



Full wwPDB NMR Structure Validation Report ⓘ

May 28, 2020 – 10:12 pm BST

PDB ID : 2JNA
Title : Solution NMR Structure of Salmonella typhimurium LT2 Secreted Protein STM0082: Northeast Structural Genomics Consortium Target StR109
Authors : Eletsky, A.; Parish, D.; Liu, G.; Sukumaran, D.; Jiang, M.; Cunningham, K.; Ma, L.; Xiao, R.; Rost, B.; Montelione, G.T.; Szyperski, T.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2006-12-31

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:

Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
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	:	2.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

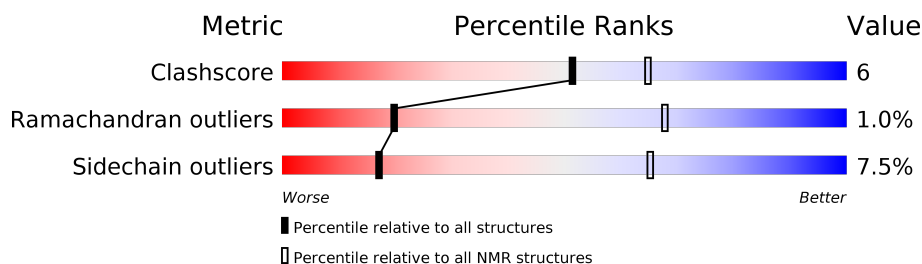
1 Overall quality at a glance

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	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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	104	 58% 11% • 31%
1	B	104	 63% 6% • 31%

2 Ensemble composition and analysis

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:22-A:93, B:222-B:293 (144)	0.57	1

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

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

The models can be grouped into 3 clusters and 4 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3200 atoms, of which 1598 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Putative secreted protein.

Mol	Chain	Residues	Atoms						Trace
1	A	104	Total	C	H	N	O	S	0
			1600	504	799	147	149	1	
1	B	104	Total	C	H	N	O	S	0
			1600	504	799	147	149	1	

There are 16 discrepancies between the modelled and reference sequences:

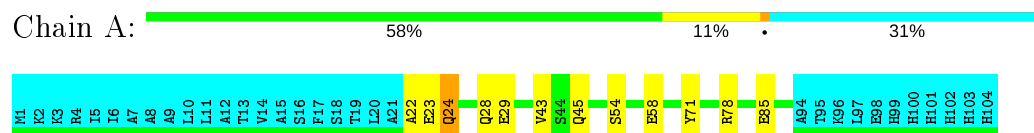
Chain	Residue	Modelled	Actual	Comment	Reference
A	97	LEU	-	EXPRESSION TAG	UNP Q7CR88
A	98	GLU	-	EXPRESSION TAG	UNP Q7CR88
A	99	HIS	-	EXPRESSION TAG	UNP Q7CR88
A	100	HIS	-	EXPRESSION TAG	UNP Q7CR88
A	101	HIS	-	EXPRESSION TAG	UNP Q7CR88
A	102	HIS	-	EXPRESSION TAG	UNP Q7CR88
A	103	HIS	-	EXPRESSION TAG	UNP Q7CR88
A	104	HIS	-	EXPRESSION TAG	UNP Q7CR88
B	297	LEU	-	EXPRESSION TAG	UNP Q7CR88
B	298	GLU	-	EXPRESSION TAG	UNP Q7CR88
B	299	HIS	-	EXPRESSION TAG	UNP Q7CR88
B	300	HIS	-	EXPRESSION TAG	UNP Q7CR88
B	301	HIS	-	EXPRESSION TAG	UNP Q7CR88
B	302	HIS	-	EXPRESSION TAG	UNP Q7CR88
B	303	HIS	-	EXPRESSION TAG	UNP Q7CR88
B	304	HIS	-	EXPRESSION TAG	UNP Q7CR88

4 Residue-property plots

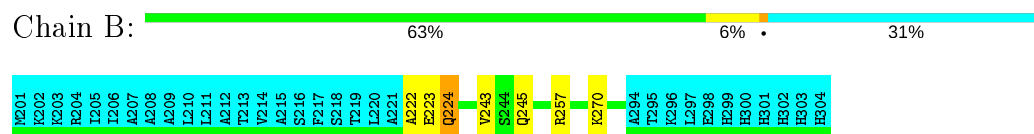
4.1 Average score per residue in the NMR ensemble

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: Putative secreted protein



- Molecule 1: Putative secreted protein

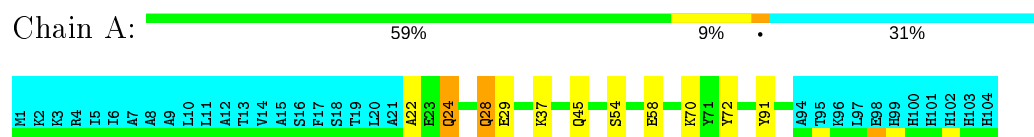


4.2 Scores per residue for each member of the ensemble

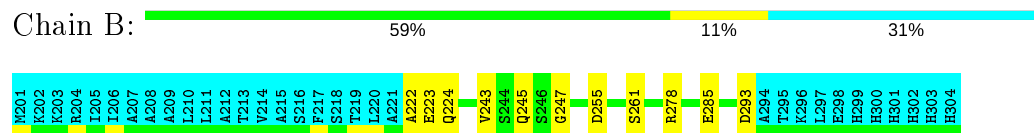
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Putative secreted protein

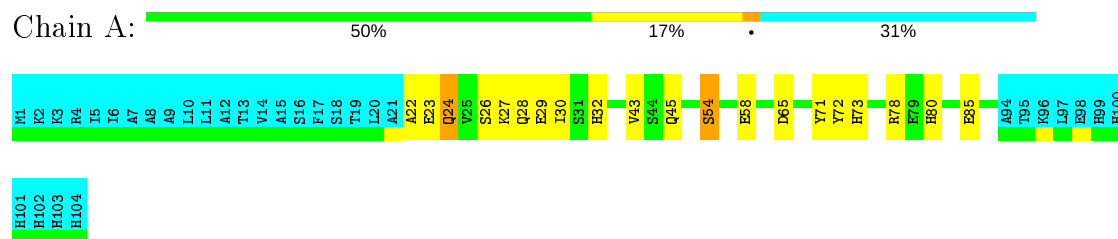


- Molecule 1: Putative secreted protein

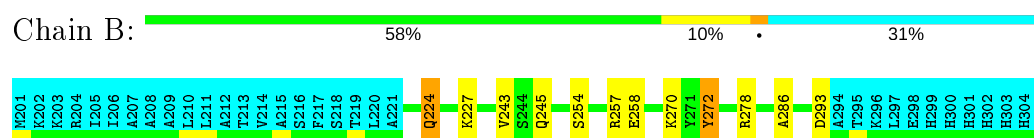


4.2.2 Score per residue for model 2

- Molecule 1: Putative secreted protein

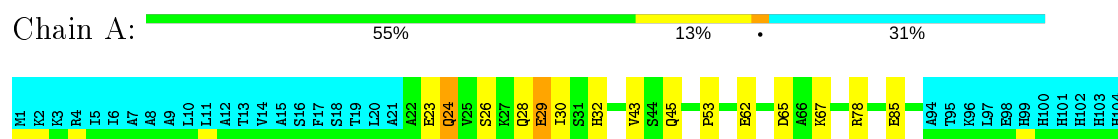


- Molecule 1: Putative secreted protein

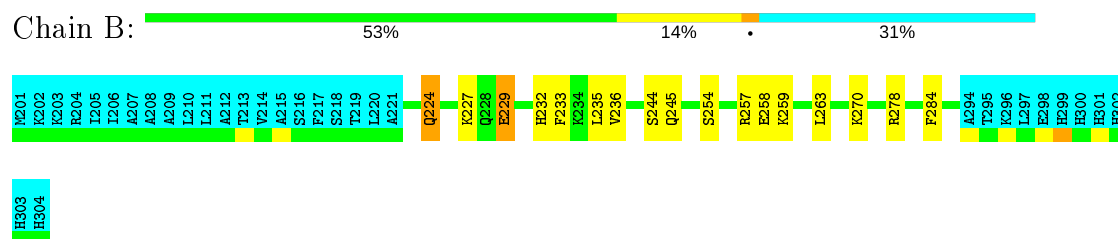


4.2.3 Score per residue for model 3

- Molecule 1: Putative secreted protein

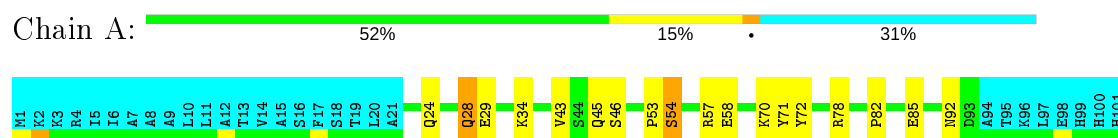


- Molecule 1: Putative secreted protein



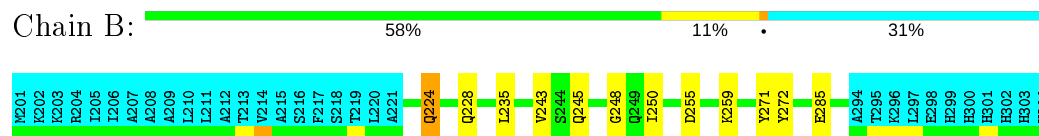
4.2.4 Score per residue for model 4

- Molecule 1: Putative secreted protein



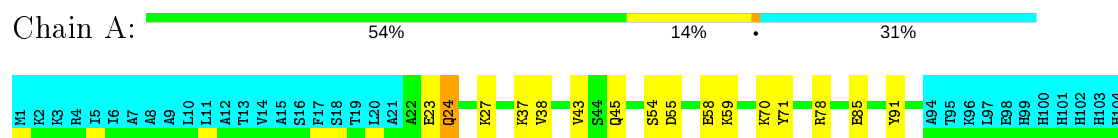
H102
H103
H104

- Molecule 1: Putative secreted protein

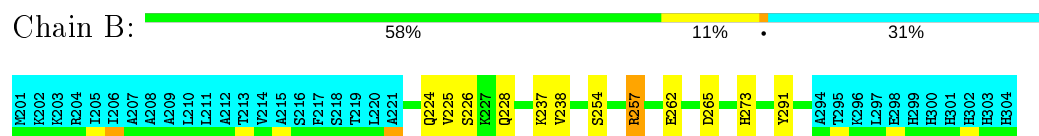


4.2.5 Score per residue for model 5

- Molecule 1: Putative secreted protein

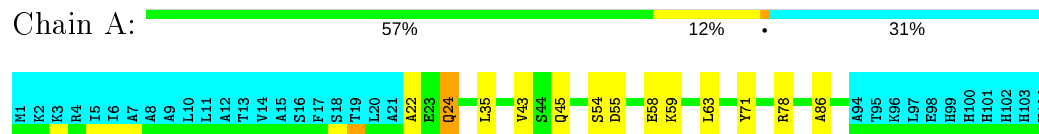


- Molecule 1: Putative secreted protein

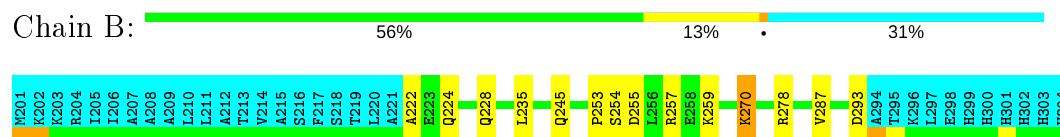


4.2.6 Score per residue for model 6

- Molecule 1: Putative secreted protein

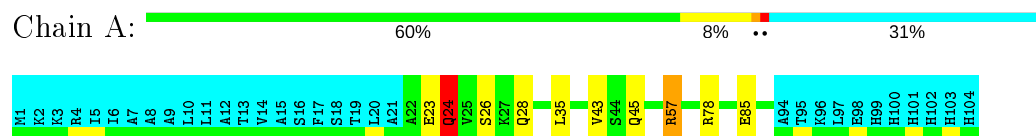


- Molecule 1: Putative secreted protein

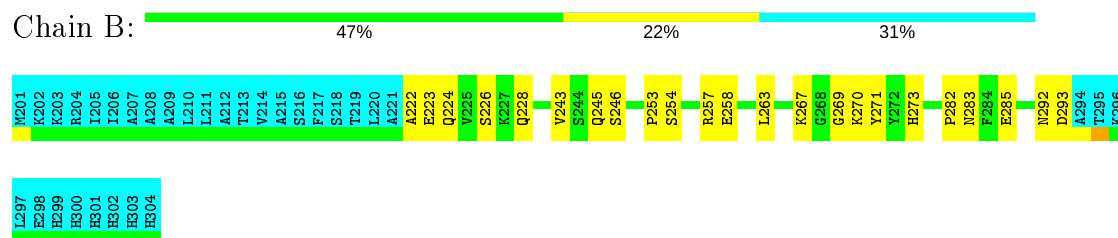


4.2.7 Score per residue for model 7

- Molecule 1: Putative secreted protein

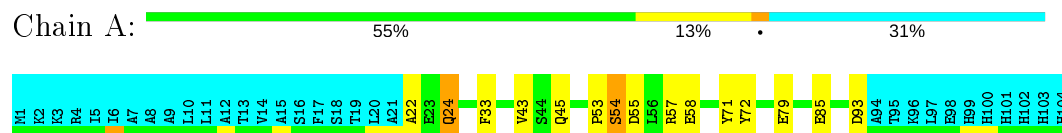


- Molecule 1: Putative secreted protein

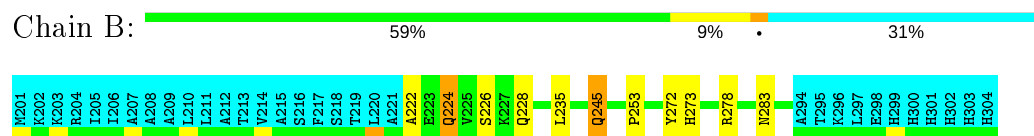


4.2.8 Score per residue for model 8

- Molecule 1: Putative secreted protein

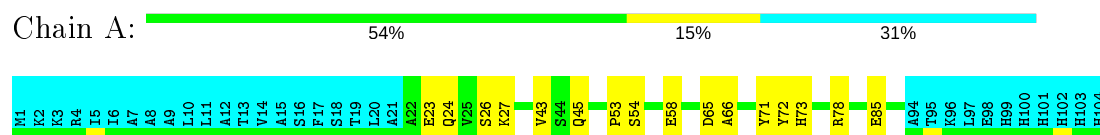


- Molecule 1: Putative secreted protein

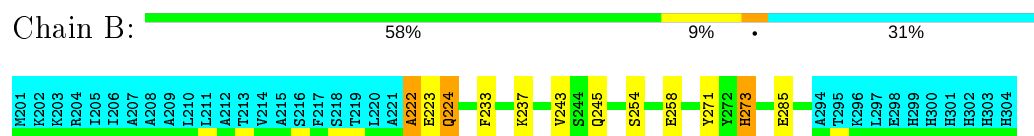


4.2.9 Score per residue for model 9

- Molecule 1: Putative secreted protein

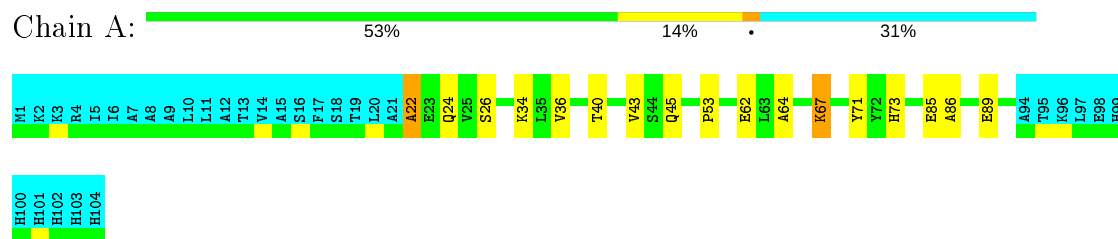


- Molecule 1: Putative secreted protein

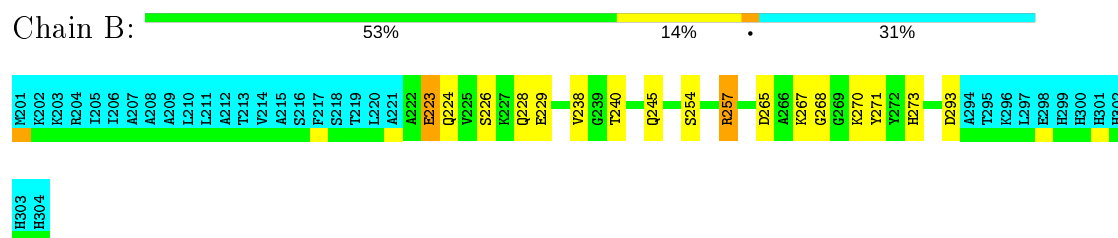


4.2.10 Score per residue for model 10

- Molecule 1: Putative secreted protein

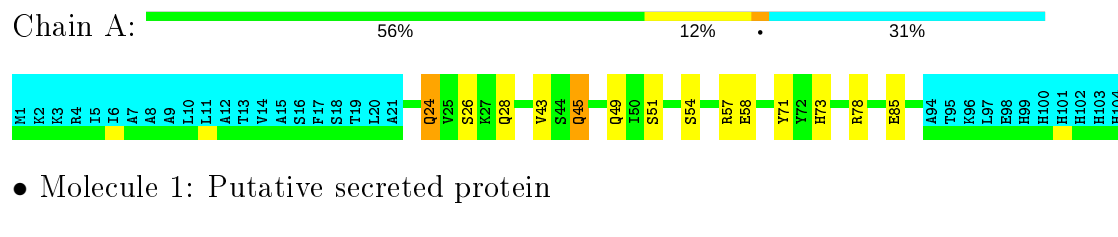


- Molecule 1: Putative secreted protein

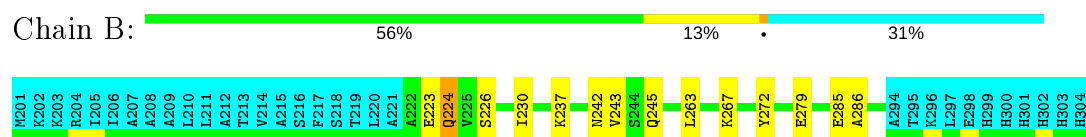


4.2.11 Score per residue for model 11

- Molecule 1: Putative secreted protein

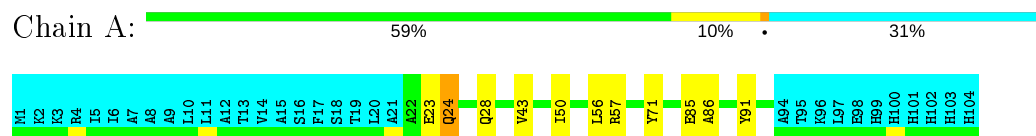


- Molecule 1: Putative secreted protein

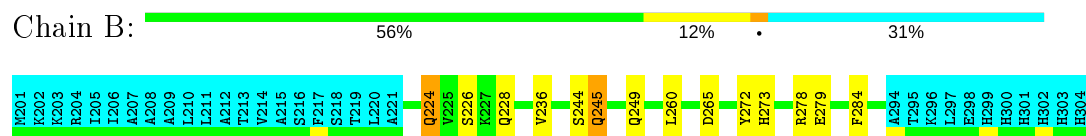


4.2.12 Score per residue for model 12

- Molecule 1: Putative secreted protein

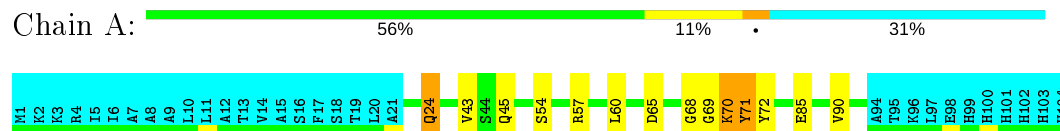


- Molecule 1: Putative secreted protein

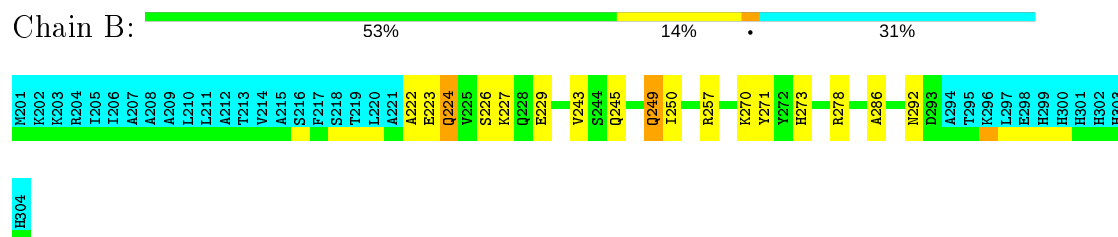


4.2.13 Score per residue for model 13

- Molecule 1: Putative secreted protein

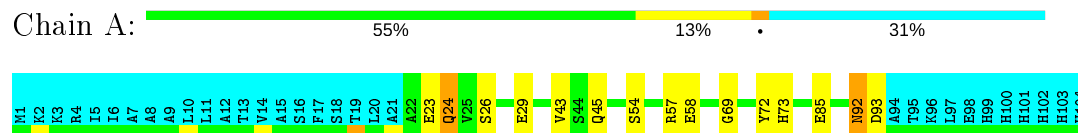


- Molecule 1: Putative secreted protein

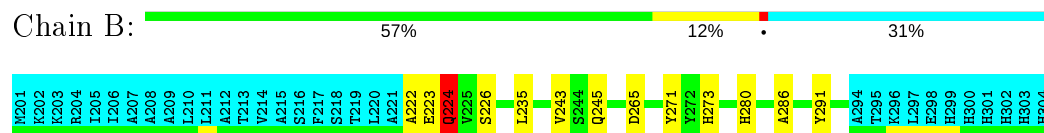


4.2.14 Score per residue for model 14

- Molecule 1: Putative secreted protein



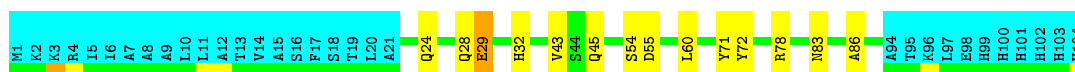
- Molecule 1: Putative secreted protein



4.2.15 Score per residue for model 15

- Molecule 1: Putative secreted protein





- Molecule 1: Putative secreted protein

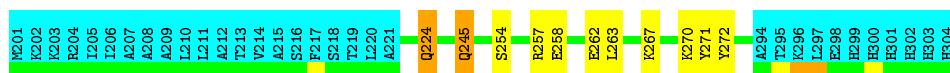


4.2.16 Score per residue for model 16

- Molecule 1: Putative secreted protein



- Molecule 1: Putative secreted protein

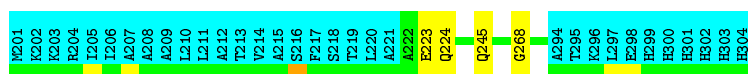


4.2.17 Score per residue for model 17

- Molecule 1: Putative secreted protein

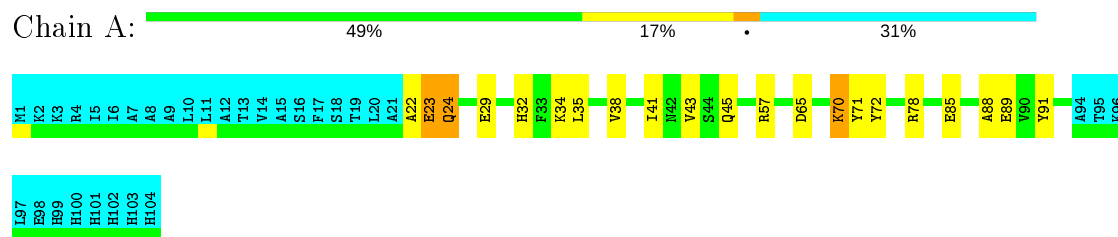


- Molecule 1: Putative secreted protein

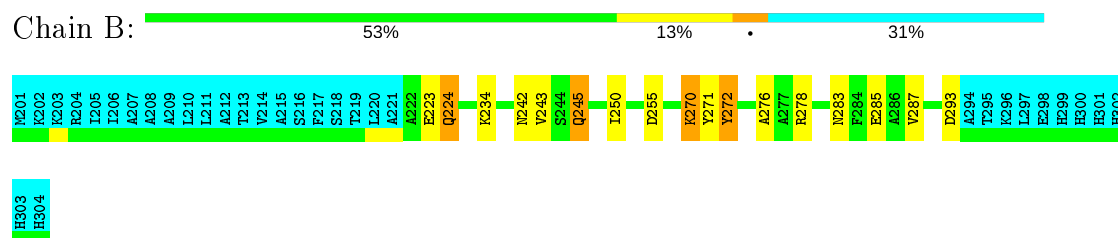


4.2.18 Score per residue for model 18

- Molecule 1: Putative secreted protein

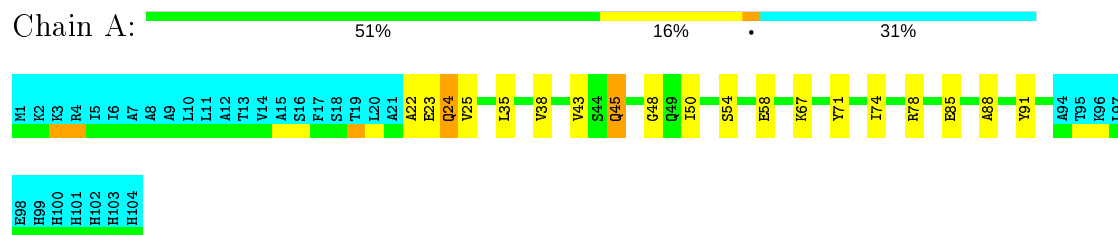


- Molecule 1: Putative secreted protein

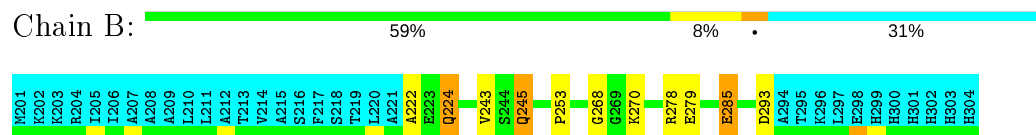


4.2.19 Score per residue for model 19

- Molecule 1: Putative secreted protein



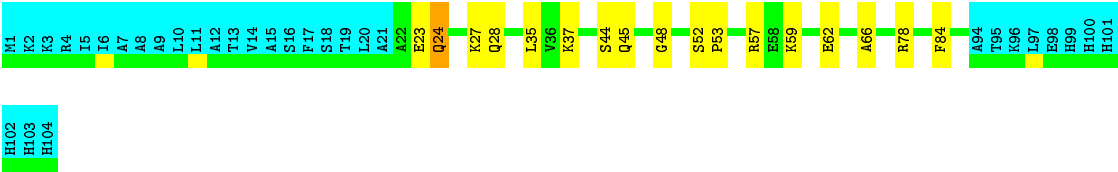
- Molecule 1: Putative secreted protein



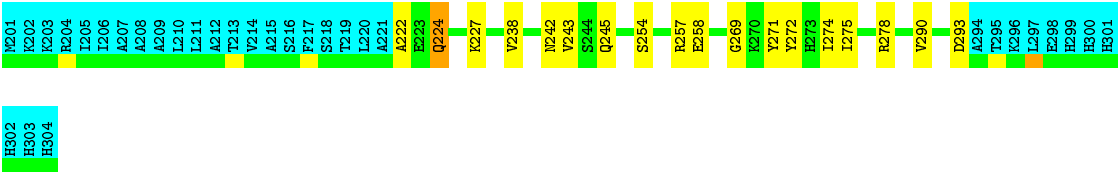
4.2.20 Score per residue for model 20

- Molecule 1: Putative secreted protein





● Molecule 1: Putative secreted protein



5 Refinement protocol and experimental data overview

The models were refined using the following method: *TORSION ANGLE DYNAMICS*, *explicit water bath refinement*.

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

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

Software name	Classification	Version
CYANA	structure solution	2.1
CYANA	refinement	2.1
CNS	refinement	1.1
CNS	structure solution	1.1

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

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	553	541	541	8±2
1	B	553	541	541	7±3
All	All	22120	21640	21640	252

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 6.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:24:GLN:HG3	1:B:224:GLN:HG3	0.99	1.34	9	2
1:A:53:PRO:HG3	1:B:235:LEU:HD21	0.73	1.59	4	1
1:A:53:PRO:HG2	1:B:235:LEU:HD21	0.71	1.63	8	1
1:B:223:GLU:HB3	1:B:271:TYR:HE2	0.70	1.45	9	1
1:B:270:LYS:HD3	1:B:293:ASP:HB2	0.70	1.62	19	2
1:B:226:SER:HA	1:B:273:HIS:CD2	0.69	2.23	7	7
1:A:35:LEU:HD21	1:B:253:PRO:HG2	0.69	1.65	6	2
1:A:24:GLN:HB3	1:B:224:GLN:CB	0.69	2.17	20	1
1:A:72:TYR:CD1	1:B:222:ALA:HB1	0.68	2.23	13	1
1:A:23:GLU:HB3	1:A:71:TYR:HE1	0.68	1.49	2	1
1:B:249:GLN:HE21	1:B:249:GLN:HA	0.67	1.50	13	1
1:A:71:TYR:CE1	1:A:91:TYR:HB2	0.66	2.26	12	2
1:A:24:GLN:HA	1:A:71:TYR:HB2	0.65	1.69	19	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:43:VAL:O	1:A:85:GLU:HA	0.64	1.93	13	15
1:A:53:PRO:HB2	1:B:293:ASP:HB2	0.64	1.70	10	1
1:B:223:GLU:HG2	1:B:271:TYR:HE1	0.63	1.54	7	1
1:A:23:GLU:O	1:A:24:GLN:HB3	0.63	1.93	17	2
1:A:53:PRO:HD3	1:B:233:PHE:HB3	0.63	1.71	9	1
1:A:70:LYS:HD2	1:A:93:ASP:HB2	0.62	1.69	16	1
1:B:223:GLU:HB3	1:B:271:TYR:HE1	0.62	1.55	13	1
1:A:23:GLU:HA	1:B:272:TYR:OH	0.61	1.95	12	1
1:B:223:GLU:HB3	1:B:271:TYR:CE2	0.59	2.29	9	1
1:B:243:VAL:O	1:B:285:GLU:HA	0.59	1.96	4	7
1:A:22:ALA:HA	1:B:223:GLU:HG3	0.59	1.74	10	1
1:A:22:ALA:HB1	1:B:272:TYR:CD1	0.58	2.33	18	1
1:A:26:SER:HA	1:A:73:HIS:CD2	0.58	2.33	10	5
1:B:254:SER:O	1:B:257:ARG:HG3	0.58	1.98	5	1
1:A:57:ARG:HD2	1:B:223:GLU:OE2	0.57	1.99	18	2
1:A:33:PHE:HB3	1:B:253:PRO:HG3	0.57	1.76	8	1
1:A:26:SER:HB2	1:A:28:GLN:OE1	0.56	2.01	3	1
1:B:237:LYS:HD3	1:B:291:TYR:CZ	0.56	2.36	5	1
1:A:70:LYS:HA	1:A:70:LYS:NZ	0.55	2.16	13	1
1:A:24:GLN:HB3	1:B:224:GLN:HB2	0.55	1.77	20	1
1:A:24:GLN:HA	1:A:71:TYR:CD1	0.54	2.37	11	1
1:B:245:GLN:HE21	1:B:245:GLN:HA	0.54	1.61	16	1
1:B:245:GLN:O	1:B:283:ASN:HA	0.53	2.02	8	2
1:A:23:GLU:HG2	1:B:222:ALA:H	0.53	1.62	19	1
1:A:54:SER:O	1:A:58:GLU:HG2	0.53	2.03	4	8
1:A:28:GLN:HG2	1:A:29:GLU:OE1	0.52	2.04	1	1
1:A:22:ALA:HB1	1:B:272:TYR:CD2	0.52	2.39	2	2
1:A:24:GLN:HB2	1:B:224:GLN:HB3	0.52	1.81	16	2
1:A:71:TYR:HA	1:B:222:ALA:CB	0.52	2.35	15	1
1:B:245:GLN:HE21	1:B:245:GLN:CA	0.52	2.18	16	1
1:B:254:SER:HA	1:B:257:ARG:NH1	0.52	2.19	10	1
1:A:26:SER:HB3	1:A:28:GLN:OE1	0.51	2.06	17	1
1:B:243:VAL:HG13	1:B:245:GLN:NE2	0.51	2.19	20	3
1:B:270:LYS:NZ	1:B:270:LYS:HA	0.51	2.21	6	1
1:B:243:VAL:HB	1:B:286:ALA:HB3	0.51	1.81	14	4
1:B:263:LEU:O	1:B:267:LYS:HG2	0.51	2.06	11	3
1:A:72:TYR:CD2	1:B:222:ALA:HB1	0.50	2.41	1	3
1:A:37:LYS:HD3	1:A:91:TYR:CE1	0.50	2.42	5	1
1:A:43:VAL:HG13	1:A:45:GLN:NE2	0.50	2.22	17	1
1:A:38:VAL:HG22	1:A:92:ASN:OD1	0.49	2.07	16	1
1:B:223:GLU:HG2	1:B:271:TYR:CE1	0.49	2.40	7	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:70:LYS:HA	1:A:70:LYS:HZ3	0.49	1.67	13	1
1:A:24:GLN:CB	1:B:224:GLN:HB3	0.49	2.37	16	1
1:B:270:LYS:HA	1:B:270:LYS:HE2	0.49	1.83	13	2
1:A:26:SER:HA	1:A:73:HIS:HD2	0.49	1.68	16	1
1:A:43:VAL:HB	1:A:86:ALA:HB3	0.49	1.84	6	4
1:B:246:SER:HA	1:B:282:PRO:O	0.48	2.08	7	1
1:A:27:LYS:HD3	1:A:27:LYS:O	0.48	2.08	17	1
1:B:238:VAL:HG12	1:B:267:LYS:HD2	0.48	1.84	10	1
1:A:45:GLN:HB3	1:A:49:GLN:HB2	0.48	1.85	11	1
1:B:254:SER:O	1:B:258:GLU:HG2	0.48	2.08	7	5
1:A:23:GLU:HG2	1:B:222:ALA:N	0.48	2.23	19	1
1:A:24:GLN:HG3	1:B:224:GLN:HB3	0.48	1.85	8	1
1:B:255:ASP:O	1:B:259:LYS:HD3	0.48	2.08	6	1
1:B:270:LYS:HZ3	1:B:270:LYS:HB3	0.48	1.69	3	1
1:A:24:GLN:HB3	1:B:224:GLN:HB3	0.48	1.83	20	1
1:A:22:ALA:HA	1:B:223:GLU:OE2	0.48	2.08	17	1
1:A:24:GLN:CG	1:B:224:GLN:HG3	0.47	2.38	5	2
1:A:46:SER:HA	1:A:82:PRO:O	0.47	2.08	4	1
1:B:229:GLU:CD	1:B:229:GLU:H	0.47	2.13	13	1
1:A:69:GLY:HA2	1:A:92:ASN:HA	0.47	1.87	14	1
1:A:55:ASP:O	1:A:59:LYS:HG2	0.47	2.10	6	2
1:A:24:GLN:HA	1:A:71:TYR:CB	0.47	2.40	13	2
1:B:224:GLN:HG3	1:B:272:TYR:O	0.47	2.09	4	1
1:B:224:GLN:HA	1:B:271:TYR:HB3	0.47	1.87	16	2
1:B:271:TYR:CZ	1:B:291:TYR:HB2	0.47	2.45	14	1
1:A:70:LYS:HG3	1:A:93:ASP:OD2	0.47	2.10	17	1
1:B:257:ARG:HD2	1:B:257:ARG:C	0.47	2.30	20	1
1:A:29:GLU:HA	1:A:32:HIS:HB3	0.47	1.86	17	5
1:A:60:LEU:HD13	1:A:72:TYR:CE2	0.47	2.45	15	1
1:A:53:PRO:HG3	1:B:233:PHE:HB3	0.46	1.87	3	1
1:A:24:GLN:HA	1:A:71:TYR:HB3	0.46	1.87	8	2
1:B:254:SER:O	1:B:257:ARG:HD2	0.46	2.10	10	1
1:B:250:ILE:HA	1:B:255:ASP:OD2	0.46	2.11	4	1
1:A:45:GLN:HG2	1:A:50:ILE:HG12	0.46	1.86	19	1
1:B:254:SER:O	1:B:257:ARG:HB3	0.46	2.11	6	1
1:A:70:LYS:HG2	1:A:92:ASN:OD1	0.46	2.10	17	1
1:B:259:LYS:HD2	1:B:259:LYS:N	0.46	2.26	4	1
1:A:24:GLN:HB2	1:B:224:GLN:HB2	0.46	1.86	13	2
1:B:244:SER:HA	1:B:284:PHE:O	0.46	2.10	12	2
1:A:54:SER:O	1:A:57:ARG:HG3	0.46	2.11	8	1
1:B:226:SER:HA	1:B:273:HIS:HD2	0.46	1.70	12	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:GLU:HB3	1:A:71:TYR:HE2	0.46	1.69	5	1
1:B:276:ALA:HB3	1:B:287:VAL:HB	0.46	1.87	18	1
1:B:224:GLN:HA	1:B:271:TYR:HD1	0.46	1.70	20	1
1:A:24:GLN:CB	1:B:224:GLN:HB2	0.46	2.41	2	2
1:A:59:LYS:O	1:A:63:LEU:HG	0.46	2.10	6	2
1:B:269:GLY:HA3	1:B:290:VAL:CG1	0.46	2.41	20	1
1:A:24:GLN:HB3	1:B:224:GLN:HG3	0.45	1.88	12	1
1:B:226:SER:O	1:B:230:ILE:HG13	0.45	2.12	11	2
1:A:24:GLN:HB2	1:B:223:GLU:H	0.45	1.70	1	1
1:A:57:ARG:HD2	1:B:223:GLU:CD	0.45	2.32	11	1
1:A:53:PRO:CD	1:B:233:PHE:HB3	0.45	2.40	9	1
1:B:229:GLU:HA	1:B:232:HIS:HB3	0.44	1.89	3	1
1:A:54:SER:O	1:A:58:GLU:HG3	0.44	2.11	9	2
1:A:22:ALA:HB2	1:B:270:LYS:O	0.44	2.13	10	2
1:A:24:GLN:CD	1:B:224:GLN:HG3	0.44	2.33	18	2
1:B:259:LYS:O	1:B:263:LEU:HG	0.44	2.13	3	1
1:A:24:GLN:HG3	1:A:72:TYR:O	0.44	2.13	18	1
1:B:254:SER:O	1:B:258:GLU:HG3	0.44	2.12	16	1
1:A:22:ALA:O	1:B:261:SER:HB3	0.44	2.13	1	1
1:B:224:GLN:HG2	1:B:225:VAL:N	0.43	2.28	5	1
1:B:245:GLN:HB3	1:B:249:GLN:OE1	0.43	2.13	12	1
1:A:37:LYS:HD3	1:A:91:TYR:CE2	0.43	2.48	1	1
1:A:23:GLU:O	1:A:24:GLN:HB2	0.43	2.12	7	2
1:A:52:SER:HB3	1:A:53:PRO:HD2	0.43	1.90	20	1
1:A:43:VAL:CG2	1:A:60:LEU:HD21	0.43	2.43	13	1
1:B:237:LYS:HD3	1:B:291:TYR:CE2	0.43	2.48	5	1
1:A:57:ARG:HD2	1:B:223:GLU:OE1	0.43	2.14	11	1
1:A:54:SER:HA	1:A:57:ARG:NE	0.43	2.29	13	1
1:A:28:GLN:HB2	1:A:29:GLU:OE2	0.42	2.13	4	1
1:B:229:GLU:H	1:B:229:GLU:CD	0.42	2.17	10	1
1:A:69:GLY:HA3	1:A:90:VAL:HG12	0.42	1.91	13	1
1:B:270:LYS:CE	1:B:270:LYS:HA	0.42	2.44	18	1
1:A:26:SER:O	1:A:30:ILE:HG13	0.42	2.14	2	2
1:A:41:ILE:HG13	1:A:88:ALA:HB3	0.42	1.90	18	1
1:A:74:ILE:HG12	1:A:88:ALA:HB2	0.42	1.90	19	1
1:A:72:TYR:OH	1:B:223:GLU:HA	0.42	2.14	15	1
1:A:71:TYR:OH	1:B:257:ARG:HD3	0.42	2.14	16	1
1:A:55:ASP:O	1:A:58:GLU:HB2	0.42	2.15	8	1
1:A:26:SER:HB3	1:A:29:GLU:OE2	0.42	2.15	16	1
1:A:27:LYS:HB2	1:A:73:HIS:CE1	0.42	2.50	2	1
1:B:227:LYS:O	1:B:227:LYS:HD3	0.42	2.15	3	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:22:ALA:HB2	1:B:271:TYR:HA	0.42	1.91	10	1
1:A:24:GLN:HB3	1:B:224:GLN:OE1	0.42	2.14	14	1
1:A:70:LYS:HA	1:A:70:LYS:HE2	0.41	1.90	5	1
1:A:64:ALA:O	1:A:67:LYS:HG3	0.41	2.15	10	1
1:A:27:LYS:HA	1:A:30:ILE:HD12	0.41	1.92	17	1
1:A:23:GLU:HB3	1:B:257:ARG:HG3	0.41	1.91	3	1
1:A:24:GLN:OE1	1:B:273:HIS:HA	0.41	2.15	9	1
1:B:260:LEU:HB3	1:B:272:TYR:CZ	0.41	2.50	12	1
1:A:27:LYS:C	1:A:27:LYS:HD3	0.41	2.36	20	1
1:B:235:LEU:HD22	1:B:293:ASP:HA	0.41	1.90	6	1
1:B:224:GLN:HG2	1:B:272:TYR:O	0.41	2.16	16	1
1:B:271:TYR:HE2	1:B:293:ASP:HB2	0.41	1.75	18	1
1:A:24:GLN:HB2	1:B:223:GLU:O	0.41	2.15	14	1
1:A:78:ARG:CG	1:A:85:GLU:HB2	0.41	2.45	19	1
1:B:227:LYS:HD3	1:B:227:LYS:C	0.41	2.36	13	1
1:A:40:THR:HG23	1:A:89:GLU:HG2	0.41	1.93	10	1
1:A:50:ILE:HD12	1:A:56:LEU:HA	0.41	1.92	12	1
1:A:25:VAL:HG22	1:A:71:TYR:CZ	0.41	2.51	19	1
1:B:245:GLN:HG2	1:B:250:ILE:HG12	0.41	1.93	18	1
1:B:227:LYS:C	1:B:227:LYS:HD3	0.41	2.35	20	1
1:A:22:ALA:CA	1:B:223:GLU:HG3	0.41	2.46	10	1
1:B:245:GLN:HG3	1:B:250:ILE:HG12	0.41	1.92	13	1
1:A:72:TYR:HD2	1:B:222:ALA:HB1	0.41	1.75	14	1
1:A:35:LEU:HD22	1:A:71:TYR:CE1	0.41	2.51	18	1
1:A:59:LYS:HA	1:A:62:GLU:HG2	0.41	1.92	20	1
1:B:269:GLY:HA2	1:B:292:ASN:OD1	0.40	2.16	7	1
1:B:245:GLN:HB3	1:B:249:GLN:HB2	0.40	1.93	13	1
1:A:57:ARG:HD3	1:B:223:GLU:OE1	0.40	2.16	7	1
1:A:89:GLU:HB3	1:A:91:TYR:CE2	0.40	2.51	18	1
1:B:235:LEU:HD13	1:B:271:TYR:CE1	0.40	2.52	14	1
1:A:35:LEU:HD21	1:B:253:PRO:HG3	0.40	1.93	19	1
1:A:44:SER:HA	1:A:84:PHE:O	0.40	2.16	20	1
1:B:272:TYR:CE2	1:B:274:ILE:HD11	0.40	2.51	20	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	72/104 (69%)	65±2 (91±3%)	6±2 (8±2%)	1±1 (1±2%)	16	63
1	B	72/104 (69%)	66±2 (92±3%)	5±2 (7±3%)	1±1 (1±1%)	24	71
All	All	2880/4160 (69%)	2632 (91%)	218 (8%)	30 (1%)	20	68

All 16 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	B	222	ALA	4
1	A	22	ALA	4
1	A	48	GLY	3
1	A	24	GLN	3
1	A	93	ASP	2
1	A	37	LYS	2
1	B	224	GLN	2
1	B	237	LYS	2
1	B	248	GLY	1
1	A	34	LYS	1
1	A	92	ASN	1
1	A	23	GLU	1
1	B	247	GLY	1
1	A	35	LEU	1
1	A	27	LYS	1
1	B	293	ASP	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	59/84 (70%)	54±2 (92±3%)	5±2 (8±3%)	16	63
1	B	59/84 (70%)	55±1 (93±3%)	4±1 (7±3%)	18	66
All	All	2360/3360 (70%)	2182 (92%)	178 (8%)	17	65

All 44 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	45	GLN	19
1	B	224	GLN	19
1	A	24	GLN	18
1	B	245	GLN	16
1	A	78	ARG	13
1	B	278	ARG	10
1	A	28	GLN	8
1	B	228	GLN	7
1	A	57	ARG	4
1	A	54	SER	4
1	B	272	TYR	4
1	A	71	TYR	4
1	B	257	ARG	4
1	A	38	VAL	3
1	A	29	GLU	3
1	B	279	GLU	3
1	A	23	GLU	2
1	B	238	VAL	2
1	B	293	ASP	2
1	B	270	LYS	2
1	B	283	ASN	2
1	A	79	GLU	2
1	B	255	ASP	2
1	A	34	LYS	2
1	B	242	ASN	2
1	A	72	TYR	2
1	A	70	LYS	2
1	A	80	HIS	1
1	A	83	ASN	1
1	B	234	LYS	1
1	B	285	GLU	1
1	A	92	ASN	1
1	A	65	ASP	1
1	B	240	THR	1
1	B	227	LYS	1
1	B	280	HIS	1
1	B	252	SER	1
1	B	223	GLU	1
1	B	249	GLN	1
1	B	273	HIS	1
1	A	26	SER	1
1	B	229	GLU	1
1	A	67	LYS	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	27	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