



Full wwPDB NMR Structure Validation Report ⓘ

Apr 27, 2016 – 12:16 AM BST

PDB ID : 2KW3
Title : Heterotrimeric interaction between RFX5 and RFXAP
Authors : Laird, K.M.; Briggs, L.L.; Boss, J.M.; Summers, M.F.; Garvie, C.W.
Deposited on : 2010-03-30

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 ⓘ 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
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

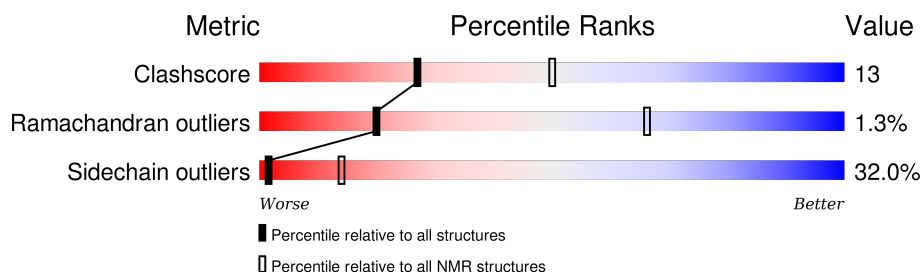
1 Overall quality at a glance

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	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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	68	
1	B	68	
2	C	62	

2 Ensemble composition and analysis

This entry contains 20 models. Model 3 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:29-A:68, B:30-B:68, C:225-C:251 (106)	0.58	3

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 6 clusters and 3 single-model clusters were found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3072 atoms, of which 1528 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called DNA-binding protein RFX5.

Mol	Chain	Residues	Atoms						Trace
1	A	68	Total	C	H	N	O	S	0
			1037	325	514	87	110	1	
1	B	68	Total	C	H	N	O	S	0
			1037	325	514	87	110	1	

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	GLY	-	EXPRESSION TAG	UNP P48382
B	23	GLY	-	EXPRESSION TAG	UNP P48382

- Molecule 2 is a protein called Regulatory factor X-associated protein.

Mol	Chain	Residues	Atoms						Trace
2	C	62	Total	C	H	N	O	S	0
			998	309	500	96	92	1	

There are 3 discrepancies between the modelled and reference sequences:

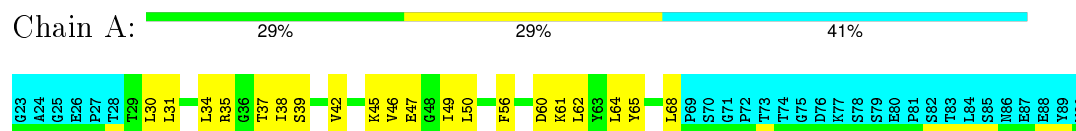
Chain	Residue	Modelled	Actual	Comment	Reference
C	211	GLY	-	EXPRESSION TAG	UNP O00287
C	212	HIS	-	EXPRESSION TAG	UNP O00287
C	213	GLY	-	EXPRESSION TAG	UNP O00287

4 Residue-property plots

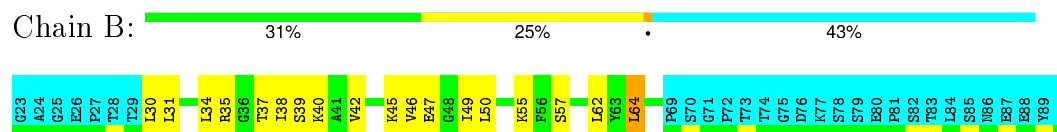
4.1 Average score per residue in the NMR ensemble

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.

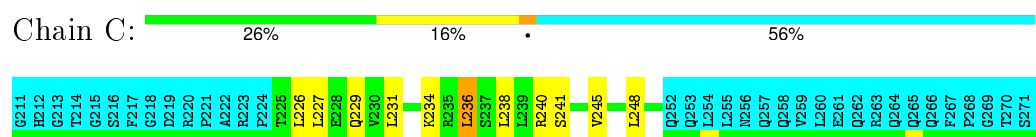
- Molecule 1: DNA-binding protein RFX5



- Molecule 1: DNA-binding protein RFX5



- Molecule 2: Regulatory factor X-associated protein

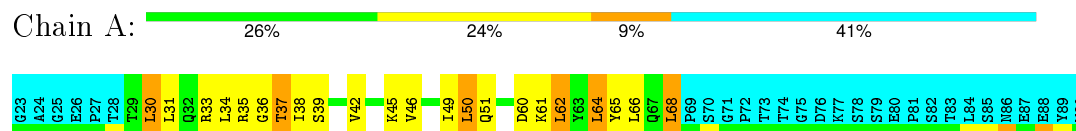


4.2 Scores per residue for each member of the ensemble

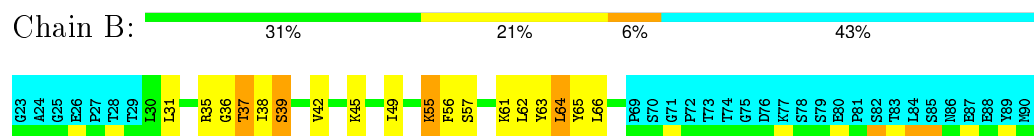
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

