



Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 07:33 AM UTC

PDB ID : 2JSW / pdb_00002jsw
Title : Solution Structure of the R13 Domain of Talin
Authors : Goult, B.T.; Gingras, A.R.; Bate, N.; Critchley, D.R.C.; Barsukov, I.L.
Deposited on : 2007-07-17

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

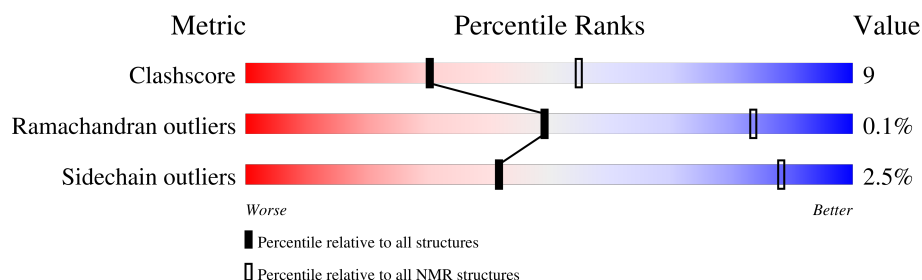
1 Overall quality at a glance

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	189	

2 Ensemble composition and analysis

This entry contains 20 models. Model 8 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:2300-A:2326, A:2340-A:2478 (166)	0.69	8

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 2 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2743 atoms, of which 1386 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Talin-1.

Mol	Chain	Residues	Atoms						Trace
1	A	189	Total	C	H	N	O	S	0
			2743	835	1386	244	274	4	

There are 6 discrepancies between the modelled and reference sequences:

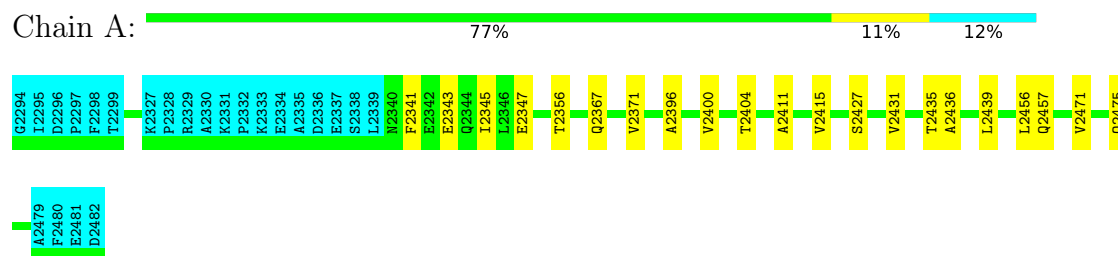
Chain	Residue	Modelled	Actual	Comment	Reference
A	2294	GLY	-	expression tag	UNP P26039
A	2295	ILE	-	expression tag	UNP P26039
A	2296	ASP	-	expression tag	UNP P26039
A	2297	PRO	-	expression tag	UNP P26039
A	2298	PHE	-	expression tag	UNP P26039
A	2299	THR	-	expression tag	UNP P26039

