WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB NMR Structure Validation Report ⓘ

Oct 31, 2021 – 04:04 PM EDT

PDB ID	:	2RMK
Title	:	Rac1/PRK1 Complex
Authors	:	Modha, R.; Campbell, L.J.; Nietlispach, D.; Buhecha, H.R.; Owen, D.; Mott, H.R.
Deposited on	:	2007-10-25

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:

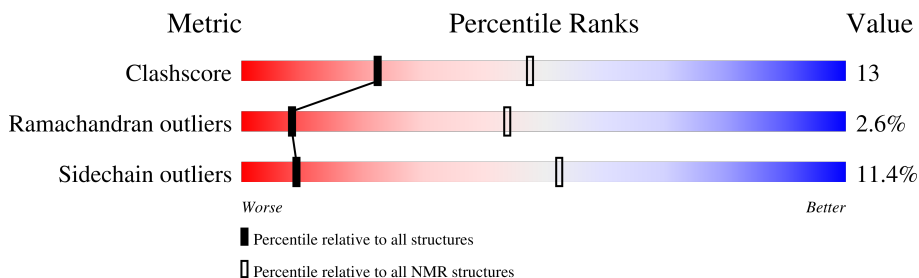|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.23.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1   Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

Metric	Percentile Ranks	Value
Clashscore		13
Ramachandran outliers		2.6%
Sidechain outliers		11.4%

Worse   *Better*

▉ Percentile relative to all structures

▯ Percentile relative to all NMR structures

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	192	59% 28% 5% 8%
2	B	81	54% 17% 28%

2 Ensemble composition and analysis ⓘ

This entry contains 25 models. Model 14 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:1-A:29, A:35-A:36, A:40-A:184, B:127-B:153, B:159-B:189 (234)	0.51	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 1 single-model cluster was found.

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

3 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 4417 atoms, of which 2248 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Ras-related C3 botulinum toxin substrate 1.

Mol	Chain	Residues	Atoms						Trace
1	A	192	Total	C	H	N	O	S	0
			3066	970	1561	252	273	10	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	61	LEU	GLN	engineered mutation	UNP P63000

- Molecule 2 is a protein called Serine/threonine-protein kinase N1.

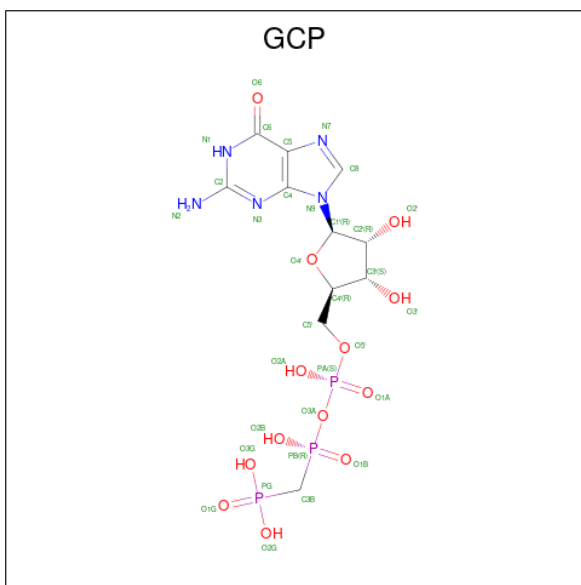| Mol	Chain	Residues	Atoms						Trace
2	B	81	Total	C	H	N	O	S	0
			1298	387	669	117	122	3	

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	119	GLY	-	expression tag	UNP Q16512
B	120	ILE	-	expression tag	UNP Q16512
B	121	PRO	-	expression tag	UNP Q16512

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	
3	A	1	Total	Mg
			1	1

- Molecule 4 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$).

GCP

Mol	Chain	Residues	Atoms					
			Total	C	H	N	O	P
4	A	1	46	11	14	5	13	3

• Molecule 5 is water.

| Mol	Chain	Residues	Atoms		
			Total	H	O
5	A	2	6	4	2

4 Residue-property plots ⓘ

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: Ras-related C3 botulinum toxin substrate 1
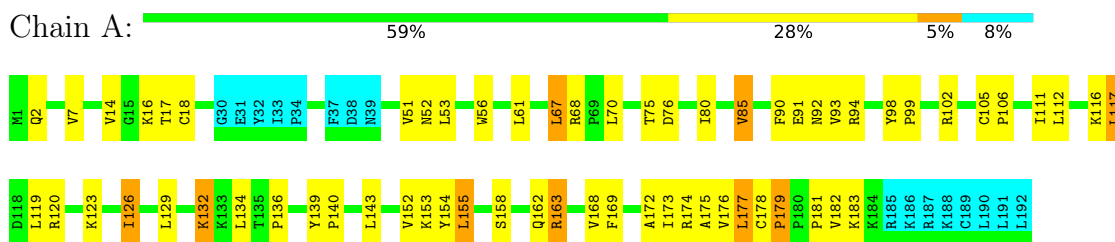
- Molecule 2: Serine/threonine-protein kinase N1
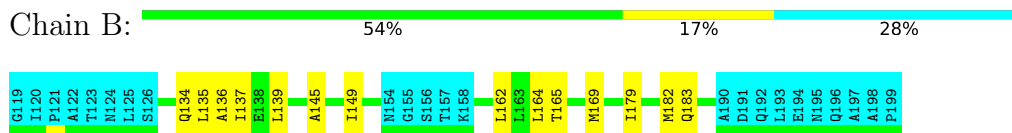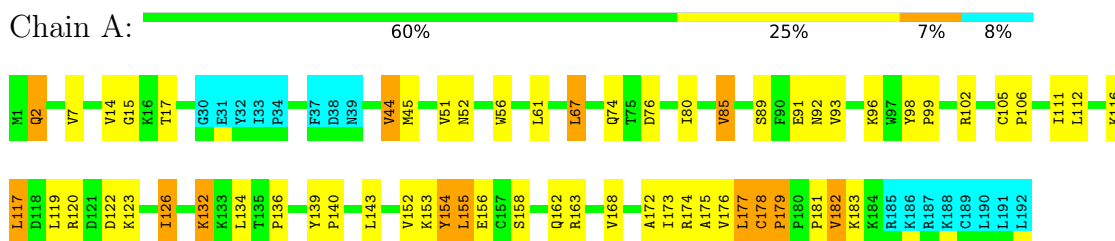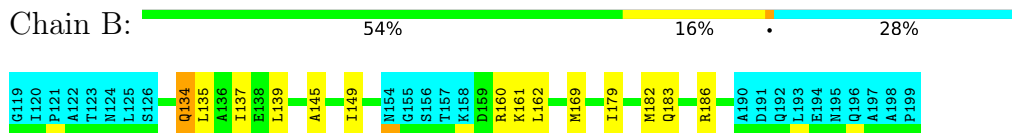

4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

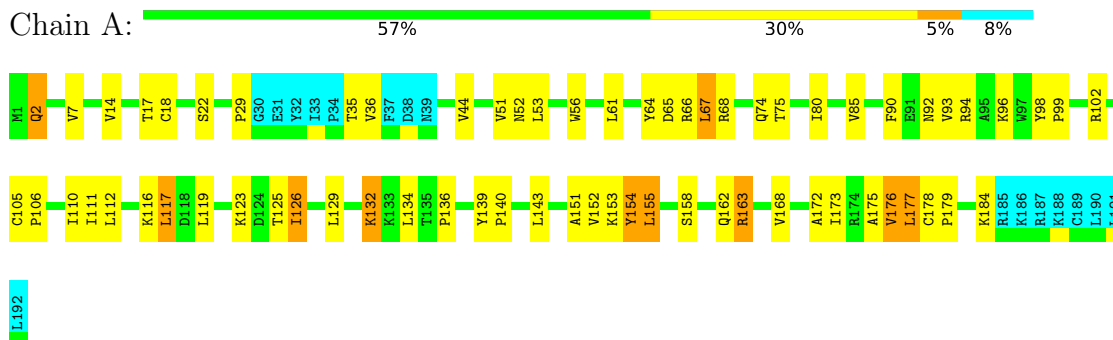- Molecule 1: Ras-related C3 botulinum toxin substrate 1

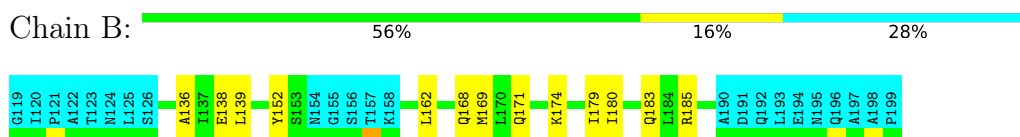- Molecule 2: Serine/threonine-protein kinase N1

Chain B: 54%   16% · 28%

G119 I120 P121 A122 T123 N124 L125 S126 Q134 L135 A136 I137 E138 L139 A145 I149 N154 G155 S156 T157 K158 D159 R160 K161 L162 M169 I179 M182 Q183 R186 A190 D191 Q192 L193 E194 N195 Q196 A197 A198 P199

4.2.2   Score per residue for model 2

• Molecule 1: Ras-related C3 botulinum toxin substrate 1

Chain A: 57%   30%   5%   8%

M1 Q2 V7 V14 T17 C18 S22 P29 G30 E31 Y32 I33 P34 T35 V36 F37 D38 N39 V44 V51 N52 L53 W56 L61 Y64 D65 R66 L67 R68 Q74 T75 I80 V85 F90 E91 N92 V93 R94 A95 K96 W97 Y98 P99 R102

C105 P106 I110 I111 L112 K116 L117 D118 L119 K123 D124 T125 I126 L129 K132 K133 L134 T135 P136 Y139 P140 L143 A151 V152 K153 V154 L155 S158 Q162 R163 V168 A172 I173 R174 A175 V176 L177 C178 P179 K184 R185 K186 R187 K188 C189 L190 L191

L192

• Molecule 2: Serine/threonine-protein kinase N1

Chain B: 56%   16%   28%

G119 I120 P121 A122 T123 N124 L125 S126 A136 I137 E138 L139 Y152 S153 N154 G155 S156 T157 K158 L162 Q168 M169 L170 Q171 K174 I179 I180 Q183 L184 R185 A190 D191 Q192 L193 E194 N195 Q196 A197 A198 P199

