WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2022 – 08:25 PM EST

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:

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		17
Ramachandran outliers		1.0%
Sidechain outliers		20.6%

Worse   *Better*

■ Percentile relative to all structures
▯ Percentile relative to all NMR structures
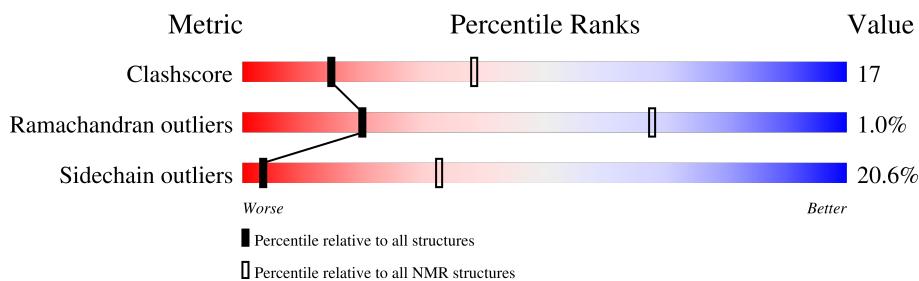
Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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	89	57% 28% • 12%
2	B	8	25% 38% 38%

WORLDWIDE wwPDB PROTEIN DATA BANK
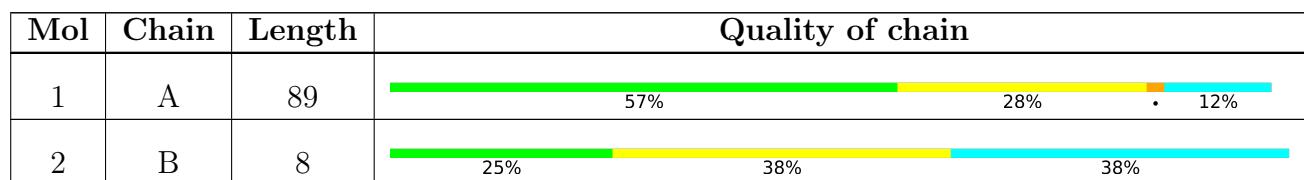
2   Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 11 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:7-A:84, B:93-B:97 (83)	0.38	11

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 2 clusters and 1 single-model cluster was found.

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1461 atoms, of which 741 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Rho guanine nucleotide exchange factor 12.

Mol	Chain	Residues	Atoms						Trace
1	A	89	Total	C	H	N	O	S	0
			1330	406	674	121	126	3	

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP Q9NZN5
A	2	SER	-	expression tag	UNP Q9NZN5
A	3	HIS	-	expression tag	UNP Q9NZN5
A	4	MET	-	expression tag	UNP Q9NZN5

- Molecule 2 is a protein called C-terminal peptide of Plexin-B1.

| Mol	Chain	Residues	Atoms					Trace
2	B	8	Total	C	H	N	O	0
			131	39	67	10	15	

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: Rho guanine nucleotide exchange factor 12

Chain A:

• Molecule 2: C-terminal peptide of Plexin-B1

Chain B:
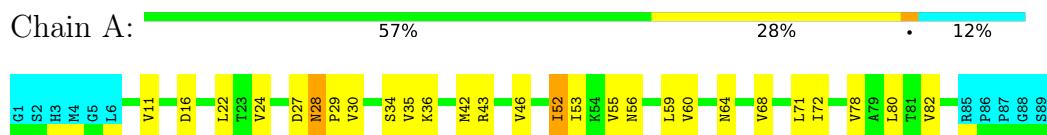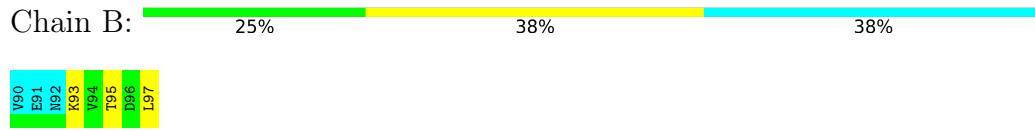
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Rho guanine nucleotide exchange factor 12

Chain A:

• Molecule 2: C-terminal peptide of Plexin-B1

Chain B:

`V90 E91 N92 K93 V94 T95 D96 L97`
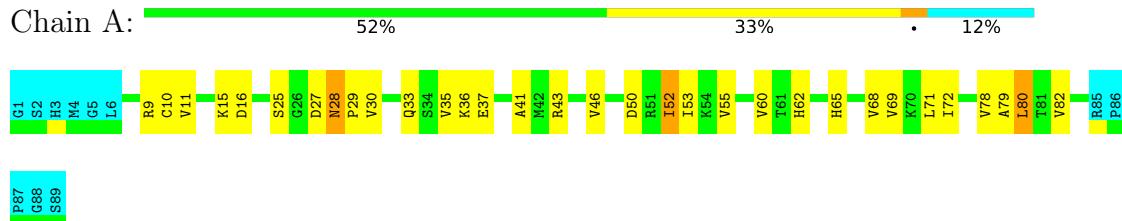
4.2.2   Score per residue for model 2

• Molecule 1: Rho guanine nucleotide exchange factor 12

Chain A:

`57%`   `28%`   `•`   `12%`

`G1 S2 H3 M4 G5 L6 V7 Q8 R9 C10 V11 D17 D27 N28 P29 V30 F31 S34 V35 K36 E37 D38 A41 M42 V46 I52 I53 K54 V55 V60 N64 V68 L71 I72 S76 Y77 V78 A79 L80 R85 P86 P87 G88 S89`

• Molecule 2: C-terminal peptide of Plexin-B1

Chain B:

`38%`   `25%`   `38%`

`V90 E91 N92 K93 V94 T95 D96 L97`
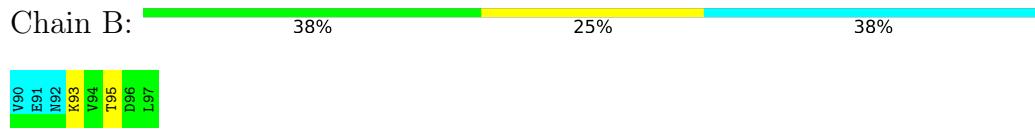
4.2.3   Score per residue for model 3

• Molecule 1: Rho guanine nucleotide exchange factor 12

Chain A:

`48%`   `31%`   `8%`   `12%`

`G1 S2 H3 M4 G5 L6 V11 I12 I13 Q14 K15 D16 L22 T23 V24 D27 N28 P29 V30 V35 D38 R43 V46 Q47 D50 R51 I52 I53 K54 V55 N56 L59 V60 T61 H62 S63 N64 V68 L71 I72 K73 S74 V78 A79 L80 T81 V82 Q83`

`G84 R85 P86 P87 G88 S89`

• Molecule 2: C-terminal peptide of Plexin-B1

Chain B:

`50%`   `12%`   `38%`

`V90 E91 N92 L97`
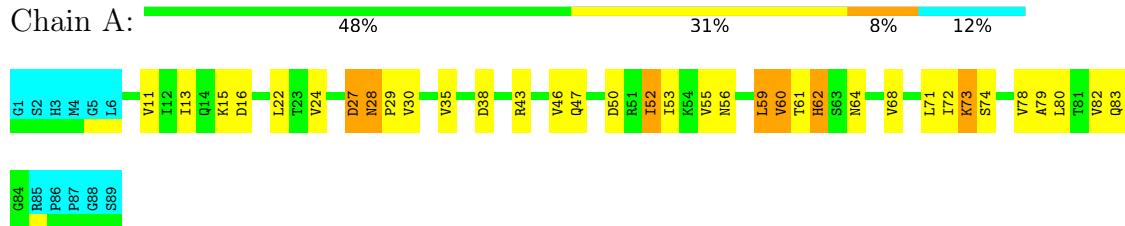
4.2.4   Score per residue for model 4

• Molecule 1: Rho guanine nucleotide exchange factor 12

Chain A:

`55%`   `31%`   `•`   `12%`

`G1 S2 H3 M4 G5 L6 K15 D16 V24 N28 P29 V30 Q33 S34 V35 D38 M42 V46 Q49 D50 R51 I52 I53 K54 V55 T58 L59 V60 N64 V68 V69 K70 L71 I72 K73 V78 A79 L80 T81 V82 R85 P86 P87 G88 S89`

• Molecule 2: C-terminal peptide of Plexin-B1

Chain B: 12%   50%   38%

V90 E91 N92 K93 V94 T95 D96 L97
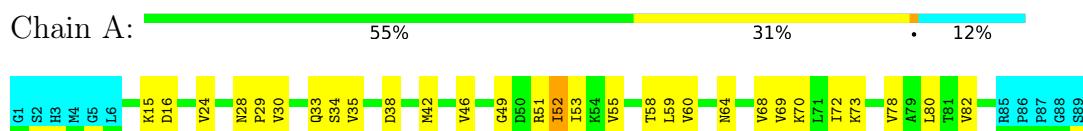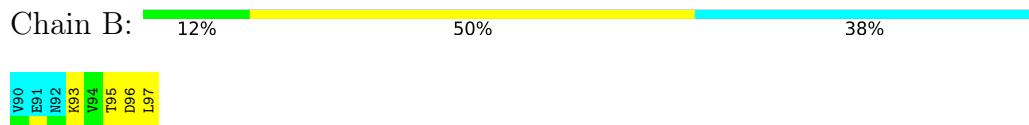
4.2.5 Score per residue for model 5

• Molecule 1: Rho guanine nucleotide exchange factor 12

Chain A: 54%   30%   •   12%

G1 S2 H3 M4 G5 L6 V11 I12 I13 L22 T23 V24 D27 N28 P29 V30 F31 V32 Q33 S34 V35 K36 A41 V46 D50 R51 I52 V55 L59 V60 T61 N64 H65 L66 E67 V68 L71 I72 K73 S74 G75 S76 A79 L80 T81 V82 R85 P86

P87 G88 S89

• Molecule 2: C-terminal peptide of Plexin-B1

Chain B: 38%   12%   12%   38%

V90 E91 N92 K93 L97
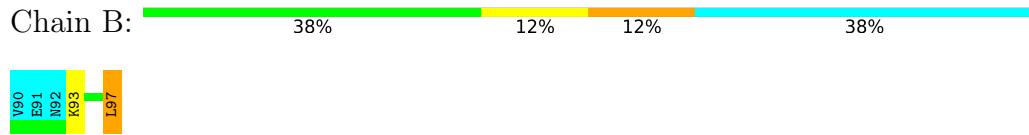
4.2.6 Score per residue for model 6

• Molecule 1: Rho guanine nucleotide exchange factor 12

Chain A: 56%   28%   •   12%

G1 S2 H3 M4 G5 L6 R9 I13 Q14 K15 D16 F20 G21 L22 D27 N28 P29 V30 Q33 S34 V35 R43 D50 R51 I52 I53 K54 V55 N56 L59 V60 T61 L66 K70 L71 S76 Y77 V78 A79 L80 T81 V82 Q83 G84 R85 P86 P87 G88 S89

• Molecule 2: C-terminal peptide of Plexin-B1

Chain B: 38%   25%   38%

V90 E91 N92 K93 L97
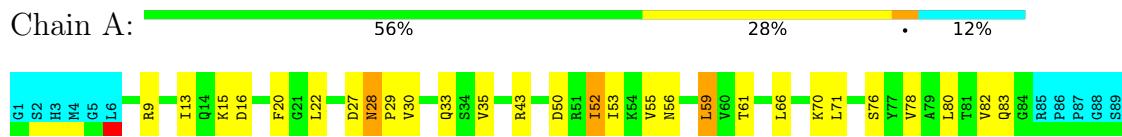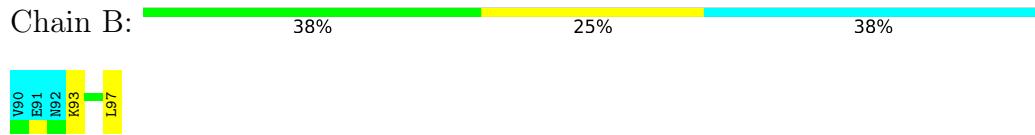
4.2.7 Score per residue for model 7

• Molecule 1: Rho guanine nucleotide exchange factor 12

Chain A: 56%   25%   7%   12%

G1 S2 H3 M4 G5 L6 V7 Q8 I13 D16 L22 T23 V24 D27 N28 P29 V30 S34 V35 A41 M42 R43 I52 V55 N56 L59 V60 T61 H62 K70 L71 V78 A79 L80 T81 V82 Q83 G84 R85 P86 P87 G88 S89

• Molecule 2: C-terminal peptide of Plexin-B1

Chain B: 50%   12%   38%

V90 E91 N92 D96 L97

4.2.8 Score per residue for model 8

• Molecule 1: Rho guanine nucleotide exchange factor 12

Chain A: 57%   29%   •   12%

G1 S2 H3 M4 G5 L6 V7 Q8 D16 V24 S25 G26 D27 N28 P29 V30 S34 V35 K36 A41 M42 R43 T48 I52 I53 K54 V60 T61 H65 V68 V69 K73 S76 Y77 V78 A79 L80 T81 V82 R85 P86 P87 G88 S89

• Molecule 2: C-terminal peptide of Plexin-B1

Chain B: 25%   38%   38%

V90 E91 N92 K93 V94 T95 D96 L97
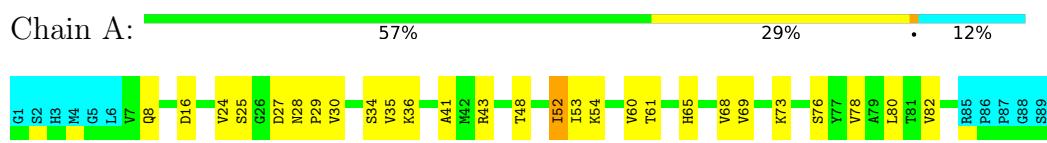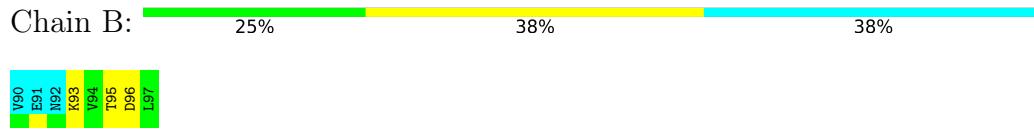
4.2.9 Score per residue for model 9

• Molecule 1: Rho guanine nucleotide exchange factor 12

Chain A: 49%   31%   7%   12%

G1 S2 H3 M4 G5 L6 Q14 K15 D16 L22 T23 V24 S25 G26 D27 N28 P29 V30 S34 V35 K36 M42 T48 Q49 D50 R51 I52 I53 K54 V55 N56 G57 T58 L59 V60 T61 H62 S63 N64 E67 V68 V78 A79 L80 T81 V82 Q83 G84 R85 P86 P87 G88 S89

• Molecule 2: C-terminal peptide of Plexin-B1

Chain B: 50%   12%   38%

V90 E91 N92 L97
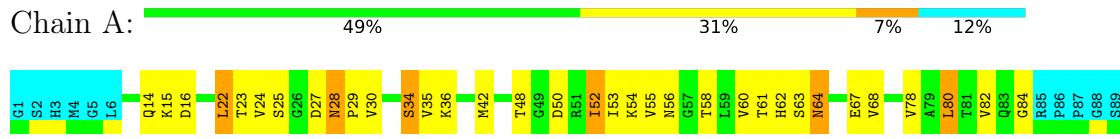
4.2.10 Score per residue for model 10

• Molecule 1: Rho guanine nucleotide exchange factor 12

Chain A: 60%   24%   •   12%

G1 S2 H3 M4 G5 L6 V7 Q8 K15 D16 L22 T23 V24 D27 N28 P29 V30 F31 V32 Q33 K36 T48 G49 D50 R51 I52 I53 K54 V55 T58 L59 V60 V69 K70 L71 I72 V78 V82 R85 P86 P87 G88 S89

• Molecule 2: C-terminal peptide of Plexin-B1

Chain B: 25% 25% 12% 38%

V90 E91 N92 K93 V94 T95 D96 L97
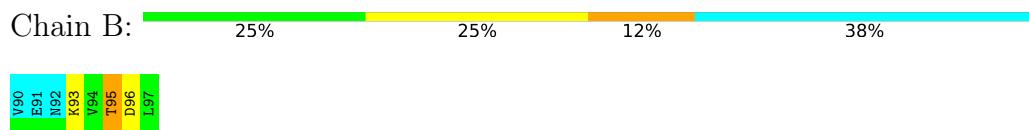
4.2.11 Score per residue for model 11 (medoid)

• Molecule 1: Rho guanine nucleotide exchange factor 12

Chain A: 53% 31% • 12%

G1 S2 H3 M4 G5 L6 V11 I12 I13 D16 T23 N28 P29 V30 Q33 S34 V35 K36 A41 M42 R43 A44 T48 R51 I52 I53 K54 V55 N56 G57 T58 L59 V60 N64 H65 L66 E67 V68 V69 K70 L71 I72 S76 L80 T81 V82 R85 P86

P87 G88 S89

• Molecule 2: C-terminal peptide of Plexin-B1

Chain B: 50% 12% 38%

V90 E91 N92 D96 L97
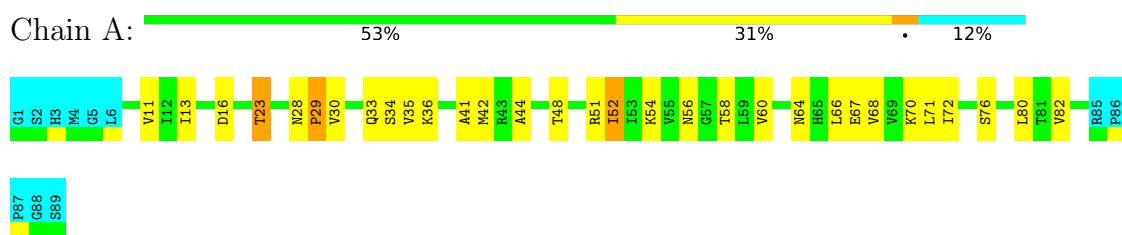
4.2.12 Score per residue for model 12

• Molecule 1: Rho guanine nucleotide exchange factor 12

Chain A: 49% 36% • 12%

G1 S2 H3 M4 G5 L6 V7 Q8 R9 C10 V11 I12 I13 Q14 K15 D16 D17 N18 L22 T23 V24 D27 N28 P29 V30 F31 V32 V35 K36 E37 D38 R43 V46 D50 R51 I52 I53 K54 V55 N56 L59 V60 T61 K70 S74 G75 S76 Y77 V78 A79 L80

