A:385:LEU:HD13	0.81	1.51	15	5
1:A:380:LEU:O	1:A:385:LEU:HD23	0.77	1.78	3	6
1:A:381:LEU:HD13	1:A:382:ASP:N	0.76	1.96	20	4
1:A:338:SER:O	1:A:381:LEU:HD12	0.76	1.81	19	4
1:A:326:LEU:HD12	1:A:328:ASP:HB2	0.68	1.66	15	7
1:A:321:ARG:C	1:A:322:ILE:HD13	0.66	2.16	10	15
1:A:359:ASN:HB3	1:A:396:ALA:HB3	0.66	1.67	8	5
1:A:322:ILE:HD11	1:A:380:LEU:CD2	0.64	2.22	7	9
1:A:363:ALA:HB3	1:A:392:VAL:CG2	0.64	2.23	10	9
1:A:323:GLN:HG3	1:A:333:THR:HG23	0.64	1.68	14	7
1:A:378:LYS:HE3	1:A:383:LEU:HD11	0.63	1.68	13	1
1:A:322:ILE:HD12	1:A:385:LEU:HD22	0.63	1.69	7	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:362:LEU:HD12	1:A:376:TYR:OH	0.62	1.95	5	2
1:A:371:PHE:CE1	1:A:383:LEU:HD13	0.62	2.30	13	1
1:A:381:LEU:HD22	1:A:381:LEU:C	0.61	2.21	20	4
1:A:363:ALA:HB2	1:A:370:GLU:HA	0.60	1.72	12	1
1:A:385:LEU:HD13	1:A:389:ALA:CB	0.59	2.28	10	3
1:A:363:ALA:O	1:A:392:VAL:HG22	0.59	1.97	5	9
1:A:326:LEU:HD13	1:A:328:ASP:HB2	0.58	1.75	16	1
1:A:364:THR:HG23	1:A:367:PRO:O	0.58	1.99	3	5
1:A:325:ARG:O	1:A:393:LEU:HD13	0.58	1.99	17	3
1:A:381:LEU:HD22	1:A:381:LEU:O	0.57	1.99	20	4
1:A:338:SER:CB	1:A:381:LEU:HD23	0.57	2.30	17	4
1:A:326:LEU:HD13	1:A:357:TYR:OH	0.57	1.99	5	2
1:A:336:PHE:HB2	1:A:380:LEU:HD22	0.56	1.77	1	8
1:A:336:PHE:CE2	1:A:345:ALA:HB2	0.56	2.36	14	1
1:A:346:ARG:HG3	1:A:362:LEU:HD11	0.56	1.78	5	7
1:A:338:SER:HB3	1:A:381:LEU:HD23	0.55	1.77	17	8
1:A:380:LEU:CB	1:A:385:LEU:HD12	0.55	2.31	1	8
1:A:326:LEU:HD12	1:A:328:ASP:CB	0.55	2.31	2	8
1:A:325:ARG:C	1:A:326:LEU:HD13	0.55	2.26	13	1
1:A:380:LEU:C	1:A:385:LEU:HD23	0.55	2.27	20	1
1:A:326:LEU:HD12	1:A:328:ASP:HB3	0.54	1.78	2	2
1:A:349:ALA:O	1:A:353:VAL:HG22	0.54	2.03	8	5
1:A:324:PHE:CE2	1:A:393:LEU:HD11	0.54	2.37	17	1
1:A:381:LEU:HD12	1:A:381:LEU:O	0.54	2.03	16	12
1:A:325:ARG:C	1:A:326:LEU:HD23	0.53	2.29	9	10
1:A:381:LEU:C	1:A:381:LEU:HD12	0.52	2.30	17	7
1:A:326:LEU:HB3	1:A:393:LEU:HD22	0.52	1.82	2	1
1:A:340:ALA:O	1:A:380:LEU:HD12	0.51	2.05	1	7
1:A:326:LEU:HD13	1:A:326:LEU:N	0.51	2.21	13	1
1:A:380:LEU:HB3	1:A:385:LEU:HD12	0.51	1.82	1	5
1:A:342:LEU:O	1:A:342:LEU:HD22	0.50	2.06	6	2
1:A:336:PHE:CB	1:A:380:LEU:HD22	0.49	2.37	10	3
1:A:342:LEU:HD12	1:A:376:TYR:HA	0.48	1.84	6	2
1:A:322:ILE:CD1	1:A:380:LEU:HD23	0.48	2.38	4	5
1:A:324:PHE:CE2	1:A:349:ALA:CB	0.48	2.97	17	4
1:A:371:PHE:CE2	1:A:383:LEU:HD13	0.48	2.43	9	3
1:A:342:LEU:C	1:A:342:LEU:HD13	0.48	2.34	14	6
1:A:342:LEU:HD22	1:A:342:LEU:O	0.47	2.09	13	4
1:A:322:ILE:HD12	1:A:385:LEU:CD1	0.47	2.21	16	2
1:A:369:ARG:CZ	1:A:383:LEU:HD22	0.47	2.39	5	1
1:A:381:LEU:HD13	1:A:381:LEU:C	0.47	2.34	14	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:375:ASP:HA	1:A:378:LYS:CD	0.47	2.40	10	2
1:A:322:ILE:CD1	1:A:385:LEU:HD13	0.47	2.40	12	5
1:A:318:THR:HG22	1:A:318:THR:O	0.47	2.10	10	2
1:A:378:LYS:HD3	1:A:383:LEU:HD11	0.46	1.86	10	1
1:A:326:LEU:HD13	1:A:328:ASP:CB	0.46	2.40	12	3
1:A:342:LEU:HD13	1:A:342:LEU:C	0.46	2.36	6	8
1:A:357:TYR:CD2	1:A:393:LEU:HD21	0.46	2.46	5	1
1:A:380:LEU:O	1:A:385:LEU:HD12	0.46	2.11	15	3
1:A:320:ALA:HB3	1:A:380:LEU:HD22	0.45	1.88	17	1
1:A:378:LYS:HE2	1:A:383:LEU:HD21	0.45	1.88	20	2
1:A:380:LEU:CA	1:A:385:LEU:HD12	0.45	2.41	2	2
1:A:380:LEU:HD23	1:A:385:LEU:CD1	0.45	2.35	15	2
1:A:364:THR:HG22	1:A:369:ARG:HG2	0.45	1.88	14	2
1:A:392:VAL:O	1:A:392:VAL:HG23	0.44	2.12	12	11
1:A:336:PHE:HB2	1:A:380:LEU:CD2	0.44	2.42	2	5
1:A:393:LEU:C	1:A:395:PRO:HD3	0.44	2.37	12	14
1:A:361:SER:HB3	1:A:394:LEU:CB	0.43	2.43	12	1
1:A:338:SER:HB3	1:A:381:LEU:CD2	0.43	2.42	11	3
1:A:321:ARG:NH1	1:A:333:THR:HG21	0.43	2.29	1	1
1:A:394:LEU:N	1:A:395:PRO:CD	0.43	2.82	19	15
1:A:371:PHE:CD1	1:A:371:PHE:C	0.43	2.96	10	1
1:A:322:ILE:HD12	1:A:385:LEU:HD13	0.43	1.89	9	4
1:A:324:PHE:CE1	1:A:393:LEU:HD11	0.43	2.49	3	1
1:A:324:PHE:HB3	1:A:332:PHE:CE2	0.43	2.49	11	4
1:A:342:LEU:HA	1:A:380:LEU:HD11	0.43	1.90	20	1
1:A:378:LYS:HE3	1:A:382:ASP:HB3	0.42	1.91	1	1
1:A:334:ASN:HB3	1:A:336:PHE:CE2	0.42	2.49	13	3
1:A:336:PHE:HB3	1:A:380:LEU:HD13	0.42	1.89	10	2
1:A:342:LEU:HD13	1:A:342:LEU:O	0.42	2.15	8	1
1:A:324:PHE:CE2	1:A:393:LEU:HD13	0.42	2.49	9	2
1:A:394:LEU:N	1:A:395:PRO:HD3	0.42	2.30	12	1
1:A:384:GLU:C	1:A:385:LEU:HD22	0.41	2.39	20	1
1:A:324:PHE:CD2	1:A:349:ALA:HB2	0.41	2.50	13	1
1:A:326:LEU:HD22	1:A:357:TYR:OH	0.41	2.15	14	1
1:A:342:LEU:HD23	1:A:380:LEU:HG	0.41	1.91	20	1
1:A:364:THR:HG21	1:A:369:ARG:CZ	0.41	2.46	3	1
1:A:324:PHE:CE1	1:A:349:ALA:CB	0.41	3.03	14	1
1:A:336:PHE:HB2	1:A:380:LEU:HD21	0.41	1.91	17	1
1:A:381:LEU:HD12	1:A:381:LEU:C	0.41	2.41	18	1
1:A:320:ALA:HB3	1:A:336:PHE:O	0.41	2.16	12	1
1:A:324:PHE:CE2	1:A:393:LEU:CD1	0.41	3.03	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:353:VAL:HG21	1:A:356:THR:HG22	0.41	1.91	20	1
1:A:392:VAL:HG23	1:A:392:VAL:O	0.40	2.16	5	1
1:A:380:LEU:C	1:A:385:LEU:HD12	0.40	2.41	17	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	79/90 (88%)	70±2 (89±3%)	8±2 (11±3%)	1±1 (1±1%)	18	68
All	All	1580/1800 (88%)	1399 (89%)	169 (11%)	12 (1%)	18	68

All 7 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	355	ASN	3
1	A	370	GLU	2
1	A	384	GLU	2
1	A	358	GLY	2
1	A	318	THR	1
1	A	365	MET	1
1	A	379	LYS	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	67/76 (88%)	48±2 (71±4%)	19±2 (29±4%)	1	18
All	All	1340/1520 (88%)	951 (71%)	389 (29%)	1	18

All 46 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	322	ILE	20
1	A	331	SER	20
1	A	377	LYS	20
1	A	391	VAL	20
1	A	373	LYS	19
1	A	326	LEU	19
1	A	394	LEU	18
1	A	381	LEU	14
1	A	335	GLN	13
1	A	323	GLN	12
1	A	393	LEU	12
1	A	368	ARG	11
1	A	378	LYS	11
1	A	372	THR	11
1	A	382	ASP	11
1	A	334	ASN	10
1	A	370	GLU	10
1	A	380	LEU	10
1	A	390	SER	9
1	A	332	PHE	8
1	A	338	SER	8
1	A	351	GLN	8
1	A	365	MET	8
1	A	333	THR	7
1	A	328	ASP	7
1	A	379	LYS	7
1	A	352	THR	6
1	A	325	ARG	6
1	A	359	ASN	6
1	A	388	SER	5
1	A	321	ARG	5
1	A	383	LEU	5
1	A	361	SER	4
1	A	347	GLN	4
1	A	384	GLU	4
1	A	374	GLU	4
1	A	330	SER	3
1	A	318	THR	2
1	A	339	ASP	2
1	A	343	GLU	2
1	A	355	ASN	2

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Mol	Chain	Res	Type	Models (Total)
1	A	392	VAL	2
1	A	356	THR	1
1	A	342	LEU	1
1	A	369	ARG	1
1	A	324	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 oligosaccharides 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