



# Full wwPDB NMR Structure Validation Report ⓘ

May 28, 2020 – 09:25 pm BST

PDB ID : 2CKN  
Title : NMR Structure of the First Ig Module of mouse FGFR1  
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Deposited on : 2006-04-20

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

<https://www.wwpdb.org/validation/2017/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 : 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

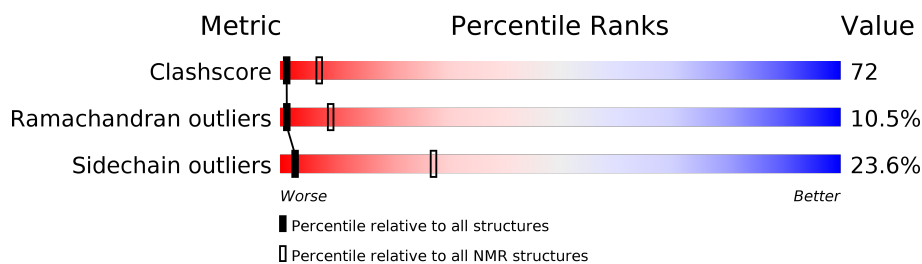
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 51%.

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  $\geq 3$ , 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	95	

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 14 is the overall representative, medoid model (most similar to other models).

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:28-A:63, A:67-A:108 (78)	0.40	14

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 3 clusters and 2 single-model clusters were found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1445 atoms, of which 711 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called BASIC FIBROBLAST GROWTH FACTOR RECEPTOR 1.

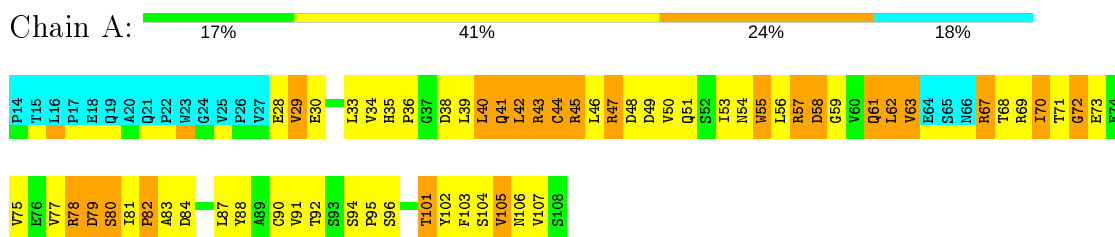
Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	95	1445	454	711	128	150	2	0

## 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: BASIC FIBROBLAST GROWTH FACTOR RECEPTOR 1

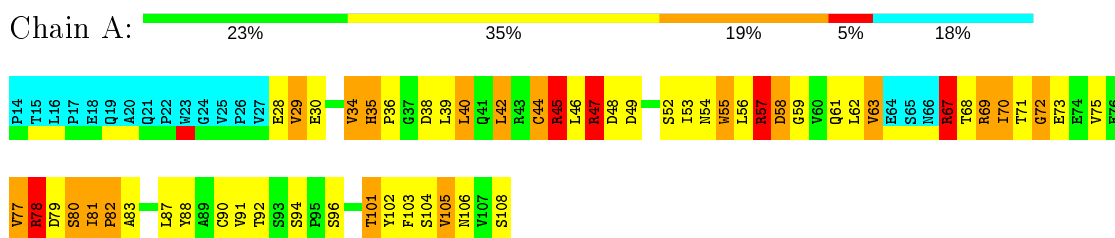


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

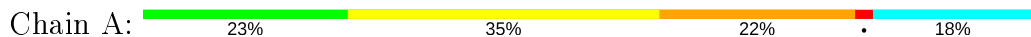
#### 4.2.1 Score per residue for model 1

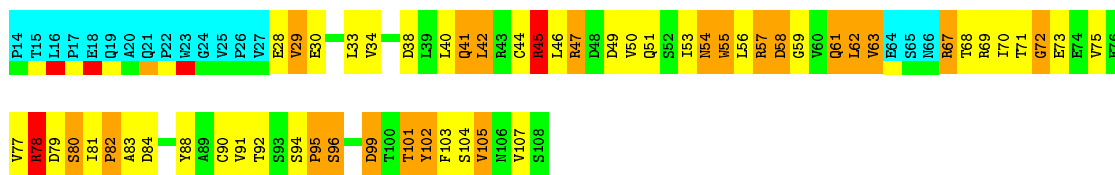
- Molecule 1: BASIC FIBROBLAST GROWTH FACTOR RECEPTOR 1



#### 4.2.2 Score per residue for model 2

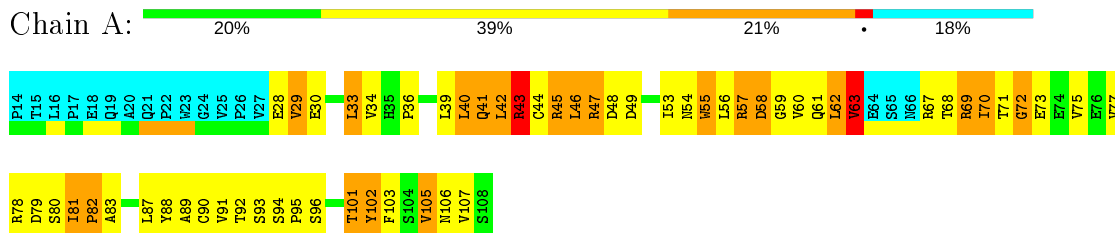
- Molecule 1: BASIC FIBROBLAST GROWTH FACTOR RECEPTOR 1





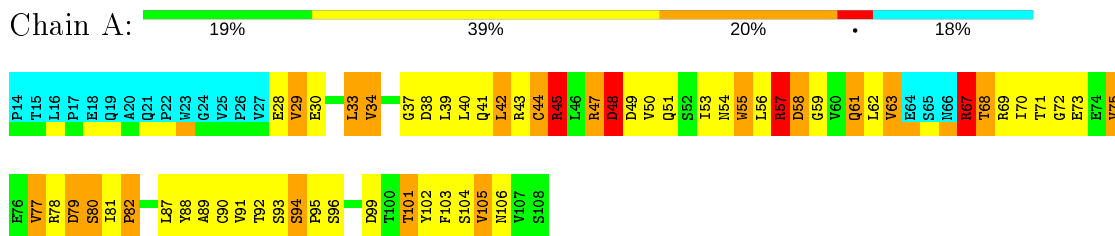
### 4.2.3 Score per residue for model 3

- Molecule 1: BASIC FIBROBLAST GROWTH FACTOR RECEPTOR 1



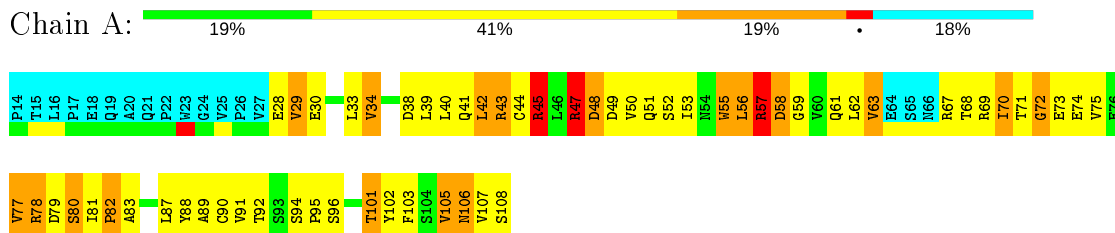
### 4.2.4 Score per residue for model 4

- Molecule 1: BASIC FIBROBLAST GROWTH FACTOR RECEPTOR 1



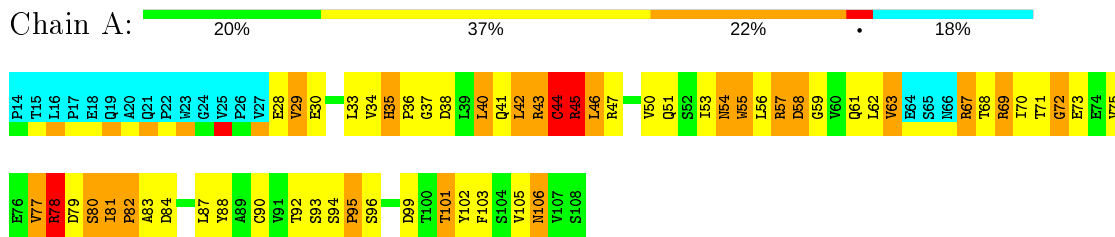
### 4.2.5 Score per residue for model 5

- Molecule 1: BASIC FIBROBLAST GROWTH FACTOR RECEPTOR 1



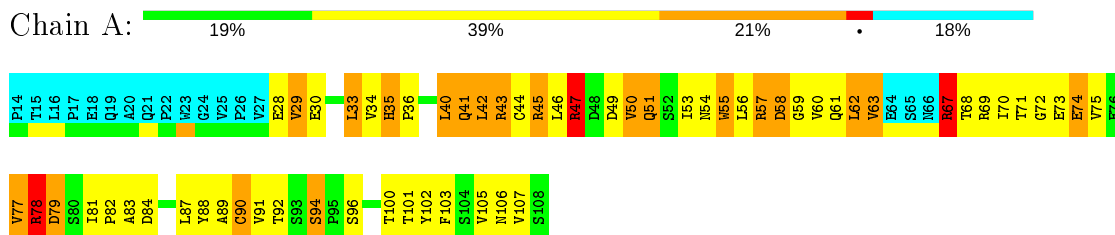
### 4.2.6 Score per residue for model 6

- Molecule 1: BASIC FIBROBLAST GROWTH FACTOR RECEPTOR 1



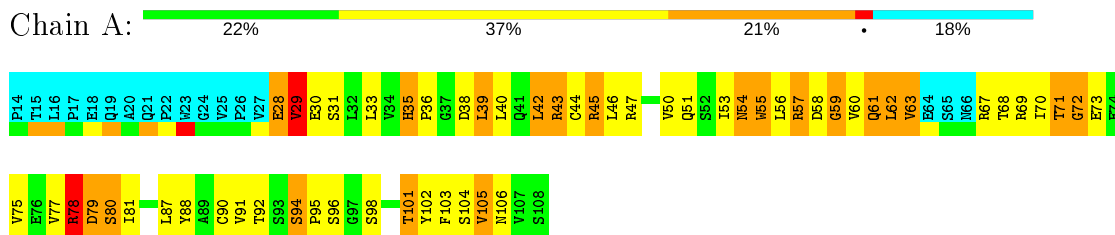
#### 4.2.7 Score per residue for model 7

- Molecule 1: BASIC FIBROBLAST GROWTH FACTOR RECEPTOR 1



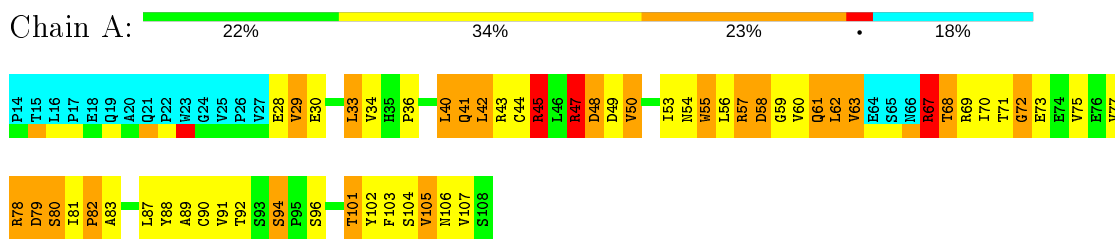
#### 4.2.8 Score per residue for model 8

- Molecule 1: BASIC FIBROBLAST GROWTH FACTOR RECEPTOR 1



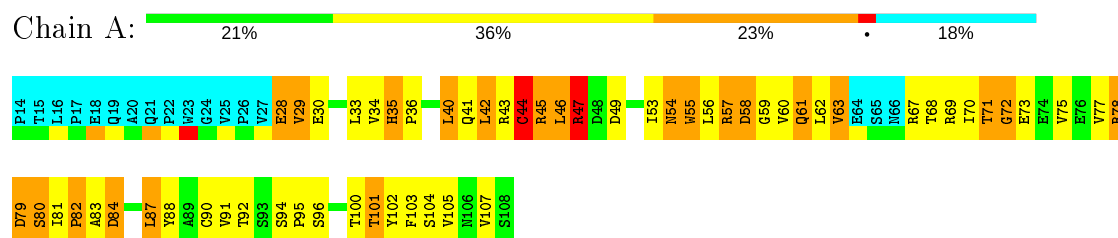
#### 4.2.9 Score per residue for model 9

- Molecule 1: BASIC FIBROBLAST GROWTH FACTOR RECEPTOR 1



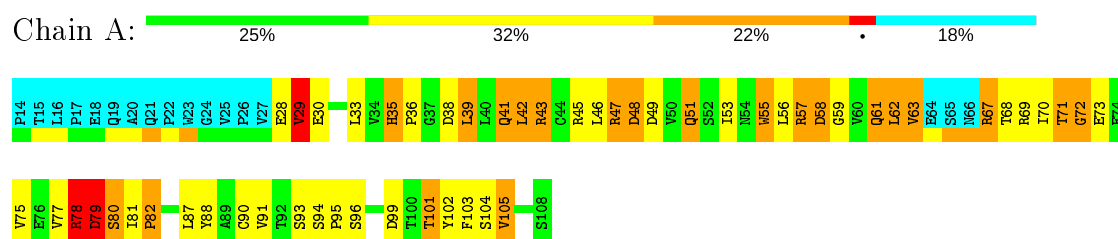
#### 4.2.10 Score per residue for model 10

- Molecule 1: BASIC FIBROBLAST GROWTH FACTOR RECEPTOR 1



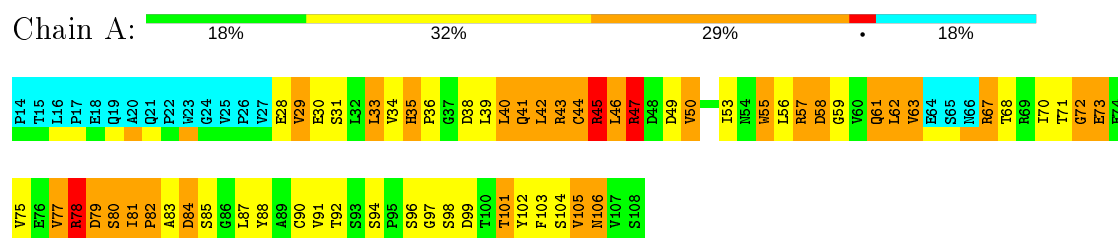
#### 4.2.11 Score per residue for model 11

- Molecule 1: BASIC FIBROBLAST GROWTH FACTOR RECEPTOR 1



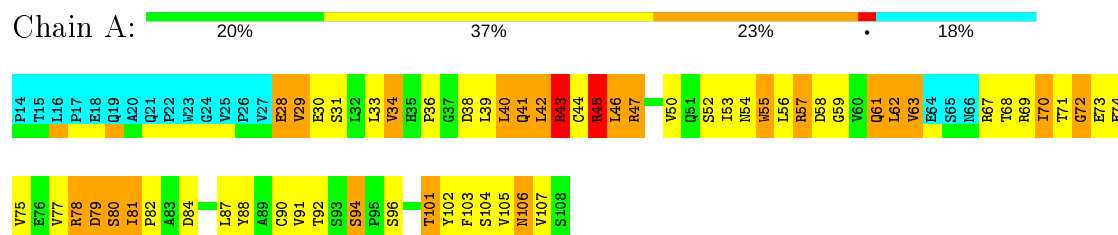
#### 4.2.12 Score per residue for model 12

- Molecule 1: BASIC FIBROBLAST GROWTH FACTOR RECEPTOR 1



#### 4.2.13 Score per residue for model 13

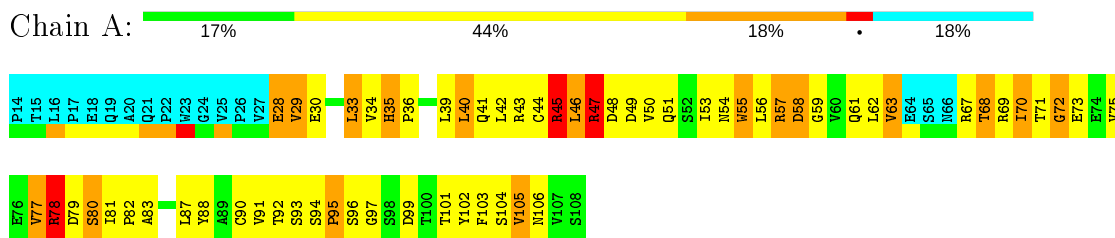
- Molecule 1: BASIC FIBROBLAST GROWTH FACTOR RECEPTOR 1





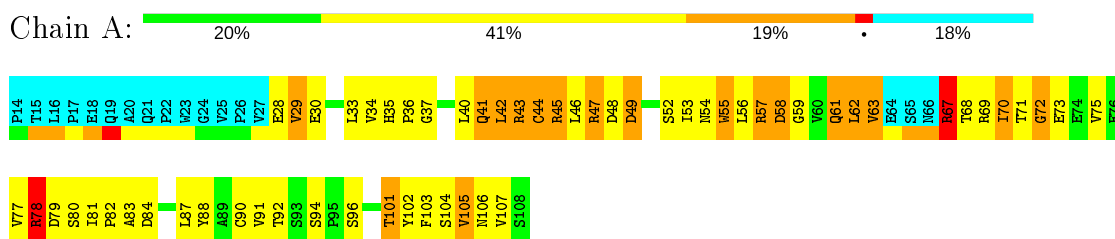
#### 4.2.14 Score per residue for model 14 (medoid)

- Molecule 1: BASIC FIBROBLAST GROWTH FACTOR RECEPTOR 1



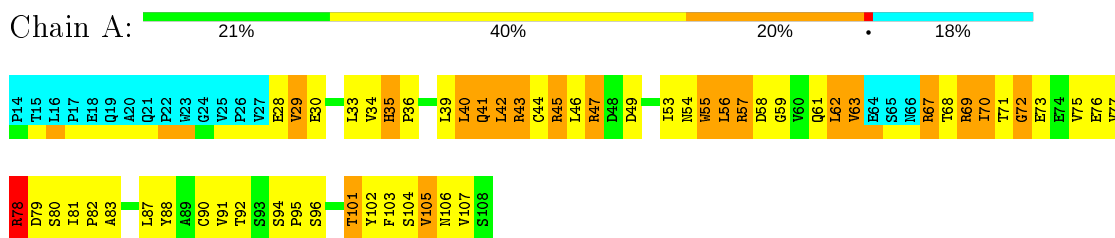
#### 4.2.15 Score per residue for model 15

- Molecule 1: BASIC FIBROBLAST GROWTH FACTOR RECEPTOR 1



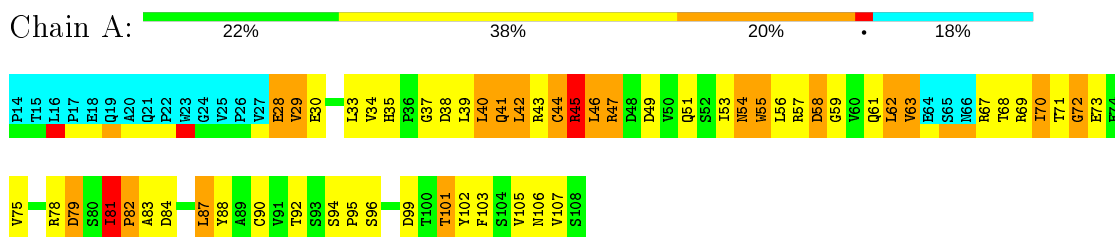
#### 4.2.16 Score per residue for model 16

- Molecule 1: BASIC FIBROBLAST GROWTH FACTOR RECEPTOR 1



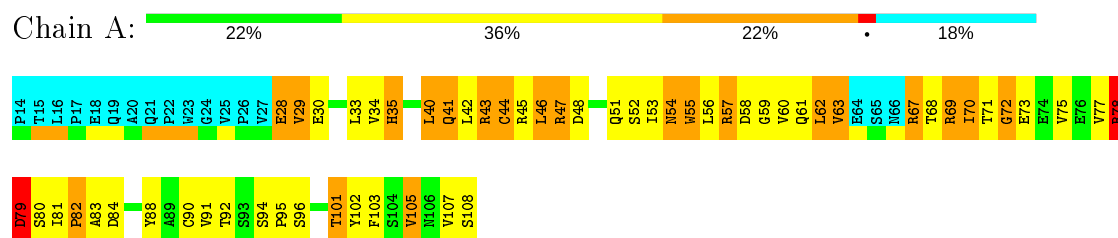
#### 4.2.17 Score per residue for model 17

- Molecule 1: BASIC FIBROBLAST GROWTH FACTOR RECEPTOR 1



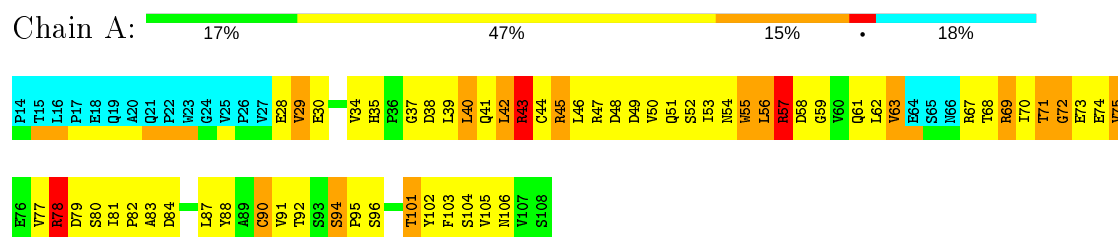
### 4.2.18 Score per residue for model 18

- Molecule 1: BASIC FIBROBLAST GROWTH FACTOR RECEPTOR 1



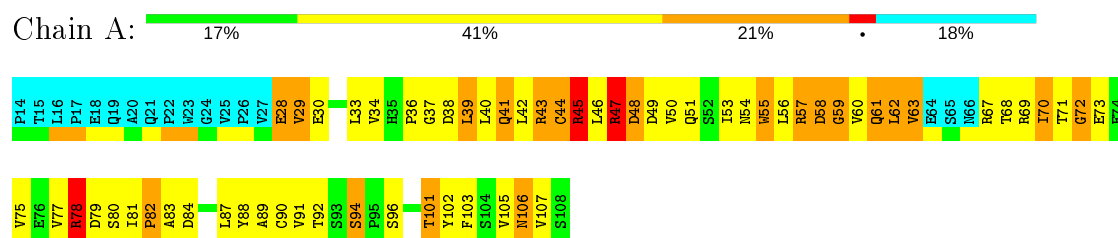
### 4.2.19 Score per residue for model 19

- Molecule 1: BASIC FIBROBLAST GROWTH FACTOR RECEPTOR 1



### 4.2.20 Score per residue for model 20

- Molecule 1: BASIC FIBROBLAST GROWTH FACTOR RECEPTOR 1



## 5 Refinement protocol and experimental data overview

Of the ? calculated structures, 20 were deposited, based on the following criterion: ?.

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

Software name	Classification	Version
X-PLOR	refinement	

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	702
Number of shifts mapped to atoms	634
Number of unparsed shifts	0
Number of shifts with mapping errors	68
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	51%

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	604	590	590	85±4
All	All	12080	11800	11800	1709

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 72.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:29:VAL:HG21	1:A:101:THR:HB	1.04	1.27	5	18

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:29:VAL:HG21	1:A:101:THR:CB	0.95	1.91	5	16
1:A:29:VAL:HG11	1:A:103:PHE:CE2	0.93	1.98	10	17
1:A:63:VAL:HB	1:A:70:ILE:HD13	0.89	1.45	2	7
1:A:71:THR:O	1:A:73:GLU:N	0.84	2.10	12	18
1:A:90:CYS:SG	1:A:101:THR:CG2	0.83	2.66	14	2
1:A:70:ILE:HG22	1:A:75:VAL:HG22	0.82	1.52	18	20
1:A:90:CYS:SG	1:A:101:THR:OG1	0.80	2.39	11	3
1:A:29:VAL:HG12	1:A:30:GLU:N	0.80	1.91	11	20
1:A:42:LEU:HD12	1:A:55:TRP:CE3	0.79	2.13	4	17
1:A:102:TYR:CD1	1:A:102:TYR:N	0.78	2.52	2	8
1:A:44:CYS:SG	1:A:92:THR:CG2	0.77	2.72	9	16
1:A:28:GLU:O	1:A:29:VAL:HG23	0.77	1.79	5	19
1:A:46:LEU:HD22	1:A:73:GLU:CB	0.76	2.11	3	1
1:A:90:CYS:SG	1:A:101:THR:HG23	0.74	2.22	14	1
1:A:55:TRP:CZ3	1:A:90:CYS:HB2	0.74	2.17	6	14
1:A:29:VAL:N	1:A:102:TYR:O	0.73	2.22	13	18
1:A:55:TRP:CD1	1:A:75:VAL:HG23	0.72	2.18	13	18
1:A:78:ARG:O	1:A:78:ARG:CD	0.72	2.38	12	3
1:A:29:VAL:HG11	1:A:103:PHE:CZ	0.72	2.19	2	20
1:A:55:TRP:CG	1:A:75:VAL:HG21	0.71	2.19	14	15
1:A:78:ARG:CD	1:A:78:ARG:O	0.70	2.39	13	3
1:A:28:GLU:CA	1:A:102:TYR:HB2	0.70	2.17	7	17
1:A:56:LEU:HD11	1:A:91:VAL:CG2	0.70	2.17	3	16
1:A:45:ARG:CZ	1:A:45:ARG:HB3	0.70	2.17	19	1
1:A:88:TYR:CD1	1:A:105:VAL:HG22	0.69	2.21	8	5
1:A:53:ILE:N	1:A:53:ILE:HD12	0.69	2.01	7	6
1:A:63:VAL:CG2	1:A:70:ILE:HD13	0.69	2.18	15	6
1:A:55:TRP:CD1	1:A:75:VAL:CG2	0.69	2.75	7	19
1:A:55:TRP:CZ3	1:A:90:CYS:HB3	0.69	2.23	14	7
1:A:42:LEU:HD12	1:A:55:TRP:CZ3	0.68	2.22	11	11
1:A:88:TYR:CE1	1:A:105:VAL:CG2	0.68	2.76	12	7
1:A:63:VAL:CB	1:A:70:ILE:HD13	0.68	2.19	2	3
1:A:54:ASN:O	1:A:54:ASN:ND2	0.67	2.27	18	1
1:A:55:TRP:CG	1:A:75:VAL:CG2	0.67	2.77	13	14
1:A:29:VAL:CG2	1:A:101:THR:HB	0.67	2.20	14	2
1:A:44:CYS:SG	1:A:53:ILE:HG23	0.67	2.30	20	3
1:A:42:LEU:HB2	1:A:55:TRP:CZ3	0.66	2.25	18	10
1:A:30:GLU:HB2	1:A:103:PHE:CD2	0.66	2.26	12	1
1:A:78:ARG:CD	1:A:78:ARG:N	0.66	2.58	20	7
1:A:45:ARG:NH2	1:A:99:ASP:CB	0.66	2.58	6	1
1:A:57:ARG:CB	1:A:62:LEU:HD22	0.66	2.21	1	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:63:VAL:HA	1:A:70:ILE:HG21	0.66	1.67	18	6
1:A:70:ILE:CD1	1:A:70:ILE:O	0.66	2.44	1	6
1:A:70:ILE:O	1:A:70:ILE:CD1	0.65	2.45	6	3
1:A:57:ARG:HG2	1:A:88:TYR:CE2	0.65	2.27	20	2
1:A:44:CYS:SG	1:A:92:THR:HG22	0.65	2.32	16	13
1:A:62:LEU:HD13	1:A:63:VAL:N	0.65	2.07	17	5
1:A:103:PHE:N	1:A:103:PHE:CD1	0.64	2.64	2	10
1:A:28:GLU:C	1:A:102:TYR:H	0.64	1.96	10	1
1:A:55:TRP:CG	1:A:75:VAL:HG23	0.64	2.27	13	2
1:A:44:CYS:HB2	1:A:55:TRP:CZ2	0.64	2.28	19	8
1:A:81:ILE:O	1:A:83:ALA:N	0.64	2.30	7	14
1:A:29:VAL:CG1	1:A:30:GLU:N	0.64	2.59	11	8
1:A:41:GLN:CD	1:A:41:GLN:N	0.64	2.51	10	4
1:A:55:TRP:NE1	1:A:75:VAL:HG23	0.64	2.07	20	17
1:A:88:TYR:CD1	1:A:105:VAL:CG2	0.64	2.80	8	7
1:A:53:ILE:CG2	1:A:90:CYS:SG	0.64	2.85	4	7
1:A:102:TYR:N	1:A:102:TYR:CD1	0.63	2.66	3	4
1:A:52:SER:C	1:A:53:ILE:HD12	0.63	2.13	18	6
1:A:63:VAL:HB	1:A:70:ILE:CD1	0.63	2.22	2	4
1:A:63:VAL:CG2	1:A:70:ILE:CD1	0.63	2.77	19	4
1:A:28:GLU:CB	1:A:102:TYR:HB2	0.63	2.23	18	10
1:A:70:ILE:O	1:A:70:ILE:HD12	0.63	1.93	6	2
1:A:53:ILE:CG1	1:A:72:GLY:O	0.63	2.47	8	15
1:A:29:VAL:CG2	1:A:101:THR:HG22	0.62	2.24	17	5
1:A:29:VAL:HB	1:A:102:TYR:C	0.62	2.15	11	18
1:A:29:VAL:HG21	1:A:101:THR:HG23	0.62	1.71	9	1
1:A:49:ASP:O	1:A:50:VAL:C	0.62	2.38	12	5
1:A:29:VAL:HG21	1:A:101:THR:CG2	0.62	2.25	9	3
1:A:62:LEU:CD1	1:A:63:VAL:H	0.61	2.08	8	2
1:A:47:ARG:O	1:A:48:ASP:C	0.61	2.38	9	4
1:A:42:LEU:HD11	1:A:75:VAL:HG11	0.61	1.72	10	5
1:A:29:VAL:CG2	1:A:101:THR:OG1	0.61	2.48	9	1
1:A:71:THR:O	1:A:72:GLY:C	0.61	2.38	11	1
1:A:71:THR:O	1:A:71:THR:OG1	0.61	2.18	12	1
1:A:84:ASP:O	1:A:106:ASN:HA	0.61	1.96	19	7
1:A:42:LEU:CD1	1:A:75:VAL:HB	0.61	2.26	8	16
1:A:55:TRP:CE2	1:A:75:VAL:HG23	0.61	2.31	20	14
1:A:46:LEU:HD22	1:A:73:GLU:HB2	0.60	1.73	3	1
1:A:45:ARG:CZ	1:A:101:THR:CG2	0.60	2.78	1	1
1:A:88:TYR:CD1	1:A:105:VAL:HB	0.60	2.30	13	4
1:A:63:VAL:HG22	1:A:70:ILE:HD13	0.60	1.73	19	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:57:ARG:CG	1:A:88:TYR:CZ	0.60	2.84	1	3
1:A:41:GLN:NE2	1:A:41:GLN:N	0.60	2.49	11	5
1:A:35:HIS:ND1	1:A:35:HIS:N	0.60	2.49	18	4
1:A:79:ASP:O	1:A:80:SER:OG	0.60	2.20	10	2
1:A:47:ARG:O	1:A:49:ASP:N	0.60	2.35	9	7
1:A:88:TYR:CE1	1:A:105:VAL:HG22	0.60	2.31	8	3
1:A:94:SER:O	1:A:96:SER:N	0.59	2.35	6	20
1:A:55:TRP:CZ3	1:A:90:CYS:CB	0.59	2.85	19	6
1:A:90:CYS:O	1:A:90:CYS:SG	0.59	2.59	19	5
1:A:28:GLU:N	1:A:102:TYR:HB2	0.59	2.13	6	5
1:A:88:TYR:CE1	1:A:105:VAL:HG21	0.59	2.33	12	6
1:A:78:ARG:HD3	1:A:78:ARG:N	0.59	2.12	20	3
1:A:53:ILE:HG23	1:A:90:CYS:SG	0.59	2.37	8	6
1:A:78:ARG:O	1:A:78:ARG:HD2	0.59	1.96	13	3
1:A:39:LEU:N	1:A:39:LEU:HD12	0.59	2.13	5	3
1:A:55:TRP:CE3	1:A:90:CYS:HB3	0.58	2.33	11	1
1:A:63:VAL:HG22	1:A:70:ILE:CD1	0.58	2.28	19	2
1:A:29:VAL:HG11	1:A:103:PHE:CE1	0.58	2.32	11	5
1:A:42:LEU:CD1	1:A:55:TRP:CE3	0.58	2.85	19	2
1:A:54:ASN:ND2	1:A:91:VAL:HB	0.58	2.13	18	4
1:A:62:LEU:HD13	1:A:63:VAL:H	0.58	1.57	3	7
1:A:40:LEU:CD2	1:A:105:VAL:HG11	0.58	2.27	10	2
1:A:29:VAL:HB	1:A:102:TYR:O	0.58	1.98	3	13
1:A:42:LEU:CB	1:A:55:TRP:CZ3	0.58	2.86	18	2
1:A:57:ARG:O	1:A:59:GLY:N	0.58	2.37	9	19
1:A:57:ARG:H	1:A:62:LEU:HB2	0.58	1.59	3	8
1:A:87:LEU:HD22	1:A:87:LEU:N	0.58	2.13	7	1
1:A:101:THR:OG1	1:A:103:PHE:CE1	0.58	2.57	8	1
1:A:57:ARG:HG3	1:A:88:TYR:CZ	0.57	2.34	4	8
1:A:35:HIS:N	1:A:35:HIS:ND1	0.57	2.53	12	2
1:A:55:TRP:CD1	1:A:75:VAL:HG21	0.57	2.34	14	8
1:A:45:ARG:CZ	1:A:45:ARG:CB	0.57	2.83	19	1
1:A:80:SER:OG	1:A:80:SER:O	0.57	2.22	8	3
1:A:56:LEU:CD1	1:A:91:VAL:HG23	0.57	2.30	14	1
1:A:45:ARG:C	1:A:46:LEU:HD23	0.57	2.20	3	3
1:A:53:ILE:HG13	1:A:72:GLY:O	0.56	2.00	9	4
1:A:46:LEU:HD23	1:A:46:LEU:N	0.56	2.15	17	4
1:A:70:ILE:HD12	1:A:70:ILE:O	0.56	2.01	17	3
1:A:30:GLU:HB3	1:A:103:PHE:CD2	0.56	2.36	5	2
1:A:57:ARG:CB	1:A:62:LEU:HD13	0.56	2.31	6	1
1:A:41:GLN:N	1:A:41:GLN:NE2	0.56	2.53	16	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:68:THR:HB	1:A:77:VAL:HA	0.56	1.78	13	2
1:A:78:ARG:HD2	1:A:78:ARG:O	0.56	2.00	12	2
1:A:84:ASP:CG	1:A:107:VAL:HB	0.55	2.21	20	1
1:A:46:LEU:HD11	1:A:73:GLU:HB2	0.55	1.77	10	1
1:A:63:VAL:HG23	1:A:70:ILE:CG1	0.55	2.32	18	8
1:A:83:ALA:O	1:A:88:TYR:CZ	0.55	2.59	20	1
1:A:50:VAL:HA	1:A:94:SER:CB	0.55	2.31	19	2
1:A:53:ILE:HD12	1:A:53:ILE:N	0.55	2.17	1	1
1:A:103:PHE:CD1	1:A:103:PHE:N	0.55	2.74	6	5
1:A:33:LEU:H	1:A:33:LEU:HD23	0.55	1.61	11	1
1:A:55:TRP:CD2	1:A:75:VAL:HG23	0.55	2.37	10	2
1:A:47:ARG:C	1:A:49:ASP:H	0.55	2.05	19	9
1:A:80:SER:O	1:A:80:SER:OG	0.55	2.24	5	2
1:A:63:VAL:HG23	1:A:70:ILE:CD1	0.54	2.32	4	4
1:A:79:ASP:O	1:A:80:SER:C	0.54	2.46	13	3
1:A:28:GLU:O	1:A:29:VAL:CG2	0.54	2.55	10	1
1:A:88:TYR:CD2	1:A:105:VAL:CG2	0.54	2.90	4	6
1:A:28:GLU:HA	1:A:102:TYR:HB2	0.54	1.78	18	11
1:A:45:ARG:NH2	1:A:99:ASP:HB2	0.54	2.18	6	1
1:A:70:ILE:HG22	1:A:75:VAL:CG2	0.54	2.31	18	6
1:A:81:ILE:HB	1:A:82:PRO:CD	0.54	2.33	16	4
1:A:40:LEU:HB3	1:A:77:VAL:CG2	0.54	2.33	8	2
1:A:28:GLU:HB3	1:A:102:TYR:HB2	0.54	1.79	19	9
1:A:45:ARG:HH11	1:A:45:ARG:H	0.54	1.44	5	1
1:A:53:ILE:HB	1:A:72:GLY:O	0.54	2.02	16	7
1:A:35:HIS:CB	1:A:36:PRO:CD	0.54	2.85	10	7
1:A:28:GLU:HA	1:A:102:TYR:CD1	0.54	2.38	2	5
1:A:40:LEU:C	1:A:40:LEU:HD12	0.54	2.23	6	3
1:A:71:THR:C	1:A:73:GLU:H	0.54	2.06	10	18
1:A:56:LEU:CD1	1:A:91:VAL:CG2	0.53	2.86	2	7
1:A:41:GLN:NE2	1:A:41:GLN:H	0.53	2.02	6	4
1:A:44:CYS:SG	1:A:53:ILE:CG2	0.53	2.97	16	1
1:A:37:GLY:N	1:A:80:SER:HA	0.53	2.19	20	1
1:A:81:ILE:CB	1:A:82:PRO:HD2	0.53	2.34	17	6
1:A:80:SER:C	1:A:107:VAL:HG21	0.53	2.24	9	2
1:A:29:VAL:CG1	1:A:103:PHE:CE2	0.53	2.91	9	11
1:A:57:ARG:CG	1:A:88:TYR:CE2	0.53	2.92	20	3
1:A:77:VAL:C	1:A:78:ARG:HD2	0.53	2.24	3	3
1:A:105:VAL:CG2	1:A:105:VAL:O	0.53	2.56	8	6
1:A:43:ARG:O	1:A:103:PHE:CZ	0.53	2.62	19	4
1:A:47:ARG:C	1:A:49:ASP:N	0.53	2.58	3	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:61:GLN:HG3	1:A:61:GLN:O	0.53	2.04	20	2
1:A:33:LEU:HD12	1:A:33:LEU:N	0.52	2.19	20	1
1:A:55:TRP:CH2	1:A:90:CYS:HB2	0.52	2.38	7	1
1:A:78:ARG:HD3	1:A:78:ARG:O	0.52	2.04	12	4
1:A:33:LEU:HA	1:A:106:ASN:ND2	0.52	2.18	5	1
1:A:29:VAL:CG2	1:A:101:THR:CG2	0.52	2.87	17	2
1:A:84:ASP:O	1:A:105:VAL:O	0.52	2.28	13	5
1:A:68:THR:OG1	1:A:77:VAL:CG1	0.52	2.57	7	2
1:A:81:ILE:C	1:A:83:ALA:N	0.52	2.62	17	2
1:A:57:ARG:CZ	1:A:58:ASP:HB2	0.52	2.35	14	7
1:A:107:VAL:HG22	1:A:107:VAL:O	0.52	2.04	5	1
1:A:78:ARG:N	1:A:78:ARG:CD	0.52	2.73	16	4
1:A:94:SER:CB	1:A:95:PRO:CD	0.52	2.88	18	3
1:A:53:ILE:N	1:A:53:ILE:CD1	0.52	2.73	7	3
1:A:40:LEU:HD12	1:A:41:GLN:N	0.52	2.20	13	11
1:A:47:ARG:CD	1:A:99:ASP:HB2	0.51	2.36	4	1
1:A:47:ARG:NH2	1:A:98:SER:CA	0.51	2.72	12	1
1:A:87:LEU:N	1:A:87:LEU:HD12	0.51	2.20	19	2
1:A:40:LEU:CD2	1:A:105:VAL:CG1	0.51	2.88	13	2
1:A:88:TYR:CD2	1:A:105:VAL:HG22	0.51	2.40	9	5
1:A:81:ILE:HB	1:A:82:PRO:HD2	0.51	1.81	16	16
1:A:63:VAL:C	1:A:70:ILE:HG21	0.51	2.25	20	1
1:A:40:LEU:HD23	1:A:77:VAL:HG21	0.51	1.82	12	1
1:A:46:LEU:HB3	1:A:53:ILE:HD11	0.51	1.83	14	1
1:A:56:LEU:HD23	1:A:61:GLN:CA	0.51	2.35	5	9
1:A:45:ARG:NE	1:A:101:THR:HG21	0.51	2.20	4	1
1:A:55:TRP:CD2	1:A:75:VAL:CG2	0.51	2.93	10	2
1:A:42:LEU:HD11	1:A:75:VAL:CG1	0.51	2.36	10	5
1:A:29:VAL:HG11	1:A:103:PHE:CD1	0.51	2.41	11	1
1:A:56:LEU:HD12	1:A:89:ALA:HB3	0.51	1.80	3	2
1:A:41:GLN:H	1:A:41:GLN:NE2	0.51	2.04	20	2
1:A:51:GLN:NE2	1:A:95:PRO:HD3	0.51	2.20	17	5
1:A:90:CYS:SG	1:A:103:PHE:HE1	0.51	2.29	11	1
1:A:38:ASP:CG	1:A:39:LEU:H	0.50	2.10	4	3
1:A:57:ARG:HB3	1:A:62:LEU:CD1	0.50	2.36	20	1
1:A:57:ARG:HB2	1:A:62:LEU:CD2	0.50	2.36	4	2
1:A:56:LEU:HD11	1:A:91:VAL:HG22	0.50	1.84	5	2
1:A:63:VAL:HB	1:A:70:ILE:HG21	0.50	1.83	10	1
1:A:57:ARG:HG2	1:A:88:TYR:CZ	0.50	2.41	1	1
1:A:51:GLN:NE2	1:A:95:PRO:CD	0.50	2.75	6	3
1:A:45:ARG:NH2	1:A:99:ASP:HB3	0.50	2.20	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:94:SER:C	1:A:96:SER:H	0.50	2.10	2	9
1:A:35:HIS:HB3	1:A:36:PRO:CD	0.50	2.37	6	1
1:A:33:LEU:N	1:A:33:LEU:HD12	0.50	2.21	8	1
1:A:79:ASP:O	1:A:80:SER:O	0.50	2.29	2	5
1:A:47:ARG:HG3	1:A:48:ASP:N	0.50	2.22	18	2
1:A:46:LEU:HD11	1:A:73:GLU:CB	0.50	2.37	10	1
1:A:84:ASP:HA	1:A:88:TYR:CE1	0.49	2.42	7	2
1:A:69:ARG:NH1	1:A:78:ARG:NH2	0.49	2.60	18	1
1:A:55:TRP:CE2	1:A:90:CYS:SG	0.49	3.05	18	1
1:A:45:ARG:CZ	1:A:101:THR:HG23	0.49	2.37	10	2
1:A:81:ILE:O	1:A:82:PRO:C	0.49	2.51	9	11
1:A:42:LEU:HD12	1:A:75:VAL:HB	0.49	1.83	14	2
1:A:53:ILE:HD12	1:A:92:THR:HG22	0.49	1.83	2	1
1:A:45:ARG:HH11	1:A:45:ARG:N	0.49	2.05	5	1
1:A:55:TRP:CE3	1:A:90:CYS:HB2	0.49	2.42	20	7
1:A:35:HIS:CG	1:A:36:PRO:HD2	0.49	2.42	8	1
1:A:49:ASP:O	1:A:51:GLN:CG	0.49	2.61	4	3
1:A:54:ASN:C	1:A:54:ASN:ND2	0.49	2.66	18	1
1:A:45:ARG:O	1:A:45:ARG:CG	0.49	2.60	13	1
1:A:34:VAL:HG21	1:A:40:LEU:HB2	0.49	1.83	1	2
1:A:105:VAL:O	1:A:105:VAL:CG2	0.49	2.61	2	5
1:A:41:GLN:O	1:A:41:GLN:NE2	0.49	2.46	7	1
1:A:78:ARG:HD2	1:A:78:ARG:C	0.49	2.28	1	1
1:A:49:ASP:O	1:A:94:SER:CB	0.49	2.60	19	4
1:A:62:LEU:CD2	1:A:63:VAL:H	0.49	2.20	20	1
1:A:62:LEU:CD1	1:A:63:VAL:N	0.49	2.76	17	4
1:A:78:ARG:HD2	1:A:78:ARG:N	0.49	2.22	18	1
1:A:55:TRP:O	1:A:62:LEU:O	0.48	2.31	15	9
1:A:89:ALA:HA	1:A:101:THR:O	0.48	2.08	7	1
1:A:35:HIS:CG	1:A:36:PRO:CD	0.48	2.96	8	1
1:A:68:THR:OG1	1:A:77:VAL:HG13	0.48	2.08	12	1
1:A:56:LEU:HD11	1:A:91:VAL:HG21	0.48	1.86	19	7
1:A:56:LEU:HD23	1:A:61:GLN:N	0.48	2.24	13	8
1:A:46:LEU:HD12	1:A:47:ARG:N	0.48	2.23	14	2
1:A:45:ARG:NE	1:A:101:THR:CG2	0.48	2.77	14	1
1:A:39:LEU:HD12	1:A:39:LEU:N	0.48	2.24	17	2
1:A:43:ARG:NE	1:A:74:GLU:HB2	0.48	2.23	19	1
1:A:78:ARG:C	1:A:78:ARG:CD	0.48	2.82	1	1
1:A:70:ILE:O	1:A:70:ILE:HD13	0.48	2.08	14	2
1:A:83:ALA:O	1:A:88:TYR:OH	0.48	2.29	2	3
1:A:28:GLU:HB3	1:A:102:TYR:O	0.48	2.08	13	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:44:CYS:HA	1:A:45:ARG:NH1	0.48	2.24	4	1
1:A:78:ARG:N	1:A:78:ARG:HD2	0.48	2.23	9	1
1:A:44:CYS:SG	1:A:92:THR:HG23	0.48	2.49	12	2
1:A:38:ASP:H	1:A:80:SER:HB3	0.48	1.69	11	2
1:A:46:LEU:HD22	1:A:53:ILE:HG12	0.48	1.85	13	1
1:A:29:VAL:HG11	1:A:103:PHE:CD2	0.48	2.44	9	4
1:A:42:LEU:HB2	1:A:55:TRP:CH2	0.48	2.44	18	1
1:A:63:VAL:CA	1:A:70:ILE:HG21	0.48	2.39	20	1
1:A:29:VAL:HG21	1:A:101:THR:OG1	0.48	2.09	8	2
1:A:53:ILE:HD13	1:A:72:GLY:O	0.47	2.09	5	4
1:A:70:ILE:HD13	1:A:70:ILE:O	0.47	2.09	5	3
1:A:90:CYS:SG	1:A:101:THR:HG21	0.47	2.44	14	1
1:A:90:CYS:SG	1:A:101:THR:HB	0.47	2.49	9	1
1:A:100:THR:HG22	1:A:102:TYR:CE1	0.47	2.44	10	1
1:A:57:ARG:NH1	1:A:58:ASP:HB2	0.47	2.24	10	1
1:A:88:TYR:CE2	1:A:105:VAL:CG2	0.47	2.98	3	2
1:A:29:VAL:CG1	1:A:103:PHE:CD2	0.47	2.97	8	4
1:A:28:GLU:HA	1:A:102:TYR:CD2	0.47	2.44	11	1
1:A:81:ILE:H	1:A:81:ILE:HD12	0.47	1.69	12	1
1:A:55:TRP:O	1:A:62:LEU:N	0.47	2.48	13	11
1:A:81:ILE:O	1:A:107:VAL:HG11	0.47	2.09	18	5
1:A:56:LEU:CD2	1:A:61:GLN:HA	0.47	2.40	1	8
1:A:29:VAL:HG23	1:A:102:TYR:N	0.47	2.25	3	3
1:A:39:LEU:HB3	1:A:78:ARG:NH1	0.47	2.23	3	1
1:A:53:ILE:CD1	1:A:72:GLY:O	0.47	2.62	7	2
1:A:57:ARG:HG2	1:A:58:ASP:N	0.47	2.24	11	3
1:A:38:ASP:H	1:A:80:SER:HB2	0.47	1.70	12	3
1:A:107:VAL:HG13	1:A:107:VAL:O	0.47	2.09	18	4
1:A:33:LEU:CB	1:A:106:ASN:HD21	0.47	2.22	15	2
1:A:45:ARG:HE	1:A:101:THR:CG2	0.47	2.23	15	2
1:A:61:GLN:O	1:A:62:LEU:HD22	0.47	2.08	7	2
1:A:57:ARG:HG3	1:A:88:TYR:OH	0.47	2.09	4	2
1:A:28:GLU:CA	1:A:102:TYR:CD1	0.47	2.97	2	1
1:A:47:ARG:NH1	1:A:99:ASP:HB3	0.47	2.23	12	1
1:A:46:LEU:HA	1:A:50:VAL:CG1	0.47	2.39	7	2
1:A:57:ARG:CB	1:A:62:LEU:CD2	0.47	2.93	1	1
1:A:78:ARG:O	1:A:78:ARG:HD3	0.47	2.09	19	2
1:A:68:THR:HB	1:A:77:VAL:CG1	0.47	2.40	1	2
1:A:77:VAL:HG23	1:A:77:VAL:O	0.46	2.10	9	4
1:A:47:ARG:NH2	1:A:99:ASP:N	0.46	2.63	12	1
1:A:41:GLN:O	1:A:42:LEU:HD23	0.46	2.10	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:42:LEU:HB3	1:A:103:PHE:CG	0.46	2.46	10	1
1:A:74:GLU:HG3	1:A:75:VAL:N	0.46	2.26	13	1
1:A:35:HIS:CD2	1:A:108:SER:CB	0.46	2.98	1	1
1:A:33:LEU:O	1:A:33:LEU:HD12	0.46	2.10	4	1
1:A:62:LEU:O	1:A:63:VAL:CG1	0.46	2.64	2	3
1:A:39:LEU:C	1:A:39:LEU:HD23	0.46	2.31	13	1
1:A:68:THR:HG23	1:A:68:THR:O	0.46	2.10	1	1
1:A:84:ASP:O	1:A:106:ASN:CA	0.46	2.63	13	2
1:A:58:ASP:HA	1:A:87:LEU:N	0.46	2.25	7	4
1:A:61:GLN:O	1:A:62:LEU:CD2	0.46	2.64	8	2
1:A:53:ILE:CD1	1:A:53:ILE:N	0.46	2.79	18	3
1:A:37:GLY:CA	1:A:79:ASP:O	0.46	2.64	4	3
1:A:40:LEU:O	1:A:77:VAL:HG22	0.46	2.10	18	2
1:A:43:ARG:N	1:A:103:PHE:CE2	0.46	2.84	8	1
1:A:56:LEU:HD23	1:A:61:GLN:HA	0.46	1.88	1	12
1:A:71:THR:C	1:A:73:GLU:N	0.46	2.69	10	17
1:A:45:ARG:CZ	1:A:101:THR:HG21	0.46	2.40	4	1
1:A:42:LEU:HD12	1:A:75:VAL:CG1	0.46	2.40	14	1
1:A:63:VAL:CG2	1:A:70:ILE:HD12	0.46	2.40	19	1
1:A:68:THR:OG1	1:A:77:VAL:HG12	0.46	2.11	7	1
1:A:68:THR:CB	1:A:77:VAL:HA	0.46	2.41	8	2
1:A:29:VAL:HB	1:A:102:TYR:N	0.46	2.26	6	1
1:A:47:ARG:CB	1:A:94:SER:HB3	0.46	2.41	7	1
1:A:39:LEU:N	1:A:39:LEU:CD1	0.46	2.79	5	1
1:A:84:ASP:HB3	1:A:105:VAL:CG1	0.46	2.41	10	1
1:A:107:VAL:O	1:A:107:VAL:HG13	0.45	2.11	7	3
1:A:57:ARG:HB3	1:A:62:LEU:HD13	0.45	1.88	6	1
1:A:57:ARG:HB2	1:A:88:TYR:CE2	0.45	2.46	14	1
1:A:29:VAL:CG2	1:A:101:THR:CB	0.45	2.94	17	3
1:A:89:ALA:HB2	1:A:102:TYR:CD2	0.45	2.46	7	1
1:A:35:HIS:O	1:A:80:SER:OG	0.45	2.30	8	1
1:A:46:LEU:O	1:A:47:ARG:HG2	0.45	2.12	16	1
1:A:28:GLU:CA	1:A:102:TYR:HD1	0.45	2.25	2	1
1:A:99:ASP:N	1:A:99:ASP:OD1	0.45	2.49	2	1
1:A:68:THR:HB	1:A:77:VAL:HG12	0.45	1.88	14	3
1:A:44:CYS:HB2	1:A:55:TRP:CH2	0.45	2.46	14	5
1:A:53:ILE:HG21	1:A:73:GLU:HA	0.45	1.88	11	1
1:A:62:LEU:C	1:A:63:VAL:HG13	0.45	2.31	2	4
1:A:94:SER:C	1:A:96:SER:N	0.45	2.70	2	8
1:A:46:LEU:C	1:A:47:ARG:HG2	0.45	2.32	16	1
1:A:90:CYS:SG	1:A:103:PHE:CE1	0.45	3.09	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:57:ARG:HB2	1:A:62:LEU:HD22	0.45	1.86	4	3
1:A:78:ARG:C	1:A:80:SER:H	0.45	2.15	20	1
1:A:28:GLU:HA	1:A:102:TYR:CB	0.45	2.42	7	1
1:A:38:ASP:O	1:A:79:ASP:N	0.45	2.50	1	6
1:A:57:ARG:NE	1:A:62:LEU:HD13	0.45	2.27	20	1
1:A:77:VAL:O	1:A:77:VAL:HG23	0.45	2.12	8	1
1:A:61:GLN:NE2	1:A:61:GLN:C	0.45	2.70	15	1
1:A:31:SER:HA	1:A:104:SER:OG	0.45	2.12	12	2
1:A:69:ARG:NE	1:A:78:ARG:NH2	0.45	2.64	16	1
1:A:53:ILE:CD1	1:A:92:THR:HG22	0.45	2.42	9	1
1:A:68:THR:CB	1:A:77:VAL:HG12	0.45	2.42	18	2
1:A:40:LEU:HD11	1:A:42:LEU:CD2	0.45	2.41	17	1
1:A:84:ASP:HB2	1:A:105:VAL:CG1	0.45	2.42	17	1
1:A:84:ASP:OD1	1:A:107:VAL:CG1	0.45	2.64	20	1
1:A:41:GLN:N	1:A:41:GLN:CD	0.45	2.70	12	6
1:A:33:LEU:HD23	1:A:33:LEU:N	0.45	2.27	12	1
1:A:53:ILE:HG22	1:A:90:CYS:SG	0.45	2.52	16	1
1:A:49:ASP:O	1:A:51:GLN:HG3	0.44	2.12	11	3
1:A:40:LEU:HG	1:A:77:VAL:HG23	0.44	1.89	6	1
1:A:81:ILE:HG13	1:A:83:ALA:CB	0.44	2.42	17	1
1:A:107:VAL:CG1	1:A:107:VAL:O	0.44	2.65	20	2
1:A:58:ASP:O	1:A:87:LEU:HB3	0.44	2.12	20	1
1:A:62:LEU:C	1:A:63:VAL:CG1	0.44	2.86	2	2
1:A:68:THR:HG22	1:A:77:VAL:HB	0.44	1.89	10	2
1:A:44:CYS:SG	1:A:45:ARG:N	0.44	2.90	9	1
1:A:45:ARG:NH2	1:A:92:THR:CG2	0.44	2.80	15	1
1:A:37:GLY:N	1:A:79:ASP:O	0.44	2.50	17	2
1:A:63:VAL:HG23	1:A:70:ILE:HD13	0.44	1.85	4	2
1:A:47:ARG:HH21	1:A:98:SER:N	0.44	2.09	12	1
1:A:62:LEU:HD12	1:A:63:VAL:H	0.44	1.71	8	1
1:A:61:GLN:C	1:A:61:GLN:NE2	0.44	2.71	11	1
1:A:40:LEU:HD22	1:A:105:VAL:HG11	0.44	1.89	20	1
1:A:40:LEU:O	1:A:77:VAL:HG23	0.44	2.13	4	1
1:A:49:ASP:H	1:A:94:SER:HB2	0.44	1.73	12	1
1:A:60:VAL:HG12	1:A:61:GLN:N	0.44	2.28	20	1
1:A:106:ASN:OD1	1:A:106:ASN:N	0.44	2.50	1	1
1:A:39:LEU:N	1:A:39:LEU:HD23	0.44	2.28	20	3
1:A:55:TRP:CE2	1:A:75:VAL:CG2	0.44	3.00	20	1
1:A:45:ARG:HB2	1:A:45:ARG:NH1	0.44	2.28	15	1
1:A:60:VAL:O	1:A:61:GLN:C	0.43	2.56	3	5
1:A:40:LEU:CD2	1:A:77:VAL:HG21	0.43	2.43	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:46:LEU:HD21	1:A:73:GLU:CB	0.43	2.43	2	1
1:A:62:LEU:O	1:A:63:VAL:HG13	0.43	2.13	13	2
1:A:90:CYS:SG	1:A:101:THR:HG22	0.43	2.54	9	1
1:A:58:ASP:O	1:A:87:LEU:CB	0.43	2.67	20	1
1:A:49:ASP:O	1:A:51:GLN:CD	0.43	2.57	7	1
1:A:29:VAL:HG11	1:A:103:PHE:CG	0.43	2.49	11	1
1:A:63:VAL:HG23	1:A:70:ILE:HG12	0.43	1.89	18	2
1:A:55:TRP:NE1	1:A:75:VAL:CG2	0.43	2.80	20	1
1:A:57:ARG:CZ	1:A:62:LEU:CD1	0.43	2.97	20	1
1:A:58:ASP:HA	1:A:87:LEU:H	0.43	1.74	7	1
1:A:84:ASP:HB3	1:A:105:VAL:HG12	0.43	1.90	10	1
1:A:43:ARG:HD3	1:A:74:GLU:OE1	0.43	2.14	5	1
1:A:50:VAL:HG11	1:A:92:THR:CB	0.43	2.43	13	3
1:A:50:VAL:HB	1:A:53:ILE:HD11	0.43	1.90	7	1
1:A:58:ASP:N	1:A:87:LEU:O	0.43	2.51	5	16
1:A:45:ARG:NH1	1:A:99:ASP:HB3	0.43	2.29	2	1
1:A:77:VAL:CG2	1:A:77:VAL:O	0.43	2.66	10	2
1:A:50:VAL:HA	1:A:94:SER:HB2	0.43	1.89	19	1
1:A:40:LEU:O	1:A:40:LEU:HG	0.43	2.14	7	1
1:A:49:ASP:O	1:A:51:GLN:NE2	0.43	2.52	7	1
1:A:46:LEU:CD2	1:A:46:LEU:N	0.43	2.81	13	1
1:A:101:THR:C	1:A:102:TYR:CD1	0.43	2.91	10	1
1:A:30:GLU:O	1:A:103:PHE:HA	0.43	2.14	17	3
1:A:40:LEU:HG	1:A:40:LEU:O	0.43	2.13	19	2
1:A:53:ILE:CB	1:A:72:GLY:O	0.43	2.66	10	2
1:A:28:GLU:HB2	1:A:102:TYR:HB2	0.43	1.90	18	1
1:A:55:TRP:CH2	1:A:90:CYS:CB	0.43	3.02	7	1
1:A:79:ASP:OD1	1:A:79:ASP:N	0.43	2.52	8	1
1:A:88:TYR:CD1	1:A:105:VAL:CG1	0.42	3.02	5	1
1:A:38:ASP:O	1:A:79:ASP:C	0.42	2.57	11	1
1:A:88:TYR:HB2	1:A:103:PHE:O	0.42	2.14	18	1
1:A:70:ILE:O	1:A:70:ILE:HG13	0.42	2.14	19	4
1:A:33:LEU:CD2	1:A:106:ASN:HD21	0.42	2.27	3	1
1:A:45:ARG:NH1	1:A:101:THR:HG21	0.42	2.29	4	1
1:A:42:LEU:HD12	1:A:75:VAL:CB	0.42	2.45	14	2
1:A:84:ASP:HB2	1:A:105:VAL:HG12	0.42	1.90	17	1
1:A:84:ASP:O	1:A:105:VAL:HG23	0.42	2.13	18	1
1:A:57:ARG:CG	1:A:88:TYR:CE1	0.42	3.02	4	1
1:A:57:ARG:HB3	1:A:62:LEU:HD22	0.42	1.90	5	1
1:A:55:TRP:CD2	1:A:90:CYS:SG	0.42	3.12	18	1
1:A:45:ARG:HD3	1:A:92:THR:HG21	0.42	1.91	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:51:GLN:NE2	1:A:95:PRO:HD2	0.42	2.30	2	1
1:A:38:ASP:CG	1:A:39:LEU:N	0.42	2.72	4	1
1:A:45:ARG:HH22	1:A:99:ASP:HB2	0.42	1.73	6	1
1:A:46:LEU:HD22	1:A:53:ILE:CG1	0.42	2.44	13	1
1:A:45:ARG:NH2	1:A:92:THR:HG23	0.42	2.30	15	1
1:A:45:ARG:NH1	1:A:101:THR:CG2	0.42	2.82	1	1
1:A:51:GLN:HE21	1:A:95:PRO:HD3	0.42	1.75	4	1
1:A:55:TRP:CZ2	1:A:90:CYS:SG	0.42	3.12	6	2
1:A:33:LEU:C	1:A:33:LEU:HD12	0.42	2.35	6	1
1:A:42:LEU:CD1	1:A:55:TRP:CZ3	0.42	3.02	19	1
1:A:88:TYR:O	1:A:103:PHE:HB2	0.42	2.14	4	1
1:A:57:ARG:HH22	1:A:83:ALA:HB1	0.42	1.75	16	1
1:A:81:ILE:CB	1:A:82:PRO:CD	0.42	2.97	16	3
1:A:79:ASP:OD1	1:A:80:SER:N	0.42	2.52	13	1
1:A:50:VAL:C	1:A:51:GLN:HG3	0.42	2.35	2	3
1:A:33:LEU:N	1:A:33:LEU:HD23	0.42	2.30	9	1
1:A:56:LEU:N	1:A:89:ALA:O	0.42	2.53	20	1
1:A:57:ARG:HG3	1:A:88:TYR:CE2	0.42	2.49	8	1
1:A:56:LEU:HA	1:A:60:VAL:O	0.42	2.15	10	1
1:A:68:THR:HG22	1:A:77:VAL:HA	0.42	1.90	10	1
1:A:45:ARG:HD3	1:A:45:ARG:N	0.42	2.29	5	1
1:A:61:GLN:NE2	1:A:63:VAL:HG12	0.42	2.30	14	1
1:A:77:VAL:O	1:A:77:VAL:CG2	0.41	2.67	3	2
1:A:40:LEU:C	1:A:40:LEU:CD1	0.41	2.87	6	1
1:A:57:ARG:C	1:A:57:ARG:HD2	0.41	2.35	6	1
1:A:57:ARG:CB	1:A:62:LEU:HG	0.41	2.44	9	1
1:A:83:ALA:C	1:A:85:SER:H	0.41	2.19	12	1
1:A:90:CYS:HB3	1:A:101:THR:HG23	0.41	1.92	8	1
1:A:57:ARG:HD3	1:A:58:ASP:CB	0.41	2.45	12	1
1:A:45:ARG:NH1	1:A:101:THR:HG23	0.41	2.29	10	1
1:A:45:ARG:O	1:A:45:ARG:HG3	0.41	2.15	13	1
1:A:54:ASN:CB	1:A:61:GLN:OE1	0.41	2.69	6	2
1:A:74:GLU:HG2	1:A:75:VAL:N	0.41	2.30	7	1
1:A:45:ARG:CD	1:A:92:THR:HG21	0.41	2.45	2	1
1:A:33:LEU:HD23	1:A:33:LEU:H	0.41	1.75	14	1
1:A:37:GLY:HA2	1:A:79:ASP:O	0.41	2.15	19	1
1:A:34:VAL:HG11	1:A:80:SER:OG	0.41	2.16	13	1
1:A:87:LEU:HD12	1:A:87:LEU:N	0.41	2.30	14	2
1:A:89:ALA:HA	1:A:102:TYR:HA	0.41	1.92	9	2
1:A:47:ARG:H	1:A:50:VAL:HG13	0.41	1.74	5	1
1:A:88:TYR:CE2	1:A:105:VAL:HG21	0.41	2.51	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:33:LEU:CA	1:A:106:ASN:ND2	0.41	2.84	5	1
1:A:106:ASN:N	1:A:106:ASN:OD1	0.41	2.53	6	1
1:A:61:GLN:NE2	1:A:62:LEU:N	0.41	2.69	11	1
1:A:79:ASP:O	1:A:80:SER:HB3	0.41	2.14	18	1
1:A:89:ALA:CA	1:A:101:THR:O	0.41	2.69	7	1
1:A:47:ARG:NH2	1:A:98:SER:C	0.41	2.74	12	1
1:A:56:LEU:HD13	1:A:91:VAL:HG23	0.41	1.92	14	1
1:A:96:SER:OG	1:A:97:GLY:N	0.41	2.54	14	1
1:A:31:SER:CB	1:A:104:SER:HB2	0.41	2.45	8	1
1:A:43:ARG:NH1	1:A:73:GLU:CD	0.41	2.74	12	1
1:A:57:ARG:HE	1:A:62:LEU:CD1	0.41	2.29	16	1
1:A:58:ASP:O	1:A:87:LEU:HB2	0.41	2.16	16	1
1:A:88:TYR:CD2	1:A:105:VAL:HB	0.41	2.50	19	1
1:A:69:ARG:CB	1:A:69:ARG:CZ	0.41	2.99	1	1
1:A:53:ILE:CD1	1:A:92:THR:HA	0.41	2.46	2	2
1:A:88:TYR:CD1	1:A:105:VAL:HG21	0.41	2.51	5	1
1:A:53:ILE:CG2	1:A:72:GLY:O	0.41	2.69	11	1
1:A:47:ARG:HB3	1:A:94:SER:OG	0.41	2.16	12	1
1:A:49:ASP:C	1:A:94:SER:HB2	0.41	2.35	16	1
1:A:94:SER:HB2	1:A:95:PRO:CD	0.41	2.46	18	1
1:A:41:GLN:CD	1:A:41:GLN:H	0.41	2.17	10	1
1:A:83:ALA:HB1	1:A:88:TYR:OH	0.41	2.16	19	1
1:A:53:ILE:HG12	1:A:72:GLY:O	0.41	2.16	7	1
1:A:50:VAL:HA	1:A:94:SER:OG	0.41	2.16	8	1
1:A:73:GLU:HG3	1:A:74:GLU:N	0.41	2.31	13	1
1:A:42:LEU:N	1:A:42:LEU:HD23	0.40	2.31	17	2
1:A:29:VAL:HG21	1:A:101:THR:CA	0.40	2.45	6	1
1:A:57:ARG:N	1:A:62:LEU:HB2	0.40	2.30	9	1
1:A:42:LEU:HA	1:A:103:PHE:CE2	0.40	2.50	7	1
1:A:30:GLU:O	1:A:103:PHE:CA	0.40	2.70	6	1
1:A:40:LEU:CG	1:A:77:VAL:HB	0.40	2.46	20	1
1:A:35:HIS:HB3	1:A:36:PRO:HD2	0.40	1.94	15	1
1:A:67:ARG:HD2	1:A:67:ARG:N	0.40	2.31	4	1
1:A:47:ARG:HH21	1:A:97:GLY:C	0.40	2.20	12	1
1:A:35:HIS:O	1:A:80:SER:CB	0.40	2.69	19	1
1:A:79:ASP:C	1:A:80:SER:OG	0.40	2.60	1	1
1:A:34:VAL:O	1:A:108:SER:N	0.40	2.54	5	1
1:A:35:HIS:CD2	1:A:36:PRO:HD3	0.40	2.52	8	1
1:A:68:THR:CB	1:A:77:VAL:CG1	0.40	2.99	1	1
1:A:47:ARG:CZ	1:A:99:ASP:HB2	0.40	2.46	12	1
1:A:46:LEU:HD13	1:A:53:ILE:CG1	0.40	2.47	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:54:ASN:HB3	1:A:61:GLN:OE1	0.40	2.16	17	1
1:A:90:CYS:O	1:A:100:THR:HA	0.40	2.17	7	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	77/95 (81%)	57±2 (74±2%)	12±2 (15±3%)	8±2 (11±2%)	<b>1</b> <b>9</b>
All	All	1540/1900 (81%)	1142 (74%)	236 (15%)	162 (11%)	<b>1</b> <b>9</b>

All 19 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	63	VAL	20
1	A	29	VAL	20
1	A	72	GLY	19
1	A	58	ASP	16
1	A	79	ASP	14
1	A	80	SER	13
1	A	82	PRO	13
1	A	48	ASP	10
1	A	95	PRO	8
1	A	28	GLU	6
1	A	67	ARG	5
1	A	36	PRO	4
1	A	50	VAL	3
1	A	59	GLY	3
1	A	44	CYS	3
1	A	84	ASP	2
1	A	73	GLU	1
1	A	81	ILE	1
1	A	47	ARG	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	71/86 (83%)	54±2 (76±2%)	17±2 (24±2%)	<b>3</b> 27
All	All	1420/1720 (83%)	1085 (76%)	335 (24%)	<b>3</b> 27

All 51 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	101	THR	18
1	A	34	VAL	18
1	A	54	ASN	17
1	A	42	LEU	17
1	A	78	ARG	15
1	A	40	LEU	14
1	A	41	GLN	14
1	A	62	LEU	13
1	A	105	VAL	13
1	A	45	ARG	12
1	A	33	LEU	12
1	A	46	LEU	11
1	A	61	GLN	10
1	A	44	CYS	10
1	A	35	HIS	10
1	A	70	ILE	10
1	A	104	SER	10
1	A	106	ASN	10
1	A	57	ARG	9
1	A	47	ARG	9
1	A	77	VAL	8
1	A	81	ILE	7
1	A	68	THR	6
1	A	39	LEU	6
1	A	93	SER	5
1	A	43	ARG	5
1	A	71	THR	4
1	A	79	ASP	3
1	A	56	LEU	3

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Mol	Chain	Res	Type	Models (Total)
1	A	99	ASP	3
1	A	67	ARG	3
1	A	69	ARG	3
1	A	87	LEU	2
1	A	75	VAL	2
1	A	90	CYS	2
1	A	92	THR	2
1	A	94	SER	2
1	A	51	GLN	2
1	A	102	TYR	2
1	A	29	VAL	2
1	A	49	ASP	1
1	A	28	GLU	1
1	A	76	GLU	1
1	A	98	SER	1
1	A	74	GLU	1
1	A	107	VAL	1
1	A	48	ASP	1
1	A	80	SER	1
1	A	96	SER	1
1	A	63	VAL	1
1	A	108	SER	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 i

The completeness of assignment taking into account all chemical shift lists is 51% for the well-defined parts and 50% 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 i

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	702
Number of shifts mapped to atoms	634
Number of unparsed shifts	0
Number of shifts with mapping errors	68
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- Residue not found in structure. All 68 occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	105	SER	HB3	3.8	0.005	2
A	107	GLU	HA	4.14	0.005	1
A	107	GLU	HG2	2.2	0.005	2
A	103	LEU	N	123.11	0.02	1
A	105	SER	HB2	3.94	0.005	2
A	107	GLU	HB2	2.04	0.005	2
A	103	LEU	HD13	0.88	0.005	2
A	103	LEU	HA	4.54	0.005	1
A	105	SER	H	8.54	0.005	1
A	5	ALA	HB1	1.34	0.005	1
A	107	GLU	N	127.79	0.02	1
A	2	ALA	HA	4.28	0.005	1
A	2	ALA	HB1	1.34	0.005	1
A	101	ASP	HA	4.56	0.005	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	102	ALA	HB2	1.26	0.005	1
A	2	ALA	H	8.33	0.005	1
A	1	GLU	HA	4.22	0.005	1
A	102	ALA	N	123.38	0.02	1
A	103	LEU	HG	1.66	0.005	1
A	3	ARG	HD2	3.16	0.005	2
A	1	GLU	N	122.54	0.02	1
A	3	ARG	N	121.63	0.02	1
A	1	GLU	HB2	1.99	0.005	2
A	4	PRO	HG2	1.99	0.005	2
A	5	ALA	N	125.84	0.02	1
A	103	LEU	HD12	0.88	0.005	2
A	101	ASP	HB3	2.54	0.005	2
A	102	ALA	HA	4.26	0.005	1
A	1	GLU	HG2	2.18	0.005	2
A	103	LEU	HB3	1.52	0.005	2
A	3	ARG	H	8.26	0.005	1
A	3	ARG	HG2	1.63	0.005	2
A	5	ALA	HA	4.52	0.005	1
A	106	SER	N	118.35	0.02	1
A	2	ALA	HB3	1.34	0.005	1
A	3	ARG	HA	4.59	0.005	1
A	103	LEU	H	8.22	0.005	1
A	5	ALA	H	8.38	0.005	1
A	1	GLU	HB3	1.86	0.005	2
A	101	ASP	H	8.54	0.005	1
A	103	LEU	HD11	0.88	0.005	2
A	5	ALA	HB2	1.34	0.005	1
A	103	LEU	HB2	1.57	0.005	2
A	106	SER	HB2	3.83	0.005	2
A	106	SER	HA	4.48	0.005	1
A	3	ARG	HB2	1.68	0.005	2
A	2	ALA	HB2	1.34	0.005	1
A	106	SER	H	8.31	0.005	1
A	104	PRO	HA	4.43	0.005	1
A	102	ALA	HB1	1.26	0.005	1
A	105	SER	HA	4.61	0.005	1
A	101	ASP	N	123.69	0.02	1
A	5	ALA	HB3	1.34	0.005	1
A	105	SER	N	116.39	0.02	1
A	101	ASP	HB2	2.64	0.005	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	104	PRO	HB3	2.28	0.005	2
A	4	PRO	HD2	3.75	0.005	2
A	102	ALA	HB3	1.26	0.005	1
A	102	ALA	H	8.23	0.005	1
A	106	SER	HB3	3.86	0.005	2
A	3	ARG	HB3	1.81	0.005	2
A	4	PRO	HA	4.38	0.005	1
A	107	GLU	HB3	1.88	0.005	2
A	1	GLU	H	8.32	0.005	1
A	104	PRO	HB2	1.9	0.005	2
A	4	PRO	HB2	1.86	0.005	2
A	107	GLU	H	8.1	0.005	1
A	2	ALA	N	125.6	0.02	1

### 6.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	0	—	None (insufficient data)
$^{13}\text{C}_\beta$	0	—	None (insufficient data)
$^{13}\text{C}'$	0	—	None (insufficient data)
$^{15}\text{N}$	96	$-1.21 \pm 0.44$	Should be applied

### 6.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 51%, i.e. 472 atoms were assigned a chemical shift out of a possible 931. 0 out of 19 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	223/384 (58%)	149/153 (97%)	0/156 (0%)	74/75 (99%)
Sidechain	228/503 (45%)	223/291 (77%)	0/186 (0%)	5/26 (19%)
Aromatic	21/44 (48%)	20/23 (87%)	0/19 (0%)	1/2 (50%)
Overall	472/931 (51%)	392/467 (84%)	0/361 (0%)	80/103 (78%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 50%, i.e. 569 atoms were assigned a chemical shift out of a possible 1130. 0 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	263/461 (57%)	177/183 (97%)	0/190 (0%)	86/88 (98%)
Sidechain	278/613 (45%)	271/357 (76%)	0/227 (0%)	7/29 (24%)
Aromatic	28/56 (50%)	26/29 (90%)	0/24 (0%)	2/3 (67%)
Overall	569/1130 (50%)	474/569 (83%)	0/441 (0%)	95/120 (79%)

### 6.1.4 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	75	VAL	HG22	-0.70	2.20 – -0.60	-5.4
1	A	75	VAL	HG23	-0.70	2.20 – -0.60	-5.4
1	A	75	VAL	HG21	-0.70	2.20 – -0.60	-5.4

### 6.1.5 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:

