Full wwPDB NMR Structure Validation Report (i)

Mar 6, 2022 – 10:50 PM EST

PDB ID	:	2KLS
Title	:	Apo-form of the second Ca2+ binding domain of NCX1.4
Authors	:	Hilge, M.; Aelen, J.; Foarce, A.; Perrakis, A.; Vuister, G.W.
Deposited on	:	2009-07-08

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:

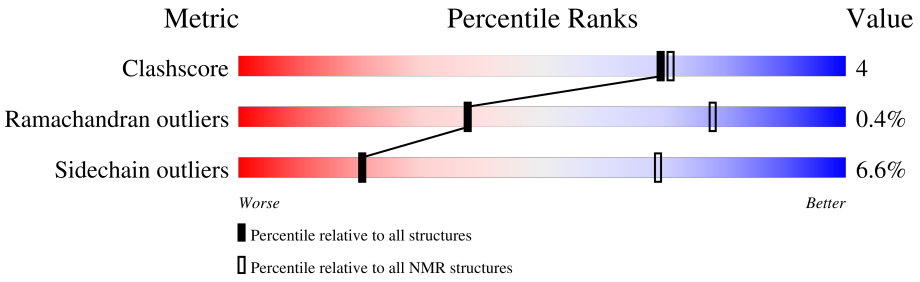
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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	164	

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:502-A:576, A:585-A:597, A:634-A:647 (102)	0.26	1

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 1 single-model cluster was found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2465 atoms, of which 1215 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Sodium/calcium exchanger 1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	157	2465	784	1215	201	261	4	0

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: Sodium/calcium exchanger 1

Chain A: 57% 5% • 34% •

MET SER HIS HIS HIS HIS HIS H501 S515 M521 E522 V523 T528 I536 V568 K569 T570 D577 D578 E579 E580 Y581 E582 K583 N584 L589 E598 M599 S600 E601 K602 K603 G604 G605 F606 T607 I608 T609 E610 E611 Y612 D613 D614 K615 Q616 P617 L618 T619 S620 K621 E622 E623

E624 E625 R626 R627 I628 A629 E630 M631 G632 R633 L636 E648 S649 Y650 E651 F652 K653 S654 T655 V656 D657

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 (medoid)

• Molecule 1: Sodium/calcium exchanger 1

Chain A: 54% 8% • 34% •

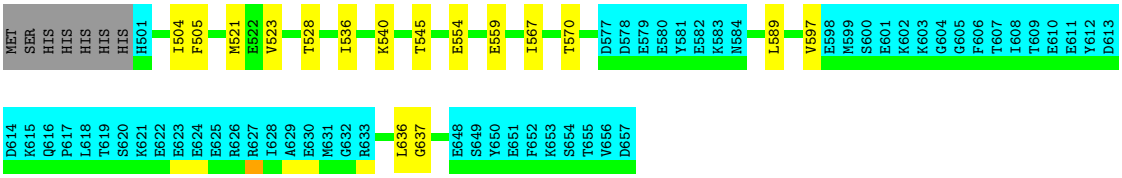
MET SER HIS HIS HIS HIS HIS H501 A502 E508 M521 E522 V523 T528 N534 R547 Q563 K569 T570 T571 D577 D578 E579 E580 Y581 E582 K583 N584 L589 E598 M599 S600 E601 K602 K603 G604 G605 F606 T607 I608 T609 E610 E611 Y612 D613 D614 K615 Q616 P617 L618

T619 S620 K621 E622 E623 E624 E625 R626 R627 I628 A629 E630 M631 G632 R633 L636 E648 S649 Y650 E651 F652 K653 S654 T655 V656 D657

4.2.2 Score per residue for model 2

• Molecule 1: Sodium/calcium exchanger 1

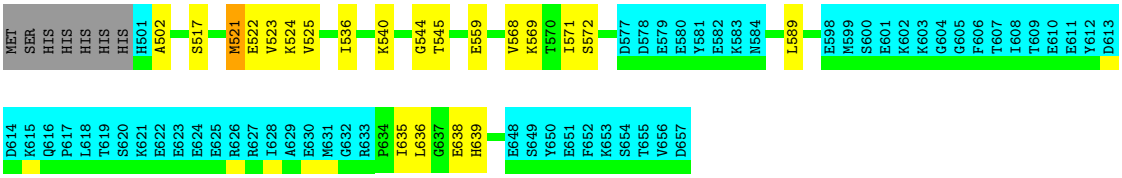
Chain A: 52% 10% 34% •



4.2.3 Score per residue for model 3

- Molecule 1: Sodium/calcium exchanger 1

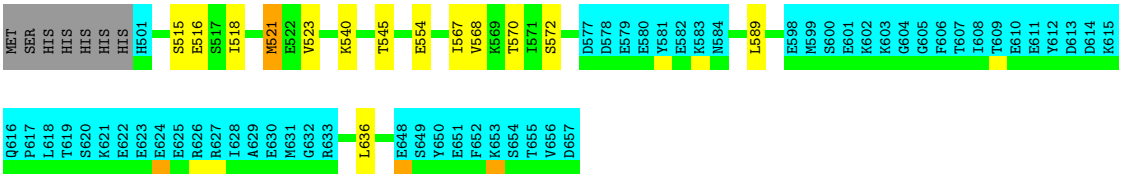
Chain A:



4.2.4 Score per residue for model 4

- Molecule 1: Sodium/calcium exchanger 1

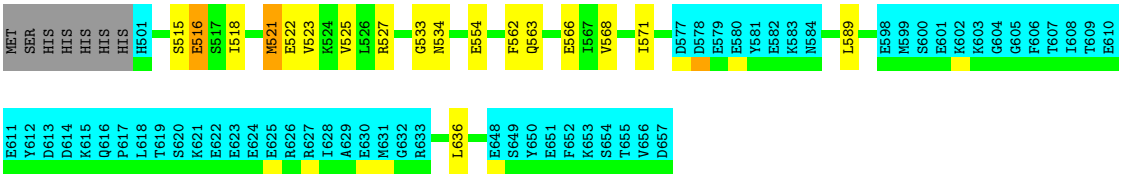
Chain A:



4.2.5 Score per residue for model 5

- Molecule 1: Sodium/calcium exchanger 1

Chain A:



4.2.6 Score per residue for model 6

- Molecule 1: Sodium/calcium exchanger 1

Chain A: 54% 8% 34% •

MET SER HIS HIS HIS HIS HIS H501 M521 E522 V523 R527 I536 E543 E554 E559 F562 T570 D577 D578 E579 E580 Y581 E582 K583 N584 L589 P594 E598 M599 S600 E601 K602 K603 G604 G605 F606 T607 I608 T609 E610 E611 Y612 D613 D614 K615 Q616 P617

L618 T619 S620 K621 E622 E623 E624 E625 R626 R627 I628 A629 E630 M631 G632 R633 P634 I635 L636 E648 S649 Y650 E651 F652 K653 S654 T655 V656 D657

4.2.7 Score per residue for model 7

• Molecule 1: Sodium/calcium exchanger 1

Chain A: 54% 8% • 34% •

MET SER HIS HIS HIS HIS HIS H501 A502 F505 E516 M521 E522 T528 A546 K569 T570 I571 D577 D578 E579 E580 Y581 E582 K583 N584 K585 L589 R595 E598 M599 S600 E601 K602 K603 G604 G605 F606 T607 I608 T609 E610 E611 Y612 D613 D614 K615 Q616 P617 L618

T619 S620 K621 E622 E623 E624 E625 R626 R627 I628 A629 E630 M631 G632 R633 L636 E648 S649 Y650 E651 F652 K653 S654 T655 V656 D657

4.2.8 Score per residue for model 8

• Molecule 1: Sodium/calcium exchanger 1

Chain A: 52% 9% • 34% •

MET SER HIS HIS HIS HIS HIS H501 E509 S515 M521 E522 V523 I536 E543 G544 T545 E554 E559 T570 I571 S572 D577 D578 E579 E580 Y581 E582 K583 N584 L589 L596 V597 E598 M599 S600 E601 K602 K603 G604 G605 F606 T607 I608 T609 E610 E611 Y612 D613

D614 K615 Q616 P617 L618 T619 S620 K621 E622 E623 E624 E625 R626 R627 I628 A629 E630 M631 G632 R633 L642 E647 E648 S649 Y650 E651 F652 K653 S654 T655 V656 D657

4.2.9 Score per residue for model 9

• Molecule 1: Sodium/calcium exchanger 1

Chain A: 51% 10% • 34% •

MET SER HIS HIS HIS HIS HIS H501 A502 S515 M521 E522 V523 K524 V525 T528 Y539 I542 R547 E554 V568 K569 T570 I571 S572 D577 D578 E579 E580 Y581 E582 K583 N584 F587 F588 L589 E590 I591 E598 M599 S600 E601 K602 K603 G604 G605 F606 T607 I608

T609 E610 E611 Y612 D613 D614 K615 Q616 P617 L618 T619 S620 K621 E622 E623 E624 E625 R626 R627 I628 A629 E630 M631 G632 R633 L636 L642 E648 S649 Y650 E651 F652 K653 S654 T655 V656 D657

4.2.10 Score per residue for model 10

- Molecule 1: Sodium/calcium exchanger 1

Chain A: 55% 7% • 34% •

MET SER HIS HIS HIS HIS HIS H501 S515 E516 S517 I518 M521 E522 V523 G544 E554 I567 V568 S572 D577 D578 E579 E580 Y581 E582 K583 N584 L589 E598 M599 S600 E601 K602 K603 G604 G605 F606 T607 I608 T609 E610 E611 Y612 D613 D614 K615 Q616 P617 L618 T619

S620 K621 E622 E623 E624 E625 R626 R627 I628 A629 E630 M631 G632 R633 L636 E648 S649 Y650 E651 F652 K653 S654 T655 V656 D657

4.2.11 Score per residue for model 11

- Molecule 1: Sodium/calcium exchanger 1

Chain A: 53% 9% • 34% •

MET SER HIS HIS HIS HIS HIS H501 A502 S515 E516 S517 I518 M521 E522 V523 T528 K569 T570 T571 S572 D577 D578 E579 E580 Y581 E582 K583 N584 K585 L589 E598 M599 S600 E601 K602 K603 G604 G605 F606 T607 I608 T609 E610 E611 Y612 D613 D614 K615 Q616 P617 L618 T619

S620 K621 E622 E623 E624 E625 R626 R627 I628 A629 E630 M631 G632 R633 L636 E648 S649 Y650 E651 F652 K653 S654 T655 V656 D657

4.2.12 Score per residue for model 12

- Molecule 1: Sodium/calcium exchanger 1

Chain A: 48% 13% • 34% •

MET SER HIS HIS HIS HIS HIS H501 S515 E516 S517 I518 M521 E522 V523 K524 V525 I536 K540 T545 E554 E559 Q563 E566 I567 V568 K569 T570 I571 S572 D577 D578 E579 E580 Y581 E582 K583 N584 K585 L589 E593 E598 M599 S600 E601 K602 K603

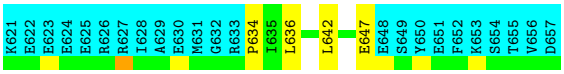
G604 G605 F606 T607 I608 T609 E610 E611 Y612 D613 D614 K615 Q616 P617 L618 T619 S620 K621 E622 E623 E624 E625 R626 R627 I628 A629 E630 M631 G632 R633 F634 I635 L636 L642 E647 E648 S649 Y650 E651 F652 K653 S654 T655 V656 D657

4.2.13 Score per residue for model 13

- Molecule 1: Sodium/calcium exchanger 1

Chain A: 54% 9% 34% •

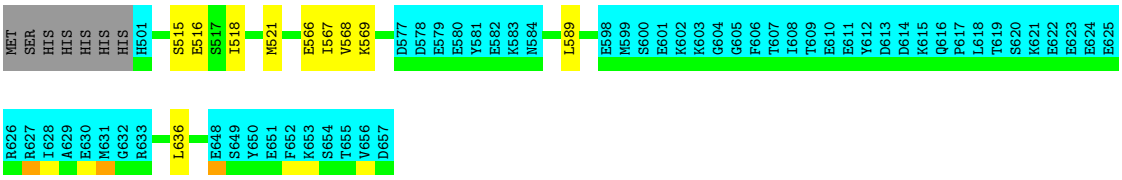
MET SER HIS HIS HIS HIS HIS H501 M521 E522 V523 I536 R547 G550 E551 E559 K569 D577 D578 E579 E580 Y581 E582 K583 N584 L589 P594 E598 M599 S600 E601 K602 K603 G604 G605 F606 T607 I608 T609 E610 E611 Y612 D613 D614 K615 Q616 P617 L618 T619 S620



4.2.14 Score per residue for model 14

- Molecule 1: Sodium/calcium exchanger 1

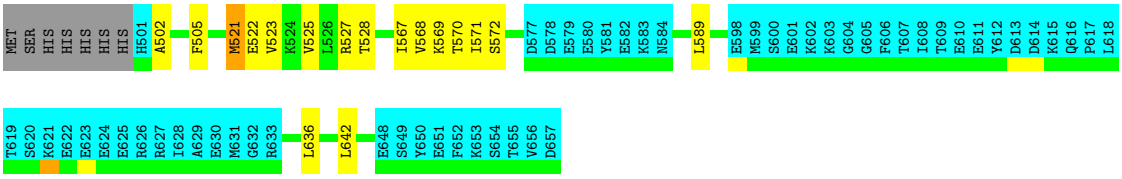
Chain A:



4.2.15 Score per residue for model 15

- Molecule 1: Sodium/calcium exchanger 1

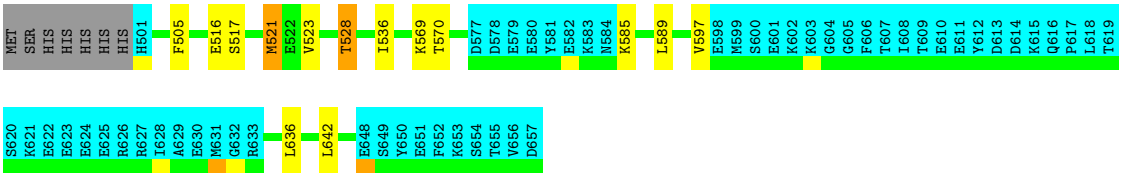
Chain A:



4.2.16 Score per residue for model 16

- Molecule 1: Sodium/calcium exchanger 1

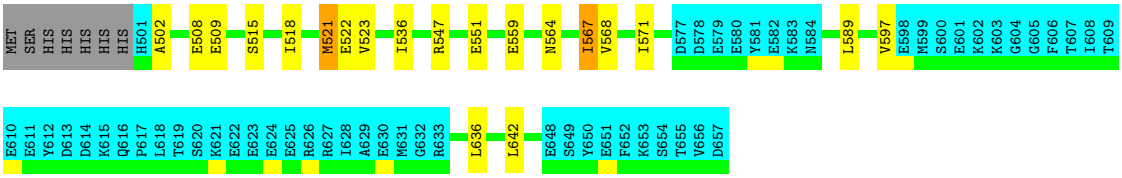
Chain A:



4.2.17 Score per residue for model 17

- Molecule 1: Sodium/calcium exchanger 1

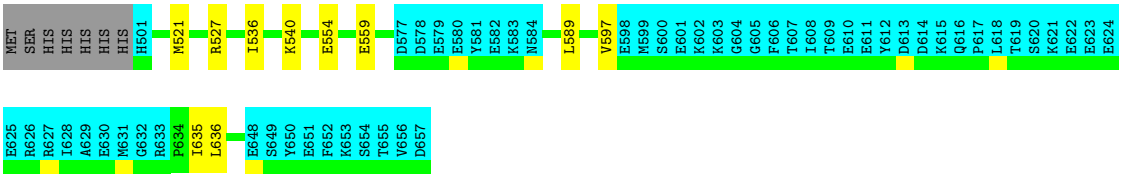
Chain A:



4.2.18 Score per residue for model 18

- Molecule 1: Sodium/calcium exchanger 1

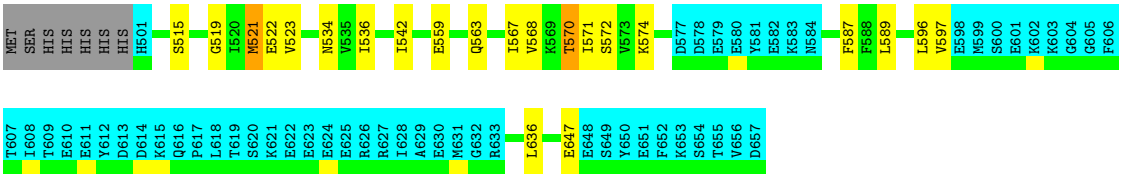
Chain A:



4.2.19 Score per residue for model 19

- Molecule 1: Sodium/calcium exchanger 1

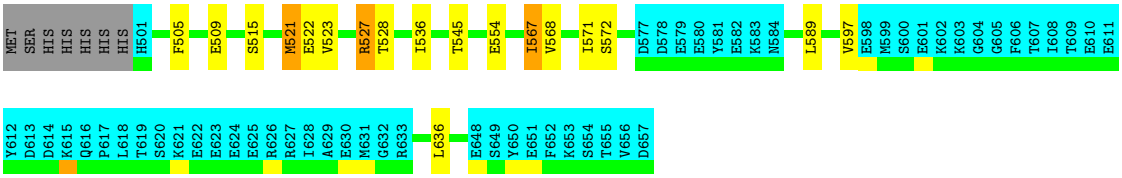
Chain A:



4.2.20 Score per residue for model 20

- Molecule 1: Sodium/calcium exchanger 1

Chain A:



5 Refinement protocol and experimental data overview (i)

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

Of the 100 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
CYANA	structure solution	2.1
X-PLOR	refinement	

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

There are no covalent bond-length or bond-angle outliers.

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	0.2±0.4
All	All	0	5

There are no bond-length outliers.

There are no bond-angle outliers.

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	547	ARG	Sidechain	2
1	A	527	ARG	Sidechain	2
1	A	595	ARG	Sidechain	1

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	789	799	799	6±2
All	All	15780	15980	15980	118

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 4.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:505:PHE:CE1	1:A:527:ARG:HA	0.61	2.31	20	1
1:A:505:PHE:CD2	1:A:528:THR:HG23	0.54	2.36	20	4
1:A:502:ALA:O	1:A:528:THR:HB	0.53	2.03	7	5
1:A:515:SER:O	1:A:518:ILE:HG22	0.52	2.05	4	5
1:A:527:ARG:CZ	1:A:562:PHE:HD1	0.50	2.19	6	1
1:A:521:MET:O	1:A:572:SER:HA	0.50	2.06	4	10
1:A:523:VAL:O	1:A:570:THR:HA	0.50	2.07	8	11
1:A:522:GLU:HA	1:A:571:ILE:O	0.49	2.07	11	9
1:A:534:ASN:ND2	1:A:563:GLN:HG2	0.48	2.24	5	3
1:A:521:MET:SD	1:A:523:VAL:HG23	0.48	2.49	3	10
1:A:536:ILE:HG12	1:A:597:VAL:CG2	0.48	2.39	2	6
1:A:505:PHE:CE2	1:A:528:THR:HG23	0.48	2.43	16	2
1:A:536:ILE:CG2	1:A:559:GLU:HB3	0.47	2.39	13	9
1:A:525:VAL:O	1:A:568:VAL:HG23	0.47	2.09	5	5
1:A:527:ARG:HB2	1:A:567:ILE:O	0.46	2.11	15	1
1:A:546:ALA:HB2	1:A:585:LYS:HB3	0.46	1.87	7	1
1:A:523:VAL:HG11	1:A:642:LEU:HD22	0.45	1.87	16	6
1:A:563:GLN:HB2	1:A:566:GLU:OE1	0.44	2.12	5	1
1:A:539:TYR:HB3	1:A:591:ILE:HG22	0.44	1.90	9	1
1:A:524:LYS:HB3	1:A:568:VAL:HG21	0.43	1.90	3	1
1:A:563:GLN:H	1:A:566:GLU:HB2	0.43	1.74	12	1
1:A:567:ILE:HG13	1:A:568:VAL:H	0.43	1.72	19	6
1:A:515:SER:HB2	1:A:518:ILE:HB	0.42	1.91	14	2
1:A:515:SER:HA	1:A:647:GLU:O	0.42	2.15	19	3
1:A:547:ARG:HD2	1:A:551:GLU:OE2	0.42	2.14	17	2
1:A:542:ILE:O	1:A:587:PHE:HB2	0.42	2.14	9	2
1:A:516:GLU:HG3	1:A:517:SER:N	0.42	2.29	16	1
1:A:527:ARG:CZ	1:A:562:PHE:HB3	0.41	2.46	5	1
1:A:533:GLY:O	1:A:563:GLN:HA	0.41	2.15	5	1
1:A:523:VAL:HG21	1:A:642:LEU:HD21	0.41	1.92	17	1
1:A:504:ILE:HG23	1:A:637:GLY:CA	0.41	2.45	2	1
1:A:593:GLU:CD	1:A:593:GLU:H	0.41	2.19	12	1
1:A:519:GLY:O	1:A:574:LYS:HA	0.41	2.15	19	1
1:A:638:GLU:HG2	1:A:639:HIS:CD2	0.41	2.51	3	1
1:A:594:PRO:HG2	1:A:634:PRO:O	0.40	2.16	13	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	102/164 (62%)	96±1 (94±1%)	5±2 (5±1%)	0±1 (0±1%)	38	78
All	All	2040/3280 (62%)	1926 (94%)	105 (5%)	9 (0%)	38	78

All 4 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	567	ILE	3
1	A	544	GLY	3
1	A	502	ALA	2
1	A	550	GLY	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	88/146 (60%)	82±1 (93±1%)	6±1 (7±1%)	20	69
All	All	1760/2920 (60%)	1643 (93%)	117 (7%)	20	69

All 21 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	521	MET	20
1	A	589	LEU	20
1	A	636	LEU	19
1	A	554	GLU	10
1	A	569	LYS	8
1	A	545	THR	6
1	A	540	LYS	5
1	A	528	THR	4
1	A	635	ILE	3
1	A	516	GLU	3
1	A	509	GLU	3
1	A	508	GLU	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	543	GLU	2
1	A	570	THR	2
1	A	596	LEU	2
1	A	515	SER	2
1	A	585	LYS	2
1	A	517	SER	1
1	A	647	GLU	1
1	A	566	GLU	1
1	A	564	ASN	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)

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 (i)

No chemical shift data were provided