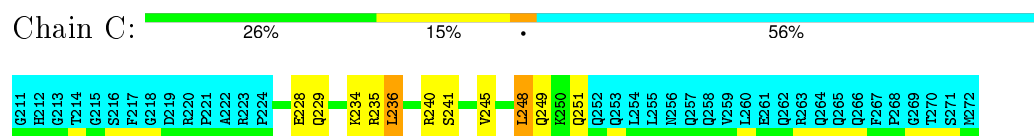
- Molecule 1: DNA-binding protein RFX5



- Molecule 1: DNA-binding protein RFX5

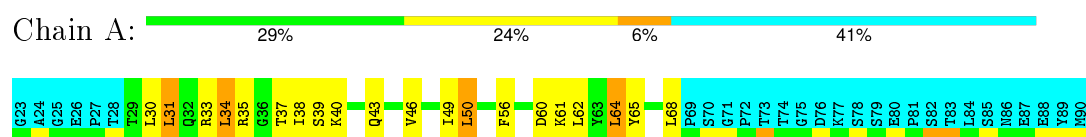


- Molecule 2: Regulatory factor X-associated protein

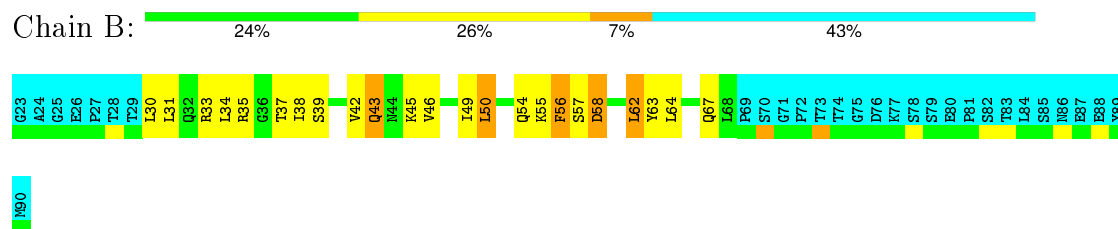


4.2.2 Score per residue for model 2

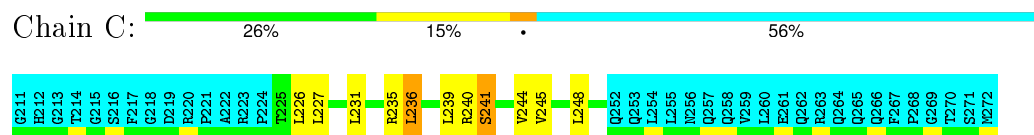
- Molecule 1: DNA-binding protein RFX5



- Molecule 1: DNA-binding protein RFX5

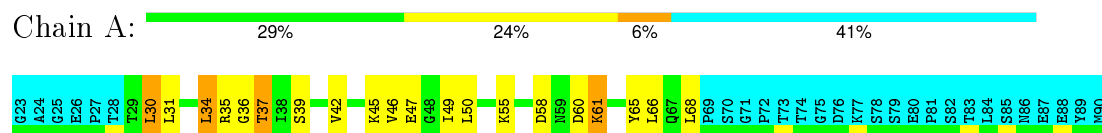


- Molecule 2: Regulatory factor X-associated protein

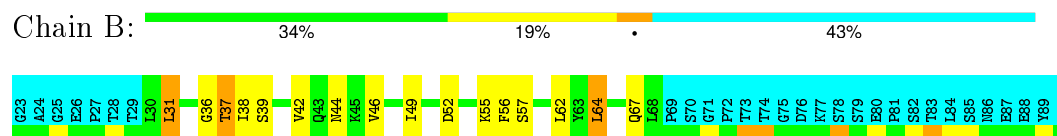


4.2.3 Score per residue for model 3 (medoid)

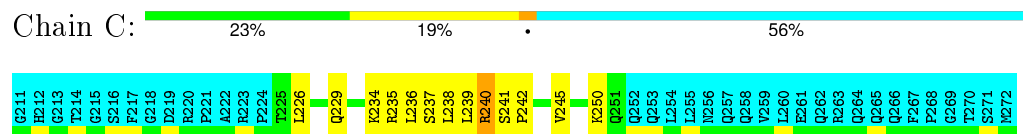
- Molecule 1: DNA-binding protein RFX5



- Molecule 1: DNA-binding protein RFX5

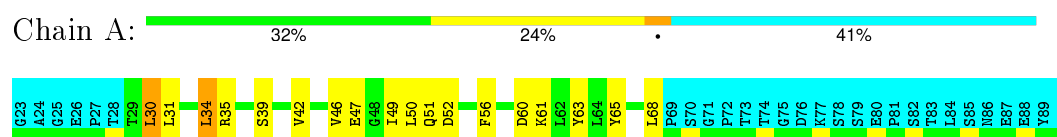


- Molecule 2: Regulatory factor X-associated protein

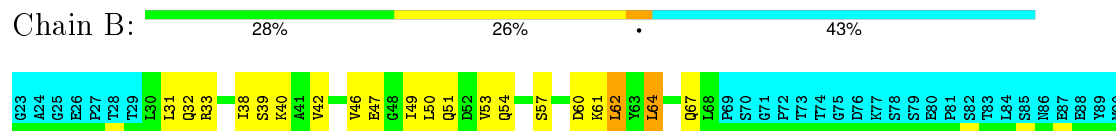


4.2.4 Score per residue for model 4

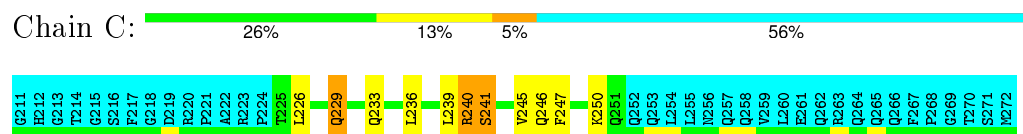
- Molecule 1: DNA-binding protein RFX5



- Molecule 1: DNA-binding protein RFX5

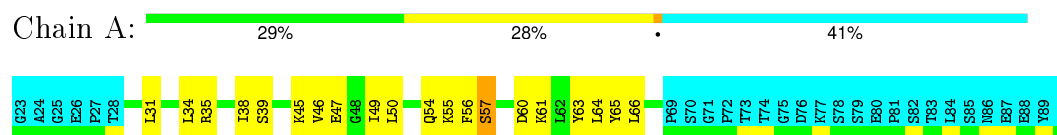


- Molecule 2: Regulatory factor X-associated protein

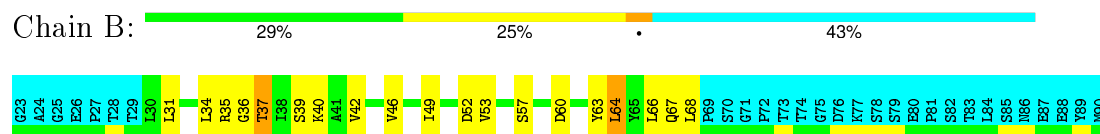


4.2.5 Score per residue for model 5

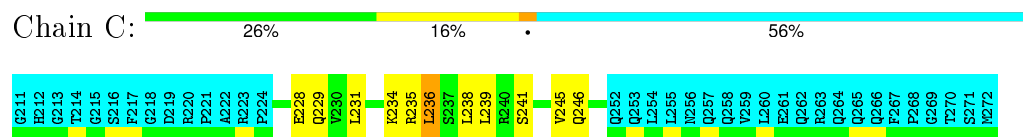
- Molecule 1: DNA-binding protein RFX5



- Molecule 1: DNA-binding protein RFX5

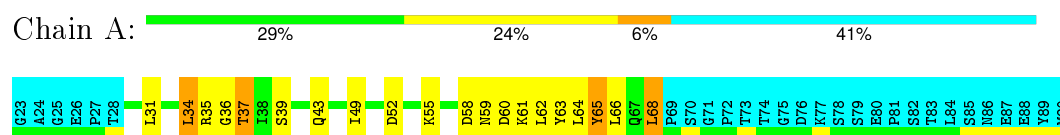


- Molecule 2: Regulatory factor X-associated protein

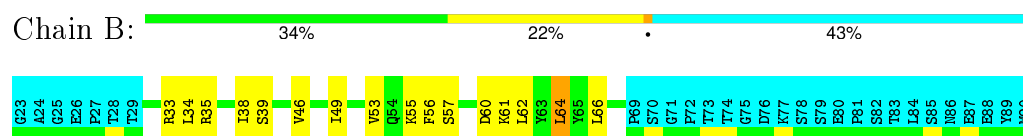


4.2.6 Score per residue for model 6

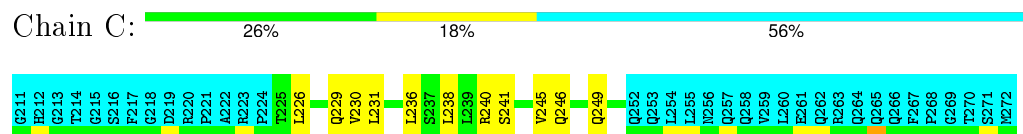
- Molecule 1: DNA-binding protein RFX5



- Molecule 1: DNA-binding protein RFX5

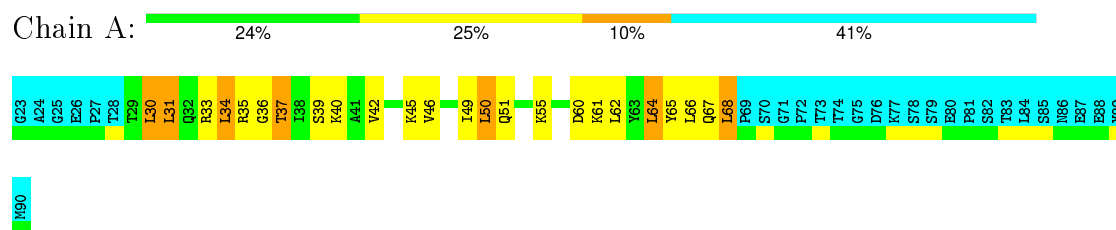


- Molecule 2: Regulatory factor X-associated protein

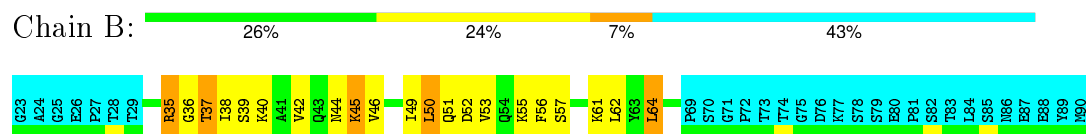


4.2.7 Score per residue for model 7

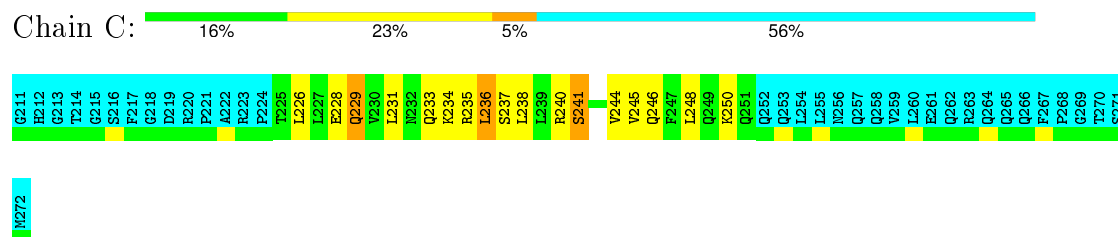
- Molecule 1: DNA-binding protein RFX5



- Molecule 1: DNA-binding protein RFX5

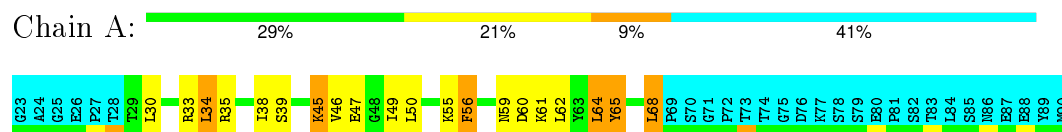


- Molecule 2: Regulatory factor X-associated protein

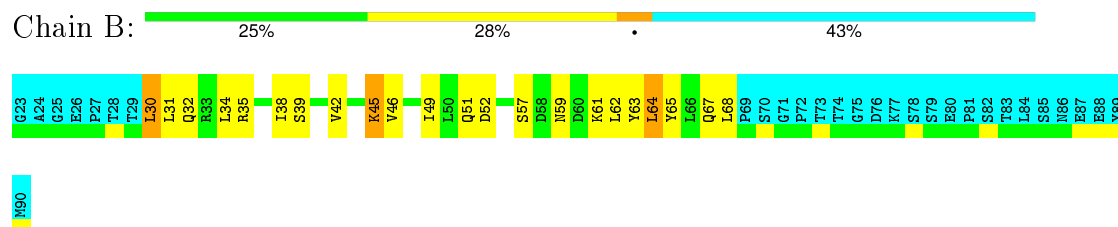


4.2.8 Score per residue for model 8

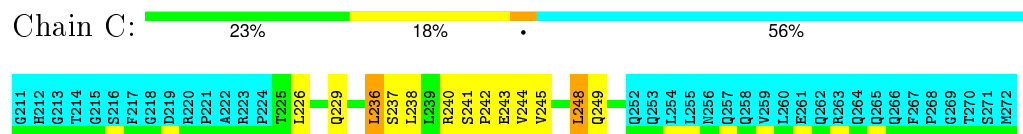
- Molecule 1: DNA-binding protein RFX5



- Molecule 1: DNA-binding protein RFX5



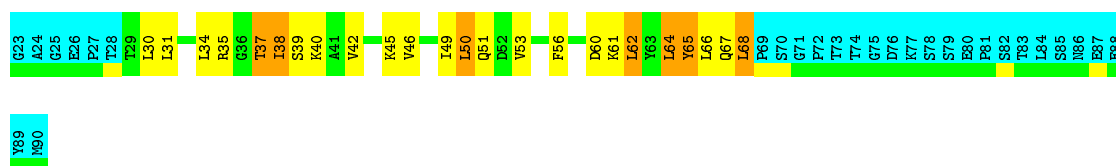
- Molecule 2: Regulatory factor X-associated protein



4.2.9 Score per residue for model 9

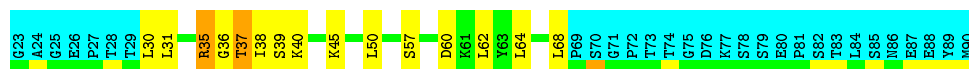
- Molecule 1: DNA-binding protein RFX5





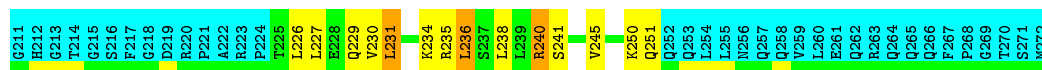
- Molecule 1: DNA-binding protein RFX5

Chain B: 35% 19% 43%



- Molecule 2: Regulatory factor X-associated protein

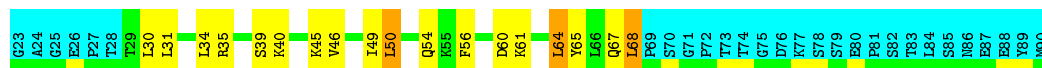
Chain C: 21% 18% 5% 56%



4.2.10 Score per residue for model 10

- Molecule 1: DNA-binding protein RFX5

Chain A: 32% 22% 41%



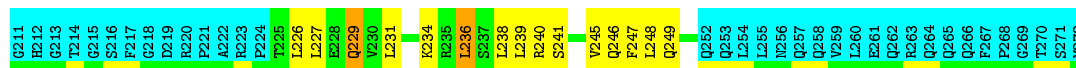
- Molecule 1: DNA-binding protein RFX5

Chain B: 29% 22% 6% 43%



- Molecule 2: Regulatory factor X-associated protein

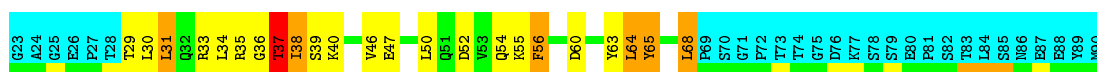
Chain C: 19% 21% 56%



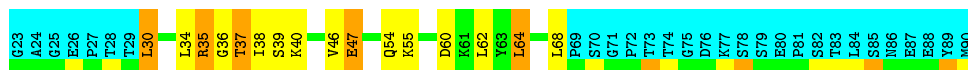
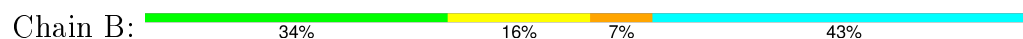
4.2.11 Score per residue for model 11

- Molecule 1: DNA-binding protein RFX5

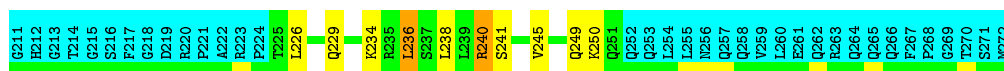
Chain A: 25% 24% 9% 41%



- Molecule 1: DNA-binding protein RFX5

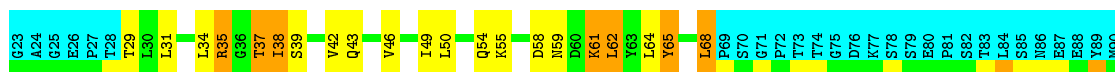
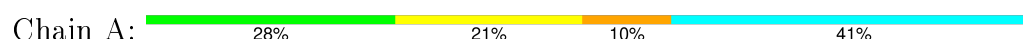


- Molecule 2: Regulatory factor X-associated protein

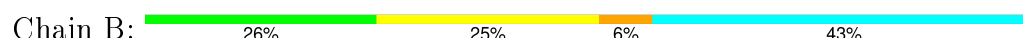


4.2.12 Score per residue for model 12

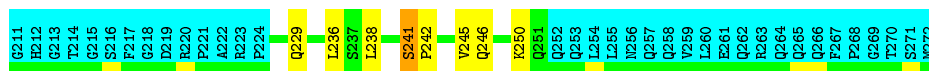
- Molecule 1: DNA-binding protein RFX5



- Molecule 1: DNA-binding protein RFX5

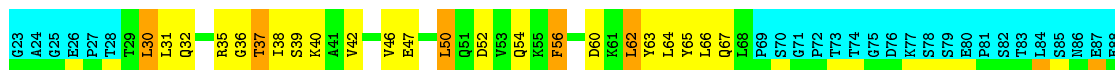
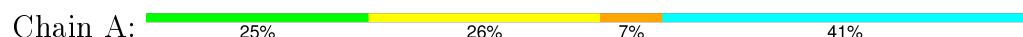


- Molecule 2: Regulatory factor X-associated protein



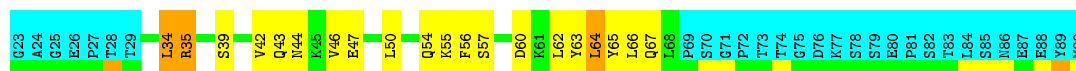
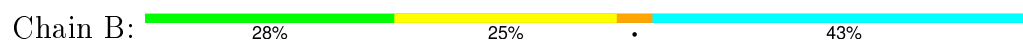
4.2.13 Score per residue for model 13

- Molecule 1: DNA-binding protein RFX5

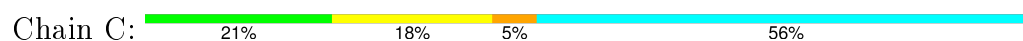




- Molecule 1: DNA-binding protein RFX5

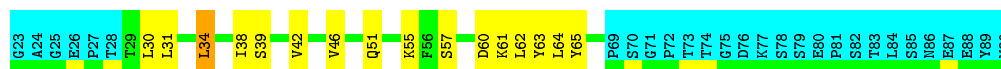


- Molecule 2: Regulatory factor X-associated protein

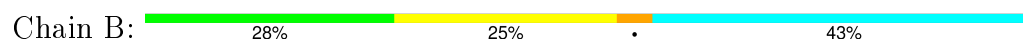


4.2.14 Score per residue for model 14

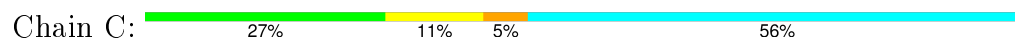
- Molecule 1: DNA-binding protein RFX5



- Molecule 1: DNA-binding protein RFX5

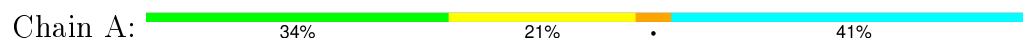


- Molecule 2: Regulatory factor X-associated protein

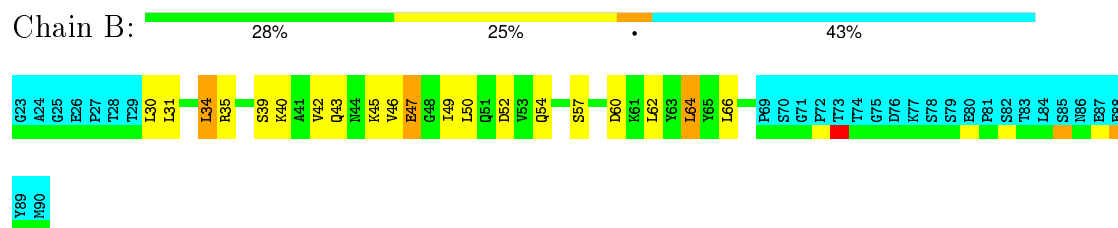


4.2.15 Score per residue for model 15

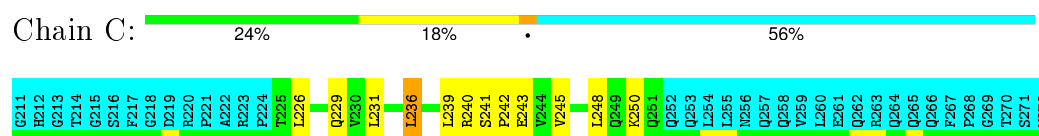
- Molecule 1: DNA-binding protein RFX5



- Molecule 1: DNA-binding protein RFX5

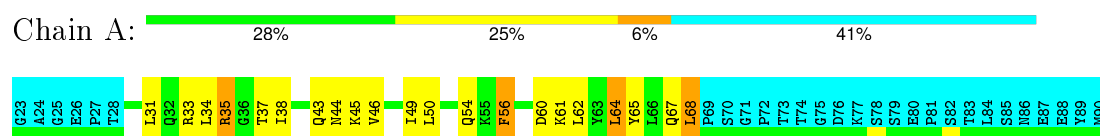


- Molecule 2: Regulatory factor X-associated protein

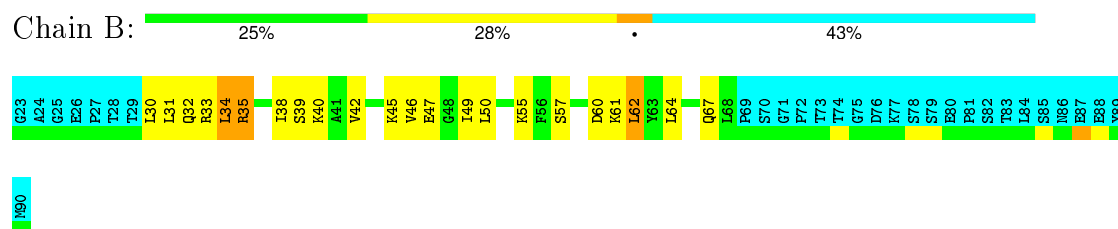


4.2.16 Score per residue for model 16

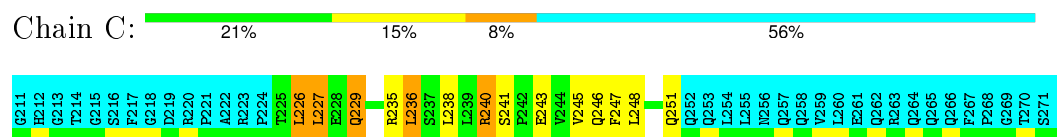
- Molecule 1: DNA-binding protein RFX5



- Molecule 1: DNA-binding protein RFX5

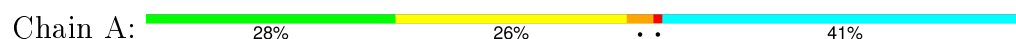


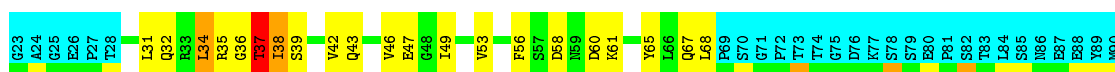
- Molecule 2: Regulatory factor X-associated protein



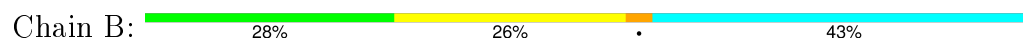
4.2.17 Score per residue for model 17

- Molecule 1: DNA-binding protein RFX5





- Molecule 1: DNA-binding protein RFX5

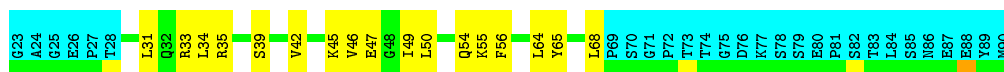


- Molecule 2: Regulatory factor X-associated protein

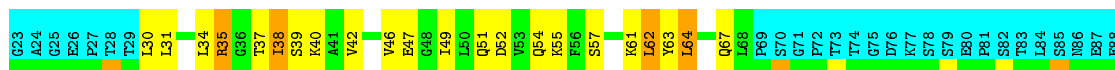
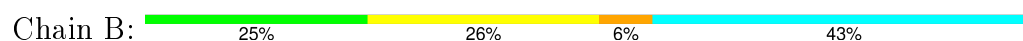


4.2.18 Score per residue for model 18

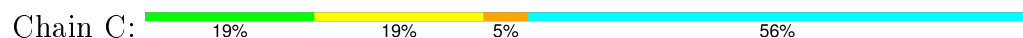
- Molecule 1: DNA-binding protein RFX5



- Molecule 1: DNA-binding protein RFX5

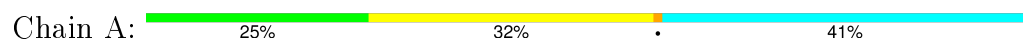


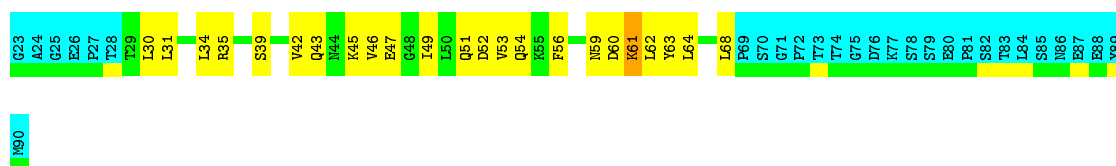
- Molecule 2: Regulatory factor X-associated protein



4.2.19 Score per residue for model 19

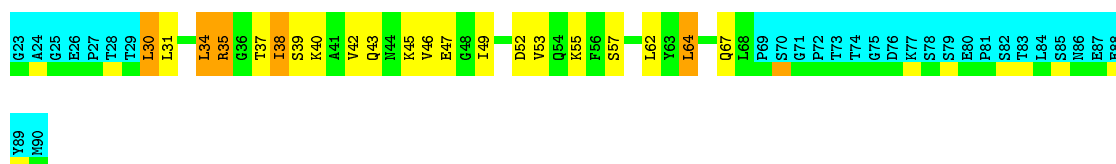
- Molecule 1: DNA-binding protein RFX5





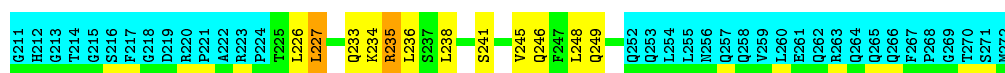
- Molecule 1: DNA-binding protein RFX5

Chain B: 26% 24% 7% 43%



- Molecule 2: Regulatory factor X-associated protein

Chain C: 24% 16% 56%



4.2.20 Score per residue for model 20

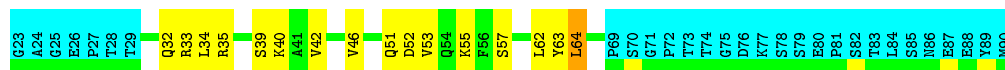
- Molecule 1: DNA-binding protein RFX5

Chain A: 29% 22% 7% 41%



- Molecule 1: DNA-binding protein RFX5

Chain B: 34% 22% 43%



- Molecule 2: Regulatory factor X-associated protein

Chain C: 21% 19% 56%



5 Refinement protocol and experimental data overview

The models were refined using the following method: *distance geometry*.