4.2.3   Score per residue for model 3

• Molecule 1: Ras-related C3 botulinum toxin substrate 1

Chain A: 64%   22%   5% · 8%

M1 Q2 A3 I4 V7 G30 E31 Y32 I33 P34 F37 D38 N39 V51 N52 L53 L61 D65 R66 L67 R68 P69 T75 D76 V85 S89 F90 E91 N92 V93 R94 A95 K96 W97 Y98 P99 R102 I111 L112 L117 R120 D121 D122 K123 I126

K132 K133 L134 T135 P136 Y139 P140 V152 K153 Y154 L155 S158 T161 Q162 R163 V168 F169 A172 I173 R174 A175 V176 L177 C178 P179 P180 P181 V182 R185 K186 R187 K188 C189 L190 L191 L192

• Molecule 2: Serine/threonine-protein kinase N1

Chain B: 51%   21%   28%

G119 I120 P121 A122 T123 N124 L125 S126 Q134 L135 A136 I137 E138 L139 Q143 G144 A145 I149 N154 G155 S156 T157 K158 D159 R160 K161 L162 T165 M169 I179 I180 R181 M182 Q183 A190 D191 Q192 L193 E194 N195 Q196 A197 A198 P199

4.2.4　Score per residue for model 4

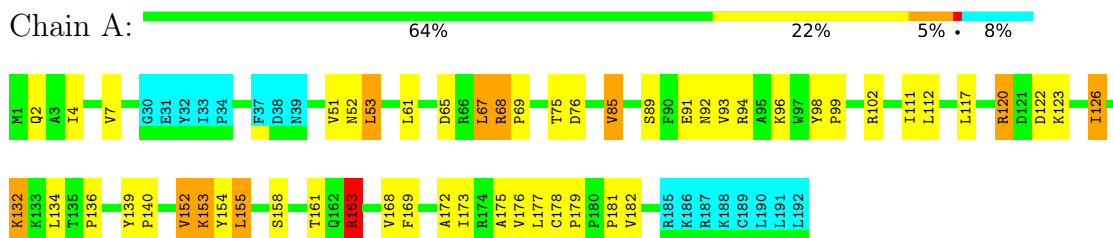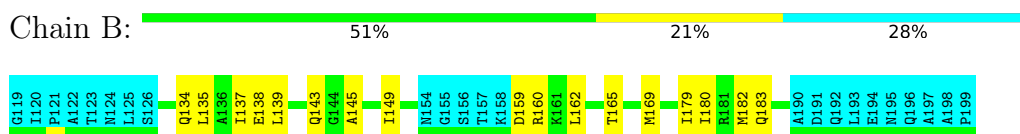• Molecule 1: Ras-related C3 botulinum toxin substrate 1
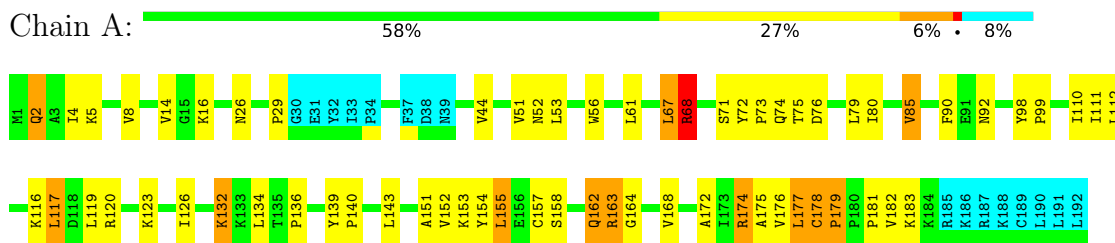
Chain A:

• Molecule 2: Serine/threonine-protein kinase N1

Chain B:

4.2.5　Score per residue for model 5

• Molecule 1: Ras-related C3 botulinum toxin substrate 1

Chain A:

• Molecule 2: Serine/threonine-protein kinase N1

Chain B:

4.2.6　Score per residue for model 6

• Molecule 1: Ras-related C3 botulinum toxin substrate 1

Chain A:

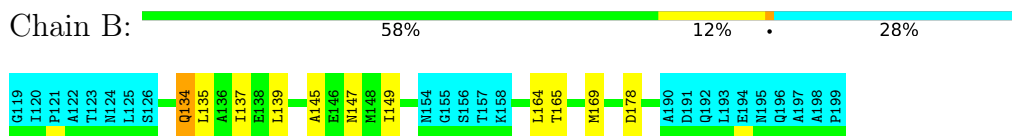• Molecule 2: Serine/threonine-protein kinase N1

Chain B:

4.2.7　Score per residue for model 7

• Molecule 1: Ras-related C3 botulinum toxin substrate 1

Chain A:

• Molecule 2: Serine/threonine-protein kinase N1

Chain B:

4.2.8　Score per residue for model 8

• Molecule 1: Ras-related C3 botulinum toxin substrate 1
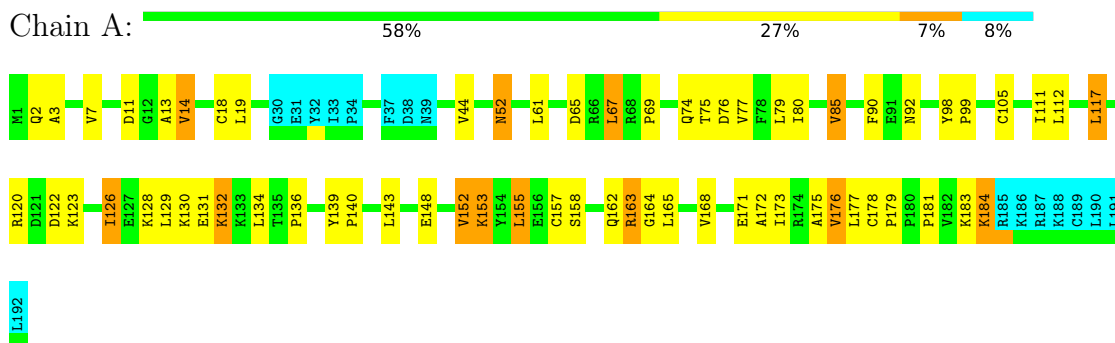
Chain A:

• Molecule 2: Serine/threonine-protein kinase N1

Chain B:

4.2.9 Score per residue for model 9

• Molecule 1: Ras-related C3 botulinum toxin substrate 1

Chain A:

• Molecule 2: Serine/threonine-protein kinase N1
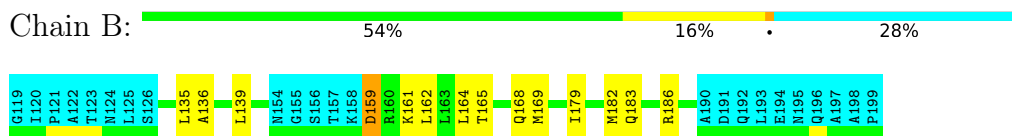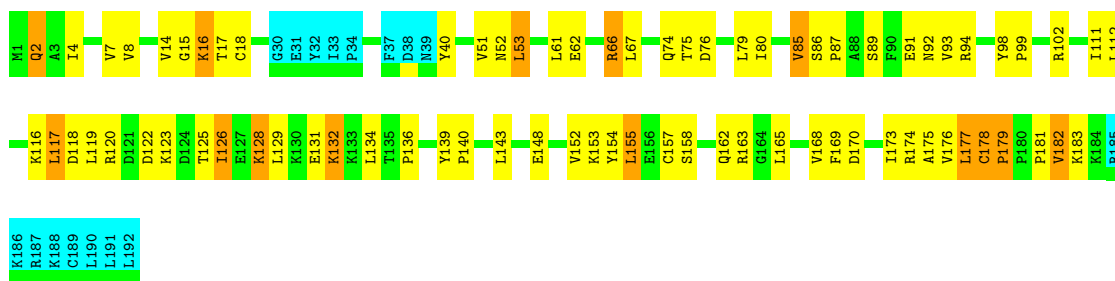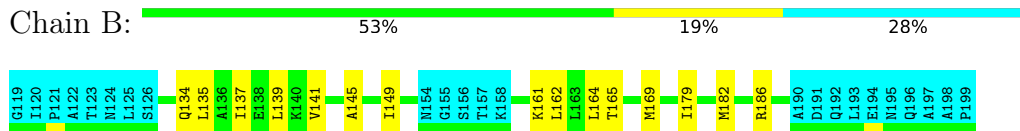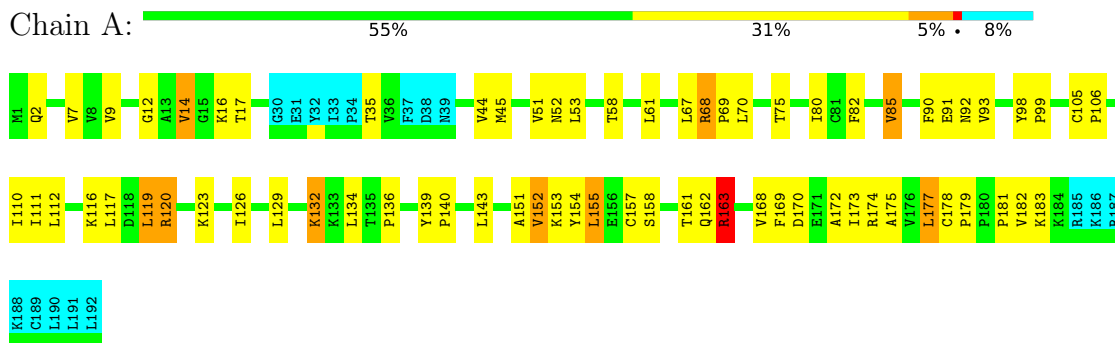
Chain B:

4.2.10 Score per residue for model 10

• Molecule 1: Ras-related C3 botulinum toxin substrate 1

Chain A:

• Molecule 2: Serine/threonine-protein kinase N1

Chain B:

G119 I120 P121 A122 T123 N124 L125 S126 Q134 L135 A136 I137 E138 L139 A145 I149 N154 G155 S156 T157 K158 L164 T165 M169 I179 Q183 A190 D191 Q192 L193 E194 N195 Q196 A197 A198 P199

4.2.11 Score per residue for model 11

• Molecule 1: Ras-related C3 botulinum toxin substrate 1

Chain A: 62% 22% 7% 8%

M1 Q2 G12 A13 V14 T17 C18 L19 G30 E31 Y32 I33 P34 F37 D38 N39 D47 N52 L61 L67 Y72 P73 Q74 T75 I80 V85 F90 E91 N92 Y98 P99 R102 C105 P106 I111 L112 K116 L117 D118 L119 K123