T81 V82 Q83 G84 R85 P86 P87 G88 S89

• Molecule 2: C-terminal peptide of Plexin-B1

Chain B: 38% 25% 38%

V90 E91 N92 T95 D96 L97
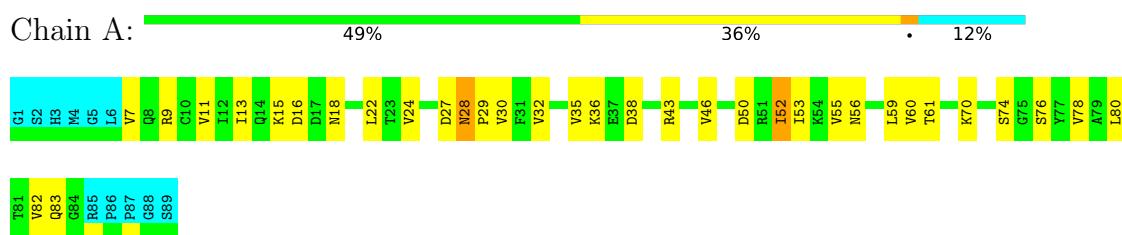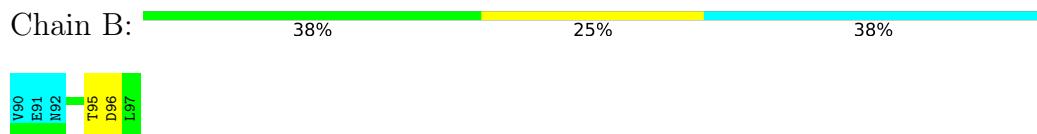
4.2.13　Score per residue for model 13

• Molecule 1: Rho guanine nucleotide exchange factor 12

Chain A:

• Molecule 2: C-terminal peptide of Plexin-B1

Chain B:
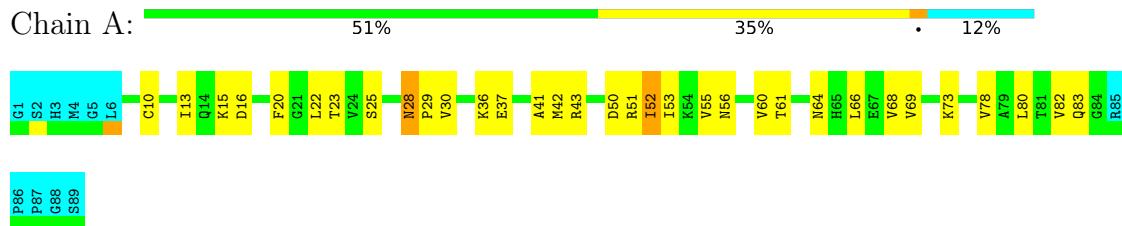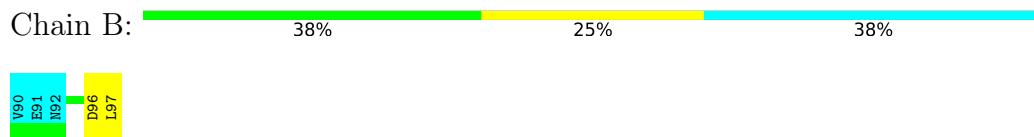
4.2.14　Score per residue for model 14

• Molecule 1: Rho guanine nucleotide exchange factor 12

Chain A:

• Molecule 2: C-terminal peptide of Plexin-B1

Chain B:
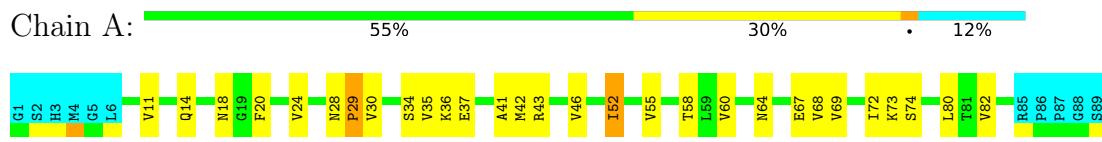
#### 4.2.15　Score per residue for model 15

• Molecule 1: Rho guanine nucleotide exchange factor 12

Chain A:

• Molecule 2: C-terminal peptide of Plexin-B1

Chain B: 25%   25%   12%   38%

V90 E91 N92 K93 V94 T95 D96 L97
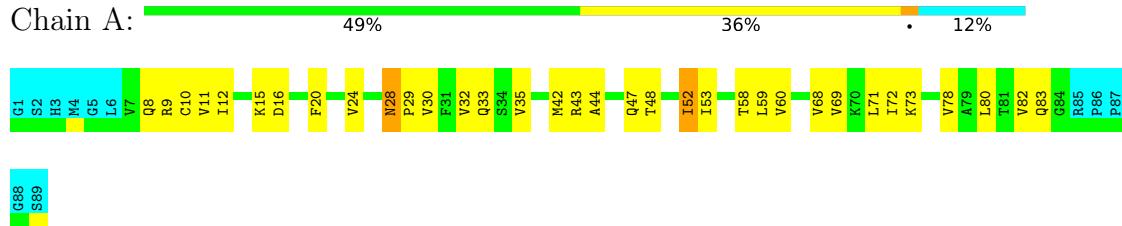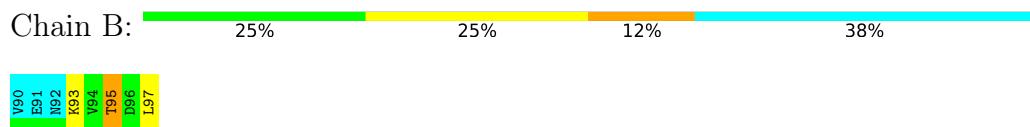
4.2.16 Score per residue for model 16

• Molecule 1: Rho guanine nucleotide exchange factor 12

Chain A: 54%   31%   •   12%

G1 S2 H3 M4 G5 L6 V11 I12 I13 D16 F20 G21 L22 D27 N28 P29 V30 V35 K36 E37 M42 R43 V46 I52 I53 K54 V55 N56 L59 V60 N64 H65 L66 E67 V68 V69 K70 L71 I72 S76 Y77 V78 A79 L80 T81 V82 R85 P86

P87 G88 S89

• Molecule 2: C-terminal peptide of Plexin-B1

Chain B: 25%   25%   12%   38%

V90 E91 N92 K93 V94 T95 D96 L97
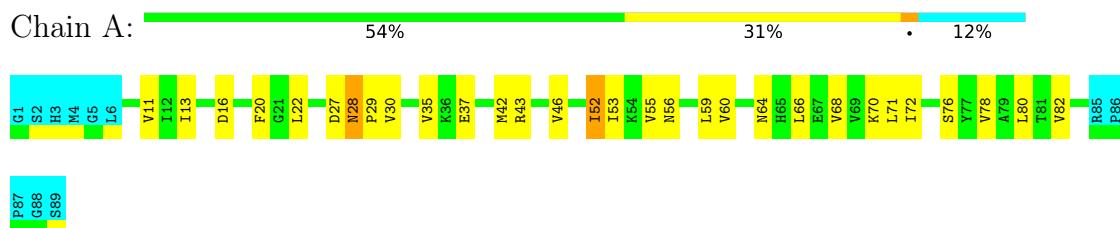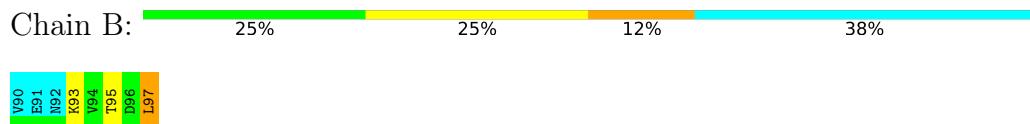
4.2.17 Score per residue for model 17

• Molecule 1: Rho guanine nucleotide exchange factor 12

Chain A: 54%   31%   •   12%

G1 S2 H3 M4 G5 L6 I12 I13 Q14 K15 D16 L22 T23 V24 S25 N28 P29 V30 F31 V32 Q33 S34 V35 K36 E37 A40 R43 A44 D50 R51 I52 I53 N56 V60 N64 H65 L66 E67 V68 V69 K70 V78 A79 L80 R85 P86 P87 G88 S89

• Molecule 2: C-terminal peptide of Plexin-B1

Chain B: 12%   25%   25%   38%

V90 E91 N92 K93 V94 T95 D96 L97
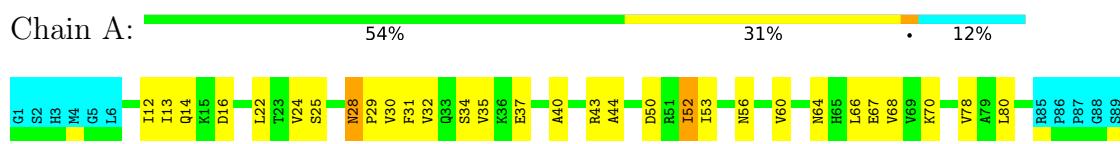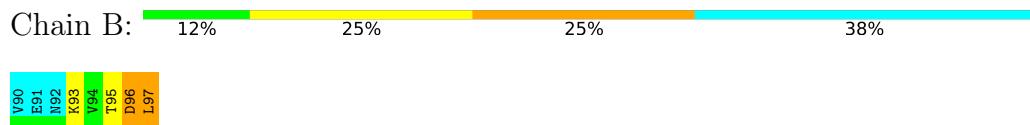
4.2.18 Score per residue for model 18

• Molecule 1: Rho guanine nucleotide exchange factor 12

Chain A: 56%   28%   •   12%

G1 S2 H3 M4 G5 L6 V11 I12 I13 D17 N18 T23 G26 D27 N28 P29 V30 Q33 E37 D38 M42 V46 R51 I52 V55 L59 V60 T61 H62 S63 N64 E67 V68 V69 K70 L71 S76 L80 T81 V82 R85 P86 P87 G88 S89

• Molecule 2: C-terminal peptide of Plexin-B1

Chain B:

38% 25% 38%

V90 E91 N92 K93 D96 L97
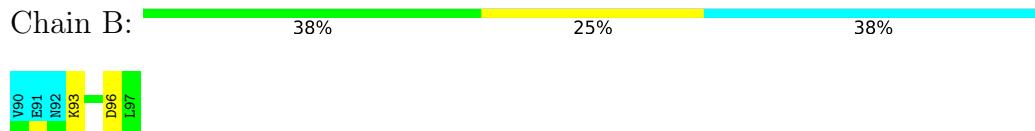
4.2.19 Score per residue for model 19

• Molecule 1: Rho guanine nucleotide exchange factor 12

Chain A:

54% 31% • 12%

G1 S2 H3 M4 G5 L6 V11 Q14 L22 N28 P29 V30 S34 V35 D38 M42 R43 V46 Q47 T48 G49 D50 R51 I52 I53 K54 V55 N56 L59 V60 T61 H62 S63 N64 E67 V68 V69 K70 L71 I72 S76 Y77 V78 A79 L80 T81 V82 R85

P86 P87 G88 S89

• Molecule 2: C-terminal peptide of Plexin-B1

Chain B:

38% 25% 38%

V90 E91 N92 K93 L97
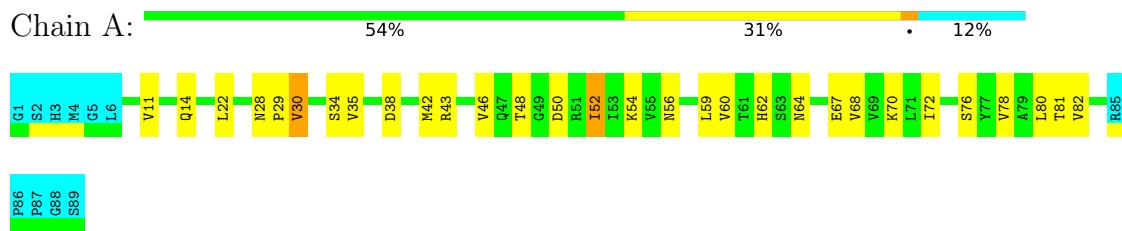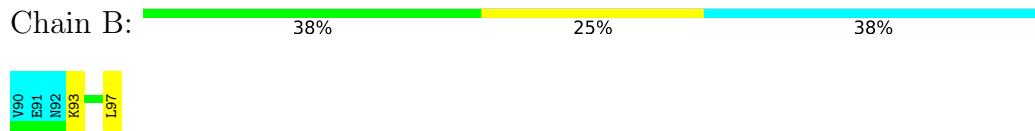
4.2.20 Score per residue for model 20

• Molecule 1: Rho guanine nucleotide exchange factor 12

Chain A:

56% 29% • 12%

G1 S2 H3 M4 G5 L6 C10 V11 D16 D27 N28 P29 V30 S34 V35 K36 M42 R43 V46 Q47 T48 R51 I52 V55 N56 L59 S63 V68 V69 K70 L71 I72 S76 Y77 V78 A79 L80 T81 V82 R85 P86 P87 G88 S89

• Molecule 2: C-terminal peptide of Plexin-B1

Chain B:

50% 12% 38%

V90 E91 N92 L97
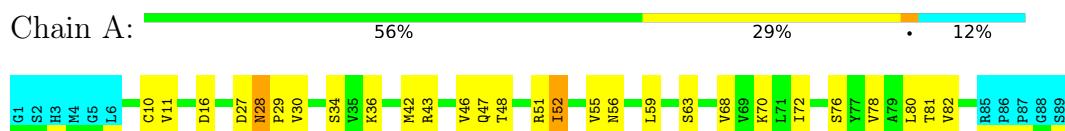
5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: *Distance geometry, simulated annealing, molecular dynamics, torsion angle dynamics.*

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy.*

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

Software name	Classification	Version
CNS	structure solution	Cns 1.1
Csi 1.0	refinement	Csi 1.0

No chemical shift data was provided.

6 Model quality ⓘ

6.1 Standard geometry ⓘ

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	580	598	596	21±3
2	B	40	44	44	1±1
All	All	12400	12840	12800	429

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 17.

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:55:VAL:HG12	1:A:80:LEU:HD23	0.99	1.35	12	4
1:A:30:VAL:HB	1:A:52:ILE:HG23	0.94	1.40	4	16
1:A:22:LEU:HD21	1:A:24:VAL:HG13	0.91	1.42	10	1
1:A:13:ILE:HD12	1:A:80:LEU:HD13	0.77	1.56	5	2
1:A:52:ILE:HD11	1:A:80:LEU:HD23	0.76	1.57	17	1
1:A:55:VAL:O	1:A:58:THR:HG22	0.75	1.82	10	1
1:A:78:VAL:HG23	1:A:80:LEU:HD11	0.74	1.58	12	5
1:A:11:VAL:HG21	1:A:46:VAL:HG22	0.73	1.60	20	5
1:A:11:VAL:HG11	1:A:46:VAL:HG22	0.71	1.60	3	5
1:A:28:ASN:CB	1:A:29:PRO:CD	0.71	2.69	13	10
1:A:55:VAL:HG21	1:A:68:VAL:HG13	0.71	1.60	14	3
1:A:80:LEU:HD12	1:A:82:VAL:CG1	0.68	2.19	1	1
1:A:30:VAL:HG23	1:A:60:VAL:HG21	0.68	1.65	4	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:55:VAL:HG12	1:A:80:LEU:HG	0.67	1.66	18	5
1:A:30:VAL:CG2	1:A:60:VAL:HG21	0.66	2.20	2	3
1:A:24:VAL:HG12	1:A:32:VAL:HA	0.66	1.66	5	1
1:A:69:VAL:HG12	1:A:73:LYS:HE3	0.66	1.67	8	1
1:A:53:ILE:HD11	1:A:83:GLN:CD	0.64	2.12	3	1
1:A:59:LEU:HD12	1:A:61:THR:OG1	0.64	1.93	18	4
1:A:30:VAL:CB	1:A:52:ILE:HG23	0.63	2.22	14	16
1:A:72:ILE:HG23	1:A:78:VAL:HG21	0.63	1.69	2	4
1:A:34:SER:HA	1:A:48:THR:HG22	0.63	1.69	19	3
1:A:55:VAL:CG1	1:A:80:LEU:HD23	0.62	2.24	9	2
1:A:64:ASN:O	1:A:68:VAL:HG23	0.62	1.94	11	12
1:A:24:VAL:CG2	1:A:30:VAL:HG12	0.61	2.24	4	3
1:A:52:ILE:HD11	1:A:55:VAL:HG13	0.61	1.71	5	7
1:A:30:VAL:HG11	1:A:52:ILE:HD12	0.61	1.70	2	1
1:A:73:LYS:HE2	2:B:97:LEU:HD11	0.61	1.72	3	2
1:A:22:LEU:HB3	1:A:35:VAL:HG12	0.61	1.71	16	3
1:A:68:VAL:HG12	1:A:72:ILE:HD11	0.60	1.73	15	5
1:A:35:VAL:HG12	1:A:48:THR:HG23	0.60	1.72	15	1
1:A:28:ASN:CB	1:A:29:PRO:HD3	0.60	2.27	6	20
1:A:13:ILE:HG12	1:A:80:LEU:HD13	0.60	1.73	11	2
1:A:78:VAL:HG13	1:A:80:LEU:HD11	0.60	1.73	19	2
1:A:59:LEU:HD22	1:A:61:THR:OG1	0.60	1.97	5	1
1:A:22:LEU:HD23	1:A:41:ALA:CB	0.60	2.26	13	1
1:A:53:ILE:O	1:A:60:VAL:HG12	0.60	1.97	16	3
1:A:56:ASN:CG	1:A:78:VAL:HG23	0.60	2.18	9	2
1:A:12:ILE:O	1:A:44:ALA:HB1	0.59	1.98	15	2
1:A:55:VAL:HB	1:A:72:ILE:HD11	0.58	1.74	4	2
1:A:35:VAL:HB	1:A:41:ALA:HB1	0.58	1.75	7	7
1:A:20:PHE:CZ	1:A:72:ILE:HG22	0.58	2.33	14	2
1:A:53:ILE:O	1:A:60:VAL:HG22	0.57	1.99	15	8
1:A:35:VAL:HG11	1:A:46:VAL:HG12	0.57	1.75	4	3
1:A:55:VAL:HG12	1:A:80:LEU:CD2	0.57	2.29	9	4
1:A:23:THR:HG23	2:B:96:ASP:HB3	0.57	1.76	13	3
1:A:80:LEU:N	1:A:80:LEU:HD12	0.57	2.15	12	4
1:A:72:ILE:HG23	1:A:78:VAL:HG11	0.57	1.77	20	2
1:A:28:ASN:HB2	1:A:29:PRO:HD3	0.57	1.77	14	5
1:A:69:VAL:HG22	1:A:73:LYS:HE3	0.57	1.77	14	3
1:A:20:PHE:HB2	2:B:97:LEU:HD22	0.56	1.76	16	1
1:A:58:THR:HG21	1:A:71:LEU:HD13	0.56	1.75	11	2
1:A:23:THR:HG23	2:B:96:ASP:CB	0.56	2.31	11	1
1:A:65:HIS:O	1:A:68:VAL:HG12	0.56	2.01	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:13:ILE:HG22	1:A:20:PHE:CD1	0.56	2.36	6	1
1:A:73:LYS:HE2	2:B:97:LEU:HD21	0.55	1.79	5	1
1:A:52:ILE:HG13	1:A:80:LEU:HD23	0.55	1.77	11	1
1:A:52:ILE:CB	1:A:82:VAL:HG12	0.55	2.31	9	16
1:A:11:VAL:HG11	1:A:46:VAL:CG2	0.55	2.30	1	1
1:A:55:VAL:HG21	1:A:68:VAL:CG1	0.55	2.32	2	1
1:A:79:ALA:C	1:A:80:LEU:HD12	0.55	2.21	5	2
1:A:13:ILE:HD13	1:A:22:LEU:CD2	0.55	2.32	16	1
1:A:24:VAL:HG12	1:A:32:VAL:HG22	0.54	1.76	15	4
1:A:11:VAL:HG21	1:A:46:VAL:CG2	0.54	2.31	20	2
1:A:52:ILE:HA	1:A:82:VAL:HG12	0.54	1.79	20	12
1:A:53:ILE:HD11	1:A:83:GLN:HB2	0.54	1.79	15	2
1:A:28:ASN:HB3	1:A:29:PRO:HD3	0.54	1.80	13	7
1:A:55:VAL:CG2	1:A:68:VAL:HG13	0.53	2.33	2	1
1:A:28:ASN:HB2	1:A:29:PRO:CD	0.53	2.32	13	6
1:A:69:VAL:HG22	2:B:95:THR:HG21	0.53	1.79	1	2
1:A:33:GLN:O	1:A:48:THR:HG23	0.53	2.04	10	1
1:A:22:LEU:HD21	1:A:35:VAL:HG12	0.53	1.79	7	1
1:A:28:ASN:OD1	1:A:61:THR:HG23	0.53	2.04	13	1
1:A:52:ILE:HB	1:A:82:VAL:HG12	0.53	1.78	8	11
1:A:22:LEU:CD2	1:A:35:VAL:HG12	0.52	2.34	7	1
1:A:22:LEU:CB	1:A:35:VAL:HG12	0.51	2.35	19	5
1:A:30:VAL:HG21	1:A:60:VAL:HG11	0.51	1.83	4	1
1:A:30:VAL:HG21	1:A:60:VAL:HG21	0.51	1.82	9	1
1:A:13:ILE:CD1	1:A:80:LEU:HD13	0.51	2.35	18	1
1:A:8:GLN:OE1	1:A:53:ILE:HD12	0.51	2.06	10	1
1:A:59:LEU:HD12	1:A:61:THR:HB	0.51	1.81	3	1
1:A:13:ILE:HD12	1:A:80:LEU:HD22	0.51	1.83	17	1
1:A:24:VAL:CG1	1:A:30:VAL:CG1	0.51	2.88	9	3
1:A:52:ILE:C	1:A:52:ILE:HD13	0.50	2.27	18	15
1:A:30:VAL:HG23	1:A:52:ILE:HG23	0.50	1.83	19	1
1:A:24:VAL:CG1	1:A:30:VAL:HG12	0.50	2.36	7	3
1:A:28:ASN:O	1:A:60:VAL:HG21	0.50	2.06	15	1
1:A:69:VAL:HG23	2:B:97:LEU:HD21	0.50	1.82	4	1
1:A:24:VAL:HB	1:A:30:VAL:HG12	0.50	1.84	15	1
1:A:54:LYS:HE3	1:A:81:THR:HG21	0.50	1.84	19	1
1:A:68:VAL:HG12	1:A:72:ILE:CD1	0.49	2.37	11	3
1:A:22:LEU:HD23	1:A:41:ALA:HB1	0.49	1.83	13	1
1:A:23:THR:HG23	2:B:96:ASP:CG	0.49	2.28	7	1
1:A:20:PHE:CD1	2:B:97:LEU:HD22	0.49	2.42	14	1
1:A:35:VAL:HG11	1:A:46:VAL:CG1	0.49	2.37	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:10:CYS:SG	1:A:79:ALA:HB1	0.49	2.48	1	1
1:A:30:VAL:HB	1:A:52:ILE:CG2	0.49	2.38	15	2
1:A:22:LEU:HD12	1:A:22:LEU:O	0.48	2.08	12	2
1:A:24:VAL:HG11	1:A:30:VAL:CG1	0.48	2.38	8	3
1:A:24:VAL:HG21	1:A:30:VAL:HG12	0.48	1.85	4	1
1:A:20:PHE:CD2	2:B:97:LEU:HD22	0.48	2.44	13	1
1:A:30:VAL:CG2	1:A:52:ILE:HG23	0.48	2.38	19	1
1:A:55:VAL:HB	1:A:80:LEU:HD22	0.48	1.85	2	1
1:A:13:ILE:CD1	1:A:80:LEU:HD22	0.48	2.38	17	1
1:A:65:HIS:O	1:A:69:VAL:HG23	0.48	2.09	1	2
1:A:14:GLN:O	1:A:40:ALA:HB1	0.48	2.09	17	1
1:A:56:ASN:ND2	1:A:78:VAL:HG12	0.47	2.24	13	5
1:A:11:VAL:HG13	1:A:44:ALA:O	0.47	2.10	11	1
1:A:24:VAL:HG12	2:B:95:THR:O	0.47	2.10	14	1
1:A:13:ILE:HD13	1:A:80:LEU:HD13	0.47	1.86	18	1
1:A:69:VAL:HB	2:B:95:THR:HG21	0.47	1.87	10	1
1:A:13:ILE:HD11	1:A:46:VAL:HG21	0.46	1.87	3	1
1:A:52:ILE:CA	1:A:82:VAL:HG12	0.46	2.40	20	6
1:A:28:ASN:O	1:A:60:VAL:HG23	0.46	2.10	1	2
1:A:55:VAL:HG22	1:A:60:VAL:HG13	0.46	1.88	12	1
1:A:56:ASN:CB	1:A:78:VAL:HG23	0.46	2.41	9	1
1:A:30:VAL:CG1	1:A:52:ILE:HG23	0.45	2.41	8	2
1:A:27:ASP:O	1:A:28:ASN:C	0.45	2.54	6	3
1:A:30:VAL:HB	1:A:52:ILE:HB	0.45	1.88	17	2
1:A:48:THR:HG23	1:A:48:THR:O	0.45	2.12	8	1
1:A:80:LEU:HD12	1:A:82:VAL:HG13	0.45	1.88	1	1
1:A:78:VAL:HG23	1:A:80:LEU:CD1	0.45	2.42	13	2
1:A:24:VAL:CG1	1:A:32:VAL:HG22	0.45	2.41	15	1
1:A:55:VAL:HG23	1:A:55:VAL:O	0.45	2.12	5	4
1:A:26:GLY:O	1:A:30:VAL:HG22	0.44	2.13	18	1
1:A:73:LYS:CE	2:B:97:LEU:HD11	0.44	2.42	3	1
1:A:68:VAL:HG22	1:A:72:ILE:HD11	0.44	1.90	1	2
1:A:59:LEU:H	1:A:59:LEU:HD23	0.44	1.73	12	2
2:B:96:ASP:C	2:B:97:LEU:HD23	0.44	2.33	17	1
1:A:24:VAL:CG2	1:A:30:VAL:CG1	0.43	2.95	14	1
1:A:22:LEU:CD1	1:A:35:VAL:HG12	0.43	2.43	9	1
1:A:27:ASP:O	1:A:29:PRO:N	0.43	2.51	20	3
1:A:22:LEU:HD11	1:A:35:VAL:HG12	0.43	1.89	9	1
1:A:55:VAL:HG22	1:A:80:LEU:HD23	0.43	1.89	3	1
1:A:55:VAL:HG12	1:A:80:LEU:CG	0.43	2.42	14	1
1:A:60:VAL:O	1:A:60:VAL:HG12	0.43	2.14	19	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
2:B:96:ASP:O	2:B:97:LEU:HD22	0.43	2.13	4	1
1:A:28:ASN:HA	1:A:61:THR:HG22	0.43	1.91	9	1
1:A:60:VAL:HG12	1:A:60:VAL:O	0.43	2.14	11	1
1:A:55:VAL:CB	1:A:80:LEU:HD22	0.43	2.44	2	1
1:A:24:VAL:HG22	1:A:30:VAL:HG12	0.43	1.90	4	1
1:A:11:VAL:HG13	1:A:82:VAL:CG2	0.42	2.44	15	1
1:A:55:VAL:HG12	1:A:80:LEU:HB3	0.42	1.90	2	1
1:A:60:VAL:O	1:A:60:VAL:HG22	0.42	2.14	8	1
1:A:12:ILE:HD12	1:A:12:ILE:N	0.42	2.30	17	1
1:A:80:LEU:HD12	1:A:82:VAL:HG11	0.41	1.89	1	1
1:A:13:ILE:HG13	1:A:80:LEU:HD13	0.41	1.91	7	1
1:A:55:VAL:HG22	1:A:60:VAL:CG1	0.41	2.45	9	1
1:A:22:LEU:HD23	1:A:22:LEU:C	0.41	2.35	10	1
1:A:34:SER:HA	1:A:48:THR:HG23	0.41	1.92	20	1
1:A:30:VAL:HG23	1:A:52:ILE:O	0.41	2.16	19	1
1:A:35:VAL:HG22	1:A:48:THR:HG23	0.41	1.91	9	1
1:A:22:LEU:HD21	1:A:24:VAL:CG1	0.41	2.30	10	1
1:A:11:VAL:CG2	1:A:46:VAL:HG22	0.41	2.46	18	1
1:A:13:ILE:CG1	1:A:80:LEU:HD13	0.40	2.46	11	1
1:A:72:ILE:CG2	2:B:97:LEU:HD21	0.40	2.47	20	1
1:A:72:ILE:HG21	2:B:97:LEU:HD21	0.40	1.92	20	1
1:A:56:ASN:N	1:A:79:ALA:O	0.40	2.54	3	1
1:A:72:ILE:CG2	1:A:78:VAL:HG11	0.40	2.45	3	1
1:A:10:CYS:SG	1:A:81:THR:HG23	0.40	2.56	20	1
1:A:30:VAL:HB	1:A:52:ILE:O	0.40	2.17	7	1
1:A:82:VAL:HG12	1:A:83:GLN:N	0.40	2.31	12	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	78/89 (88%)	69±2 (89±2%)	8±2 (10±2%)	1±1 (1±1%)	18	66
2	B	4/8 (50%)	3±0 (81±11%)	1±0 (19±11%)	0±0 (0±0%)	100	100
All	All	1640/1940 (85%)	1449 (88%)	174 (11%)	17 (1%)	20	68

All 6 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	28	ASN	6
1	A	62	HIS	4
1	A	29	PRO	4
1	A	36	LYS	1
1	A	60	VAL	1
1	A	49	GLY	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	65/73 (89%)	52±2 (80±3%)	13±2 (20±3%)	4	34
2	B	5/8 (62%)	3±1 (66±24%)	2±1 (34±24%)	1	10
All	All	1400/1620 (86%)	1111 (79%)	289 (21%)	3	32

All 47 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	52	ILE	20
1	A	16	ASP	15
1	A	43	ARG	13
2	B	93	LYS	12
1	A	42	MET	12
1	A	36	LYS	11
1	A	50	ASP	10
1	A	71	LEU	10
1	A	76	SER	10
1	A	70	LYS	10
1	A	15	LYS	9
2	B	97	LEU	9
1	A	27	ASP	9
2	B	95	THR	9
1	A	59	LEU	9
1	A	34	SER	8

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Mol	Chain	Res	Type	Models (Total)
1	A	28	ASN	7
1	A	33	GLN	6
1	A	37	GLU	6
1	A	38	ASP	6
1	A	66	LEU	6
1	A	67	GLU	6
1	A	9	ARG	5
1	A	25	SER	5
1	A	51	ARG	5
1	A	62	HIS	4
1	A	80	LEU	4
1	A	8	GLN	4
1	A	74	SER	4
1	A	58	THR	4
1	A	23	THR	4
2	B	96	ASP	4
1	A	47	GLN	3
1	A	22	LEU	3
1	A	56	ASN	3
1	A	54	LYS	3
1	A	14	GLN	3
1	A	18	ASN	3
1	A	17	ASP	2
1	A	31	PHE	2
1	A	73	LYS	2
1	A	64	ASN	2
1	A	63	SER	2
1	A	10	CYS	2
1	A	83	GLN	1
1	A	61	THR	1
1	A	30	VAL	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 ⓘ

There are no ligands in this entry.

6.7 Other polymers ⓘ

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation ⓘ

No chemical shift data were provided