WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB NMR Structure Validation Report (i)

Apr 26, 2016 – 10:57 PM BST

PDB ID	:	2KBG
Title	:	Solution structure of the second Fibronectin type-III module of NCAM2
Authors	:	Rasmussen, K.K.; Teilum, K.; Kulahin, N.; Clausen, O.; Berezin, V.; Bock, E.; Walmod, P.S.; Poulsen, F.M.
Deposited on	:	2008-11-28

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
http://wwpdb.org/validation/2016/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:

|		
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027457

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		16
Ramachandran outliers		6.3%
Sidechain outliers		10.1%

Worse   *Better*

▮ Percentile relative to all structures

▯ Percentile relative to all NMR structures
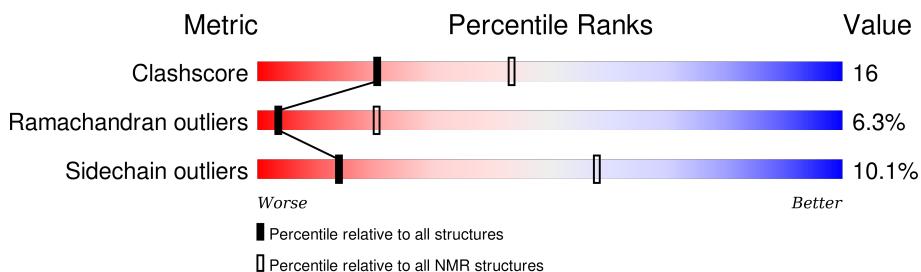
Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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	114	51% 29% • 8% 11%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 7 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:5-A:97 (93)	0.25	7

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

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

The models can be grouped into 3 clusters and 2 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1637 atoms, of which 815 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Neural cell adhesion molecule 2.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	102	1637	524	815	139	157	2	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLU	-	EXPRESSION TAG	UNP O15394
A	-4	ALA	-	EXPRESSION TAG	UNP O15394
A	-3	GLU	-	EXPRESSION TAG	UNP O15394
A	-2	ALA	-	EXPRESSION TAG	UNP O15394
A	-1	SER	-	EXPRESSION TAG	UNP O15394
A	0	MET	-	EXPRESSION TAG	UNP O15394
A	103	HIS	-	EXPRESSION TAG	UNP O15394
A	104	HIS	-	EXPRESSION TAG	UNP O15394
A	105	HIS	-	EXPRESSION TAG	UNP O15394
A	106	HIS	-	EXPRESSION TAG	UNP O15394
A	107	HIS	-	EXPRESSION TAG	UNP O15394
A	108	HIS	-	EXPRESSION TAG	UNP O15394

4 Residue-property plots ⓘ

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: Neural cell adhesion molecule 2

Chain A:

51% 29% • 8% 11%

GLU ALA GLU ALA SER MET R1 E2 P3 S4 P5 P6 S7 S13 F18 K24 Q25 D26 D27 G28 G29 I32 Y35 I36 V37 R40 S41 K44 E45 D46 K51 K52 V53 D58 H59 H64 L65 Q66 A77 A78 N79 R80 L81 G82 Y83 S84 E85 P86 T87

V88 Y89 E90 F91 N98 I99 I100 K101 D102 HIS HIS HIS HIS HIS HIS
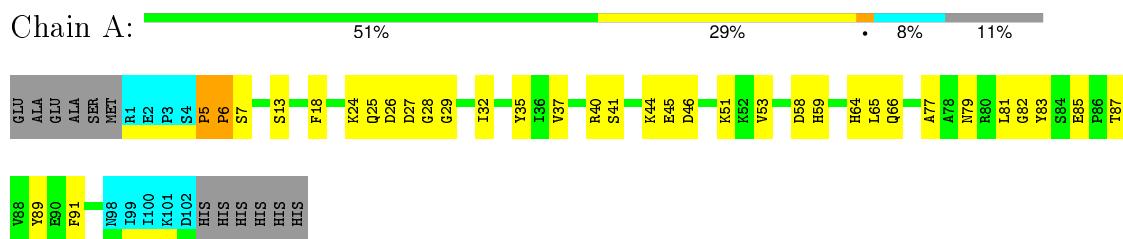
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Neural cell adhesion molecule 2

Chain A:

53% 26% • 8% 11%

GLU ALA GLU ALA SER MET R1 E2 P3 S4 P5 P6 S13 S14 F18 K24 Q25 I32 L33 E34 Y35 I36 V37 K38 Y39 R40 S41 K44 L49 E50 K51 K52 V53 H59 I60 L65 Q66 Y71 I75 T76 A77 A78 N79 R80 L81 G82 Y83 T87 V88

Y89 E90 F91 N98 I99 I100 K101 D102 HIS HIS HIS HIS HIS HIS
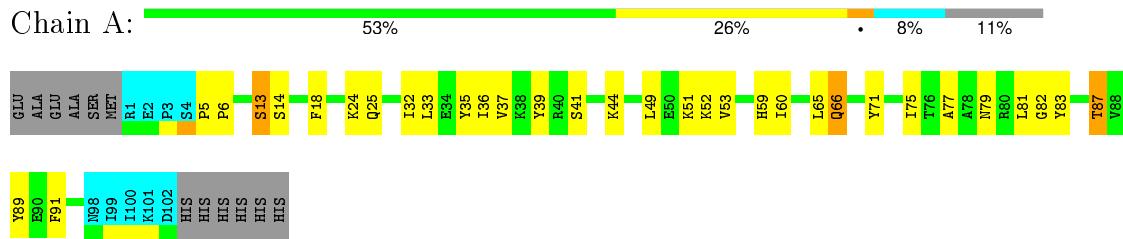
4.2.2 Score per residue for model 2

- Molecule 1: Neural cell adhesion molecule 2

Chain A:

54% 25% •• 8% 11%
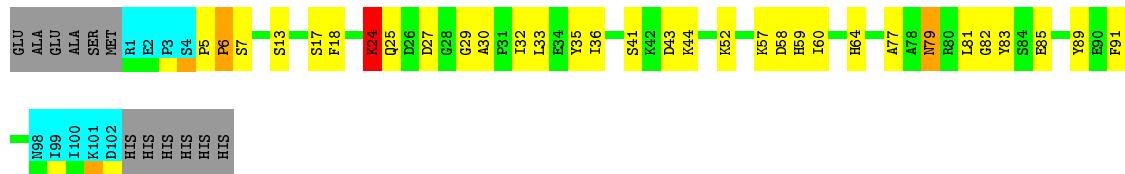
### 4.2.3 Score per residue for model 3

• Molecule 1: Neural cell adhesion molecule 2
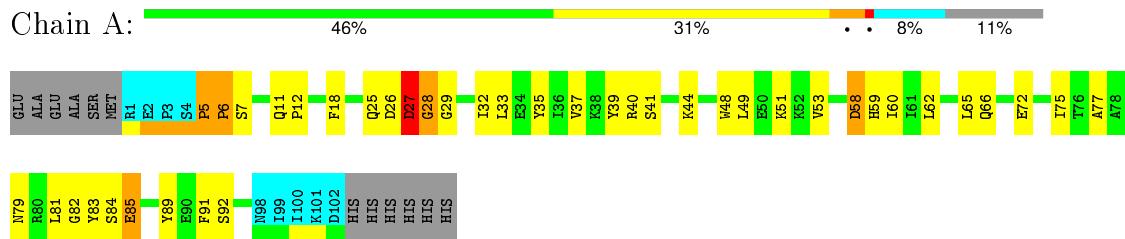
4.2.4 Score per residue for model 4

• Molecule 1: Neural cell adhesion molecule 2
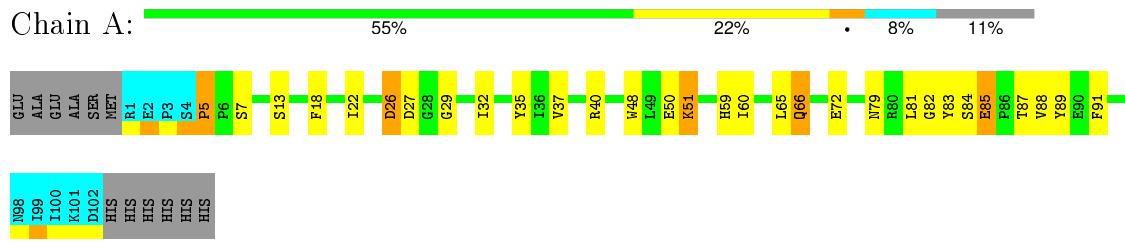
4.2.5 Score per residue for model 5

• Molecule 1: Neural cell adhesion molecule 2
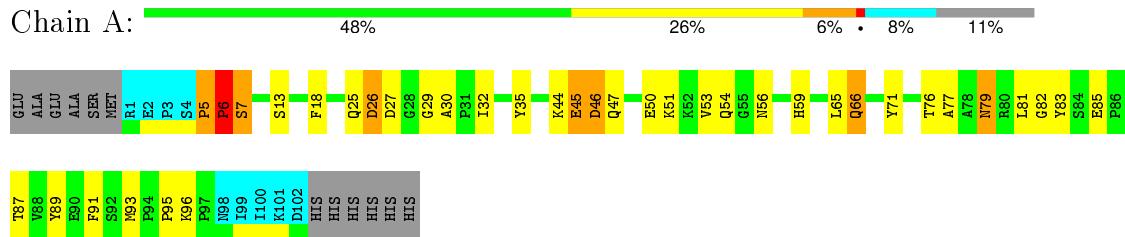
4.2.6 Score per residue for model 6

• Molecule 1: Neural cell adhesion molecule 2

Chain A:
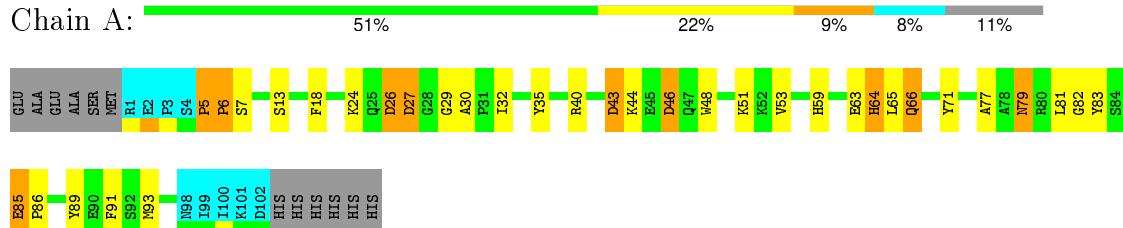
4.2.7 Score per residue for model 7 (medoid)

• Molecule 1: Neural cell adhesion molecule 2

Chain A:
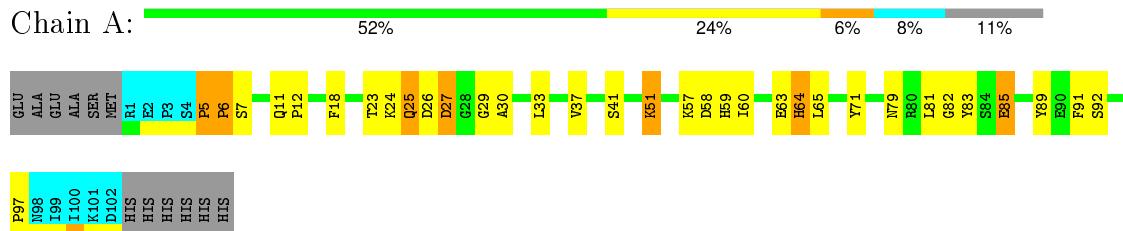
4.2.8 Score per residue for model 8

• Molecule 1: Neural cell adhesion molecule 2

Chain A:
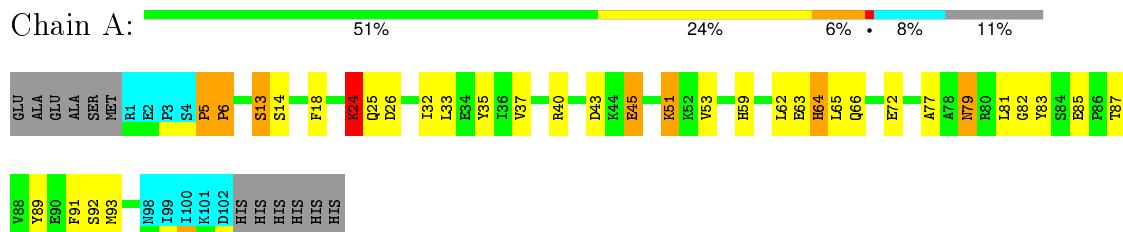
4.2.9 Score per residue for model 9

• Molecule 1: Neural cell adhesion molecule 2

Chain A:
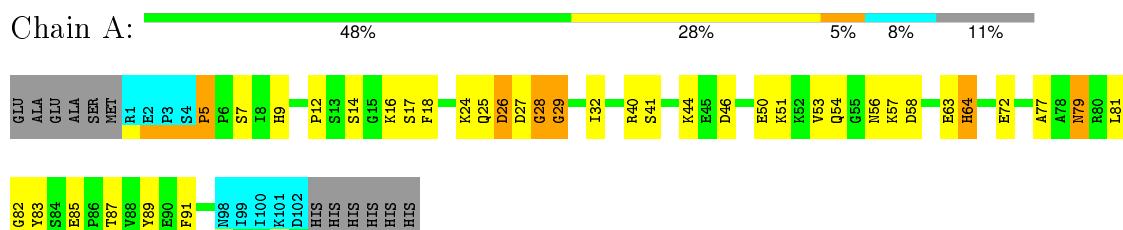
4.2.10 Score per residue for model 10

• Molecule 1: Neural cell adhesion molecule 2
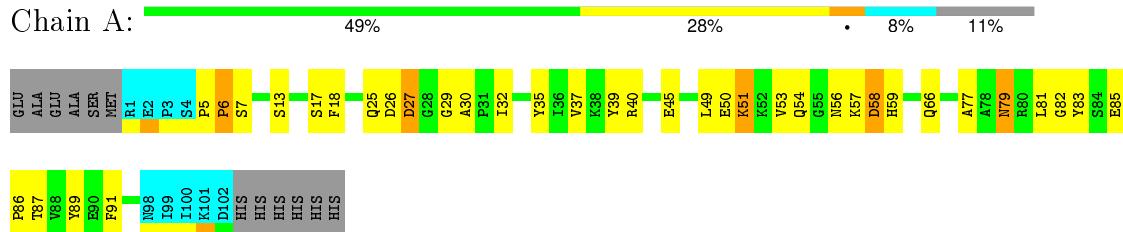
4.2.11 Score per residue for model 11

• Molecule 1: Neural cell adhesion molecule 2
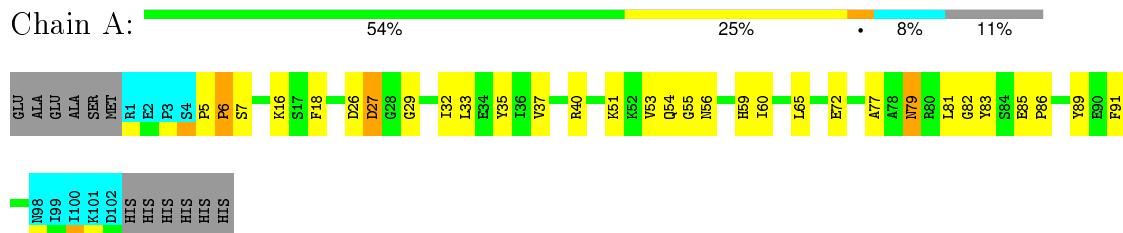

4.2.12 Score per residue for model 12

• Molecule 1: Neural cell adhesion molecule 2
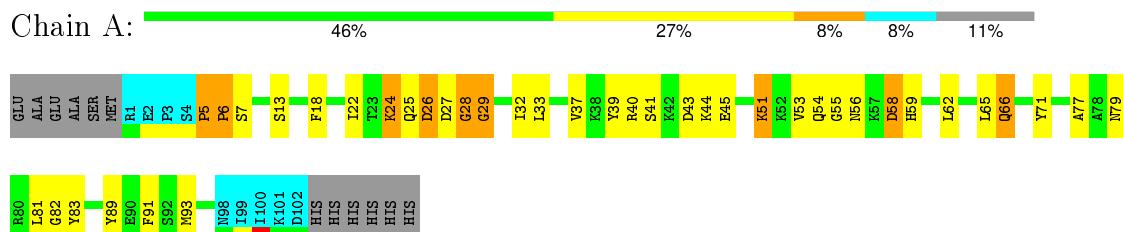
4.2.13 Score per residue for model 13

• Molecule 1: Neural cell adhesion molecule 2
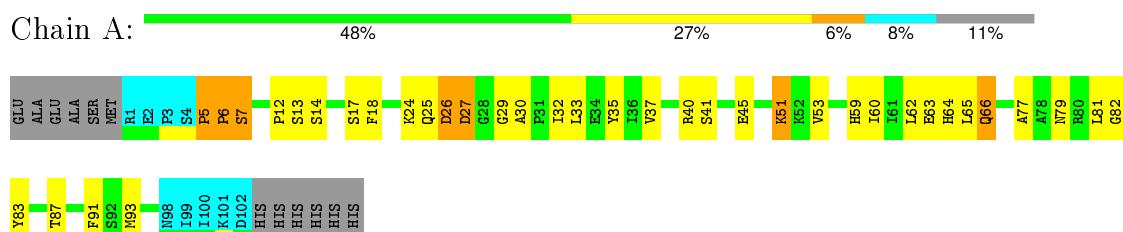
4.2.14 Score per residue for model 14

• Molecule 1: Neural cell adhesion molecule 2
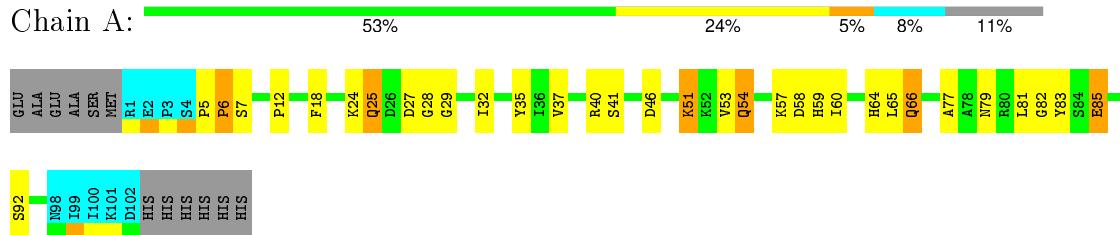
4.2.15 Score per residue for model 15

• Molecule 1: Neural cell adhesion molecule 2

4.2.16 Score per residue for model 16

• Molecule 1: Neural cell adhesion molecule 2
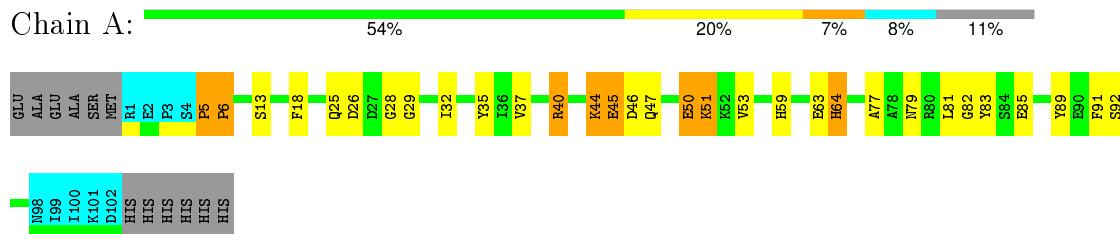
4.2.17 Score per residue for model 17

• Molecule 1: Neural cell adhesion molecule 2

4.2.18 Score per residue for model 18

• Molecule 1: Neural cell adhesion molecule 2
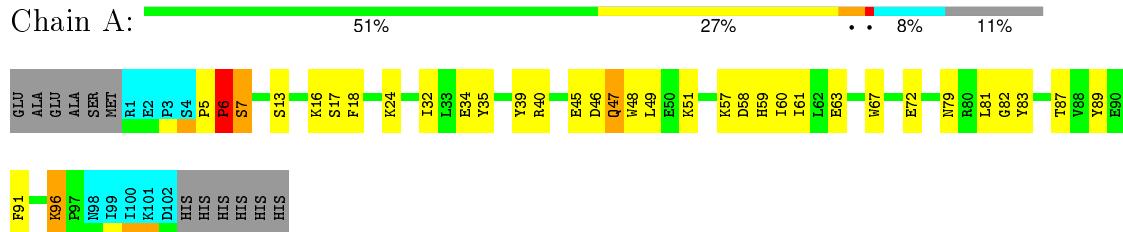
4.2.19 Score per residue for model 19

• Molecule 1: Neural cell adhesion molecule 2
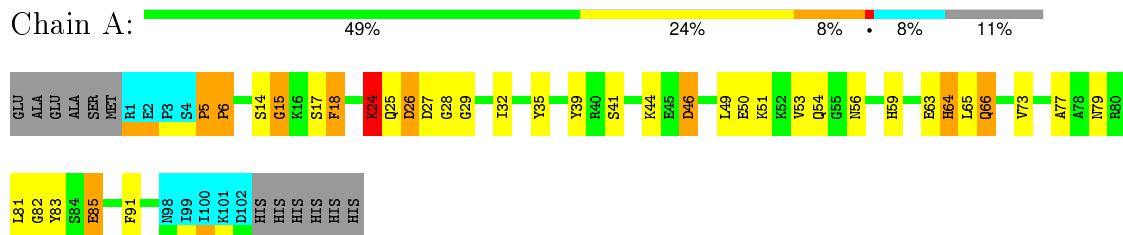

4.2.20 Score per residue for model 20

• Molecule 1: Neural cell adhesion molecule 2
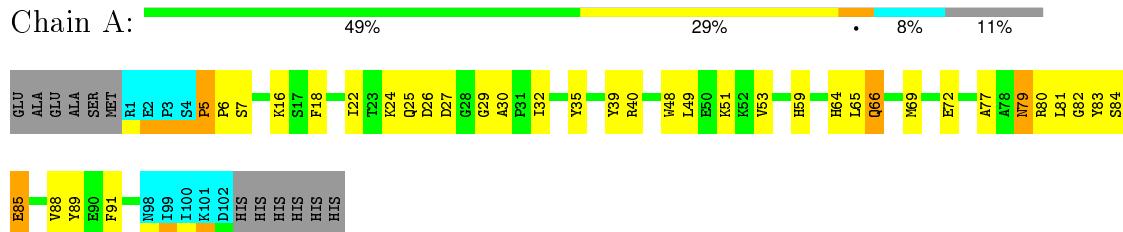
5 Refinement protocol and experimental data overview (i)

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

Of the 100 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
X-PLOR NIH	structure solution	2.19
X-PLOR NIH	refinement	2.19

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality (i)

6.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.68±0.01	0±0/770 (0.0±0.0%)	0.76±0.01	0±0/1042 (0.0±0.0%)
All	All	0.68	0/15400 (0.0%)	0.76	2/20840 (0.0%)

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	35	TYR	CB-CG-CD2	-5.56	117.67	121.00	10	2

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	748	739	739	24±3
All	All	14960	14780	14780	474

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 16.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:33:LEU:HD22	1:A:33:LEU:N	0.68	2.03	13	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:16:LYS:HZ2	1:A:67:TRP:HE1	0.68	1.29	18	1
1:A:79:ASN:ND2	1:A:79:ASN:H	0.67	1.87	8	2
1:A:40:ARG:HH21	1:A:47:GLN:H	0.67	1.33	16	1
1:A:79:ASN:N	1:A:79:ASN:ND2	0.64	2.46	2	4
1:A:65:LEU:HD13	1:A:71:TYR:OH	0.64	1.93	5	2
1:A:16:LYS:NZ	1:A:66:GLN:H	0.63	1.92	20	1
1:A:89:TYR:CE2	1:A:91:PHE:CD1	0.62	2.88	2	16
1:A:40:ARG:NH2	1:A:47:GLN:H	0.62	1.91	16	1
1:A:67:TRP:NE1	1:A:96:LYS:CE	0.61	2.63	18	1
1:A:63:GLU:O	1:A:64:HIS:CG	0.61	2.54	6	2
1:A:79:ASN:H	1:A:79:ASN:ND2	0.60	1.92	20	5
1:A:79:ASN:ND2	1:A:79:ASN:N	0.60	2.49	10	3
1:A:81:LEU:N	1:A:81:LEU:HD22	0.59	2.13	15	6
1:A:85:GLU:OE1	1:A:85:GLU:N	0.59	2.36	6	1
1:A:40:ARG:NE	1:A:41:SER:O	0.59	2.36	15	3
1:A:81:LEU:HD22	1:A:81:LEU:N	0.58	2.13	16	8
1:A:77:ALA:HB3	1:A:85:GLU:OE2	0.58	1.99	20	1
1:A:54:GLN:HE21	1:A:56:ASN:HD22	0.58	1.42	11	1
1:A:32:ILE:HG21	1:A:35:TYR:CE1	0.57	2.34	18	14
1:A:33:LEU:N	1:A:33:LEU:CD2	0.57	2.67	13	4
1:A:27:ASP:O	1:A:29:GLY:N	0.57	2.37	12	5
1:A:74:GLN:NE2	1:A:75:ILE:O	0.56	2.38	17	1
1:A:40:ARG:NH2	1:A:44:LYS:O	0.56	2.38	16	1
1:A:54:GLN:NE2	1:A:56:ASN:HD22	0.56	1.98	11	1
1:A:79:ASN:O	1:A:82:GLY:N	0.56	2.39	9	8
1:A:27:ASP:OD2	1:A:79:ASN:ND2	0.56	2.39	5	3
1:A:79:ASN:N	1:A:79:ASN:OD1	0.56	2.39	3	7
1:A:40:ARG:NE	1:A:48:TRP:CZ2	0.55	2.75	18	5
1:A:65:LEU:CD2	1:A:65:LEU:N	0.55	2.69	13	2
1:A:40:ARG:NE	1:A:47:GLN:O	0.55	2.39	16	1
1:A:24:LYS:H	1:A:24:LYS:CD	0.55	2.14	12	1
1:A:44:LYS:O	1:A:46:ASP:N	0.55	2.39	16	1
1:A:79:ASN:OD1	1:A:79:ASN:N	0.55	2.38	4	6
1:A:65:LEU:O	1:A:93:MET:SD	0.54	2.66	8	4
1:A:25:GLN:NE2	1:A:85:GLU:O	0.54	2.41	2	1
1:A:66:GLN:O	1:A:93:MET:SD	0.53	2.66	12	5
1:A:41:SER:OG	1:A:71:TYR:CE2	0.53	2.61	7	1
1:A:25:GLN:NE2	1:A:85:GLU:OE1	0.53	2.40	19	1
1:A:11:GLN:O	1:A:13:SER:N	0.53	2.42	17	1
1:A:40:ARG:NH2	1:A:72:GLU:OE2	0.53	2.42	11	5
1:A:7:SER:OG	1:A:7:SER:O	0.53	2.26	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:27:ASP:OD1	1:A:79:ASN:ND2	0.53	2.41	2	2
1:A:91:PHE:CD2	1:A:91:PHE:O	0.53	2.62	13	1
1:A:7:SER:O	1:A:7:SER:OG	0.53	2.26	12	1
1:A:40:ARG:NH2	1:A:72:GLU:OE1	0.53	2.42	4	3
1:A:16:LYS:NZ	1:A:67:TRP:HE1	0.53	1.99	18	1
1:A:40:ARG:NH2	1:A:41:SER:O	0.52	2.42	14	2
1:A:18:PHE:CD2	1:A:91:PHE:CE2	0.52	2.98	19	1
1:A:81:LEU:N	1:A:81:LEU:CD2	0.51	2.74	10	5
1:A:25:GLN:CD	1:A:25:GLN:H	0.51	2.09	14	1
1:A:74:GLN:OE1	1:A:88:VAL:HG22	0.51	2.06	17	1
1:A:58:ASP:O	1:A:58:ASP:CG	0.51	2.48	3	2
1:A:57:LYS:O	1:A:58:ASP:OD1	0.51	2.29	10	2
1:A:84:SER:O	1:A:85:GLU:C	0.51	2.49	4	3
1:A:63:GLU:O	1:A:64:HIS:CB	0.50	2.58	6	7
1:A:50:GLU:OE1	1:A:50:GLU:N	0.50	2.44	15	1
1:A:5:PRO:O	1:A:6:PRO:O	0.50	2.30	10	15
1:A:65:LEU:HD13	1:A:71:TYR:CZ	0.50	2.42	6	2
1:A:81:LEU:CD2	1:A:81:LEU:N	0.50	2.75	8	8
1:A:16:LYS:CE	1:A:65:LEU:O	0.50	2.60	17	1
1:A:82:GLY:C	1:A:83:TYR:CG	0.50	2.85	2	20
1:A:46:ASP:OD1	1:A:46:ASP:N	0.50	2.44	9	2
1:A:65:LEU:HD22	1:A:65:LEU:N	0.50	2.21	13	1
1:A:27:ASP:OD1	1:A:30:ALA:N	0.50	2.45	20	1
1:A:27:ASP:OD1	1:A:29:GLY:N	0.50	2.43	11	1
1:A:25:GLN:O	1:A:26:ASP:C	0.49	2.50	9	2
1:A:81:LEU:HD12	1:A:81:LEU:N	0.49	2.22	14	5
1:A:50:GLU:N	1:A:50:GLU:OE1	0.49	2.46	9	1
1:A:63:GLU:OE1	1:A:63:GLU:N	0.49	2.45	18	1
1:A:7:SER:OG	1:A:25:GLN:NE2	0.49	2.46	5	1
1:A:40:ARG:NH2	1:A:72:GLU:CD	0.49	2.66	3	4
1:A:23:THR:O	1:A:25:GLN:NE2	0.49	2.46	7	1
1:A:63:GLU:CD	1:A:64:HIS:N	0.49	2.66	8	1
1:A:27:ASP:C	1:A:29:GLY:H	0.49	2.11	14	3
1:A:33:LEU:HD12	1:A:33:LEU:N	0.48	2.23	3	2
1:A:82:GLY:C	1:A:83:TYR:CD1	0.48	2.87	3	10
1:A:85:GLU:N	1:A:86:PRO:CD	0.48	2.76	17	5
1:A:43:ASP:OD1	1:A:43:ASP:N	0.48	2.47	6	1
1:A:40:ARG:NH1	1:A:44:LYS:C	0.48	2.67	16	1
1:A:81:LEU:N	1:A:81:LEU:CD1	0.48	2.77	20	3
1:A:33:LEU:N	1:A:33:LEU:HD22	0.47	2.23	7	2
1:A:50:GLU:N	1:A:50:GLU:CD	0.47	2.68	4	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:91:PHE:CG	1:A:91:PHE:O	0.47	2.67	13	3
1:A:79:ASN:N	1:A:79:ASN:HD22	0.47	2.07	6	2
1:A:25:GLN:O	1:A:27:ASP:N	0.47	2.47	13	4
1:A:79:ASN:HD22	1:A:79:ASN:H	0.47	1.51	8	1
1:A:62:LEU:N	1:A:62:LEU:HD22	0.47	2.24	3	1
1:A:53:VAL:HG21	1:A:60:ILE:CG2	0.47	2.40	13	1
1:A:65:LEU:CB	1:A:93:MET:SD	0.47	3.03	12	4
1:A:39:TYR:CE2	1:A:49:LEU:HD12	0.47	2.45	18	6
1:A:88:VAL:HG23	1:A:88:VAL:O	0.47	2.09	4	1
1:A:24:LYS:CG	1:A:24:LYS:O	0.47	2.62	17	1
1:A:79:ASN:HD22	1:A:79:ASN:N	0.47	2.05	2	1
1:A:57:LYS:O	1:A:58:ASP:CG	0.47	2.53	7	5
1:A:25:GLN:C	1:A:27:ASP:N	0.47	2.67	2	3
1:A:46:ASP:O	1:A:47:GLN:CB	0.47	2.62	18	1
1:A:65:LEU:O	1:A:66:GLN:O	0.47	2.33	13	6
1:A:13:SER:OG	1:A:14:SER:N	0.46	2.48	1	3
1:A:27:ASP:C	1:A:29:GLY:N	0.46	2.69	3	3
1:A:14:SER:H	1:A:17:SER:HG	0.46	1.53	9	1
1:A:40:ARG:NH1	1:A:45:GLU:CB	0.46	2.79	10	1
1:A:24:LYS:H	1:A:24:LYS:HD3	0.46	1.70	2	1
1:A:32:ILE:HG12	1:A:77:ALA:HB1	0.46	1.88	12	15
1:A:26:ASP:O	1:A:85:GLU:OE1	0.46	2.33	15	2
1:A:37:VAL:O	1:A:51:LYS:N	0.46	2.47	14	9
1:A:25:GLN:O	1:A:26:ASP:O	0.46	2.33	19	1
1:A:81:LEU:CD1	1:A:81:LEU:N	0.46	2.78	14	3
1:A:40:ARG:HH21	1:A:47:GLN:N	0.46	2.07	16	1
1:A:25:GLN:O	1:A:85:GLU:OE1	0.46	2.34	5	1
1:A:24:LYS:O	1:A:24:LYS:CG	0.46	2.64	8	1
1:A:85:GLU:OE1	1:A:85:GLU:O	0.45	2.34	20	1
1:A:85:GLU:CA	1:A:85:GLU:OE1	0.45	2.64	6	1
1:A:62:LEU:N	1:A:62:LEU:HD12	0.45	2.27	17	3
1:A:27:ASP:OD2	1:A:30:ALA:O	0.45	2.35	13	6
1:A:41:SER:O	1:A:44:LYS:O	0.45	2.35	2	7
1:A:62:LEU:HD12	1:A:62:LEU:N	0.45	2.27	8	1
1:A:67:TRP:NE1	1:A:96:LYS:HE2	0.45	2.25	18	1
1:A:63:GLU:O	1:A:64:HIS:CD2	0.45	2.70	6	1
1:A:40:ARG:HH12	1:A:44:LYS:C	0.44	2.15	16	1
1:A:37:VAL:HG21	1:A:60:ILE:HD13	0.44	1.89	1	1
1:A:17:SER:OG	1:A:61:ILE:HG22	0.44	2.11	18	1
1:A:54:GLN:C	1:A:56:ASN:H	0.44	2.16	11	6
1:A:65:LEU:C	1:A:93:MET:SD	0.44	2.96	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:45:GLU:O	1:A:46:ASP:OD1	0.44	2.36	16	2
1:A:13:SER:OG	1:A:17:SER:OG	0.44	2.35	10	2
1:A:40:ARG:NH2	1:A:47:GLN:O	0.44	2.50	16	1
1:A:27:ASP:O	1:A:27:ASP:OD1	0.44	2.35	20	2
1:A:46:ASP:O	1:A:47:GLN:NE2	0.44	2.51	5	1
1:A:91:PHE:O	1:A:91:PHE:CG	0.44	2.70	3	3
1:A:33:LEU:O	1:A:55:GLY:N	0.44	2.51	12	1
1:A:5:PRO:CB	1:A:6:PRO:CD	0.44	2.94	20	1
1:A:26:ASP:N	1:A:26:ASP:OD1	0.44	2.49	4	1
1:A:43:ASP:O	1:A:45:GLU:OE2	0.44	2.36	8	1
1:A:50:GLU:CD	1:A:50:GLU:N	0.44	2.71	10	1
1:A:24:LYS:CD	1:A:24:LYS:H	0.44	2.25	19	1
1:A:46:ASP:O	1:A:47:GLN:HB2	0.44	2.13	18	1
1:A:36:ILE:HG23	1:A:52:LYS:HZ3	0.43	1.72	17	1
1:A:58:ASP:CG	1:A:58:ASP:O	0.43	2.55	10	1
1:A:45:GLU:O	1:A:46:ASP:CG	0.43	2.57	5	1
1:A:26:ASP:O	1:A:27:ASP:O	0.43	2.36	13	3
1:A:39:TYR:N	1:A:39:TYR:CD1	0.43	2.86	12	1
1:A:26:ASP:OD1	1:A:26:ASP:O	0.43	2.36	3	1
1:A:83:TYR:CD1	1:A:83:TYR:N	0.43	2.87	16	2
1:A:41:SER:OG	1:A:71:TYR:CZ	0.43	2.69	7	1
1:A:84:SER:O	1:A:85:GLU:OE2	0.43	2.35	20	1
1:A:25:GLN:OE1	1:A:85:GLU:OE1	0.43	2.35	10	2
1:A:63:GLU:C	1:A:64:HIS:CG	0.43	2.91	13	1
1:A:82:GLY:O	1:A:83:TYR:CD1	0.43	2.72	8	1
1:A:62:LEU:N	1:A:62:LEU:CD1	0.43	2.80	12	2
1:A:33:LEU:CD2	1:A:33:LEU:N	0.43	2.81	1	1
1:A:45:GLU:O	1:A:45:GLU:OE1	0.43	2.36	16	1
1:A:26:ASP:O	1:A:85:GLU:OE2	0.43	2.37	6	2
1:A:43:ASP:O	1:A:43:ASP:OD1	0.43	2.37	12	1
1:A:25:GLN:HE22	1:A:87:THR:HG23	0.43	1.74	1	1
1:A:16:LYS:O	1:A:65:LEU:HD12	0.43	2.14	11	1
1:A:62:LEU:CD1	1:A:62:LEU:N	0.42	2.81	8	1
1:A:58:ASP:OD1	1:A:58:ASP:O	0.42	2.37	10	1
1:A:16:LYS:HZ2	1:A:66:GLN:H	0.42	1.55	20	1
1:A:37:VAL:HG21	1:A:60:ILE:CD1	0.42	2.45	11	2
1:A:40:ARG:CZ	1:A:72:GLU:CD	0.42	2.88	4	1
1:A:83:TYR:N	1:A:83:TYR:CD1	0.42	2.88	15	1
1:A:25:GLN:N	1:A:25:GLN:CD	0.42	2.73	14	1
1:A:25:GLN:C	1:A:27:ASP:H	0.42	2.17	2	2
1:A:16:LYS:HZ1	1:A:64:HIS:HA	0.42	1.74	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Models Total
1:A:54:GLN:O	1:A:56:ASN:N	0.42	2.52	11	1
1:A:14:SER:N	1:A:17:SER:OG	0.42	2.51	9	1
1:A:27:ASP:O	1:A:28:GLY:C	0.42	2.58	12	2
1:A:37:VAL:HG22	1:A:75:ILE:HG13	0.42	1.92	1	2
1:A:40:ARG:NH1	1:A:72:GLU:CD	0.41	2.73	4	1
1:A:36:ILE:HG12	1:A:52:LYS:HZ2	0.41	1.75	1	1
1:A:82:GLY:O	1:A:83:TYR:CD2	0.41	2.73	2	1
1:A:65:LEU:O	1:A:66:GLN:C	0.41	2.58	19	4
1:A:40:ARG:NH1	1:A:45:GLU:CG	0.41	2.83	13	1
1:A:44:LYS:O	1:A:45:GLU:O	0.41	2.39	5	1
1:A:85:GLU:CD	1:A:85:GLU:O	0.41	2.58	20	2
1:A:46:ASP:OD1	1:A:46:ASP:O	0.41	2.38	6	1
1:A:46:ASP:N	1:A:46:ASP:OD1	0.41	2.53	14	1
1:A:36:ILE:HG23	1:A:52:LYS:NZ	0.41	2.30	2	1
1:A:26:ASP:O	1:A:27:ASP:CG	0.41	2.59	20	2
1:A:22:ILE:HG21	1:A:35:TYR:CE2	0.41	2.51	20	1
1:A:53:VAL:HG12	1:A:54:GLN:N	0.41	2.30	14	1
1:A:82:GLY:O	1:A:83:TYR:CG	0.41	2.74	10	1
1:A:50:GLU:CD	1:A:50:GLU:H	0.41	2.18	10	1
1:A:22:ILE:O	1:A:58:ASP:CG	0.41	2.59	12	1
1:A:14:SER:O	1:A:15:GLY:C	0.41	2.57	19	1
1:A:58:ASP:OD1	1:A:58:ASP:C	0.41	2.58	10	1
1:A:32:ILE:CD1	1:A:77:ALA:HB1	0.40	2.46	3	2
1:A:64:HIS:O	1:A:64:HIS:CD2	0.40	2.74	13	1
1:A:13:SER:O	1:A:14:SER:C	0.40	2.60	13	1
1:A:13:SER:OG	1:A:17:SER:O	0.40	2.38	13	1
1:A:33:LEU:N	1:A:33:LEU:CD1	0.40	2.84	3	1
1:A:95:PRO:O	1:A:96:LYS:C	0.40	2.59	5	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	93/114 (82%)	76±2 (82±2%)	11±2 (12±3%)	6±2 (6±2%)	3	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1860/2280 (82%)	1528 (82%)	215 (12%)	117 (6%)	3	20

All 19 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	6	PRO	17
1	A	5	PRO	14
1	A	29	GLY	10
1	A	66	GLN	10
1	A	13	SER	10
1	A	64	HIS	9
1	A	24	LYS	7
1	A	26	ASP	7
1	A	12	PRO	6
1	A	27	ASP	6
1	A	28	GLY	5
1	A	45	GLU	4
1	A	7	SER	3
1	A	46	ASP	3
1	A	85	GLU	2
1	A	44	LYS	1
1	A	15	GLY	1
1	A	55	GLY	1
1	A	47	GLN	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	83/102 (81%)	75±2 (90±2%)	8±2 (10±2%)	14	58
All	All	1660/2040 (81%)	1492 (90%)	168 (10%)	14	58

All 35 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	PHE	20
1	A	51	LYS	18
1	A	59	HIS	18
1	A	53	VAL	14
1	A	7	SER	12
1	A	24	LYS	10
1	A	87	THR	10
1	A	79	ASN	9
1	A	60	ILE	7
1	A	25	GLN	6
1	A	92	SER	6
1	A	85	GLU	5
1	A	58	ASP	4
1	A	40	ARG	3
1	A	50	GLU	2
1	A	43	ASP	2
1	A	6	PRO	2
1	A	11	GLN	2
1	A	76	THR	2
1	A	54	GLN	1
1	A	9	HIS	1
1	A	22	ILE	1
1	A	26	ASP	1
1	A	73	VAL	1
1	A	27	ASP	1
1	A	34	GLU	1
1	A	88	VAL	1
1	A	44	LYS	1
1	A	69	MET	1
1	A	66	GLN	1
1	A	45	GLU	1
1	A	17	SER	1
1	A	96	LYS	1
1	A	80	ARG	1
1	A	16	LYS	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 carbohydrates 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 ⓘ

No chemical shift data were provided