I126 L129 K132 K133 L134 T135 P136 Y139 P140 L143 V152 K153 V154 L155 S158 Q162 R163 G164 L165 K166 T167 V168 E171 A172 I173 R174 A175 V176 L177 C178 P179 P180 P181 K184 K185 K186 R187 K188 C189 L190 L191 L192

• Molecule 2: Serine/threonine-protein kinase N1

Chain B: 53% 19% 28%

G119 I120 P121 A122 T123 N124 L125 S126 Q134 L135 A136 I137 E138 L139 G144 A145 E146 N147 M148 I149 S153 N154 G155 S156 T157 K158 L162 L163 L164 Q168 I179 Q183 A190 D191 Q192 L193 E194 N195 Q196 A197 A198 P199

4.2.12 Score per residue for model 12

• Molecule 1: Ras-related C3 botulinum toxin substrate 1

Chain A: 58% 26% 8% 8%

M1 Q2 V7 V14 C18 G30 E31 Y32 I33 P34 F37 D38 N39 N52 W56 L61 D65 R66 L67 R68 P69 L70 S71 Y72 P73 Q74 T75 D76 I80 V85 S86 P87 E91 N92 V93 R94 A95 Y98 P99 R102 C105 P106 P109 I110

I111 L112 L117 R120 K123 I126 E127 K128 L129 K130 E131 K132 K133 L134 Y139 P140 Q141 A151 V152 K153 Y154 L155 E156 C157 S158 Q162 R163 V168 R174 A175 V176 L177 C178 P179 P180 P181 V182 K183 K184 R185 K186 R187 K188 C189 L190 L191 L192

• Molecule 2: Serine/threonine-protein kinase N1

Chain B: 54% 17% 28%

G119 I120 P121 A122 T123 N124 L125 S126 Q134 L135 A136 I137 E138 L139 A145 I149 N154 G155 S156 T157 K158 T165 M169 D178 I179 I180 R181 M182 Q183 A190 D191 Q192 L193 E194 N195 Q196 A197 A198 P199

4.2.13 Score per residue for model 13

• Molecule 1: Ras-related C3 botulinum toxin substrate 1

Chain A: 56% 28% 8% 8%

• Molecule 2: Serine/threonine-protein kinase N1

Chain B:

4.2.14 Score per residue for model 14 (medoid)

• Molecule 1: Ras-related C3 botulinum toxin substrate 1

Chain A:

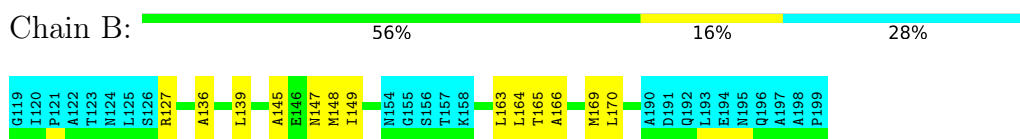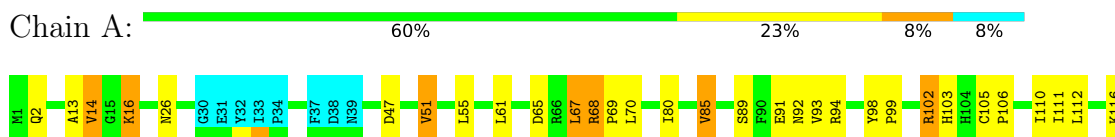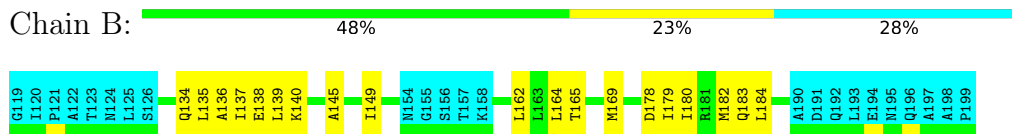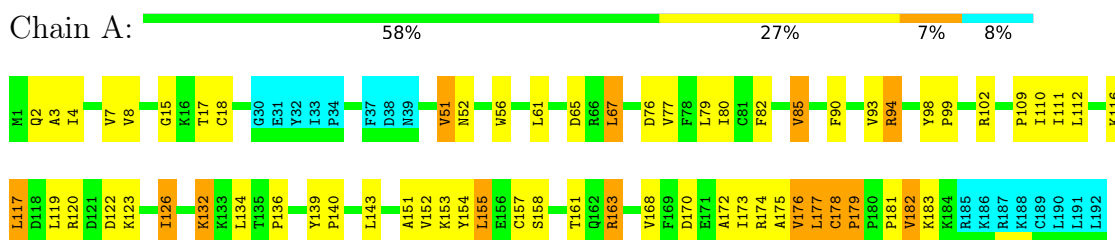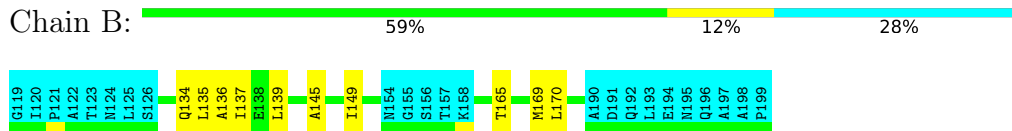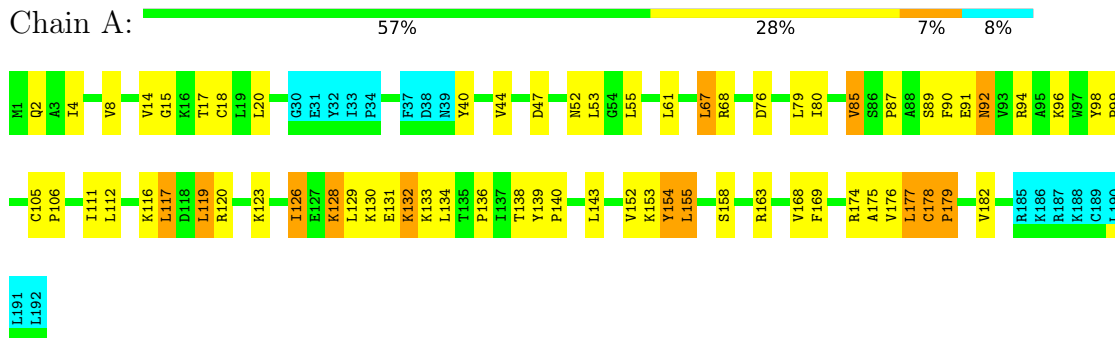• Molecule 2: Serine/threonine-protein kinase N1
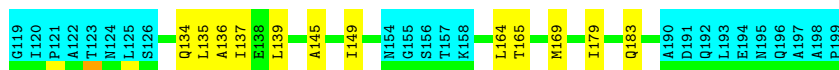
Chain B:
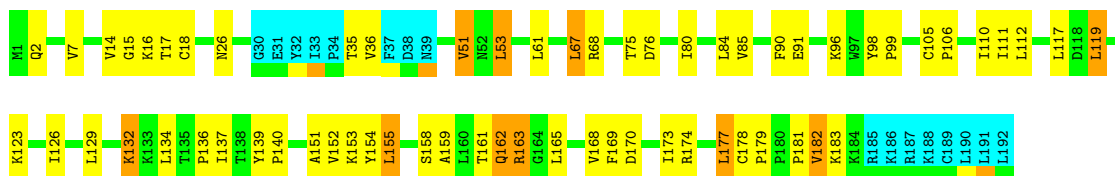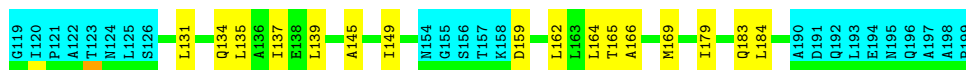
4.2.15 Score per residue for model 15

• Molecule 1: Ras-related C3 botulinum toxin substrate 1

Chain A:

• Molecule 2: Serine/threonine-protein kinase N1

Chain B: 63%   9%   28%

G119 I120 P121 A122 T123 N124 L125 S126 L135 L139 N154 G155 S156 T157 K158 L164 M169 I179 M182 Q183 A190 D191 Q192 L193 E194 N195 Q196 A197 A198 P199

4.2.16 Score per residue for model 16

• Molecule 1: Ras-related C3 botulinum toxin substrate 1

Chain A: 64%   23%   5%   8%

M1 D11 G15 C18 G30 E31 Y32 I33 P34 T35 V36 F37 D38 N39 Y40 L53 L61 R66 L67 Q74 T75 D76 I80 V85 F90 E91 N92 V93 R94 Y98 P99 I110 I111 L112 K116 L117 D118 L119 K123 I126 K132 K133 L134

T135 P136 Y139 P140 L143 A151 V152 K153 V154 L155 E156 C157 S158 Q162 R163 G164 L165 V168 F169 A172 I173 R174 A175 V176 L177 C178 P179 V182 R185 K186 R187 K188 C189 L190 L191 L192

• Molecule 2: Serine/threonine-protein kinase N1

Chain B: 52%   19%   •   28%

G119 I120 P121 A122 T123 N124 L125 S126 Q134 L135 A136 I137 E138 L139 A145 E146 N147 M148 I149 N154 G155 S156 T157 K158 L162 L163 L164 Q168 M169 D178 I179 M182 Q183 R186 A190 D191 Q192 L193 E194 N195 Q196 A197 A198 P199

4.2.17 Score per residue for model 17

• Molecule 1: Ras-related C3 botulinum toxin substrate 1

Chain A: 57%   28%   7%   8%

M1 Q2 A3 I4 V7 A13 V14 C18 L19 L20 I21 G30 E31 Y32 I33 P34 F37 D38 N39 V44 V51 N52 L53 W56 L61 E62 D63 L67 R68 S71 Y72 T75 D76 V77 I80 V85 F90 E91 N92 V93 R94 A95 Y98 P99

R102 I111 L112 K116 L117 D118 L119 R120 K123 I126 L129 K132 K133 L134 T135 P136 Y139 P140 L143 V152 K153 Y154 L155 S158 R163 V168 F169 D170 E171 A172 I173 R174 A175 V176 L177 C178 P179 P180 P181 V182 R185 K186 R187 K188 C189 L190

L191 L192

• Molecule 2: Serine/threonine-protein kinase N1

Chain B: 52%   17%   •   28%

G119 I120 P121 A122 T123 N124 L125 S126 R127 V128 Q134 L135 A136 I137 E138 L139 A145 I149 N154 G155 S156 T157 K158 L162 L163 L164 Q168 M169 I180 R185 R186 A187 A190 D191 Q192 L193 E194 N195 Q196 A197 A198 P199
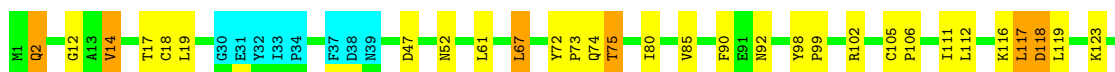
4.2.18　Score per residue for model 18

• Molecule 1: Ras-related C3 botulinum toxin substrate 1

Chain A:

• Molecule 2: Serine/threonine-protein kinase N1

Chain B:
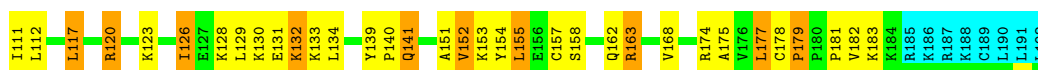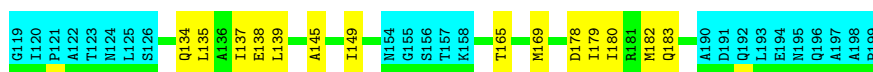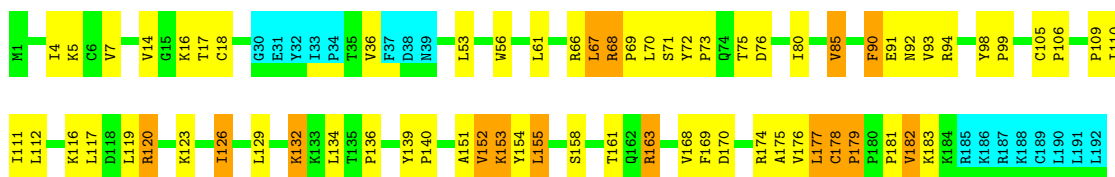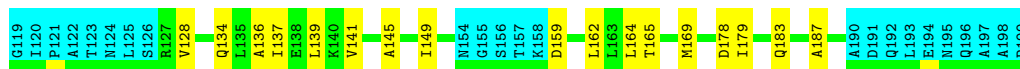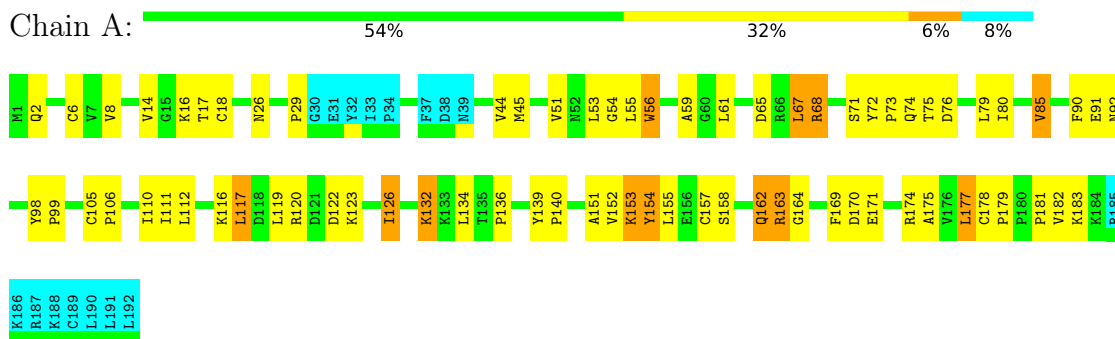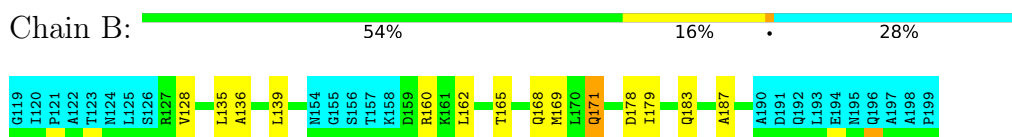

4.2.19　Score per residue for model 19

• Molecule 1: Ras-related C3 botulinum toxin substrate 1

Chain A:

• Molecule 2: Serine/threonine-protein kinase N1

Chain B:
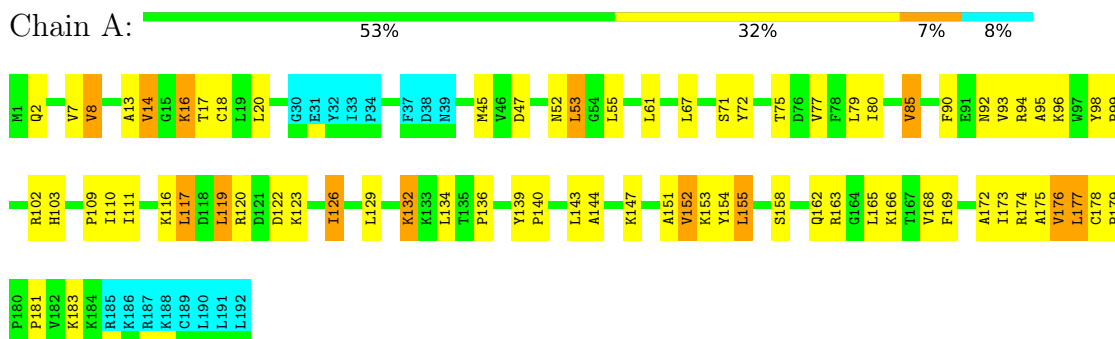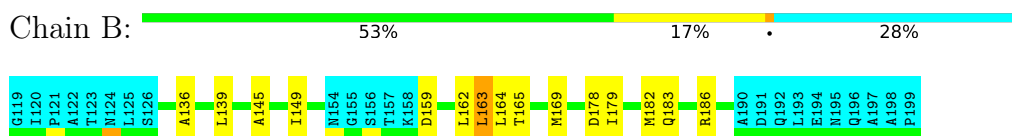
4.2.20　Score per residue for model 20

• Molecule 1: Ras-related C3 botulinum toxin substrate 1

Chain A:　　　　53%　　　　31%　　　7%　　8%
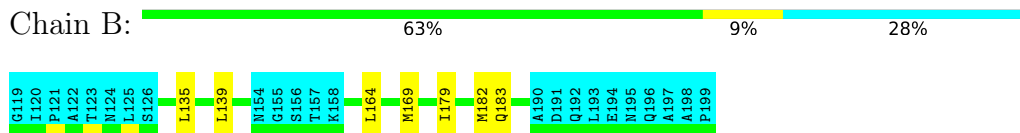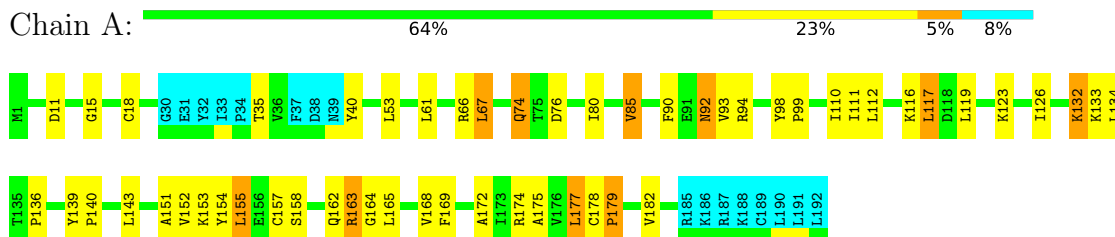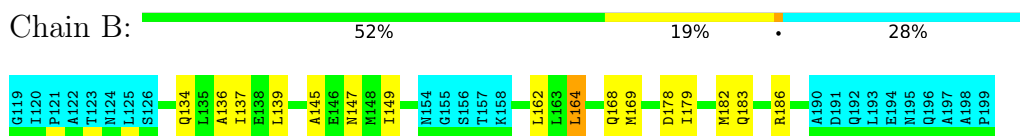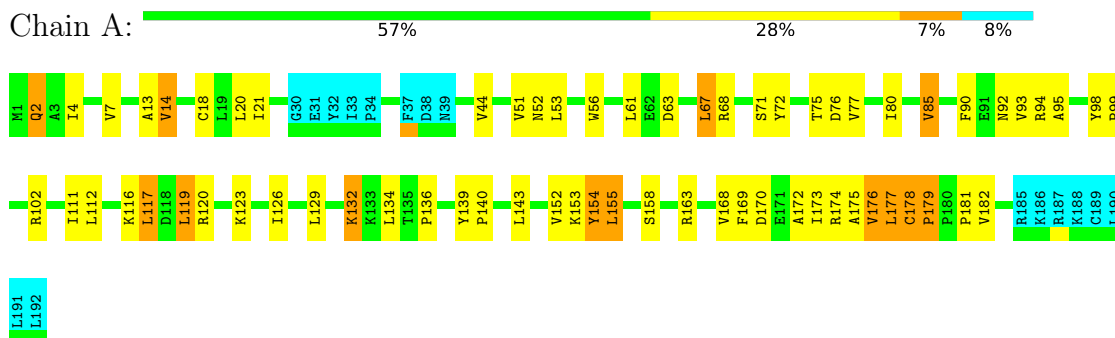
M1 Q2 A3 I4 K5 C6 V7 V14 G15 K16 T17 C18 G30 E31 Y32 I33 P34 T35 V36 F37 D38 N39 V44 D47 N52 L53 W56 L61 E62 D63 Y64 L67 R68 P69 L70 S71 Y72 T75 D76 V77 F78 L79 I80 V85 S86 P87 F90 E91

R94 A95 K96 W97 Y98 P99 R102 H103 I111 L112 K116 L117 D118 L119 R120 K123 I126 L129 K132 K133 L134 T135 P136 Y139 P140 L143 V152 K153 Y154 L155 E156 C157 S158 A159 Q162 R163 G164 L165 V168 F169 D170 I173 R174 A175 V176 L177 C178

P179 P180 P181 V182 K183 K184 R185 K186 R187 K188 C189 L190 L191 L192

• Molecule 2: Serine/threonine-protein kinase N1

Chain B:　　　　56%　　　　16%　　　28%

G119 I120 P121 A122 T123 N124 L125 S126 L135 L139 K140 V141 A145 N154 G155 S156 T157 K158 L164 T165 A166 Q167 Q168 M169 I179 M182 Q183 R186 A190 D191 Q192 L193 E194 N195 Q196 A197 A198 P199

4.2.21　Score per residue for model 21

• Molecule 1: Ras-related C3 botulinum toxin substrate 1

Chain A:　　　　56%　　　　28%　　　7%　　8%

M1 Q2 V7 V8 V14 G15 K16 T17 C18 L19 L20 G30 E31 Y32 I33 P34 T35 V36 F37 D38 N39 V51 L55 W56 L61 E62 D63 Y64 D65 R66 L67 R68 P69 L70 S71 Y72 P73 Q74 T75 D76 V77 F78 L79 I80 V85 F90 R94 Y98 P99

R102 C105 P106 I111 L112 K116 L117 D118 L119 R120 D121 D122 K123 I126 K132 K133 L134 T135 P136 Y139 P140 L143 V152 K153 Y154 L155 S158 R163 V168 F169 D170 R174 A175 V176 L177 C178 P179 P180 P181 V182 K183 K184 R185 K186 R187 K188 C189 L190

L191 L192

• Molecule 2: Serine/threonine-protein kinase N1

Chain B:　　　　54%　　　　17%　　　28%

G119 I120 P121 A122 T123 N124 L125 S126 L135 L139 N147 M148 N154 G155 S156 T157 K158 D159 L162 L163 L164 T165 M169 D178 I179 M182 Q183 R186 A190 D191 Q192 L193 E194 N195 Q196 A197 A198 P199

4.2.22　Score per residue for model 22

• Molecule 1: Ras-related C3 botulinum toxin substrate 1

Chain A:　　　　55%　　　　28%　　　9%　　8%

M1 Q2 V7 G12 A13 V14 G15 K16 T17 P29 G30 E31 Y32 I33 P34 F37 D38 N39 V51 N52 L53 A59 G60 L61 L67 R68 P69 L70 T75 D76 I80 C81 F82 V85 F90 E91 N92 V93 R94 A95 K96 W97 Y98 P99 R102 H103 H104 C105

P106 P109 I110 I111 L112 K116 L117 D118 L119 R120 K123 I126 L129 K132 K133 L134 T135 P136 Y139 P140 L143 V152 K153 Y154 L155 S158 Q162 R163 G164 L165 V168 F169 D170 E171 A172 I173 R174 A175 V176 L177 C178 P179 P180 P181 V182 K183 R184 R185

K186 R187 K188 C189 L190 L191 L192

• Molecule 2: Serine/threonine-protein kinase N1

Chain B: 53% 17% • 28%

G119 I120 P121 A122 T123 N124 L125 S126 Q134 L135 A136 I137 E138 L139 K140 V141 A145 I149 N154 G155 S156 T157 K158 D159 L162 T165 Q168 M169 D178 I179 M182 A190 D191 Q192 L193 E194 N195 Q196 A197 A198 P199

4.2.23 Score per residue for model 23

• Molecule 1: Ras-related C3 botulinum toxin substrate 1

Chain A: 57% 27% 8% 8%

M1 Q2 A3 I4 V14 G15 K16 T17 C18 G30 E31 Y32 I33 P34 T35 V36 F37 D38 N39 Y40 V44 V51 N52 L53 L61 E62 D63 L67 R68 P69 L70 S71 Y72 P73 Q74 T75 D76 V77 F78 V85 F90 E91 W97 Y98 P99 E100 V101 R102 I111

L117 D118 L119 R120 K123 D124 T125 I126 L129 K132 K133 L134 T135 P136 Y139 P140 L143 V152 K153 Y154 L155 S158 Q162 R163 G164 L165 V168 F169 D170 E171 A172 I173 R174 A175 V176 L177 C178 P179 K184 R185 K186 R187 K188 C189 L190 L191 L192

• Molecule 2: Serine/threonine-protein kinase N1

Chain B: 56% 16% 28%

G119 I120 P121 A122 T123 N124 L125 S126 Q134 L135 A136 I137 E138 L139 K140 V141 N154 G155 S156 T157 K158 T165 Q168 M169 I179 M182 Q183 R186 A190 D191 Q192 L193 E194 N195 Q196 A197 A198 P199

4.2.24 Score per residue for model 24

• Molecule 1: Ras-related C3 botulinum toxin substrate 1

Chain A: 57% 29% 5% 8%

M1 Q2 A3 G12 A13 V14 T17 C18 L19 L20 P29 G30 E31 Y32 I33 P34 T35 V36 F37 D38 N39 Y40 D47 V51 N52 L53 A59 G60 L61 E62 D63 L67 L70 D76 I80 V85 S89 F90 E91 N92 V93 R94 A95 K96 W97 Y98 P99

R102 P109 L112 K116 L117 D118 L119 R120 K123 D124 T125 I126 L129 K132 K133 L134 T135 P136 Y139 P140 L143 E148 V152 K153 Y154 L155 S158 Q162 R163 T167 V168 F169 D170 E171 A172 A175 V176 L177 C178 P179 V182 K183 K184 R185 K186

R187 K188 C189 L190 L191 L192

• Molecule 2: Serine/threonine-protein kinase N1

Chain B:

52%   19%   •   28%

G119 I120 P121 A122 T123 N124 L125 S126 L131 Q134 L135 A136 L139 A145 I149 N154 G155 S156 T157 K158 Q167 Q168 M169 L170 Q171 I179 M182 Q183 L184 R185 R186 A190 D191 Q192 L193 E194 N195 Q196 A197 A198 P199

4.2.25 Score per residue for model 25

• Molecule 1: Ras-related C3 botulinum toxin substrate 1

Chain A:

60%   26%   6%   8%

M1 Q2 A3 I4 V7 G12 A13 V14 G15 K16 G30 E31 Y32 I33 P34 F37 D38 N39 Y40 N52 L53 Q54 L55 W56 L61 L67 R68 P69 L70 S71 T75 I80 V85 E91 N92 Y98 P99 R102 C105 P106 I111 L112 K116 L117

D118 L119 R120 K123 I126 E127 K128 L129 K130 E131 K132 K133 L134 T135 P136 Y139 P140 L143 E148 V152 V153 Y154 L155 E156 C157 S158 Q162 R163 V168 R174 A175 V176 L177 C178 P179 K183 K184 R185 K186 R187 K188 C189 L190 L191 L192

• Molecule 2: Serine/threonine-protein kinase N1

Chain B:

48%   21%   •   28%

G119 I120 P121 A122 T123 N124 L125 S126 L131 Q134 L135 A136 L139 K140 V141 K142 N147 M148 I149 N154 G155 S156 T157 K158 L162 L163 L164 T165 M169 I179 M182 Q183 L184 R185 R186 A190 D191 Q192 L193 E194 N195 Q196 A197 A198 P199

5 Refinement protocol and experimental data overview ⓘ

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

Of the 100 calculated structures, 25 were deposited, based on the following criterion: *structures with the lowest energy.*

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

Software name	Classification	Version
CNS	structure solution	1.1
CNS	refinement	1.1

No chemical shift data was provided.

6 Model quality ⓘ

6.1 Standard geometry ⓘ

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

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 ⓘ

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	1367	1416	1414	41±5
2	B	468	513	513	9±2
4	A	32	14	14	3±1
All	All	46750	48675	48525	1196

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 13.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Models Total
1:A:67:LEU:HD22	2:B:169:MET:SD	0.74	2.23	22	14
1:A:153:LYS:HZ3	1:A:155:LEU:HD22	0.73	1.42	21	17
1:A:153:LYS:HD2	1:A:154:TYR:N	0.70	2.01	24	1
1:A:4:ILE:HD12	1:A:176:VAL:HG21	0.70	1.61	3	4
1:A:70:LEU:HD22	2:B:169:MET:HE1	0.67	1.66	21	1
1:A:175:ALA:O	1:A:179:PRO:HG2	0.65	1.92	24	15
1:A:70:LEU:HD23	1:A:70:LEU:H	0.65	1.51	21	1
1:A:162:GLN:HG3	1:A:165:LEU:HD12	0.63	1.70	19	7
1:A:153:LYS:NZ	1:A:155:LEU:HD22	0.62	2.09	17	17
1:A:76:ASP:HB3	1:A:176:VAL:HG11	0.62	1.71	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:14:VAL:HG22	4:A:193:GCP:H5'1	0.62	1.71	19	1
1:A:64:TYR:HB3	2:B:141:VAL:HG22	0.61	1.72	20	1
1:A:14:VAL:HG12	4:A:193:GCP:H5'1	0.61	1.71	11	4
1:A:70:LEU:HD21	2:B:148:MET:SD	0.61	2.35	21	1
2:B:165:THR:HG22	2:B:169:MET:SD	0.61	2.36	7	3
1:A:159:ALA:HA	1:A:165:LEU:HD11	0.60	1.71	15	3
1:A:128:LYS:O	1:A:131:GLU:HG3	0.60	1.97	10	2
1:A:70:LEU:HD12	2:B:165:THR:HB	0.59	1.74	21	1
1:A:132:LYS:HB2	1:A:134:LEU:HD12	0.59	1.75	16	25
1:A:116:LYS:HB3	1:A:119:LEU:HD21	0.59	1.74	7	3
1:A:5:LYS:HB2	1:A:56:TRP:HE1	0.58	1.58	13	2
1:A:111:ILE:HD11	1:A:175:ALA:HB2	0.58	1.75	11	7
1:A:128:LYS:HG3	1:A:129:LEU:N	0.58	2.13	6	2
1:A:178:CYS:HB3	1:A:179:PRO:HD3	0.58	1.76	19	9
1:A:70:LEU:HD13	2:B:165:THR:HB	0.58	1.74	23	1
2:B:131:LEU:HB2	2:B:184:LEU:HD23	0.58	1.76	24	2
2:B:165:THR:HG22	2:B:169:MET:HE3	0.57	1.75	10	12
1:A:67:LEU:HD11	2:B:145:ALA:HB2	0.57	1.77	4	4
4:A:193:GCP:H8	4:A:193:GCP:H5'2	0.57	1.76	8	3
1:A:176:VAL:HG22	1:A:177:LEU:HD23	0.57	1.77	1	3
1:A:111:ILE:HD12	1:A:171:GLU:OE1	0.57	2.00	11	1
1:A:54:GLY:O	1:A:55:LEU:HD22	0.57	1.99	18	1
1:A:117:LEU:HB3	1:A:158:SER:HB2	0.57	1.77	18	24
1:A:3:ALA:HA	1:A:52:ASN:HB3	0.57	1.77	5	1
1:A:175:ALA:HA	1:A:179:PRO:HG2	0.56	1.76	4	3
1:A:76:ASP:HA	1:A:182:VAL:HG21	0.56	1.77	16	10
1:A:85:VAL:HG12	1:A:120:ARG:HA	0.56	1.75	13	15
2:B:135:LEU:O	2:B:139:LEU:HD13	0.56	2.01	15	19
1:A:117:LEU:HD23	1:A:163:ARG:CG	0.56	2.30	13	2
1:A:2:GLN:O	1:A:51:VAL:HG23	0.56	2.00	8	5
1:A:15:GLY:HA2	4:A:193:GCP:H5'1	0.56	1.76	10	1
1:A:13:ALA:O	1:A:14:VAL:HG13	0.56	2.01	17	2
1:A:111:ILE:HG23	1:A:153:LYS:HD3	0.56	1.78	22	22
1:A:18:CYS:HB2	4:A:193:GCP:H5'2	0.56	1.77	10	1
1:A:126:ILE:HG12	1:A:136:PRO:HG3	0.56	1.78	15	9
1:A:105:CYS:N	1:A:106:PRO:HD3	0.55	2.16	7	5
1:A:77:VAL:HG21	1:A:111:ILE:HG12	0.55	1.78	17	4
1:A:18:CYS:HB2	4:A:193:GCP:H5'1	0.55	1.79	5	3
1:A:72:TYR:HB3	1:A:73:PRO:HD3	0.55	1.78	23	8
1:A:6:CYS:O	1:A:56:TRP:CE3	0.55	2.59	18	1
1:A:14:VAL:HB	4:A:193:GCP:H5'1	0.55	1.79	8	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
2:B:166:ALA:HA	2:B:169:MET:SD	0.55	2.42	7	3
1:A:155:LEU:HD21	1:A:168:VAL:HG22	0.54	1.78	22	23
1:A:74:GLN:HG3	2:B:162:LEU:HD21	0.54	1.79	5	6
1:A:116:LYS:HB3	1:A:119:LEU:HD11	0.54	1.79	2	17
1:A:119:LEU:HD13	1:A:119:LEU:H	0.54	1.62	10	2
1:A:167:THR:O	1:A:171:GLU:HG3	0.54	2.02	11	1
1:A:2:GLN:O	1:A:51:VAL:HG13	0.54	2.03	4	7
1:A:7:VAL:HG22	1:A:75:THR:HG21	0.54	1.79	17	6
1:A:117:LEU:HD23	1:A:163:ARG:HG3	0.54	1.79	7	2
1:A:80:ILE:HB	1:A:112:LEU:HD23	0.54	1.79	18	17
1:A:117:LEU:O	1:A:117:LEU:HD13	0.53	2.04	23	20
1:A:76:ASP:HA	1:A:182:VAL:HG11	0.53	1.80	12	7
1:A:8:VAL:HG22	1:A:79:LEU:HD12	0.53	1.80	18	5
1:A:15:GLY:N	4:A:193:GCP:H5'1	0.53	2.18	6	3
1:A:172:ALA:O	1:A:175:ALA:HB3	0.53	2.04	5	13
1:A:128:LYS:HA	1:A:131:GLU:HG3	0.53	1.81	25	2
1:A:117:LEU:HD12	1:A:120:ARG:HG2	0.53	1.81	13	2
1:A:8:VAL:HB	1:A:79:LEU:HD12	0.53	1.80	4	2
1:A:98:TYR:N	1:A:99:PRO:HD2	0.52	2.20	15	25
1:A:70:LEU:HB2	2:B:165:THR:HG21	0.52	1.81	21	1
1:A:44:VAL:HG11	1:A:173:ILE:HD11	0.52	1.81	1	2
2:B:136:ALA:HA	2:B:139:LEU:HG	0.52	1.82	7	6
1:A:7:VAL:HG12	1:A:56:TRP:HB2	0.52	1.81	2	7
1:A:173:ILE:O	1:A:176:VAL:HG13	0.51	2.04	5	6
1:A:5:LYS:CB	1:A:56:TRP:HE1	0.51	2.19	4	1
1:A:17:THR:HB	4:A:193:GCP:O1A	0.51	2.06	18	16
1:A:7:VAL:HG12	1:A:75:THR:HG21	0.51	1.82	3	7
1:A:67:LEU:HD23	2:B:141:VAL:HG23	0.51	1.82	22	1
2:B:134:GLN:HA	2:B:137:ILE:HD12	0.50	1.83	10	15
1:A:157:CYS:HA	1:A:163:ARG:HB2	0.50	1.83	18	11
1:A:153:LYS:HZ2	1:A:171:GLU:HG3	0.50	1.66	8	3
2:B:149:ILE:HG23	2:B:163:LEU:HD11	0.50	1.83	7	2
1:A:53:LEU:HD11	1:A:169:PHE:HB3	0.50	1.84	19	8
1:A:16:LYS:HE3	1:A:59:ALA:HB3	0.50	1.84	22	1
1:A:2:GLN:HB3	1:A:51:VAL:HB	0.49	1.84	24	5
1:A:85:VAL:HG11	1:A:119:LEU:HG	0.49	1.82	23	1
1:A:4:ILE:HD13	1:A:176:VAL:HG21	0.49	1.83	4	1
1:A:66:ARG:HD2	1:A:67:LEU:N	0.49	2.22	6	1
1:A:67:LEU:HD22	2:B:169:MET:HE2	0.49	1.82	7	1
1:A:70:LEU:HD11	2:B:169:MET:SD	0.49	2.47	22	4
2:B:162:LEU:H	2:B:162:LEU:HD22	0.49	1.68	21	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:74:GLN:O	1:A:75:THR:C	0.49	2.50	23	4
1:A:2:GLN:O	1:A:52:ASN:N	0.49	2.45	2	16
2:B:134:GLN:HE21	2:B:134:GLN:HA	0.49	1.68	4	3
1:A:18:CYS:SG	4:A:193:GCP:H3'	0.49	2.48	11	12
1:A:59:ALA:H	1:A:68:ARG:HD2	0.49	1.68	22	1
2:B:128:VAL:HG22	2:B:187:ALA:HB1	0.49	1.85	17	3
1:A:85:VAL:HA	1:A:136:PRO:HA	0.48	1.85	3	24
1:A:67:LEU:HD13	2:B:141:VAL:HG13	0.48	1.84	6	1
1:A:67:LEU:O	1:A:68:ARG:HB2	0.48	2.09	21	1
1:A:110:ILE:HG13	1:A:151:ALA:HA	0.48	1.84	19	12
1:A:105:CYS:N	1:A:106:PRO:CD	0.48	2.77	12	8
1:A:175:ALA:O	1:A:179:PRO:CG	0.48	2.62	5	1
1:A:70:LEU:HD22	2:B:169:MET:CE	0.48	2.37	21	1
1:A:153:LYS:HD2	1:A:171:GLU:HB2	0.48	1.86	11	1
1:A:67:LEU:HD21	2:B:145:ALA:HB2	0.48	1.85	14	4
1:A:153:LYS:HG2	1:A:154:TYR:N	0.48	2.23	18	9
1:A:178:CYS:HB3	1:A:179:PRO:CD	0.48	2.39	17	16
1:A:68:ARG:HB3	1:A:69:PRO:HD3	0.48	1.84	13	8
1:A:53:LEU:HD21	1:A:169:PHE:CD2	0.48	2.44	10	2
1:A:125:THR:O	1:A:129:LEU:HG	0.48	2.09	6	1
1:A:117:LEU:HD12	1:A:163:ARG:HD2	0.47	1.87	6	1
2:B:165:THR:HA	2:B:168:GLN:HE21	0.47	1.68	23	3
2:B:145:ALA:O	2:B:149:ILE:HG13	0.47	2.10	3	16
1:A:85:VAL:HG11	1:A:119:LEU:HD23	0.47	1.87	8	3
1:A:153:LYS:HZ1	1:A:155:LEU:HB3	0.47	1.69	13	3
1:A:61:LEU:HD23	1:A:63:ASP:HB3	0.47	1.87	17	2
2:B:159:ASP:HB2	2:B:162:LEU:HD23	0.47	1.85	22	3
1:A:71:SER:O	1:A:72:TYR:C	0.47	2.53	23	8
1:A:87:PRO:O	1:A:91:GLU:HG2	0.47	2.10	10	4
1:A:161:THR:OG1	1:A:163:ARG:HG2	0.47	2.10	13	2
1:A:153:LYS:HE2	1:A:171:GLU:HG3	0.47	1.87	24	1
1:A:15:GLY:HA2	4:A:193:GCP:H5'2	0.46	1.85	22	3
1:A:126:ILE:HA	1:A:129:LEU:HD12	0.46	1.85	6	3
2:B:138:GLU:HG3	2:B:180:ILE:HD12	0.46	1.87	3	5
1:A:163:ARG:HA	1:A:163:ARG:HE	0.46	1.71	16	7
1:A:126:ILE:O	1:A:130:LYS:HG2	0.46	2.10	10	3
2:B:131:LEU:HB2	2:B:184:LEU:HG	0.46	1.85	14	1
1:A:5:LYS:O	1:A:75:THR:HG23	0.46	2.10	20	1
1:A:85:VAL:HG22	1:A:120:ARG:HA	0.46	1.87	12	3
1:A:99:PRO:HA	1:A:102:ARG:NE	0.46	2.24	23	1
1:A:174:ARG:HA	1:A:177:LEU:HG	0.46	1.88	22	19

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:152:VAL:HG11	1:A:179:PRO:HG3	0.46	1.88	5	1
1:A:18:CYS:CB	4:A:193:GCP:H5'2	0.46	2.40	10	1
1:A:20:LEU:HB2	1:A:55:LEU:HD12	0.46	1.88	19	1
1:A:26:ASN:HA	1:A:162:GLN:NE2	0.46	2.26	18	5
1:A:18:CYS:SG	4:A:193:GCP:H2'	0.46	2.51	14	2
1:A:175:ALA:O	1:A:179:PRO:HB2	0.46	2.10	19	2
1:A:111:ILE:HG22	1:A:112:LEU:N	0.46	2.26	6	19
1:A:66:ARG:O	1:A:69:PRO:HD2	0.46	2.11	13	1
1:A:70:LEU:HD22	2:B:165:THR:CG2	0.46	2.41	23	1
1:A:111:ILE:HD13	1:A:152:VAL:HG23	0.46	1.88	22	6
1:A:117:LEU:HB3	1:A:163:ARG:HG3	0.46	1.87	6	6
1:A:139:TYR:HB3	1:A:140:PRO:HD3	0.45	1.88	21	25
1:A:109:PRO:HB2	1:A:152:VAL:HG21	0.45	1.87	19	1
2:B:149:ILE:HG23	2:B:163:LEU:HD21	0.45	1.86	19	1
1:A:15:GLY:HA2	4:A:193:GCP:O2A	0.45	2.12	25	1
1:A:13:ALA:O	1:A:14:VAL:HB	0.45	2.11	19	2
1:A:128:LYS:O	1:A:131:GLU:HG2	0.45	2.12	6	3
1:A:71:SER:O	1:A:74:GLN:N	0.45	2.50	23	1
1:A:51:VAL:HG21	1:A:173:ILE:HD13	0.45	1.89	14	2
1:A:178:CYS:CB	1:A:179:PRO:CD	0.45	2.94	1	15
1:A:175:ALA:CA	1:A:179:PRO:HG2	0.45	2.42	4	1
1:A:117:LEU:CB	1:A:163:ARG:HG3	0.45	2.40	6	1
1:A:20:LEU:HD12	1:A:21:ILE:N	0.45	2.27	17	1
1:A:51:VAL:HG11	1:A:173:ILE:HG21	0.45	1.87	3	1
1:A:118:ASP:HA	1:A:163:ARG:HH21	0.45	1.72	6	1
1:A:174:ARG:O	1:A:179:PRO:HD2	0.45	2.11	19	2
1:A:69:PRO:HB2	1:A:72:TYR:HB2	0.45	1.89	15	1
1:A:153:LYS:HD2	1:A:171:GLU:HB3	0.45	1.87	18	1
1:A:51:VAL:HG11	1:A:173:ILE:HD13	0.45	1.89	15	5
1:A:183:LYS:HG2	1:A:184:LYS:H	0.45	1.72	20	2
1:A:82:PHE:HB3	1:A:93:VAL:HG11	0.45	1.89	9	3
1:A:20:LEU:HD22	1:A:55:LEU:HG	0.45	1.89	21	1
1:A:153:LYS:HE3	1:A:155:LEU:HB3	0.44	1.89	24	3
1:A:67:LEU:O	1:A:68:ARG:CB	0.44	2.64	21	1
2:B:182:MET:O	2:B:186:ARG:HG2	0.44	2.12	21	10
1:A:19:LEU:HD22	1:A:165:LEU:HD21	0.44	1.87	11	1
1:A:89:SER:O	1:A:93:VAL:HG13	0.44	2.12	3	5
1:A:157:CYS:HB2	1:A:164:GLY:H	0.44	1.72	16	3
1:A:117:LEU:CB	1:A:158:SER:HB2	0.44	2.42	19	11
1:A:129:LEU:HB3	1:A:134:LEU:HB2	0.44	1.90	12	2
2:B:135:LEU:HD12	2:B:136:ALA:N	0.44	2.27	24	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:9:VAL:HG12	1:A:58:THR:HG23	0.44	1.90	7	1
1:A:4:ILE:HD12	1:A:176:VAL:HG11	0.44	1.87	20	3
1:A:68:ARG:N	1:A:69:PRO:HD2	0.44	2.28	20	1
1:A:68:ARG:HB2	1:A:69:PRO:HD3	0.44	1.89	21	1
1:A:14:VAL:HA	4:A:193:GCP:O1B	0.44	2.13	14	4
1:A:141:GLN:HA	1:A:141:GLN:HE21	0.44	1.73	12	1
2:B:134:GLN:HA	2:B:134:GLN:HE21	0.44	1.73	1	1
1:A:80:ILE:N	1:A:80:ILE:HD12	0.44	2.28	19	13
1:A:4:ILE:HD13	1:A:176:VAL:CG2	0.44	2.43	4	1
1:A:85:VAL:CG1	1:A:119:LEU:HD23	0.44	2.43	7	2
1:A:70:LEU:HD11	2:B:169:MET:CE	0.44	2.43	15	1
1:A:120:ARG:O	1:A:126:ILE:HD11	0.44	2.13	24	1
1:A:132:LYS:N	1:A:132:LYS:HD3	0.44	2.28	15	11
2:B:164:LEU:O	2:B:168:GLN:HG2	0.44	2.12	16	4
1:A:53:LEU:HD21	1:A:169:PHE:HB3	0.44	1.89	18	1
1:A:89:SER:HA	1:A:92:ASN:OD1	0.43	2.11	10	2
1:A:93:VAL:HG23	1:A:94:ARG:N	0.43	2.28	17	9
1:A:125:THR:O	1:A:129:LEU:HD22	0.43	2.12	2	3
1:A:155:LEU:HD11	1:A:168:VAL:HG22	0.43	1.90	19	6
2:B:179:ILE:O	2:B:183:GLN:HG3	0.43	2.13	19	19
1:A:119:LEU:HD13	1:A:119:LEU:N	0.43	2.27	10	1
1:A:15:GLY:N	4:A:193:GCP:O2A	0.43	2.51	16	1
1:A:54:GLY:O	1:A:56:TRP:CZ3	0.43	2.72	18	1
1:A:153:LYS:HG2	1:A:171:GLU:HB3	0.43	1.88	24	1
1:A:16:LYS:H	1:A:16:LYS:HD3	0.43	1.72	6	2
2:B:136:ALA:O	2:B:139:LEU:HB2	0.43	2.12	17	7
2:B:179:ILE:O	2:B:182:MET:HG2	0.43	2.13	16	11
1:A:85:VAL:HB	1:A:129:LEU:HD11	0.43	1.88	23	9
1:A:16:LYS:HE3	1:A:16:LYS:H	0.43	1.73	8	2
1:A:158:SER:HB3	1:A:163:ARG:HG2	0.43	1.91	6	1
1:A:53:LEU:HD21	1:A:169:PHE:CD1	0.43	2.48	7	2
2:B:185:ARG:HA	2:B:185:ARG:HE	0.43	1.74	17	1
1:A:144:ALA:HA	1:A:147:LYS:HD2	0.43	1.89	19	1
2:B:159:ASP:HB3	2:B:162:LEU:HD23	0.43	1.89	19	4
1:A:85:VAL:HG12	1:A:136:PRO:HG3	0.43	1.91	16	2
1:A:117:LEU:HD12	1:A:163:ARG:CD	0.43	2.43	6	1
1:A:70:LEU:HD13	2:B:148:MET:SD	0.43	2.54	25	2
1:A:5:LYS:HB2	1:A:56:TRP:NE1	0.42	2.29	4	2
1:A:14:VAL:HG23	4:A:193:GCP:O3A	0.42	2.14	5	1
1:A:22:SER:OG	1:A:162:GLN:NE2	0.42	2.52	2	1
2:B:141:VAL:CG2	2:B:142:LYS:N	0.42	2.82	25	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:7:VAL:HG22	1:A:56:TRP:HB2	0.42	1.90	1	2
1:A:64:TYR:O	1:A:66:ARG:N	0.42	2.52	2	2
1:A:112:LEU:HB2	1:A:154:TYR:HB2	0.42	1.90	11	3
2:B:167:GLN:O	2:B:171:GLN:HG2	0.42	2.15	24	1
1:A:122:ASP:O	1:A:126:ILE:HD12	0.42	2.14	5	9
1:A:2:GLN:HB3	1:A:51:VAL:HG22	0.42	1.89	4	1
1:A:117:LEU:CG	1:A:163:ARG:HD2	0.42	2.44	2	1
1:A:153:LYS:HE2	1:A:155:LEU:HD22	0.42	1.91	13	2
1:A:67:LEU:HD23	2:B:141:VAL:HG13	0.42	1.92	13	2
1:A:153:LYS:HD2	1:A:154:TYR:H	0.42	1.69	24	1
1:A:117:LEU:HG	1:A:163:ARG:HD2	0.42	1.92	2	1
1:A:173:ILE:HG22	1:A:177:LEU:HD11	0.42	1.90	2	1
1:A:4:ILE:HD12	1:A:176:VAL:CG2	0.42	2.40	3	1
1:A:162:GLN:O	1:A:163:ARG:C	0.42	2.57	7	1
1:A:97:TRP:O	1:A:101:VAL:HG23	0.42	2.14	23	1
1:A:16:LYS:H	1:A:16:LYS:HD2	0.42	1.74	7	1
1:A:68:ARG:H	1:A:69:PRO:HD2	0.42	1.74	20	1
2:B:165:THR:O	2:B:169:MET:HG2	0.42	2.13	5	2
1:A:15:GLY:HA2	4:A:193:GCP:H8	0.42	1.92	23	2
1:A:70:LEU:HB3	2:B:165:THR:CB	0.42	2.45	23	1
1:A:158:SER:O	1:A:162:GLN:HA	0.41	2.15	25	2
2:B:171:GLN:HA	2:B:174:LYS:HE2	0.41	1.91	2	1
1:A:79:LEU:HD23	1:A:111:ILE:HB	0.41	1.92	5	1
2:B:168:GLN:O	2:B:171:GLN:HG3	0.41	2.15	24	2
1:A:153:LYS:CE	1:A:155:LEU:HB3	0.41	2.46	11	1
1:A:40:TYR:HB2	1:A:55:LEU:HD12	0.41	1.93	25	1
1:A:117:LEU:HG	1:A:163:ARG:HH11	0.41	1.75	2	1
2:B:145:ALA:HB3	2:B:170:LEU:HD23	0.41	1.90	7	3
4:A:193:GCP:O2B	4:A:193:GCP:O1A	0.41	2.38	25	1
2:B:162:LEU:HD22	2:B:162:LEU:N	0.41	2.31	14	4
1:A:76:ASP:HB3	1:A:176:VAL:HB	0.41	1.92	5	1
1:A:109:PRO:HB3	1:A:152:VAL:HG11	0.41	1.91	12	3
2:B:164:LEU:HD13	2:B:164:LEU:O	0.41	2.16	13	1
1:A:119:LEU:HB2	1:A:125:THR:HG21	0.41	1.92	23	1
1:A:70:LEU:H	1:A:70:LEU:HD12	0.41	1.74	24	1
1:A:138:THR:OG1	1:A:140:PRO:HD2	0.41	2.16	10	1
2:B:179:ILE:HG22	2:B:183:GLN:NE2	0.41	2.31	13	1
1:A:11:ASP:HB3	1:A:92:ASN:HD21	0.41	1.76	16	1
1:A:119:LEU:HD23	1:A:120:ARG:N	0.41	2.31	23	1
1:A:71:SER:HA	2:B:162:LEU:HD11	0.41	1.93	25	1
1:A:96:LYS:N	1:A:96:LYS:HD2	0.41	2.31	15	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:4:ILE:HD12	1:A:173:ILE:HG23	0.41	1.91	23	2
1:A:109:PRO:HG3	1:A:175:ALA:O	0.41	2.14	19	3
1:A:20:LEU:HB3	1:A:55:LEU:HD23	0.41	1.92	21	2
1:A:118:ASP:CG	4:A:193:GCP:HN21	0.41	2.19	15	2
1:A:95:ALA:O	1:A:99:PRO:HG3	0.41	2.15	12	3
2:B:164:LEU:O	2:B:164:LEU:HD13	0.41	2.16	7	1
1:A:163:ARG:HE	1:A:163:ARG:HA	0.41	1.76	25	2
1:A:75:THR:HG21	1:A:78:PHE:HB3	0.41	1.93	23	1
1:A:2:GLN:HG3	1:A:51:VAL:HG13	0.41	1.91	2	1
1:A:3:ALA:HA	1:A:52:ASN:O	0.41	2.16	24	2
1:A:118:ASP:OD2	1:A:160:LEU:HB3	0.41	2.16	15	1
1:A:102:ARG:HD3	1:A:103:HIS:N	0.40	2.31	8	1
1:A:90:PHE:O	1:A:93:VAL:HG22	0.40	2.16	13	1
1:A:99:PRO:HA	1:A:102:ARG:HE	0.40	1.76	15	1
1:A:153:LYS:HE2	1:A:155:LEU:HB3	0.40	1.93	25	1
1:A:132:LYS:HD3	1:A:132:LYS:N	0.40	2.31	7	1
1:A:171:GLU:OE1	1:A:172:ALA:N	0.40	2.55	11	1
2:B:135:LEU:C	2:B:135:LEU:HD13	0.40	2.37	12	1
1:A:155:LEU:HD13	1:A:167:THR:HG22	0.40	1.92	24	1
1:A:117:LEU:CD1	1:A:163:ARG:HD2	0.40	2.47	2	1
1:A:153:LYS:HZ1	1:A:168:VAL:HA	0.40	1.76	9	1
1:A:80:ILE:HD12	1:A:80:ILE:N	0.40	2.31	21	1
1:A:68:ARG:NE	1:A:68:ARG:HA	0.40	2.30	4	1
1:A:84:LEU:O	1:A:137:ILE:HG12	0.40	2.17	14	1
1:A:17:THR:O	1:A:20:LEU:HG	0.40	2.16	24	1
1:A:16:LYS:HD3	1:A:16:LYS:N	0.40	2.32	6	1
2:B:162:LEU:N	2:B:162:LEU:HD22	0.40	2.31	11	1
1:A:61:LEU:HD12	1:A:63:ASP:HB3	0.40	1.91	23	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	175/192 (91%)	153±3 (87±1%)	16±2 (9±1%)	6±2 (3±1%)	6	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	58/81 (72%)	57±1 (99±1%)	0±1 (1±1%)	0±0 (0±0%)	54	85
All	All	5825/6825 (85%)	5262 (90%)	412 (7%)	151 (3%)	8	44

All 24 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	181	PRO	19
1	A	68	ARG	16
1	A	183	LYS	15
1	A	179	PRO	14
1	A	178	CYS	12
1	A	182	VAL	11
1	A	2	GLN	10
1	A	65	ASP	9
1	A	14	VAL	8
1	A	35	THR	6
1	A	29	PRO	5
1	A	12	GLY	5
1	A	184	LYS	4
1	A	36	VAL	2
1	A	163	ARG	2
1	A	67	LEU	2
1	A	69	PRO	2
1	A	75	THR	2
1	A	59	ALA	2
1	A	105	CYS	1
2	B	159	ASP	1
2	B	153	SER	1
1	A	164	GLY	1
1	A	72	TYR	1

6.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	153/168 (91%)	132±2 (86±2%)	21±2 (14±2%)	6	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	51/68 (75%)	49±1 (96±2%)	2±1 (4±2%)	37	85
All	All	5100/5900 (86%)	4519 (89%)	581 (11%)	9	52

All 79 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	123	LYS	25
1	A	126	ILE	25
1	A	132	LYS	25
1	A	152	VAL	25
1	A	177	LEU	25
1	A	61	LEU	24
1	A	163	ARG	24
1	A	67	LEU	23
1	A	155	LEU	23
1	A	117	LEU	21
1	A	154	TYR	21
1	A	92	ASN	19
1	A	143	LEU	18
1	A	90	PHE	18
1	A	85	VAL	17
1	A	102	ARG	15
1	A	91	GLU	12
2	B	164	LEU	11
1	A	16	LYS	10
1	A	170	ASP	10
1	A	44	VAL	9
1	A	96	LYS	9
1	A	53	LEU	9
1	A	176	VAL	9
1	A	94	ARG	9
1	A	162	GLN	9
2	B	178	ASP	9
1	A	119	LEU	8
1	A	153	LYS	7
2	B	147	ASN	6
1	A	40	TYR	6
1	A	47	ASP	6
1	A	45	MET	5
1	A	148	GLU	5
1	A	51	VAL	5

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Mol	Chain	Res	Type	Models (Total)
1	A	133	LYS	5
2	B	134	GLN	4
1	A	120	ARG	4
2	B	160	ARG	3
1	A	68	ARG	3
1	A	161	THR	3
1	A	62	GLU	3
1	A	70	LEU	3
1	A	103	HIS	3
2	B	185	ARG	2
1	A	174	ARG	2
1	A	77	VAL	2
2	B	161	LYS	2
1	A	66	ARG	2
1	A	128	LYS	2
1	A	14	VAL	2
1	A	55	LEU	2
1	A	118	ASP	2
1	A	74	GLN	2
1	A	36	VAL	2
1	A	78	PHE	2
2	B	141	VAL	2
1	A	156	GLU	1
2	B	168	GLN	1
2	B	143	GLN	1
1	A	11	ASP	1
1	A	19	LEU	1
1	A	52	ASN	1
1	A	86	SER	1
2	B	127	ARG	1
2	B	140	LYS	1
2	B	184	LEU	1
1	A	171	GLU	1
1	A	141	GLN	1
1	A	24	THR	1
1	A	49	LYS	1
2	B	162	LEU	1
1	A	56	TRP	1
2	B	171	GLN	1
1	A	8	VAL	1
1	A	166	LYS	1
2	B	163	LEU	1

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Mol	Chain	Res	Type	Models (Total)
1	A	122	ASP	1
1	A	184	LYS	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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
4	GCP	A	193	3	26,34,34	2.37±0.01	8±0 (29±1%)

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
4	GCP	A	193	3	31,54,54	1.92±0.01	6±0 (19±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
4	GCP	A	193	3	-	0±0,18,38,38	0±0,3,3,3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
4	A	193	GCP	C4-N9	7.48	1.37	1.47	4	25
4	A	193	GCP	C5-C6	6.16	1.42	1.52	14	25
4	A	193	GCP	C6-N1	4.14	1.40	1.33	4	25
4	A	193	GCP	PB-O2B	3.29	1.48	1.56	10	25
4	A	193	GCP	C5-C4	2.42	1.38	1.53	20	25
4	A	193	GCP	C8-N9	2.34	1.37	1.45	6	25
4	A	193	GCP	PG-O2G	2.19	1.59	1.54	23	16
4	A	193	GCP	PG-O3G	2.16	1.59	1.54	13	25

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

| Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	193	GCP	C4-C5-N7	6.36	110.90	102.46	6	25
4	A	193	GCP	C5-C6-N1	5.12	111.87	118.19	11	25
4	A	193	GCP	O6-C6-C5	4.20	128.43	119.86	20	25
4	A	193	GCP	PA-O3A-PB	4.19	119.29	132.56	4	25
4	A	193	GCP	O2B-PB-O1B	2.72	119.14	110.07	12	25
4	A	193	GCP	O6-C6-N1	2.27	119.64	122.69	15	25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand GCP A 193

Bond lengths   Bond angles   Torsions   Rings
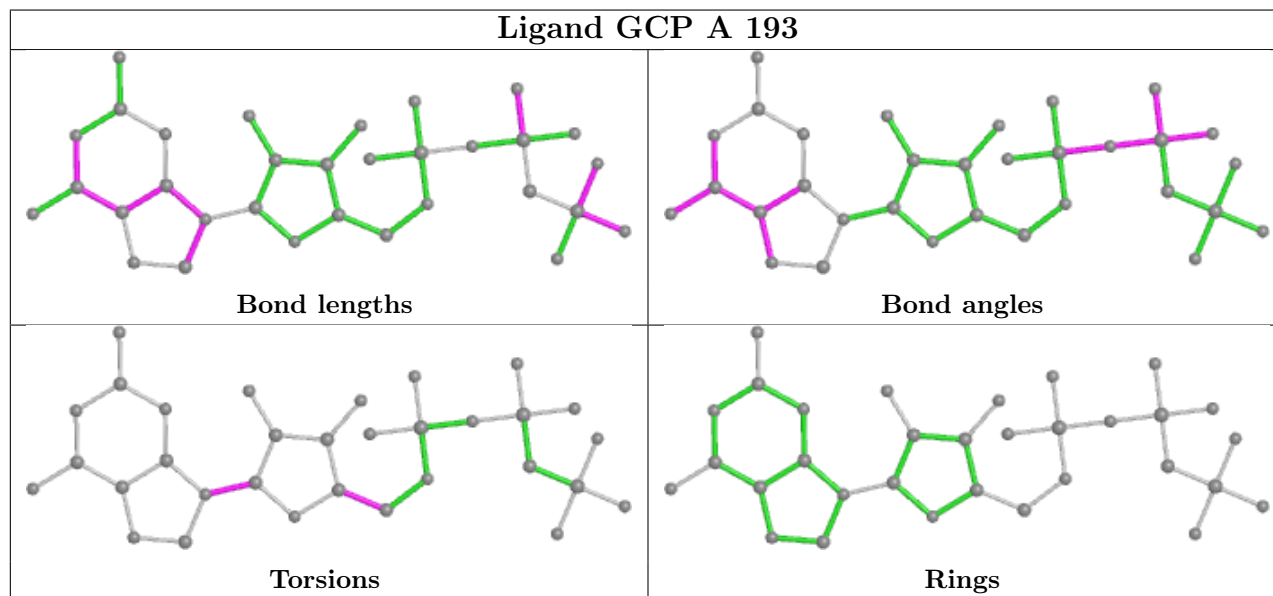
6.7 Other polymers ⓘ

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation (i)

No chemical shift data were provided