



Full wwPDB NMR Structure Validation Report ⓘ

Oct 11, 2021 – 01:32 PM EDT

PDB ID : 2G9J
Title : Complex of TM1a(1-14)Zip with TM9a(251-284): a model for the polymerization domain ("overlap region") of tropomyosin, Northeast Structural Genomics Target OR9
Authors : Greenfield, N.J.; Huang, Y.J.; Swapna, G.V.T.; Bhattacharya, A.; Singh, A.; Montelione, G.T.; Hitchcock-DeGregori, S.E.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2006-03-06

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

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

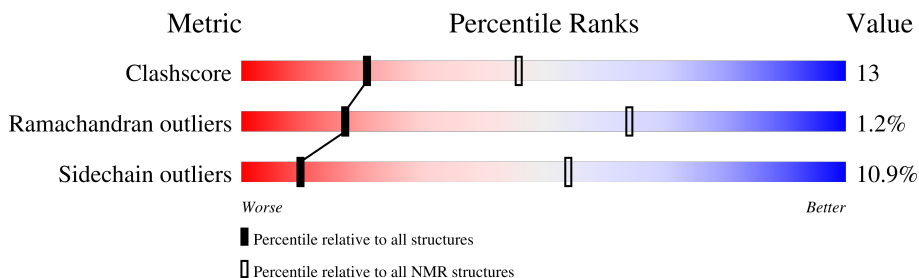
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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



Metric	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	C	37	
1	D	37	
2	A	33	
2	B	33	

2 Ensemble composition and analysis

This entry contains 10 models. Model 9 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	C:270-C:284, A:0-A:31, D:270-D:284, B:0-B:32 (95)	0.65	9

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	2, 7, 8
2	3, 9, 10
3	4, 5
Single-model clusters	1; 6

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2295 atoms, of which 1171 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Tropomyosin 1 alpha chain.

Mol	Chain	Residues	Atoms					Trace	
			Total	C	H	N	O		S
1	C	37	580	181	289	45	63	2	0
1	D	37	581	181	290	45	63	2	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	248	GLY	-	cloning artifact	UNP Q63609
C	249	CYS	-	cloning artifact	UNP Q63609
C	250	GLY	-	cloning artifact	UNP Q63609
C	279	LYS	ASN	engineered mutation	UNP Q63609
D	248	GLY	-	cloning artifact	UNP Q63609
D	249	CYS	-	cloning artifact	UNP Q63609
D	250	GLY	-	cloning artifact	UNP Q63609
D	279	LYS	ASN	engineered mutation	UNP Q63609

- Molecule 2 is a protein called Tropomyosin 1 alpha chain/General control protein GCN4.

Mol	Chain	Residues	Atoms					Trace	
			Total	C	H	N	O		S
2	A	33	567	170	296	50	48	3	0
2	B	33	567	170	296	50	48	3	0

There are 2 discrepancies between the modelled and reference sequences:

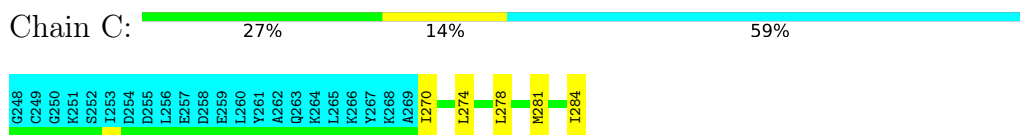
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	cloning artifact	UNP Q63609
B	0	GLY	-	cloning artifact	UNP Q63609

4 Residue-property plots

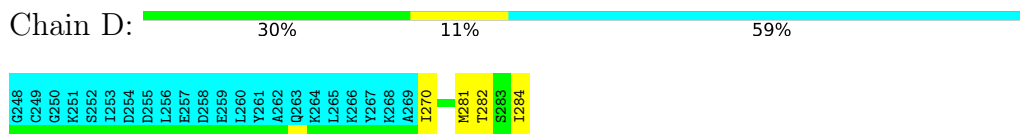
4.1 Average score per residue in the NMR ensemble

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

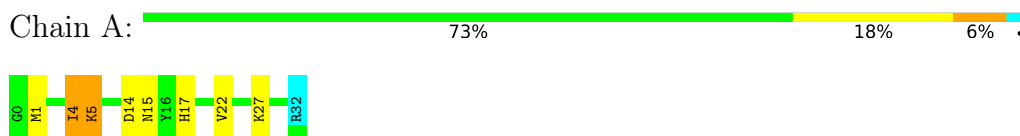
- Molecule 1: Tropomyosin 1 alpha chain



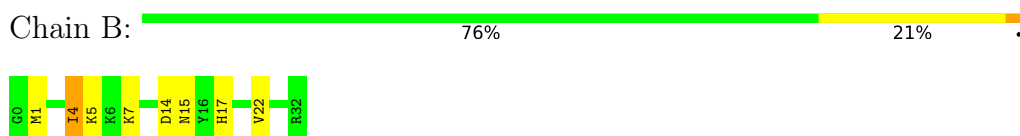
- Molecule 1: Tropomyosin 1 alpha chain



- Molecule 2: Tropomyosin 1 alpha chain/General control protein GCN4



- Molecule 2: Tropomyosin 1 alpha chain/General control protein GCN4

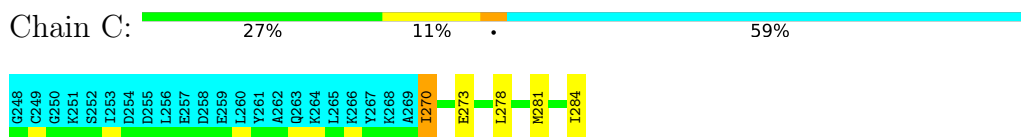


4.2 Scores per residue for each member of the ensemble

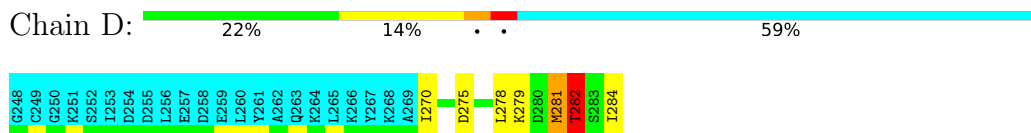
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

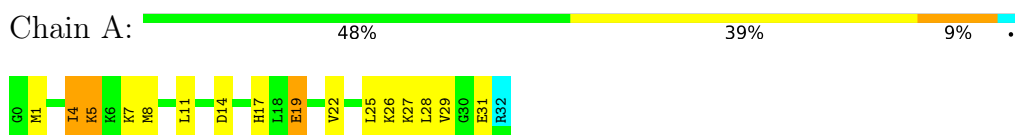
- Molecule 1: Tropomyosin 1 alpha chain



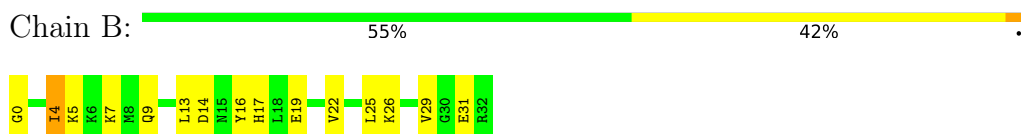
- Molecule 1: Tropomyosin 1 alpha chain



- Molecule 2: Tropomyosin 1 alpha chain/General control protein GCN4

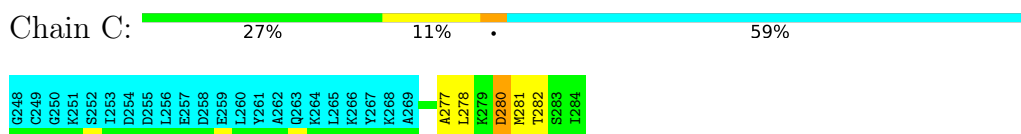


- Molecule 2: Tropomyosin 1 alpha chain/General control protein GCN4

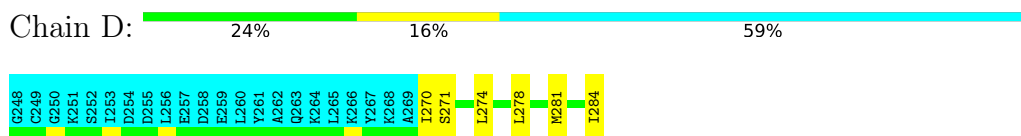


4.2.2 Score per residue for model 2

- Molecule 1: Tropomyosin 1 alpha chain



- Molecule 1: Tropomyosin 1 alpha chain

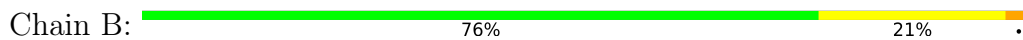


- Molecule 2: Tropomyosin 1 alpha chain/General control protein GCN4



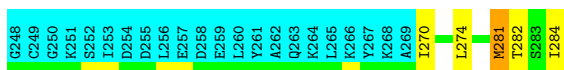


- Molecule 2: Tropomyosin 1 alpha chain/General control protein GCN4

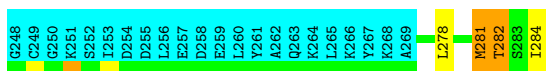


4.2.3 Score per residue for model 3

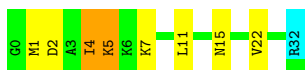
- Molecule 1: Tropomyosin 1 alpha chain



- Molecule 1: Tropomyosin 1 alpha chain



- Molecule 2: Tropomyosin 1 alpha chain/General control protein GCN4



- Molecule 2: Tropomyosin 1 alpha chain/General control protein GCN4

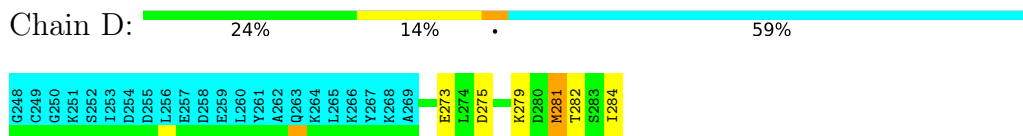


4.2.4 Score per residue for model 4

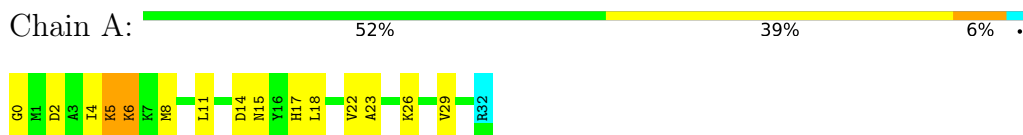
- Molecule 1: Tropomyosin 1 alpha chain



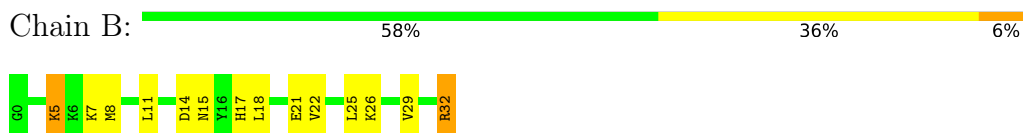
- Molecule 1: Tropomyosin 1 alpha chain



- Molecule 2: Tropomyosin 1 alpha chain/General control protein GCN4

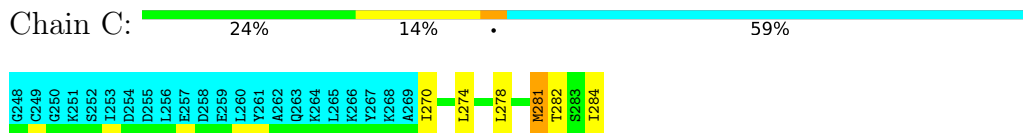


- Molecule 2: Tropomyosin 1 alpha chain/General control protein GCN4

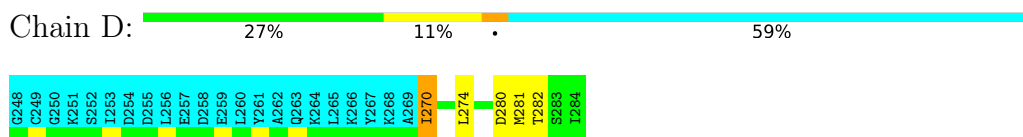


4.2.5 Score per residue for model 5

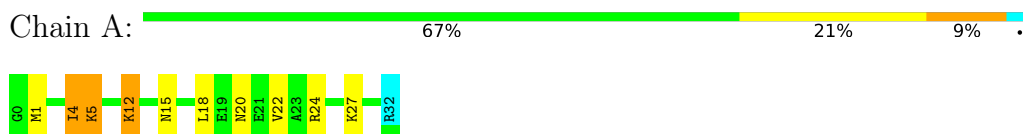
- Molecule 1: Tropomyosin 1 alpha chain



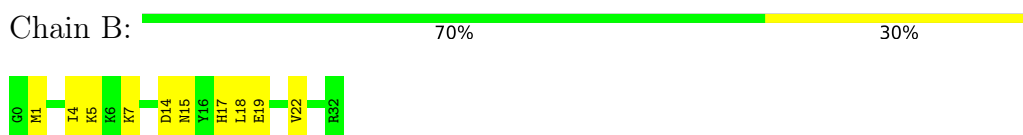
- Molecule 1: Tropomyosin 1 alpha chain



- Molecule 2: Tropomyosin 1 alpha chain/General control protein GCN4

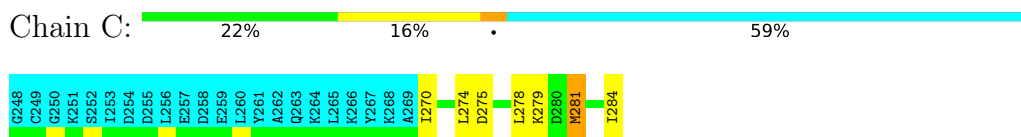


- Molecule 2: Tropomyosin 1 alpha chain/General control protein GCN4

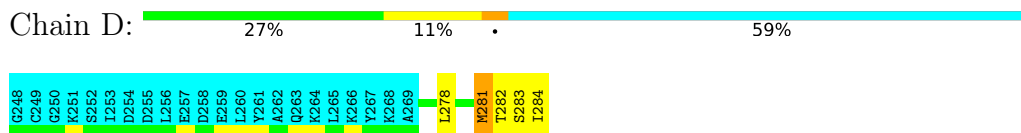


4.2.6 Score per residue for model 6

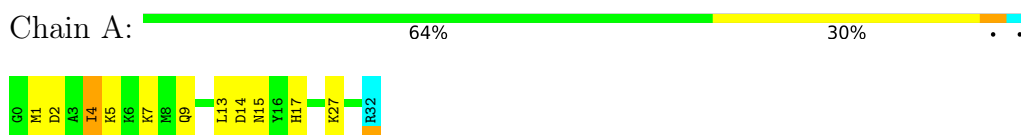
- Molecule 1: Tropomyosin 1 alpha chain



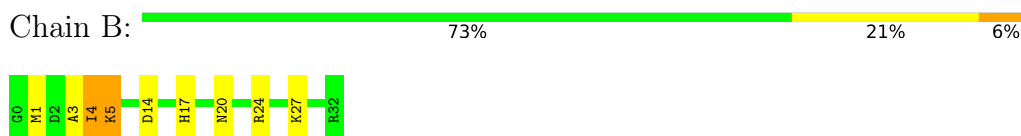
- Molecule 1: Tropomyosin 1 alpha chain



- Molecule 2: Tropomyosin 1 alpha chain/General control protein GCN4

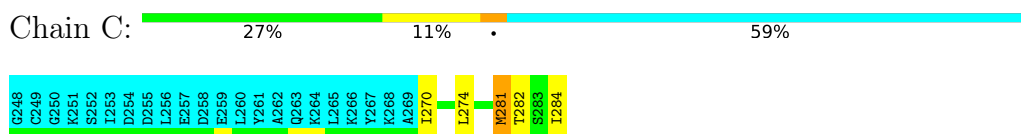


- Molecule 2: Tropomyosin 1 alpha chain/General control protein GCN4

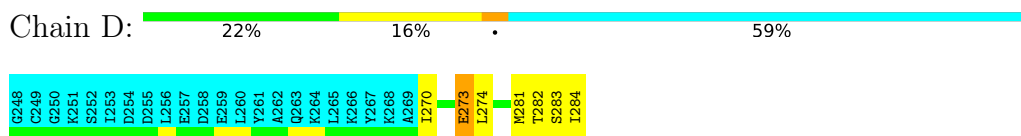


4.2.7 Score per residue for model 7

- Molecule 1: Tropomyosin 1 alpha chain



- Molecule 1: Tropomyosin 1 alpha chain



- Molecule 2: Tropomyosin 1 alpha chain/General control protein GCN4





- Molecule 2: Tropomyosin 1 alpha chain/General control protein GCN4

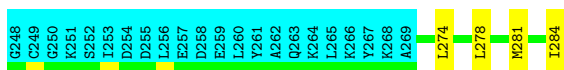
Chain B: 64% 33%



4.2.8 Score per residue for model 8

- Molecule 1: Tropomyosin 1 alpha chain

Chain C: 30% 11% 59%



- Molecule 1: Tropomyosin 1 alpha chain

Chain D: 24% 14% 59%



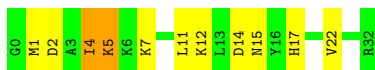
- Molecule 2: Tropomyosin 1 alpha chain/General control protein GCN4

Chain A: 61% 33% 6%



- Molecule 2: Tropomyosin 1 alpha chain/General control protein GCN4

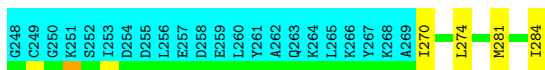
Chain B: 67% 27% 6%



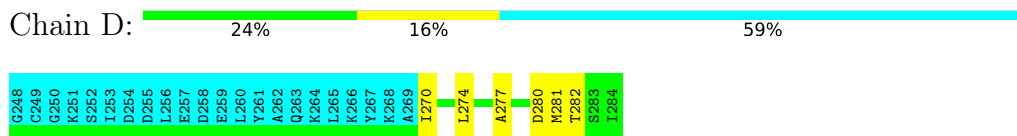
4.2.9 Score per residue for model 9 (medoid)

- Molecule 1: Tropomyosin 1 alpha chain

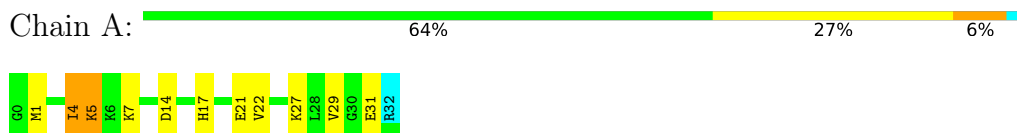
Chain C: 30% 11% 59%



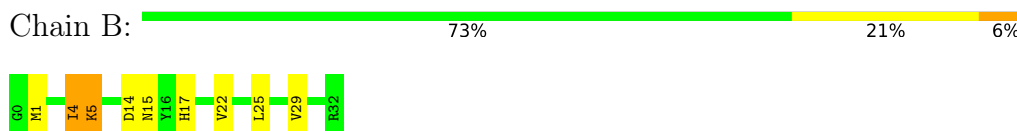
- Molecule 1: Tropomyosin 1 alpha chain



- Molecule 2: Tropomyosin 1 alpha chain/General control protein GCN4

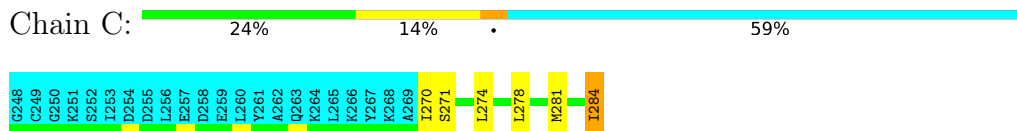


- Molecule 2: Tropomyosin 1 alpha chain/General control protein GCN4

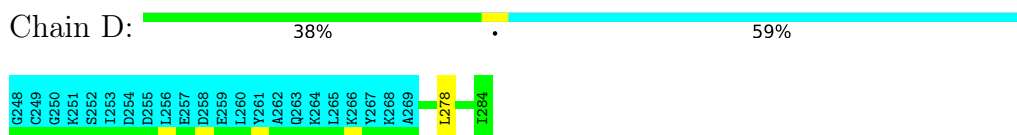


4.2.10 Score per residue for model 10

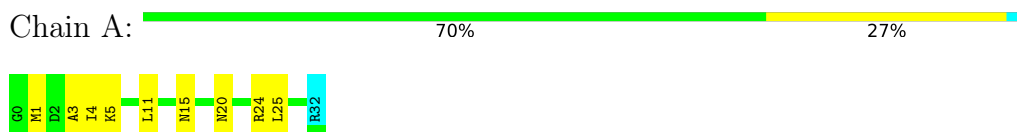
- Molecule 1: Tropomyosin 1 alpha chain



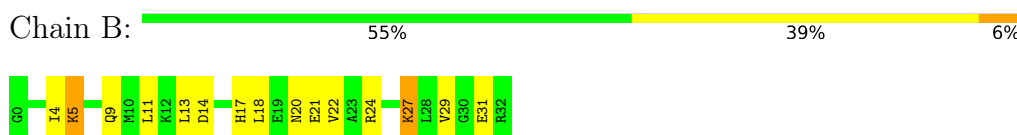
- Molecule 1: Tropomyosin 1 alpha chain



- Molecule 2: Tropomyosin 1 alpha chain/General control protein GCN4



- Molecule 2: Tropomyosin 1 alpha chain/General control protein GCN4



5 Refinement protocol and experimental data overview

The models were refined using the following method: *Initial structure was calculated with Torsion Angle Dynamics and refined with simulated annealing and included a term for explicit solvent in the refinement protocol.*

Of the 196 calculated structures, 10 were deposited, based on the following criterion: *10 structures from initial DYANA calculations with the lowest target functions were refined using CNS. The structures back calculated data agree with experimental NOESY spectra. The structures have acceptable covalent geometry, favorable non-bond energy, the lowest energy and the fewest restraint violations.*

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

Software name	Classification	Version
DYANA	structure solution	1.5
CNS	refinement	1.1

No chemical shift data was provided.

6 Model quality

6.1 Standard geometry

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	C	118	116	115	4±2
1	D	118	116	115	5±2
2	A	259	283	282	10±3
2	B	271	296	295	10±3
All	All	7660	8110	8070	210

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:4:ILE:HD12	2:B:4:ILE:HB	0.82	1.52	3	5
2:B:12:LYS:HA	2:B:12:LYS:HE2	0.80	1.53	2	2
2:B:5:LYS:HA	2:B:5:LYS:HE2	0.79	1.51	3	4
2:A:14:ASP:HA	2:A:17:HIS:HD2	0.75	1.41	2	2
2:A:14:ASP:HA	2:A:17:HIS:CD2	0.73	2.18	2	6
2:A:11:LEU:HD21	2:B:11:LEU:HD21	0.73	1.60	8	3
2:A:5:LYS:HE2	2:A:5:LYS:HA	0.72	1.60	2	3
1:D:284:ILE:HG12	2:B:7:LYS:HD2	0.70	1.62	1	1
2:A:11:LEU:HD11	2:B:11:LEU:HD21	0.69	1.64	3	1
1:C:281:MET:HE3	1:C:284:ILE:HG21	0.68	1.66	4	1
1:D:284:ILE:HG13	2:B:11:LEU:HD22	0.68	1.65	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:14:ASP:HA	2:B:17:HIS:CD2	0.67	2.23	7	9
2:A:12:LYS:HA	2:A:12:LYS:HE3	0.67	1.65	5	1
2:B:14:ASP:HA	2:B:17:HIS:CE1	0.66	2.26	9	1
2:A:25:LEU:HD11	2:B:29:VAL:HG11	0.66	1.68	7	1
2:A:14:ASP:HA	2:A:17:HIS:ND1	0.64	2.08	7	1
1:C:270:ILE:O	1:C:274:LEU:HG	0.64	1.93	3	4
2:A:5:LYS:HA	2:A:5:LYS:HE2	0.62	1.72	5	1
1:D:270:ILE:O	1:D:274:LEU:HG	0.60	1.97	9	2
2:A:29:VAL:HB	2:B:29:VAL:HG22	0.60	1.74	9	1
2:A:5:LYS:HE2	1:D:281:MET:SD	0.59	2.38	8	2
1:C:281:MET:HG2	1:C:282:THR:N	0.58	2.13	7	1
1:C:281:MET:HG3	1:C:284:ILE:HG23	0.57	1.76	7	1
2:A:14:ASP:HA	2:A:17:HIS:CE1	0.56	2.35	7	1
2:A:22:VAL:HB	2:B:22:VAL:HG22	0.56	1.77	8	2
2:B:14:ASP:HA	2:B:17:HIS:HD2	0.56	1.61	10	4
2:B:27:LYS:HA	2:B:27:LYS:HE2	0.56	1.76	10	1
1:D:281:MET:HG2	1:D:282:THR:N	0.56	2.16	4	2
1:D:274:LEU:HB2	2:B:1:MET:HE3	0.55	1.78	2	1
1:D:284:ILE:HG23	2:B:7:LYS:HE3	0.55	1.76	7	1
2:A:17:HIS:O	2:A:21:GLU:HB2	0.54	2.01	9	1
2:B:19:GLU:HA	2:B:22:VAL:HG12	0.54	1.80	1	1
1:C:281:MET:O	1:C:284:ILE:HG22	0.54	2.03	1	3
2:B:20:ASN:O	2:B:24:ARG:HG2	0.54	2.03	3	3
1:C:274:LEU:HG	2:B:1:MET:CE	0.53	2.33	5	1
2:A:29:VAL:CG2	2:B:29:VAL:HG22	0.53	2.34	1	1
2:A:8:MET:SD	1:D:281:MET:HG2	0.53	2.44	1	1
2:A:26:LYS:HA	2:A:29:VAL:HG12	0.52	1.81	8	2
1:C:281:MET:HG2	1:C:282:THR:H	0.52	1.63	7	1
2:A:4:ILE:HD12	2:B:4:ILE:CB	0.52	2.35	2	3
2:A:20:ASN:O	2:A:24:ARG:HG2	0.52	2.05	5	2
2:A:5:LYS:HE2	2:A:5:LYS:CA	0.52	2.31	2	1
2:B:18:LEU:O	2:B:22:VAL:HG23	0.52	2.04	4	4
2:B:14:ASP:HA	2:B:17:HIS:ND1	0.52	2.19	9	1
1:C:281:MET:HE3	2:B:8:MET:SD	0.52	2.45	7	1
1:C:278:LEU:HD12	2:A:4:ILE:HB	0.52	1.82	2	1
1:D:284:ILE:HG23	2:B:7:LYS:NZ	0.51	2.20	3	1
2:A:18:LEU:O	2:A:22:VAL:HG23	0.51	2.05	4	2
2:A:5:LYS:O	2:A:8:MET:HG2	0.51	2.06	1	1
2:A:28:LEU:O	2:A:31:GLU:HG2	0.51	2.06	1	1
2:B:16:TYR:HA	2:B:19:GLU:HG2	0.51	1.82	1	1
1:C:275:ASP:O	1:C:279:LYS:HB2	0.51	2.04	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:284:ILE:HG13	2:A:11:LEU:HD22	0.51	1.83	4	1
2:A:4:ILE:HB	2:B:4:ILE:HD12	0.51	1.83	1	1
2:B:18:LEU:O	2:B:22:VAL:HG13	0.51	2.05	3	1
2:A:8:MET:SD	1:D:281:MET:HE3	0.51	2.46	7	1
2:A:1:MET:HG3	2:A:4:ILE:CG2	0.51	2.36	2	1
2:A:22:VAL:HG22	2:B:22:VAL:HB	0.50	1.82	7	1
1:D:281:MET:O	1:D:284:ILE:HG22	0.50	2.06	2	3
2:A:29:VAL:HG11	2:B:25:LEU:HD11	0.50	1.80	4	2
2:A:25:LEU:O	2:A:29:VAL:HG23	0.50	2.06	1	1
2:A:1:MET:O	2:A:5:LYS:HG2	0.50	2.06	6	2
2:A:22:VAL:HG22	2:A:26:LYS:HE3	0.50	1.84	1	1
1:D:284:ILE:OXT	2:B:7:LYS:HB3	0.50	2.06	4	2
1:C:278:LEU:CD1	2:A:4:ILE:HB	0.49	2.37	5	3
2:A:2:ASP:HA	2:A:5:LYS:HB2	0.49	1.84	3	2
2:A:1:MET:HG3	2:A:4:ILE:HG22	0.49	1.83	6	2
1:C:281:MET:SD	1:C:282:THR:N	0.49	2.84	5	2
2:B:5:LYS:HE2	2:B:5:LYS:CA	0.49	2.36	10	2
2:A:25:LEU:HD11	2:B:29:VAL:HG21	0.49	1.84	10	2
2:A:0:GLY:HA2	1:D:273:GLU:CD	0.49	2.29	4	1
1:D:274:LEU:HB2	2:B:1:MET:SD	0.48	2.49	5	2
1:D:278:LEU:HD11	2:B:4:ILE:HB	0.48	1.84	1	1
1:C:270:ILE:HD13	1:D:270:ILE:HD12	0.48	1.86	5	1
2:B:25:LEU:O	2:B:29:VAL:HG23	0.48	2.08	1	2
2:A:27:LYS:O	2:A:31:GLU:HB2	0.48	2.09	2	2
2:B:14:ASP:O	2:B:18:LEU:HG	0.48	2.09	3	1
2:A:11:LEU:CD2	2:B:11:LEU:HD21	0.47	2.39	10	1
1:C:278:LEU:HD11	2:A:4:ILE:HB	0.47	1.86	5	1
2:B:2:ASP:HA	2:B:5:LYS:HB2	0.47	1.87	8	1
1:C:270:ILE:HD11	1:D:274:LEU:HD11	0.47	1.86	9	1
1:D:281:MET:HG3	1:D:282:THR:H	0.47	1.69	9	1
1:D:284:ILE:HG23	2:B:7:LYS:HZ1	0.47	1.69	3	1
1:C:278:LEU:HD21	2:A:1:MET:SD	0.47	2.49	1	1
2:A:8:MET:HG3	1:D:284:ILE:HD12	0.46	1.87	4	1
1:C:278:LEU:HD13	2:A:3:ALA:HB3	0.46	1.87	10	1
1:D:278:LEU:HD13	1:D:281:MET:SD	0.46	2.50	2	1
1:D:282:THR:O	2:B:7:LYS:HE2	0.46	2.11	5	1
1:C:281:MET:SD	2:B:5:LYS:HE2	0.46	2.51	6	1
1:C:273:GLU:CD	2:B:0:GLY:HA2	0.46	2.31	1	1
2:B:26:LYS:HA	2:B:29:VAL:HG12	0.46	1.87	4	1
1:D:273:GLU:HG3	1:D:274:LEU:N	0.46	2.25	7	1
1:C:281:MET:HE1	2:B:4:ILE:HG13	0.46	1.88	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:284:ILE:HD11	1:D:284:ILE:HD11	0.46	1.86	6	1
2:A:4:ILE:O	2:A:8:MET:HB3	0.46	2.11	1	1
2:A:4:ILE:HG13	2:A:5:LYS:HE3	0.45	1.88	1	1
2:A:22:VAL:HG11	2:B:22:VAL:HG12	0.45	1.88	3	1
1:C:271:SER:O	1:C:274:LEU:HG	0.45	2.11	10	1
2:A:9:GLN:O	2:A:13:LEU:HG	0.45	2.12	6	2
2:A:5:LYS:HE3	1:D:281:MET:HE1	0.45	1.86	6	1
2:B:9:GLN:O	2:B:13:LEU:HG	0.45	2.12	1	2
1:C:274:LEU:HD13	2:A:1:MET:CE	0.45	2.42	3	1
1:C:284:ILE:HG22	2:B:8:MET:HG3	0.45	1.89	3	1
1:D:270:ILE:O	1:D:270:ILE:HD13	0.45	2.11	5	1
1:D:278:LEU:HD12	2:B:4:ILE:HB	0.44	1.87	6	1
1:D:277:ALA:HA	1:D:280:ASP:OD2	0.44	2.12	9	1
1:C:274:LEU:O	1:C:278:LEU:HD22	0.44	2.13	4	1
1:D:275:ASP:O	1:D:279:LYS:HB2	0.44	2.12	1	2
2:B:12:LYS:HA	2:B:12:LYS:CE	0.44	2.35	2	1
1:D:270:ILE:HD13	1:D:270:ILE:O	0.44	2.12	8	1
2:A:4:ILE:CD1	2:B:4:ILE:HG13	0.44	2.42	8	1
1:C:284:ILE:HG23	2:A:7:LYS:HD3	0.44	1.89	1	1
1:D:281:MET:O	1:D:282:THR:HG22	0.44	2.12	1	2
1:C:284:ILE:O	2:A:7:LYS:HB3	0.44	2.12	6	1
1:D:281:MET:C	1:D:283:SER:H	0.44	2.16	6	2
2:A:19:GLU:HA	2:A:22:VAL:HG12	0.44	1.89	1	1
2:A:23:ALA:HA	2:A:26:LYS:HG2	0.44	1.89	4	1
2:A:4:ILE:HD12	2:B:4:ILE:CG1	0.43	2.43	7	1
1:D:278:LEU:HG	2:B:1:MET:SD	0.43	2.53	3	1
2:A:4:ILE:CD1	2:B:4:ILE:HB	0.43	2.43	2	1
1:C:270:ILE:HD13	1:C:270:ILE:O	0.43	2.14	1	1
1:D:281:MET:HG2	1:D:282:THR:H	0.42	1.75	4	1
1:C:284:ILE:O	1:C:284:ILE:HG12	0.42	2.14	6	1
2:A:4:ILE:HD12	2:B:4:ILE:HD12	0.42	1.90	9	1
2:B:1:MET:O	2:B:5:LYS:HD2	0.42	2.14	9	1
2:A:27:LYS:HB2	2:A:27:LYS:NZ	0.42	2.29	8	1
1:C:281:MET:HB2	1:C:284:ILE:HB	0.42	1.92	10	1
2:A:1:MET:SD	1:D:278:LEU:HD21	0.42	2.55	10	1
1:C:284:ILE:OXT	1:C:284:ILE:HG13	0.41	2.15	5	1
1:C:277:ALA:O	1:C:280:ASP:HB2	0.41	2.14	2	1
2:A:8:MET:O	2:A:12:LYS:HG3	0.41	2.15	2	1
1:D:271:SER:O	1:D:274:LEU:HG	0.41	2.15	2	1
2:A:2:ASP:O	2:A:6:LYS:HB2	0.41	2.15	4	1
2:B:32:ARG:HG2	2:B:32:ARG:OXT	0.41	2.16	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:281:MET:O	1:C:283:SER:N	0.41	2.54	4	1
1:C:278:LEU:HD12	1:C:281:MET:CE	0.41	2.45	4	1
2:A:1:MET:HB3	2:A:5:LYS:NZ	0.41	2.30	7	1
2:A:8:MET:HA	2:A:11:LEU:HB3	0.40	1.91	1	1
2:B:26:LYS:HA	2:B:29:VAL:HG23	0.40	1.92	1	1
2:B:7:LYS:NZ	2:B:7:LYS:CB	0.40	2.85	3	1
1:C:284:ILE:HG23	2:A:7:LYS:HE2	0.40	1.92	9	1
1:C:281:MET:HB2	2:B:8:MET:SD	0.40	2.56	4	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	C	14/37 (38%)	12±1 (84±4%)	2±1 (14±6%)	0±1 (2±5%)	10	50
1	D	14/37 (38%)	12±1 (84±6%)	2±1 (14±6%)	0±0 (2±3%)	10	50
2	A	31/33 (94%)	30±1 (95±3%)	1±1 (4±3%)	0±0 (1±1%)	20	68
2	B	31/33 (94%)	30±1 (96±2%)	1±1 (3±2%)	0±1 (1±2%)	29	74
All	All	900/1400 (64%)	830 (92%)	59 (7%)	11 (1%)	17	64

All 7 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	D	282	THR	3
1	C	282	THR	2
2	A	1	MET	2
1	C	283	SER	1
2	B	1	MET	1
2	B	3	ALA	1
2	A	3	ALA	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	C	14/32 (44%)	12±1 (89±5%)	2±1 (11±5%)	10	54
1	D	14/32 (44%)	12±1 (89±7%)	2±1 (11±7%)	10	54
2	A	28/29 (97%)	25±1 (89±4%)	3±1 (11±4%)	9	52
2	B	29/29 (100%)	26±1 (89±3%)	3±1 (11±3%)	10	54
All	All	850/1220 (70%)	757 (89%)	93 (11%)	10	54

All 30 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)
2	A	4	ILE	9
2	A	15	ASN	8
2	A	5	LYS	7
2	B	4	ILE	7
2	B	5	LYS	7
1	C	281	MET	7
2	B	15	ASN	7
1	D	281	MET	5
1	D	270	ILE	4
2	A	27	LYS	3
1	D	282	THR	3
1	C	270	ILE	2
2	B	31	GLU	2
2	B	32	ARG	2
2	B	21	GLU	2
1	D	280	ASP	2
2	B	27	LYS	2
1	C	284	ILE	2
2	A	19	GLU	1
1	C	280	ASP	1
2	A	7	LYS	1
1	C	278	LEU	1
1	C	279	LYS	1
2	A	6	LYS	1
2	A	12	LYS	1

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Mol	Chain	Res	Type	Models (Total)
2	B	19	GLU	1
2	A	18	LEU	1
1	D	273	GLU	1
1	C	274	LEU	1
2	B	12	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 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

No chemical shift data were provided