Of the 600 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
CYANA	refinement	
CYANA	structure solution	

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	327	347	347	15±4
1	B	320	340	340	14±3
2	C	225	247	247	9±3
All	All	17440	18680	18680	468

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:C:236:LEU:HD13	2:C:248:LEU:HD13	0.99	1.32	13	4
1:A:49:ILE:HD11	1:B:49:ILE:HD13	0.91	1.40	15	2
1:A:38:ILE:HD11	1:B:68:LEU:HD11	0.89	1.43	8	4
2:C:236:LEU:HD13	2:C:248:LEU:HD22	0.84	1.48	8	2
1:A:68:LEU:HD11	1:B:38:ILE:HD11	0.81	1.52	8	8
1:A:46:VAL:HG12	1:A:50:LEU:HD12	0.79	1.52	2	3
1:A:49:ILE:HD13	1:B:49:ILE:HD11	0.75	1.57	8	4
1:A:46:VAL:HG22	1:B:49:ILE:HG21	0.74	1.60	18	1
1:A:68:LEU:HD13	1:B:38:ILE:HD11	0.68	1.65	19	4
1:B:38:ILE:HG21	2:C:227:LEU:HD22	0.68	1.64	2	1
2:C:244:VAL:HG12	2:C:248:LEU:HD12	0.68	1.65	2	2
1:A:37:THR:HG22	1:A:38:ILE:HD12	0.67	1.64	12	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:65:TYR:CD1	2:C:231:LEU:HD11	0.67	2.25	5	5
1:A:46:VAL:HG22	1:B:49:ILE:HG23	0.66	1.67	17	1
1:A:50:LEU:HD13	2:C:240:ARG:HG2	0.65	1.68	9	6
1:A:50:LEU:HD22	2:C:240:ARG:HG3	0.65	1.69	18	8
1:B:42:VAL:O	1:B:46:VAL:HG23	0.64	1.93	5	15
1:A:68:LEU:CD1	1:B:38:ILE:HD11	0.63	2.24	17	12
1:A:65:TYR:OH	1:B:38:ILE:HG23	0.63	1.94	12	11
1:A:49:ILE:CD1	1:B:49:ILE:HD11	0.63	2.24	8	4
1:B:46:VAL:HG11	2:C:226:LEU:O	0.62	1.94	11	8
1:A:49:ILE:HD13	1:B:49:ILE:CG1	0.62	2.24	5	1
1:A:42:VAL:O	1:A:46:VAL:HG23	0.62	1.95	13	10
1:A:64:LEU:HD11	1:B:35:ARG:HG3	0.62	1.71	20	8
1:A:46:VAL:HG22	1:B:49:ILE:CG2	0.62	2.24	17	1
1:B:45:LYS:O	1:B:49:ILE:HD12	0.62	1.94	10	5
1:A:64:LEU:HD11	1:B:35:ARG:CG	0.62	2.25	14	10
1:A:56:PHE:CZ	1:B:34:LEU:HD22	0.61	2.30	15	8
1:A:38:ILE:HD11	1:B:68:LEU:CD1	0.61	2.25	14	5
1:A:64:LEU:HD11	1:B:35:ARG:CD	0.61	2.26	15	2
1:A:35:ARG:O	1:B:64:LEU:HD11	0.60	1.96	9	12
1:A:45:LYS:O	1:A:49:ILE:HD12	0.60	1.95	19	10
1:B:53:VAL:HG21	2:C:246:GLN:OE1	0.60	1.95	10	2
1:B:38:ILE:HG12	2:C:227:LEU:HD13	0.60	1.71	2	1
1:A:35:ARG:O	1:B:64:LEU:HD21	0.59	1.97	12	6
1:A:46:VAL:HG11	2:C:242:PRO:HB3	0.59	1.72	12	4
1:A:56:PHE:CE2	1:B:34:LEU:HD22	0.59	2.32	13	3
1:A:65:TYR:OH	1:B:34:LEU:HD23	0.59	1.98	2	3
1:A:49:ILE:HG12	1:B:49:ILE:HD11	0.58	1.76	1	1
1:B:53:VAL:HG21	2:C:246:GLN:CD	0.58	2.19	19	3
1:A:46:VAL:HG12	1:A:50:LEU:CD1	0.58	2.28	8	6
1:A:65:TYR:CE2	2:C:227:LEU:HD23	0.58	2.34	9	1
1:B:53:VAL:HG11	2:C:246:GLN:CG	0.57	2.29	4	4
1:A:49:ILE:CD1	1:B:49:ILE:HD13	0.57	2.26	15	2
1:A:30:LEU:HD12	1:A:31:LEU:N	0.57	2.14	2	1
1:A:47:GLU:HA	1:A:50:LEU:HD12	0.57	1.76	20	2
1:B:50:LEU:HD21	2:C:229:GLN:HG2	0.57	1.77	16	2
1:B:39:SER:OG	1:B:42:VAL:HG23	0.56	2.01	1	4
1:A:65:TYR:HA	1:A:68:LEU:HD12	0.56	1.77	7	7
1:A:64:LEU:HD11	1:B:35:ARG:HG2	0.56	1.78	18	3
1:A:66:LEU:HG	2:C:231:LEU:HD13	0.56	1.78	5	2
1:A:62:LEU:HG	1:A:66:LEU:HD12	0.56	1.78	1	2
1:A:31:LEU:HD23	1:A:35:ARG:HG3	0.56	1.77	11	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:C:236:LEU:HD13	2:C:248:LEU:CD2	0.55	2.31	15	1
1:A:65:TYR:O	1:A:68:LEU:HD12	0.55	2.01	6	2
1:A:49:ILE:HG21	1:B:49:ILE:HD11	0.55	1.78	6	3
1:B:38:ILE:HD13	2:C:227:LEU:HD22	0.55	1.78	19	2
1:A:49:ILE:HG13	1:B:49:ILE:HD11	0.55	1.77	4	2
1:A:50:LEU:HD13	2:C:240:ARG:CG	0.55	2.31	9	4
2:C:236:LEU:HD11	2:C:245:VAL:HA	0.54	1.78	13	12
1:B:50:LEU:HD22	2:C:226:LEU:HD11	0.54	1.79	2	1
1:B:47:GLU:HA	2:C:226:LEU:HD22	0.54	1.78	4	5
1:A:34:LEU:HD12	1:B:61:LYS:HD2	0.54	1.78	8	1
1:B:38:ILE:HG21	2:C:227:LEU:HD11	0.54	1.79	16	1
1:A:46:VAL:HG12	1:A:50:LEU:HD11	0.54	1.79	8	2
1:B:62:LEU:HD22	2:C:247:PHE:CE2	0.54	2.38	16	4
1:A:49:ILE:CG1	1:B:49:ILE:HD11	0.53	2.33	1	2
2:C:227:LEU:O	2:C:231:LEU:HD12	0.53	2.03	9	1
1:B:62:LEU:HD12	2:C:247:PHE:CD2	0.53	2.39	4	1
1:A:65:TYR:CD2	2:C:231:LEU:HD21	0.53	2.38	10	2
1:B:50:LEU:HD11	2:C:229:GLN:HG2	0.53	1.80	7	1
1:A:49:ILE:HD13	1:B:49:ILE:CD1	0.53	2.34	19	2
1:B:50:LEU:HD21	2:C:229:GLN:CG	0.53	2.34	16	2
1:A:35:ARG:HG3	1:B:64:LEU:HD13	0.53	1.79	17	1
2:C:236:LEU:HD13	2:C:248:LEU:CD1	0.52	2.29	10	2
1:A:64:LEU:HD11	1:B:35:ARG:HA	0.52	1.81	12	1
2:C:236:LEU:CD1	2:C:248:LEU:HD13	0.52	2.34	8	2
1:B:65:TYR:O	1:B:68:LEU:HD12	0.52	2.04	12	2
1:B:47:GLU:HB2	2:C:226:LEU:HD13	0.52	1.81	18	5
1:A:49:ILE:O	1:A:53:VAL:HG23	0.52	2.05	9	1
1:B:53:VAL:HG11	2:C:246:GLN:HG2	0.52	1.80	4	3
2:C:241:SER:O	2:C:245:VAL:HG23	0.52	2.05	7	20
1:A:50:LEU:HD22	2:C:240:ARG:CG	0.52	2.34	4	2
1:B:38:ILE:CG1	2:C:227:LEU:HD13	0.52	2.34	2	1
1:A:37:THR:HG22	1:A:38:ILE:CD1	0.51	2.35	12	1
1:A:38:ILE:HD11	1:B:68:LEU:HD13	0.51	1.82	14	2
2:C:236:LEU:HD22	2:C:248:LEU:HD22	0.51	1.81	13	2
2:C:233:GLN:NE2	2:C:245:VAL:HG12	0.51	2.21	7	1
1:A:68:LEU:HD21	1:B:38:ILE:HD11	0.51	1.82	12	1
1:A:58:ASP:O	1:A:62:LEU:HD23	0.51	2.06	12	1
1:A:34:LEU:HD13	1:B:56:PHE:CD2	0.50	2.41	1	3
1:A:45:LYS:HB3	1:B:49:ILE:HD12	0.50	1.82	16	1
1:A:30:LEU:HD22	1:B:55:LYS:CG	0.50	2.37	1	1
1:B:30:LEU:O	1:B:34:LEU:HD12	0.50	2.06	17	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:50:LEU:HD21	2:C:229:GLN:HB3	0.50	1.83	7	1
1:A:34:LEU:HD21	1:A:42:VAL:HG21	0.50	1.82	17	1
1:B:38:ILE:HG21	2:C:227:LEU:HD23	0.49	1.84	19	1
1:A:46:VAL:O	1:A:50:LEU:HD12	0.49	2.07	1	2
1:A:65:TYR:CB	2:C:231:LEU:HD21	0.49	2.37	9	1
2:C:236:LEU:CD1	2:C:248:LEU:HD22	0.49	2.33	15	1
1:A:66:LEU:HD23	2:C:231:LEU:HD13	0.49	1.84	6	2
1:B:50:LEU:HD11	2:C:229:GLN:CD	0.49	2.27	14	1
1:B:53:VAL:HG11	2:C:246:GLN:HB2	0.48	1.85	7	1
1:A:64:LEU:HD21	1:B:35:ARG:CG	0.48	2.38	13	1
1:A:35:ARG:HD2	1:B:64:LEU:HD13	0.48	1.84	9	1
1:A:61:LYS:NZ	1:A:64:LEU:HD13	0.48	2.22	19	1
1:A:37:THR:C	1:A:38:ILE:HD12	0.48	2.29	9	3
1:A:49:ILE:HD11	1:B:45:LYS:HG3	0.48	1.85	8	1
1:A:66:LEU:CD2	2:C:231:LEU:HD13	0.48	2.39	9	1
1:B:50:LEU:HD11	2:C:229:GLN:NE2	0.48	2.24	16	1
1:B:38:ILE:HD13	2:C:227:LEU:CD2	0.47	2.38	18	1
1:A:30:LEU:O	1:A:34:LEU:HD12	0.47	2.08	1	5
1:A:34:LEU:HD12	1:B:61:LYS:CD	0.47	2.39	8	1
1:A:34:LEU:HD22	1:B:56:PHE:CZ	0.47	2.44	14	1
1:A:57:SER:HB3	1:B:31:LEU:HD21	0.47	1.86	15	2
2:C:236:LEU:CD1	2:C:244:VAL:HG12	0.47	2.40	7	2
1:A:36:GLY:O	1:A:37:THR:HG23	0.47	2.10	11	8
1:B:53:VAL:HG21	2:C:246:GLN:NE2	0.47	2.25	19	2
1:B:53:VAL:HG11	2:C:246:GLN:OE1	0.46	2.09	19	1
2:C:233:GLN:HB3	2:C:245:VAL:HG11	0.46	1.86	19	3
1:A:49:ILE:HG13	1:B:49:ILE:HD13	0.46	1.86	7	2
1:A:46:VAL:O	1:A:50:LEU:HD23	0.46	2.10	5	1
1:A:56:PHE:CD2	1:B:30:LEU:HD23	0.46	2.45	11	1
1:A:35:ARG:CD	1:B:64:LEU:HD13	0.46	2.41	9	1
1:B:58:ASP:O	1:B:62:LEU:HD23	0.46	2.10	2	1
1:A:64:LEU:HD23	1:A:65:TYR:CD1	0.46	2.46	2	1
1:A:65:TYR:HB2	2:C:231:LEU:HD22	0.46	1.86	2	1
1:A:64:LEU:HD21	1:B:35:ARG:HG3	0.46	1.86	15	2
1:A:53:VAL:HG13	1:A:56:PHE:CZ	0.46	2.46	17	2
1:B:53:VAL:HG11	2:C:246:GLN:HG3	0.46	1.87	6	2
1:A:64:LEU:HD11	1:B:35:ARG:HD3	0.45	1.87	15	1
1:B:46:VAL:HG11	2:C:230:VAL:HB	0.45	1.88	18	1
1:A:49:ILE:CB	1:B:49:ILE:HD11	0.45	2.41	5	2
1:A:62:LEU:HA	2:C:231:LEU:HD23	0.45	1.88	2	1
2:C:236:LEU:HD13	2:C:248:LEU:HG	0.45	1.88	1	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:46:VAL:HG11	2:C:230:VAL:CG2	0.45	2.42	18	1
1:B:61:LYS:HE2	1:B:64:LEU:HD22	0.45	1.88	14	1
1:A:30:LEU:HD22	1:B:55:LYS:HG2	0.45	1.88	1	1
1:A:50:LEU:HD11	2:C:237:SER:OG	0.45	2.12	7	1
1:A:62:LEU:HD23	1:A:63:TYR:N	0.44	2.27	6	2
1:A:35:ARG:HA	1:B:64:LEU:HD13	0.44	1.89	2	1
1:B:50:LEU:HD13	2:C:229:GLN:CD	0.44	2.33	4	2
1:A:38:ILE:HG23	1:B:65:TYR:OH	0.44	2.12	1	2
1:B:46:VAL:HG11	2:C:230:VAL:CB	0.44	2.43	18	1
1:A:34:LEU:HD13	1:B:56:PHE:CE1	0.44	2.47	2	1
1:B:31:LEU:HD13	1:B:31:LEU:O	0.44	2.12	12	1
1:A:61:LYS:HE3	1:B:31:LEU:HD23	0.44	1.89	3	1
1:B:50:LEU:HD22	2:C:226:LEU:CD1	0.44	2.43	9	1
1:A:55:LYS:HB3	1:B:30:LEU:HD22	0.43	1.90	8	1
1:A:65:TYR:CG	2:C:231:LEU:HD21	0.43	2.48	13	1
1:A:49:ILE:HD11	1:B:49:ILE:CD1	0.43	2.37	10	1
1:A:49:ILE:CG2	1:B:49:ILE:HD11	0.43	2.44	6	2
1:A:49:ILE:HG21	1:B:49:ILE:CD1	0.43	2.43	6	2
1:B:47:GLU:HA	2:C:226:LEU:HD23	0.43	1.89	13	2
2:C:244:VAL:HG12	2:C:248:LEU:CD1	0.43	2.41	2	2
1:A:65:TYR:HD1	2:C:231:LEU:HD11	0.43	1.73	13	3
1:A:49:ILE:HG21	1:B:46:VAL:HG22	0.43	1.90	2	1
1:A:46:VAL:HG11	2:C:242:PRO:CB	0.42	2.44	12	1
1:B:50:LEU:HD12	2:C:229:GLN:HG2	0.42	1.91	10	1
1:A:31:LEU:HD22	1:B:56:PHE:HB3	0.42	1.91	7	1
1:B:43:GLN:HG3	2:C:227:LEU:HD21	0.42	1.91	2	1
1:A:49:ILE:HD13	1:B:49:ILE:HG13	0.42	1.92	5	1
1:B:46:VAL:HG13	2:C:230:VAL:HB	0.42	1.90	6	1
1:B:36:GLY:O	1:B:37:THR:HG23	0.42	2.15	12	7
1:A:30:LEU:HD23	1:B:56:PHE:CD1	0.41	2.50	13	1
1:A:49:ILE:HD12	1:B:45:LYS:HB3	0.41	1.91	17	1
1:A:37:THR:HG22	1:B:68:LEU:CD2	0.41	2.45	11	1
1:A:35:ARG:HA	1:B:64:LEU:HD22	0.41	1.91	2	1
1:B:50:LEU:HD13	2:C:229:GLN:HG2	0.41	1.89	13	1
1:A:62:LEU:HD21	2:C:235:ARG:HB2	0.41	1.93	19	1
1:B:43:GLN:CD	2:C:227:LEU:HD21	0.41	2.36	17	1
1:B:38:ILE:CD1	2:C:227:LEU:HD22	0.41	2.45	19	1
1:A:55:LYS:CB	1:B:30:LEU:HD22	0.41	2.46	8	1
1:A:61:LYS:HE2	1:A:64:LEU:HD22	0.40	1.92	12	1
1:A:64:LEU:HD23	1:A:64:LEU:O	0.40	2.16	15	1
1:A:62:LEU:O	1:A:66:LEU:HD12	0.40	2.16	13	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:46:VAL:HG11	2:C:242:PRO:HA	0.40	1.94	15	1
2:C:226:LEU:O	2:C:230:VAL:HG23	0.40	2.17	9	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	40/68 (59%)	36±2 (89±4%)	4±1 (9±3%)	1±1 (2±2%)	17	61
1	B	39/68 (57%)	37±1 (95±3%)	2±1 (5±2%)	0±1 (1±2%)	29	74
2	C	27/62 (44%)	23±2 (84±7%)	4±1 (15±5%)	0±1 (1±2%)	18	63
All	All	2120/3960 (54%)	1903 (90%)	190 (9%)	27 (1%)	20	66

All 8 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	C	240	ARG	7
1	A	38	ILE	6
1	A	37	THR	5
1	A	56	PHE	2
1	B	56	PHE	2
1	B	37	THR	2
1	B	38	ILE	2
2	C	225	THR	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	37/60 (62%)	25±2 (66±6%)	13±2 (34±6%)	1	11
1	B	36/60 (60%)	24±2 (66±5%)	12±2 (34±5%)	1	11
2	C	27/56 (48%)	20±2 (73±6%)	7±2 (27±6%)	2	23
All	All	2000/3520 (57%)	1360 (68%)	640 (32%)	1	14

All 78 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	C	236	LEU	20
1	A	39	SER	19
1	B	57	SER	19
1	A	34	LEU	18
1	B	62	LEU	18
1	A	60	ASP	18
1	A	31	LEU	18
1	B	39	SER	18
1	A	61	LYS	16
1	B	64	LEU	15
2	C	238	LEU	15
2	C	229	GLN	15
1	B	55	LYS	14
1	A	30	LEU	12
1	B	31	LEU	12
2	C	234	LYS	11
1	B	40	LYS	11
1	B	35	ARG	11
1	A	68	LEU	10
1	A	47	GLU	10
1	B	63	TYR	10
1	B	67	GLN	10
1	B	34	LEU	10
2	C	250	LYS	9
1	B	60	ASP	9
1	A	37	THR	9
1	B	37	THR	9
2	C	239	LEU	9
2	C	235	ARG	9
1	A	55	LYS	9
1	A	62	LEU	9
1	B	30	LEU	9
1	B	52	ASP	9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
2	C	240	ARG	8
2	C	249	GLN	8
1	A	33	ARG	8
1	A	67	GLN	8
1	A	64	LEU	8
1	A	54	GLN	8
1	A	56	PHE	8
2	C	241	SER	8
1	B	54	GLN	8
1	B	51	GLN	7
1	B	61	LYS	7
1	A	43	GLN	7
1	B	43	GLN	7
1	A	40	LYS	6
1	A	51	GLN	6
1	A	65	TYR	6
1	A	50	LEU	6
2	C	248	LEU	6
1	A	63	TYR	6
1	B	45	LYS	6
2	C	228	GLU	5
1	A	52	ASP	5
1	B	32	GLN	5
1	B	66	LEU	5
2	C	227	LEU	5
1	A	59	ASN	5
1	B	33	ARG	5
1	B	47	GLU	4
2	C	251	GLN	4
2	C	243	GLU	4
2	C	237	SER	3
1	A	58	ASP	3
2	C	226	LEU	3
1	A	45	LYS	3
1	B	50	LEU	3
1	A	32	GLN	3
1	B	44	ASN	3
1	A	35	ARG	2
1	A	57	SER	2
1	B	58	ASP	1
1	A	44	ASN	1
1	B	59	ASN	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	66	LEU	1
2	C	246	GLN	1
2	C	231	LEU	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