



# Full wwPDB NMR Structure Validation Report ⓘ

Feb 13, 2017 – 12:10 am GMT

PDB ID : 2LLA  
Title : NMR solution structure ensemble of domain 11 of the echidna M6P/IGF2R receptor  
Authors : Strickland, M.; Crump, M.P.; Williams, C.; Rezgui, D.; Ellis, R.Z.; Hoppe, H.; Frago, S.; Prince, S.N.; Zaccheo, O.J.; Forbes, B.E.; Jones, E.; Hassan, A.Z.; Wattana-Amorn, P.  
Deposited on : 2011-11-05

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

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

Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	trunk28760
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

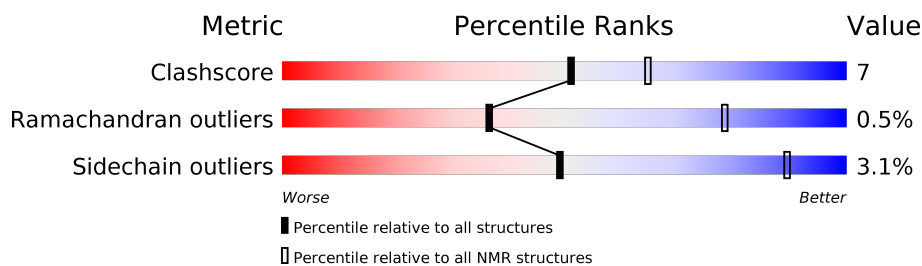
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 91%.

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	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

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  $\geq 3$ , 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	140	

## 2 Ensemble composition and analysis

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: *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:1493-A:1625 (133)	0.64	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 4 single-model clusters were found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2111 atoms, of which 1041 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Mannose-6-phosphate/insulin-like growth factor II receptor.

Mol	Chain	Residues	Atoms						Trace
1	A	140	Total	C	H	N	O	S	0
			2111	673	1041	178	210	9	

There are 2 discrepancies between the modelled and reference sequences:

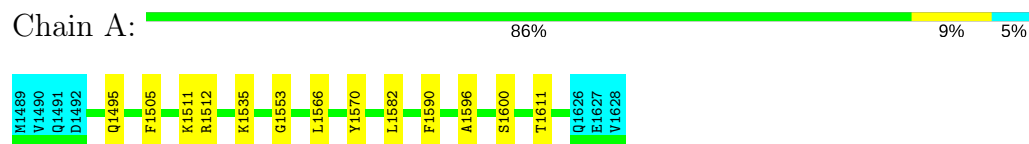
Chain	Residue	Modelled	Actual	Comment	Reference
A	1489	MET	-	EXPRESSION TAG	UNP Q95LC7
A	1607	VAL	MET	CONFLICT	UNP Q95LC7

## 4 Residue-property plots

### 4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA 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: Mannose-6-phosphate/insulin-like growth factor II receptor

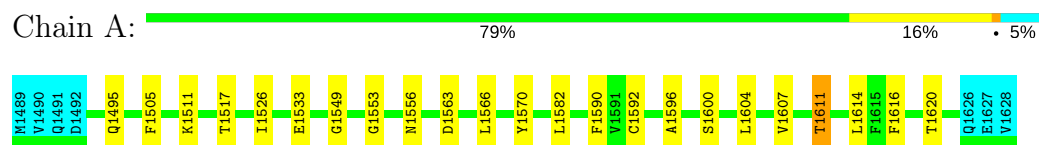


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

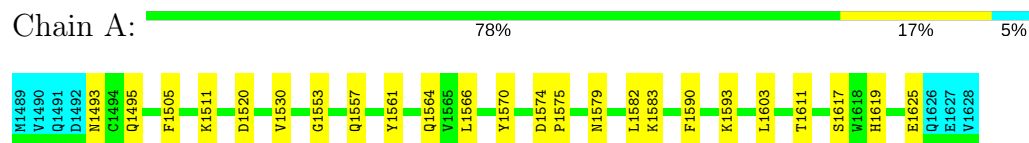
#### 4.2.1 Score per residue for model 1

- Molecule 1: Mannose-6-phosphate/insulin-like growth factor II receptor



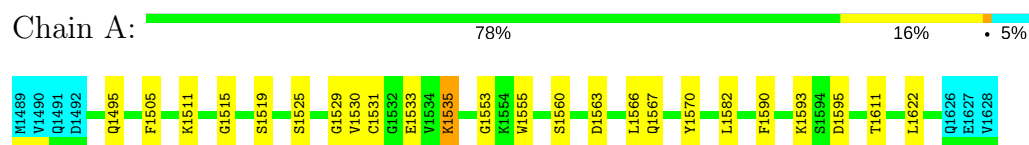
#### 4.2.2 Score per residue for model 2

- Molecule 1: Mannose-6-phosphate/insulin-like growth factor II receptor



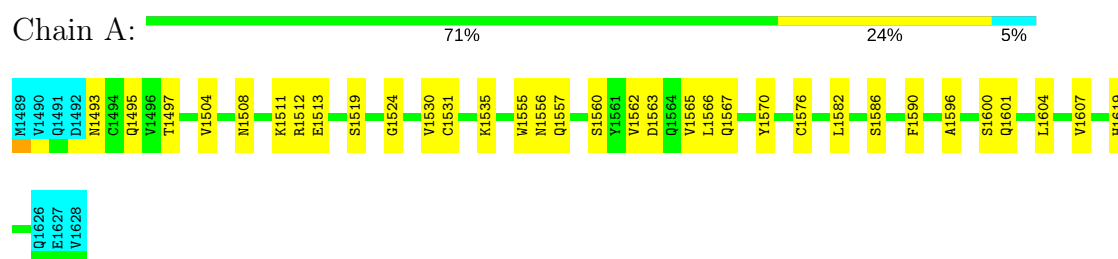
### 4.2.3 Score per residue for model 3

- Molecule 1: Mannose-6-phosphate/insulin-like growth factor II receptor



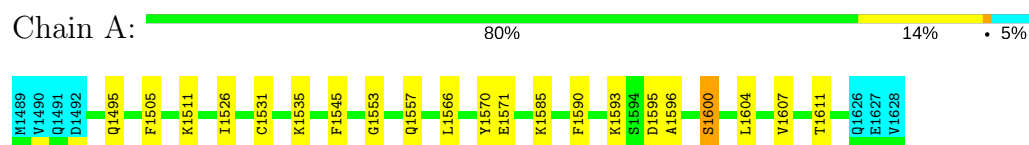
### 4.2.4 Score per residue for model 4

- Molecule 1: Mannose-6-phosphate/insulin-like growth factor II receptor



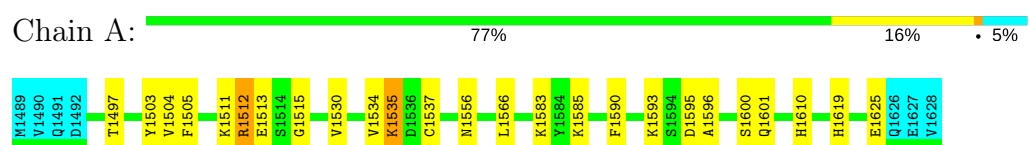
### 4.2.5 Score per residue for model 5

- Molecule 1: Mannose-6-phosphate/insulin-like growth factor II receptor



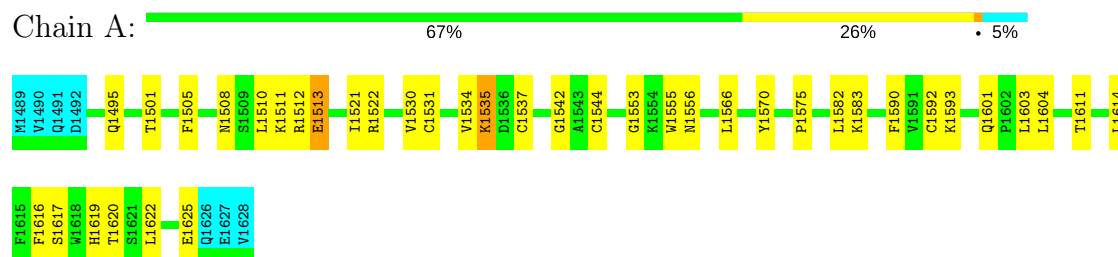
### 4.2.6 Score per residue for model 6

- Molecule 1: Mannose-6-phosphate/insulin-like growth factor II receptor



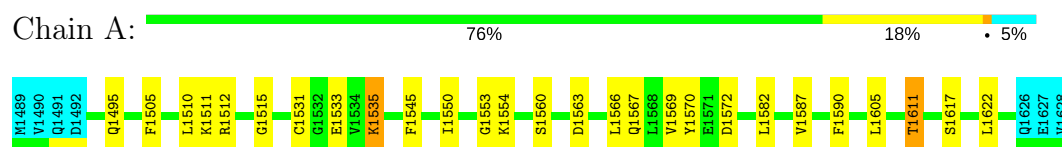
### 4.2.7 Score per residue for model 7

- Molecule 1: Mannose-6-phosphate/insulin-like growth factor II receptor



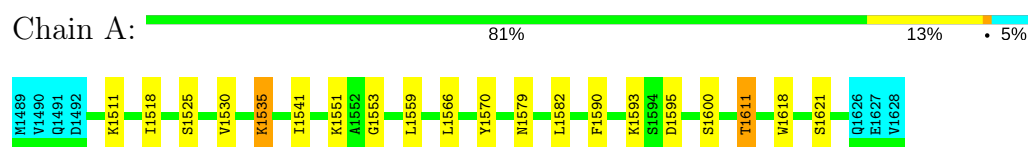
#### 4.2.8 Score per residue for model 8

- Molecule 1: Mannose-6-phosphate/insulin-like growth factor II receptor



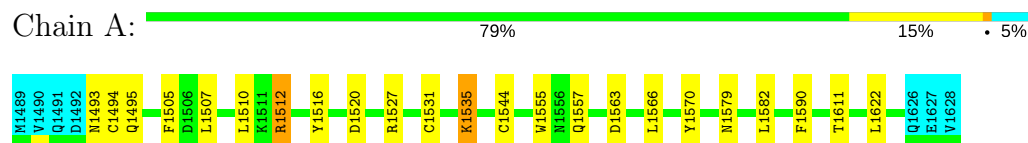
#### 4.2.9 Score per residue for model 9

- Molecule 1: Mannose-6-phosphate/insulin-like growth factor II receptor



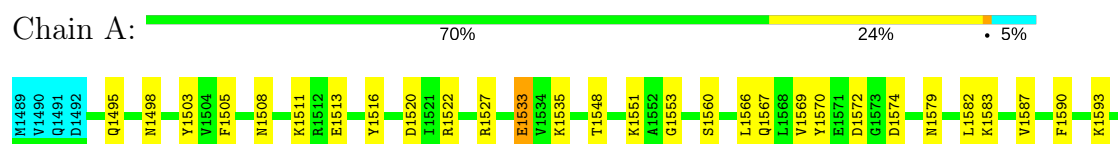
#### 4.2.10 Score per residue for model 10

- Molecule 1: Mannose-6-phosphate/insulin-like growth factor II receptor



#### 4.2.11 Score per residue for model 11

- Molecule 1: Mannose-6-phosphate/insulin-like growth factor II receptor





#### 4.2.12 Score per residue for model 12

- Molecule 1: Mannose-6-phosphate/insulin-like growth factor II receptor

Chain A: 83% 11% 5%



#### 4.2.13 Score per residue for model 13

- Molecule 1: Mannose-6-phosphate/insulin-like growth factor II receptor

Chain A: 76% 19% 5%



#### 4.2.14 Score per residue for model 14

- Molecule 1: Mannose-6-phosphate/insulin-like growth factor II receptor

Chain A: 76% 19% 5%



#### 4.2.15 Score per residue for model 15

- Molecule 1: Mannose-6-phosphate/insulin-like growth factor II receptor

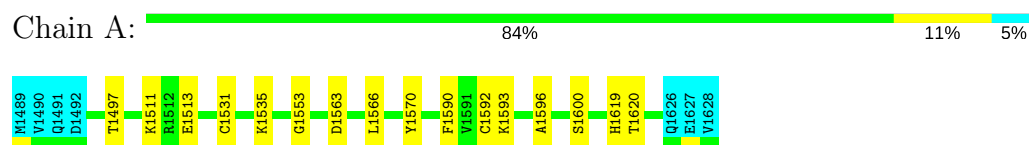
Chain A: 76% 19% 5%





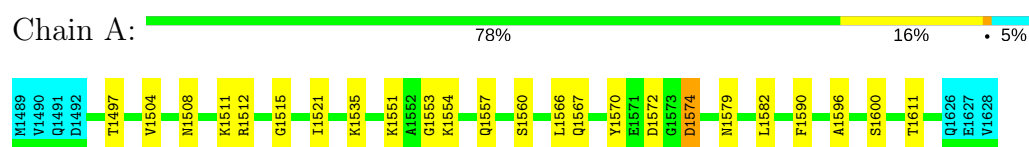
#### 4.2.16 Score per residue for model 16

- Molecule 1: Mannose-6-phosphate/insulin-like growth factor II receptor



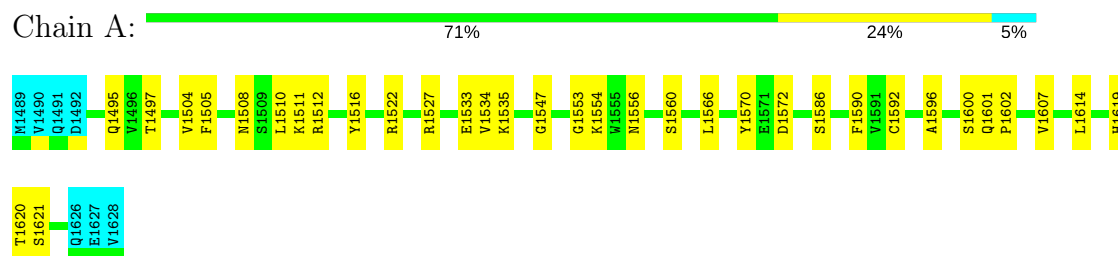
#### 4.2.17 Score per residue for model 17 (medoid)

- Molecule 1: Mannose-6-phosphate/insulin-like growth factor II receptor



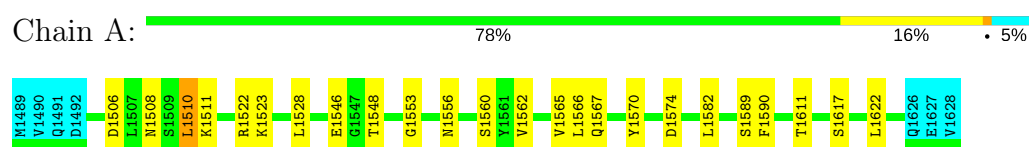
#### 4.2.18 Score per residue for model 18

- Molecule 1: Mannose-6-phosphate/insulin-like growth factor II receptor



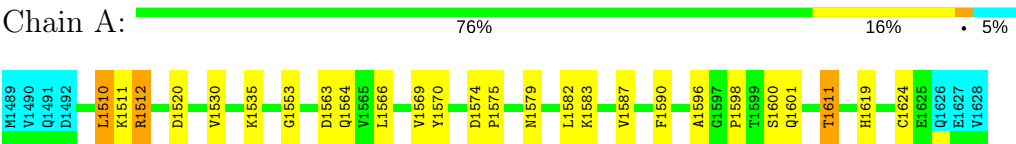
#### 4.2.19 Score per residue for model 19

- Molecule 1: Mannose-6-phosphate/insulin-like growth factor II receptor



#### 4.2.20 Score per residue for model 20

- Molecule 1: Mannose-6-phosphate/insulin-like growth factor II receptor



## 5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *STRUCTURES WITH THE LOWEST ENER*.

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
ProcheckNMR	refinement	
Analysis	refinement	2.1

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)	2lla_cs.str
Number of chemical shift lists	1
Total number of shifts	1680
Number of shifts mapped to atoms	1680
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	91%

No validations of the models with respect to experimental NMR restraints is performed at this time.

## 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±0.4
All	All	0	3

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	1522	ARG	Sidechain	2
1	A	1512	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	1012	986	983	13±4
All	All	20240	19720	19660	268

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 7.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1582:LEU:HD13	1:A:1611:THR:HA	0.76	1.56	9	14
1:A:1596:ALA:HB1	1:A:1600:SER:HA	0.76	1.58	6	10
1:A:1566:LEU:HB3	1:A:1590:PHE:HB2	0.73	1.60	7	9
1:A:1553:GLY:HA3	1:A:1570:TYR:HB3	0.73	1.57	18	17
1:A:1579:ASN:HB2	1:A:1582:LEU:HG	0.69	1.64	2	4
1:A:1566:LEU:HB2	1:A:1590:PHE:HB2	0.68	1.65	11	11
1:A:1579:ASN:HB3	1:A:1582:LEU:HG	0.68	1.65	15	5
1:A:1560:SER:HB2	1:A:1567:GLN:HB2	0.66	1.65	3	4
1:A:1560:SER:HB3	1:A:1567:GLN:HB2	0.65	1.66	19	2
1:A:1601:GLN:HB2	1:A:1619:HIS:HB2	0.63	1.68	4	5
1:A:1494:CYS:HB3	1:A:1507:LEU:HB3	0.62	1.72	10	1
1:A:1512:ARG:HD3	1:A:1534:VAL:HG12	0.62	1.70	18	1
1:A:1497:THR:HG23	1:A:1504:VAL:HG22	0.61	1.71	6	3
1:A:1593:LYS:HB2	1:A:1619:HIS:HB3	0.60	1.73	11	3
1:A:1522:ARG:HH22	1:A:1607:VAL:HG11	0.60	1.55	18	1
1:A:1601:GLN:HG3	1:A:1619:HIS:HB2	0.59	1.71	11	2
1:A:1604:LEU:HD21	1:A:1607:VAL:HG23	0.59	1.74	5	3
1:A:1526:ILE:HB	1:A:1545:PHE:HD1	0.58	1.57	5	1
1:A:1575:PRO:HA	1:A:1583:LYS:HG2	0.58	1.75	7	3
1:A:1531:CYS:HA	1:A:1555:TRP:NE1	0.58	2.14	3	2
1:A:1590:PHE:HD1	1:A:1618:TRP:HE3	0.58	1.42	9	1
1:A:1535:LYS:H	1:A:1535:LYS:HD3	0.58	1.57	7	2
1:A:1562:VAL:HG23	1:A:1565:VAL:HB	0.57	1.74	15	1
1:A:1593:LYS:HE3	1:A:1595:ASP:HB3	0.57	1.76	9	3
1:A:1531:CYS:HA	1:A:1555:TRP:CZ3	0.56	2.35	4	1
1:A:1561:TYR:CZ	1:A:1564:GLN:HA	0.56	2.36	2	2
1:A:1511:LYS:HB2	1:A:1530:VAL:O	0.56	2.00	3	2
1:A:1526:ILE:HB	1:A:1545:PHE:CD1	0.55	2.37	5	1
1:A:1572:ASP:HA	1:A:1583:LYS:HD3	0.55	1.77	11	2
1:A:1511:LYS:HA	1:A:1530:VAL:HB	0.54	1.78	6	1
1:A:1495:GLN:HA	1:A:1505:PHE:O	0.54	2.03	18	11
1:A:1535:LYS:H	1:A:1535:LYS:HD2	0.53	1.61	15	4
1:A:1521:ILE:HB	1:A:1604:LEU:HD21	0.53	1.79	7	1
1:A:1506:ASP:HB2	1:A:1508:ASN:HD22	0.53	1.64	19	1
1:A:1515:GLY:HA2	1:A:1529:GLY:HA2	0.52	1.80	15	2
1:A:1511:LYS:HD3	1:A:1531:CYS:HB2	0.52	1.81	4	3
1:A:1545:PHE:HB3	1:A:1550:ILE:HG13	0.52	1.81	8	1
1:A:1551:LYS:HD2	1:A:1574:ASP:HB2	0.52	1.82	11	1
1:A:1517:THR:HA	1:A:1526:ILE:O	0.52	2.05	1	1
1:A:1519:SER:HA	1:A:1525:SER:HA	0.51	1.82	3	3
1:A:1592:CYS:HA	1:A:1620:THR:O	0.51	2.04	1	5
1:A:1512:ARG:NE	1:A:1512:ARG:HA	0.51	2.21	7	1

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1603:LEU:HB3	1:A:1617:SER:HB3	0.51	1.82	7	1
1:A:1542:GLY:HA3	1:A:1570:TYR:CE1	0.51	2.41	7	2
1:A:1508:ASN:HA	1:A:1511:LYS:HG3	0.51	1.83	11	4
1:A:1546:GLU:HG3	1:A:1548:THR:HG23	0.51	1.81	19	1
1:A:1551:LYS:HG2	1:A:1574:ASP:OD1	0.51	2.06	17	2
1:A:1576:CYS:HB3	1:A:1582:LEU:HB2	0.51	1.83	4	1
1:A:1569:VAL:HG22	1:A:1587:VAL:HG23	0.51	1.83	20	3
1:A:1516:TYR:O	1:A:1527:ARG:HA	0.50	2.05	18	3
1:A:1564:GLN:HB2	1:A:1624:CYS:SG	0.50	2.46	20	1
1:A:1497:THR:HA	1:A:1503:TYR:O	0.50	2.07	6	1
1:A:1570:TYR:HB2	1:A:1586:SER:HB2	0.50	1.84	4	1
1:A:1582:LEU:HD22	1:A:1611:THR:HG22	0.48	1.86	8	1
1:A:1600:SER:HB3	1:A:1619:HIS:O	0.48	2.08	13	2
1:A:1614:LEU:HB3	1:A:1616:PHE:HE1	0.48	1.67	14	2
1:A:1614:LEU:HB3	1:A:1616:PHE:CE2	0.48	2.43	1	1
1:A:1511:LYS:CD	1:A:1531:CYS:HB2	0.48	2.38	4	2
1:A:1562:VAL:CG2	1:A:1565:VAL:HB	0.48	2.39	15	1
1:A:1494:CYS:SG	1:A:1507:LEU:HB3	0.48	2.48	13	2
1:A:1531:CYS:HA	1:A:1557:GLN:OE1	0.48	2.08	15	1
1:A:1551:LYS:HG3	1:A:1573:GLY:HA2	0.48	1.84	15	1
1:A:1562:VAL:HB	1:A:1565:VAL:HB	0.48	1.84	4	1
1:A:1572:ASP:HA	1:A:1583:LYS:HD2	0.47	1.84	15	1
1:A:1527:ARG:HB3	1:A:1544:CYS:SG	0.47	2.49	10	1
1:A:1534:VAL:HG23	1:A:1537:CYS:HB2	0.47	1.87	7	3
1:A:1590:PHE:CD1	1:A:1618:TRP:HE3	0.47	2.26	9	1
1:A:1614:LEU:HB3	1:A:1616:PHE:CE1	0.47	2.45	7	2
1:A:1562:VAL:O	1:A:1565:VAL:HG12	0.47	2.09	19	1
1:A:1505:PHE:HZ	1:A:1625:GLU:HA	0.46	1.71	6	1
1:A:1497:THR:HB	1:A:1504:VAL:HG22	0.46	1.86	18	1
1:A:1511:LYS:HA	1:A:1530:VAL:HG23	0.46	1.86	7	1
1:A:1511:LYS:CB	1:A:1530:VAL:HB	0.46	2.41	2	2
1:A:1512:ARG:HD3	1:A:1515:GLY:O	0.45	2.12	17	1
1:A:1533:GLU:HB2	1:A:1535:LYS:HD2	0.45	1.89	8	1
1:A:1510:LEU:HB2	1:A:1622:LEU:HD12	0.45	1.88	19	3
1:A:1512:ARG:HG3	1:A:1515:GLY:CA	0.45	2.42	8	1
1:A:1604:LEU:HD11	1:A:1607:VAL:HG23	0.44	1.88	1	1
1:A:1520:ASP:OD2	1:A:1522:ARG:HB2	0.44	2.12	11	1
1:A:1593:LYS:HB3	1:A:1596:ALA:HB2	0.44	1.89	11	1
1:A:1535:LYS:HD3	1:A:1535:LYS:H	0.44	1.72	12	1
1:A:1603:LEU:HB3	1:A:1617:SER:HB2	0.44	1.90	2	1
1:A:1531:CYS:HA	1:A:1557:GLN:HE22	0.44	1.73	10	1

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1493:ASN:HB2	1:A:1495:GLN:HG2	0.44	1.89	10	1
1:A:1512:ARG:HA	1:A:1512:ARG:NE	0.44	2.28	20	1
1:A:1493:ASN:HB2	1:A:1557:GLN:OE1	0.44	2.13	4	1
1:A:1519:SER:HA	1:A:1524:GLY:O	0.43	2.13	4	1
1:A:1604:LEU:HG	1:A:1616:PHE:CE2	0.43	2.48	14	1
1:A:1555:TRP:HA	1:A:1570:TYR:HE1	0.43	1.74	10	1
1:A:1508:ASN:HA	1:A:1511:LYS:HE3	0.43	1.89	19	1
1:A:1605:LEU:HD21	1:A:1617:SER:HB2	0.43	1.90	8	1
1:A:1589:SER:O	1:A:1617:SER:HA	0.43	2.14	19	1
1:A:1533:GLU:O	1:A:1535:LYS:HD3	0.43	2.13	3	1
1:A:1579:ASN:HB3	1:A:1582:LEU:CG	0.43	2.41	15	1
1:A:1523:LYS:HE2	1:A:1607:VAL:HG11	0.43	1.90	13	1
1:A:1508:ASN:O	1:A:1511:LYS:HG2	0.43	2.13	7	2
1:A:1534:VAL:HG21	1:A:1544:CYS:SG	0.43	2.53	7	1
1:A:1518:ILE:O	1:A:1525:SER:HA	0.43	2.14	9	1
1:A:1511:LYS:HE2	1:A:1531:CYS:SG	0.42	2.54	8	1
1:A:1512:ARG:HG3	1:A:1515:GLY:HA2	0.42	1.91	6	1
1:A:1625:GLU:CD	1:A:1625:GLU:H	0.42	2.17	6	1
1:A:1493:ASN:HB2	1:A:1557:GLN:HB2	0.42	1.90	2	1
1:A:1586:SER:HB3	1:A:1614:LEU:HD12	0.42	1.91	18	1
1:A:1535:LYS:HD2	1:A:1535:LYS:H	0.42	1.73	6	2
1:A:1498:ASN:ND2	1:A:1503:TYR:HB3	0.42	2.30	11	1
1:A:1531:CYS:HA	1:A:1555:TRP:CH2	0.42	2.50	7	1
1:A:1511:LYS:HB2	1:A:1530:VAL:HB	0.42	1.92	20	2
1:A:1511:LYS:HD2	1:A:1530:VAL:O	0.42	2.15	20	1
1:A:1554:LYS:HD3	1:A:1572:ASP:O	0.42	2.14	8	1
1:A:1512:ARG:HD2	1:A:1530:VAL:H	0.42	1.75	6	1
1:A:1512:ARG:H	1:A:1530:VAL:HB	0.42	1.75	4	1
1:A:1513:GLU:CD	1:A:1513:GLU:H	0.42	2.19	7	1
1:A:1510:LEU:HD22	1:A:1598:PRO:HA	0.42	1.92	20	1
1:A:1541:ILE:HD12	1:A:1551:LYS:HG2	0.42	1.92	9	1
1:A:1614:LEU:HB3	1:A:1616:PHE:HE2	0.41	1.74	1	1
1:A:1511:LYS:HB2	1:A:1531:CYS:HB2	0.41	1.92	5	1
1:A:1593:LYS:HE3	1:A:1595:ASP:HB2	0.41	1.92	6	1
1:A:1494:CYS:HA	1:A:1559:LEU:HD11	0.41	1.92	13	1
1:A:1533:GLU:HG3	1:A:1535:LYS:HE3	0.41	1.93	18	1
1:A:1541:ILE:HG21	1:A:1544:CYS:SG	0.41	2.55	14	1
1:A:1554:LYS:HG3	1:A:1572:ASP:O	0.41	2.15	18	2
1:A:1563:ASP:O	1:A:1564:GLN:HG2	0.41	2.15	20	1
1:A:1535:LYS:HD2	1:A:1535:LYS:N	0.41	2.31	18	1
1:A:1622:LEU:HD13	1:A:1622:LEU:O	0.41	2.15	11	1

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1580:LEU:H	1:A:1580:LEU:HD22	0.41	1.75	15	1
1:A:1583:LYS:O	1:A:1585:LYS:HD2	0.41	2.16	6	1
1:A:1501:THR:OG1	1:A:1625:GLU:HG2	0.40	2.17	7	1
1:A:1607:VAL:HG13	1:A:1614:LEU:HD23	0.40	1.91	18	1
1:A:1593:LYS:HG2	1:A:1601:GLN:OE1	0.40	2.15	7	1
1:A:1622:LEU:HD23	1:A:1622:LEU:O	0.40	2.16	7	1
1:A:1571:GLU:HA	1:A:1585:LYS:HG2	0.40	1.92	5	1
1:A:1579:ASN:OD1	1:A:1581:HIS:HB3	0.40	2.16	14	1
1:A:1512:ARG:HD3	1:A:1534:VAL:CG1	0.40	2.44	18	1
1:A:1593:LYS:CB	1:A:1619:HIS:HB3	0.40	2.46	14	2
1:A:1533:GLU:CD	1:A:1533:GLU:H	0.40	2.20	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	133/140 (95%)	120±3 (90±2%)	12±2 (9±2%)	1±1 (1±1%)	37	78
All	All	2660/2800 (95%)	2401 (90%)	245 (9%)	14 (1%)	37	78

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	1563	ASP	7
1	A	1600	SER	2
1	A	1547	GLY	2
1	A	1511	LYS	1
1	A	1521	ILE	1
1	A	1549	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	114/121 (94%)	111±1 (97±1%)	4±1 (3±1%)	49	89
All	All	2280/2420 (94%)	2210 (97%)	70 (3%)	49	89

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	1535	LYS	14
1	A	1556	ASN	7
1	A	1611	THR	6
1	A	1574	ASP	5
1	A	1513	GLU	5
1	A	1510	LEU	5
1	A	1557	GLN	4
1	A	1520	ASP	4
1	A	1512	ARG	3
1	A	1528	LEU	3
1	A	1621	SER	2
1	A	1585	LYS	2
1	A	1533	GLU	2
1	A	1625	GLU	1
1	A	1602	PRO	1
1	A	1559	LEU	1
1	A	1560	SER	1
1	A	1622	LEU	1
1	A	1548	THR	1
1	A	1610	HIS	1
1	A	1523	LYS	1

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.5 Carbohydrates [i](#)

There are no carbohydrates 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

The completeness of assignment taking into account all chemical shift lists is 91% for the well-defined parts and 91% for the entire structure.

### 7.1 Chemical shift list 1

File name: 2lla\_cs.str

Chemical shift list name: *assigned\_chem\_shift\_list\_1*

#### 7.1.1 Bookkeeping

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	1680
Number of shifts mapped to atoms	1680
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	139	$0.35 \pm 0.18$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	127	$0.79 \pm 0.14$	Should be applied
$^{13}\text{C}'$	133	$0.17 \pm 0.14$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	133	$-1.04 \pm 0.49$	Should be applied

#### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 91%, i.e. 1411 atoms were assigned a chemical shift out of a possible 1550. 0 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	647/653 (99%)	260/260 (100%)	260/266 (98%)	127/127 (100%)
Sidechain	679/764 (89%)	417/448 (93%)	252/288 (88%)	10/28 (36%)

*Continued on next page...*

Continued from previous page...

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	85/133 (64%)	48/69 (70%)	36/56 (64%)	1/8 (12%)
Overall	1411/1550 (91%)	725/777 (93%)	548/610 (90%)	138/163 (85%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 91%, i.e. 1489 atoms were assigned a chemical shift out of a possible 1636. 0 out of 25 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	678/688 (99%)	273/274 (100%)	272/280 (97%)	133/134 (99%)
Sidechain	726/815 (89%)	446/477 (94%)	268/308 (87%)	12/30 (40%)
Aromatic	85/133 (64%)	48/69 (70%)	36/56 (64%)	1/8 (12%)
Overall	1489/1636 (91%)	767/820 (94%)	576/644 (89%)	146/172 (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.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	1532	GLY	HA3	1.95	5.80 – 2.00	-5.1

#### 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.

Random coil index (RCI) for chain A:

