Full wwPDB NMR Structure Validation Report (i)

Feb 20, 2022 – 01:50 AM EST

PDB ID	:	1V27
Title	:	Solution structure of the first C2 domain of RIM2
Authors	:	Nagashima, T.; Hayashi, F.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2003-10-07

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

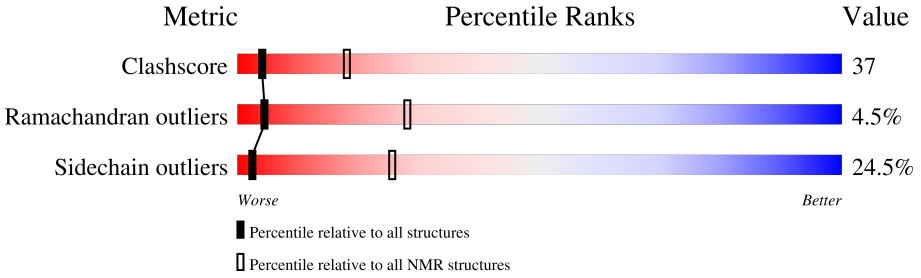
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

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	141	25% 39% 7% 29%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 2 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:8-A:33, A:42-A:51, A:60-A:99, A:109-A:132 (100)	0.22	2

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. No single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2314 atoms, of which 1153 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Regulating synaptic membrane exocytosis protein 2.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	141	2314	735	1153	208	217	1	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	cloning artifact	UNP Q9UQ26
A	2	SER	-	cloning artifact	UNP Q9UQ26
A	3	SER	-	cloning artifact	UNP Q9UQ26
A	4	GLY	-	cloning artifact	UNP Q9UQ26
A	5	SER	-	cloning artifact	UNP Q9UQ26
A	6	SER	-	cloning artifact	UNP Q9UQ26
A	7	GLY	-	cloning artifact	UNP Q9UQ26
A	136	SER	-	cloning artifact	UNP Q9UQ26
A	137	GLY	-	cloning artifact	UNP Q9UQ26
A	138	PRO	-	cloning artifact	UNP Q9UQ26
A	139	SER	-	cloning artifact	UNP Q9UQ26
A	140	SER	-	cloning artifact	UNP Q9UQ26
A	141	GLY	-	cloning artifact	UNP Q9UQ26

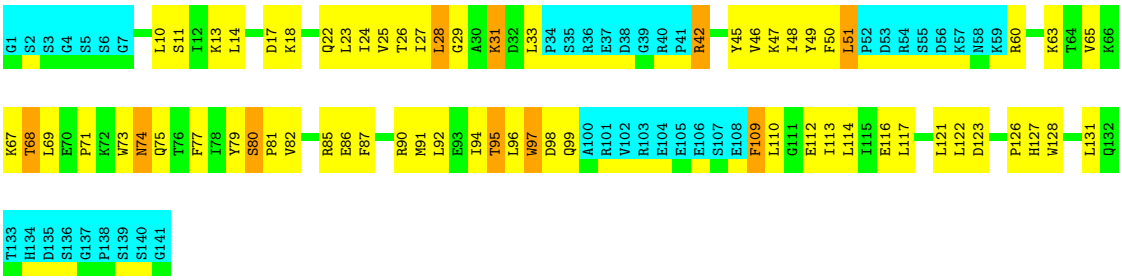
4 Residue-property plots (i)

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: Regulating synaptic membrane exocytosis protein 2

Chain A: 25% 39% 7% 29%



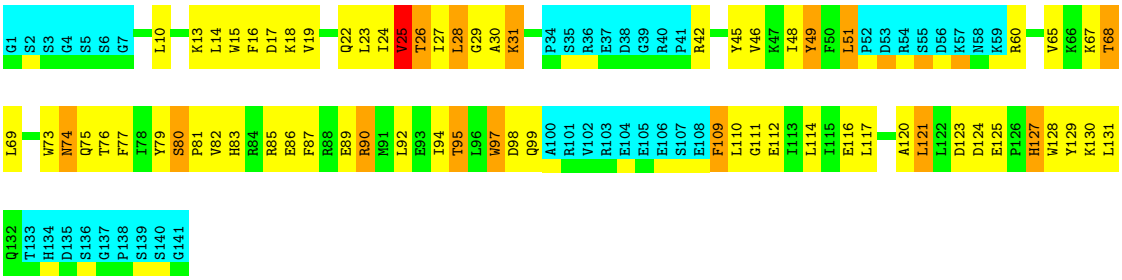
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Regulating synaptic membrane exocytosis protein 2

Chain A: 23% 37% 10% • 29%



4.2.2 Score per residue for model 2 (medoid)

• Molecule 1: Regulating synaptic membrane exocytosis protein 2

Chain A: 32% 30% 9% 29%

G1 S2 S3 G4 S5 S6 G7 L10 K13 L14 K18 V19 Q22 L23 I24 V25 T26 I27 L28 G29 A30 K31 P34 S35 R36 E37 D38 G39 R40 P41 R42 Y45 V46 K47 I48 Y49 F50 L51 P52 D53 R54 S55 D56 K57 N58 K59 R60 K63 T64 V65 K66 K67 T68

L69 E70 W73 N74 F77 I78 Y79 S80 P81 V82 H83 R84 R85 E86 F87 R90 M91 L92 E93 I94 T95 L96 W97 D98 Q99 A100 R101 V102 R103 E104 E105 E106 S107 E108 F109 L110 G111 E112 I113 L114 L117 L121 L122 D123 D124 E125 P126 H127 W128 T133 H134 D135 S136 G137

P138 S139 S140 G141

4.2.3 Score per residue for model 3

• Molecule 1: Regulating synaptic membrane exocytosis protein 2

Chain A: 25% 36% 9% • 29%

G1 S2 S3 G4 S5 S6 G7 L10 S11 I12 K13 L14 W15 F16 D17 K18 V19 Q22 L23 I24 V25 T26 I27 L28 G29 A30 K31 D32 L33 P34 S35 R36 E37 D38 G39 R40 P41 R42 Y45 V46 K47 I48 Y49 F50 L51 P52 D53 R54 S55 D56 K57 N58 K59 V65 K66 K67

T68 L69 E70 P71 K72 W73 N74 Q75 T76 F77 I78 Y79 S80 P81 V82 H83 R84 R85 E86 F87 R90 M91 L92 E93 I94 T95 L96 W97 D98 Q99 A100 R101 V102 R103 E104 E105 E106 S107 E108 F109 L110 G111 E112 I113 L114 I115 E116 L117 D123 D124 E125 P126 H127 W128 L131 Q132 T133

H134 D135 S136 G137 P138 S139 S140 G141

4.2.4 Score per residue for model 4

• Molecule 1: Regulating synaptic membrane exocytosis protein 2

Chain A: 28% 32% 9% • 29%

G1 S2 S3 G4 S5 S6 G7 L10 S11 I12 K13 L14 W15 F16 D17 K18 Q22 L23 I24 V25 T26 I27 L28 G29 A30 K31 D32 L33 P34 S35 R36 E37 D38 G39 R40 P41 R42 N43 P44 Y45 V46 K47 I48 Y49 F50 L51 P52 D53 R54 S55 D56 K57 N58 K59 R60 R61 T62

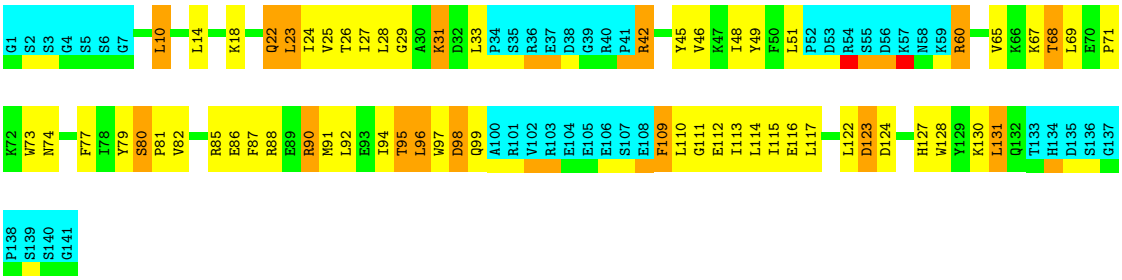
V65 T68 L69 E70 P71 K72 W73 N74 Q75 I78 Y79 S80 P81 V82 H83 R84 R85 E86 F87 R88 E89 R90 M91 L92 E93 I94 T95 L96 W97 D98 Q99 A100 R101 V102 R103 E104 E105 E106 S107 E108 E112 I113 L114 I115 E116 L117 A120 L121 L122 D123 D124 E125 W128 L131

Q132 T133 H134 D135 S136 G137 P138 S139 S140 G141

4.2.5 Score per residue for model 5

• Molecule 1: Regulating synaptic membrane exocytosis protein 2

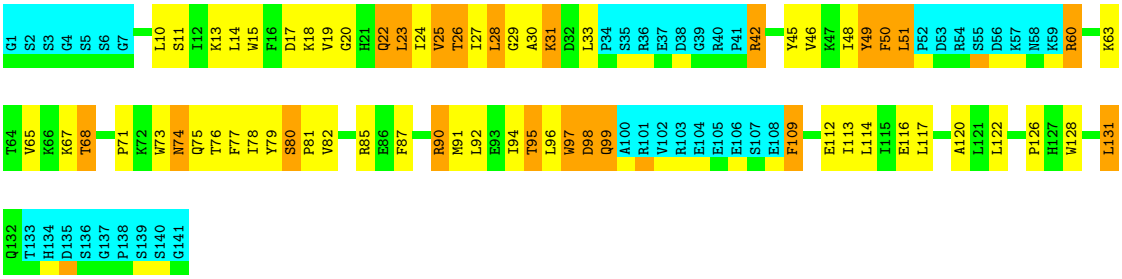
Chain A: 28% 33% 11% 29%



4.2.6 Score per residue for model 6

• Molecule 1: Regulating synaptic membrane exocytosis protein 2

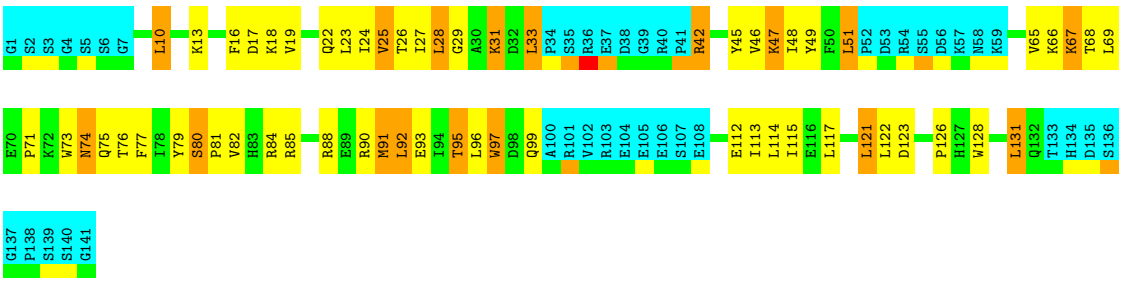
Chain A: 25% 31% 15% 29%



4.2.7 Score per residue for model 7

• Molecule 1: Regulating synaptic membrane exocytosis protein 2

Chain A: 28% 30% 12% 29%



4.2.8 Score per residue for model 8

- Molecule 1: Regulating synaptic membrane exocytosis protein 2

Chain A: 29% 31% 11% 29%

G1 S2 S3 G4 S5 S6 G7 L10 S11 I12 K13 F16 D17 K18 Q22 L23 I24 V25 T26 I27 L28 K31 D32 L33 P34 S35 R36 E37 D38 G39 R40 P41 R42 Y45 V46 K47 I48 Y49 F50 L51 P52 D53 R54 S55 D56 K57 N58 K59 K63 T64 V65 T68 L69

E70 P71 K72 W73 N74 Q75 Y79 S80 P81 V82 R85 E86 F87 R90 M91 I94 T95 L96 W97 D98 Q99 A100 R101 V102 R103 E104 E105 E106 S107 E108 F109 L110 G111 E112 I113 L114 I115 E116 L117 A120 L121 L122 D123 D124 E125 P126 H127 W128 Y129 K130 L131 Q132 T133 H134 D135

S136 G137 P138 S139 S140 G141

4.2.9 Score per residue for model 9

- Molecule 1: Regulating synaptic membrane exocytosis protein 2

Chain A: 26% 35% 9% • 29%

G1 S2 S3 G4 S5 S6 G7 L10 K13 L14 D17 K18 Q22 L23 I24 V25 T26 I27 L28 G29 A30 K31 D32 L33 P34 S35 R36 E37 D38 G39 R40 P41 R42 Y45 V46 K47 I48 Y49 F50 L51 P52 D53 R54 S55 D56 K57 N58 K59 R60 V65 K66 K67 T68 L69

E70 P71 K72 W73 N74 Q75 T76 F77 T78 Y79 S80 P81 V82 R85 E89 R90 M91 L92 E93 I94 T95 L96 W97 D98 Q99 A100 R101 V102 R103 E104 E105 E106 S107 E108 F109 L110 G111 E112 I113 L114 I115 E116 T119 A120 L121 L122 H127 W128 Y129 K130 L131 Q132 T133 H134 D135 S136

G137 P138 S139 S140 G141

4.2.10 Score per residue for model 10

- Molecule 1: Regulating synaptic membrane exocytosis protein 2

Chain A: 23% 35% 11% • 29%

G1 S2 S3 G4 S5 S6 G7 L10 S11 I12 K13 L14 D17 K18 Q22 L23 I24 V25 T26 I27 L28 G29 A30 K31 P34 S35 R36 E37 D38 G39 R40 P41 R42 Y45 V46 K47 I48 Y49 F50 L51 P52 D53 R54 S55 D56 K57 N58 K59 R60 R61 T62 K63 T64 V65 K66

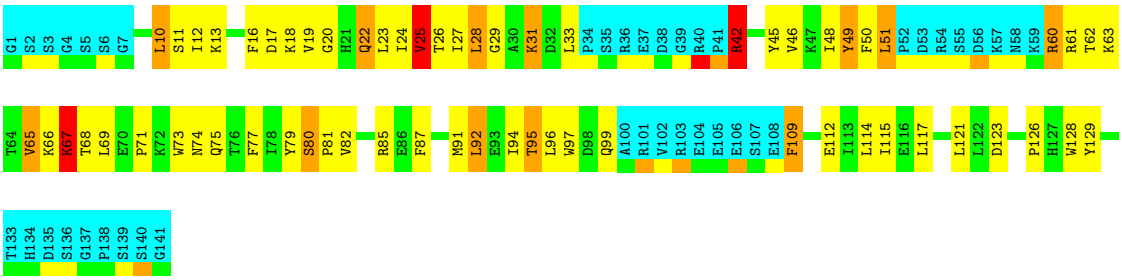
K67 T68 L69 E70 P71 K72 W73 N74 Q75 T76 F77 T78 Y79 S80 P81 V82 R85 E86 F87 R90 M91 L92 E93 I94 T95 L96 W97 D98 Q99 A100 R101 V102 R103 E104 E105 E106 S107 E108 F109 E112 I113 L114 I115 E116 L117 E118 T119 A120 L121 L122 D123 D124 E125 P126 H127 W128

L131 Q132 T133 H134 D135 S136 G137 P138 S139 S140 G141

4.2.11 Score per residue for model 11

- Molecule 1: Regulating synaptic membrane exocytosis protein 2

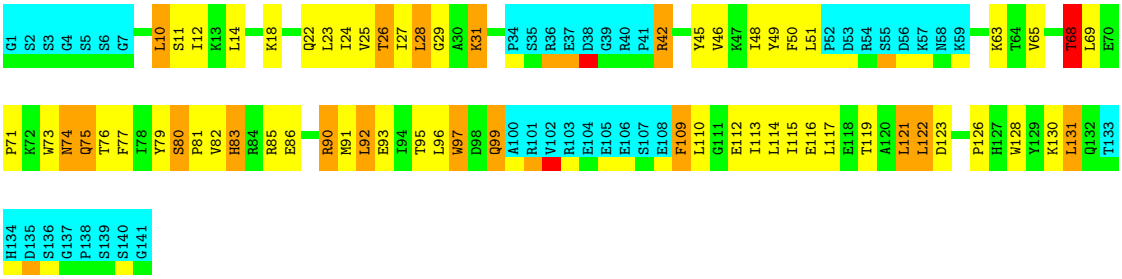
Chain A: 26% 34% 9% • 29%



4.2.12 Score per residue for model 12

- Molecule 1: Regulating synaptic membrane exocytosis protein 2

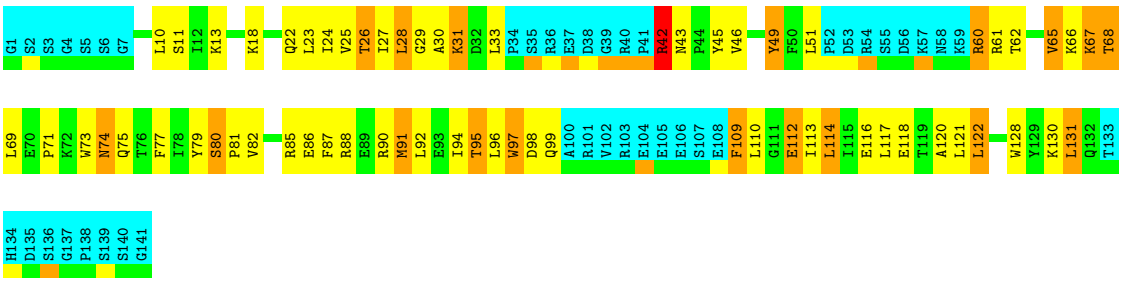
Chain A: 27% 31% 12% • 29%



4.2.13 Score per residue for model 13

- Molecule 1: Regulating synaptic membrane exocytosis protein 2

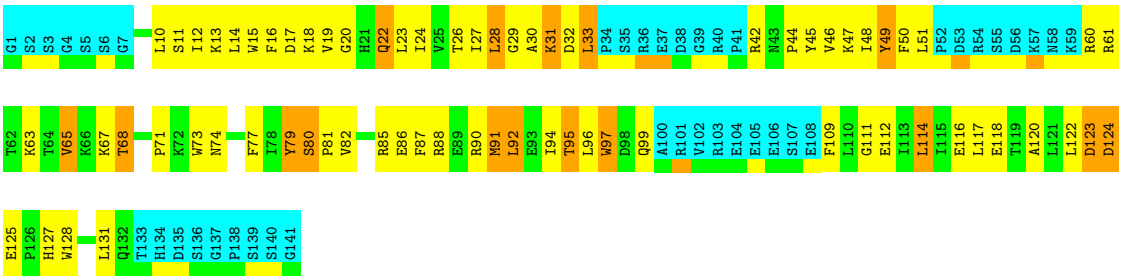
Chain A: 25% 33% 13% • 29%



4.2.14 Score per residue for model 14

• Molecule 1: Regulating synaptic membrane exocytosis protein 2

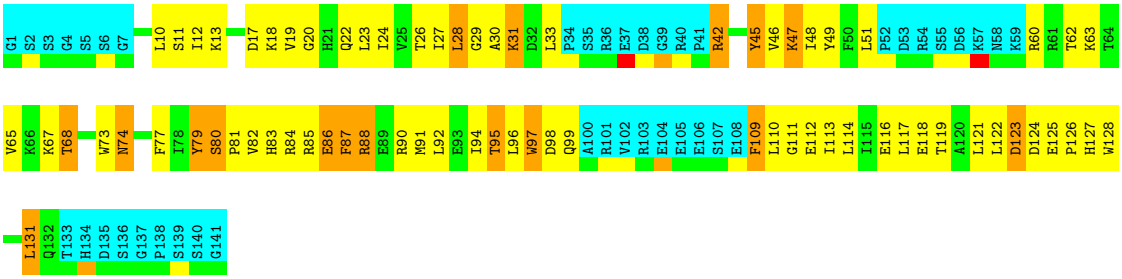
Chain A: 20% 40% 11% 29%



4.2.15 Score per residue for model 15

• Molecule 1: Regulating synaptic membrane exocytosis protein 2

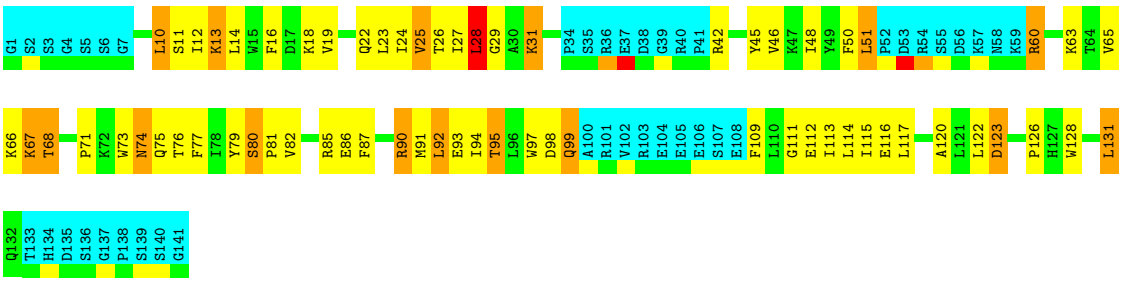
Chain A: 20% 39% 12% 29%



4.2.16 Score per residue for model 16

• Molecule 1: Regulating synaptic membrane exocytosis protein 2

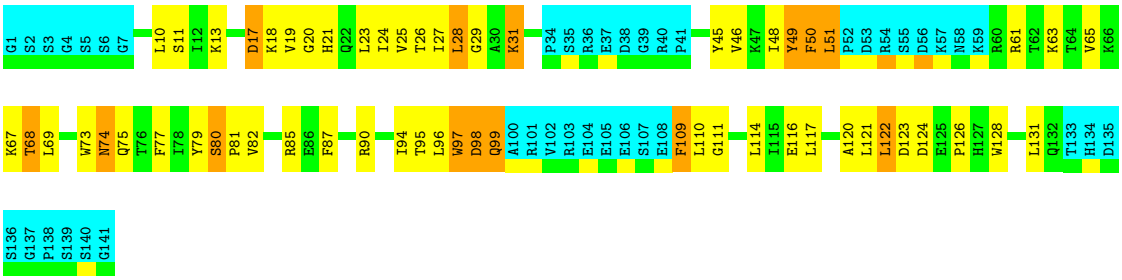
Chain A: 25% 34% 11% • 29%



4.2.17 Score per residue for model 17

• Molecule 1: Regulating synaptic membrane exocytosis protein 2

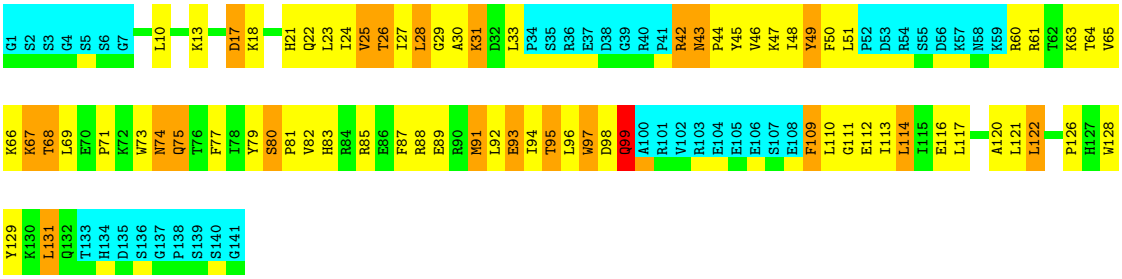
Chain A: 29% 32% 10% 29%



4.2.18 Score per residue for model 18

• Molecule 1: Regulating synaptic membrane exocytosis protein 2

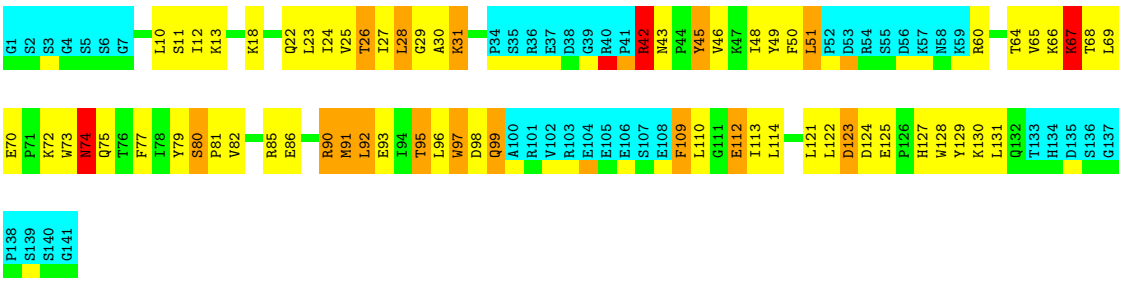
Chain A: 19% 36% 15% • 29%



4.2.19 Score per residue for model 19

• Molecule 1: Regulating synaptic membrane exocytosis protein 2

Chain A: 24% 34% 11% • 29%



4.2.20 Score per residue for model 20

- Molecule 1: Regulating synaptic membrane exocytosis protein 2

Chain A: 26% 35% 10% 29%

G1 S2 S3 G4 S5 S6 G7 L10 K13 L14 W15 F16 D17 K18 H21 Q22 L23 T24 V25 T26 I27 L28 G29 A30 K31 D32 L33 P34 S35 R36 E37 D38 G39 R40 P41 R42 Y45 V46 K47 I48 Y49 F50 L51 P52 D53 R54 S55 D56 K57 N58 K59 R60 R61 T62 K63 T64

V65 K66 K67 T68 W73 N74 F77 I78 Y79 S80 P81 V82 R85 E86 F87 R88 E89 R90 M91 L92 E93 I94 T95 L96 W97 D98 Q99 A100 R101 V102 R103 E104 E105 E106 S107 E108 F109 L110 G111 E112 I113 L114 I115 E116 L117 A120 L121 L122 D123 D124 E125 P126 H127 W128 L131

Q132 T133 H134 D135 S136 G137 P138 S139 S140 G141

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *torsion angle dynamics*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the least restraint violations, target function*.

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

Software name	Classification	Version
CYANA	structure solution	1.0.7
CYANA	refinement	1.0.7

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

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	862	886	886	64±11
All	All	17240	17720	17720	1279

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 37.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:10:LEU:HD23	1:A:12:ILE:HD11	0.99	1.34	14	3
1:A:121:LEU:HD12	1:A:121:LEU:O	0.94	1.62	10	5
1:A:27:ILE:HG22	1:A:73:TRP:CE3	0.93	1.98	9	20
1:A:121:LEU:C	1:A:122:LEU:HD13	0.89	1.88	17	3
1:A:46:VAL:HG22	1:A:96:LEU:HD13	0.87	1.45	20	14
1:A:23:LEU:C	1:A:23:LEU:HD13	0.86	1.90	6	1
1:A:33:LEU:HD22	1:A:69:LEU:O	0.86	1.69	3	5
1:A:92:LEU:HD23	1:A:117:LEU:HD21	0.83	1.49	7	5
1:A:26:THR:HG23	1:A:75:GLN:O	0.83	1.74	8	13
1:A:65:VAL:HG11	1:A:68:THR:HG21	0.81	1.53	18	16
1:A:96:LEU:HD13	1:A:97:TRP:N	0.79	1.90	5	1
1:A:23:LEU:HB2	1:A:82:VAL:HG11	0.79	1.54	11	18
1:A:27:ILE:HG13	1:A:48:ILE:HD11	0.79	1.53	18	19
1:A:122:LEU:HD22	1:A:122:LEU:N	0.77	1.94	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:64:THR:HG21	1:A:99:GLN:OE1	0.76	1.81	19	2
1:A:46:VAL:HG23	1:A:73:TRP:CH2	0.75	2.15	20	17
1:A:10:LEU:CD2	1:A:12:ILE:HD11	0.75	2.11	14	1
1:A:94:ILE:HD12	1:A:94:ILE:N	0.74	1.97	17	16
1:A:23:LEU:HD22	1:A:24:ILE:N	0.74	1.96	5	2
1:A:27:ILE:CG1	1:A:48:ILE:HD11	0.73	2.13	10	19
1:A:16:PHE:HB2	1:A:122:LEU:HD13	0.72	1.61	8	4
1:A:23:LEU:CB	1:A:82:VAL:HG11	0.72	2.15	6	2
1:A:28:LEU:HD21	1:A:126:PRO:HB3	0.72	1.60	16	2
1:A:23:LEU:CD1	1:A:25:VAL:HG23	0.72	2.15	5	1
1:A:65:VAL:HG21	1:A:71:PRO:HB3	0.71	1.62	18	10
1:A:46:VAL:CG2	1:A:73:TRP:CH2	0.71	2.74	8	20
1:A:46:VAL:HG23	1:A:73:TRP:CZ2	0.71	2.20	6	20
1:A:92:LEU:HD12	1:A:117:LEU:HD21	0.71	1.63	18	9
1:A:91:MET:CE	1:A:114:LEU:HD12	0.71	2.16	18	1
1:A:13:LYS:CE	1:A:28:LEU:HD21	0.70	2.15	18	16
1:A:10:LEU:HD13	1:A:30:ALA:HB2	0.69	1.64	6	7
1:A:131:LEU:N	1:A:131:LEU:CD2	0.69	2.55	5	6
1:A:45:TYR:O	1:A:96:LEU:HD12	0.69	1.87	19	4
1:A:26:THR:HG22	1:A:28:LEU:HD12	0.69	1.64	16	2
1:A:23:LEU:HD11	1:A:25:VAL:CG2	0.69	2.18	5	1
1:A:50:PHE:CD1	1:A:92:LEU:HD21	0.69	2.23	9	5
1:A:15:TRP:O	1:A:23:LEU:HD22	0.68	1.88	6	1
1:A:113:ILE:HD11	1:A:131:LEU:CD2	0.67	2.20	15	6
1:A:131:LEU:CD2	1:A:131:LEU:N	0.66	2.58	15	1
1:A:26:THR:HG22	1:A:28:LEU:CD1	0.66	2.21	16	2
1:A:33:LEU:HD23	1:A:42:ARG:NH2	0.65	2.07	6	1
1:A:23:LEU:CD1	1:A:25:VAL:HG12	0.65	2.21	6	1
1:A:33:LEU:HD21	1:A:96:LEU:HD21	0.65	1.66	6	2
1:A:23:LEU:C	1:A:24:ILE:HD12	0.65	2.11	6	2
1:A:14:LEU:HB2	1:A:122:LEU:HD23	0.65	1.67	10	3
1:A:17:ASP:CG	1:A:19:VAL:HG22	0.65	2.13	15	1
1:A:19:VAL:HG23	1:A:20:GLY:H	0.64	1.52	15	4
1:A:30:ALA:HB1	1:A:33:LEU:HD21	0.64	1.67	18	2
1:A:50:PHE:CD2	1:A:92:LEU:HD21	0.64	2.28	19	2
1:A:117:LEU:HD12	1:A:117:LEU:N	0.64	2.08	20	2
1:A:12:ILE:CG2	1:A:14:LEU:HD11	0.63	2.23	10	1
1:A:13:LYS:HE2	1:A:28:LEU:HD21	0.63	1.70	17	5
1:A:24:ILE:HD12	1:A:24:ILE:N	0.63	2.08	17	19
1:A:14:LEU:CB	1:A:122:LEU:HD23	0.63	2.22	10	6
1:A:46:VAL:CG2	1:A:96:LEU:HD13	0.63	2.23	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:47:LYS:CD	1:A:49:TYR:CE2	0.63	2.82	2	4
1:A:33:LEU:O	1:A:69:LEU:HD22	0.63	1.93	3	1
1:A:23:LEU:HD21	1:A:92:LEU:HD11	0.63	1.70	1	1
1:A:95:THR:HG22	1:A:112:GLU:CB	0.63	2.24	10	16
1:A:113:ILE:HD11	1:A:131:LEU:HD22	0.62	1.70	15	4
1:A:28:LEU:HD21	1:A:126:PRO:CB	0.62	2.23	16	2
1:A:45:TYR:O	1:A:45:TYR:CD1	0.62	2.52	19	4
1:A:45:TYR:O	1:A:45:TYR:CG	0.62	2.53	4	16
1:A:43:ASN:HD22	1:A:43:ASN:N	0.62	1.93	18	1
1:A:42:ARG:NH1	1:A:110:LEU:HD21	0.62	2.09	20	2
1:A:95:THR:HG22	1:A:112:GLU:HB2	0.62	1.70	12	9
1:A:23:LEU:HD11	1:A:25:VAL:HG12	0.62	1.71	6	1
1:A:65:VAL:HG21	1:A:71:PRO:CB	0.62	2.25	18	4
1:A:23:LEU:HD11	1:A:25:VAL:HG23	0.61	1.71	5	1
1:A:94:ILE:HD13	1:A:115:ILE:HD12	0.61	1.73	16	3
1:A:50:PHE:CE2	1:A:92:LEU:HD21	0.61	2.31	19	2
1:A:109:PHE:CE1	1:A:111:GLY:C	0.61	2.74	16	4
1:A:45:TYR:CD1	1:A:45:TYR:O	0.61	2.53	18	14
1:A:91:MET:CE	1:A:114:LEU:HD23	0.61	2.26	19	2
1:A:45:TYR:CD1	1:A:45:TYR:C	0.60	2.75	19	12
1:A:87:PHE:CD2	1:A:117:LEU:O	0.60	2.54	13	12
1:A:15:TRP:CE3	1:A:124:ASP:CG	0.60	2.74	14	1
1:A:122:LEU:HD13	1:A:122:LEU:N	0.60	2.11	17	2
1:A:109:PHE:CZ	1:A:111:GLY:C	0.60	2.75	14	4
1:A:11:SER:OG	1:A:128:TRP:CZ3	0.60	2.54	3	5
1:A:11:SER:OG	1:A:128:TRP:CE3	0.59	2.55	3	7
1:A:14:LEU:CD2	1:A:25:VAL:HG22	0.59	2.27	4	1
1:A:50:PHE:CE1	1:A:92:LEU:HD21	0.59	2.32	9	2
1:A:125:GLU:O	1:A:127:HIS:CD2	0.59	2.56	20	2
1:A:92:LEU:CD2	1:A:117:LEU:HD21	0.59	2.25	7	2
1:A:27:ILE:CG2	1:A:73:TRP:CE3	0.58	2.84	1	11
1:A:50:PHE:CZ	1:A:117:LEU:HD11	0.58	2.33	18	3
1:A:97:TRP:CD1	1:A:97:TRP:N	0.58	2.71	19	14
1:A:83:HIS:O	1:A:87:PHE:CE1	0.58	2.56	15	1
1:A:131:LEU:N	1:A:131:LEU:HD23	0.58	2.13	12	7
1:A:14:LEU:HB3	1:A:122:LEU:HD23	0.57	1.75	14	6
1:A:109:PHE:CE1	1:A:111:GLY:O	0.57	2.56	2	4
1:A:66:LYS:O	1:A:67:LYS:C	0.57	2.43	18	2
1:A:31:LYS:CG	1:A:128:TRP:CZ3	0.57	2.88	20	11
1:A:28:LEU:HD11	1:A:126:PRO:HB3	0.57	1.77	17	9
1:A:93:GLU:HG3	1:A:114:LEU:HD11	0.56	1.76	9	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:79:TYR:O	1:A:82:VAL:CG2	0.56	2.53	6	20
1:A:24:ILE:N	1:A:24:ILE:CD1	0.56	2.68	17	18
1:A:46:VAL:CG2	1:A:73:TRP:CZ2	0.56	2.88	6	2
1:A:50:PHE:CE1	1:A:117:LEU:HD11	0.56	2.35	6	1
1:A:11:SER:OG	1:A:128:TRP:CH2	0.56	2.56	4	7
1:A:46:VAL:CG2	1:A:73:TRP:CZ3	0.56	2.89	10	2
1:A:27:ILE:O	1:A:74:ASN:N	0.55	2.39	16	14
1:A:31:LYS:HG2	1:A:128:TRP:CZ3	0.55	2.36	15	17
1:A:67:LYS:CG	1:A:67:LYS:O	0.55	2.55	18	1
1:A:68:THR:CG2	1:A:68:THR:O	0.55	2.54	9	13
1:A:11:SER:OG	1:A:128:TRP:CD2	0.55	2.60	8	5
1:A:76:THR:O	1:A:77:PHE:CD1	0.55	2.59	1	6
1:A:96:LEU:CD1	1:A:110:LEU:HD12	0.55	2.31	5	1
1:A:46:VAL:HG21	1:A:73:TRP:CZ3	0.55	2.37	10	3
1:A:11:SER:OG	1:A:128:TRP:CZ2	0.55	2.59	4	3
1:A:94:ILE:HD12	1:A:94:ILE:H	0.55	1.61	13	13
1:A:94:ILE:H	1:A:94:ILE:HD12	0.54	1.61	2	1
1:A:122:LEU:N	1:A:122:LEU:CD2	0.54	2.66	18	1
1:A:23:LEU:C	1:A:23:LEU:CD1	0.54	2.66	6	1
1:A:17:ASP:CG	1:A:19:VAL:CG2	0.54	2.76	15	1
1:A:11:SER:OG	1:A:128:TRP:CE2	0.54	2.60	4	4
1:A:42:ARG:NH2	1:A:69:LEU:HD22	0.54	2.17	12	1
1:A:50:PHE:CE2	1:A:90:ARG:HG2	0.54	2.38	9	1
1:A:91:MET:HE1	1:A:114:LEU:HD12	0.54	1.80	18	1
1:A:49:TYR:O	1:A:51:LEU:HD13	0.54	2.02	5	3
1:A:122:LEU:HD22	1:A:122:LEU:H	0.54	1.58	18	3
1:A:47:LYS:HD2	1:A:49:TYR:CE2	0.54	2.38	2	3
1:A:22:GLN:O	1:A:24:ILE:CD1	0.54	2.56	6	2
1:A:19:VAL:HG23	1:A:20:GLY:N	0.53	2.18	11	4
1:A:20:GLY:CA	1:A:22:GLN:OE1	0.53	2.56	6	1
1:A:28:LEU:CD1	1:A:28:LEU:N	0.53	2.72	10	2
1:A:116:GLU:O	1:A:120:ALA:N	0.53	2.41	14	7
1:A:23:LEU:HD11	1:A:25:VAL:CG1	0.53	2.33	6	1
1:A:29:GLY:HA2	1:A:73:TRP:CZ3	0.53	2.38	16	18
1:A:83:HIS:N	1:A:83:HIS:CD2	0.53	2.77	12	3
1:A:16:PHE:CD1	1:A:87:PHE:CZ	0.52	2.98	11	4
1:A:10:LEU:CB	1:A:113:ILE:CD1	0.52	2.87	5	3
1:A:96:LEU:HD13	1:A:97:TRP:H	0.52	1.60	5	1
1:A:50:PHE:CZ	1:A:117:LEU:CD1	0.52	2.93	18	1
1:A:96:LEU:HD12	1:A:110:LEU:HD12	0.52	1.80	5	1
1:A:23:LEU:HD13	1:A:23:LEU:O	0.52	2.04	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:50:PHE:CE2	1:A:90:ARG:CD	0.52	2.93	3	1
1:A:46:VAL:CG1	1:A:94:ILE:CG2	0.52	2.88	16	4
1:A:121:LEU:O	1:A:121:LEU:CD1	0.52	2.51	11	4
1:A:17:ASP:OD2	1:A:19:VAL:CG2	0.52	2.58	17	2
1:A:71:PRO:HG2	1:A:73:TRP:CH2	0.52	2.40	13	13
1:A:60:ARG:HG2	1:A:77:PHE:CD1	0.52	2.39	10	4
1:A:71:PRO:HG2	1:A:73:TRP:CZ2	0.52	2.40	8	8
1:A:50:PHE:CE1	1:A:90:ARG:HB3	0.52	2.40	14	1
1:A:30:ALA:HB1	1:A:33:LEU:HD11	0.51	1.82	13	1
1:A:33:LEU:HD12	1:A:69:LEU:O	0.51	2.05	8	2
1:A:43:ASN:N	1:A:43:ASN:ND2	0.51	2.59	18	1
1:A:10:LEU:HD11	1:A:73:TRP:CZ3	0.51	2.40	15	7
1:A:121:LEU:CD1	1:A:121:LEU:O	0.51	2.59	2	5
1:A:60:ARG:CG	1:A:77:PHE:CD1	0.51	2.94	10	1
1:A:96:LEU:HG	1:A:110:LEU:HD12	0.51	1.82	15	3
1:A:94:ILE:N	1:A:94:ILE:CD1	0.51	2.69	17	6
1:A:98:ASP:OD1	1:A:98:ASP:N	0.51	2.44	10	1
1:A:29:GLY:CA	1:A:71:PRO:O	0.51	2.59	13	4
1:A:113:ILE:HG13	1:A:131:LEU:HD23	0.51	1.81	19	1
1:A:97:TRP:CE3	1:A:109:PHE:HB2	0.50	2.42	10	3
1:A:10:LEU:HD11	1:A:73:TRP:HZ3	0.50	1.66	6	5
1:A:26:THR:CG2	1:A:75:GLN:O	0.50	2.58	13	8
1:A:122:LEU:N	1:A:122:LEU:HD22	0.50	2.21	13	2
1:A:13:LYS:HB2	1:A:28:LEU:HD11	0.50	1.84	10	2
1:A:68:THR:O	1:A:68:THR:CG2	0.50	2.60	2	5
1:A:50:PHE:CZ	1:A:90:ARG:HD2	0.50	2.42	3	1
1:A:71:PRO:HB2	1:A:73:TRP:CZ2	0.49	2.41	18	6
1:A:31:LYS:HG2	1:A:128:TRP:CH2	0.49	2.42	20	17
1:A:91:MET:HA	1:A:117:LEU:CD1	0.49	2.38	8	2
1:A:13:LYS:C	1:A:14:LEU:HD13	0.49	2.28	10	1
1:A:67:LYS:O	1:A:67:LYS:HG3	0.49	2.07	18	1
1:A:27:ILE:HB	1:A:62:THR:HG21	0.49	1.85	13	1
1:A:90:ARG:HB3	1:A:117:LEU:HD12	0.49	1.84	17	1
1:A:51:LEU:HD11	1:A:93:GLU:HB2	0.49	1.83	18	1
1:A:30:ALA:HB3	1:A:71:PRO:HD2	0.49	1.82	13	3
1:A:121:LEU:HD11	1:A:129:TYR:OH	0.49	2.07	18	2
1:A:91:MET:SD	1:A:114:LEU:HD12	0.49	2.48	18	2
1:A:97:TRP:CZ3	1:A:109:PHE:HB2	0.49	2.42	5	2
1:A:33:LEU:HD23	1:A:42:ARG:HH21	0.49	1.66	6	1
1:A:17:ASP:OD1	1:A:21:HIS:N	0.48	2.46	17	1
1:A:117:LEU:N	1:A:117:LEU:CD1	0.48	2.75	20	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:10:LEU:CD1	1:A:30:ALA:HB2	0.48	2.39	14	1
1:A:92:LEU:CD1	1:A:117:LEU:HD21	0.48	2.38	5	2
1:A:117:LEU:HA	1:A:120:ALA:HB2	0.48	1.84	17	4
1:A:45:TYR:CZ	1:A:97:TRP:CD1	0.48	3.01	12	1
1:A:10:LEU:HD12	1:A:29:GLY:O	0.48	2.07	9	1
1:A:93:GLU:CG	1:A:114:LEU:HD11	0.48	2.39	12	4
1:A:91:MET:CG	1:A:92:LEU:N	0.48	2.76	5	3
1:A:11:SER:HB2	1:A:128:TRP:CZ3	0.48	2.44	16	3
1:A:23:LEU:HD13	1:A:25:VAL:HG23	0.48	1.84	5	1
1:A:125:GLU:O	1:A:127:HIS:CE1	0.48	2.66	14	1
1:A:91:MET:HE3	1:A:116:GLU:CG	0.48	2.39	13	2
1:A:23:LEU:CD1	1:A:25:VAL:CG2	0.48	2.87	5	1
1:A:50:PHE:CZ	1:A:117:LEU:HD21	0.48	2.44	20	2
1:A:17:ASP:OD1	1:A:19:VAL:CG2	0.48	2.61	14	2
1:A:86:GLU:O	1:A:88:ARG:N	0.48	2.47	15	1
1:A:17:ASP:OD1	1:A:19:VAL:HG22	0.47	2.08	15	2
1:A:88:ARG:N	1:A:118:GLU:OE1	0.47	2.47	14	1
1:A:27:ILE:CG2	1:A:46:VAL:HG21	0.47	2.38	10	1
1:A:17:ASP:OD2	1:A:20:GLY:N	0.47	2.47	11	1
1:A:12:ILE:CG2	1:A:13:LYS:N	0.47	2.76	16	1
1:A:24:ILE:CD1	1:A:24:ILE:N	0.47	2.77	6	1
1:A:45:TYR:CE2	1:A:97:TRP:HB2	0.47	2.45	12	14
1:A:65:VAL:CG1	1:A:68:THR:HG21	0.47	2.39	3	12
1:A:10:LEU:HD23	1:A:12:ILE:CD1	0.47	2.25	14	1
1:A:14:LEU:HD23	1:A:25:VAL:HB	0.47	1.87	16	1
1:A:60:ARG:HG2	1:A:77:PHE:CE1	0.47	2.44	6	1
1:A:62:THR:HG22	1:A:77:PHE:CZ	0.47	2.45	10	1
1:A:12:ILE:HG22	1:A:13:LYS:N	0.47	2.24	16	1
1:A:80:SER:CB	1:A:81:PRO:HA	0.47	2.39	4	18
1:A:121:LEU:O	1:A:121:LEU:HD13	0.47	2.10	1	5
1:A:11:SER:HB2	1:A:128:TRP:CH2	0.47	2.45	10	3
1:A:14:LEU:CD2	1:A:25:VAL:HG13	0.47	2.40	20	1
1:A:45:TYR:CZ	1:A:97:TRP:HB2	0.47	2.45	5	6
1:A:73:TRP:O	1:A:74:ASN:C	0.47	2.53	19	17
1:A:50:PHE:CD2	1:A:92:LEU:CD2	0.47	2.97	19	1
1:A:47:LYS:HD3	1:A:49:TYR:CE2	0.47	2.45	3	4
1:A:62:THR:HB	1:A:73:TRP:CD1	0.47	2.45	11	2
1:A:97:TRP:CZ3	1:A:109:PHE:CD1	0.47	3.03	13	5
1:A:60:ARG:HD2	1:A:77:PHE:CD1	0.47	2.44	9	7
1:A:28:LEU:O	1:A:73:TRP:N	0.47	2.48	19	1
1:A:116:GLU:O	1:A:120:ALA:HB2	0.46	2.09	8	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:12:ILE:CG2	1:A:14:LEU:CD1	0.46	2.93	10	1
1:A:92:LEU:CD2	1:A:117:LEU:HD11	0.46	2.40	10	2
1:A:10:LEU:HB2	1:A:113:ILE:HD11	0.46	1.86	5	2
1:A:16:PHE:CE2	1:A:84:ARG:HD3	0.46	2.45	3	3
1:A:89:GLU:O	1:A:90:ARG:NE	0.46	2.49	4	1
1:A:28:LEU:CD2	1:A:126:PRO:CB	0.46	2.93	10	2
1:A:91:MET:HE3	1:A:116:GLU:HG2	0.46	1.87	3	3
1:A:10:LEU:HD13	1:A:12:ILE:HD11	0.46	1.87	12	2
1:A:86:GLU:O	1:A:90:ARG:N	0.46	2.49	12	7
1:A:45:TYR:C	1:A:45:TYR:CD1	0.46	2.89	2	1
1:A:95:THR:HB	1:A:97:TRP:CZ2	0.46	2.46	5	3
1:A:20:GLY:N	1:A:22:GLN:OE1	0.46	2.49	6	1
1:A:86:GLU:OE1	1:A:90:ARG:NH1	0.46	2.49	14	2
1:A:109:PHE:CE2	1:A:111:GLY:HA2	0.46	2.46	14	3
1:A:23:LEU:N	1:A:79:TYR:O	0.46	2.49	17	1
1:A:87:PHE:CG	1:A:117:LEU:HB3	0.46	2.46	1	3
1:A:113:ILE:HG22	1:A:115:ILE:HD11	0.46	1.87	9	3
1:A:21:HIS:CE1	1:A:83:HIS:CE1	0.46	3.04	18	1
1:A:113:ILE:HD11	1:A:131:LEU:HG	0.45	1.87	18	4
1:A:91:MET:HE1	1:A:114:LEU:HB3	0.45	1.89	8	2
1:A:25:VAL:HG22	1:A:25:VAL:O	0.45	2.10	9	3
1:A:123:ASP:C	1:A:125:GLU:N	0.45	2.69	14	3
1:A:50:PHE:CE2	1:A:117:LEU:HD11	0.45	2.46	18	1
1:A:88:ARG:O	1:A:89:GLU:CB	0.45	2.64	18	1
1:A:13:LYS:HG3	1:A:126:PRO:CD	0.45	2.41	10	1
1:A:23:LEU:HD22	1:A:117:LEU:HD13	0.45	1.86	7	1
1:A:51:LEU:N	1:A:91:MET:O	0.45	2.49	18	1
1:A:112:GLU:OE2	1:A:114:LEU:HD13	0.45	2.11	7	3
1:A:14:LEU:HB3	1:A:122:LEU:CD2	0.45	2.41	10	2
1:A:49:TYR:O	1:A:51:LEU:CD1	0.45	2.64	8	1
1:A:15:TRP:CE3	1:A:124:ASP:HB2	0.45	2.47	4	2
1:A:12:ILE:HG22	1:A:14:LEU:CD1	0.45	2.42	10	1
1:A:93:GLU:HG3	1:A:114:LEU:CD1	0.45	2.42	19	3
1:A:127:HIS:HB3	1:A:129:TYR:CE1	0.45	2.47	9	1
1:A:123:ASP:O	1:A:125:GLU:N	0.45	2.50	14	2
1:A:10:LEU:HB3	1:A:113:ILE:HD12	0.45	1.89	15	1
1:A:87:PHE:O	1:A:90:ARG:O	0.44	2.34	15	6
1:A:42:ARG:NH1	1:A:98:ASP:OD2	0.44	2.50	15	2
1:A:14:LEU:CB	1:A:122:LEU:CD2	0.44	2.94	10	1
1:A:25:VAL:HG13	1:A:77:PHE:HB2	0.44	1.89	1	1
1:A:92:LEU:HD12	1:A:117:LEU:CD2	0.44	2.42	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:27:ILE:CG2	1:A:62:THR:HG21	0.44	2.42	4	1
1:A:17:ASP:OD1	1:A:17:ASP:C	0.44	2.56	17	1
1:A:10:LEU:HD11	1:A:46:VAL:CG2	0.44	2.42	20	1
1:A:69:LEU:N	1:A:69:LEU:HD23	0.44	2.28	7	1
1:A:116:GLU:O	1:A:119:THR:N	0.44	2.51	9	4
1:A:73:TRP:O	1:A:75:GLN:N	0.44	2.50	19	2
1:A:45:TYR:CE1	1:A:97:TRP:CD1	0.44	3.05	9	2
1:A:60:ARG:HD2	1:A:77:PHE:CE1	0.44	2.47	11	3
1:A:92:LEU:N	1:A:92:LEU:CD2	0.44	2.80	16	1
1:A:10:LEU:HB3	1:A:113:ILE:CD1	0.44	2.42	12	4
1:A:15:TRP:N	1:A:24:ILE:O	0.44	2.46	6	1
1:A:23:LEU:HD13	1:A:24:ILE:N	0.44	2.27	6	1
1:A:10:LEU:HB2	1:A:113:ILE:CD1	0.44	2.43	5	1
1:A:33:LEU:C	1:A:69:LEU:HD22	0.44	2.33	3	1
1:A:14:LEU:HD23	1:A:25:VAL:HG22	0.44	1.90	4	1
1:A:50:PHE:CE1	1:A:117:LEU:HD21	0.44	2.47	8	1
1:A:23:LEU:HD22	1:A:23:LEU:C	0.44	2.34	5	1
1:A:25:VAL:N	1:A:77:PHE:O	0.44	2.51	17	2
1:A:109:PHE:CZ	1:A:111:GLY:CA	0.43	3.01	14	2
1:A:14:LEU:CD2	1:A:25:VAL:HG23	0.43	2.43	6	1
1:A:87:PHE:CD1	1:A:117:LEU:HB3	0.43	2.48	6	2
1:A:98:ASP:OD1	1:A:98:ASP:C	0.43	2.56	5	4
1:A:92:LEU:CD2	1:A:92:LEU:N	0.43	2.82	10	1
1:A:10:LEU:HD23	1:A:11:SER:N	0.43	2.28	16	1
1:A:24:ILE:N	1:A:24:ILE:HD12	0.43	2.29	5	1
1:A:27:ILE:O	1:A:28:LEU:O	0.43	2.37	16	3
1:A:27:ILE:HG22	1:A:73:TRP:HE3	0.43	1.63	1	1
1:A:11:SER:O	1:A:28:LEU:HB2	0.43	2.13	16	2
1:A:11:SER:HB2	1:A:128:TRP:CZ2	0.43	2.48	16	1
1:A:29:GLY:HA2	1:A:73:TRP:CE3	0.43	2.49	7	3
1:A:30:ALA:HB1	1:A:33:LEU:CD1	0.43	2.43	6	1
1:A:66:LYS:O	1:A:67:LYS:O	0.43	2.37	10	7
1:A:14:LEU:HD22	1:A:25:VAL:HG22	0.43	1.90	5	1
1:A:25:VAL:O	1:A:77:PHE:N	0.43	2.52	20	1
1:A:46:VAL:HG22	1:A:96:LEU:CD2	0.43	2.43	5	1
1:A:88:ARG:CB	1:A:118:GLU:OE1	0.43	2.67	13	1
1:A:11:SER:HB2	1:A:128:TRP:CE2	0.43	2.49	16	1
1:A:13:LYS:O	1:A:26:THR:N	0.42	2.48	1	2
1:A:73:TRP:C	1:A:75:GLN:N	0.42	2.72	4	3
1:A:46:VAL:HG22	1:A:96:LEU:HD23	0.42	1.91	5	1
1:A:17:ASP:O	1:A:21:HIS:N	0.42	2.52	18	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:86:GLU:OE1	1:A:90:ARG:NE	0.42	2.52	19	1
1:A:96:LEU:C	1:A:97:TRP:CD1	0.42	2.93	19	2
1:A:123:ASP:O	1:A:124:ASP:C	0.42	2.58	3	5
1:A:50:PHE:CD1	1:A:92:LEU:CD2	0.42	3.02	12	2
1:A:17:ASP:N	1:A:22:GLN:O	0.42	2.48	11	2
1:A:26:THR:O	1:A:28:LEU:HD13	0.42	2.15	16	1
1:A:33:LEU:HD23	1:A:42:ARG:HH12	0.42	1.73	14	1
1:A:22:GLN:CB	1:A:78:ILE:HG23	0.42	2.44	6	2
1:A:94:ILE:O	1:A:113:ILE:N	0.42	2.49	6	1
1:A:28:LEU:HD13	1:A:28:LEU:H	0.42	1.75	16	1
1:A:48:ILE:CD1	1:A:77:PHE:CE2	0.42	3.03	1	1
1:A:91:MET:CE	1:A:116:GLU:HG2	0.42	2.45	9	1
1:A:121:LEU:O	1:A:122:LEU:HD13	0.42	2.14	13	1
1:A:86:GLU:C	1:A:88:ARG:N	0.42	2.72	15	1
1:A:44:PRO:CG	1:A:68:THR:O	0.41	2.68	4	2
1:A:42:ARG:O	1:A:67:LYS:CA	0.41	2.68	18	1
1:A:93:GLU:HG3	1:A:114:LEU:HD21	0.41	1.91	3	1
1:A:92:LEU:HD21	1:A:117:LEU:HD11	0.41	1.92	10	1
1:A:42:ARG:NH1	1:A:110:LEU:CD2	0.41	2.83	1	1
1:A:80:SER:HA	1:A:81:PRO:C	0.41	2.35	6	9
1:A:124:ASP:CG	1:A:124:ASP:O	0.41	2.58	10	1
1:A:87:PHE:CA	1:A:117:LEU:HB2	0.41	2.45	15	1
1:A:50:PHE:CE2	1:A:90:ARG:HD3	0.41	2.51	3	1
1:A:26:THR:OG1	1:A:75:GLN:O	0.41	2.37	10	1
1:A:86:GLU:O	1:A:87:PHE:C	0.41	2.58	15	1
1:A:23:LEU:O	1:A:79:TYR:N	0.41	2.53	17	1
1:A:42:ARG:O	1:A:67:LYS:N	0.41	2.54	13	1
1:A:42:ARG:NH1	1:A:69:LEU:HD12	0.41	2.30	13	1
1:A:43:ASN:HA	1:A:65:VAL:O	0.41	2.14	13	1
1:A:17:ASP:O	1:A:22:GLN:N	0.41	2.48	14	1
1:A:25:VAL:HG13	1:A:77:PHE:O	0.41	2.14	16	1
1:A:51:LEU:HD11	1:A:93:GLU:CB	0.41	2.46	16	1
1:A:62:THR:HG22	1:A:77:PHE:CE2	0.41	2.50	15	1
1:A:42:ARG:O	1:A:67:LYS:HA	0.41	2.14	18	1
1:A:127:HIS:HB2	1:A:129:TYR:CZ	0.41	2.51	19	1
1:A:14:LEU:CD2	1:A:25:VAL:HB	0.41	2.46	3	2
1:A:86:GLU:O	1:A:89:GLU:N	0.41	2.53	1	1
1:A:50:PHE:CZ	1:A:90:ARG:CD	0.41	3.03	3	1
1:A:31:LYS:O	1:A:32:ASP:C	0.41	2.59	9	2
1:A:127:HIS:HB3	1:A:129:TYR:CZ	0.41	2.51	1	1
1:A:42:ARG:O	1:A:44:PRO:HD3	0.41	2.16	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:109:PHE:CZ	1:A:112:GLU:N	0.41	2.89	5	1
1:A:23:LEU:HD22	1:A:24:ILE:H	0.41	1.75	6	1
1:A:25:VAL:O	1:A:25:VAL:HG22	0.41	2.15	7	1
1:A:91:MET:CE	1:A:114:LEU:HD13	0.41	2.46	8	1
1:A:28:LEU:H	1:A:28:LEU:HD13	0.41	1.76	10	1
1:A:19:VAL:CG2	1:A:20:GLY:N	0.41	2.84	11	1
1:A:65:VAL:HG11	1:A:68:THR:CG2	0.41	2.37	18	1
1:A:93:GLU:HG3	1:A:114:LEU:CD2	0.41	2.46	20	1
1:A:98:ASP:O	1:A:99:GLN:C	0.41	2.59	8	1
1:A:48:ILE:HD13	1:A:77:PHE:CD2	0.40	2.51	1	1
1:A:111:GLY:O	1:A:131:LEU:CD2	0.40	2.69	9	1
1:A:27:ILE:CB	1:A:62:THR:HG21	0.40	2.46	13	1
1:A:91:MET:CE	1:A:114:LEU:CD1	0.40	2.97	18	1
1:A:79:TYR:O	1:A:82:VAL:HG23	0.40	2.15	15	1
1:A:87:PHE:HB3	1:A:117:LEU:CB	0.40	2.46	15	1
1:A:88:ARG:O	1:A:89:GLU:HB2	0.40	2.14	18	1
1:A:123:ASP:CB	1:A:125:GLU:OE2	0.40	2.69	2	1
1:A:95:THR:HB	1:A:97:TRP:CE2	0.40	2.51	8	1
1:A:28:LEU:CD2	1:A:126:PRO:HB3	0.40	2.43	10	1
1:A:12:ILE:O	1:A:126:PRO:HA	0.40	2.16	10	1
1:A:92:LEU:HD23	1:A:117:LEU:CD2	0.40	2.44	16	1
1:A:17:ASP:OD1	1:A:17:ASP:O	0.40	2.39	17	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	100/141 (71%)	87±2 (87±2%)	9±2 (9±2%)	4±1 (4±1%)	4 28
All	All	2000/2820 (71%)	1736 (87%)	174 (9%)	90 (4%)	4 28

All 12 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	LEU	20
1	A	67	LYS	17
1	A	109	PHE	14
1	A	123	ASP	11
1	A	99	GLN	7
1	A	19	VAL	6
1	A	42	ARG	6
1	A	25	VAL	3
1	A	74	ASN	2
1	A	68	THR	2
1	A	124	ASP	1
1	A	87	PHE	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	94/128 (73%)	71±2 (75±2%)	23±2 (25±2%)	2 25
All	All	1880/2560 (73%)	1419 (75%)	461 (25%)	2 25

All 59 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	18	LYS	20
1	A	31	LYS	20
1	A	80	SER	20
1	A	85	ARG	20
1	A	95	THR	19
1	A	22	GLN	18
1	A	68	THR	18
1	A	99	GLN	18
1	A	74	ASN	17
1	A	97	TRP	16
1	A	114	LEU	16
1	A	131	LEU	15
1	A	26	THR	14
1	A	25	VAL	13

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Mol	Chain	Res	Type	Models (Total)
1	A	10	LEU	13
1	A	63	LYS	12
1	A	91	MET	12
1	A	49	TYR	10
1	A	51	LEU	10
1	A	42	ARG	10
1	A	90	ARG	9
1	A	60	ARG	8
1	A	92	LEU	8
1	A	17	ASP	7
1	A	121	LEU	7
1	A	127	HIS	7
1	A	130	LYS	7
1	A	47	LYS	7
1	A	33	LEU	7
1	A	61	ARG	7
1	A	65	VAL	7
1	A	122	LEU	7
1	A	123	ASP	5
1	A	50	PHE	5
1	A	98	ASP	5
1	A	125	GLU	4
1	A	112	GLU	4
1	A	75	GLN	4
1	A	79	TYR	3
1	A	88	ARG	3
1	A	70	GLU	2
1	A	86	GLU	2
1	A	23	LEU	2
1	A	72	LYS	2
1	A	89	GLU	2
1	A	13	LYS	2
1	A	28	LEU	2
1	A	67	LYS	2
1	A	45	TYR	2
1	A	43	ASN	2
1	A	32	ASP	1
1	A	96	LEU	1
1	A	69	LEU	1
1	A	14	LEU	1
1	A	83	HIS	1
1	A	84	ARG	1

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Mol	Chain	Res	Type	Models (Total)
1	A	118	GLU	1
1	A	124	ASP	1
1	A	93	GLU	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)

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

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)

No chemical shift data were provided