Full wwPDB NMR Structure Validation Report (i)

Jun 15, 2024 – 05:50 PM EDT

PDB ID	:	2MRK
BMRB ID	:	25082
Title	:	Fyn SH2 domain in complex with the natural inhibitory phosphotyrosine peptide
Authors	:	Huculeci, R.; Buts, L.; Lenaerts, A.J.; van Nuland, N.
Deposited on	:	2014-07-09

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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

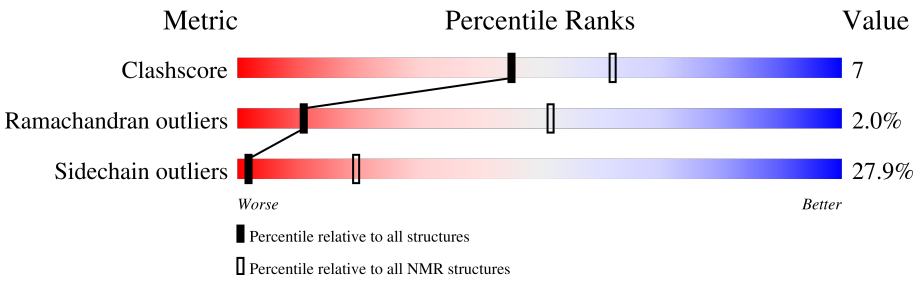
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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	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 <=5%

Mol	Chain	Length	Quality of chain
1	A	100	63% 32%
2	B	10	100%

2 Ensemble composition and analysis (i)

This entry contains 27 models. Model 1 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:149-A:244 (96)	0.53	1

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 4 clusters and 4 single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 5, 6, 7, 10, 11, 14, 15, 17
2	8, 9, 12, 13, 18
3	19, 20, 21, 25
4	23, 24
Single-model clusters	16; 22; 26; 27

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1800 atoms, of which 890 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Tyrosine-protein kinase Fyn.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	100	1641	520	818	152	147	4	0

- Molecule 2 is a protein called C-terminal Tyrosine-protein kinase Fyn.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	P	
2	B	10	159	51	72	13	22	1	0

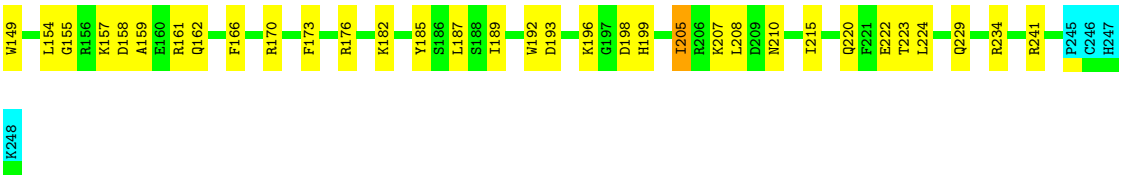
4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide 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.

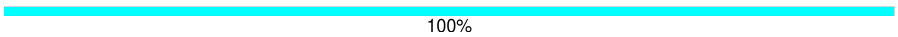
• Molecule 1: Tyrosine-protein kinase Fyn

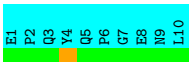
Chain A:



• Molecule 2: C-terminal Tyrosine-protein kinase Fyn

Chain B:





4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

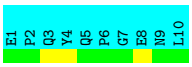
4.2.1 Score per residue for model 1 (medoid)

• Molecule 1: Tyrosine-protein kinase Fyn

Chain A:

• Molecule 2: C-terminal Tyrosine-protein kinase Fyn

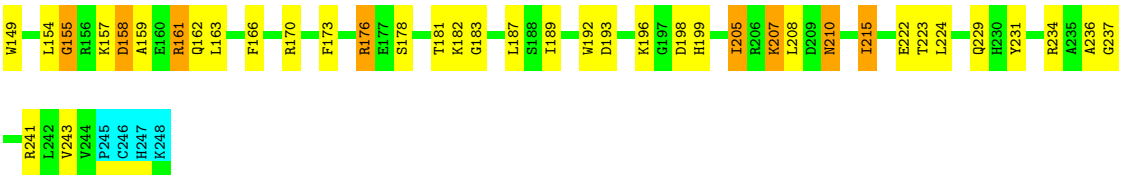
Chain B: 100%



4.2.2 Score per residue for model 2

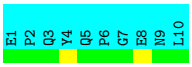
- Molecule 1: Tyrosine-protein kinase Fyn

Chain A: 57% 31% 8%



- Molecule 2: C-terminal Tyrosine-protein kinase Fyn

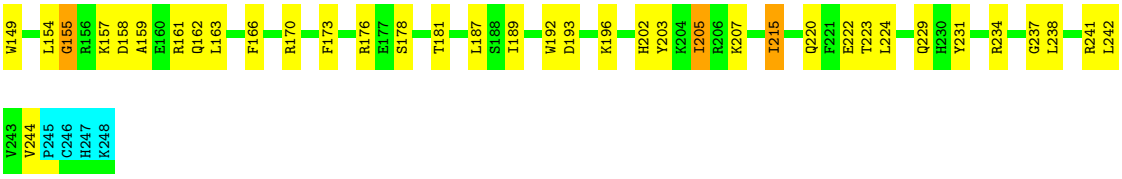
Chain B: 100%



4.2.3 Score per residue for model 3

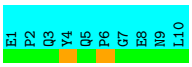
- Molecule 1: Tyrosine-protein kinase Fyn

Chain A: 59% 34%



- Molecule 2: C-terminal Tyrosine-protein kinase Fyn

Chain B: 100%



4.2.4 Score per residue for model 4

- Molecule 1: Tyrosine-protein kinase Fyn

Chain A: 61% 30% 5% •

W149 L154 G155 R156 K157 D158 A159 Q162 L163 L164 S165 F166 R170 F173 R176 E177 S178 T181 K182 L187 S188 I189 W192 D193 K196 G197 D198 I205 R206 K207 L208 D209 N210 I215 Q220 F221 E222 T223 L224 Q229 R234 G237 R241

P245 C246 H247 K248

• Molecule 2: C-terminal Tyrosine-protein kinase Fyn

Chain B: 100%

E1 P2 Q3 Y4 Q5 P6 G7 E8 N9 L10

4.2.5 Score per residue for model 5

• Molecule 1: Tyrosine-protein kinase Fyn

Chain A: 57% 35% • •

W149 L154 G155 R156 K157 D158 A159 Q162 L163 F166 R170 F173 R176 E177 S178 T181 K182 L187 S188 I189 W192 D193 K196 G197 D198 H199 I205 R206 K207 L208 D209 N210 I215 R218 A219 Q220 F221 E222 T223 L224 Q229 R234 G237 L238

C239 C240 R241 L242 V243 V244 P245 C246 H247 K248

• Molecule 2: C-terminal Tyrosine-protein kinase Fyn

Chain B: 100%

E1 P2 Q3 Y4 Q5 P6 G7 E8 N9 L10

4.2.6 Score per residue for model 6

• Molecule 1: Tyrosine-protein kinase Fyn

Chain A: 52% 37% 7% •

W149 K153 L154 G155 R156 K157 D158 A159 E160 R161 Q162 L163 F166 R170 F173 R176 E179 K182 G183 A184 Y185 S186 L187 S188 I189 W192 D193 K196 G197 D198 H199 K204 I205 R206 K207 L208 D209 N210 I215 Q220 F221 E222 T223 L224 Q225 Q226 L227

Y231 R234 G237 C240 R241 L242 V243 V244 P245 C246 H247 K248

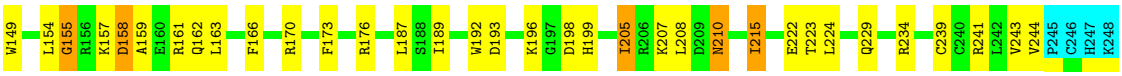
• Molecule 2: C-terminal Tyrosine-protein kinase Fyn

Chain B: 100%

4.2.7 Score per residue for model 7

- Molecule 1: Tyrosine-protein kinase Fyn

Chain A: 62% 29% 5% •



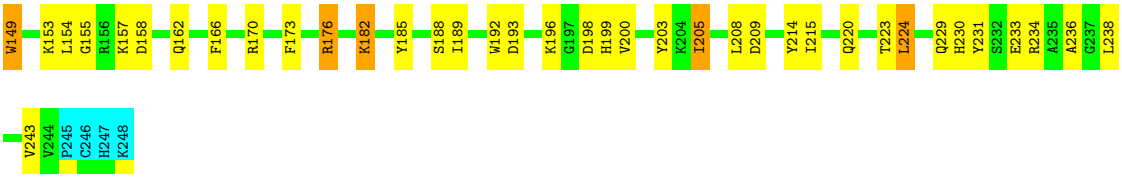
- Molecule 2: C-terminal Tyrosine-protein kinase Fyn

Chain B: 100%

4.2.8 Score per residue for model 8

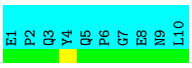
- Molecule 1: Tyrosine-protein kinase Fyn

Chain A: 58% 33% 5% •



- Molecule 2: C-terminal Tyrosine-protein kinase Fyn

Chain B: 100%



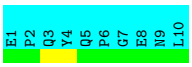
4.2.9 Score per residue for model 9

- Molecule 1: Tyrosine-protein kinase Fyn

Chain A: 64% 27% 5% •

• Molecule 2: C-terminal Tyrosine-protein kinase Fyn

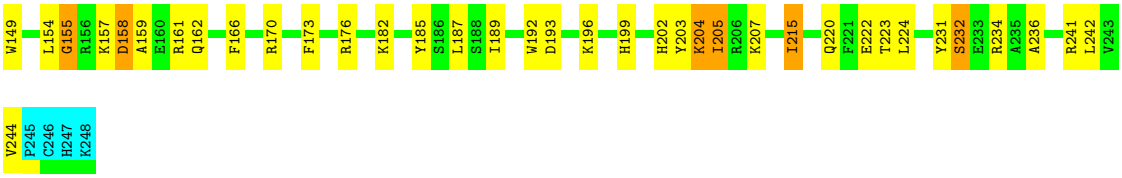
Chain B: 100%



4.2.10 Score per residue for model 10

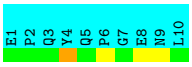
• Molecule 1: Tyrosine-protein kinase Fyn

Chain A: 59% 31% 6% •



• Molecule 2: C-terminal Tyrosine-protein kinase Fyn

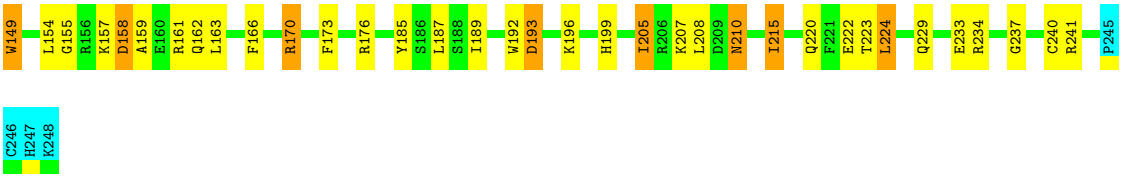
Chain B: 100%



4.2.11 Score per residue for model 11

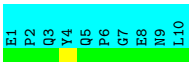
• Molecule 1: Tyrosine-protein kinase Fyn

Chain A: 61% 27% 8% •



• Molecule 2: C-terminal Tyrosine-protein kinase Fyn

Chain B: 100%



4.2.12 Score per residue for model 12

- Molecule 1: Tyrosine-protein kinase Fyn

Chain A: 61% 29% 6% •

W149 K153 L154 G155 R156 K157 D158 L163 F166 R170 F173 R176 K182 Y185 I189 W192 D193 K196 G197 D198 H199 V200 Y203 K204 I205 L208 Y214 I215 Q220 F221 E222 T223 L224 Y231 R234 A235 A236 G237 L238 V243 V244 P245

C246 H247 K248

- Molecule 2: C-terminal Tyrosine-protein kinase Fyn

Chain B: 100%

E1 P2 Q3 Y4 Q5 P6 G7 E8 N9 L10

4.2.13 Score per residue for model 13

- Molecule 1: Tyrosine-protein kinase Fyn

Chain A: 69% 23% • •

W149 K153 L154 G155 R156 K157 D158 A159 E160 R161 Q162 L163 F166 R170 R176 K182 Y185 W192 D193 K196 H199 V200 I205 I215 Q220 F221 E222 T223 L224 Q229 R234 P245 C246 H247 K248

- Molecule 2: C-terminal Tyrosine-protein kinase Fyn

Chain B: 100%

E1 P2 Q3 Y4 Q5 P6 G7 E8 N9 L10

4.2.14 Score per residue for model 14

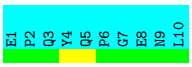
- Molecule 1: Tyrosine-protein kinase Fyn

Chain A: 65% 27% • •

W149 L154 G155 R156 K157 D158 Q162 F166 R170 F173 R176 S186 L187 S188 I189 W192 D193 K196 H199 I205 R206 K207 L208 D209 N210 I215 Q220 F221 E222 T223 L224 Q229 E233 R234 R241 V244 P245 C246 H247 K248

- Molecule 2: C-terminal Tyrosine-protein kinase Fyn

Chain B: 100%



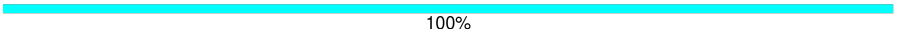
4.2.15 Score per residue for model 15

• Molecule 1: Tyrosine-protein kinase Fyn

Chain A:

• Molecule 2: C-terminal Tyrosine-protein kinase Fyn

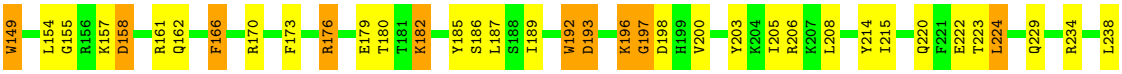
Chain B:

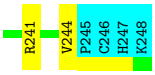


4.2.16 Score per residue for model 16

• Molecule 1: Tyrosine-protein kinase Fyn

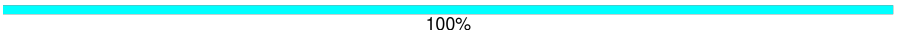
Chain A:

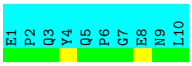




• Molecule 2: C-terminal Tyrosine-protein kinase Fyn

Chain B:

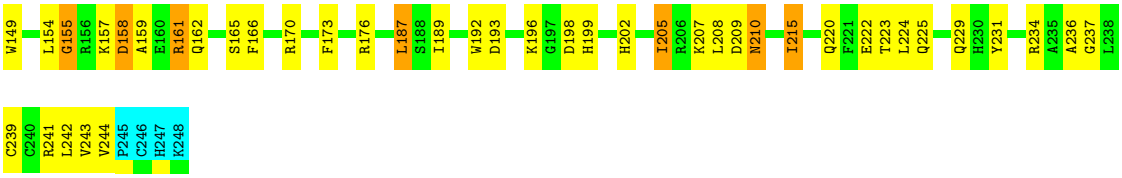




4.2.17 Score per residue for model 17

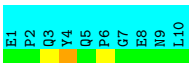
• Molecule 1: Tyrosine-protein kinase Fyn

Chain A:



• Molecule 2: C-terminal Tyrosine-protein kinase Fyn

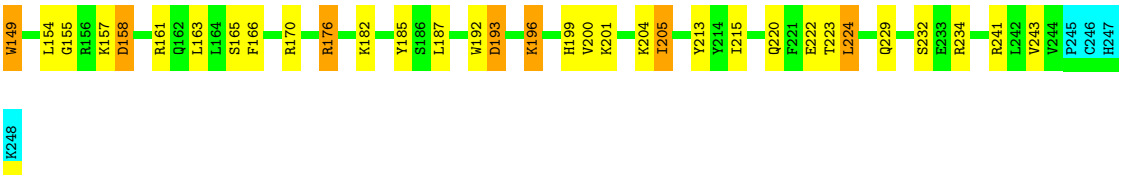
Chain B: 100%



4.2.18 Score per residue for model 18

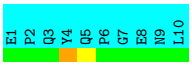
• Molecule 1: Tyrosine-protein kinase Fyn

Chain A: 63% 26% 7% •



• Molecule 2: C-terminal Tyrosine-protein kinase Fyn

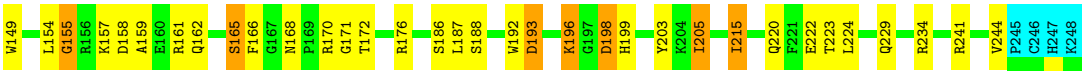
Chain B: 100%



4.2.19 Score per residue for model 19

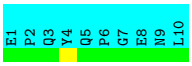
• Molecule 1: Tyrosine-protein kinase Fyn

Chain A: 62% 27% 7% •



• Molecule 2: C-terminal Tyrosine-protein kinase Fyn

Chain B: 100%



4.2.20 Score per residue for model 20

- Molecule 1: Tyrosine-protein kinase Fyn

Chain A: 68% 22% 6% •

W149 G155 R156 K157 D158 A159 Q162 F166 R170 F173 R176 Y185 S186 L187 S188 I189 W192 D193 K196 H202 Y203 K204 I205 L208 D209 N210 I215 Q220 T223 L224 Q229 R234 L242 P245 C246 H247 K248

- Molecule 2: C-terminal Tyrosine-protein kinase Fyn

Chain B: 100%

E1 P2 Q3 Y4 Q5 P6 G7 E8 N9 L10

4.2.21 Score per residue for model 21

- Molecule 1: Tyrosine-protein kinase Fyn

Chain A: 66% 25% 5% •

W149 L154 G155 R156 K157 D158 R161 Q162 S165 F166 R170 R176 E177 Y185 S186 L187 W192 D193 K196 Y203 K204 I205 L208 D209 N210 I215 Q220 F221 E222 T223 L224 Q229 R234 G237 P245 C246 H247 K248

- Molecule 2: C-terminal Tyrosine-protein kinase Fyn

Chain B: 100%

E1 P2 Q3 Y4 Q5 P6 G7 E8 N9 L10

4.2.22 Score per residue for model 22

- Molecule 1: Tyrosine-protein kinase Fyn

Chain A: 59% 37% •

W149 Y150 F151 G152 K153 L154 G155 R156 K157 D158 R161 Q162 S165 F166 R170 R176 E177 S178 E179 T180 Y185 S186 L187 W192 K196 H199 V200 I205 R206 K207 L208 D209 N210 Y214 Q220 T223 L224 Q229 S232 E233 R234 R241 L242 V243 V244

P245 C246 H247 K248

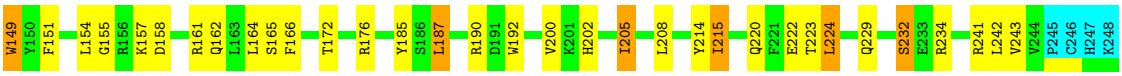
- Molecule 2: C-terminal Tyrosine-protein kinase Fyn

Chain B: 100%

4.2.23 Score per residue for model 23

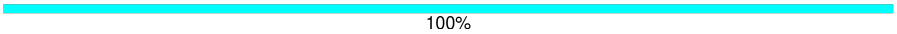
• Molecule 1: Tyrosine-protein kinase Fyn

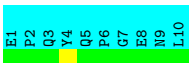
Chain A:



• Molecule 2: C-terminal Tyrosine-protein kinase Fyn

Chain B:

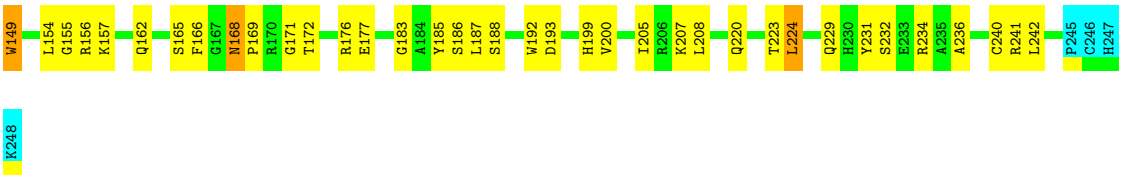




4.2.24 Score per residue for model 24

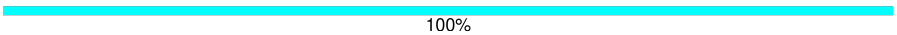
• Molecule 1: Tyrosine-protein kinase Fyn

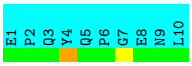
Chain A:



• Molecule 2: C-terminal Tyrosine-protein kinase Fyn

Chain B:

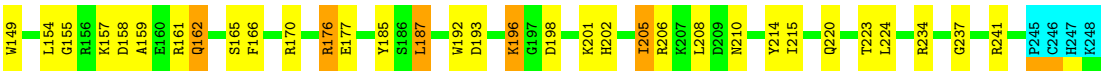




4.2.25 Score per residue for model 25

• Molecule 1: Tyrosine-protein kinase Fyn

Chain A:



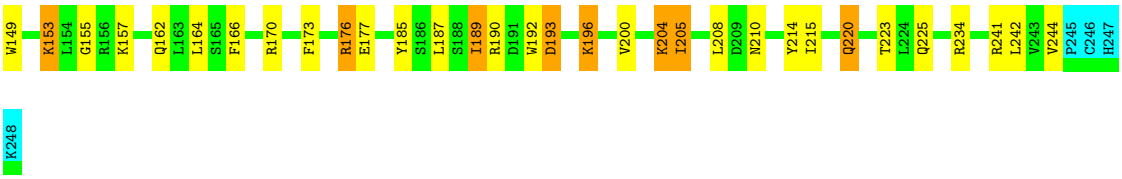
• Molecule 2: C-terminal Tyrosine-protein kinase Fyn

Chain B: 100%

4.2.26 Score per residue for model 26

- Molecule 1: Tyrosine-protein kinase Fyn

Chain A: 64% 24% 8% •



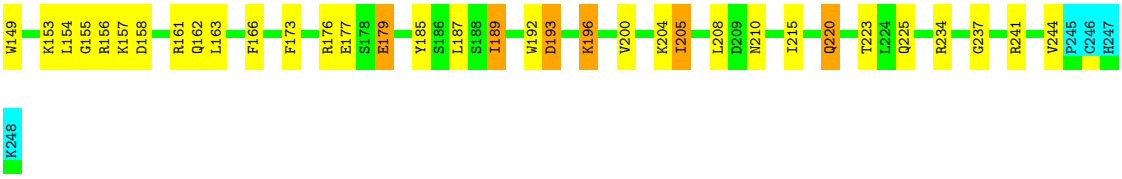
- Molecule 2: C-terminal Tyrosine-protein kinase Fyn

Chain B: 100%

4.2.27 Score per residue for model 27

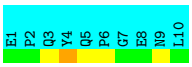
- Molecule 1: Tyrosine-protein kinase Fyn

Chain A: 62% 28% 6% •



- Molecule 2: C-terminal Tyrosine-protein kinase Fyn

Chain B: 100%



5 Refinement protocol and experimental data overview (i)

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

Of the 200 calculated structures, 27 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
HADDOCK	structure solution	
HADDOCK	refinement	
CNS	structure solution	
CNS	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	57
Number of shifts mapped to atoms	57
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	0%

6 Model quality (i)

6.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PTR

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	790	785	779	11±2
2	B	0	0	0	0±0
All	All	21330	21195	21033	284

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:173:PHE:CG	1:A:189:ILE:HG22	0.77	2.15	15	12
1:A:208:LEU:HD11	1:A:220:GLN:HB2	0.69	1.66	27	5
1:A:176:ARG:O	1:A:185:TYR:HB2	0.68	1.89	10	12
1:A:193:ASP:OD1	1:A:196:LYS:HD3	0.64	1.92	27	10
1:A:205:ILE:HD11	1:A:215:ILE:HG12	0.63	1.70	17	14
1:A:154:LEU:O	1:A:176:ARG:HB3	0.62	1.95	9	24
1:A:203:TYR:CE2	1:A:238:LEU:HD22	0.60	2.31	3	1
1:A:208:LEU:HB3	1:A:210:ASN:ND2	0.56	2.14	4	10
1:A:185:TYR:CE2	1:A:205:ILE:HD13	0.56	2.35	20	9
1:A:161:ARG:O	1:A:165:SER:HB2	0.56	2.01	25	4
1:A:168:ASN:HD22	1:A:172:THR:HG21	0.56	1.61	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:149:TRP:CH2	1:A:224:LEU:HB3	0.55	2.37	24	8
1:A:173:PHE:CD1	1:A:189:ILE:HG22	0.54	2.38	5	10
1:A:208:LEU:HD13	1:A:210:ASN:HD21	0.53	1.63	11	13
1:A:158:ASP:O	1:A:161:ARG:HG2	0.53	2.03	6	12
1:A:230:HIS:HA	1:A:233:GLU:OE2	0.53	2.03	8	2
1:A:178:SER:HB3	1:A:181:THR:O	0.53	2.04	4	6
1:A:192:TRP:CG	1:A:197:GLY:HA2	0.52	2.40	16	1
1:A:187:LEU:O	1:A:202:HIS:HA	0.52	2.04	20	4
1:A:173:PHE:HB3	1:A:189:ILE:HG23	0.52	1.81	27	2
1:A:185:TYR:CZ	1:A:205:ILE:HG21	0.52	2.39	10	3
1:A:155:GLY:HA3	1:A:176:ARG:CG	0.51	2.36	10	1
1:A:170:ARG:HD3	1:A:240:CYS:SG	0.50	2.47	11	2
1:A:192:TRP:CD1	1:A:197:GLY:HA2	0.50	2.42	16	1
1:A:208:LEU:HG	1:A:214:TYR:CD1	0.50	2.42	8	7
1:A:159:ALA:O	1:A:162:GLN:HG3	0.49	2.07	25	1
1:A:186:SER:HA	1:A:203:TYR:O	0.49	2.07	21	3
1:A:176:ARG:NH1	1:A:178:SER:HA	0.49	2.22	22	1
1:A:159:ALA:O	1:A:163:LEU:HB2	0.49	2.08	7	6
1:A:231:TYR:CE2	1:A:236:ALA:HB3	0.48	2.43	17	4
1:A:185:TYR:H	1:A:205:ILE:HG22	0.48	1.69	9	2
1:A:203:TYR:CD2	1:A:238:LEU:HD22	0.48	2.44	8	3
1:A:231:TYR:CE1	1:A:236:ALA:HB3	0.48	2.44	15	4
1:A:155:GLY:HA3	1:A:176:ARG:CB	0.47	2.39	20	1
1:A:154:LEU:HB2	1:A:158:ASP:CG	0.47	2.29	4	10
1:A:155:GLY:HA2	1:A:159:ALA:HB2	0.47	1.86	10	10
1:A:171:GLY:HA2	1:A:241:ARG:O	0.47	2.10	19	2
1:A:156:ARG:NH1	1:A:179:GLU:HB2	0.47	2.24	27	1
1:A:185:TYR:CE1	1:A:224:LEU:HD21	0.46	2.45	24	3
1:A:155:GLY:HA3	1:A:176:ARG:CD	0.46	2.39	10	1
1:A:171:GLY:C	1:A:244:VAL:HB	0.46	2.31	19	1
1:A:164:LEU:HD23	1:A:190:ARG:NH1	0.46	2.25	26	2
1:A:154:LEU:HB2	1:A:158:ASP:HB2	0.46	1.88	5	1
1:A:193:ASP:CG	1:A:196:LYS:HD3	0.45	2.32	27	2
1:A:232:SER:HA	1:A:242:LEU:O	0.45	2.12	22	5
1:A:168:ASN:ND2	1:A:172:THR:HG21	0.45	2.26	19	1
1:A:155:GLY:HA2	1:A:159:ALA:CB	0.45	2.42	10	4
1:A:185:TYR:CE1	1:A:205:ILE:HG21	0.45	2.47	20	3
1:A:176:ARG:NH1	1:A:179:GLU:HG3	0.45	2.27	6	1
1:A:149:TRP:CD1	1:A:149:TRP:N	0.44	2.86	24	2
1:A:182:LYS:HD2	1:A:182:LYS:O	0.44	2.13	12	3
1:A:154:LEU:HB2	1:A:158:ASP:HB3	0.44	1.89	23	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:176:ARG:HD2	1:A:177:GLU:O	0.44	2.13	4	2
1:A:173:PHE:CG	1:A:242:LEU:HG	0.43	2.48	20	2
1:A:198:ASP:O	1:A:199:HIS:HB2	0.43	2.14	19	1
1:A:172:THR:HA	1:A:244:VAL:HG11	0.43	1.91	1	1
1:A:153:LYS:HB3	1:A:177:GLU:OE2	0.43	2.14	26	1
1:A:241:ARG:HG3	1:A:243:VAL:HG22	0.43	1.90	18	1
1:A:231:TYR:HB3	1:A:242:LEU:HD13	0.42	1.92	3	2
1:A:164:LEU:HD22	1:A:198:ASP:OD1	0.42	2.13	4	1
1:A:183:GLY:O	1:A:207:LYS:HG3	0.42	2.14	2	2
1:A:227:LEU:O	1:A:231:TYR:HD1	0.42	1.98	6	1
1:A:166:PHE:CD1	1:A:166:PHE:N	0.42	2.87	9	3
1:A:155:GLY:HA3	1:A:176:ARG:HG2	0.41	1.92	6	1
1:A:173:PHE:HB3	1:A:189:ILE:HG22	0.41	1.91	16	3
1:A:185:TYR:CE1	1:A:205:ILE:HD13	0.41	2.51	26	1
1:A:170:ARG:HD2	1:A:170:ARG:O	0.41	2.15	20	1
1:A:183:GLY:O	1:A:207:LYS:HD3	0.41	2.16	24	1
1:A:168:ASN:OD1	1:A:168:ASN:N	0.41	2.50	1	1
1:A:189:ILE:HD11	1:A:203:TYR:CE1	0.41	2.50	20	1
1:A:182:LYS:O	1:A:182:LYS:HD2	0.40	2.16	8	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	95/100 (95%)	85±2 (89±2%)	8±2 (9±2%)	2±1 (2±1%)	11 52
2	B	0	-	-	-	-
All	All	2565/2970 (86%)	2287 (89%)	227 (9%)	51 (2%)	11 52

