



Full wwPDB NMR Structure Validation Report ⓘ

May 28, 2020 – 10:52 pm BST

PDB ID : 2L29
Title : Complex structure of E4 mutant human IGF2R domain 11 bound to IGF-II
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/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 : 20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : 2.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

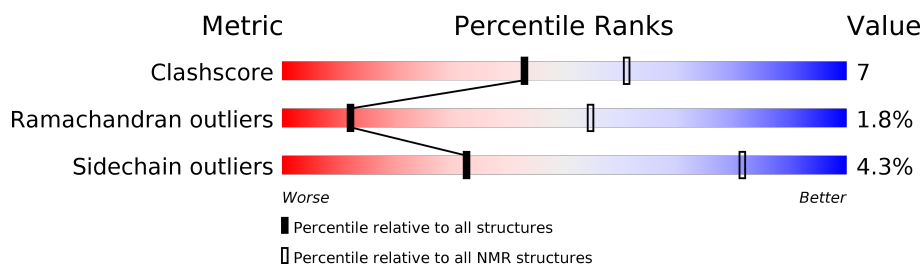
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 83%.

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	142	
2	B	67	

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:1647, B:10-B:28, B:41-B:60 (172)	0.60	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. No single-model clusters were found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3146 atoms, of which 1548 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

- Molecule 2 is a protein called Insulin-like growth factor II.

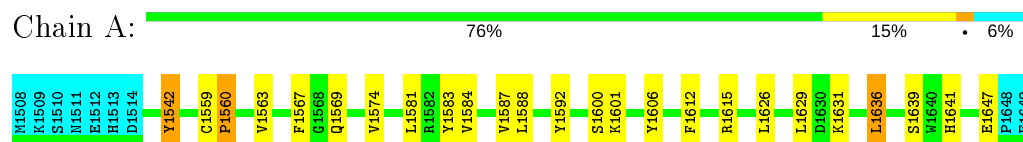
Mol	Chain	Residues	Atoms						Trace
2	B	67	Total	C	H	N	O	S	0
			1020	321	499	93	101	6	

4 Residue-property plots

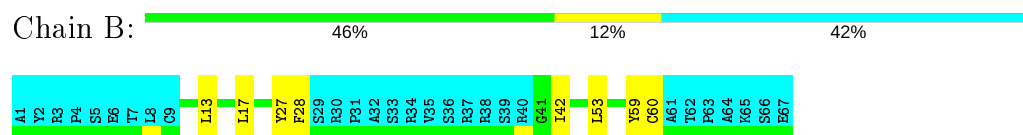
4.1 Average score per residue in the NMR ensemble

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



- Molecule 2: Insulin-like growth factor II

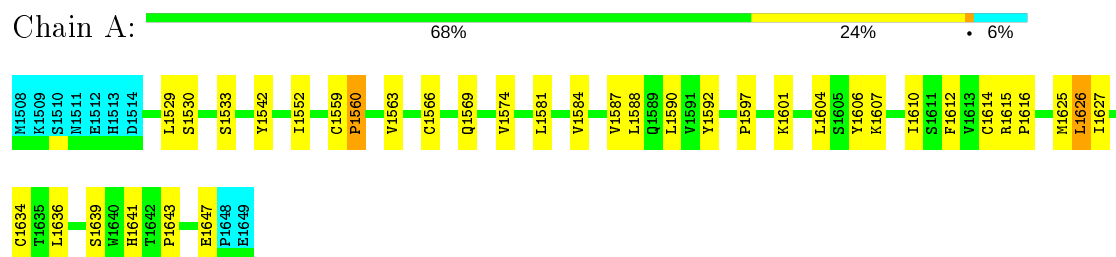


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

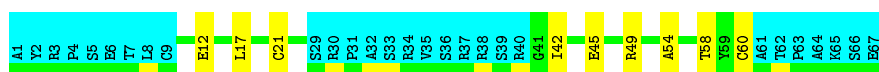
4.2.1 Score per residue for model 1

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



- Molecule 2: Insulin-like growth factor II



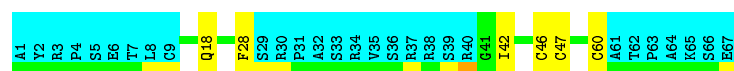


4.2.2 Score per residue for model 2

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

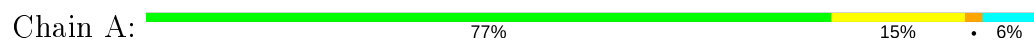


- Molecule 2: Insulin-like growth factor II

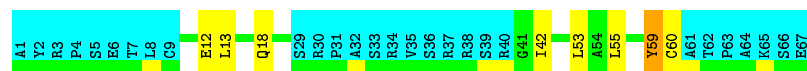


4.2.3 Score per residue for model 3

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

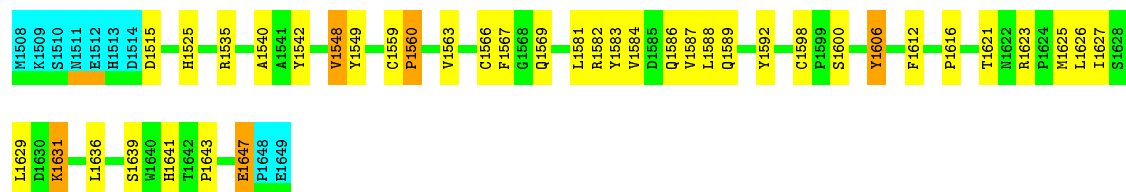


- Molecule 2: Insulin-like growth factor II

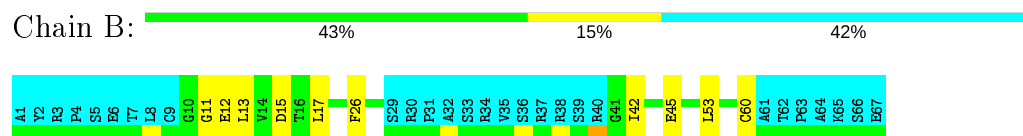


4.2.4 Score per residue for model 4

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

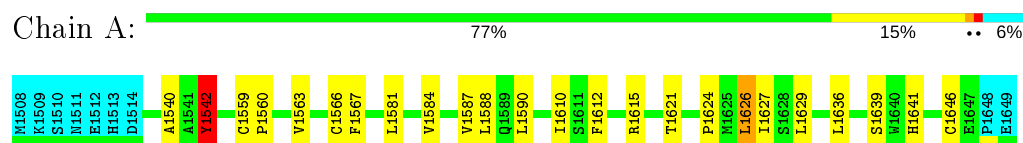


- Molecule 2: Insulin-like growth factor II

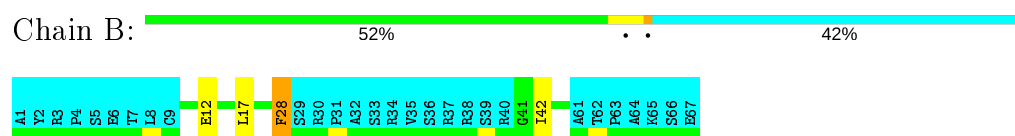


4.2.5 Score per residue for model 5

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

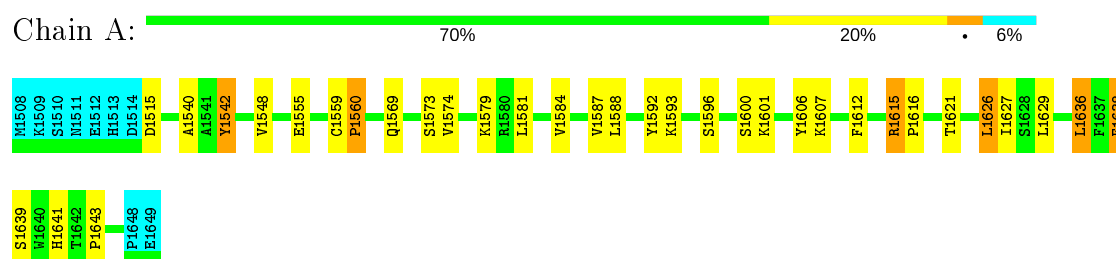


- Molecule 2: Insulin-like growth factor II

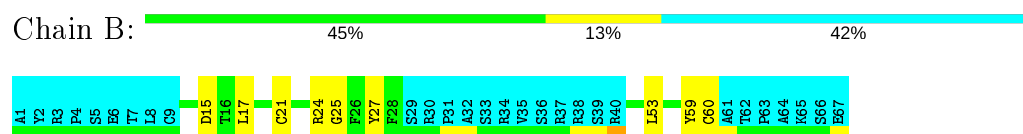


4.2.6 Score per residue for model 6

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

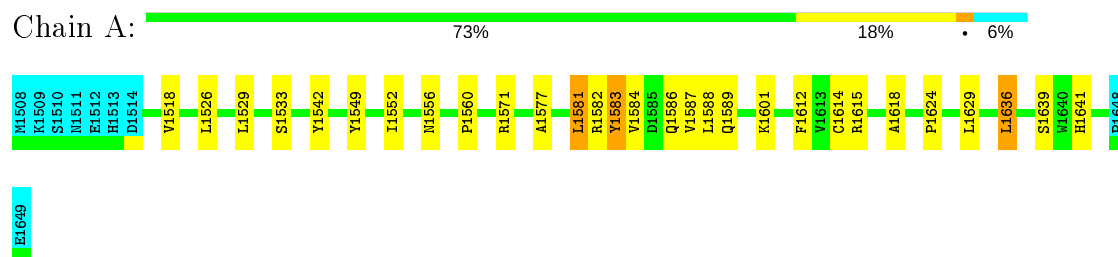


- Molecule 2: Insulin-like growth factor II

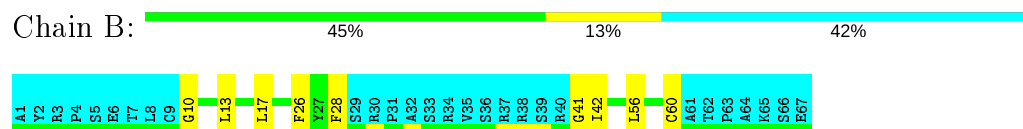


4.2.7 Score per residue for model 7

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

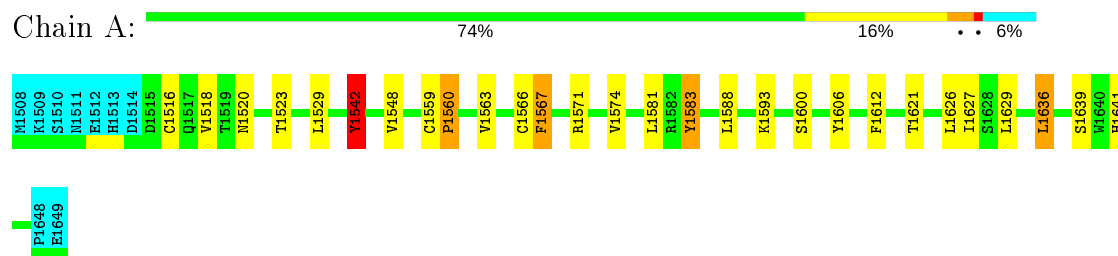


- Molecule 2: Insulin-like growth factor II

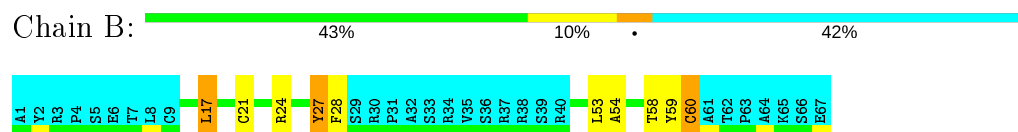


4.2.8 Score per residue for model 8

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

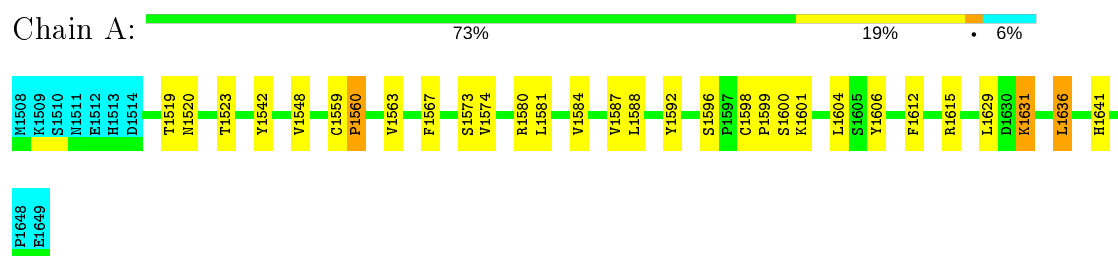


- Molecule 2: Insulin-like growth factor II

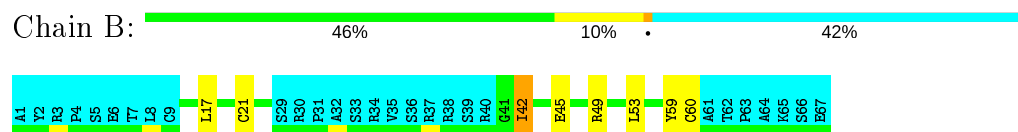


4.2.9 Score per residue for model 9

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

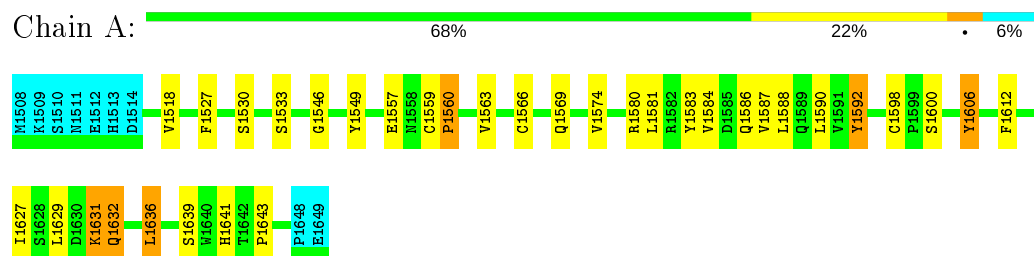


- Molecule 2: Insulin-like growth factor II

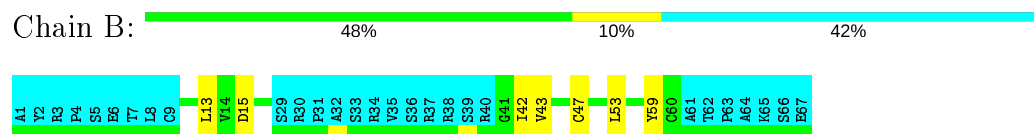


4.2.10 Score per residue for model 10 (medoid)

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

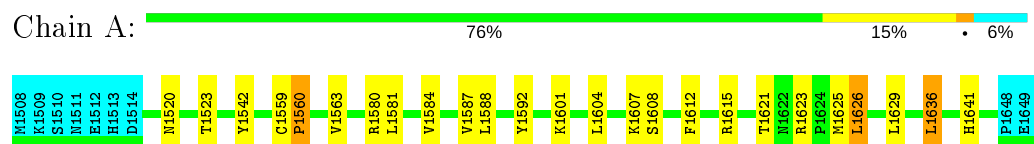


- Molecule 2: Insulin-like growth factor II

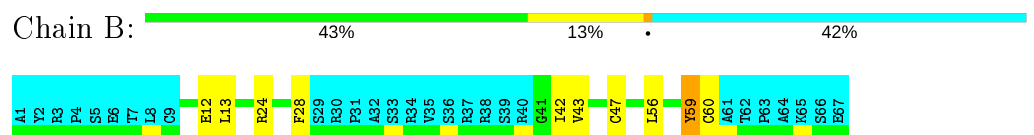


4.2.11 Score per residue for model 11

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



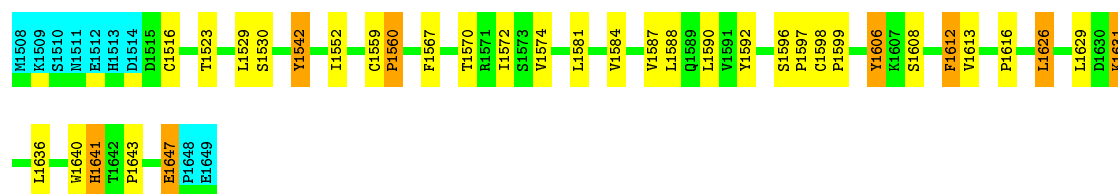
- Molecule 2: Insulin-like growth factor II