4 Residue-property plots

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: Talin-1

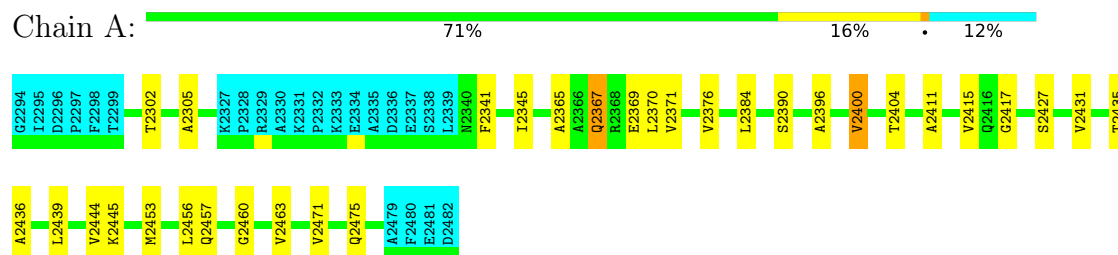


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Talin-1



4.2.2 Score per residue for model 2

- Molecule 1: Talin-1

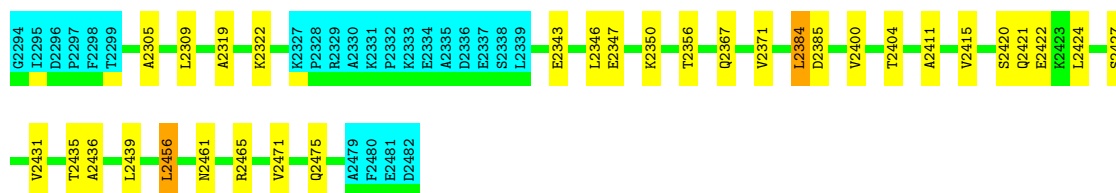




4.2.3 Score per residue for model 3

- Molecule 1: Talin-1

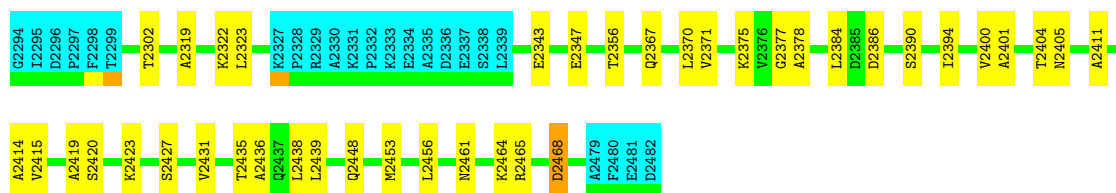
Chain A: 71% 15% 12%



4.2.4 Score per residue for model 4

- Molecule 1: Talin-1

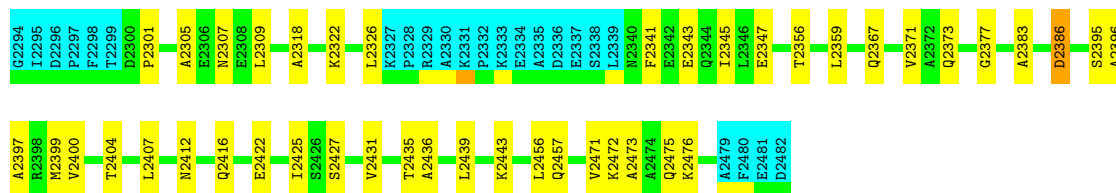
Chain A: 67% 21% 12%



4.2.5 Score per residue for model 5

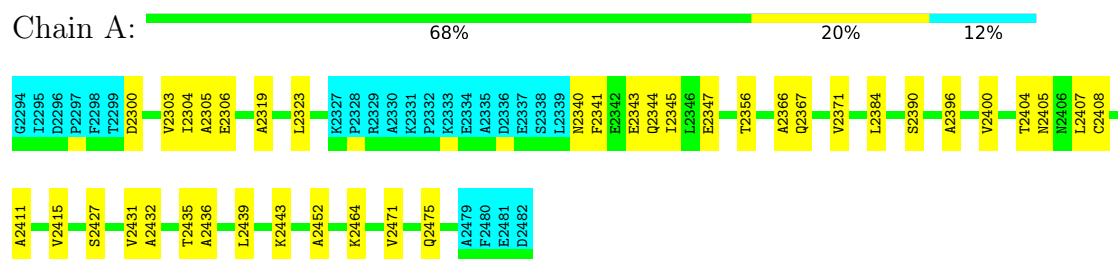
- Molecule 1: Talin-1

Chain A: 65% 22% 12%



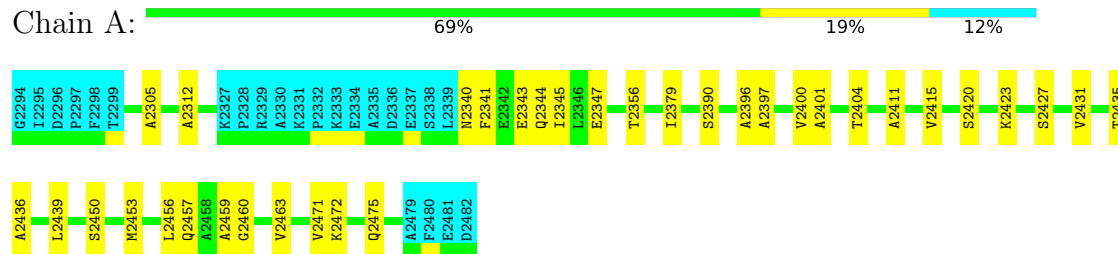
4.2.6 Score per residue for model 6

- Molecule 1: Talin-1



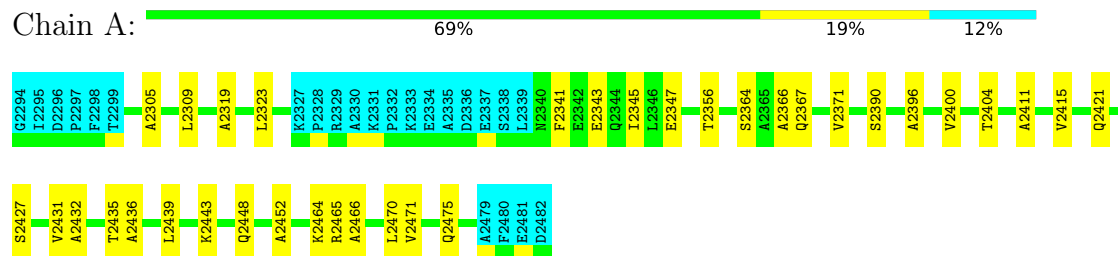
4.2.7 Score per residue for model 7

- Molecule 1: Talin-1



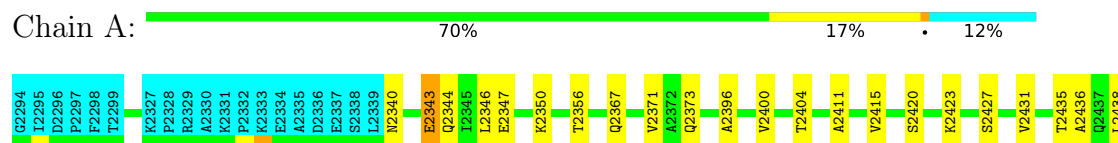
4.2.8 Score per residue for model 8 (medoid)

- Molecule 1: Talin-1



4.2.9 Score per residue for model 9

- Molecule 1: Talin-1





4.2.10 Score per residue for model 10

- Molecule 1: Talin-1

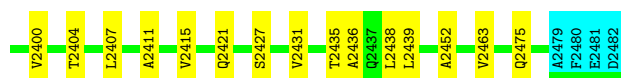
Chain A: 66% 21% 12%



4.2.11 Score per residue for model 11

- Molecule 1: Talin-1

Chain A: 68% 20% 12%



4.2.12 Score per residue for model 12

- Molecule 1: Talin-1

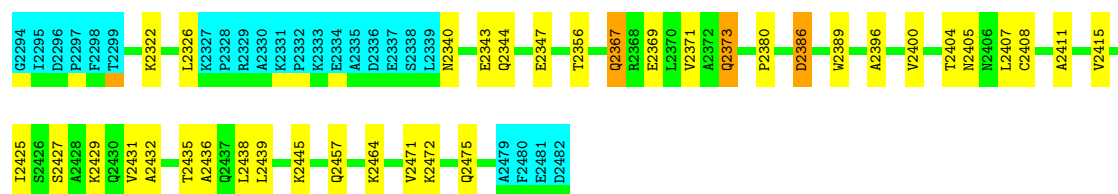
Chain A: 74% 14% 12%



4.2.13 Score per residue for model 13

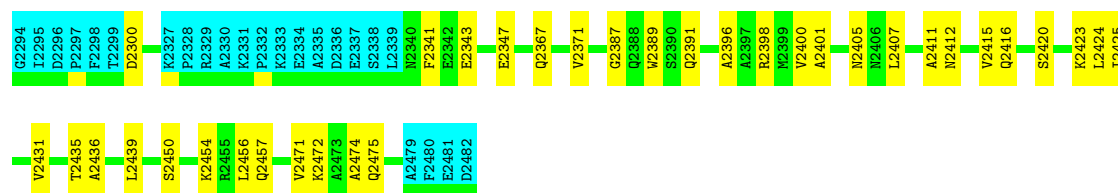
- Molecule 1: Talin-1

Chain A: 68% 18% 12%



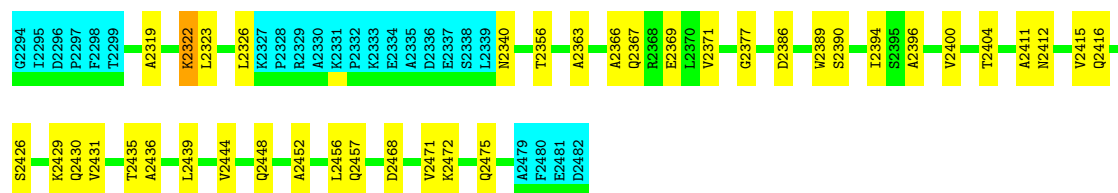
4.2.14 Score per residue for model 14

- Molecule 1: Talin-1



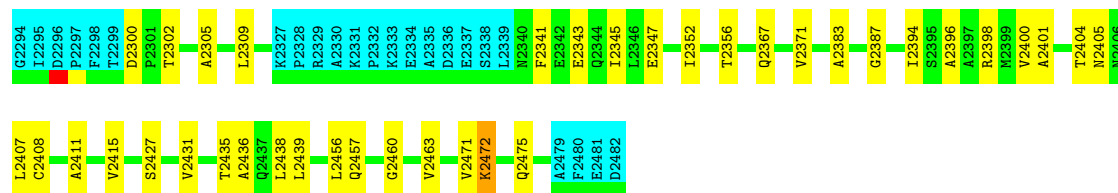
4.2.15 Score per residue for model 15

- Molecule 1: Talin-1



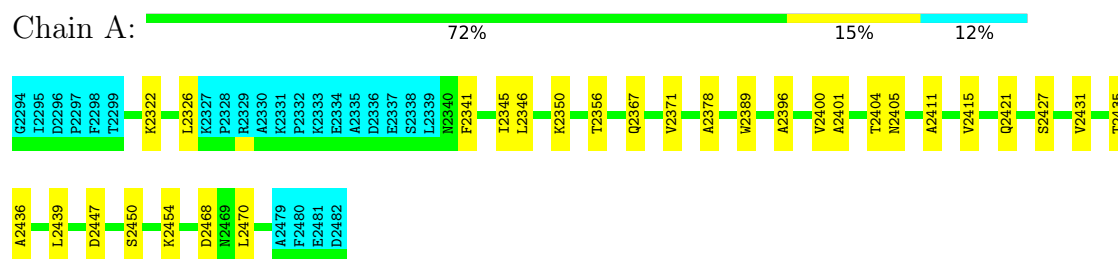
4.2.16 Score per residue for model 16

- Molecule 1: Talin-1



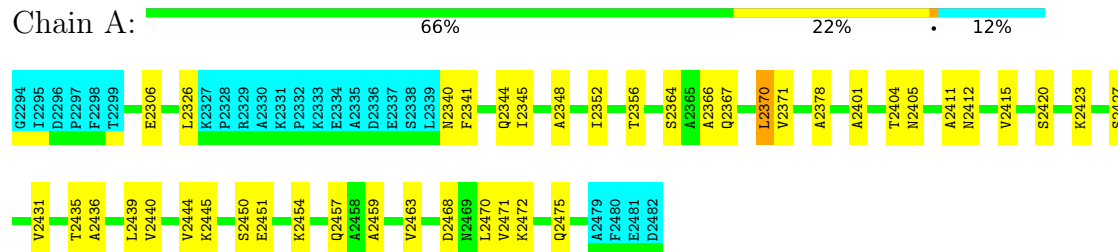
4.2.17 Score per residue for model 17

- Molecule 1: Talin-1



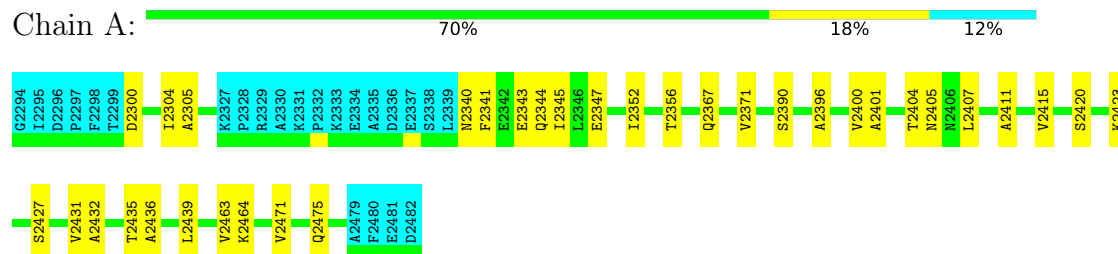
4.2.18 Score per residue for model 18

- Molecule 1: Talin-1



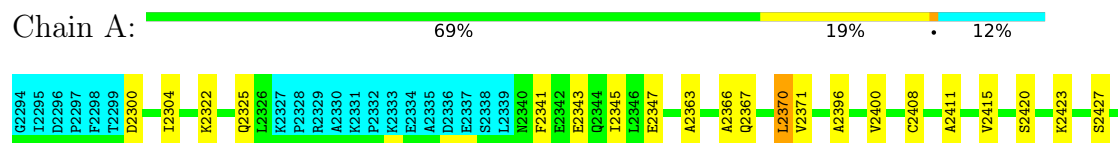
4.2.19 Score per residue for model 19

- Molecule 1: Talin-1



4.2.20 Score per residue for model 20

- Molecule 1: Talin-1



V2431	
T2435	
A2436	
Q2437	
L2438	
L2439	
S2450	
M2453	
L2456	
Q2457	
K2464	
D2468	
V2471	
K2472	
A2473	
A2474	
Q2475	
K2476	
A2479	
F2480	
E2481	
D2482	

5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
ARIA	structure solution	1.2
ARIA	refinement	1.2
CYANA	structure solution	2.1
TALOS	geometry optimization	

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	1176	1211	1211	21±3
All	All	23520	24220	24220	428

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 9.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:2377:GLY:HA3	1:A:2386:ASP:HB2	0.73	1.59	11	2
1:A:2370:LEU:HB3	1:A:2376:VAL:HB	0.63	1.71	1	1
1:A:2448:GLN:HA	1:A:2453:MET:CB	0.63	2.24	10	1
1:A:2473:ALA:O	1:A:2476:LYS:HG2	0.62	1.93	20	2
1:A:2386:ASP:HA	1:A:2445:LYS:NZ	0.62	2.10	13	1
1:A:2404:THR:HG22	1:A:2431:VAL:HG13	0.61	1.72	1	9
1:A:2473:ALA:HA	1:A:2476:LYS:HE2	0.60	1.73	5	1
1:A:2371:VAL:HG22	1:A:2378:ALA:HB2	0.60	1.72	12	1
1:A:2400:VAL:HG12	1:A:2435:THR:HA	0.59	1.74	16	12
1:A:2322:LYS:O	1:A:2326:LEU:HG	0.59	1.97	17	5
1:A:2432:ALA:HB1	1:A:2464:LYS:HD2	0.59	1.73	6	3
1:A:2439:LEU:HD23	1:A:2457:GLN:HA	0.58	1.74	18	10
1:A:2369:GLU:HG3	1:A:2452:ALA:HB2	0.58	1.74	11	1
1:A:2390:SER:O	1:A:2394:ILE:HG12	0.58	1.98	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:2305:ALA:HB2	1:A:2390:SER:HB3	0.58	1.76	10	3
1:A:2352:ILE:HG23	1:A:2463:VAL:HG13	0.58	1.76	16	3
1:A:2400:VAL:HG22	1:A:2435:THR:HA	0.58	1.75	2	2
1:A:2420:SER:HB2	1:A:2423:LYS:HG2	0.58	1.75	7	4
1:A:2436:ALA:HA	1:A:2439:LEU:HD13	0.57	1.76	2	20
1:A:2420:SER:HB2	1:A:2423:LYS:HE2	0.57	1.76	14	2
1:A:2439:LEU:HG	1:A:2456:LEU:HD22	0.57	1.76	15	2
1:A:2356:THR:HG21	1:A:2404:THR:HG21	0.57	1.76	8	16
1:A:2435:THR:HG21	1:A:2463:VAL:HG21	0.57	1.76	2	2
1:A:2448:GLN:HA	1:A:2453:MET:HB3	0.57	1.77	4	2
1:A:2305:ALA:HB2	1:A:2390:SER:HB2	0.56	1.77	19	3
1:A:2367:GLN:O	1:A:2371:VAL:HG23	0.56	2.00	8	17
1:A:2343:GLU:O	1:A:2347:GLU:HG2	0.55	2.01	5	16
1:A:2396:ALA:O	1:A:2400:VAL:HG13	0.55	2.01	5	14
1:A:2319:ALA:HA	1:A:2322:LYS:HE3	0.55	1.77	3	1
1:A:2447:ASP:HB3	1:A:2450:SER:OG	0.55	2.02	17	2
1:A:2377:GLY:CA	1:A:2386:ASP:HB2	0.54	2.32	11	1
1:A:2341:PHE:O	1:A:2345:ILE:HG12	0.54	2.03	19	13
1:A:2439:LEU:HG	1:A:2456:LEU:CD2	0.53	2.33	4	12
1:A:2432:ALA:HB1	1:A:2464:LYS:HG2	0.53	1.79	13	1
1:A:2421:GLN:HE21	1:A:2475:GLN:HA	0.53	1.63	3	1
1:A:2450:SER:HB3	1:A:2453:MET:SD	0.53	2.44	20	2
1:A:2425:ILE:HG23	1:A:2471:VAL:HG13	0.53	1.81	5	2
1:A:2472:LYS:HA	1:A:2475:GLN:HE21	0.53	1.64	16	2
1:A:2400:VAL:CG1	1:A:2435:THR:HA	0.52	2.34	5	14
1:A:2371:VAL:HG13	1:A:2378:ALA:HB1	0.52	1.81	11	4
1:A:2443:LYS:HE2	1:A:2448:GLN:HG2	0.52	1.81	8	1
1:A:2366:ALA:HA	1:A:2452:ALA:HB1	0.52	1.80	15	3
1:A:2450:SER:OG	1:A:2453:MET:HB3	0.52	2.05	7	1
1:A:2412:ASN:O	1:A:2416:GLN:HG2	0.52	2.04	5	4
1:A:2411:ALA:O	1:A:2415:VAL:HG23	0.51	2.06	18	19
1:A:2427:SER:O	1:A:2431:VAL:HG23	0.51	2.06	11	17
1:A:2465:ARG:HD3	1:A:2466:ALA:N	0.51	2.20	8	1
1:A:2384:LEU:HD13	1:A:2385:ASP:H	0.51	1.64	3	1
1:A:2471:VAL:O	1:A:2475:GLN:HG3	0.51	2.06	18	15
1:A:2366:ALA:O	1:A:2370:LEU:HD22	0.50	2.06	18	2
1:A:2371:VAL:HG13	1:A:2378:ALA:CB	0.50	2.36	10	2
1:A:2356:THR:HG22	1:A:2435:THR:HG21	0.49	1.82	12	5
1:A:2319:ALA:O	1:A:2322:LYS:HG2	0.49	2.07	3	1
1:A:2345:ILE:HG23	1:A:2470:LEU:HD11	0.49	1.84	17	3
1:A:2320:ALA:O	1:A:2324:GLU:HG3	0.49	2.08	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:2405:ASN:O	1:A:2408:CYS:HB3	0.48	2.08	13	3
1:A:2450:SER:O	1:A:2454:LYS:HG2	0.48	2.08	18	2
1:A:2407:LEU:HB2	1:A:2431:VAL:HG21	0.48	1.84	19	7
1:A:2435:THR:CG2	1:A:2463:VAL:HG21	0.48	2.39	2	1
1:A:2305:ALA:O	1:A:2309:LEU:HG	0.48	2.09	11	5
1:A:2340:ASN:O	1:A:2344:GLN:HG3	0.48	2.09	18	7
1:A:2352:ILE:HD12	1:A:2407:LEU:HD21	0.48	1.86	16	1
1:A:2401:ALA:O	1:A:2405:ASN:HB2	0.47	2.08	14	7
1:A:2301:PRO:HG3	1:A:2383:ALA:HA	0.47	1.85	10	2
1:A:2375:LYS:HG3	1:A:2447:ASP:HB2	0.47	1.86	2	1
1:A:2300:ASP:O	1:A:2304:ILE:HG12	0.47	2.09	20	2
1:A:2439:LEU:HD11	1:A:2460:GLY:HA3	0.47	1.86	7	1
1:A:2322:LYS:HB2	1:A:2322:LYS:NZ	0.47	2.25	15	1
1:A:2453:MET:SD	1:A:2453:MET:N	0.47	2.87	20	1
1:A:2440:VAL:O	1:A:2444:VAL:HG23	0.47	2.10	18	1
1:A:2400:VAL:HG11	1:A:2438:LEU:HB2	0.47	1.86	20	6
1:A:2425:ILE:O	1:A:2429:LYS:HG3	0.47	2.08	13	1
1:A:2367:GLN:HG2	1:A:2389:TRP:CH2	0.47	2.45	17	2
1:A:2439:LEU:HD21	1:A:2460:GLY:HA3	0.47	1.86	16	5
1:A:2346:LEU:HG	1:A:2350:LYS:HE3	0.46	1.86	17	3
1:A:2384:LEU:HD22	1:A:2385:ASP:N	0.46	2.26	3	1
1:A:2407:LEU:HD22	1:A:2431:VAL:HG21	0.46	1.87	6	2
1:A:2303:VAL:HA	1:A:2306:GLU:HG2	0.46	1.86	6	1
1:A:2387:GLY:O	1:A:2391:GLN:HB2	0.46	2.11	14	1
1:A:2439:LEU:CD2	1:A:2457:GLN:HA	0.46	2.39	15	4
1:A:2396:ALA:O	1:A:2400:VAL:HG23	0.46	2.11	14	1
1:A:2444:VAL:O	1:A:2445:LYS:HB2	0.45	2.10	1	1
1:A:2366:ALA:HA	1:A:2452:ALA:CB	0.45	2.42	6	1
1:A:2439:LEU:HG	1:A:2456:LEU:HD23	0.45	1.88	7	5
1:A:2318:ALA:O	1:A:2322:LYS:HG3	0.45	2.11	5	1
1:A:2394:ILE:O	1:A:2398:ARG:HD3	0.45	2.12	16	2
1:A:2376:VAL:HG23	1:A:2445:LYS:HG2	0.45	1.88	1	1
1:A:2461:ASN:O	1:A:2465:ARG:HG3	0.45	2.12	4	2
1:A:2389:TRP:CD1	1:A:2444:VAL:HB	0.45	2.47	15	1
1:A:2363:ALA:O	1:A:2367:GLN:HG3	0.44	2.13	20	2
1:A:2389:TRP:CG	1:A:2445:LYS:HD2	0.44	2.46	13	1
1:A:2370:LEU:CD1	1:A:2375:LYS:HB2	0.44	2.43	2	1
1:A:2420:SER:O	1:A:2424:LEU:HB2	0.44	2.11	3	1
1:A:2421:GLN:OE1	1:A:2475:GLN:HA	0.44	2.12	11	1
1:A:2370:LEU:HG	1:A:2445:LYS:O	0.44	2.12	18	1
1:A:2359:LEU:HD12	1:A:2456:LEU:HD12	0.43	1.89	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:2443:LYS:HB2	1:A:2453:MET:HE2	0.43	1.90	9	1
1:A:2341:PHE:CE1	1:A:2474:ALA:HA	0.43	2.48	14	1
1:A:2348:ALA:O	1:A:2352:ILE:HG13	0.43	2.14	2	2
1:A:2306:GLU:HG3	1:A:2364:SER:OG	0.43	2.14	18	2
1:A:2400:VAL:HG21	1:A:2438:LEU:HB2	0.43	1.91	2	1
1:A:2395:SER:O	1:A:2399:MET:HB2	0.43	2.14	5	1
1:A:2302:THR:OG1	1:A:2378:ALA:HA	0.42	2.14	10	1
1:A:2369:GLU:O	1:A:2373:GLN:HB3	0.42	2.14	13	1
1:A:2426:SER:O	1:A:2430:GLN:HG2	0.42	2.14	15	1
1:A:2448:GLN:HA	1:A:2453:MET:HB2	0.42	1.89	10	1
1:A:2305:ALA:HB2	1:A:2390:SER:OG	0.42	2.14	1	1
1:A:2322:LYS:HD2	1:A:2408:CYS:SG	0.42	2.55	20	1
1:A:2390:SER:O	1:A:2394:ILE:HG13	0.42	2.14	11	2
1:A:2312:ALA:HB1	1:A:2401:ALA:HB2	0.42	1.90	7	1
1:A:2459:ALA:O	1:A:2463:VAL:HG23	0.42	2.15	7	2
1:A:2323:LEU:HD11	1:A:2408:CYS:SG	0.42	2.54	10	1
1:A:2370:LEU:HD11	1:A:2375:LYS:HB2	0.42	1.91	2	1
1:A:2421:GLN:NE2	1:A:2475:GLN:HA	0.42	2.29	3	1
1:A:2473:ALA:O	1:A:2476:LYS:HB2	0.42	2.14	9	1
1:A:2300:ASP:O	1:A:2304:ILE:HG13	0.42	2.15	19	1
1:A:2420:SER:HB3	1:A:2423:LYS:HG2	0.42	1.91	19	2
1:A:2370:LEU:HG	1:A:2375:LYS:HB3	0.42	1.92	4	1
1:A:2443:LYS:NZ	1:A:2443:LYS:HB3	0.41	2.30	6	1
1:A:2397:ALA:O	1:A:2400:VAL:HG22	0.41	2.15	7	2
1:A:2422:GLU:H	1:A:2422:GLU:CD	0.41	2.22	3	2
1:A:2377:GLY:C	1:A:2379:ILE:H	0.41	2.22	10	1
1:A:2304:ILE:HA	1:A:2307:ASN:ND2	0.41	2.31	12	1
1:A:2383:ALA:O	1:A:2387:GLY:HA3	0.41	2.16	16	1
1:A:2377:GLY:H	1:A:2386:ASP:CG	0.41	2.23	5	2
1:A:2319:ALA:O	1:A:2323:LEU:HD13	0.41	2.16	6	2
1:A:2356:THR:HG21	1:A:2404:THR:CG2	0.41	2.46	11	1
1:A:2341:PHE:CE1	1:A:2345:ILE:HD11	0.41	2.51	6	1
1:A:2319:ALA:O	1:A:2323:LEU:HG	0.41	2.16	8	2
1:A:2379:ILE:N	1:A:2379:ILE:HD12	0.41	2.30	7	1
1:A:2326:LEU:HD21	1:A:2412:ASN:ND2	0.41	2.31	18	1
1:A:2365:ALA:O	1:A:2369:GLU:HG2	0.41	2.16	1	1
1:A:2451:GLU:O	1:A:2455:ARG:HD3	0.41	2.16	2	1
1:A:2414:ALA:HA	1:A:2419:ALA:HB2	0.40	1.93	4	1
1:A:2464:LYS:O	1:A:2468:ASP:HB2	0.40	2.16	4	1
1:A:2370:LEU:HD12	1:A:2375:LYS:HB2	0.40	1.92	11	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	166/189 (88%)	163±1 (98±1%)	2±1 (2±1%)	0±0 (0±0%)	49	83
All	All	3320/3780 (88%)	3268 (98%)	50 (2%)	2 (0%)	49	83

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
1	A	2340	ASN	2

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	112/131 (85%)	109±2 (98±2%)	3±2 (2±2%)	42	88
All	All	2240/2620 (85%)	2185 (98%)	55 (2%)	42	88

All 28 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	2472	LYS	8
1	A	2384	LEU	5
1	A	2468	ASP	5
1	A	2302	THR	4
1	A	2373	GLN	3
1	A	2367	GLN	2
1	A	2456	LEU	2
1	A	2322	LYS	2
1	A	2386	ASP	2
1	A	2421	GLN	2

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Mol	Chain	Res	Type	Models (Total)
1	A	2470	LEU	2
1	A	2370	LEU	2
1	A	2400	VAL	1
1	A	2453	MET	1
1	A	2408	CYS	1
1	A	2307	ASN	1
1	A	2443	LYS	1
1	A	2364	SER	1
1	A	2343	GLU	1
1	A	2398	ARG	1
1	A	2424	LEU	1
1	A	2369	GLU	1
1	A	2429	LYS	1
1	A	2448	GLN	1
1	A	2454	LYS	1
1	A	2451	GLU	1
1	A	2325	GLN	1
1	A	2464	LYS	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 ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided