Full wwPDB NMR Structure Validation Report (i)

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Title	:	NMR solution structure ensemble of 3-4D mutant domain 11 IGF2R
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Deposited on	:	2013-04-09

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:

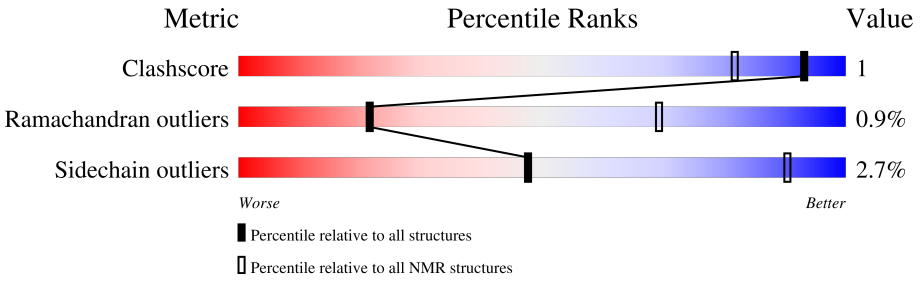
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 85%.

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	142	80% • 18%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 17 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:1516-A:1542, A:1547-A:1598, A:1604-A:1616, A:1623-A:1646 (116)	0.81	17

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 6 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2129 atoms, of which 1051 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Insulin-like growth factor 2 receptor variant.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	142	2129	676	1051	187	204	11	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1543	ALA	SER	ENGINEERED MUTATION	UNP Q59EZ3
A	1544	LYS	GLU	ENGINEERED MUTATION	UNP Q59EZ3
A	1545	GLY	LYS	ENGINEERED MUTATION	UNP Q59EZ3
A	1546	TRP	GLY	ENGINEERED MUTATION	UNP Q59EZ3
A	1547	GLY	LEU	ENGINEERED MUTATION	UNP Q59EZ3
A	1648	LEU	GLN	ENGINEERED MUTATION	UNP Q59EZ3

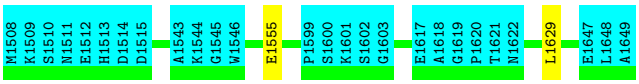
4 Residue-property plots (i)

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: Insulin-like growth factor 2 receptor variant

Chain A:



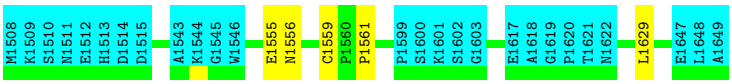
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Insulin-like growth factor 2 receptor variant

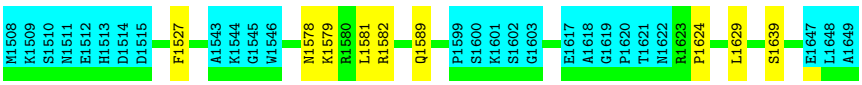
Chain A:



4.2.2 Score per residue for model 2

• Molecule 1: Insulin-like growth factor 2 receptor variant

Chain A:



4.2.3 Score per residue for model 3

- Molecule 1: Insulin-like growth factor 2 receptor variant

Chain A: 76% 5% • 18%

M1508 K1509 S1510 N1511 E1512 H1513 D1514 D1515 A1543 K1544 G1545 W1546 G1547 E1555 P1561 R1580 P1599 S1600 K1601 S1602 G1603 L1604 C1614 E1617 A1618 G1619 P1620 T1621 N1622 L1629 T1642 E1647 L1648 A1649

4.2.4 Score per residue for model 4

- Molecule 1: Insulin-like growth factor 2 receptor variant

Chain A: 77% 5% 18%

M1508 K1509 S1510 N1511 E1512 H1513 D1514 D1515 D1528 R1535 A1536 G1537 A1543 K1544 G1545 W1546 G1547 M1550 N1556 P1599 S1600 K1601 S1602 G1603 E1617 A1618 G1619 P1620 T1621 N1622 L1629 E1647 L1648 A1649

4.2.5 Score per residue for model 5

- Molecule 1: Insulin-like growth factor 2 receptor variant

Chain A: 77% • 18%

M1508 K1509 S1510 N1511 E1512 H1513 D1514 D1515 C1516 Q1517 F1527 S1533 A1543 K1544 G1545 W1546 I1552 N1558 P1561 P1599 S1600 K1601 S1602 G1603 E1617 A1618 G1619 P1620 T1621 N1622 E1647 L1648 A1649

4.2.6 Score per residue for model 6

- Molecule 1: Insulin-like growth factor 2 receptor variant

Chain A: 70% 11% • 18%

M1508 K1509 S1510 N1511 E1512 H1513 D1514 D1515 C1516 T1523 S1533 A1543 K1544 G1545 W1546 I1552 E1555 C1559 R1571 A1577 N1578 K1579 Y1583 Q1586 P1599 S1600 K1601 S1602 G1603 L1604 S1605 R1615 P1616 E1617 A1618 G1619 P1620 T1621 N1622 M1625 L1629 E1647 L1648 A1649

4.2.7 Score per residue for model 7

- Molecule 1: Insulin-like growth factor 2 receptor variant

Chain A: 73% 8% 18%

M1508 K1509 S1510 N1511 E1512 H1513 D1514 D1515 C1516 F1527 D1528 L1529 G1537 A1543 K1544 G1545 W1546 M1550 E1555 P1561 K1579 L1588 P1599 S1600 K1601 S1602 G1603 E1617 A1618 G1619 P1620 T1621 N1622 L1629 H1641 E1647 L1648 A1649

4.2.8 Score per residue for model 8

- Molecule 1: Insulin-like growth factor 2 receptor variant

Chain A: 75% 6% 18%

M1508 K1509 S1510 N1511 E1512 H1513 D1514 D1515 T1539 A1543 K1544 G1545 W1546 G1547 V1548 E1555 P1561 V1574 Y1583 Q1586 P1599 S1600 K1601 S1602 G1603 Y1606 E1617 A1618 G1619 P1620 T1621 N1622 L1629 E1647 L1648 A1649

4.2.9 Score per residue for model 9

- Molecule 1: Insulin-like growth factor 2 receptor variant

Chain A: 77% • 18%

M1508 K1509 S1510 N1511 E1512 H1513 D1514 D1515 A1543 K1544 G1545 W1546 V1574 Y1583 Q1586 P1599 S1600 K1601 S1602 G1603 Y1606 C1614 E1617 A1618 G1619 P1620 T1621 N1622 L1629 E1647 L1648 A1649

4.2.10 Score per residue for model 10

- Molecule 1: Insulin-like growth factor 2 receptor variant

Chain A: 75% 7% 18%

M1508 K1509 S1510 N1511 E1512 H1513 D1514 D1515 R1535 A1543 K1544 G1545 W1546 E1555 N1556 V1574 P1599 S1600 K1601 S1602 G1603 L1604 S1605 Y1606 E1617 A1618 G1619 P1620 T1621 N1622 L1629 P1643 C1646 E1647 L1648 A1649

4.2.11 Score per residue for model 11

- Molecule 1: Insulin-like growth factor 2 receptor variant

Chain A: 77% • • 18%

M1508 K1509 S1510 N1511 E1512 H1513 D1514 D1515 R1535 A1543 K1544 G1545 W1546 G1547 E1555 N1556 P1561 S1596 P1599 S1600 K1601 S1602 G1603 L1604 S1605 E1617 A1618 G1619 P1620 T1621 N1622 E1647 L1648 A1649

4.2.12 Score per residue for model 12

- Molecule 1: Insulin-like growth factor 2 receptor variant

Chain A: 76% 5% • 18%

M1508 K1509 S1510 N1511 E1512 H1513 D1514 D1515 C1516 Q1517 F1527 A1543 K1544 G1545 W1546 E1555 N1578 K1579 P1599 S1600 K1601 S1602 G1603 C1614 R1615 P1616 E1617 A1618 G1619 P1620 T1621 N1622 L1629 E1647 L1648 A1649

4.2.13 Score per residue for model 13

• Molecule 1: Insulin-like growth factor 2 receptor variant

Chain A: 75% 6% 18%

M1508 K1509 S1510 N1511 E1512 H1513 D1514 D1515 S1533 A1543 K1544 G1545 W1546 I1552 E1555 P1599 S1600 K1601 S1602 G1603 L1604 S1605 Y1606 K1607 E1617 A1618 G1619 P1620 T1621 N1622 L1629 C1634 T1635 E1647 L1648 A1649

4.2.14 Score per residue for model 14

• Molecule 1: Insulin-like growth factor 2 receptor variant

Chain A: 79% • 18%

M1508 K1509 S1510 N1511 E1512 H1513 D1514 D1515 A1543 K1544 G1545 W1546 N1578 L1581 L1588 P1599 S1600 K1601 S1602 G1603 E1617 A1618 G1619 P1620 T1621 N1622 L1629 E1647 L1648 A1649

4.2.15 Score per residue for model 15

• Molecule 1: Insulin-like growth factor 2 receptor variant

Chain A: 75% 6% 18%

M1508 K1509 S1510 N1511 E1512 H1513 D1514 D1515 S1533 A1543 K1544 G1545 W1546 I1552 E1555 A1577 N1578 K1593 P1599 S1600 K1601 S1602 G1603 C1614 E1617 A1618 G1619 P1620 T1621 N1622 L1629 T1642 E1647 L1648 A1649

4.2.16 Score per residue for model 16

• Molecule 1: Insulin-like growth factor 2 receptor variant

Chain A: 76% 6% 18%

M1508 K1509 S1510 N1511 E1512 H1513 D1514 D1515 S1530 S1533 A1543 K1544 G1545 W1546 G1547 R1571 Y1583 Q1586 P1599 S1600 K1601 S1602 G1603 R1615 P1616 E1617 A1618 G1619 P1620 T1621 N1622 L1629 E1647 L1648 A1649

4.2.17 Score per residue for model 17 (medoid)

• Molecule 1: Insulin-like growth factor 2 receptor variant

Chain A: 79% • 18%

M1508 K1509 S1510 N1511 E1512 H1513 D1514 D1515 A1543 K1544 G1545 W1546 G1547 V1548 C1566 P1599 S1600 K1601 S1602 G1603 C1614 E1617 A1618 G1619 P1620 T1621 N1622 T1642 E1647 L1648 A1649

4.2.18 Score per residue for model 18

- Molecule 1: Insulin-like growth factor 2 receptor variant

Chain A: 75% 6% 18%

M1508 K1509 S1510 N1511 E1512 H1513 D1514 D1515 C1516 Q1517 F1527 R1535 A1543 K1544 G1545 W1546 N1556 T1570 K1579 D1594 P1599 S1600 K1601 S1602 G1603 L1604 E1617 A1618 G1619 P1620 T1621 N1622 L1629 E1647 L1648 A1649

4.2.19 Score per residue for model 19

- Molecule 1: Insulin-like growth factor 2 receptor variant

Chain A: 71% 11% 18%

M1508 K1509 S1510 N1511 E1512 H1513 D1514 D1515 C1516 Q1517 L1526 L1529 R1535 A1536 G1537 A1543 K1544 G1545 W1546 G1547 M1550 E1555 N1556 P1599 S1600 K1601 S1602 G1603 C1614 E1617 A1618 G1619 P1620 T1621 N1622 R1623 P1624 L1629 S1639 T1642 E1647 L1648 A1649

4.2.20 Score per residue for model 20

- Molecule 1: Insulin-like growth factor 2 receptor variant

Chain A: 75% 6% 18%

M1508 K1509 S1510 N1511 E1512 H1513 D1514 D1515 A1543 K1544 G1545 W1546 G1547 E1555 P1561 A1577 N1578 L1581 P1599 S1600 K1601 S1602 G1603 L1604 E1617 A1618 G1619 P1620 T1621 N1622 L1629 H1641 E1647 L1648 A1649

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *DGSA-distance geometry simulated annealing*.

Of the 250 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	refinement	2.2
ARIA	structure solution	2.2
CING	refinement	iCing
TALOS	geometry optimization	TALOS+

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	1563
Number of shifts mapped to atoms	1563
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	85%

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	0.1±0.2
All	All	0	1

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	1580	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	885	874	872	2±1
All	All	17700	17480	17440	47

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 1.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1574:VAL:HG23	1:A:1606:TYR:HB3	0.62	1.72	8	3
1:A:1517:GLN:HA	1:A:1527:PHE:O	0.60	1.96	12	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1516:CYS:SG	1:A:1529:LEU:HB2	0.58	2.38	19	2
1:A:1643:PRO:HA	1:A:1646:CYS:SG	0.57	2.40	10	1
1:A:1614:CYS:HA	1:A:1642:THR:O	0.53	2.04	17	4
1:A:1533:SER:HA	1:A:1552:ILE:O	0.52	2.04	13	4
1:A:1555:GLU:OE1	1:A:1561:PRO:HA	0.50	2.06	11	1
1:A:1614:CYS:O	1:A:1615:ARG:HD2	0.50	2.06	12	1
1:A:1537:GLY:HA3	1:A:1550:MET:O	0.48	2.06	19	3
1:A:1615:ARG:HA	1:A:1615:ARG:NE	0.47	2.24	16	2
1:A:1581:LEU:HD11	1:A:1588:LEU:HB3	0.47	1.87	14	1
1:A:1535:ARG:O	1:A:1556:ASN:HA	0.47	2.10	10	5
1:A:1583:TYR:CZ	1:A:1586:GLN:HA	0.46	2.46	8	3
1:A:1548:VAL:HA	1:A:1566:CYS:O	0.46	2.10	17	1
1:A:1607:LYS:O	1:A:1635:THR:HA	0.46	2.11	13	1
1:A:1606:TYR:CD2	1:A:1634:CYS:HB3	0.45	2.47	13	1
1:A:1596:SER:O	1:A:1605:SER:HA	0.45	2.11	11	1
1:A:1516:CYS:SG	1:A:1579:LYS:HB2	0.45	2.52	6	1
1:A:1624:PRO:HA	1:A:1639:SER:O	0.44	2.12	19	2
1:A:1583:TYR:CE1	1:A:1586:GLN:HA	0.44	2.48	6	1
1:A:1539:THR:HA	1:A:1548:VAL:O	0.42	2.14	8	1
1:A:1556:ASN:HB3	1:A:1559:CYS:SG	0.42	2.55	1	1
1:A:1559:CYS:SG	1:A:1571:ARG:HB3	0.41	2.54	6	1
1:A:1517:GLN:HB2	1:A:1526:LEU:HD11	0.41	1.92	19	1
1:A:1582:ARG:NH2	1:A:1589:GLN:HG2	0.41	2.30	2	1
1:A:1530:SER:HA	1:A:1533:SER:OG	0.41	2.16	16	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	116/142 (82%)	110±2 (95±1%)	5±1 (4±1%)	1±1 (1±1%)	21	69
All	All	2320/2840 (82%)	2196 (95%)	103 (4%)	21 (1%)	21	69

All 6 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	1561	PRO	6
1	A	1547	GLY	6
1	A	1577	ALA	3
1	A	1605	SER	3
1	A	1614	CYS	2
1	A	1594	ASP	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	100/120 (83%)	97±2 (97±2%)	3±2 (3±2%)	48 90
All	All	2000/2400 (83%)	1946 (97%)	54 (3%)	48 90

All 14 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	1629	LEU	17
1	A	1555	GLU	11
1	A	1604	LEU	6
1	A	1578	ASN	5
1	A	1579	LYS	4
1	A	1581	LEU	2
1	A	1528	ASP	2
1	A	1558	ASN	1
1	A	1523	THR	1
1	A	1625	MET	1
1	A	1588	LEU	1
1	A	1593	LYS	1
1	A	1571	ARG	1
1	A	1570	THR	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)

The completeness of assignment taking into account all chemical shift lists is 85% for the well-defined parts and 85% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

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	1563
Number of shifts mapped to atoms	1563
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
$^{13}C_{\alpha}$	142	-0.27 ± 0.12	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	129	-0.21 ± 0.22	None needed (< 0.5 ppm)
$^{13}C'$	132	-0.44 ± 0.14	None needed (< 0.5 ppm)
^{15}N	132	-0.42 ± 0.42	None needed (< 0.5 ppm)

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 85%, i.e. 1292 atoms were assigned a chemical shift out of a possible 1526. 0 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	568/576 (99%)	235/235 (100%)	224/232 (97%)	109/109 (100%)
Sidechain	620/817 (76%)	377/536 (70%)	228/249 (92%)	15/32 (47%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	104/133 (78%)	58/64 (91%)	45/64 (70%)	1/5 (20%)
Overall	1292/1526 (85%)	670/835 (80%)	497/545 (91%)	125/146 (86%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 85%, i.e. 1560 atoms were assigned a chemical shift out of a possible 1831. 0 out of 21 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	693/705 (98%)	287/288 (100%)	274/284 (96%)	132/133 (99%)
Sidechain	749/973 (77%)	459/635 (72%)	273/301 (91%)	17/37 (46%)
Aromatic	118/153 (77%)	66/74 (89%)	50/71 (70%)	2/8 (25%)
Overall	1560/1831 (85%)	812/997 (81%)	597/656 (91%)	151/178 (85%)

7.1.4 Statistically unusual chemical shifts (i)

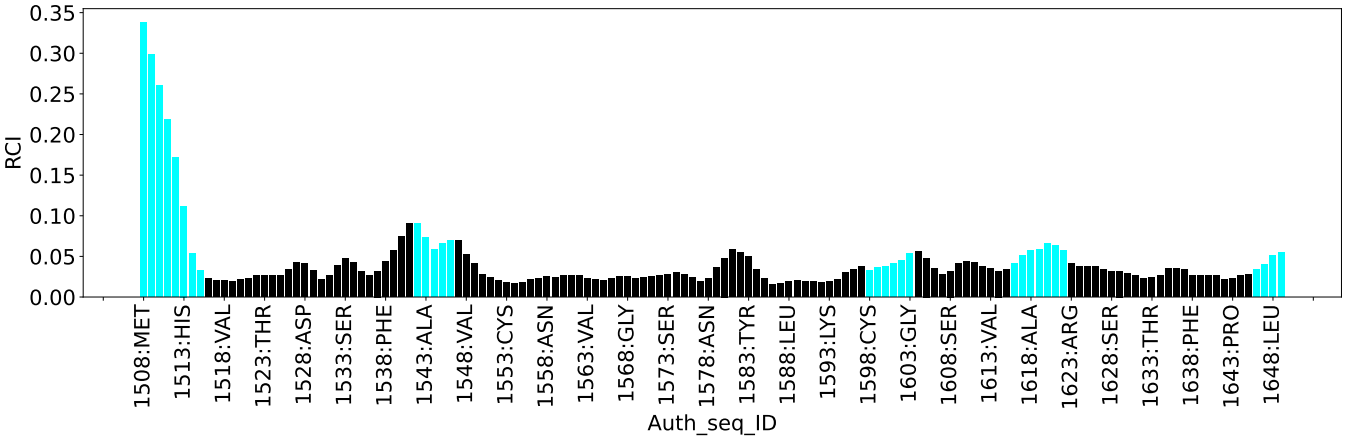
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	1635	THR	HG21	-0.02	0.08 – 2.19	-5.5
1	A	1529	LEU	HD11	-0.66	-0.61 – 2.12	-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
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
1508:MET
1513:HIS
1518:VAL
1523:THR
1528:ASP
1533:SER
1538:PHE
1543:ALA
1548:VAL
1553:CYS
1558:ASN
1563:VAL
1568:GLY
1573:SER
1578:ASN
1583:TYR
1588:LEU
1593:LYS
1598:CYS
1603:GLY
1608:SER
1613:VAL
1618:ALA
1623:ARG
1628:SER
1633:THR
1638:PHE
1643:PRO
1648:LEU
Auth_seq_ID