



# Full wwPDB NMR Structure Validation Report ⓘ

Apr 27, 2016 – 12:32 AM BST

PDB ID : 2L2G  
Title : Solution structure of Opossum Domain 11  
Authors : Williams, C.; Hoppe, H.; Rezgui, D.; Rezgui, M.; Frago, S.; Ellis, R.Z.; Wattana-Amorn, P.; Prince, S.N.; Zaccheo, O.J.; Forbes, B.; Jones, E.Y.; Crump, M.P.; Bassim, A.H.  
Deposited on : 2010-08-18

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.

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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  
Mogul : unknown  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : rb-20027457  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027457

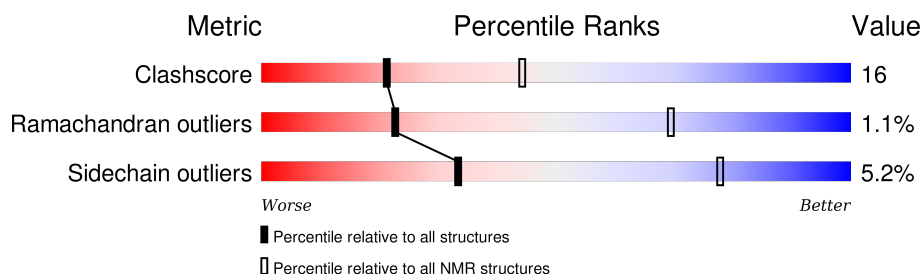
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment 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	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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	151	<div> <div>56%</div> <div>28%</div> <div>13%</div> <div>.</div> </div>

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 10 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:1531-A:1614, A:1620-A:1662 (127)	0.26	10

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 5 clusters and 4 single-model clusters were found.

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

### 3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 2215 atoms, of which 1089 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called IGF2R DOMAIN 11.

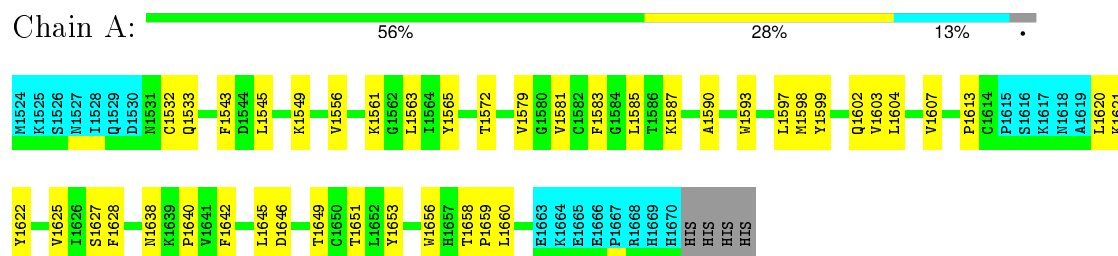
Mol	Chain	Residues	Atoms							Trace
1	A	147	Total	C	H	N	O	S		0
			2215	709	1089	190	217	10		

## 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: IGF2R DOMAIN 11

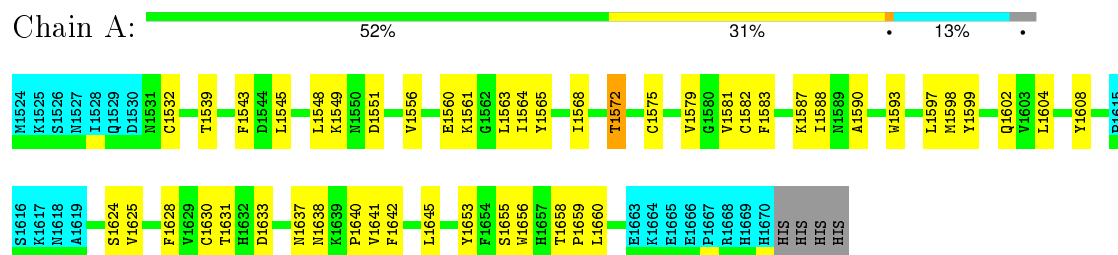


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

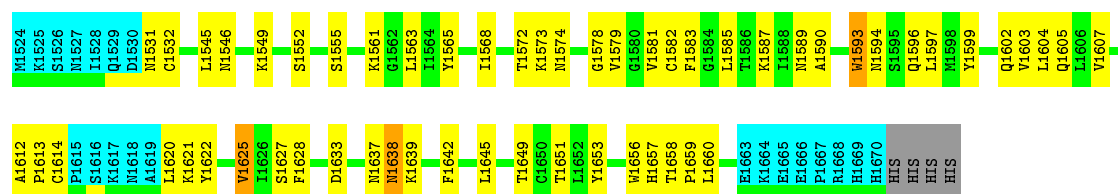
- Molecule 1: IGF2R DOMAIN 11



#### 4.2.2 Score per residue for model 2

- Molecule 1: IGF2R DOMAIN 11





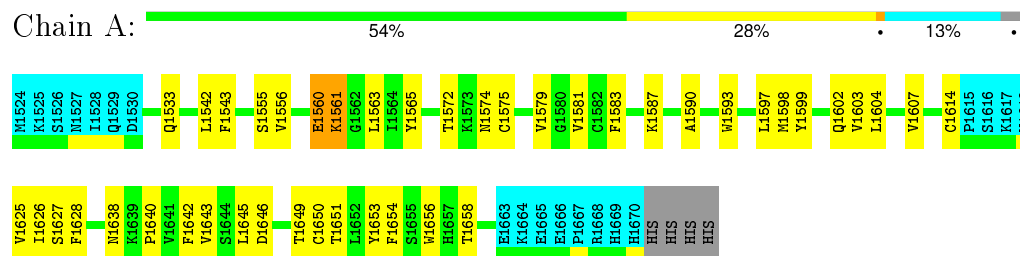
### 4.2.3 Score per residue for model 3

- Molecule 1: IGF2R DOMAIN 11



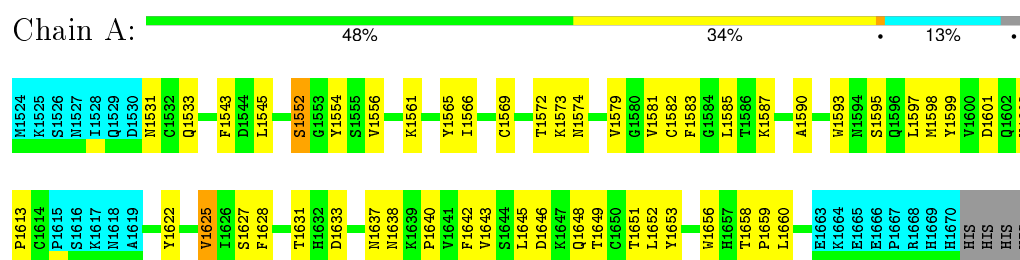
### 4.2.4 Score per residue for model 4

- Molecule 1: IGF2R DOMAIN 11



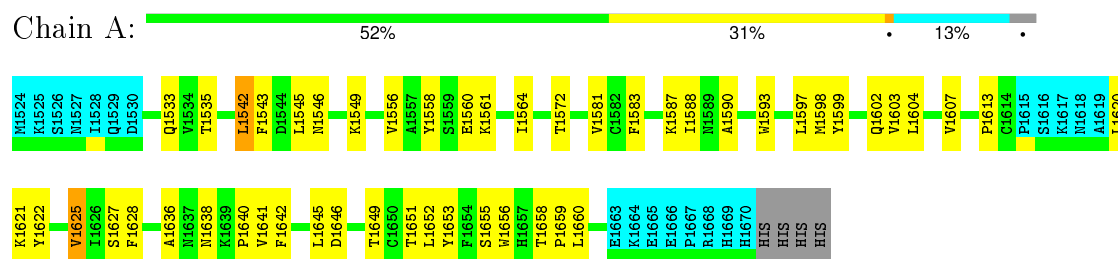
### 4.2.5 Score per residue for model 5

- Molecule 1: IGF2R DOMAIN 11



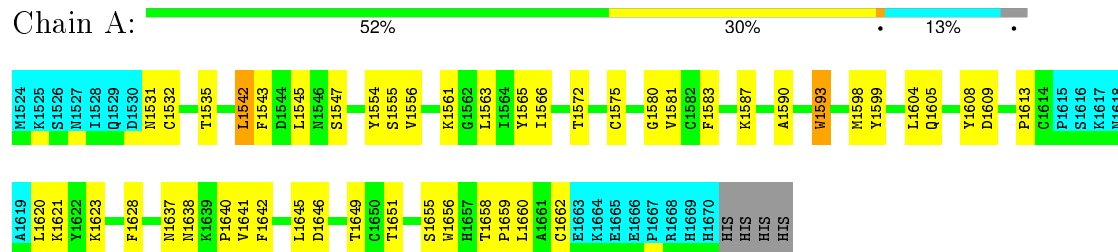
### 4.2.6 Score per residue for model 6

- Molecule 1: IGF2R DOMAIN 11



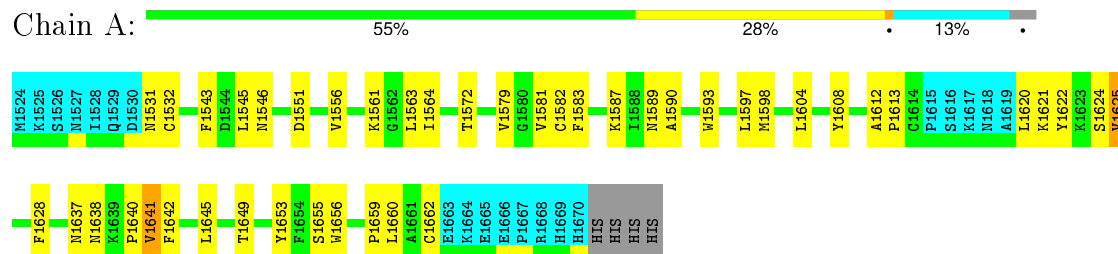
### 4.2.7 Score per residue for model 7

- Molecule 1: IGF2R DOMAIN 11



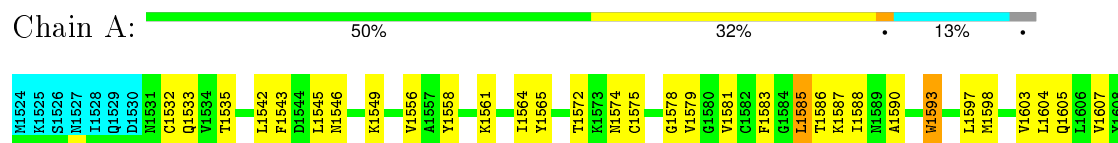
### 4.2.8 Score per residue for model 8

- Molecule 1: IGF2R DOMAIN 11



### 4.2.9 Score per residue for model 9

- Molecule 1: IGF2R DOMAIN 11





#### 4.2.10 Score per residue for model 10 (medoid)

- Molecule 1: IGF2R DOMAIN 11

Chain A: 47% 36% 13%



#### 4.2.11 Score per residue for model 11

- Molecule 1: IGF2R DOMAIN 11

Chain A: 47% 36% 13%



#### 4.2.12 Score per residue for model 12

- Molecule 1: IGF2R DOMAIN 11

Chain A: 60% 25% 13%



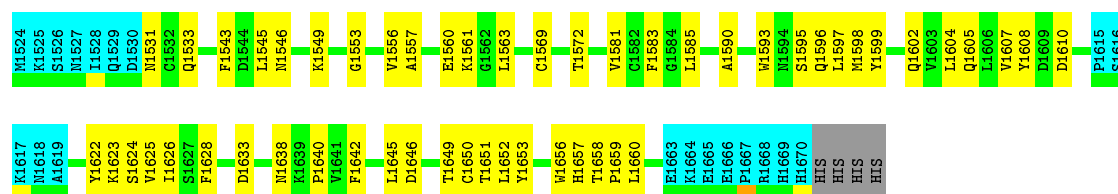
#### 4.2.13 Score per residue for model 13

- Molecule 1: IGF2R DOMAIN 11

Chain A: 50% 34% 13%



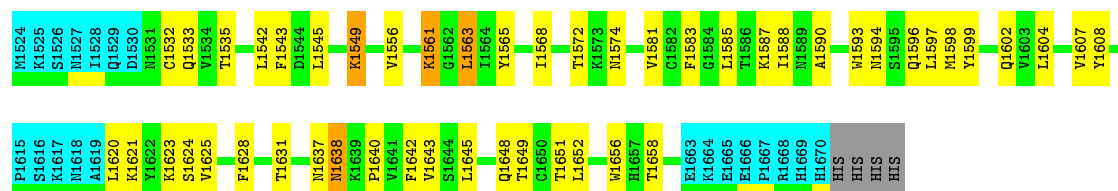




#### 4.2.14 Score per residue for model 14

- Molecule 1: IGF2R DOMAIN 11

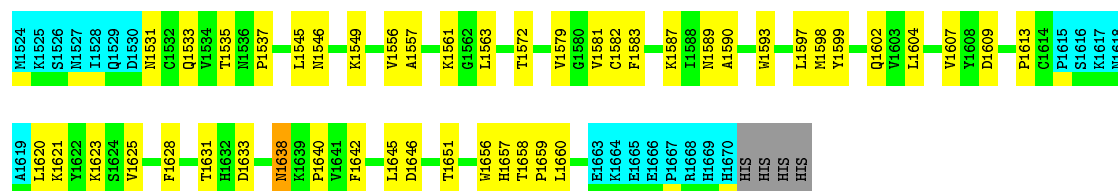
Chain A: 52% 30% 13%



#### 4.2.15 Score per residue for model 15

- Molecule 1: IGF2R DOMAIN 11

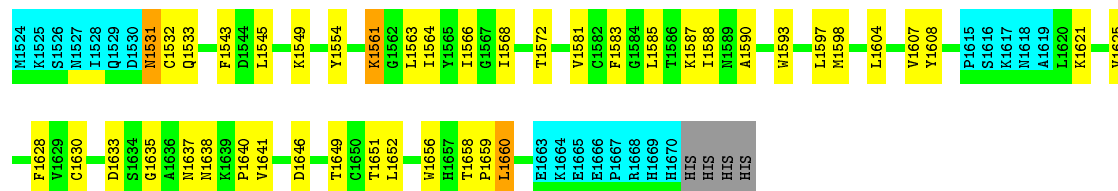
Chain A: 54% 30% 13%



#### 4.2.16 Score per residue for model 16

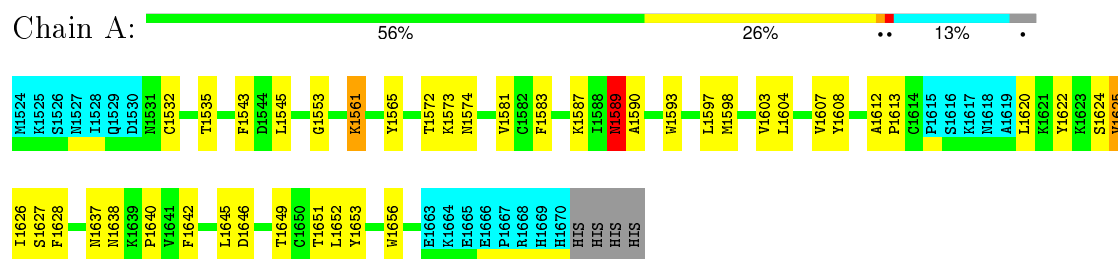
- Molecule 1: IGF2R DOMAIN 11

Chain A: 56% 26% 13%



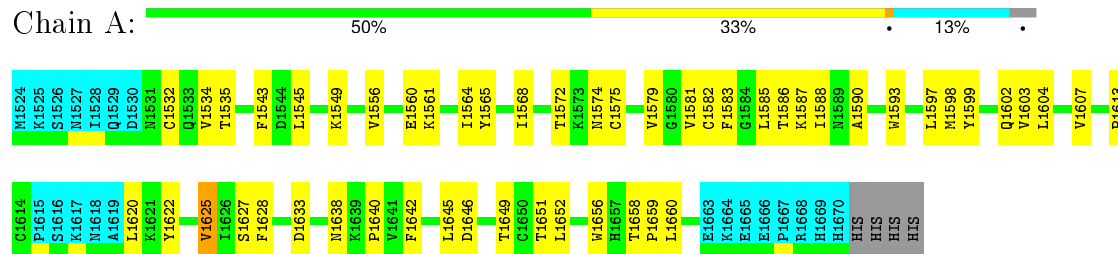
## 4.2.17 Score per residue for model 17

- Molecule 1: IGF2R DOMAIN 11



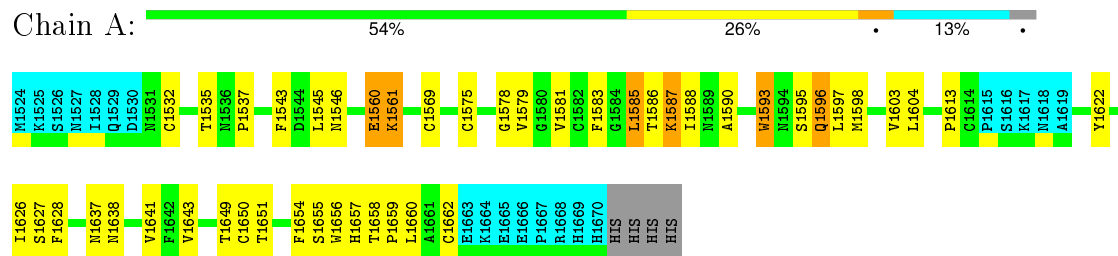
## 4.2.18 Score per residue for model 18

- Molecule 1: IGF2R DOMAIN 11



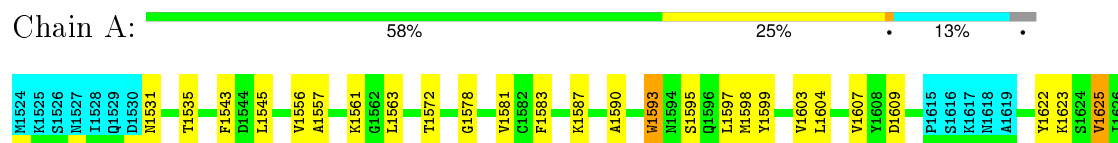
## 4.2.19 Score per residue for model 19

- Molecule 1: IGF2R DOMAIN 11



## 4.2.20 Score per residue for model 20

- Molecule 1: IGF2R DOMAIN 11



S1627	F1628	M1637	M1638	K1639	P1640	D1646	T1649	C1650	T1651	L1652	V1653	W1656	H1657	T1658	P1659	L1660	A1661	C1662	E1663	K1664	E1665	E1666	P1667	L1668	H1669	H1670	HIS	HIS	HIS	HIS
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## 5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
ARIA	structure solution	1.2
ARIA	refinement	1.2
CNS	refinement	1.2
CNS	structure solution	1.2
iCing	refinement	r765
TALOS	geometry optimization	

No chemical shift data was provided. 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](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.97±0.02	0±0/985 (0.0±0.0%)	0.73±0.01	0±0/1343 (0.0±0.0%)
All	All	0.97	1/19700 (0.0%)	0.73	1/26860 (0.0%)

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	1660	LEU	N-CA	-5.30	1.35	1.46	16	1

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	1660	LEU	N-CA-CB	-5.58	99.25	110.40	16	1

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	961	928	925	29±4
All	All	19220	18560	18500	586

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 16.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1604:LEU:HB2	1:A:1628:PHE:HB2	0.89	1.44	9	20
1:A:1656:TRP:CD1	1:A:1658:THR:HB	0.76	2.16	19	18
1:A:1623:LYS:HB2	1:A:1651:THR:HG23	0.75	1.56	14	1
1:A:1556:VAL:HG22	1:A:1640:PRO:HB2	0.73	1.61	4	16
1:A:1560:GLU:HB3	1:A:1561:LYS:HD2	0.71	1.62	12	3
1:A:1642:PHE:HZ	1:A:1645:LEU:HB2	0.69	1.46	18	17
1:A:1552:SER:HA	1:A:1573:LYS:HE2	0.68	1.65	2	3
1:A:1658:THR:OG1	1:A:1660:LEU:HG	0.68	1.88	3	10
1:A:1565:TYR:HB2	1:A:1575:CYS:SG	0.67	2.29	1	3
1:A:1613:PRO:HA	1:A:1621:LYS:HA	0.67	1.66	7	7
1:A:1531:ASN:HB3	1:A:1533:GLN:HG2	0.67	1.65	16	2
1:A:1581:VAL:HG12	1:A:1590:ALA:HB3	0.66	1.68	3	20
1:A:1633:ASP:HB2	1:A:1659:PRO:HG3	0.66	1.67	16	10
1:A:1597:LEU:HD11	1:A:1604:LEU:HB3	0.64	1.67	8	16
1:A:1582:CYS:HA	1:A:1589:ASN:HA	0.64	1.67	2	3
1:A:1596:GLN:HE21	1:A:1596:GLN:HA	0.64	1.52	19	1
1:A:1607:VAL:HG22	1:A:1625:VAL:HG22	0.64	1.70	16	3
1:A:1583:PHE:O	1:A:1587:LYS:HA	0.63	1.94	16	18
1:A:1569:CYS:SG	1:A:1595:SER:HA	0.63	2.33	19	3
1:A:1646:ASP:HB3	1:A:1651:THR:HB	0.62	1.69	5	11
1:A:1531:ASN:HB2	1:A:1533:GLN:HG2	0.62	1.72	5	2
1:A:1608:TYR:HB2	1:A:1624:SER:HB3	0.62	1.70	14	4
1:A:1543:PHE:HB3	1:A:1604:LEU:HD21	0.61	1.70	5	17
1:A:1532:CYS:SG	1:A:1545:LEU:HB2	0.60	2.37	1	10
1:A:1607:VAL:HG22	1:A:1625:VAL:HG12	0.60	1.74	3	12
1:A:1580:GLY:CA	1:A:1593:TRP:HB3	0.59	2.26	7	2
1:A:1545:LEU:HD23	1:A:1660:LEU:HD22	0.58	1.74	16	1
1:A:1599:TYR:CZ	1:A:1602:GLN:HA	0.57	2.35	15	11
1:A:1561:LYS:HE2	1:A:1585:LEU:HD21	0.57	1.77	16	1
1:A:1545:LEU:CD2	1:A:1660:LEU:HD11	0.56	2.31	1	8
1:A:1641:VAL:HG12	1:A:1655:SER:OG	0.54	2.03	8	1
1:A:1605:GLN:OE1	1:A:1625:VAL:HB	0.54	2.02	13	1
1:A:1620:LEU:HD22	1:A:1649:THR:HA	0.53	1.79	2	11
1:A:1625:VAL:HG23	1:A:1653:TYR:HA	0.53	1.79	13	13
1:A:1588:ILE:HG21	1:A:1622:TYR:CE2	0.53	2.39	19	2
1:A:1642:PHE:CZ	1:A:1645:LEU:HB2	0.53	2.34	8	10
1:A:1533:GLN:HG3	1:A:1542:LEU:HD21	0.52	1.82	4	1
1:A:1622:TYR:HA	1:A:1650:CYS:HB3	0.52	1.81	3	1
1:A:1590:ALA:HA	1:A:1622:TYR:CB	0.52	2.35	3	13
1:A:1583:PHE:HB2	1:A:1588:ILE:HB	0.51	1.82	18	1
1:A:1641:VAL:HB	1:A:1655:SER:OG	0.51	2.04	3	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1548:LEU:HD22	1:A:1637:ASN:HB3	0.51	1.82	1	1
1:A:1640:PRO:HB3	1:A:1656:TRP:CE3	0.51	2.40	16	3
1:A:1603:VAL:HG11	1:A:1627:SER:HB2	0.51	1.81	2	3
1:A:1603:VAL:HG11	1:A:1627:SER:HB3	0.51	1.83	11	9
1:A:1551:ASP:HA	1:A:1572:THR:HA	0.51	1.83	1	2
1:A:1545:LEU:HD23	1:A:1660:LEU:HD11	0.50	1.81	2	7
1:A:1545:LEU:HD23	1:A:1660:LEU:CD1	0.50	2.36	13	8
1:A:1533:GLN:HB2	1:A:1542:LEU:HD11	0.50	1.84	14	1
1:A:1649:THR:HG23	1:A:1651:THR:OG1	0.50	2.06	7	11
1:A:1563:LEU:HD21	1:A:1565:TYR:CD1	0.50	2.41	14	1
1:A:1546:ASN:O	1:A:1549:LYS:HG2	0.50	2.06	6	1
1:A:1646:ASP:CB	1:A:1651:THR:HB	0.50	2.37	5	3
1:A:1579:VAL:HG13	1:A:1589:ASN:HB2	0.50	1.81	15	3
1:A:1599:TYR:HD1	1:A:1604:LEU:HD12	0.50	1.66	7	9
1:A:1549:LYS:HG2	1:A:1568:ILE:O	0.50	2.07	16	8
1:A:1598:MET:O	1:A:1604:LEU:HA	0.49	2.07	16	16
1:A:1626:ILE:HG23	1:A:1654:PHE:CD2	0.49	2.41	19	1
1:A:1546:ASN:O	1:A:1549:LYS:HB2	0.49	2.07	15	1
1:A:1545:LEU:HD23	1:A:1660:LEU:CD2	0.49	2.37	16	1
1:A:1593:TRP:HA	1:A:1608:TYR:CD1	0.49	2.43	7	2
1:A:1583:PHE:HB3	1:A:1585:LEU:HG	0.49	1.84	13	1
1:A:1556:VAL:CG2	1:A:1640:PRO:HB2	0.49	2.38	7	13
1:A:1547:SER:HB2	1:A:1660:LEU:HD21	0.49	1.84	7	1
1:A:1614:CYS:HB3	1:A:1622:TYR:CZ	0.49	2.42	4	1
1:A:1637:ASN:HB2	1:A:1656:TRP:CZ2	0.49	2.43	8	7
1:A:1609:ASP:HA	1:A:1623:LYS:HB2	0.49	1.84	9	7
1:A:1625:VAL:HG22	1:A:1651:THR:HG22	0.48	1.85	13	3
1:A:1589:ASN:HB3	1:A:1612:ALA:HB2	0.48	1.85	17	1
1:A:1565:TYR:CD1	1:A:1574:ASN:HB3	0.48	2.44	4	7
1:A:1560:GLU:HB3	1:A:1561:LYS:HD3	0.48	1.84	19	2
1:A:1590:ALA:HB1	1:A:1652:LEU:HG	0.48	1.85	18	4
1:A:1557:ALA:HA	1:A:1563:LEU:CB	0.48	2.39	13	4
1:A:1631:THR:O	1:A:1659:PRO:HA	0.47	2.09	5	2
1:A:1599:TYR:OH	1:A:1602:GLN:HA	0.47	2.10	15	1
1:A:1558:TYR:CD1	1:A:1564:ILE:HD11	0.47	2.44	9	1
1:A:1583:PHE:CZ	1:A:1652:LEU:HD11	0.47	2.45	18	8
1:A:1575:CYS:SG	1:A:1579:VAL:HG12	0.47	2.50	9	5
1:A:1638:ASN:HB3	1:A:1657:HIS:HB2	0.47	1.86	19	5
1:A:1531:ASN:HA	1:A:1595:SER:HB2	0.47	1.85	20	1
1:A:1545:LEU:HA	1:A:1660:LEU:HD23	0.47	1.87	8	6
1:A:1576:PRO:HD2	1:A:1582:CYS:SG	0.46	2.50	11	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1583:PHE:CD1	1:A:1588:ILE:HB	0.46	2.45	9	6
1:A:1594:ASN:HB3	1:A:1596:GLN:HG2	0.46	1.86	2	1
1:A:1535:THR:HA	1:A:1542:LEU:HA	0.46	1.87	7	3
1:A:1599:TYR:CD1	1:A:1604:LEU:HD12	0.46	2.46	18	7
1:A:1554:TYR:HB2	1:A:1566:ILE:HB	0.45	1.87	16	3
1:A:1532:CYS:SG	1:A:1549:LYS:HD2	0.45	2.51	9	1
1:A:1578:GLY:C	1:A:1593:TRP:HB2	0.45	2.32	2	4
1:A:1564:ILE:HD13	1:A:1652:LEU:HD12	0.45	1.88	18	1
1:A:1553:GLY:HA3	1:A:1572:THR:OG1	0.45	2.12	11	5
1:A:1659:PRO:HA	1:A:1662:CYS:SG	0.45	2.52	19	4
1:A:1654:PHE:CE2	1:A:1656:TRP:HE3	0.44	2.30	19	1
1:A:1654:PHE:HE2	1:A:1656:TRP:HE3	0.44	1.54	19	1
1:A:1557:ALA:HA	1:A:1563:LEU:HA	0.44	1.87	20	4
1:A:1612:ALA:HB1	1:A:1613:PRO:HD2	0.44	1.88	2	2
1:A:1590:ALA:HA	1:A:1622:TYR:HB2	0.44	1.90	5	1
1:A:1533:GLN:HA	1:A:1543:PHE:O	0.43	2.13	9	1
1:A:1568:ILE:HA	1:A:1608:TYR:HH	0.43	1.73	16	1
1:A:1579:VAL:HG11	1:A:1582:CYS:HB3	0.43	1.89	1	3
1:A:1558:TYR:H	1:A:1563:LEU:HA	0.43	1.73	3	1
1:A:1626:ILE:HA	1:A:1654:PHE:HB2	0.43	1.89	4	1
1:A:1608:TYR:HB2	1:A:1624:SER:HB2	0.43	1.90	1	1
1:A:1585:LEU:HD12	1:A:1586:THR:HG23	0.43	1.91	19	2
1:A:1637:ASN:HA	1:A:1656:TRP:NE1	0.43	2.28	19	2
1:A:1555:SER:HB3	1:A:1563:LEU:HD13	0.43	1.91	7	4
1:A:1546:ASN:HA	1:A:1549:LYS:HG3	0.43	1.90	13	2
1:A:1558:TYR:HB2	1:A:1564:ILE:HG13	0.43	1.91	3	2
1:A:1533:GLN:CA	1:A:1597:LEU:HD23	0.42	2.45	4	1
1:A:1614:CYS:HB3	1:A:1622:TYR:CE2	0.42	2.48	4	1
1:A:1645:LEU:HD13	1:A:1646:ASP:N	0.42	2.29	4	1
1:A:1633:ASP:O	1:A:1659:PRO:HB3	0.42	2.15	1	3
1:A:1565:TYR:HB2	1:A:1582:CYS:SG	0.42	2.55	2	1
1:A:1533:GLN:HB2	1:A:1542:LEU:HD22	0.42	1.91	9	2
1:A:1532:CYS:HB2	1:A:1546:ASN:ND2	0.42	2.28	19	1
1:A:1631:THR:HG21	1:A:1638:ASN:OD1	0.42	2.15	14	1
1:A:1635:GLY:H	1:A:1659:PRO:HB2	0.42	1.75	9	2
1:A:1532:CYS:HB3	1:A:1546:ASN:ND2	0.42	2.30	8	1
1:A:1590:ALA:HA	1:A:1622:TYR:HB3	0.42	1.92	3	1
1:A:1638:ASN:HB3	1:A:1657:HIS:O	0.42	2.14	15	1
1:A:1565:TYR:HB3	1:A:1574:ASN:HB3	0.41	1.92	17	1
1:A:1564:ILE:HG21	1:A:1654:PHE:HZ	0.41	1.75	11	2
1:A:1556:VAL:CG1	1:A:1642:PHE:HB2	0.41	2.46	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1565:TYR:CG	1:A:1574:ASN:HB3	0.41	2.51	14	1
1:A:1563:LEU:HD11	1:A:1565:TYR:CD1	0.41	2.51	1	1
1:A:1608:TYR:HE2	1:A:1626:ILE:HD12	0.41	1.76	17	1
1:A:1561:LYS:N	1:A:1561:LYS:HD3	0.41	2.31	14	1
1:A:1563:LEU:HD12	1:A:1564:ILE:N	0.41	2.31	16	3
1:A:1623:LYS:O	1:A:1651:THR:HA	0.40	2.15	13	1
1:A:1658:THR:HA	1:A:1659:PRO:HD3	0.40	1.76	2	1
1:A:1636:ALA:H	1:A:1659:PRO:CD	0.40	2.29	6	1
1:A:1545:LEU:HA	1:A:1660:LEU:HD13	0.40	1.92	19	1
1:A:1589:ASN:OD1	1:A:1612:ALA:HB2	0.40	2.17	8	1
1:A:1594:ASN:OD1	1:A:1596:GLN:HG2	0.40	2.16	14	1
1:A:1605:GLN:HA	1:A:1626:ILE:O	0.40	2.15	13	1
1:A:1561:LYS:HD3	1:A:1561:LYS:N	0.40	2.32	16	1
1:A:1556:VAL:HG12	1:A:1642:PHE:HB2	0.40	1.93	1	1

## 6.3 Torsion angles

### 6.3.1 Protein backbone

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	127/151 (84%)	113±1 (89±1%)	13±2 (10±1%)	1±1 (1±1%)	23	69
All	All	2540/3020 (84%)	2258 (89%)	254 (10%)	28 (1%)	23	69

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	1638	ASN	16
1	A	1560	GLU	4
1	A	1531	ASN	4
1	A	1586	THR	1
1	A	1549	LYS	1
1	A	1589	ASN	1
1	A	1561	LYS	1

### 6.3.2 Protein sidechains ⓘ

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	109/132 (83%)	103±2 (95±2%)	6±2 (5±2%)	33	78
All	All	2180/2640 (83%)	2067 (95%)	113 (5%)	33	78

All 26 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	1593	TRP	20
1	A	1561	LYS	17
1	A	1572	THR	15
1	A	1625	VAL	11
1	A	1585	LEU	9
1	A	1643	VAL	7
1	A	1605	GLN	4
1	A	1621	LYS	4
1	A	1630	CYS	2
1	A	1546	ASN	2
1	A	1610	ASP	2
1	A	1648	GLN	2
1	A	1587	LYS	2
1	A	1641	VAL	2
1	A	1542	LEU	2
1	A	1639	LYS	2
1	A	1552	SER	1
1	A	1589	ASN	1
1	A	1596	GLN	1
1	A	1601	ASP	1
1	A	1563	LEU	1
1	A	1637	ASN	1
1	A	1574	ASN	1
1	A	1631	THR	1
1	A	1620	LEU	1
1	A	1573	LYS	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 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

No chemical shift data were provided