



# Full wwPDB NMR Structure Validation Report ⓘ

Feb 12, 2017 – 11:36 pm GMT

PDB ID : 2L2A  
Title : Mutated Domain 11 of the Cytoplasmic region of the Cation-independent mannose-6-phosphate receptor  
Authors : Williams, C.; Hoppe, H.; Rezgui, D.; Strickland, M.; Frago, S.; Ellis, R.Z.; Wattana-Amorn, P.; Prince, S.N.; Zaccheo, O.J.; Forbes, B.; Jones, E.Y.; Crump, M.P.; Hassan, A.B.  
Deposited on : 2010-08-13

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  
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

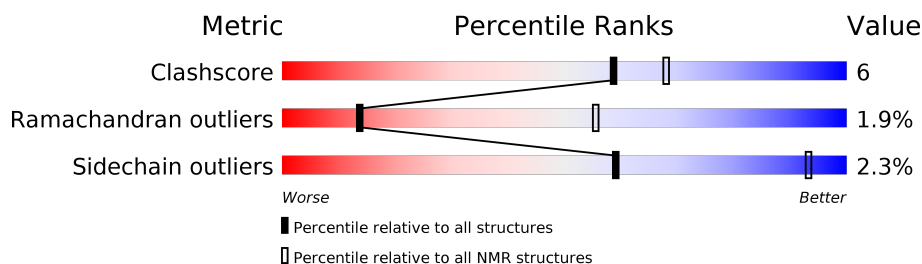
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment 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	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	142	

## 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:1515-A:1617, A:1622-A:1647 (129)	0.67	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 4 clusters and 1 single-model cluster was found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2126 atoms, of which 1049 are hydrogens and 0 are deuteriums.

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

Mol	Chain	Residues	Atoms						Trace
1	A	142	Total	C	H	N	O	S	0
			2126	672	1049	186	208	11	

There are 5 discrepancies between the modelled and reference sequences:

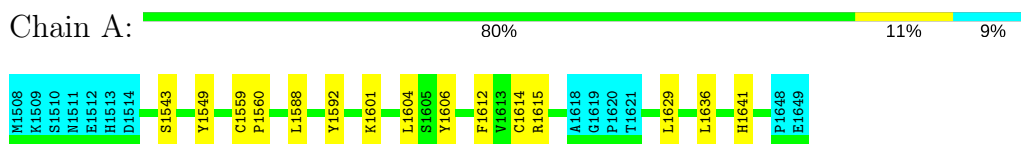
Chain	Residue	Modelled	Actual	Comment	Reference
A	1544	LYS	GLU	ENGINEERED MUTATION	UNP Q59EZ3
A	1545	SER	LYS	ENGINEERED MUTATION	UNP Q59EZ3
A	1547	VAL	LEU	ENGINEERED MUTATION	UNP Q59EZ3
A	1648	PRO	-	EXPRESSION TAG	UNP Q59EZ3
A	1649	GLU	-	EXPRESSION TAG	UNP Q59EZ3

## 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: Insulin-like growth factor 2 receptor variant

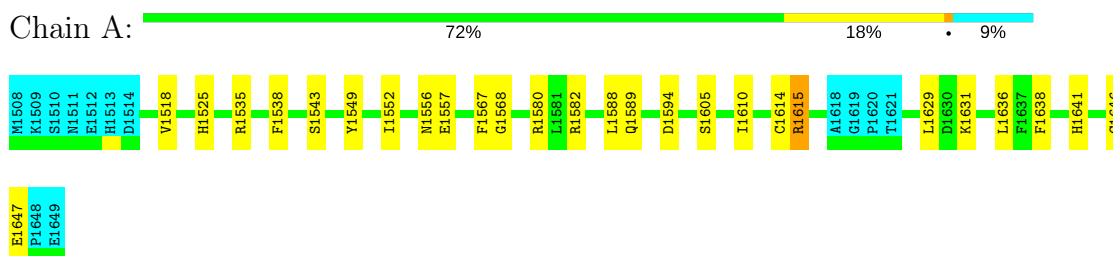


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

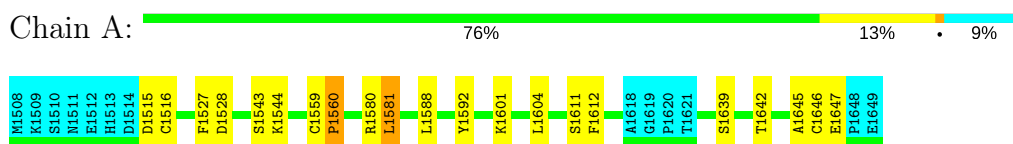
#### 4.2.1 Score per residue for model 1

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



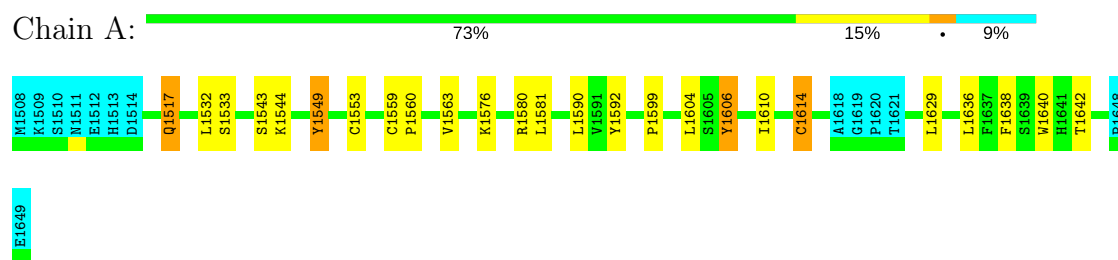
#### 4.2.2 Score per residue for model 2

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



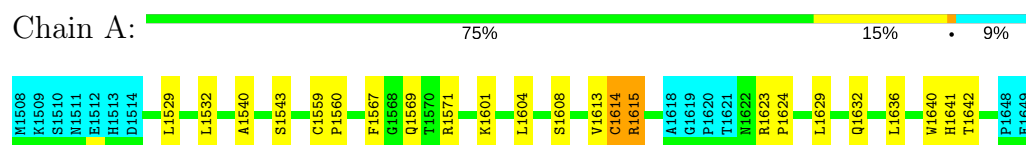
### 4.2.3 Score per residue for model 3

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



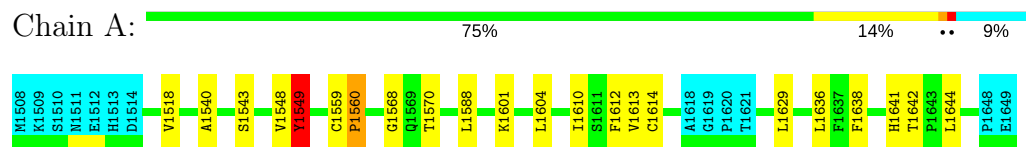
### 4.2.4 Score per residue for model 4

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



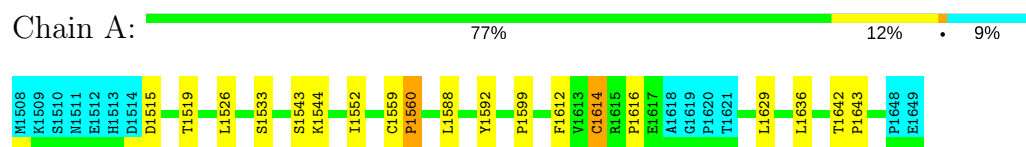
### 4.2.5 Score per residue for model 5

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



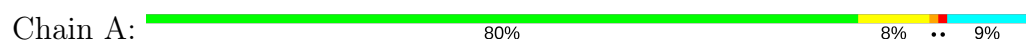
### 4.2.6 Score per residue for model 6

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



### 4.2.7 Score per residue for model 7

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

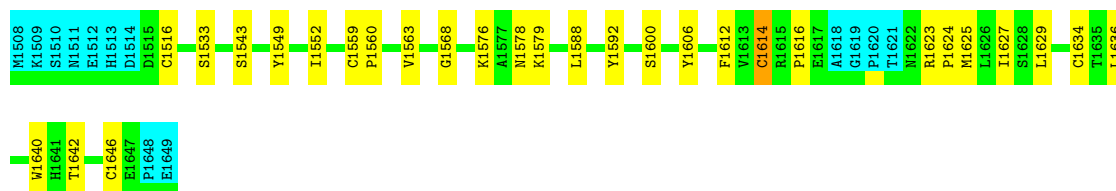




#### 4.2.8 Score per residue for model 8

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

Chain A: 70% 20% 9%



#### 4.2.9 Score per residue for model 9

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

Chain A: 76% 14% 9%



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

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

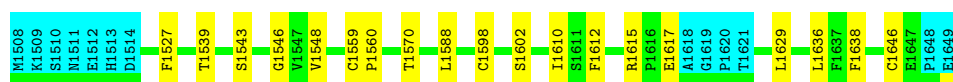
Chain A: 66% 24% 9%



#### 4.2.11 Score per residue for model 11

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

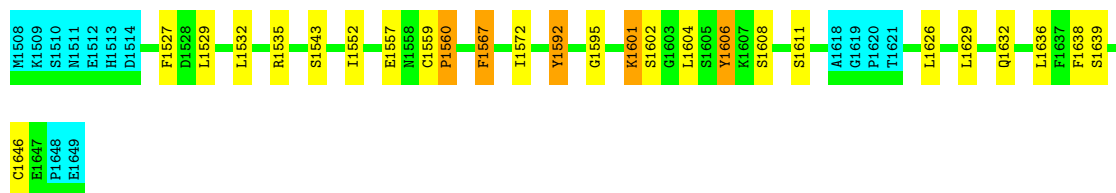
Chain A: 77% 13% 9%



#### 4.2.12 Score per residue for model 12

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

Chain A: 73% 15% 9%



#### 4.2.13 Score per residue for model 13

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

Chain A: 73% 15% 9%



#### 4.2.14 Score per residue for model 14

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

Chain A: 74% 16% 9%



#### 4.2.15 Score per residue for model 15

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

Chain A: 73% 16% 9%

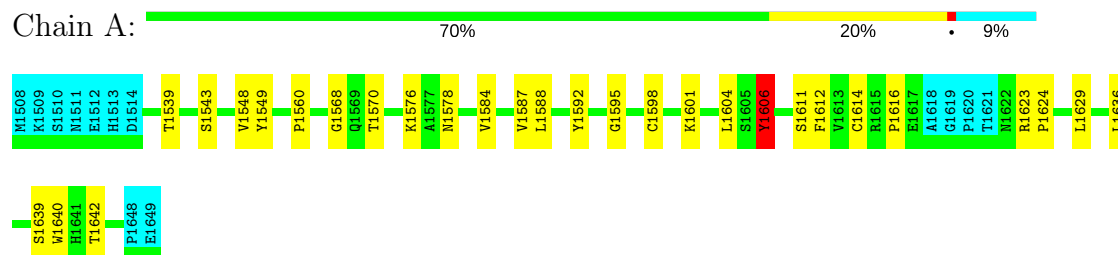






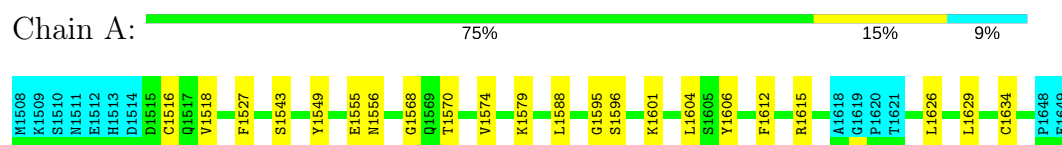
#### 4.2.16 Score per residue for model 16

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



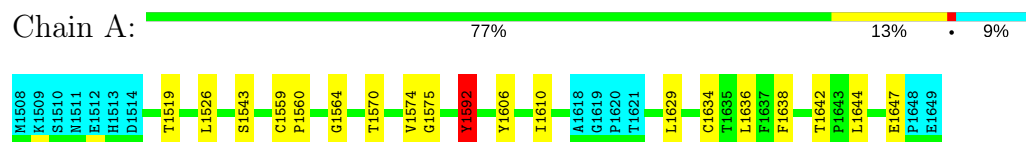
#### 4.2.17 Score per residue for model 17

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



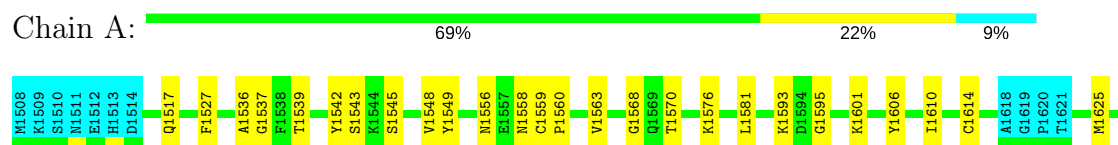
#### 4.2.18 Score per residue for model 18

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



#### 4.2.19 Score per residue for model 19

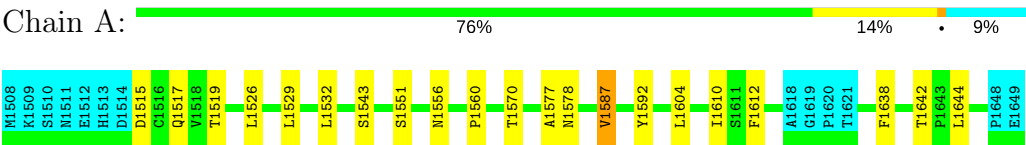
- Molecule 1: Insulin-like growth factor 2 receptor variant





4.2.20 Score per residue for model 20

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



## 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
CNS	refinement	
CNS	structure solution	
TALOS	geometry optimization	
iCing	refinement	r765
ARIA	refinement	2.2
ARIA	structure solution	2.2

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

### 6.1 Standard geometry

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	0.86±0.04	1±1/1002 (0.1±0.1%)	0.69±0.02	0±0/1359 (0.0±0.0%)
All	All	0.87	21/20040 (0.1%)	0.69	0/27180 (0.0%)

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	0.9±0.9
All	All	0	18

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	1549	TYR	CE2-CZ	-9.01	1.26	1.38	5	3
1	A	1606	TYR	CE1-CZ	8.91	1.50	1.38	16	3
1	A	1606	TYR	CE2-CZ	-8.68	1.27	1.38	16	3
1	A	1592	TYR	CE1-CZ	-8.35	1.27	1.38	2	3
1	A	1549	TYR	CE1-CZ	8.11	1.49	1.38	5	2
1	A	1592	TYR	CE2-CZ	-7.88	1.28	1.38	18	4
1	A	1583	TYR	CE1-CZ	-7.10	1.29	1.38	15	1
1	A	1583	TYR	CE2-CZ	6.30	1.46	1.38	15	1
1	A	1567	PHE	CE1-CZ	5.65	1.48	1.37	12	1

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	1606	TYR	Sidechain	4
1	A	1592	TYR	Sidechain	4
1	A	1549	TYR	Sidechain	3
1	A	1567	PHE	Sidechain	2
1	A	1612	PHE	Sidechain	1
1	A	1615	ARG	Sidechain	1
1	A	1542	TYR	Sidechain	1
1	A	1580	ARG	Sidechain	1
1	A	1583	TYR	Sidechain	1

## 6.2 Too-close contacts

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	979	961	959	11±3
All	All	19580	19220	19180	216

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 6.

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:HA	1:A:1596:SER:HB3	0.80	1.51	17	1
1:A:1629:LEU:HG	1:A:1636:LEU:HG	0.79	1.54	15	8
1:A:1629:LEU:HD13	1:A:1636:LEU:HG	0.76	1.56	5	4
1:A:1601:LYS:HB3	1:A:1604:LEU:HD12	0.73	1.60	16	6
1:A:1533:SER:HB2	1:A:1552:ILE:HG22	0.72	1.62	6	1
1:A:1588:LEU:HB2	1:A:1612:PHE:HB2	0.68	1.64	7	12
1:A:1554:GLY:HA2	1:A:1579:LYS:HE2	0.68	1.65	10	1
1:A:1615:ARG:HB3	1:A:1641:HIS:HB3	0.67	1.64	10	3
1:A:1559:CYS:HB3	1:A:1560:PRO:HD2	0.64	1.70	3	13
1:A:1535:ARG:HG3	1:A:1557:GLU:HG3	0.64	1.68	12	1
1:A:1601:LYS:HD2	1:A:1632:GLN:HA	0.63	1.71	12	1
1:A:1601:LYS:HG2	1:A:1604:LEU:HD12	0.63	1.70	15	1
1:A:1610:ILE:HG13	1:A:1638:PHE:HB2	0.62	1.71	3	8
1:A:1535:ARG:HD3	1:A:1557:GLU:HG3	0.62	1.70	1	1
1:A:1542:TYR:HB3	1:A:1546:GLY:HA3	0.61	1.72	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1602:SER:HB3	1:A:1604:LEU:HD22	0.61	1.73	12	1
1:A:1553:CYS:SG	1:A:1579:LYS:HE3	0.60	2.36	15	1
1:A:1615:ARG:HB2	1:A:1641:HIS:HB3	0.60	1.72	15	1
1:A:1518:VAL:HG21	1:A:1588:LEU:HD11	0.59	1.74	1	1
1:A:1529:LEU:HA	1:A:1532:LEU:HD13	0.58	1.75	4	2
1:A:1629:LEU:HD13	1:A:1636:LEU:HD13	0.58	1.76	4	1
1:A:1615:ARG:HB2	1:A:1641:HIS:HB2	0.58	1.74	14	1
1:A:1575:GLY:HA3	1:A:1592:TYR:HB3	0.57	1.75	18	1
1:A:1582:ARG:HB2	1:A:1589:GLN:HB3	0.57	1.74	10	1
1:A:1628:SER:HB2	1:A:1637:PHE:HB2	0.57	1.75	14	1
1:A:1540:ALA:HB3	1:A:1548:VAL:HG13	0.57	1.77	10	2
1:A:1519:THR:HA	1:A:1526:LEU:HA	0.57	1.77	6	3
1:A:1533:SER:HB2	1:A:1552:ILE:HB	0.56	1.76	8	1
1:A:1608:SER:HA	1:A:1636:LEU:HB2	0.56	1.77	10	2
1:A:1577:ALA:HA	1:A:1592:TYR:CE2	0.56	2.36	15	1
1:A:1567:PHE:O	1:A:1571:ARG:HA	0.56	2.01	4	1
1:A:1516:CYS:SG	1:A:1579:LYS:HE3	0.55	2.40	15	2
1:A:1614:CYS:HA	1:A:1642:THR:O	0.55	2.01	8	6
1:A:1615:ARG:HG3	1:A:1617:GLU:HG2	0.55	1.79	10	1
1:A:1642:THR:HG22	1:A:1644:LEU:HG	0.54	1.79	5	1
1:A:1529:LEU:HG	1:A:1532:LEU:HD12	0.54	1.79	12	1
1:A:1613:VAL:O	1:A:1641:HIS:HA	0.54	2.02	5	5
1:A:1642:THR:OG1	1:A:1644:LEU:HG	0.54	2.03	18	2
1:A:1642:THR:HG23	1:A:1645:ALA:HB2	0.54	1.78	2	1
1:A:1615:ARG:HB3	1:A:1641:HIS:HB2	0.54	1.78	13	2
1:A:1549:TYR:CD1	1:A:1568:GLY:HA3	0.53	2.39	1	1
1:A:1598:CYS:O	1:A:1602:SER:HA	0.53	2.04	11	1
1:A:1559:CYS:SG	1:A:1560:PRO:HD2	0.52	2.44	5	1
1:A:1516:CYS:HA	1:A:1581:LEU:HD23	0.52	1.81	2	1
1:A:1527:PHE:CE1	1:A:1646:CYS:HA	0.51	2.40	12	2
1:A:1551:SER:CB	1:A:1556:ASN:HB3	0.51	2.34	13	1
1:A:1584:VAL:O	1:A:1587:VAL:HG12	0.51	2.06	16	2
1:A:1590:LEU:HB2	1:A:1612:PHE:HE1	0.51	1.66	15	1
1:A:1560:PRO:O	1:A:1563:VAL:HG22	0.51	2.05	19	1
1:A:1598:CYS:HA	1:A:1606:TYR:HE1	0.51	1.66	16	1
1:A:1529:LEU:HA	1:A:1532:LEU:HD23	0.51	1.81	14	1
1:A:1538:PHE:CD1	1:A:1552:ILE:HD13	0.50	2.41	1	1
1:A:1564:GLY:HA3	1:A:1592:TYR:CE2	0.50	2.42	18	1
1:A:1518:VAL:HB	1:A:1581:LEU:HD11	0.50	1.82	15	1
1:A:1540:ALA:HA	1:A:1623:ARG:HD3	0.49	1.85	4	1
1:A:1542:TYR:HD2	1:A:1545:SER:HB2	0.49	1.67	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1516:CYS:HB3	1:A:1529:LEU:HB2	0.49	1.85	13	1
1:A:1549:TYR:CE1	1:A:1568:GLY:HA3	0.48	2.43	1	2
1:A:1549:TYR:HB3	1:A:1556:ASN:HD21	0.48	1.67	1	1
1:A:1542:TYR:CD2	1:A:1545:SER:HB2	0.48	2.44	19	1
1:A:1564:GLY:HA3	1:A:1592:TYR:CD2	0.48	2.43	13	1
1:A:1624:PRO:HB3	1:A:1640:TRP:HB2	0.48	1.85	4	2
1:A:1576:LYS:HG3	1:A:1595:GLY:HA2	0.48	1.85	19	1
1:A:1626:LEU:HD21	1:A:1629:LEU:HD23	0.48	1.84	17	1
1:A:1601:LYS:HD2	1:A:1604:LEU:HG	0.48	1.86	2	1
1:A:1527:PHE:HE1	1:A:1646:CYS:HA	0.47	1.69	12	1
1:A:1636:LEU:HB3	1:A:1638:PHE:CE2	0.47	2.44	10	1
1:A:1543:SER:HB3	1:A:1546:GLY:N	0.47	2.24	11	1
1:A:1551:SER:HB2	1:A:1556:ASN:HB3	0.47	1.86	20	1
1:A:1574:VAL:HB	1:A:1606:TYR:HB2	0.47	1.87	9	2
1:A:1629:LEU:HG	1:A:1636:LEU:HD13	0.47	1.86	3	1
1:A:1552:ILE:O	1:A:1592:TYR:OH	0.46	2.30	12	1
1:A:1515:ASP:HB3	1:A:1517:GLN:HG2	0.46	1.86	20	1
1:A:1549:TYR:CD2	1:A:1568:GLY:HA2	0.46	2.45	7	2
1:A:1577:ALA:HA	1:A:1592:TYR:CE1	0.46	2.45	20	1
1:A:1549:TYR:HD2	1:A:1568:GLY:HA3	0.46	1.70	19	1
1:A:1594:ASP:HA	1:A:1605:SER:CB	0.46	2.41	1	1
1:A:1520:ASN:HB2	1:A:1527:PHE:CE2	0.46	2.46	10	1
1:A:1549:TYR:HE1	1:A:1568:GLY:HA3	0.46	1.70	15	1
1:A:1533:SER:HA	1:A:1553:CYS:O	0.46	2.11	14	1
1:A:1574:VAL:HA	1:A:1596:SER:CB	0.45	2.34	17	1
1:A:1582:ARG:HB3	1:A:1589:GLN:HB3	0.45	1.88	1	1
1:A:1566:CYS:SG	1:A:1571:ARG:HA	0.45	2.51	10	1
1:A:1613:VAL:HG12	1:A:1615:ARG:HG2	0.45	1.87	14	1
1:A:1537:GLY:HA3	1:A:1556:ASN:ND2	0.45	2.26	19	1
1:A:1549:TYR:CE2	1:A:1568:GLY:HA2	0.44	2.46	17	1
1:A:1563:VAL:HA	1:A:1576:LYS:HA	0.44	1.89	8	2
1:A:1611:SER:O	1:A:1639:SER:HA	0.44	2.12	12	3
1:A:1629:LEU:CD2	1:A:1636:LEU:HG	0.44	2.41	14	1
1:A:1606:TYR:HA	1:A:1634:CYS:O	0.44	2.13	17	2
1:A:1600:SER:HB3	1:A:1634:CYS:SG	0.44	2.52	8	1
1:A:1557:GLU:CD	1:A:1558:ASN:H	0.44	2.15	13	1
1:A:1629:LEU:HD22	1:A:1631:LYS:HG2	0.44	1.89	1	1
1:A:1532:LEU:HD13	1:A:1640:TRP:CZ3	0.44	2.48	3	1
1:A:1580:ARG:O	1:A:1590:LEU:HA	0.44	2.12	3	1
1:A:1629:LEU:CD1	1:A:1636:LEU:HG	0.44	2.43	9	1
1:A:1591:VAL:HG12	1:A:1609:VAL:HG22	0.44	1.90	10	1

*Continued on next page...*

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1539:THR:HA	1:A:1548:VAL:O	0.44	2.13	19	3
1:A:1612:PHE:HE1	1:A:1640:TRP:HE3	0.44	1.56	10	1
1:A:1518:VAL:HB	1:A:1527:PHE:HB2	0.43	1.90	17	1
1:A:1535:ARG:O	1:A:1557:GLU:HB2	0.43	2.12	1	1
1:A:1601:LYS:HG3	1:A:1633:THR:HG22	0.43	1.89	9	1
1:A:1615:ARG:HD2	1:A:1617:GLU:OE2	0.43	2.13	11	1
1:A:1629:LEU:HD22	1:A:1636:LEU:HG	0.43	1.90	14	1
1:A:1616:PRO:HA	1:A:1643:PRO:HD3	0.43	1.90	10	1
1:A:1592:TYR:HB2	1:A:1608:SER:HB3	0.43	1.91	12	1
1:A:1517:GLN:HA	1:A:1527:PHE:O	0.43	2.14	19	2
1:A:1588:LEU:CB	1:A:1612:PHE:HB2	0.42	2.41	7	1
1:A:1587:VAL:HA	1:A:1612:PHE:O	0.42	2.14	20	1
1:A:1581:LEU:HD13	1:A:1590:LEU:HB2	0.42	1.91	9	1
1:A:1590:LEU:HG	1:A:1612:PHE:HE1	0.42	1.75	13	1
1:A:1616:PRO:HB3	1:A:1643:PRO:HB3	0.41	1.91	6	1
1:A:1601:LYS:HG3	1:A:1632:GLN:O	0.41	2.15	19	1
1:A:1599:PRO:HD2	1:A:1606:TYR:OH	0.41	2.14	15	2
1:A:1590:LEU:HG	1:A:1612:PHE:CE1	0.41	2.50	13	1
1:A:1549:TYR:CD2	1:A:1568:GLY:HA3	0.41	2.49	19	1
1:A:1590:LEU:HB2	1:A:1610:ILE:HB	0.41	1.92	13	1
1:A:1614:CYS:HB3	1:A:1646:CYS:HB2	0.41	1.62	1	1
1:A:1589:GLN:HA	1:A:1610:ILE:O	0.41	2.15	13	1
1:A:1516:CYS:HB2	1:A:1579:LYS:HD2	0.41	1.93	8	1
1:A:1525:HIS:CE1	1:A:1647:GLU:HB2	0.41	2.51	1	1
1:A:1527:PHE:CE2	1:A:1646:CYS:HA	0.41	2.51	2	1
1:A:1542:TYR:HB3	1:A:1546:GLY:CA	0.41	2.43	9	1
1:A:1551:SER:HB3	1:A:1556:ASN:HB3	0.41	1.91	13	1
1:A:1549:TYR:CE2	1:A:1568:GLY:HA3	0.41	2.51	8	1
1:A:1533:SER:OG	1:A:1553:CYS:HB2	0.40	2.16	3	1
1:A:1615:ARG:HA	1:A:1615:ARG:NE	0.40	2.31	1	1
1:A:1525:HIS:HE1	1:A:1647:GLU:HB2	0.40	1.76	1	1
1:A:1623:ARG:HB3	1:A:1640:TRP:CG	0.40	2.51	16	1
1:A:1549:TYR:CZ	1:A:1568:GLY:HA2	0.40	2.51	5	1
1:A:1626:LEU:HG	1:A:1638:PHE:CE1	0.40	2.52	12	1
1:A:1606:TYR:HA	1:A:1634:CYS:HB3	0.40	1.92	18	1
1:A:1629:LEU:HG	1:A:1636:LEU:CD1	0.40	2.47	3	1
1:A:1623:ARG:HB3	1:A:1640:TRP:CD1	0.40	2.52	8	1
1:A:1625:MET:HG3	1:A:1627:ILE:HG23	0.40	1.93	8	1
1:A:1576:LYS:HG2	1:A:1595:GLY:HA2	0.40	1.93	16	1
1:A:1543:SER:HB3	1:A:1546:GLY:H	0.40	1.74	11	1
1:A:1536:ALA:HB1	1:A:1558:ASN:HD21	0.40	1.76	19	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	129/142 (91%)	116±2 (90±2%)	11±3 (8±2%)	2±1 (2±1%)	14	55
All	All	2580/2840 (91%)	2315 (90%)	216 (8%)	49 (2%)	14	55

All 15 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	1543	SER	19
1	A	1560	PRO	9
1	A	1544	LYS	3
1	A	1556	ASN	2
1	A	1624	PRO	2
1	A	1587	VAL	2
1	A	1595	GLY	2
1	A	1515	ASP	2
1	A	1616	PRO	2
1	A	1614	CYS	1
1	A	1601	LYS	1
1	A	1585	ASP	1
1	A	1572	ILE	1
1	A	1557	GLU	1
1	A	1558	ASN	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	112/123 (91%)	109±1 (98±1%)	3±1 (2±1%)	59	93
All	All	2240/2460 (91%)	2189 (98%)	51 (2%)	59	93

All 25 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	1570	THR	9
1	A	1614	CYS	5
1	A	1578	ASN	5
1	A	1517	GLN	3
1	A	1604	LEU	3
1	A	1641	HIS	2
1	A	1581	LEU	2
1	A	1528	ASP	2
1	A	1615	ARG	2
1	A	1555	GLU	2
1	A	1647	GLU	2
1	A	1646	CYS	1
1	A	1530	SER	1
1	A	1599	PRO	1
1	A	1560	PRO	1
1	A	1557	GLU	1
1	A	1625	MET	1
1	A	1642	THR	1
1	A	1588	LEU	1
1	A	1623	ARG	1
1	A	1569	GLN	1
1	A	1559	CYS	1
1	A	1593	LYS	1
1	A	1632	GLN	1
1	A	1549	TYR	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 ⓘ

There are no carbohydrates in this entry.

## 6.6 Ligand geometry

There are no ligands in this entry.

## 6.7 Other polymers

There are no such molecules in this entry.

## 6.8 Polymer linkage issues

There are no chain breaks in this entry.

## 7 Chemical shift validation

No chemical shift data were provided