All 7 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	155	GLY	27
1	A	237	GLY	10

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Mol	Chain	Res	Type	Models (Total)
1	A	198	ASP	10
1	A	197	GLY	1
1	A	165	SER	1
1	A	243	VAL	1
1	A	169	PRO	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	82/86 (95%)	59±3 (72±4%)	23±3 (28±4%)	2 19
2	B	0	-	-	-
All	All	2214/2538 (87%)	1597 (72%)	617 (28%)	2 19

All 53 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	149	TRP	27
1	A	157	LYS	27
1	A	166	PHE	27
1	A	192	TRP	27
1	A	223	THR	27
1	A	234	ARG	27
1	A	205	ILE	25
1	A	220	GLN	25
1	A	170	ARG	24
1	A	215	ILE	24
1	A	224	LEU	24
1	A	162	GLN	23
1	A	196	LYS	23
1	A	187	LEU	22
1	A	193	ASP	21
1	A	229	GLN	20
1	A	222	GLU	18
1	A	241	ARG	18
1	A	158	ASP	17

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Mol	Chain	Res	Type	Models (Total)
1	A	199	HIS	16
1	A	176	ARG	13
1	A	182	LYS	12
1	A	207	LYS	12
1	A	200	VAL	11
1	A	210	ASN	10
1	A	243	VAL	10
1	A	244	VAL	9
1	A	153	LYS	8
1	A	177	GLU	6
1	A	161	ARG	5
1	A	186	SER	5
1	A	163	LEU	5
1	A	165	SER	5
1	A	232	SER	4
1	A	225	GLN	4
1	A	239	CYS	3
1	A	188	SER	3
1	A	201	LYS	3
1	A	233	GLU	3
1	A	206	ARG	3
1	A	168	ASN	2
1	A	240	CYS	2
1	A	209	ASP	2
1	A	204	LYS	2
1	A	198	ASP	2
1	A	179	GLU	2
1	A	180	THR	2
1	A	189	ILE	2
1	A	218	ARG	1
1	A	214	TYR	1
1	A	213	TYR	1
1	A	172	THR	1
1	A	208	LEU	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	PTR	B	4	2	15,16,17	0.79±0.02	0±0 (0±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	PTR	B	4	2	17,22,24	0.98±0.03	1±0 (5±0%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PTR	B	4	2	-	0±0,10,11,13	0±0,1,1,1

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	4	PTR	O2P-P-OH	3.15	114.63	105.32	7	27

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

The completeness of assignment taking into account all chemical shift lists is 0% for the well-defined parts and 3% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 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	57
Number of shifts mapped to atoms	57
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing (i)

No chemical shift referencing corrections were calculated (not enough data).

7.1.3 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 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 1368. 0 out of 14 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	**^{1}H**	**^{13}C**	**^{15}N**
Backbone	0/487 (0%)	0/200 (0%)	0/192 (0%)	0/95 (0%)
Sidechain	0/739 (0%)	0/475 (0%)	0/223 (0%)	0/41 (0%)
Aromatic	0/142 (0%)	0/68 (0%)	0/66 (0%)	0/8 (0%)
Overall	0/1368 (0%)	0/743 (0%)	0/481 (0%)	0/144 (0%)

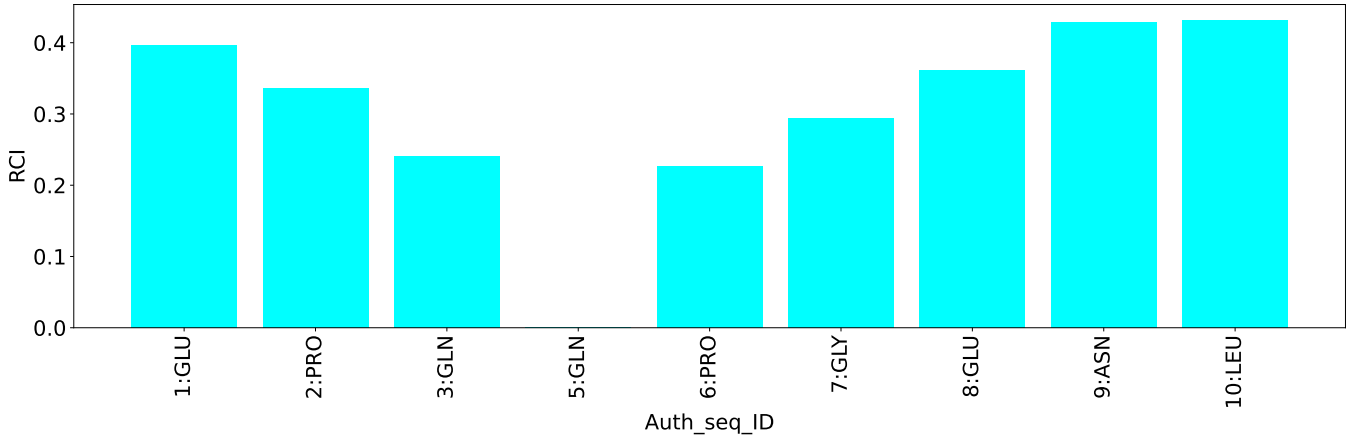
The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 3%, i.e. 53 atoms were assigned a chemical shift out of a possible 1536. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	14/547 (3%)	14/224 (6%)	0/218 (0%)	0/105 (0%)
Sidechain	39/839 (5%)	39/538 (7%)	0/256 (0%)	0/45 (0%)
Aromatic	0/150 (0%)	0/72 (0%)	0/68 (0%)	0/10 (0%)
Overall	53/1536 (3%)	53/834 (6%)	0/542 (0%)	0/160 (0%)

7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots (i)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain B: