Full wwPDB NMR Structure Validation Report (i)

Apr 11, 2024 – 04:07 PM EDT

PDB ID	:	1KBF
BMRB ID	:	5203
Title	:	Solution Structure of the Cysteine-Rich C1 Domain of Kinase Suppressor of Ras
Authors	:	Zhou, M.; Horita, D.A.; Waugh, D.S.; Byrd, R.A.; Morrison, D.K.
Deposited on	:	2001-11-06

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 (i) 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 (i)) were used in the production of this report:

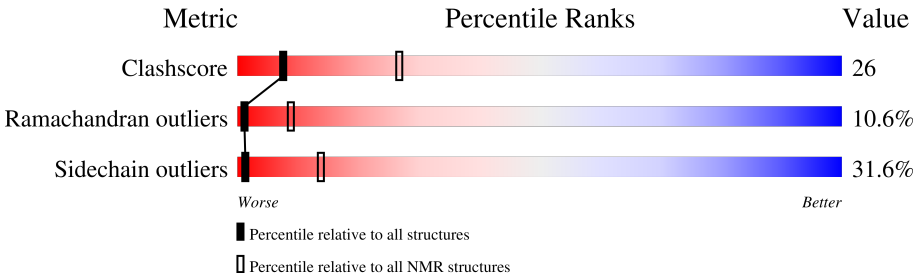
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.1

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 is 69%.

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	49	27% 47% 8% • 16%

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 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:334-A:340, A:344-A:377 (41)	0.68	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 3 single-model clusters were found.

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 778 atoms, of which 392 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Kinase suppressor of Ras 1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	49	776	236	392	76	64	8	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	330	GLY	-	expression tag	UNP Q61097

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	
			Total	Zn
2	A	2	2	2

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: Kinase suppressor of Ras 1

Chain A: 27% 47% 8% • 16%

G330 S331 V332 T333 H334 R335 F336 S337 W341 L342 S343 Q344 V345 C346 N347 V348 C349 Q350 K351 S352 M353 I354 F355 G356 V357 K358 C359 K360 H361 C362 R363 C366 H367 N368 K369 C370 T371 K372 E373 A374 C377 R378

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: Kinase suppressor of Ras 1

Chain A: 51% 22% 8% • 16%

G330 S331 V332 T333 H334 R335 F336 S337 W341 L342 S343 C346 Q350 M353 I354 F355 G356 V357 K358 C359 K360 H361 C362 C366 H367 N368 K369 C377 R378

4.2.2 Score per residue for model 2

• Molecule 1: Kinase suppressor of Ras 1

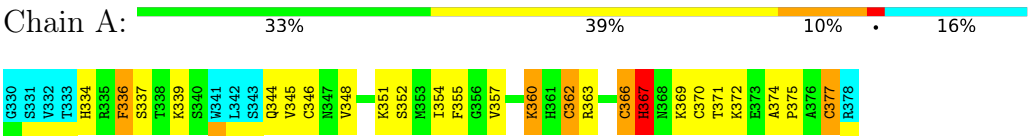
Chain A: 37% 35% 10% • 16%

G330 S331 V332 T333 H334 R335 F336 S337 T338 W341 L342 S343 Q344 V345 C346 N347 V348 C349 Q350 K351 S352 M353 V357 K358 C359 K360 H361 C362 K365 C366 H367 N368 K369 C370 T371 K372 E373 A374 R378

4.2.3 Score per residue for model 3

- Molecule 1: Kinase suppressor of Ras 1

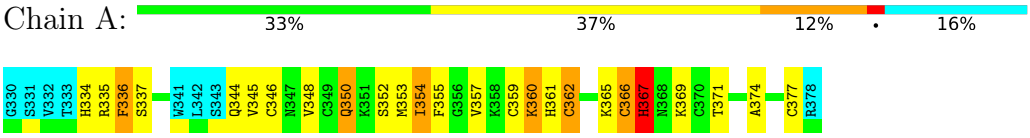
Chain A:



4.2.4 Score per residue for model 4

- Molecule 1: Kinase suppressor of Ras 1

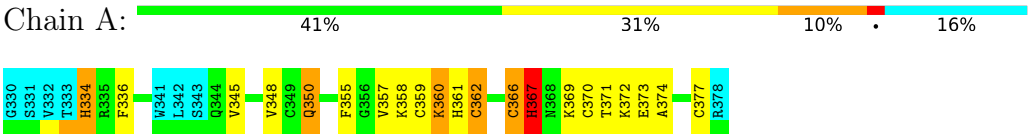
Chain A:



4.2.5 Score per residue for model 5 (medoid)

- Molecule 1: Kinase suppressor of Ras 1

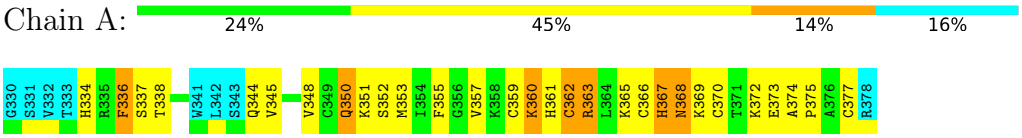
Chain A:



4.2.6 Score per residue for model 6

- Molecule 1: Kinase suppressor of Ras 1

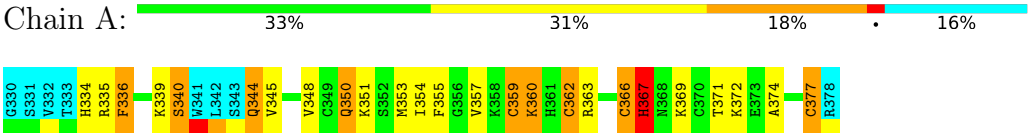
Chain A:



4.2.7 Score per residue for model 7

- Molecule 1: Kinase suppressor of Ras 1

Chain A:



4.2.8 Score per residue for model 8

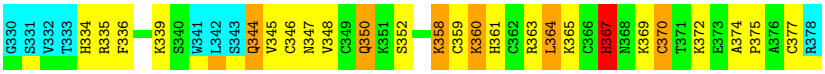
- Molecule 1: Kinase suppressor of Ras 1

Chain A: 37% 29% 14% • 16%

4.2.9 Score per residue for model 9

- Molecule 1: Kinase suppressor of Ras 1

Chain A: 33% 37% 12% • 16%



4.2.10 Score per residue for model 10

- Molecule 1: Kinase suppressor of Ras 1

Chain A: 27% 41% 12% • 16%

4.2.11 Score per residue for model 11

- Molecule 1: Kinase suppressor of Ras 1

Chain A: 39% 31% 14% 16%

4.2.12 Score per residue for model 12

- Molecule 1: Kinase suppressor of Ras 1

Chain A: 20% 45% 16% • 16%

4.2.13 Score per residue for model 13

- Molecule 1: Kinase suppressor of Ras 1

Chain A: 39% 27% 18% 16%

4.2.14 Score per residue for model 14

- Molecule 1: Kinase suppressor of Ras 1

Chain A: 33% 33% 18% 16%

4.2.15 Score per residue for model 15

- Molecule 1: Kinase suppressor of Ras 1

Chain A: 33% 35% 16% 16%

4.2.16 Score per residue for model 16

- Molecule 1: Kinase suppressor of Ras 1

Chain A: 35% 33% 14% • 16%

4.2.17 Score per residue for model 17

- Molecule 1: Kinase suppressor of Ras 1

Chain A: 39% 31% 10% • 16%

4.2.18 Score per residue for model 18

- Molecule 1: Kinase suppressor of Ras 1

Chain A: 31% 39% 14% 16%

G330 S331 V332 T333 H334 R335 F336 W341 L342 S343 Q344 V345 C346 N347 V348 C349 Q350 K351 S352 M353 I354 F355 G356 V357 K358 C359 K360 H361 C362 R363 L364 K365 C366 H367 N368 K369 C370 T371 A374 P375 A376 C377 R378

4.2.19 Score per residue for model 19

- Molecule 1: Kinase suppressor of Ras 1

Chain A: 31% 37% 12% • 16%

G330 S331 V332 T333 H334 R335 F336 W341 L342 S343 Q344 V345 C346 N347 Q350 K351 S352 M353 I354 F355 G356 V357 K358 C359 K360 H361 C362 R363 C366 H367 N368 K369 C370 T371 A374 P375 A376 C377 R378

4.2.20 Score per residue for model 20

- Molecule 1: Kinase suppressor of Ras 1

Chain A: 35% 33% 12% • 16%

G330 S331 V332 T333 H334 R335 F336 S337 W341 L342 S343 Q344 V345 V348 C349 Q350 K351 S352 M353 I354 F355 G356 V357 K358 C359 K360 H361 C362 R363 L364 K365 C366 H367 K372 E373 A374 C377 R378

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *molecular 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	refinement	1.0

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	452
Number of shifts mapped to atoms	452
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	69%

6 Model quality (i)

6.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	320	327	326	17±4
All	All	6440	6540	6520	335

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 26.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:348:VAL:HG21	1:A:374:ALA:HB2	0.90	1.41	7	9
1:A:357:VAL:HG22	1:A:366:CYS:O	0.84	1.72	14	15
1:A:336:PHE:CE1	1:A:357:VAL:HG23	0.79	2.13	13	13
1:A:374:ALA:HB1	1:A:375:PRO:HD2	0.73	1.60	16	8
1:A:338:THR:HA	1:A:357:VAL:HG12	0.73	1.61	14	4
1:A:357:VAL:HG21	1:A:366:CYS:O	0.70	1.85	16	1
1:A:369:LYS:HG3	1:A:371:THR:HG22	0.70	1.63	18	1
1:A:345:VAL:HG12	1:A:350:GLN:HA	0.69	1.62	2	6
1:A:348:VAL:HG22	1:A:374:ALA:HB2	0.68	1.64	16	5
1:A:366:CYS:O	1:A:368:ASN:N	0.67	2.28	16	2
1:A:348:VAL:CG2	1:A:374:ALA:HB2	0.65	2.21	14	13
1:A:354:ILE:HG23	1:A:354:ILE:O	0.65	1.91	12	8

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:345:VAL:HG22	1:A:350:GLN:HA	0.64	1.70	10	6
1:A:348:VAL:HG11	1:A:373:GLU:HB2	0.62	1.69	13	1
1:A:357:VAL:HG23	1:A:366:CYS:O	0.62	1.94	10	1
1:A:348:VAL:HG21	1:A:374:ALA:CB	0.62	2.25	12	1
1:A:359:CYS:O	1:A:363:ARG:N	0.61	2.34	18	4
1:A:337:SER:O	1:A:357:VAL:HA	0.61	1.96	12	6
1:A:348:VAL:CG1	1:A:374:ALA:HB2	0.60	2.26	3	4
1:A:345:VAL:HG23	1:A:353:MET:CE	0.60	2.26	14	1
1:A:338:THR:OG1	1:A:357:VAL:HG12	0.60	1.96	12	1
1:A:348:VAL:HG11	1:A:374:ALA:HB2	0.59	1.74	18	2
1:A:336:PHE:CD1	1:A:357:VAL:HG23	0.58	2.33	6	4
1:A:368:ASN:O	1:A:369:LYS:HB2	0.57	1.99	15	1
1:A:369:LYS:HD2	1:A:371:THR:HG23	0.57	1.75	12	2
1:A:348:VAL:HG11	1:A:373:GLU:CB	0.56	2.30	13	1
1:A:360:LYS:N	1:A:360:LYS:HE3	0.56	2.15	19	1
1:A:345:VAL:HG23	1:A:353:MET:HE1	0.56	1.76	14	1
1:A:374:ALA:HB1	1:A:375:PRO:CD	0.56	2.29	16	1
1:A:364:LEU:HD23	1:A:366:CYS:SG	0.55	2.41	20	1
1:A:360:LYS:N	1:A:360:LYS:CD	0.55	2.70	9	2
1:A:360:LYS:N	1:A:360:LYS:HE2	0.54	2.17	20	1
1:A:346:CYS:CB	1:A:367:HIS:CE1	0.54	2.91	15	3
1:A:363:ARG:O	1:A:363:ARG:CG	0.53	2.57	10	3
1:A:345:VAL:HG13	1:A:351:LYS:O	0.53	2.03	12	6
1:A:363:ARG:O	1:A:363:ARG:HG3	0.53	2.03	10	3
1:A:345:VAL:HG12	1:A:350:GLN:CA	0.53	2.34	2	3
1:A:334:HIS:CD2	1:A:334:HIS:N	0.53	2.76	4	13
1:A:336:PHE:CD1	1:A:357:VAL:HB	0.52	2.39	10	6
1:A:367:HIS:O	1:A:369:LYS:N	0.52	2.41	16	1
1:A:348:VAL:HG11	1:A:370:CYS:O	0.51	2.05	6	1
1:A:338:THR:HG21	1:A:355:PHE:CD2	0.51	2.41	12	1
1:A:346:CYS:HB2	1:A:367:HIS:CE1	0.51	2.40	16	3
1:A:360:LYS:HD3	1:A:360:LYS:N	0.51	2.20	18	1
1:A:353:MET:HG3	1:A:367:HIS:NE2	0.49	2.23	18	2
1:A:353:MET:CE	1:A:367:HIS:NE2	0.49	2.75	17	1
1:A:348:VAL:HG11	1:A:374:ALA:N	0.49	2.22	4	4
1:A:336:PHE:CE1	1:A:359:CYS:HB3	0.48	2.43	15	9
1:A:351:LYS:O	1:A:352:SER:C	0.48	2.51	14	1
1:A:358:LYS:O	1:A:358:LYS:HG2	0.48	2.09	19	2
1:A:364:LEU:HD22	1:A:377:CYS:HA	0.48	1.84	16	1
1:A:336:PHE:CZ	1:A:359:CYS:CB	0.48	2.97	20	2
1:A:354:ILE:O	1:A:354:ILE:CG2	0.48	2.62	17	8

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:348:VAL:HG13	1:A:374:ALA:HB2	0.48	1.84	9	2
1:A:348:VAL:HG21	1:A:370:CYS:HB3	0.48	1.85	16	1
1:A:355:PHE:CB	1:A:367:HIS:CD2	0.47	2.98	6	7
1:A:336:PHE:CE1	1:A:359:CYS:N	0.47	2.82	2	4
1:A:357:VAL:HG22	1:A:367:HIS:O	0.47	2.10	18	1
1:A:366:CYS:O	1:A:367:HIS:O	0.47	2.33	18	4
1:A:359:CYS:O	1:A:363:ARG:CA	0.46	2.64	20	3
1:A:357:VAL:CG2	1:A:366:CYS:O	0.46	2.62	16	1
1:A:336:PHE:CZ	1:A:359:CYS:HB3	0.46	2.45	20	11
1:A:334:HIS:N	1:A:334:HIS:CD2	0.46	2.82	18	5
1:A:360:LYS:N	1:A:360:LYS:CE	0.46	2.79	20	1
1:A:334:HIS:CE1	1:A:362:CYS:SG	0.46	3.09	2	7
1:A:334:HIS:CE1	1:A:361:HIS:CB	0.46	2.99	13	3
1:A:367:HIS:HB2	1:A:370:CYS:HB2	0.46	1.87	16	1
1:A:369:LYS:N	1:A:369:LYS:CD	0.46	2.79	16	1
1:A:336:PHE:CE2	1:A:359:CYS:HB3	0.45	2.47	16	1
1:A:369:LYS:HZ3	1:A:371:THR:CB	0.45	2.24	11	1
1:A:346:CYS:SG	1:A:367:HIS:CG	0.45	3.09	12	1
1:A:348:VAL:HG11	1:A:370:CYS:HB3	0.45	1.87	9	2
1:A:360:LYS:C	1:A:362:CYS:H	0.45	2.15	1	15
1:A:338:THR:CA	1:A:357:VAL:HG12	0.45	2.39	6	2
1:A:358:LYS:HA	1:A:364:LEU:O	0.45	2.11	10	3
1:A:357:VAL:N	1:A:366:CYS:O	0.45	2.50	1	3
1:A:357:VAL:HG13	1:A:367:HIS:O	0.45	2.12	11	1
1:A:357:VAL:HG23	1:A:366:CYS:SG	0.45	2.52	18	1
1:A:359:CYS:O	1:A:363:ARG:HA	0.45	2.12	9	3
1:A:336:PHE:CE1	1:A:359:CYS:CB	0.44	3.00	20	1
1:A:344:GLN:N	1:A:354:ILE:HD11	0.44	2.27	8	1
1:A:346:CYS:HB3	1:A:367:HIS:CE1	0.44	2.48	15	1
1:A:348:VAL:HG13	1:A:373:GLU:O	0.44	2.13	6	1
1:A:353:MET:HG3	1:A:367:HIS:HE2	0.44	1.73	11	1
1:A:362:CYS:O	1:A:363:ARG:CB	0.44	2.66	17	5
1:A:362:CYS:O	1:A:363:ARG:CG	0.43	2.66	10	1
1:A:351:LYS:O	1:A:351:LYS:HG2	0.43	2.13	14	1
1:A:345:VAL:HG23	1:A:351:LYS:O	0.43	2.14	3	1
1:A:360:LYS:O	1:A:362:CYS:N	0.43	2.51	7	4
1:A:346:CYS:HB2	1:A:367:HIS:CD2	0.42	2.49	18	1
1:A:369:LYS:O	1:A:371:THR:N	0.42	2.52	18	2
1:A:357:VAL:CG2	1:A:367:HIS:O	0.42	2.68	10	1
1:A:353:MET:CG	1:A:354:ILE:N	0.42	2.83	12	1
1:A:346:CYS:CB	1:A:367:HIS:ND1	0.42	2.82	3	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:366:CYS:SG	1:A:371:THR:HG23	0.42	2.54	16	1
1:A:348:VAL:HG12	1:A:373:GLU:HB3	0.41	1.92	5	1
1:A:346:CYS:O	1:A:350:GLN:CA	0.41	2.69	2	1
1:A:357:VAL:HG22	1:A:366:CYS:C	0.41	2.35	11	1
1:A:348:VAL:HG22	1:A:374:ALA:CB	0.41	2.41	16	1
1:A:353:MET:HE1	1:A:367:HIS:CD2	0.41	2.50	17	1
1:A:348:VAL:CG1	1:A:373:GLU:CB	0.41	2.99	20	1
1:A:353:MET:SD	1:A:367:HIS:CD2	0.41	3.14	12	1
1:A:355:PHE:HB2	1:A:367:HIS:CD2	0.41	2.51	20	5
1:A:354:ILE:O	1:A:355:PHE:CD1	0.41	2.74	18	2
1:A:355:PHE:CD2	1:A:368:ASN:HB3	0.41	2.51	12	1
1:A:347:ASN:HB2	1:A:365:LYS:O	0.41	2.16	14	1
1:A:334:HIS:ND1	1:A:361:HIS:CB	0.41	2.84	18	1
1:A:334:HIS:CE1	1:A:361:HIS:HB3	0.40	2.51	9	1
1:A:334:HIS:CE1	1:A:377:CYS:SG	0.40	3.15	9	1
1:A:334:HIS:CE1	1:A:377:CYS:O	0.40	2.75	13	1
1:A:359:CYS:O	1:A:359:CYS:SG	0.40	2.79	19	1
1:A:368:ASN:C	1:A:369:LYS:CD	0.40	2.89	2	1
1:A:349:CYS:O	1:A:350:GLN:CG	0.40	2.69	12	1
1:A:367:HIS:O	1:A:368:ASN:C	0.40	2.59	2	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	41/49 (84%)	26±2 (62±5%)	11±2 (27±4%)	4±1 (11±3%)	1 9
All	All	820/980 (84%)	512 (62%)	221 (27%)	87 (11%)	1 9

All 14 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	350	GLN	18
1	A	367	HIS	18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	344	GLN	10
1	A	370	CYS	8
1	A	352	SER	8
1	A	363	ARG	6
1	A	369	LYS	4
1	A	377	CYS	3
1	A	346	CYS	3
1	A	368	ASN	2
1	A	348	VAL	2
1	A	360	LYS	2
1	A	361	HIS	2
1	A	376	ALA	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	38/45 (84%)	26±2 (68±6%)	12±2 (32±6%)	1 14
All	All	760/900 (84%)	520 (68%)	240 (32%)	1 14

All 30 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	336	PHE	20
1	A	360	LYS	20
1	A	362	CYS	18
1	A	367	HIS	16
1	A	353	MET	15
1	A	377	CYS	15
1	A	372	LYS	13
1	A	344	GLN	10
1	A	369	LYS	9
1	A	365	LYS	9
1	A	370	CYS	9
1	A	371	THR	9
1	A	361	HIS	9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	363	ARG	8
1	A	358	LYS	7
1	A	337	SER	6
1	A	359	CYS	6
1	A	351	LYS	6
1	A	366	CYS	5
1	A	335	ARG	5
1	A	364	LEU	5
1	A	339	LYS	4
1	A	347	ASN	4
1	A	352	SER	3
1	A	354	ILE	3
1	A	340	SER	2
1	A	334	HIS	1
1	A	368	ASN	1
1	A	357	VAL	1
1	A	355	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)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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)

The completeness of assignment taking into account all chemical shift lists is 69% for the well-defined parts and 68% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *shift_set*

7.1.1 Bookkeeping (i)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	452
Number of shifts mapped to atoms	452
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	48	-0.32 ± 0.26	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	47	0.07 ± 0.27	None needed (< 0.5 ppm)
$^{13}C'$	0	—	None (insufficient data)
^{15}N	44	1.01 ± 0.75	None needed (imprecise)

7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 69%, i.e. 384 atoms were assigned a chemical shift out of a possible 554. 0 out of 4 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	159/204 (78%)	80/82 (98%)	41/82 (50%)	38/40 (95%)
Sidechain	223/308 (72%)	147/198 (74%)	76/93 (82%)	0/17 (0%)

Continued on next page...

Continued from previous page...

	Total	^{1}H	^{13}C	^{15}N
Aromatic	2/42 (5%)	2/22 (9%)	0/16 (0%)	0/4 (0%)
Overall	384/554 (69%)	229/302 (76%)	117/191 (61%)	38/61 (62%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 68%, i.e. 452 atoms were assigned a chemical shift out of a possible 663. 0 out of 6 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	185/245 (76%)	93/99 (94%)	48/98 (49%)	44/48 (92%)
Sidechain	265/364 (73%)	175/235 (74%)	90/109 (83%)	0/20 (0%)
Aromatic	2/54 (4%)	2/28 (7%)	0/21 (0%)	0/5 (0%)
Overall	452/663 (68%)	270/362 (75%)	138/228 (61%)	44/73 (60%)

7.1.4 Statistically unusual chemical shifts (i)

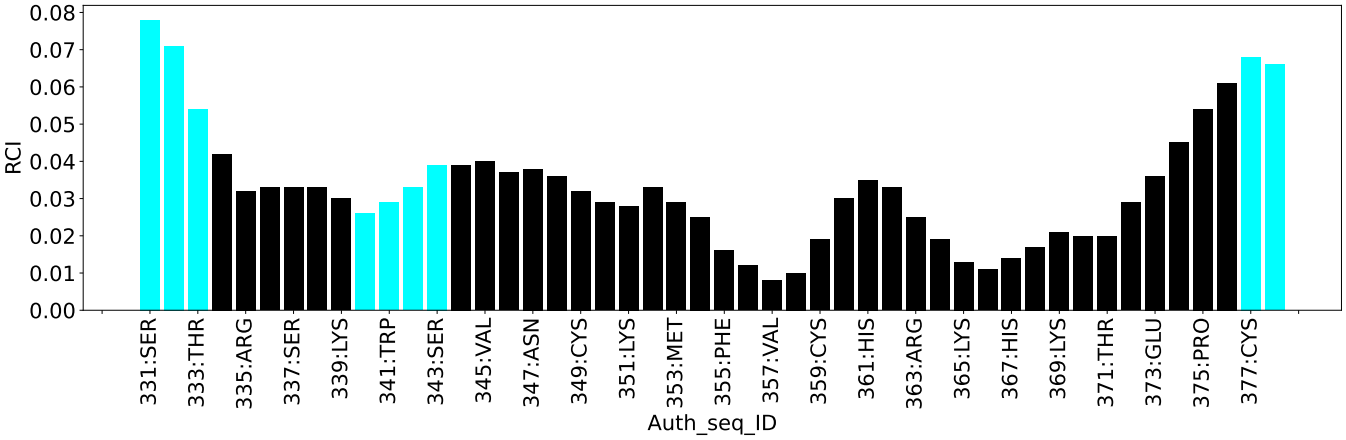
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	351	LYS	HD2	3.14	0.58 – 2.64	7.4
1	A	344	GLN	HG3	0.86	0.91 – 3.68	-5.2

7.1.5 Random Coil Index (RCI) plots (i)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:


RCI
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0.00
331:SER
333:THR
335:ARG
337:SER
339:LYS
341:TRP
343:SER
345:VAL
347:ASN
349:CYS
351:LYS
353:MET
355:PHE
357:VAL
359:CYS
361:HIS
363:ARG
365:LYS
367:HIS
369:LYS
371:THR
373:GLU
375:PRO
377:CYS
Auth_seq_ID