Full wwPDB NMR Structure Validation Report (i)

Mar 5, 2022 – 09:11 AM EST

PDB ID	:	2K3H
Title	:	Structural determinants for Ca2+ and PIP2 binding by the C2A domain of rabphilin-3A
Authors	:	Coudevylle, N.; Montaville, P.; Leonov, A.; Zweckstetter, M.; Becker, S.
Deposited on	:	2008-05-08

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

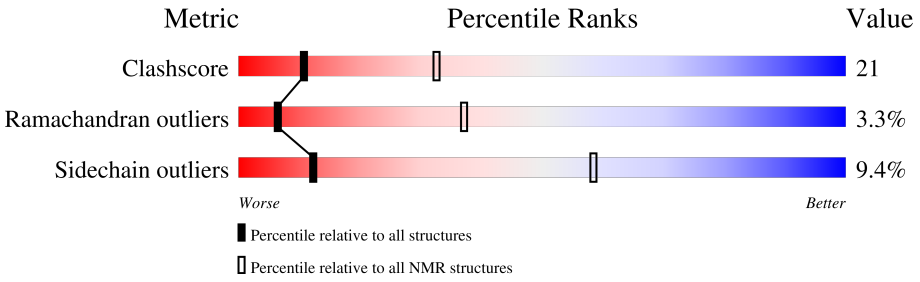
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

1 Overall quality at a glance (i)

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	140	49% 32% • 6% 9%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 13 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest violations*.

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:385-A:476, A:481-A:506 (118)	0.17	13

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 9 single-model clusters were found.

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2078 atoms, of which 1048 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Rabphilin-3A.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	127	2076	643	1048	189	191	5	0

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	
			Total	Ca
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: Rabphilin-3A

Chain A: 49% 32% • 6% 9%

GLU ALA ASN SER TYR ASP SER ASP GLU ALA THR THR LEU G384 F388 S389 L390 L391 Y392 D393 Q394 D395 N396 S397 N398 L399 Q400 C401 T402 R405 G408 L409 K410 P411 M412 D413 S414 N415 G416 Y421 V422 H425 L426 A430 S431 K432 S433 N434 K435 T438 L441 R442

N443 T444 R445 N446 P447 V448 H456 D462 C473 D474 E475 D476 K477 F478 G479 H480 N481 L494 N497 Q498 N501 F502 N503 I504 E507 R508 V509 I510

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: Rabphilin-3A

Chain A: 49% 31% • 6% 9%

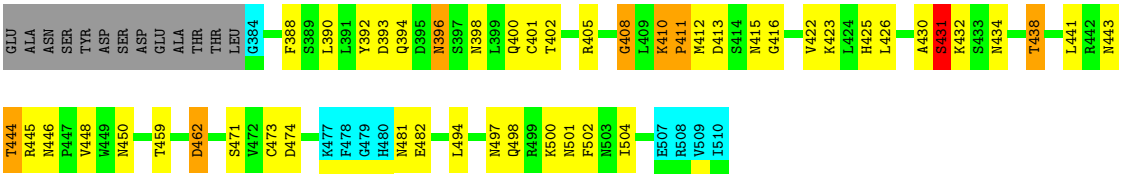
GLU ALA ASN SER TYR ASP SER ASP GLU ALA THR THR LEU G384 F388 S389 L390 L391 Y392 D393 N396 S397 N398 L399 Q400 C401 T402 R405 A406 K407 G408 L409 K410 P411 M412 D413 S414 N415 G416 Y421 V422 H425 L426 A430 S431 K432 S433 N434 K435 T438 L441 R442

N443 T444 R445 N446 P447 V448 T459 D462 C473 D474 E475 D476 K477 F478 G479 H480 N481 E486 S490 L494 N497 Q498 R499 F502 N503 I504 E507 R508 V509 I510

4.2.2 Score per residue for model 2

• Molecule 1: Rabphilin-3A

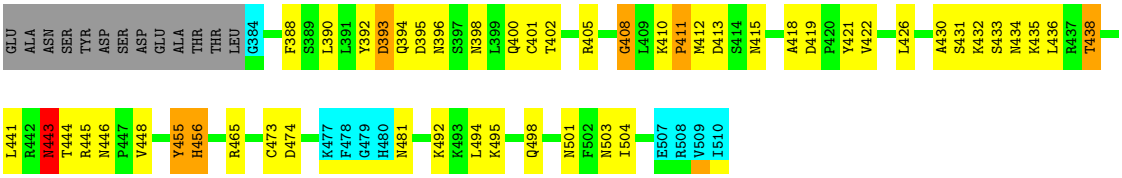
Chain A: 50% 29% 5% • 6% 9%



4.2.3 Score per residue for model 3

- Molecule 1: Rabphilin-3A

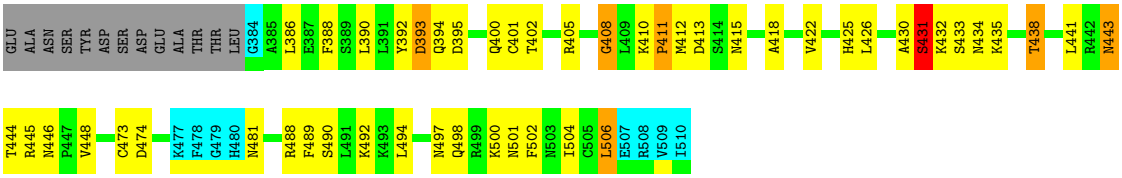
Chain A:



4.2.4 Score per residue for model 4

- Molecule 1: Rabphilin-3A

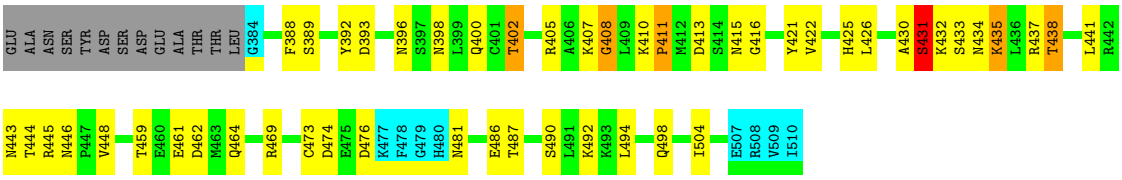
Chain A:



4.2.5 Score per residue for model 5

- Molecule 1: Rabphilin-3A

Chain A:



4.2.6 Score per residue for model 6

- Molecule 1: Rabphilin-3A

Chain A: 48% 33% • 6% 9%

GLU ALA ASN SER TYR ASP SER ASP GLU ALA THR THR LEU G384 F388 S389 L390 L391 Y392 D393 Q394 D395 N396 S397 N398 L399 Q400 C401 T402 R405 G408 L409 K410 P411 M412 D413 S414 N415 G416 Y421 V422 K423 L424 H425 L426 A430 S431 K432 S433 N434 K435 T438 K439 T440

L441 R442 N443 T444 R445 N446 P447 V448 H456 T459 D462 C473 D474 K477 F478 G479 H480 N481 S490 L494 N497 Q498 N501 F502 N503 I504 E507 R508 V509 I510

4.2.7 Score per residue for model 7

- Molecule 1: Rabphilin-3A

Chain A: 50% 29% 6% 6% 9%

GLU ALA ASN SER TYR ASP SER ASP GLU ALA THR THR LEU G384 F388 S389 L390 L391 Y392 D393 Q394 D395 Q400 C401 T402 R405 A406 K407 G408 L409 K410 P411 M412 D413 S414 N415 G416 L417 A418 V422 K423 L424 H425 L426 A430 S431 K432 S433 N434 K435 T438 N443 T444

R445 N446 P447 V448 H456 R469 C473 D474 K477 F478 G479 H480 N481 R488 F489 S490 L491 K492 K493 L494 Q498 F502 N503 I504 E507 R508 V509 I510

4.2.8 Score per residue for model 8

- Molecule 1: Rabphilin-3A

Chain A: 45% 32% 7% 6% 9%

GLU ALA ASN SER TYR ASP SER ASP GLU ALA THR THR LEU G384 E387 F388 S389 L390 L391 Y392 D393 Q394 D395 N396 S397 N398 L399 Q400 C401 T402 R405 A406 K407 G408 L409 K410 P411 M412 D413 S414 N415 G416 Y421 V422 L426 L427 A430 S431 K432 S433 N434 K435 T438

L441 R442 N443 T444 R445 N446 P447 V448 W449 T452 H456 T459 D462 T467 C473 D474 E475 D476 K477 F478 G479 H480 N481 E482 F483 T487 R488 F489 Q498 N501 F502 N503 I504 E507 R508 V509 I510

4.2.9 Score per residue for model 9

- Molecule 1: Rabphilin-3A

Chain A: 53% 29% • 6% 9%

GLU ALA ASN SER TYR ASP SER ASP GLU ALA THR THR LEU G384 E387 F388 S389 L390 L391 Y392 D393 Q394 D395 N396 S397 N398 L399 Q400 C401 T402 R405 G408 L409 K410 P411 M412 D413 S414 N415 G416 Y421 V422 H425 L426 A430 S431 K432 S433 N434 T438 L441 R442

N443 T444 R445 V448 T452 H456 C473 D474 E475 D476 K477 F478 G479 H480 N481 L494 N497 Q498 F502 N503 I504 E507 R508 V509 I510

4.2.10 Score per residue for model 10

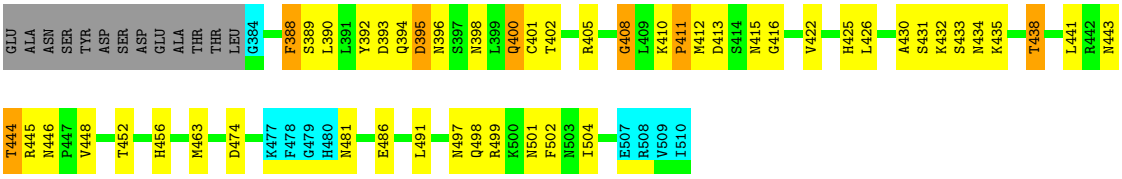
- Molecule 1: Rabphilin-3A

Chain A: 51% 31% • 6% 9%

4.2.11 Score per residue for model 11

- Molecule 1: Rabphilin-3A

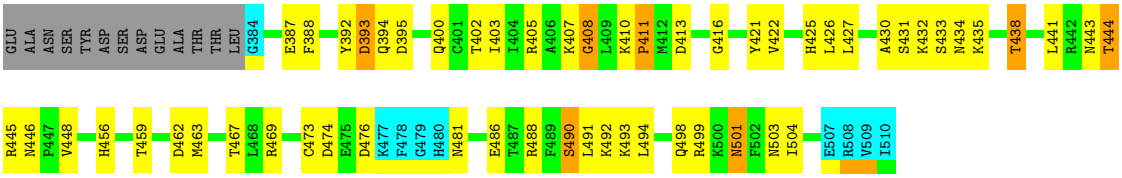
Chain A: 49% 30% 5% 6% 9%



4.2.12 Score per residue for model 12

- Molecule 1: Rabphilin-3A

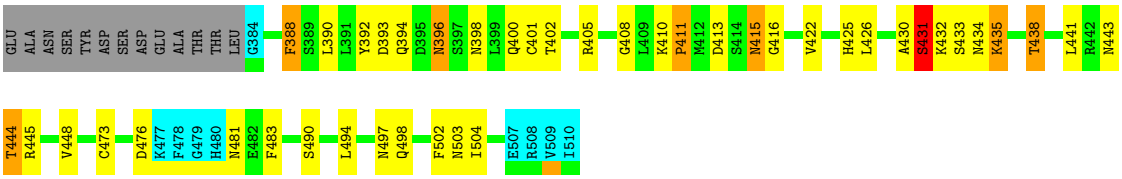
Chain A: 44% 35% 5% 6% 9%



4.2.13 Score per residue for model 13 (medoid)

- Molecule 1: Rabphilin-3A

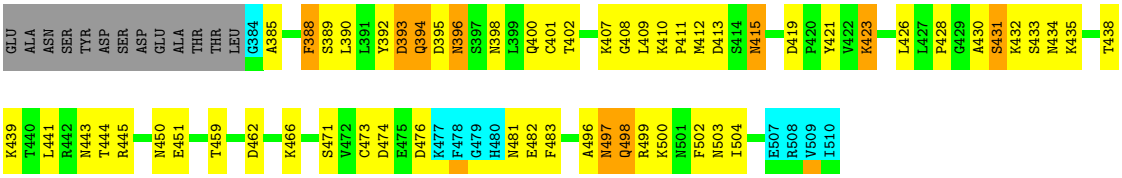
Chain A: 54% 25% 5% • 6% 9%



4.2.14 Score per residue for model 14

- Molecule 1: Rabphilin-3A

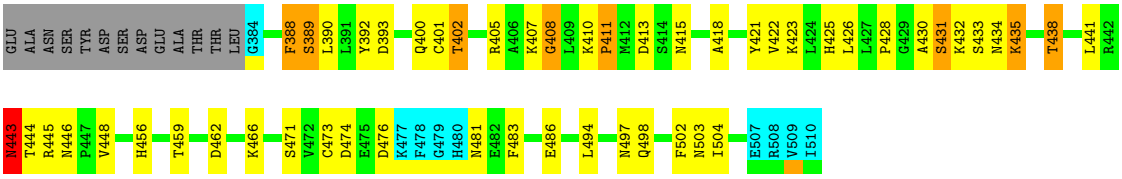
Chain A: 43% 35% 6% 6% 9%



4.2.15 Score per residue for model 15

- Molecule 1: Rabphilin-3A

Chain A: 47% 31% 6% • 6% 9%



4.2.16 Score per residue for model 16

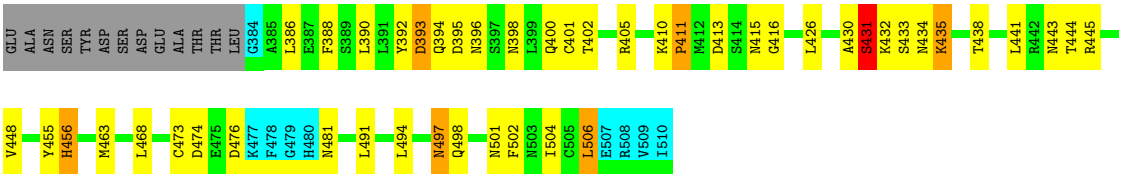
- Molecule 1: Rabphilin-3A

Chain A: 52% 29% • 6% 9%

4.2.17 Score per residue for model 17

- Molecule 1: Rabphilin-3A

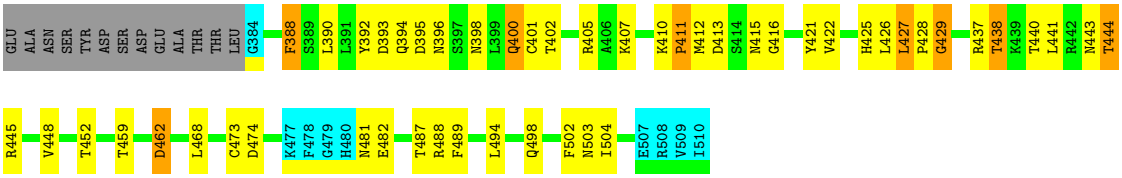
Chain A: 51% 29% • • 6% 9%



4.2.18 Score per residue for model 18

- Molecule 1: Rabphilin-3A

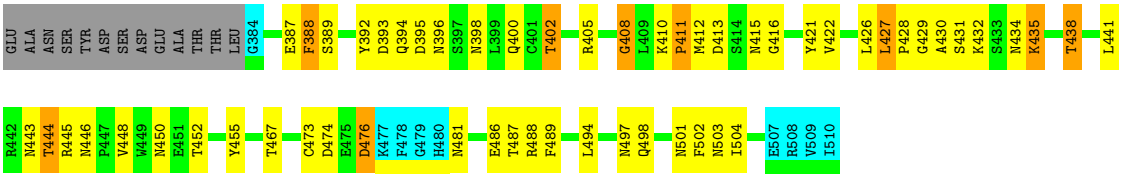
Chain A: 49% 30% 6% 6% 9%



4.2.19 Score per residue for model 19

- Molecule 1: Rabphilin-3A

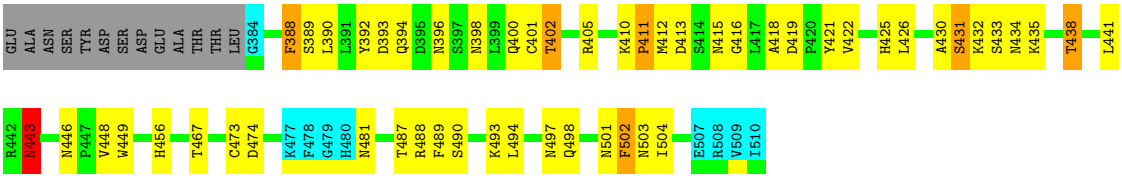
Chain A: 44% 34% 6% 6% 9%



4.2.20 Score per residue for model 20

- Molecule 1: Rabphilin-3A

Chain A: 46% 33% • • 6% 9%



5 Refinement protocol and experimental data overview (i)

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

Of the 200 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
CYANA	structure solution	
X-PLOR NIH	refinement	

No chemical shift data was provided.

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: CA

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	955	973	971	40±5
All	All	19140	19460	19420	801

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 21.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:427:LEU:H	1:A:427:LEU:HD22	0.92	1.21	18	1
1:A:427:LEU:N	1:A:427:LEU:HD22	0.92	1.79	19	1
1:A:427:LEU:HD22	1:A:427:LEU:H	0.87	1.28	19	1
1:A:427:LEU:HD22	1:A:427:LEU:N	0.85	1.87	18	1
1:A:426:LEU:C	1:A:427:LEU:HD13	0.75	2.02	18	2
1:A:473:CYS:SG	1:A:474:ASP:N	0.61	2.73	15	17
1:A:427:LEU:N	1:A:427:LEU:CD2	0.61	2.53	19	2
1:A:456:HIS:CD2	1:A:456:HIS:H	0.60	2.12	16	3
1:A:396:ASN:O	1:A:398:ASN:ND2	0.60	2.35	18	14
1:A:427:LEU:N	1:A:427:LEU:HD13	0.60	2.12	18	2
1:A:388:PHE:CE1	1:A:502:PHE:CD1	0.60	2.90	16	3
1:A:473:CYS:SG	1:A:483:PHE:CD2	0.59	2.96	13	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:501:ASN:HD22	1:A:502:PHE:N	0.59	1.94	11	3
1:A:394:GLN:NE2	1:A:497:ASN:HD21	0.59	1.95	13	1
1:A:502:PHE:CD1	1:A:502:PHE:N	0.59	2.70	20	11
1:A:388:PHE:CD1	1:A:388:PHE:N	0.58	2.72	18	16
1:A:469:ARG:NH2	1:A:488:ARG:HH21	0.57	1.96	12	2
1:A:499:ARG:NH1	1:A:501:ASN:HD21	0.57	1.97	12	1
1:A:501:ASN:ND2	1:A:502:PHE:N	0.57	2.52	11	2
1:A:443:ASN:HD22	1:A:443:ASN:N	0.57	1.98	15	2
1:A:412:MET:SD	1:A:474:ASP:CB	0.56	2.93	14	6
1:A:413:ASP:O	1:A:416:GLY:N	0.55	2.39	18	15
1:A:461:GLU:H	1:A:461:GLU:CD	0.55	2.02	5	1
1:A:469:ARG:CZ	1:A:488:ARG:NH2	0.55	2.69	12	1
1:A:430:ALA:O	1:A:434:ASN:ND2	0.55	2.40	14	18
1:A:444:THR:OG1	1:A:445:ARG:N	0.55	2.40	10	19
1:A:431:SER:O	1:A:435:LYS:NZ	0.54	2.41	8	6
1:A:394:GLN:CD	1:A:395:ASP:N	0.54	2.61	11	10
1:A:425:HIS:CE1	1:A:434:ASN:OD1	0.54	2.61	6	8
1:A:499:ARG:NH1	1:A:501:ASN:ND2	0.54	2.56	12	1
1:A:425:HIS:CD2	1:A:434:ASN:OD1	0.53	2.62	1	6
1:A:388:PHE:O	1:A:501:ASN:ND2	0.53	2.42	11	3
1:A:393:ASP:OD2	1:A:396:ASN:ND2	0.53	2.42	14	1
1:A:387:GLU:OE1	1:A:405:ARG:NH2	0.53	2.42	19	1
1:A:425:HIS:NE2	1:A:434:ASN:OD1	0.53	2.42	20	4
1:A:486:GLU:N	1:A:486:GLU:OE1	0.53	2.42	11	1
1:A:469:ARG:NH2	1:A:488:ARG:NH2	0.53	2.57	12	1
1:A:396:ASN:CB	1:A:398:ASN:HD22	0.53	2.17	14	1
1:A:430:ALA:O	1:A:432:LYS:N	0.53	2.42	19	12
1:A:388:PHE:CZ	1:A:502:PHE:CB	0.52	2.92	1	1
1:A:387:GLU:OE2	1:A:405:ARG:NH2	0.52	2.42	19	1
1:A:389:SER:OG	1:A:499:ARG:NH2	0.52	2.42	11	3
1:A:412:MET:CB	1:A:418:ALA:HB2	0.52	2.35	10	5
1:A:394:GLN:NE2	1:A:497:ASN:OD1	0.52	2.43	9	2
1:A:415:ASN:O	1:A:415:ASN:ND2	0.52	2.42	13	6
1:A:435:LYS:CB	1:A:435:LYS:NZ	0.52	2.72	19	1
1:A:392:TYR:O	1:A:497:ASN:N	0.52	2.42	11	6
1:A:494:LEU:CD2	1:A:494:LEU:N	0.52	2.73	3	16
1:A:418:ALA:O	1:A:443:ASN:N	0.52	2.42	20	3
1:A:394:GLN:CG	1:A:497:ASN:HD21	0.52	2.16	17	2
1:A:459:THR:N	1:A:462:ASP:OD2	0.51	2.42	8	2
1:A:394:GLN:OE1	1:A:497:ASN:ND2	0.51	2.42	20	1
1:A:405:ARG:CZ	1:A:407:LYS:NZ	0.51	2.73	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:459:THR:HG1	1:A:462:ASP:CG	0.51	2.08	18	2
1:A:427:LEU:HA	1:A:429:GLY:H	0.51	1.64	19	1
1:A:493:LYS:CB	1:A:493:LYS:NZ	0.51	2.74	20	2
1:A:390:LEU:CD2	1:A:401:CYS:SG	0.51	2.99	20	17
1:A:428:PRO:O	1:A:466:LYS:NZ	0.51	2.42	14	3
1:A:492:LYS:NZ	1:A:492:LYS:CB	0.50	2.74	4	1
1:A:481:ASN:N	1:A:481:ASN:OD1	0.50	2.43	13	10
1:A:405:ARG:NH2	1:A:446:ASN:OD1	0.50	2.45	16	1
1:A:502:PHE:N	1:A:502:PHE:CD1	0.50	2.78	11	1
1:A:464:GLN:C	1:A:492:LYS:HZ2	0.50	2.09	5	1
1:A:406:ALA:HB2	1:A:449:TRP:CZ3	0.50	2.42	8	1
1:A:410:LYS:CB	1:A:410:LYS:NZ	0.49	2.75	2	1
1:A:430:ALA:C	1:A:432:LYS:H	0.49	2.11	16	19
1:A:494:LEU:N	1:A:494:LEU:HD22	0.49	2.21	2	15
1:A:400:GLN:NE2	1:A:452:THR:CG2	0.49	2.75	10	6
1:A:421:TYR:OH	1:A:473:CYS:SG	0.49	2.70	20	9
1:A:430:ALA:C	1:A:434:ASN:HD22	0.49	2.11	16	17
1:A:430:ALA:C	1:A:434:ASN:ND2	0.48	2.66	17	11
1:A:439:LYS:NZ	1:A:451:GLU:OE2	0.48	2.44	14	1
1:A:436:LEU:HD12	1:A:455:TYR:CE2	0.48	2.43	3	1
1:A:469:ARG:NH2	1:A:486:GLU:OE1	0.48	2.46	5	1
1:A:501:ASN:OD1	1:A:501:ASN:N	0.48	2.45	8	1
1:A:456:HIS:CD2	1:A:456:HIS:N	0.48	2.81	16	2
1:A:394:GLN:CD	1:A:497:ASN:ND2	0.48	2.67	13	2
1:A:408:GLY:H	1:A:446:ASN:ND2	0.48	2.06	7	13
1:A:500:LYS:CG	1:A:502:PHE:CZ	0.48	2.96	14	3
1:A:501:ASN:HD22	1:A:502:PHE:H	0.48	1.52	11	2
1:A:402:THR:CG2	1:A:452:THR:OG1	0.48	2.62	19	2
1:A:396:ASN:ND2	1:A:396:ASN:N	0.48	2.61	14	1
1:A:490:SER:OG	1:A:492:LYS:NZ	0.48	2.42	12	2
1:A:412:MET:SD	1:A:474:ASP:CG	0.47	2.93	14	7
1:A:430:ALA:C	1:A:432:LYS:N	0.47	2.66	19	19
1:A:486:GLU:N	1:A:486:GLU:CD	0.47	2.68	12	4
1:A:441:LEU:N	1:A:441:LEU:HD12	0.47	2.25	13	19
1:A:394:GLN:CD	1:A:497:ASN:HD21	0.47	2.13	20	2
1:A:413:ASP:C	1:A:415:ASN:N	0.47	2.68	20	15
1:A:462:ASP:OD1	1:A:462:ASP:N	0.47	2.47	8	1
1:A:463:MET:SD	1:A:491:LEU:HD22	0.47	2.49	17	3
1:A:422:VAL:O	1:A:438:THR:OG1	0.47	2.30	20	16
1:A:394:GLN:OE1	1:A:395:ASP:N	0.47	2.48	11	5
1:A:459:THR:O	1:A:462:ASP:N	0.47	2.46	12	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:504:ILE:HD12	1:A:504:ILE:O	0.47	2.10	10	20
1:A:413:ASP:OD1	1:A:413:ASP:N	0.46	2.49	16	8
1:A:439:LYS:NZ	1:A:451:GLU:CD	0.46	2.68	14	1
1:A:443:ASN:N	1:A:443:ASN:HD22	0.46	2.06	20	2
1:A:429:GLY:C	1:A:434:ASN:HD22	0.46	2.14	19	1
1:A:391:LEU:HD12	1:A:498:GLN:O	0.46	2.10	8	1
1:A:392:TYR:C	1:A:392:TYR:CD1	0.46	2.88	13	20
1:A:387:GLU:CG	1:A:503:ASN:ND2	0.46	2.79	19	4
1:A:437:ARG:NH2	1:A:440:THR:OG1	0.46	2.49	18	1
1:A:462:ASP:N	1:A:462:ASP:OD1	0.46	2.48	18	1
1:A:426:LEU:N	1:A:426:LEU:CD1	0.46	2.79	8	20
1:A:486:GLU:N	1:A:486:GLU:OE2	0.46	2.49	12	1
1:A:421:TYR:CD1	1:A:473:CYS:O	0.46	2.68	9	4
1:A:434:ASN:O	1:A:434:ASN:OD1	0.45	2.35	3	2
1:A:388:PHE:HB3	1:A:403:ILE:HD12	0.45	1.87	12	1
1:A:421:TYR:C	1:A:421:TYR:CD1	0.45	2.90	14	1
1:A:426:LEU:HD11	1:A:468:LEU:HD12	0.45	1.89	17	3
1:A:473:CYS:SG	1:A:483:PHE:CE2	0.45	3.09	14	1
1:A:434:ASN:OD1	1:A:434:ASN:O	0.45	2.35	9	13
1:A:406:ALA:O	1:A:446:ASN:ND2	0.45	2.49	10	1
1:A:394:GLN:NE2	1:A:395:ASP:OD1	0.45	2.49	11	1
1:A:410:LYS:O	1:A:411:PRO:C	0.45	2.54	10	20
1:A:465:ARG:C	1:A:492:LYS:NZ	0.45	2.69	3	1
1:A:385:ALA:HB3	1:A:407:LYS:HB3	0.45	1.87	10	2
1:A:405:ARG:HB3	1:A:448:VAL:HG22	0.45	1.89	18	2
1:A:427:LEU:CA	1:A:429:GLY:H	0.45	2.25	18	1
1:A:405:ARG:CB	1:A:448:VAL:HG22	0.45	2.42	12	17
1:A:386:LEU:HB2	1:A:506:LEU:HD21	0.45	1.89	4	2
1:A:389:SER:CB	1:A:499:ARG:NH2	0.45	2.80	14	2
1:A:439:LYS:HZ3	1:A:451:GLU:CD	0.44	2.15	14	1
1:A:427:LEU:O	1:A:467:THR:N	0.44	2.51	8	2
1:A:388:PHE:C	1:A:388:PHE:CD1	0.44	2.91	9	1
1:A:425:HIS:CE1	1:A:427:LEU:HD12	0.44	2.47	18	1
1:A:450:ASN:O	1:A:450:ASN:ND2	0.44	2.50	14	1
1:A:394:GLN:NE2	1:A:395:ASP:N	0.44	2.64	6	2
1:A:388:PHE:CD1	1:A:388:PHE:C	0.44	2.91	16	2
1:A:389:SER:OG	1:A:499:ARG:CZ	0.44	2.66	11	2
1:A:433:SER:C	1:A:435:LYS:H	0.44	2.16	17	14
1:A:427:LEU:N	1:A:427:LEU:CD1	0.44	2.77	18	1
1:A:486:GLU:OE1	1:A:488:ARG:NH2	0.44	2.51	19	1
1:A:428:PRO:O	1:A:429:GLY:O	0.44	2.36	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:434:ASN:N	1:A:434:ASN:OD1	0.44	2.50	19	1
1:A:431:SER:O	1:A:432:LYS:C	0.43	2.57	17	7
1:A:456:HIS:ND1	1:A:456:HIS:N	0.43	2.66	17	3
1:A:488:ARG:O	1:A:489:PHE:CD1	0.43	2.72	19	4
1:A:413:ASP:OD1	1:A:476:ASP:OD1	0.43	2.37	16	9
1:A:434:ASN:OD1	1:A:434:ASN:C	0.43	2.57	20	16
1:A:421:TYR:CD1	1:A:421:TYR:N	0.43	2.87	8	4
1:A:419:ASP:O	1:A:474:ASP:OD1	0.43	2.36	14	1
1:A:446:ASN:O	1:A:446:ASN:OD1	0.43	2.36	20	1
1:A:435:LYS:N	1:A:455:TYR:OH	0.43	2.51	3	1
1:A:459:THR:OG1	1:A:461:GLU:OE1	0.43	2.36	5	1
1:A:461:GLU:OE2	1:A:461:GLU:N	0.43	2.42	5	1
1:A:389:SER:O	1:A:402:THR:N	0.43	2.41	1	5
1:A:423:LYS:O	1:A:471:SER:OG	0.43	2.36	2	3
1:A:387:GLU:CD	1:A:405:ARG:NH2	0.43	2.71	19	1
1:A:388:PHE:O	1:A:501:ASN:OD1	0.43	2.37	20	1
1:A:412:MET:O	1:A:482:GLU:OE2	0.43	2.37	10	3
1:A:403:ILE:O	1:A:403:ILE:HG23	0.43	2.14	12	1
1:A:474:ASP:OD2	1:A:476:ASP:OD1	0.43	2.37	14	1
1:A:496:ALA:O	1:A:498:GLN:N	0.43	2.52	14	1
1:A:413:ASP:OD1	1:A:476:ASP:OD2	0.43	2.37	19	1
1:A:394:GLN:OE1	1:A:497:ASN:OD1	0.43	2.37	16	2
1:A:412:MET:O	1:A:482:GLU:OE1	0.42	2.36	14	1
1:A:412:MET:SD	1:A:474:ASP:OD2	0.42	2.78	2	2
1:A:415:ASN:O	1:A:415:ASN:OD1	0.42	2.37	9	4
1:A:459:THR:OG1	1:A:462:ASP:OD1	0.42	2.36	18	2
1:A:443:ASN:HD22	1:A:443:ASN:H	0.42	1.56	15	1
1:A:443:ASN:N	1:A:443:ASN:ND2	0.42	2.67	3	2
1:A:504:ILE:HD12	1:A:504:ILE:C	0.42	2.35	9	7
1:A:394:GLN:NE2	1:A:497:ASN:ND2	0.42	2.66	13	1
1:A:467:THR:HG23	1:A:489:PHE:O	0.42	2.14	8	3
1:A:422:VAL:HG23	1:A:449:TRP:CE2	0.42	2.49	20	1
1:A:405:ARG:HB2	1:A:448:VAL:HG22	0.42	1.91	9	2
1:A:425:HIS:C	1:A:426:LEU:HD12	0.42	2.35	18	2
1:A:465:ARG:CA	1:A:492:LYS:NZ	0.42	2.83	3	1
1:A:393:ASP:OD1	1:A:393:ASP:C	0.42	2.59	14	2
1:A:410:LYS:O	1:A:411:PRO:O	0.41	2.38	18	1
1:A:413:ASP:N	1:A:413:ASP:OD1	0.41	2.52	4	2
1:A:469:ARG:CZ	1:A:488:ARG:HH21	0.41	2.26	12	1
1:A:393:ASP:O	1:A:393:ASP:OD1	0.41	2.38	8	5
1:A:483:PHE:CD1	1:A:483:PHE:N	0.41	2.87	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:388:PHE:CE2	1:A:502:PHE:CG	0.41	3.09	1	1
1:A:387:GLU:OE2	1:A:503:ASN:ND2	0.41	2.54	8	1
1:A:433:SER:O	1:A:455:TYR:OH	0.40	2.36	3	1
1:A:418:ALA:HB3	1:A:444:THR:O	0.40	2.16	15	1
1:A:494:LEU:N	1:A:494:LEU:CD2	0.40	2.83	17	1
1:A:415:ASN:OD1	1:A:415:ASN:O	0.40	2.40	5	2
1:A:439:LYS:NZ	1:A:439:LYS:CB	0.40	2.84	6	1
1:A:393:ASP:OD1	1:A:393:ASP:O	0.40	2.38	9	1
1:A:394:GLN:CG	1:A:395:ASP:N	0.40	2.85	8	2

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	118/140 (84%)	103±1 (87±1%)	11±1 (9±1%)	4±0 (3±0%)	6	37
All	All	2360/2800 (84%)	2059 (87%)	224 (9%)	77 (3%)	6	37

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	443	ASN	20
1	A	411	PRO	19
1	A	431	SER	18
1	A	408	GLY	17
1	A	497	ASN	1
1	A	429	GLY	1
1	A	428	PRO	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	108/126 (86%)	98±2 (91±2%)	10±2 (9±2%)	12 58
All	All	2160/2520 (86%)	1957 (91%)	203 (9%)	12 58

All 35 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	393	ASP	20
1	A	402	THR	20
1	A	438	THR	20
1	A	498	GLN	20
1	A	400	GLN	19
1	A	444	THR	9
1	A	503	ASN	9
1	A	490	SER	8
1	A	388	PHE	8
1	A	456	HIS	7
1	A	501	ASN	6
1	A	435	LYS	6
1	A	431	SER	5
1	A	487	THR	5
1	A	462	ASP	4
1	A	396	ASN	3
1	A	450	ASN	3
1	A	443	ASN	3
1	A	455	TYR	3
1	A	423	LYS	3
1	A	415	ASN	3
1	A	419	ASP	2
1	A	495	LYS	2
1	A	506	LEU	2
1	A	395	ASP	2
1	A	427	LEU	2
1	A	410	LYS	1
1	A	437	ARG	1
1	A	424	LEU	1
1	A	394	GLN	1
1	A	409	LEU	1
1	A	389	SER	1
1	A	497	ASN	1
1	A	476	ASP	1

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Mol	Chain	Res	Type	Models (Total)
1	A	502	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)

No chemical shift data were provided