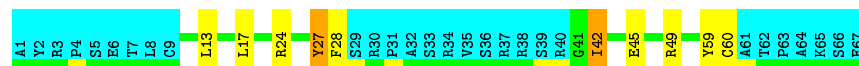
4.2.12 Score per residue for model 12

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



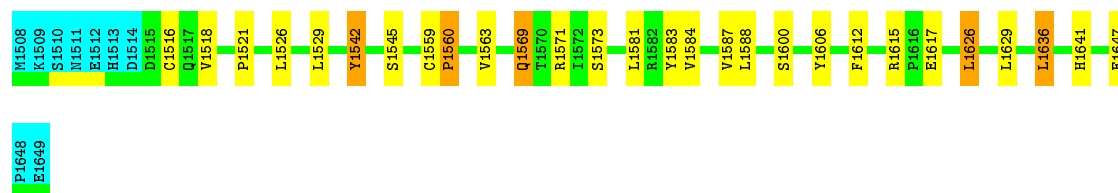


- Molecule 2: Insulin-like growth factor II

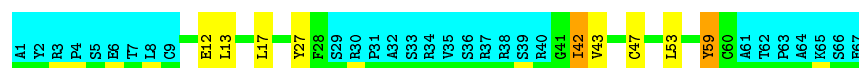


4.2.13 Score per residue for model 13

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

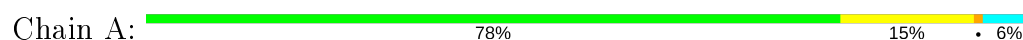


- Molecule 2: Insulin-like growth factor II

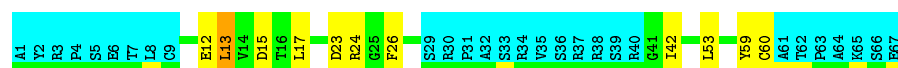


4.2.14 Score per residue for model 14

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

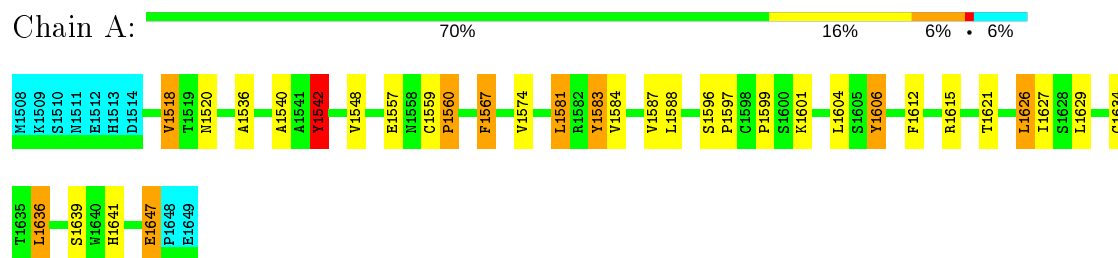


- Molecule 2: Insulin-like growth factor II

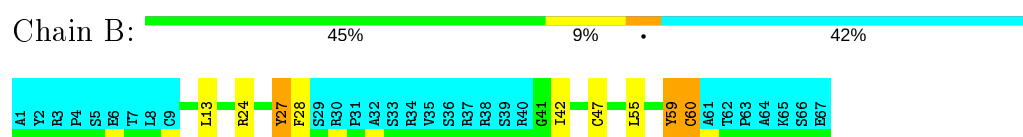


4.2.15 Score per residue for model 15

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

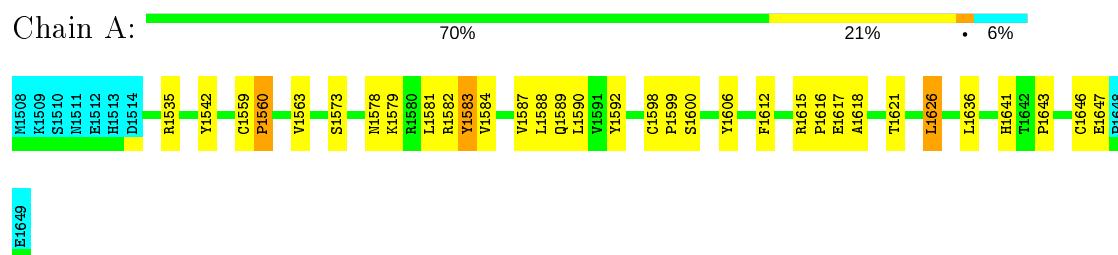


- Molecule 2: Insulin-like growth factor II

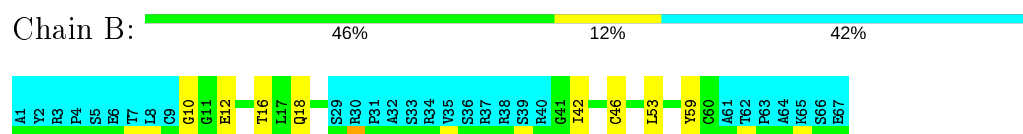


4.2.16 Score per residue for model 16

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

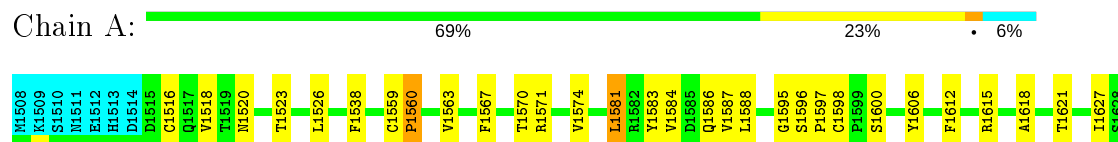


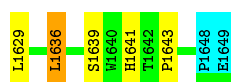
- Molecule 2: Insulin-like growth factor II



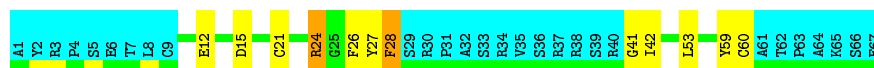
4.2.17 Score per residue for model 17

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



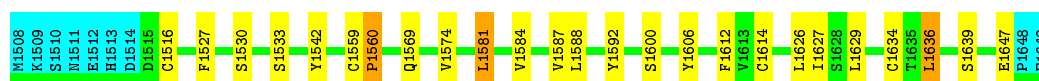


- Molecule 2: Insulin-like growth factor II



4.2.18 Score per residue for model 18

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



- Molecule 2: Insulin-like growth factor II



4.2.19 Score per residue for model 19

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

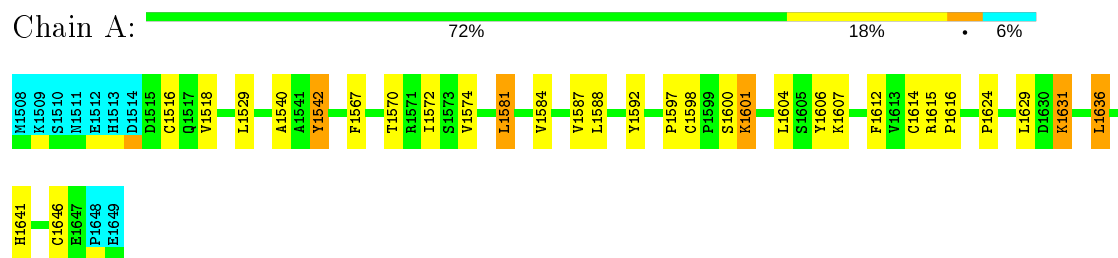


- Molecule 2: Insulin-like growth factor II

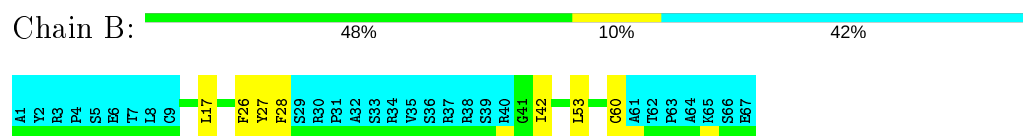


4.2.20 Score per residue for model 20

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



- Molecule 2: Insulin-like growth factor II



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
TALOS	geometry optimization	
iCing	refinement	r765
ARIA	refinement	2.2
ARIA	structure solution	2.2
CNS	refinement	1.2
CNS	structure solution	1.2

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 6 of this report.

Chemical shift file(s)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	2265
Number of shifts mapped to atoms	2265
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	83%

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

COVALENT-GEOMETRY INFOmissingINFO

5.1 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	1002	983	981	16±4
2	B	303	276	276	3±2
All	All	26100	25180	25140	365

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:1629:LEU:HD13	1:A:1636:LEU:HG	0.87	1.44	13	10
1:A:1588:LEU:HB2	1:A:1612:PHE:HB2	0.85	1.45	1	19
1:A:1629:LEU:HG	1:A:1636:LEU:HG	0.78	1.54	7	3
1:A:1533:SER:HA	1:A:1536:ALA:HB2	0.77	1.56	19	1
1:A:1563:VAL:HG21	1:A:1573:SER:HB2	0.76	1.58	13	2
1:A:1548:VAL:HB	1:A:1567:PHE:CE1	0.75	2.16	8	3
1:A:1600:SER:HA	2:B:53:LEU:HB2	0.73	1.59	17	5
1:A:1567:PHE:HB3	1:A:1569:GLN:HG2	0.73	1.60	4	1
1:A:1616:PRO:HA	1:A:1643:PRO:HB3	0.73	1.60	12	9
1:A:1516:CYS:HB3	1:A:1529:LEU:HB2	0.70	1.63	3	2
1:A:1621:THR:HB	1:A:1641:HIS:HB2	0.69	1.63	6	9
1:A:1627:ILE:HD11	1:A:1639:SER:HB2	0.69	1.65	1	10
1:A:1559:CYS:SG	1:A:1560:PRO:HD2	0.67	2.30	4	12
1:A:1613:VAL:HB	1:A:1641:HIS:HB3	0.67	1.65	12	1
1:A:1600:SER:HA	2:B:53:LEU:HB3	0.66	1.66	14	2
2:B:17:LEU:HD21	2:B:42:ILE:HD11	0.66	1.65	5	4
1:A:1629:LEU:HD23	1:A:1636:LEU:HG	0.65	1.68	6	1
1:A:1601:LYS:HE3	1:A:1601:LYS:HA	0.64	1.70	7	1
1:A:1632:GLN:HE21	1:A:1632:GLN:HA	0.64	1.52	10	1
1:A:1542:TYR:HE2	1:A:1626:LEU:HG	0.63	1.51	5	3
1:A:1615:ARG:HB2	1:A:1641:HIS:HB3	0.62	1.70	14	14
1:A:1629:LEU:HD13	1:A:1636:LEU:HD23	0.62	1.71	5	2
1:A:1544:LYS:HG3	2:B:23:ASP:HB3	0.61	1.71	14	1
1:A:1584:VAL:O	1:A:1587:VAL:HB	0.61	1.96	5	18
2:B:45:GLU:O	2:B:49:ARG:HG2	0.60	1.96	1	1
1:A:1542:TYR:HE1	1:A:1626:LEU:HG	0.60	1.56	15	1
2:B:53:LEU:HD12	2:B:53:LEU:H	0.59	1.58	9	1
1:A:1631:LYS:HD3	1:A:1631:LYS:H	0.59	1.58	10	2
1:A:1600:SER:HB3	2:B:53:LEU:HB2	0.59	1.74	8	2
1:A:1574:VAL:HA	1:A:1606:TYR:HB2	0.57	1.76	12	13
1:A:1596:SER:HB2	1:A:1597:PRO:HD2	0.57	1.75	12	2
1:A:1559:CYS:HB3	1:A:1563:VAL:HG11	0.57	1.75	9	4
1:A:1601:LYS:HE3	2:B:53:LEU:HB3	0.56	1.77	19	1
2:B:43:VAL:O	2:B:47:CYS:HB2	0.56	2.01	19	5
1:A:1583:TYR:CE1	1:A:1586:GLN:HA	0.56	2.35	2	5
1:A:1563:VAL:HG11	1:A:1566:CYS:HB2	0.55	1.78	1	6
1:A:1600:SER:HB3	2:B:53:LEU:HD13	0.55	1.76	6	1
1:A:1516:CYS:HA	1:A:1581:LEU:HB2	0.55	1.77	8	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1529:LEU:HG	1:A:1581:LEU:HD21	0.55	1.77	7	3
1:A:1559:CYS:HB3	1:A:1560:PRO:HD2	0.55	1.79	6	5
1:A:1573:SER:HB3	1:A:1596:SER:HB2	0.55	1.78	6	1
1:A:1582:ARG:HB2	1:A:1589:GLN:HB3	0.55	1.79	16	2
1:A:1516:CYS:SG	1:A:1529:LEU:HB2	0.55	2.42	13	1
2:B:55:LEU:O	2:B:59:TYR:HB2	0.54	2.03	15	2
1:A:1570:THR:HB	1:A:1572:ILE:HG13	0.54	1.80	20	2
1:A:1542:TYR:CE2	1:A:1626:LEU:HG	0.54	2.36	5	8
1:A:1540:ALA:HB3	1:A:1548:VAL:HG23	0.53	1.80	4	1
1:A:1590:LEU:HB3	1:A:1610:ILE:HB	0.53	1.80	1	2
1:A:1598:CYS:HA	1:A:1606:TYR:CE1	0.53	2.39	20	2
1:A:1567:PHE:HB2	1:A:1570:THR:OG1	0.53	2.04	20	2
1:A:1583:TYR:OH	1:A:1647:GLU:OE1	0.52	2.25	16	1
2:B:17:LEU:HB3	2:B:26:PHE:HB3	0.52	1.82	20	2
1:A:1600:SER:HB2	2:B:53:LEU:HG	0.52	1.81	9	1
1:A:1614:CYS:HB2	1:A:1646:CYS:HA	0.52	1.81	20	1
2:B:42:ILE:HA	2:B:45:GLU:HG2	0.51	1.83	4	1
1:A:1542:TYR:CE1	1:A:1626:LEU:HG	0.51	2.40	15	2
2:B:54:ALA:O	2:B:58:THR:HG22	0.51	2.06	1	2
1:A:1574:VAL:HA	1:A:1606:TYR:CB	0.51	2.34	19	3
1:A:1598:CYS:HA	1:A:1606:TYR:CE2	0.51	2.40	16	4
1:A:1540:ALA:HB2	1:A:1624:PRO:HG2	0.50	1.81	5	2
1:A:1569:GLN:HB3	2:B:15:ASP:OD1	0.50	2.06	18	3
2:B:26:PHE:HA	2:B:60:CYS:SG	0.50	2.47	14	2
1:A:1643:PRO:HA	1:A:1646:CYS:SG	0.50	2.46	2	3
1:A:1601:LYS:HG2	1:A:1604:LEU:HD22	0.50	1.83	20	2
1:A:1520:ASN:ND2	1:A:1583:TYR:OH	0.50	2.45	15	1
1:A:1604:LEU:HD23	1:A:1634:CYS:SG	0.50	2.47	14	3
1:A:1599:PRO:HD3	1:A:1606:TYR:OH	0.50	2.07	3	1
1:A:1523:THR:HG21	1:A:1647:GLU:HG3	0.49	1.84	3	2
1:A:1536:ALA:HB1	1:A:1552:ILE:H	0.49	1.68	19	1
1:A:1569:GLN:HB2	2:B:15:ASP:OD2	0.49	2.07	10	1
1:A:1599:PRO:HD2	1:A:1606:TYR:HE1	0.49	1.67	12	1
1:A:1583:TYR:CZ	1:A:1586:GLN:HA	0.49	2.43	3	1
1:A:1631:LYS:HB2	2:B:53:LEU:HD21	0.49	1.83	4	1
1:A:1516:CYS:HA	1:A:1581:LEU:HD23	0.49	1.83	20	1
1:A:1530:SER:HA	1:A:1533:SER:OG	0.49	2.07	18	3
1:A:1552:ILE:HG13	1:A:1640:TRP:HZ3	0.49	1.67	12	1
1:A:1596:SER:HB3	1:A:1597:PRO:HD2	0.49	1.85	17	1
1:A:1560:PRO:O	1:A:1563:VAL:HG12	0.49	2.08	14	1
1:A:1533:SER:HA	1:A:1552:ILE:HB	0.49	1.84	1	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:17:LEU:O	2:B:21:CYS:HB2	0.49	2.06	8	4
1:A:1631:LYS:HB2	2:B:53:LEU:CD2	0.48	2.37	4	1
1:A:1518:VAL:HG21	1:A:1583:TYR:HB2	0.48	1.85	15	4
1:A:1601:LYS:HA	1:A:1601:LYS:HE2	0.48	1.85	20	1
1:A:1598:CYS:HA	1:A:1606:TYR:HE1	0.48	1.67	12	1
1:A:1600:SER:HB3	2:B:53:LEU:HB3	0.48	1.83	16	1
1:A:1546:GLY:HA3	1:A:1569:GLN:HG2	0.48	1.86	10	1
1:A:1599:PRO:HB2	2:B:16:THR:HB	0.48	1.84	16	1
1:A:1629:LEU:HG	1:A:1636:LEU:CD2	0.48	2.38	12	1
2:B:42:ILE:HA	2:B:45:GLU:CG	0.47	2.38	4	1
1:A:1563:VAL:HG21	1:A:1573:SER:CB	0.47	2.37	13	1
1:A:1625:MET:HB2	1:A:1639:SER:HB3	0.47	1.86	1	1
1:A:1631:LYS:HB3	2:B:53:LEU:HD22	0.47	1.87	9	1
1:A:1631:LYS:H	1:A:1631:LYS:HD3	0.47	1.69	12	1
2:B:11:GLY:O	2:B:15:ASP:HB2	0.47	2.10	4	1
1:A:1560:PRO:O	1:A:1563:VAL:HB	0.47	2.10	11	1
1:A:1593:LYS:HB3	1:A:1607:LYS:HD3	0.47	1.85	6	1
1:A:1545:SER:HB2	1:A:1569:GLN:HG2	0.47	1.85	13	1
1:A:1600:SER:HB2	1:A:1634:CYS:SG	0.47	2.50	18	1
1:A:1516:CYS:O	1:A:1529:LEU:HB2	0.46	2.11	12	1
1:A:1632:GLN:CA	1:A:1632:GLN:HE21	0.46	2.23	10	1
1:A:1592:TYR:O	1:A:1607:LYS:HG3	0.46	2.10	1	1
1:A:1615:ARG:CB	1:A:1641:HIS:HB3	0.46	2.41	16	1
2:B:28:PHE:O	2:B:41:GLY:HA3	0.46	2.10	17	1
1:A:1612:PHE:HE1	1:A:1640:TRP:CE3	0.46	2.28	12	1
2:B:13:LEU:O	2:B:17:LEU:HD23	0.46	2.10	18	2
1:A:1563:VAL:CG1	1:A:1566:CYS:HB2	0.46	2.40	1	3
1:A:1614:CYS:SG	1:A:1616:PRO:HD3	0.46	2.50	20	2
1:A:1529:LEU:HG	1:A:1581:LEU:HD11	0.46	1.87	1	1
1:A:1599:PRO:HD2	1:A:1606:TYR:CE1	0.45	2.46	12	1
2:B:28:PHE:HA	2:B:59:TYR:HE2	0.45	1.71	12	1
1:A:1525:HIS:CE1	1:A:1647:GLU:HB3	0.45	2.46	4	1
2:B:17:LEU:HB3	2:B:26:PHE:CB	0.45	2.42	7	1
1:A:1592:TYR:HB2	1:A:1608:SER:HB3	0.45	1.89	12	1
1:A:1599:PRO:HD2	1:A:1606:TYR:OH	0.45	2.12	15	1
1:A:1597:PRO:HA	1:A:1604:LEU:O	0.45	2.12	1	2
1:A:1560:PRO:HD2	1:A:1571:ARG:HB3	0.45	1.89	8	1
1:A:1623:ARG:O	1:A:1625:MET:HG3	0.44	2.12	11	2
1:A:1583:TYR:HE1	1:A:1586:GLN:HA	0.44	1.71	7	1
2:B:24:ARG:HG2	2:B:60:CYS:SG	0.44	2.52	8	1
2:B:45:GLU:O	2:B:49:ARG:HB2	0.44	2.12	12	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1533:SER:HA	1:A:1552:ILE:O	0.44	2.12	7	1
1:A:1598:CYS:SG	1:A:1600:SER:HB2	0.44	2.53	17	1
1:A:1515:ASP:O	1:A:1579:LYS:HB3	0.44	2.13	6	1
1:A:1570:THR:HA	2:B:15:ASP:OD2	0.44	2.12	17	1
1:A:1582:ARG:HD2	1:A:1589:GLN:OE1	0.43	2.13	4	1
1:A:1618:ALA:HB2	1:A:1643:PRO:HG3	0.43	1.89	17	1
1:A:1629:LEU:HD13	1:A:1636:LEU:CD2	0.43	2.43	4	2
1:A:1583:TYR:OH	1:A:1647:GLU:OE2	0.43	2.32	15	1
1:A:1629:LEU:CG	1:A:1636:LEU:HG	0.43	2.36	7	1
1:A:1615:ARG:HG3	1:A:1617:GLU:HB3	0.43	1.89	16	1
1:A:1518:VAL:CG2	1:A:1581:LEU:HD12	0.43	2.44	7	2
2:B:24:ARG:HD2	2:B:60:CYS:SG	0.43	2.54	15	1
1:A:1569:GLN:NE2	2:B:18:GLN:HE22	0.43	2.12	19	1
2:B:53:LEU:HD23	2:B:53:LEU:H	0.42	1.74	3	1
1:A:1536:ALA:HA	1:A:1557:GLU:HG2	0.42	1.92	15	1
1:A:1600:SER:HB3	2:B:53:LEU:CB	0.42	2.44	16	1
1:A:1606:TYR:HD1	1:A:1636:LEU:HD11	0.42	1.74	17	1
1:A:1542:TYR:HE2	1:A:1626:LEU:HD13	0.42	1.73	18	1
2:B:28:PHE:HD2	2:B:41:GLY:H	0.42	1.57	7	1
1:A:1631:LYS:HD3	1:A:1631:LYS:N	0.42	2.30	20	1
1:A:1520:ASN:OD1	1:A:1523:THR:HG22	0.42	2.14	11	4
1:A:1629:LEU:CD1	1:A:1636:LEU:HG	0.42	2.44	8	1
1:A:1592:TYR:HB2	1:A:1608:SER:HB2	0.42	1.92	11	1
1:A:1578:ASN:O	1:A:1592:TYR:HE1	0.42	1.98	16	1
2:B:21:CYS:HA	2:B:24:ARG:HB3	0.41	1.92	17	1
2:B:28:PHE:HA	2:B:59:TYR:CE2	0.41	2.50	12	1
1:A:1549:TYR:HB3	1:A:1556:ASN:ND2	0.41	2.30	7	1
1:A:1624:PRO:HA	1:A:1639:SER:O	0.41	2.15	7	1
1:A:1542:TYR:HD2	1:A:1567:PHE:CZ	0.41	2.34	4	1
1:A:1581:LEU:HA	1:A:1589:GLN:O	0.41	2.16	2	1
1:A:1567:PHE:CE2	1:A:1574:VAL:HG11	0.41	2.51	12	1
1:A:1540:ALA:HB3	1:A:1548:VAL:CG1	0.41	2.45	15	1
1:A:1540:ALA:HB3	1:A:1548:VAL:HG12	0.41	1.91	6	1
1:A:1580:ARG:NE	1:A:1580:ARG:HA	0.41	2.31	2	1
2:B:21:CYS:HB2	2:B:26:PHE:HB3	0.41	1.92	18	1
1:A:1601:LYS:HB3	1:A:1604:LEU:HD22	0.41	1.93	11	1
1:A:1573:SER:O	1:A:1596:SER:HB3	0.40	2.16	6	1
1:A:1601:LYS:HE3	1:A:1604:LEU:HD13	0.40	1.92	15	1
1:A:1536:ALA:HB1	1:A:1552:ILE:N	0.40	2.31	19	1
1:A:1573:SER:HB3	1:A:1596:SER:OG	0.40	2.16	9	1
1:A:1563:VAL:CG2	1:A:1573:SER:HB2	0.40	2.40	13	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1592:TYR:O	1:A:1607:LYS:HA	0.40	2.16	20	1
1:A:1615:ARG:HD2	1:A:1617:GLU:OE1	0.40	2.16	13	1

5.2 Torsion angles [i](#)

5.2.1 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	133/142 (94%)	119±3 (89±2%)	13±3 (10±2%)	1±1 (1±1%)	18	66
2	B	39/67 (58%)	34±2 (87±5%)	3±2 (9±4%)	2±1 (4±2%)	4	28
All	All	3440/4180 (82%)	3048 (89%)	329 (10%)	63 (2%)	12	54

All 10 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	1560	PRO	17
2	B	42	ILE	16
2	B	60	CYS	14
1	A	1618	ALA	4
2	B	28	PHE	3
1	A	1595	GLY	3
2	B	10	GLY	2
1	A	1542	TYR	2
1	A	1515	ASP	1
1	A	1577	ALA	1

5.2.2 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	114/123 (93%)	109±2 (95±2%)	5±2 (5±2%)	31	79
2	B	33/57 (58%)	32±1 (97±2%)	1±1 (3±2%)	42	88
All	All	2940/3600 (82%)	2813 (96%)	127 (4%)	33	81

All 36 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	1581	LEU	18
1	A	1636	LEU	15
1	A	1626	LEU	11
2	B	13	LEU	10
1	A	1647	GLU	9
1	A	1631	LYS	7
1	A	1542	TYR	5
2	B	18	GLN	4
1	A	1569	GLN	4
1	A	1580	ARG	4
1	A	1601	LYS	4
1	A	1590	LEU	3
2	B	56	LEU	2
1	A	1570	THR	2
1	A	1518	VAL	2
1	A	1526	LEU	2
1	A	1614	CYS	2
1	A	1555	GLU	2
1	A	1530	SER	2
1	A	1571	ARG	2
1	A	1632	GLN	2
1	A	1548	VAL	1
2	B	59	TYR	1
1	A	1604	LEU	1
2	B	26	PHE	1
1	A	1607	LYS	1
1	A	1535	ARG	1
2	B	17	LEU	1
1	A	1641	HIS	1
1	A	1593	LYS	1
1	A	1615	ARG	1
1	A	1557	GLU	1
2	B	24	ARG	1
2	B	28	PHE	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	1544	LYS	1
1	A	1574	VAL	1

5.2.3 RNA [i](#)

There are no RNA molecules in this entry.

5.3 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.4 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.5 Ligand geometry [i](#)

There are no ligands in this entry.

5.6 Other polymers [i](#)

There are no such molecules in this entry.

5.7 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 83% for the well-defined parts and 83% for the entire structure.

6.1 Chemical shift list 1

File name: input_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

6.1.1 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	2265
Number of shifts mapped to atoms	2265
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

6.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	198	-0.06 ± 0.11	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	172	0.27 ± 0.11	None needed (< 0.5 ppm)
$^{13}\text{C}'$	178	0.21 ± 0.13	None needed (< 0.5 ppm)
^{15}N	188	0.47 ± 0.19	None needed (< 0.5 ppm)

6.1.3 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 83%, i.e. 1669 atoms were assigned a chemical shift out of a possible 2004. 0 out of 29 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	785/842 (93%)	320/335 (96%)	306/344 (89%)	159/163 (98%)
Sidechain	755/988 (76%)	473/584 (81%)	263/362 (73%)	19/42 (45%)

Continued on next page...

Continued from previous page...

	Total	¹ H	¹³ C	¹⁵ N
Aromatic	129/174 (74%)	82/92 (89%)	46/77 (60%)	1/5 (20%)
Overall	1669/2004 (83%)	875/1011 (87%)	615/783 (79%)	179/210 (85%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 83%, i.e. 2048 atoms were assigned a chemical shift out of a possible 2475. 0 out of 31 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	949/1019 (93%)	385/405 (95%)	376/418 (90%)	188/196 (96%)
Sidechain	966/1266 (76%)	609/753 (81%)	331/450 (74%)	26/63 (41%)
Aromatic	133/190 (70%)	86/100 (86%)	46/83 (55%)	1/7 (14%)
Overall	2048/2475 (83%)	1080/1258 (86%)	753/951 (79%)	215/266 (81%)

6.1.4 Statistically unusual chemical shifts ⓘ

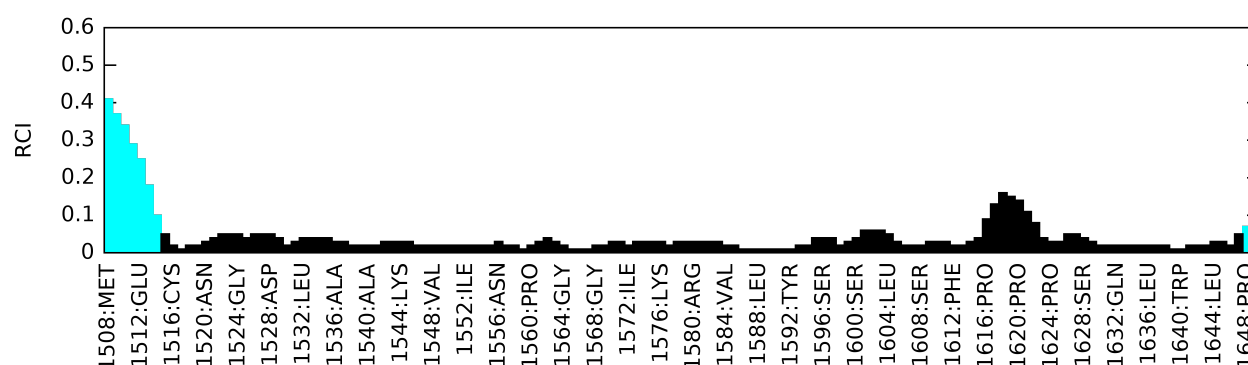
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	1572	ILE	HB	0.06	3.24 – 0.34	-6.0

6.1.5 Random Coil Index (RCI) plots ⓘ

The images below report *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:



Random coil index (RCI) for chain B:

