Full wwPDB NMR Structure Validation Report (i)

May 28, 2020 – 08:16 pm BST

PDB ID	:	1P4Q
Title	:	Solution structure of the CITED2 transactivation domain in complex with the p300 CH1 domain
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Deposited on	:	2003-04-23

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

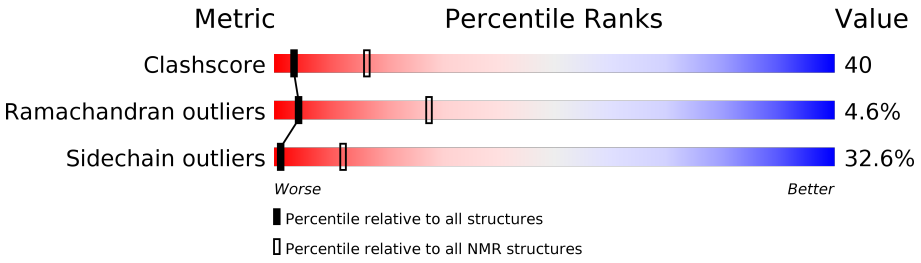
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.11
Ideal geometry (proteins)	:	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 <=5%

Mol	Chain	Length	Quality of chain
1	A	52	27% 44% 6% 23%
2	B	101	30% 45% 10% 16%

2 Ensemble composition and analysis

This entry contains 17 models. Model 12 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:10-A:49, B:109-B:184, B:189-B:197 (125)	0.44	12

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 5 clusters and 3 single-model clusters were found.

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

3 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2371 atoms, of which 1172 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Cbp/p300-interacting transactivator 2.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	52	788	256	382	60	87	3	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	CLONING ARTIFACT	UNP Q99967
A	2	SER	-	CLONING ARTIFACT	UNP Q99967
A	3	GLY	-	CLONING ARTIFACT	UNP Q99967
A	4	SER	-	CLONING ARTIFACT	UNP Q99967
A	5	GLY	-	CLONING ARTIFACT	UNP Q99967
A	6	SER	-	CLONING ARTIFACT	UNP Q99967
A	7	GLY	-	CLONING ARTIFACT	UNP Q99967
A	8	SER	-	CLONING ARTIFACT	UNP Q99967

- Molecule 2 is a protein called E1A-associated protein p300.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	B	101	1580	475	790	164	139	12	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
			Total	Zn
3	B	3	3	3

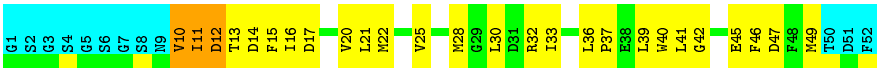
4 Residue-property plots (i)

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.

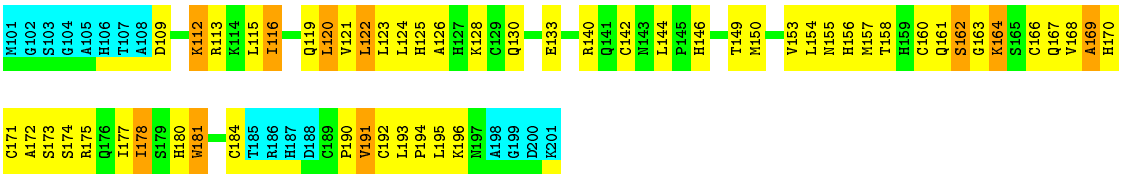
• Molecule 1: Cbp/p300-interacting transactivator 2

Chain A:



• Molecule 2: E1A-associated protein p300

Chain B:



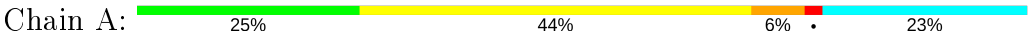
4.2 Scores per residue for each member of the ensemble

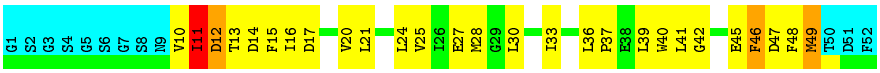
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Cbp/p300-interacting transactivator 2

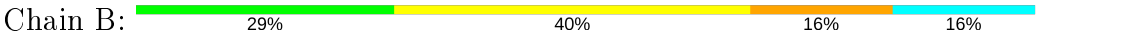
Chain A:

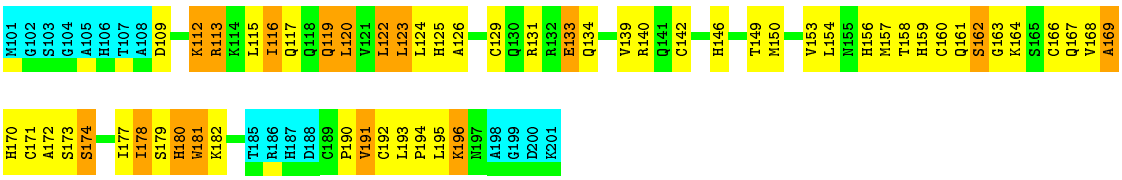




• Molecule 2: E1A-associated protein p300

Chain B:

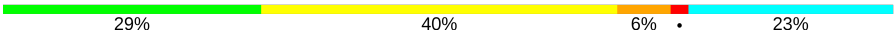




4.2.2 Score per residue for model 2

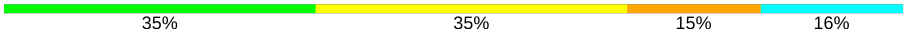
- Molecule 1: Cbp/p300-interacting transactivator 2

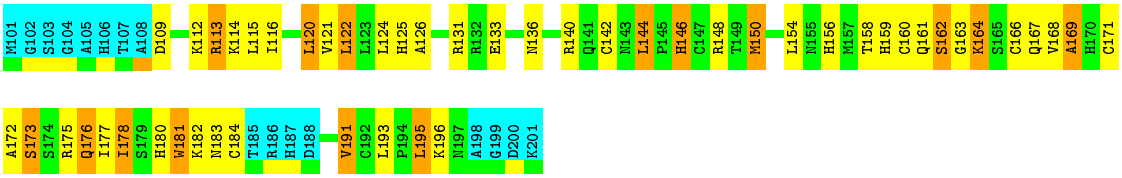
Chain A:



- Molecule 2: E1A-associated protein p300

Chain B:

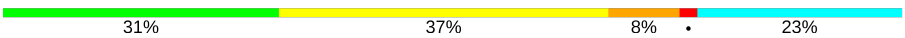




4.2.3 Score per residue for model 3

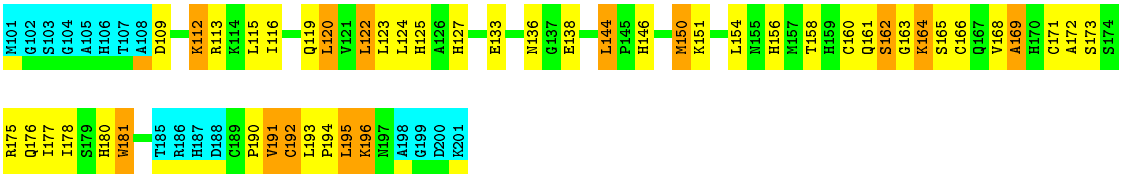
- Molecule 1: Cbp/p300-interacting transactivator 2

Chain A:



- Molecule 2: E1A-associated protein p300

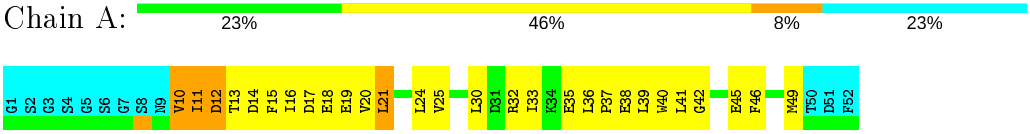
Chain B:



4.2.4 Score per residue for model 4

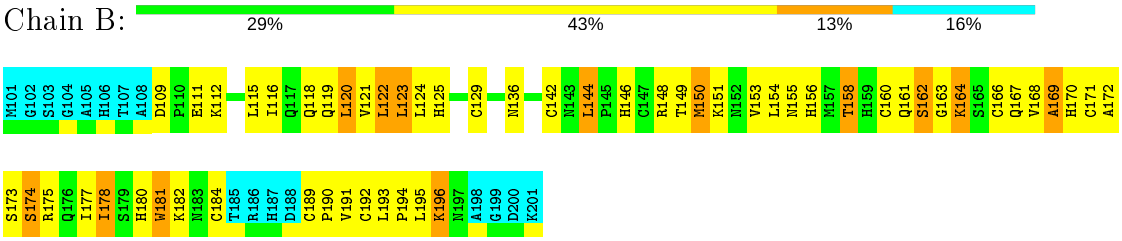
- Molecule 1: Cbp/p300-interacting transactivator 2

Chain A:



• Molecule 2: E1A-associated protein p300

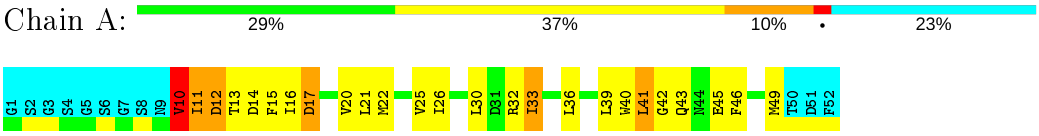
Chain B:



4.2.5 Score per residue for model 5

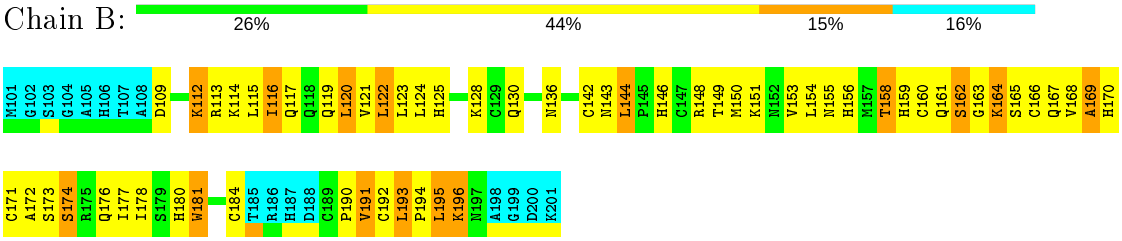
• Molecule 1: Cbp/p300-interacting transactivator 2

Chain A:



• Molecule 2: E1A-associated protein p300

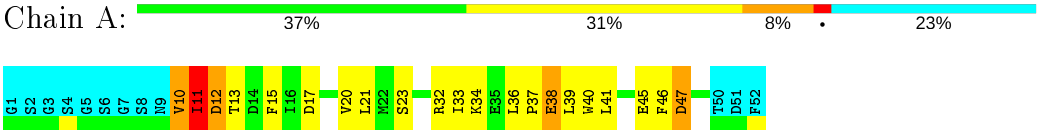
Chain B:



4.2.6 Score per residue for model 6

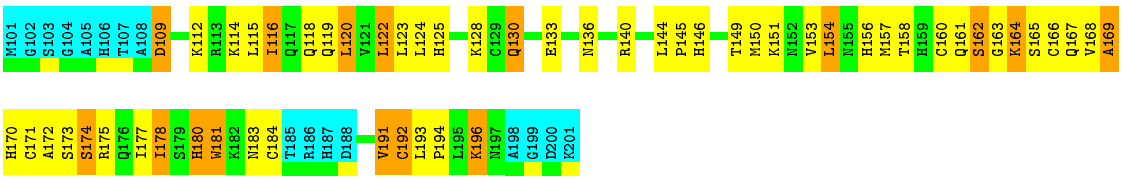
• Molecule 1: Cbp/p300-interacting transactivator 2

Chain A:



• Molecule 2: E1A-associated protein p300

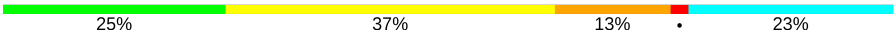
Chain B:



4.2.7 Score per residue for model 7

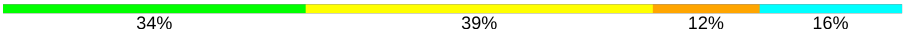
- Molecule 1: Cbp/p300-interacting transactivator 2

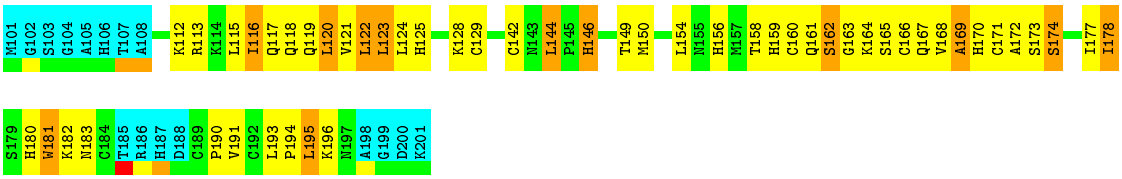
Chain A:



- Molecule 2: E1A-associated protein p300

Chain B:

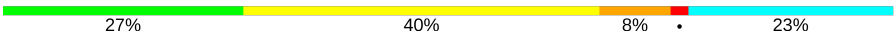




4.2.8 Score per residue for model 8

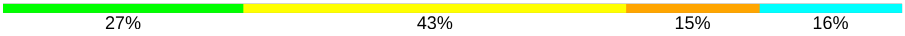
- Molecule 1: Cbp/p300-interacting transactivator 2

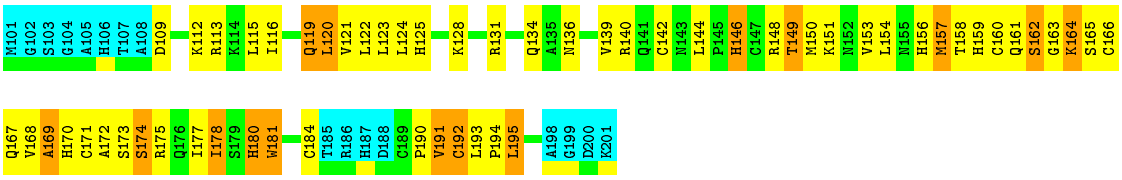
Chain A:



- Molecule 2: E1A-associated protein p300

Chain B:

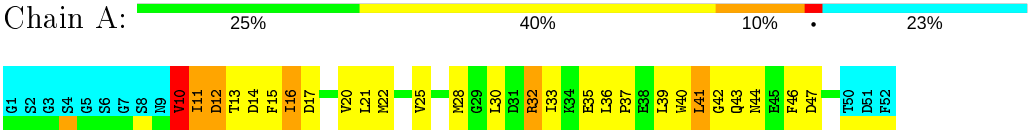




4.2.9 Score per residue for model 9

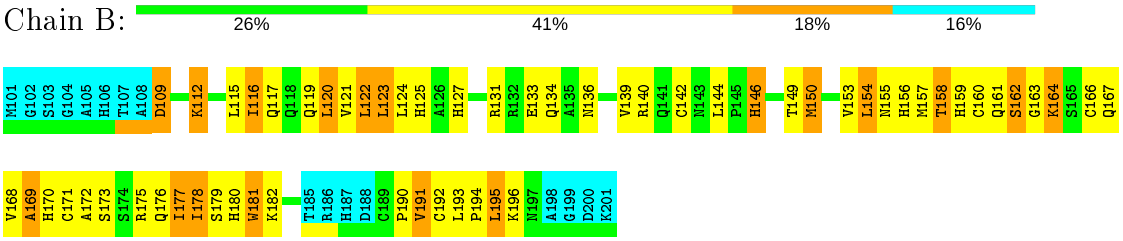
- Molecule 1: Cbp/p300-interacting transactivator 2

Chain A:



- Molecule 2: E1A-associated protein p300

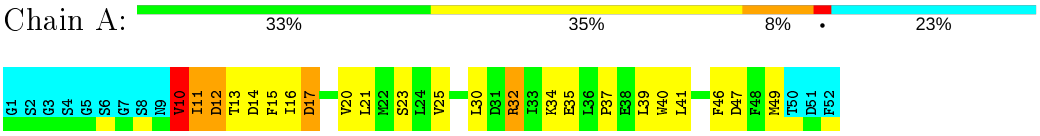
Chain B:



4.2.10 Score per residue for model 10

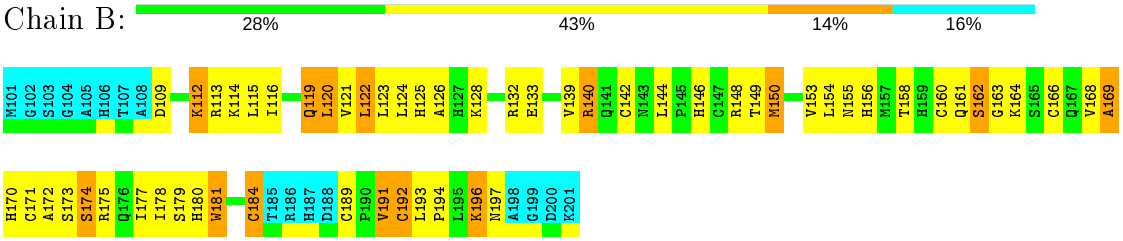
- Molecule 1: Cbp/p300-interacting transactivator 2

Chain A:



- Molecule 2: E1A-associated protein p300

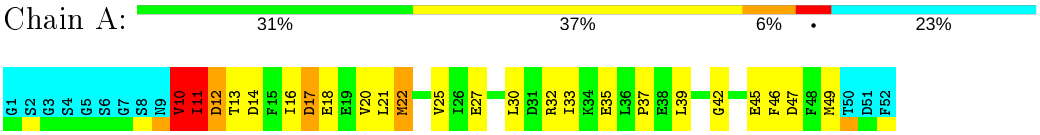
Chain B:



4.2.11 Score per residue for model 11

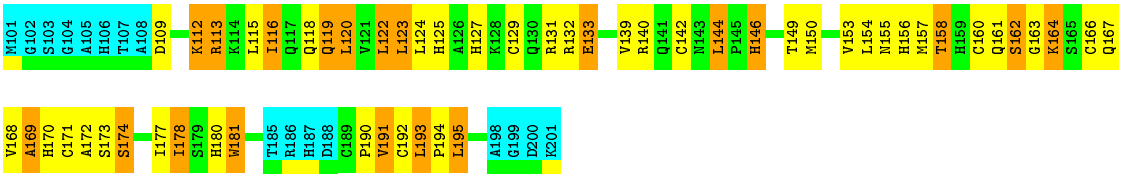
- Molecule 1: Cbp/p300-interacting transactivator 2

Chain A:



- Molecule 2: E1A-associated protein p300

Chain B:



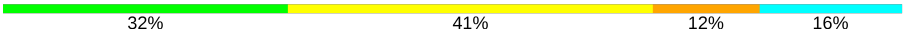
4.2.12 Score per residue for model 12 (medoid)

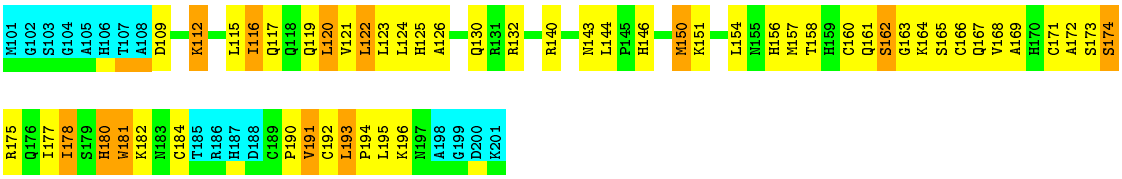
- Molecule 1: Cbp/p300-interacting transactivator 2

Chain A:

- Molecule 2: E1A-associated protein p300

Chain B:

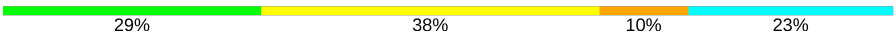




4.2.13 Score per residue for model 13

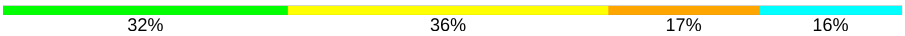
- Molecule 1: Cbp/p300-interacting transactivator 2

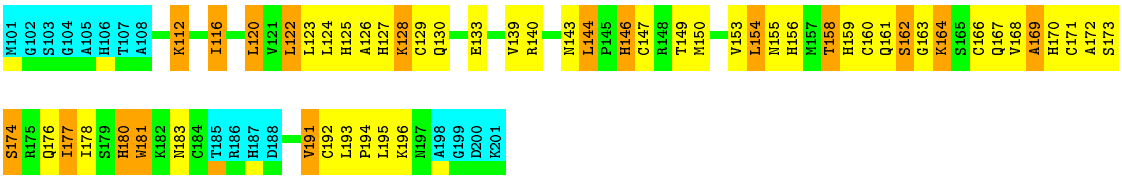
Chain A:



- Molecule 2: E1A-associated protein p300

Chain B:

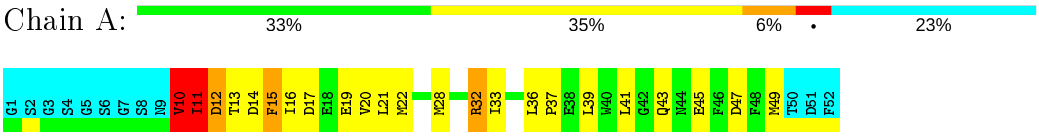




4.2.14 Score per residue for model 14

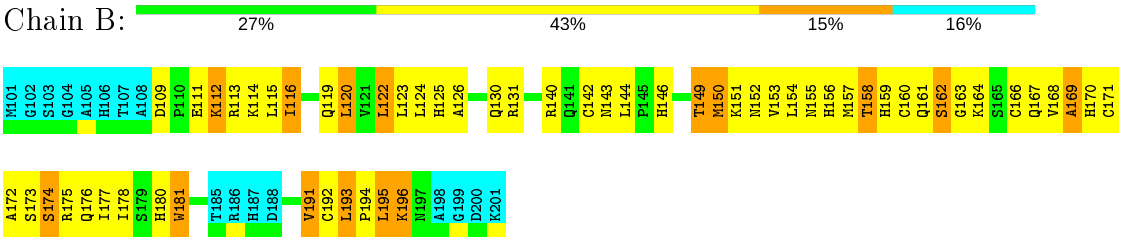
- Molecule 1: Cbp/p300-interacting transactivator 2

Chain A:



• Molecule 2: E1A-associated protein p300

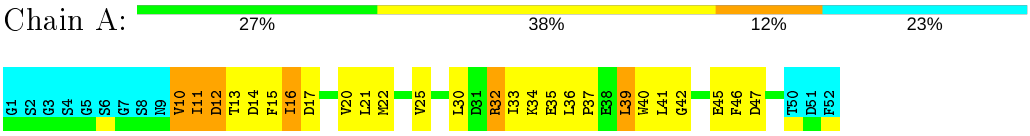
Chain B:



4.2.15 Score per residue for model 15

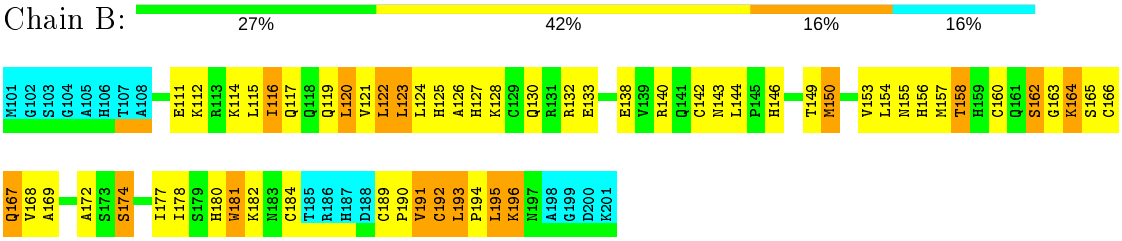
• Molecule 1: Cbp/p300-interacting transactivator 2

Chain A:



• Molecule 2: E1A-associated protein p300

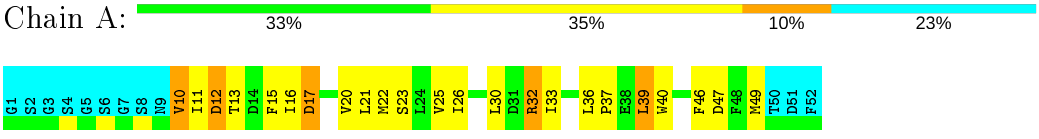
Chain B:



4.2.16 Score per residue for model 16

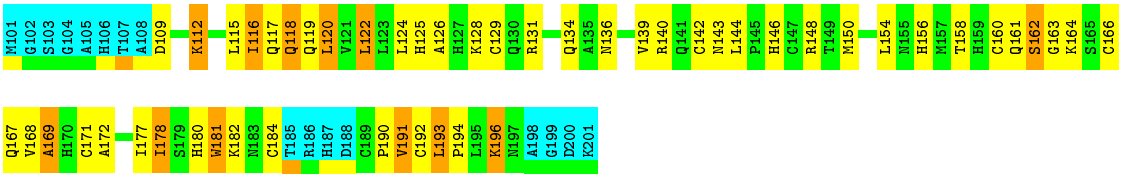
• Molecule 1: Cbp/p300-interacting transactivator 2

Chain A:



• Molecule 2: E1A-associated protein p300

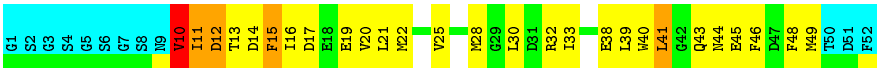
Chain B:



4.2.17 Score per residue for model 17

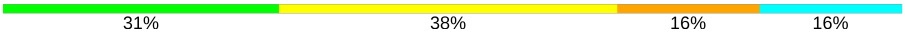
- Molecule 1: Cbp/p300-interacting transactivator 2

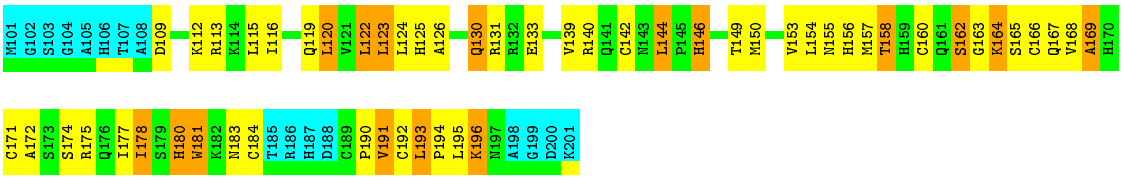
Chain A:



- Molecule 2: E1A-associated protein p300

Chain B:





5 Refinement protocol and experimental data overview

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

Of the 25 calculated structures, 17 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	structure solution	1.0.4
X-PLOR	refinement	3.1

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

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	331	322	322	38±4
2	B	678	686	682	65±7
All	All	17204	17136	17068	1358

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 40.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:33:ILE:HD12	2:B:146:HIS:CD2	0.87	2.03	14	13
1:A:49:MET:HE1	2:B:116:ILE:HD13	0.86	1.45	17	7
2:B:166:CYS:O	2:B:172:ALA:HB2	0.85	1.70	2	17
1:A:11:ILE:CG2	1:A:13:THR:HG23	0.84	2.01	11	14
1:A:11:ILE:CG2	1:A:13:THR:HG22	0.83	2.03	2	2
1:A:25:VAL:HG11	2:B:144:LEU:HD22	0.82	1.49	5	3
1:A:11:ILE:HG21	1:A:13:THR:HG23	0.82	1.50	11	14
1:A:49:MET:CE	2:B:116:ILE:HD13	0.80	2.06	4	7
1:A:25:VAL:HG11	2:B:144:LEU:HD11	0.78	1.53	7	5
1:A:36:LEU:HD23	2:B:149:THR:HG21	0.77	1.55	7	1
2:B:149:THR:O	2:B:153:VAL:HG23	0.76	1.79	17	12

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:37:PRO:CG	2:B:115:LEU:HD13	0.75	2.10	15	6
2:B:124:LEU:HD21	2:B:181:TRP:CH2	0.75	2.17	15	2
1:A:17:ASP:HB3	1:A:20:VAL:HG23	0.74	1.60	2	17
2:B:153:VAL:HG12	2:B:157:MET:SD	0.73	2.23	8	1
2:B:123:LEU:HD11	2:B:174:SER:OG	0.73	1.84	7	11
2:B:112:LYS:CE	2:B:116:ILE:HD11	0.73	2.14	4	3
2:B:122:LEU:HD12	2:B:150:MET:SD	0.73	2.24	10	7
1:A:39:LEU:HD21	2:B:116:ILE:HD12	0.72	1.61	9	2
1:A:39:LEU:HD21	2:B:116:ILE:CD1	0.72	2.14	9	4
2:B:123:LEU:HD13	2:B:178:ILE:CD1	0.72	2.15	4	2
2:B:113:ARG:HA	2:B:116:ILE:HD12	0.71	1.62	17	3
2:B:112:LYS:HD3	2:B:116:ILE:HD11	0.71	1.62	17	2
1:A:39:LEU:HD22	2:B:112:LYS:HB2	0.70	1.62	9	3
2:B:123:LEU:HD22	2:B:178:ILE:HD11	0.70	1.63	15	3
2:B:120:LEU:HD22	2:B:177:ILE:CG2	0.70	2.17	7	16
1:A:33:ILE:HD12	2:B:146:HIS:NE2	0.70	2.02	4	11
1:A:39:LEU:HD22	1:A:39:LEU:N	0.69	2.01	15	4
2:B:112:LYS:O	2:B:116:ILE:N	0.69	2.25	8	17
1:A:11:ILE:HG21	1:A:13:THR:HG22	0.69	1.65	1	2
2:B:180:HIS:CE1	2:B:191:VAL:HG21	0.69	2.23	11	12
2:B:112:LYS:O	2:B:116:ILE:HD12	0.68	1.89	6	4
1:A:21:LEU:HD13	2:B:125:HIS:HA	0.68	1.64	15	4
2:B:181:TRP:CZ2	2:B:195:LEU:HD22	0.68	2.22	15	5
1:A:37:PRO:CB	2:B:115:LEU:HD13	0.68	2.18	7	6
2:B:120:LEU:O	2:B:124:LEU:N	0.67	2.27	1	17
1:A:25:VAL:HG11	2:B:144:LEU:HD21	0.67	1.66	3	2
2:B:122:LEU:HD12	2:B:150:MET:HG2	0.67	1.67	11	5
2:B:123:LEU:HD22	2:B:178:ILE:CD1	0.67	2.20	17	4
2:B:112:LYS:HE2	2:B:116:ILE:HD11	0.66	1.66	8	3
1:A:11:ILE:HD12	2:B:178:ILE:HG13	0.66	1.66	6	10
1:A:11:ILE:HG23	1:A:12:ASP:N	0.66	2.06	7	16
2:B:127:HIS:CE1	2:B:154:LEU:HD21	0.66	2.26	13	1
2:B:123:LEU:HD13	2:B:178:ILE:HD13	0.65	1.68	4	3
1:A:10:VAL:HG22	1:A:11:ILE:N	0.65	2.07	10	16
1:A:11:ILE:HD11	2:B:120:LEU:CD1	0.64	2.21	11	7
2:B:124:LEU:HD22	2:B:195:LEU:CD2	0.64	2.22	15	1
1:A:39:LEU:HD23	2:B:115:LEU:HB3	0.64	1.67	10	3
1:A:39:LEU:N	1:A:39:LEU:HD22	0.64	2.08	4	1
1:A:39:LEU:HD21	2:B:116:ILE:HG12	0.64	1.69	3	2
2:B:117:GLN:HG2	2:B:191:VAL:HG13	0.63	1.70	15	2
1:A:21:LEU:HD13	2:B:121:VAL:HG13	0.63	1.70	7	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:120:LEU:O	2:B:124:LEU:CD1	0.63	2.47	15	4
1:A:39:LEU:HD23	2:B:116:ILE:HD12	0.63	1.68	16	1
2:B:181:TRP:HE1	2:B:191:VAL:HG12	0.63	1.53	2	17
1:A:40:TRP:CH2	2:B:172:ALA:HB3	0.63	2.28	5	9
2:B:180:HIS:NE2	2:B:191:VAL:HG21	0.63	2.09	9	12
2:B:117:GLN:O	2:B:121:VAL:HG23	0.63	1.92	15	2
1:A:36:LEU:HD12	1:A:37:PRO:HD2	0.62	1.70	9	8
1:A:10:VAL:HG13	1:A:11:ILE:H	0.62	1.55	13	16
2:B:112:LYS:CD	2:B:116:ILE:HD11	0.62	2.25	4	2
2:B:120:LEU:O	2:B:124:LEU:HG	0.61	1.94	1	15
1:A:39:LEU:HD11	2:B:116:ILE:CD1	0.61	2.25	10	3
1:A:39:LEU:C	1:A:39:LEU:HD13	0.61	2.16	10	4
1:A:41:LEU:HD11	2:B:176:GLN:NE2	0.60	2.11	5	1
1:A:11:ILE:HD11	2:B:178:ILE:HG13	0.60	1.72	13	1
1:A:39:LEU:HD23	2:B:116:ILE:CD1	0.60	2.25	16	1
2:B:112:LYS:CE	2:B:116:ILE:HD13	0.60	2.26	1	1
1:A:21:LEU:HD11	2:B:125:HIS:HB2	0.59	1.75	8	10
1:A:39:LEU:CG	2:B:177:ILE:HD11	0.59	2.27	9	7
2:B:120:LEU:O	2:B:124:LEU:CG	0.59	2.51	13	15
1:A:39:LEU:HD13	1:A:39:LEU:C	0.58	2.18	3	3
2:B:120:LEU:O	2:B:124:LEU:HD13	0.58	1.97	15	2
1:A:49:MET:HE2	2:B:116:ILE:HD13	0.58	1.74	4	2
1:A:37:PRO:HG2	2:B:115:LEU:HD21	0.58	1.72	3	4
1:A:39:LEU:HD12	2:B:177:ILE:HD11	0.58	1.75	5	7
1:A:37:PRO:HB2	2:B:115:LEU:HD13	0.58	1.73	7	6
2:B:124:LEU:HD21	2:B:181:TRP:CZ3	0.58	2.34	5	1
2:B:154:LEU:HD12	2:B:154:LEU:C	0.58	2.19	17	1
1:A:39:LEU:HG	2:B:177:ILE:HD11	0.58	1.74	9	7
1:A:39:LEU:HD11	2:B:115:LEU:HB3	0.58	1.76	16	3
1:A:11:ILE:HD11	2:B:120:LEU:HD12	0.57	1.73	11	6
2:B:156:HIS:HE2	2:B:171:CYS:CB	0.57	2.10	16	15
2:B:180:HIS:CD2	2:B:181:TRP:N	0.57	2.72	2	17
1:A:39:LEU:HD11	2:B:116:ILE:HD11	0.57	1.76	10	4
1:A:39:LEU:CD1	2:B:177:ILE:HD11	0.57	2.29	14	7
1:A:30:LEU:N	1:A:30:LEU:HD23	0.57	2.14	13	7
1:A:39:LEU:HD21	2:B:112:LYS:O	0.57	2.00	14	3
1:A:25:VAL:HG13	1:A:30:LEU:HB2	0.56	1.76	13	9
2:B:191:VAL:O	2:B:195:LEU:HD23	0.56	2.00	12	2
1:A:39:LEU:HD11	2:B:115:LEU:CB	0.56	2.30	17	5
1:A:39:LEU:HD21	2:B:116:ILE:CG1	0.56	2.31	9	4
1:A:39:LEU:HB3	2:B:177:ILE:HD11	0.56	1.76	17	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:120:LEU:CD2	2:B:181:TRP:CD1	0.55	2.89	11	16
2:B:126:ALA:HB3	2:B:154:LEU:CD1	0.55	2.31	13	1
2:B:115:LEU:O	2:B:119:GLN:N	0.55	2.36	16	10
1:A:37:PRO:HG2	2:B:115:LEU:HD11	0.55	1.76	3	4
1:A:38:GLU:C	1:A:39:LEU:HD22	0.55	2.20	2	6
2:B:120:LEU:C	2:B:124:LEU:HD12	0.55	2.22	17	13
1:A:21:LEU:HD13	2:B:125:HIS:CA	0.55	2.32	15	3
2:B:123:LEU:HD23	2:B:154:LEU:CD1	0.55	2.31	9	1
2:B:115:LEU:HD23	2:B:118:GLN:CD	0.55	2.22	7	1
2:B:123:LEU:HD11	2:B:174:SER:HB3	0.55	1.79	4	1
2:B:133:GLU:CD	2:B:139:VAL:HG22	0.55	2.23	10	1
1:A:39:LEU:HD21	2:B:116:ILE:HG13	0.54	1.79	11	5
2:B:123:LEU:HD21	2:B:174:SER:OG	0.54	2.02	14	7
1:A:10:VAL:HG13	1:A:11:ILE:N	0.54	2.16	1	1
1:A:21:LEU:HD13	2:B:125:HIS:HB2	0.54	1.77	11	3
1:A:39:LEU:HD22	2:B:177:ILE:CD1	0.54	2.32	16	1
2:B:154:LEU:HD12	2:B:155:ASN:N	0.54	2.18	17	1
2:B:193:LEU:CB	2:B:194:PRO:HD3	0.54	2.33	3	5
2:B:133:GLU:OE2	2:B:139:VAL:HG13	0.54	2.03	1	1
2:B:133:GLU:HB3	2:B:139:VAL:HG22	0.54	1.80	1	1
1:A:39:LEU:HD11	2:B:116:ILE:CG1	0.54	2.33	13	2
1:A:25:VAL:HG22	1:A:30:LEU:HB2	0.54	1.80	16	5
2:B:117:GLN:CG	2:B:191:VAL:HG13	0.54	2.32	15	1
1:A:21:LEU:O	1:A:25:VAL:HG23	0.53	2.03	7	1
1:A:17:ASP:CB	1:A:20:VAL:HG23	0.53	2.33	15	8
2:B:122:LEU:HD21	2:B:144:LEU:HD13	0.53	1.79	5	1
1:A:13:THR:CG2	2:B:124:LEU:HD23	0.53	2.34	17	8
1:A:39:LEU:HD21	2:B:116:ILE:HA	0.53	1.80	16	1
1:A:39:LEU:HD11	2:B:116:ILE:HG13	0.52	1.81	14	3
2:B:162:SER:O	2:B:164:LYS:N	0.52	2.42	15	17
2:B:181:TRP:CZ2	2:B:192:CYS:HA	0.52	2.39	16	12
2:B:120:LEU:HG	2:B:181:TRP:CD1	0.52	2.40	1	12
1:A:37:PRO:HG3	2:B:115:LEU:HD22	0.52	1.81	15	2
1:A:39:LEU:HD21	2:B:116:ILE:CA	0.52	2.34	16	1
2:B:112:LYS:HE2	2:B:116:ILE:HD13	0.52	1.81	1	1
2:B:124:LEU:CD1	2:B:195:LEU:HD23	0.52	2.35	4	1
1:A:21:LEU:N	1:A:21:LEU:HD13	0.52	2.19	4	1
1:A:39:LEU:HD11	2:B:119:GLN:HB2	0.52	1.80	6	1
2:B:120:LEU:CD1	2:B:178:ILE:HD12	0.52	2.35	16	7
1:A:13:THR:HG22	2:B:124:LEU:HD23	0.52	1.82	5	1
2:B:156:HIS:CE1	2:B:168:VAL:HG11	0.51	2.39	3	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:120:LEU:HD22	2:B:177:ILE:HG23	0.51	1.81	11	8
1:A:39:LEU:HD11	2:B:119:GLN:CB	0.51	2.36	6	1
1:A:40:TRP:O	1:A:42:GLY:N	0.51	2.42	1	8
1:A:13:THR:CB	2:B:124:LEU:HD22	0.51	2.35	1	1
1:A:41:LEU:H	1:A:41:LEU:HD22	0.51	1.65	2	1
1:A:36:LEU:HD22	2:B:146:HIS:CE1	0.51	2.41	8	3
2:B:133:GLU:CD	2:B:139:VAL:HG13	0.50	2.27	1	1
1:A:15:PHE:CD1	2:B:196:LYS:CG	0.50	2.94	16	9
2:B:130:GLN:NE2	2:B:154:LEU:HD11	0.50	2.22	17	1
2:B:156:HIS:NE2	2:B:171:CYS:HB2	0.50	2.22	5	15
1:A:40:TRP:O	2:B:116:ILE:HD11	0.50	2.06	2	1
1:A:39:LEU:HD21	2:B:119:GLN:HG2	0.50	1.83	1	1
1:A:11:ILE:HG12	2:B:181:TRP:CE3	0.50	2.41	11	15
1:A:39:LEU:HD22	2:B:112:LYS:CB	0.50	2.35	9	2
1:A:13:THR:HG22	2:B:124:LEU:CD2	0.50	2.35	17	6
2:B:112:LYS:CD	2:B:113:ARG:N	0.50	2.74	14	3
1:A:46:PHE:CZ	2:B:113:ARG:CD	0.50	2.95	7	1
2:B:127:HIS:CE1	2:B:154:LEU:CD2	0.50	2.94	13	1
1:A:15:PHE:CE1	2:B:196:LYS:CB	0.49	2.95	5	6
2:B:130:GLN:OE1	2:B:154:LEU:HD22	0.49	2.07	13	1
2:B:122:LEU:HD21	2:B:144:LEU:CD2	0.49	2.37	2	2
1:A:39:LEU:CD2	1:A:39:LEU:N	0.49	2.73	15	3
1:A:10:VAL:CG1	1:A:11:ILE:N	0.49	2.76	1	1
1:A:36:LEU:CD2	2:B:149:THR:HG21	0.49	2.37	5	1
2:B:155:ASN:O	2:B:158:THR:HG22	0.49	2.06	17	8
2:B:156:HIS:HE2	2:B:168:VAL:HB	0.49	1.65	17	2
2:B:112:LYS:C	2:B:116:ILE:HD12	0.49	2.27	14	3
1:A:11:ILE:CG2	1:A:12:ASP:N	0.49	2.75	16	9
1:A:40:TRP:CZ3	2:B:172:ALA:HB3	0.49	2.42	16	2
2:B:123:LEU:O	2:B:127:HIS:CD2	0.49	2.66	13	1
2:B:193:LEU:CB	2:B:194:PRO:CD	0.49	2.90	1	13
1:A:15:PHE:CZ	2:B:196:LYS:CG	0.49	2.95	1	3
2:B:156:HIS:O	2:B:160:CYS:N	0.49	2.45	17	17
2:B:120:LEU:C	2:B:124:LEU:HD13	0.49	2.28	15	2
2:B:120:LEU:O	2:B:124:LEU:HD12	0.48	2.08	17	8
2:B:112:LYS:HG3	2:B:113:ARG:N	0.48	2.23	7	3
1:A:10:VAL:CG2	1:A:11:ILE:N	0.48	2.76	3	9
1:A:38:GLU:O	1:A:39:LEU:HD22	0.48	2.08	6	1
1:A:46:PHE:CD2	2:B:113:ARG:CG	0.48	2.96	1	1
1:A:33:ILE:HD12	2:B:146:HIS:HB2	0.48	1.85	6	1
1:A:11:ILE:HG23	1:A:13:THR:H	0.48	1.67	5	13

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:40:TRP:O	2:B:112:LYS:HG3	0.48	2.09	9	1
2:B:122:LEU:HD11	2:B:146:HIS:C	0.48	2.29	6	1
2:B:173:SER:O	2:B:177:ILE:N	0.48	2.38	2	1
2:B:125:HIS:O	2:B:129:CYS:N	0.48	2.47	13	6
2:B:162:SER:HB3	2:B:166:CYS:N	0.48	2.24	17	2
2:B:120:LEU:CD2	2:B:177:ILE:CG2	0.47	2.92	10	17
1:A:12:ASP:O	1:A:15:PHE:CZ	0.47	2.67	13	6
2:B:120:LEU:HD11	2:B:178:ILE:HD12	0.47	1.85	16	2
1:A:24:LEU:HD12	2:B:121:VAL:HG21	0.47	1.84	4	1
1:A:39:LEU:HD22	2:B:177:ILE:HD11	0.47	1.86	16	1
2:B:168:VAL:O	2:B:171:CYS:N	0.47	2.46	14	16
2:B:122:LEU:HD21	2:B:144:LEU:HD21	0.47	1.85	17	1
2:B:124:LEU:HD13	2:B:195:LEU:HD22	0.47	1.87	3	2
2:B:190:PRO:O	2:B:194:PRO:CG	0.47	2.62	1	10
1:A:30:LEU:HA	1:A:33:ILE:HD11	0.47	1.86	3	1
2:B:115:LEU:O	2:B:119:GLN:CB	0.47	2.62	11	8
1:A:33:ILE:CD1	2:B:146:HIS:CD2	0.47	2.98	5	1
2:B:190:PRO:O	2:B:194:PRO:HG3	0.47	2.09	8	3
2:B:156:HIS:NE2	2:B:171:CYS:CB	0.47	2.78	1	9
2:B:181:TRP:NE1	2:B:191:VAL:HG12	0.47	2.24	1	1
1:A:21:LEU:HD13	2:B:121:VAL:CG1	0.47	2.40	2	1
1:A:29:GLY:C	1:A:30:LEU:HD23	0.47	2.30	13	1
1:A:37:PRO:CG	2:B:115:LEU:HD11	0.47	2.40	3	2
1:A:11:ILE:CG1	2:B:181:TRP:CE3	0.47	2.98	17	5
1:A:12:ASP:O	1:A:15:PHE:CE2	0.46	2.69	1	1
1:A:49:MET:HE1	2:B:116:ILE:CD1	0.46	2.40	3	2
1:A:36:LEU:HD21	2:B:149:THR:HG21	0.46	1.86	5	1
2:B:193:LEU:HB3	2:B:194:PRO:CD	0.46	2.40	4	2
2:B:116:ILE:HG22	2:B:117:GLN:N	0.46	2.25	1	3
1:A:15:PHE:CE1	2:B:196:LYS:CG	0.46	2.99	6	6
1:A:41:LEU:HD12	1:A:47:ASP:OD1	0.46	2.11	6	1
2:B:189:CYS:O	2:B:193:LEU:CB	0.46	2.64	4	1
1:A:16:ILE:CD1	2:B:195:LEU:HD23	0.46	2.40	15	1
1:A:39:LEU:CD2	2:B:116:ILE:HD12	0.46	2.39	16	1
2:B:174:SER:O	2:B:178:ILE:HD13	0.46	2.10	15	1
1:A:10:VAL:O	1:A:11:ILE:O	0.46	2.34	1	1
1:A:21:LEU:HD13	2:B:125:HIS:CB	0.46	2.41	14	3
1:A:40:TRP:O	2:B:112:LYS:CD	0.46	2.64	8	2
2:B:154:LEU:HA	2:B:157:MET:CE	0.46	2.41	17	1
1:A:11:ILE:HG23	1:A:13:THR:HG22	0.46	1.83	2	2
1:A:12:ASP:O	1:A:15:PHE:CE1	0.46	2.69	7	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:120:LEU:HD21	2:B:181:TRP:CD1	0.46	2.46	11	4
1:A:41:LEU:N	1:A:41:LEU:HD13	0.45	2.26	2	1
1:A:33:ILE:HD13	2:B:146:HIS:CD2	0.45	2.47	5	1
1:A:39:LEU:C	1:A:39:LEU:CD1	0.45	2.85	10	1
2:B:120:LEU:HG	2:B:181:TRP:NE1	0.45	2.27	7	6
1:A:39:LEU:HD11	2:B:115:LEU:HB2	0.45	1.88	15	2
1:A:41:LEU:HD21	2:B:176:GLN:CD	0.45	2.32	3	1
2:B:173:SER:O	2:B:177:ILE:HG13	0.45	2.12	10	2
1:A:41:LEU:HD23	1:A:41:LEU:N	0.45	2.27	6	1
2:B:115:LEU:HD12	2:B:118:GLN:CD	0.45	2.32	11	1
1:A:37:PRO:CG	2:B:115:LEU:HD22	0.45	2.42	1	4
1:A:39:LEU:HD12	2:B:116:ILE:HD13	0.45	1.88	1	1
2:B:124:LEU:CD2	2:B:181:TRP:CH2	0.45	2.97	5	1
2:B:133:GLU:OE1	2:B:139:VAL:HG13	0.45	2.12	9	1
2:B:154:LEU:HA	2:B:157:MET:HE2	0.45	1.89	17	1
2:B:139:VAL:CG2	2:B:140:ARG:N	0.44	2.80	17	3
1:A:21:LEU:HA	1:A:24:LEU:HD12	0.44	1.89	1	1
2:B:122:LEU:HD12	2:B:150:MET:CG	0.44	2.41	11	1
2:B:111:GLU:O	2:B:115:LEU:N	0.44	2.40	4	1
1:A:39:LEU:CD1	1:A:39:LEU:C	0.44	2.85	3	1
1:A:36:LEU:CD2	2:B:146:HIS:CE1	0.44	3.01	6	1
1:A:11:ILE:HG23	1:A:13:THR:HG23	0.44	1.89	7	3
1:A:49:MET:HE1	2:B:116:ILE:HG13	0.44	1.88	10	1
1:A:15:PHE:CG	2:B:196:LYS:CG	0.44	3.01	15	1
2:B:170:HIS:O	2:B:173:SER:N	0.44	2.51	14	11
1:A:15:PHE:CE1	2:B:196:LYS:HA	0.44	2.47	7	1
2:B:139:VAL:HG22	2:B:140:ARG:N	0.44	2.27	17	3
2:B:112:LYS:HE2	2:B:116:ILE:CD1	0.44	2.43	12	1
1:A:49:MET:HE3	2:B:116:ILE:HD13	0.44	1.88	13	1
1:A:46:PHE:CZ	2:B:113:ARG:HG3	0.44	2.47	7	1
2:B:156:HIS:NE2	2:B:168:VAL:HB	0.44	2.28	15	2
1:A:10:VAL:CG2	2:B:178:ILE:CG2	0.44	2.96	6	5
1:A:39:LEU:N	1:A:39:LEU:CD2	0.44	2.78	8	2
2:B:120:LEU:O	2:B:124:LEU:CB	0.44	2.65	13	1
2:B:156:HIS:HE2	2:B:171:CYS:HB2	0.43	1.67	3	6
2:B:180:HIS:NE2	2:B:191:VAL:CG2	0.43	2.80	5	12
2:B:133:GLU:HB3	2:B:139:VAL:HB	0.43	1.90	11	1
1:A:30:LEU:HD23	1:A:30:LEU:N	0.43	2.28	11	1
1:A:33:ILE:HG22	1:A:34:LYS:N	0.43	2.28	15	1
1:A:39:LEU:HD23	2:B:119:GLN:OE1	0.43	2.13	8	1
2:B:116:ILE:CG2	2:B:117:GLN:N	0.43	2.81	7	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:124:LEU:O	2:B:128:LYS:HG3	0.43	2.13	13	1
2:B:123:LEU:HD13	2:B:178:ILE:HD11	0.43	1.89	4	1
1:A:41:LEU:HD11	2:B:176:GLN:OE1	0.43	2.14	2	1
1:A:11:ILE:CD1	2:B:120:LEU:HD12	0.43	2.43	11	1
2:B:168:VAL:O	2:B:169:ALA:C	0.43	2.57	11	15
1:A:38:GLU:O	2:B:112:LYS:HG2	0.43	2.14	2	1
2:B:156:HIS:CD2	2:B:171:CYS:SG	0.43	3.10	9	5
1:A:11:ILE:HD13	2:B:124:LEU:HD23	0.43	1.89	13	1
2:B:113:ARG:CA	2:B:116:ILE:HD12	0.43	2.39	17	1
2:B:126:ALA:CB	2:B:150:MET:CB	0.43	2.97	10	6
2:B:120:LEU:CD2	2:B:177:ILE:HG23	0.43	2.44	2	1
2:B:190:PRO:O	2:B:194:PRO:HG2	0.43	2.13	3	1
2:B:112:LYS:O	2:B:115:LEU:N	0.43	2.52	9	2
1:A:13:THR:CG2	2:B:124:LEU:CD2	0.43	2.97	17	7
1:A:21:LEU:HA	1:A:24:LEU:HD21	0.43	1.91	7	1
1:A:16:ILE:HD11	2:B:195:LEU:CD2	0.43	2.42	8	1
2:B:139:VAL:HG12	2:B:140:ARG:N	0.43	2.29	10	3
2:B:122:LEU:O	2:B:126:ALA:CB	0.43	2.67	17	4
2:B:180:HIS:C	2:B:180:HIS:CD2	0.43	2.93	8	4
2:B:167:GLN:O	2:B:167:GLN:CG	0.43	2.67	11	7
2:B:109:ASP:O	2:B:112:LYS:CG	0.43	2.67	6	1
2:B:156:HIS:CD2	2:B:171:CYS:HB2	0.43	2.49	17	1
2:B:180:HIS:CD2	2:B:180:HIS:C	0.42	2.92	9	6
1:A:12:ASP:HB3	1:A:15:PHE:CZ	0.42	2.49	6	2
2:B:121:VAL:HG22	2:B:195:LEU:HD21	0.42	1.90	8	2
1:A:40:TRP:CZ3	2:B:173:SER:N	0.42	2.87	12	1
1:A:36:LEU:HD11	2:B:146:HIS:CE1	0.42	2.49	5	1
1:A:26:ILE:HD12	1:A:26:ILE:N	0.42	2.29	12	1
1:A:40:TRP:O	1:A:41:LEU:C	0.42	2.58	17	2
1:A:37:PRO:HG2	2:B:115:LEU:CD1	0.42	2.44	11	2
2:B:121:VAL:CG2	2:B:195:LEU:HD21	0.42	2.44	2	1
1:A:38:GLU:O	2:B:112:LYS:CD	0.42	2.68	6	1
1:A:15:PHE:CD1	2:B:196:LYS:HG2	0.42	2.50	10	4
1:A:22:MET:HE2	1:A:22:MET:HA	0.42	1.89	11	1
1:A:30:LEU:N	1:A:30:LEU:CD2	0.42	2.82	13	1
2:B:126:ALA:CB	2:B:154:LEU:CD1	0.42	2.97	13	1
2:B:167:GLN:CG	2:B:167:GLN:O	0.42	2.68	4	8
1:A:49:MET:CE	2:B:116:ILE:CD1	0.42	2.97	12	2
2:B:126:ALA:CB	2:B:150:MET:HB2	0.42	2.44	16	1
2:B:123:LEU:O	2:B:127:HIS:HB2	0.42	2.15	3	1
2:B:156:HIS:O	2:B:160:CYS:HB2	0.42	2.15	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:ILE:HG21	2:B:124:LEU:HD23	0.42	1.92	13	1
2:B:166:CYS:O	2:B:172:ALA:CB	0.42	2.65	15	1
1:A:46:PHE:CD2	2:B:113:ARG:HG3	0.42	2.50	1	1
1:A:16:ILE:HD11	2:B:195:LEU:HD23	0.42	1.92	9	1
1:A:39:LEU:HD22	2:B:112:LYS:HA	0.42	1.92	14	2
1:A:15:PHE:CE1	2:B:196:LYS:HG3	0.42	2.50	12	2
1:A:15:PHE:CZ	2:B:196:LYS:HG2	0.41	2.50	1	1
1:A:39:LEU:O	1:A:40:TRP:CE3	0.41	2.73	1	1
2:B:122:LEU:CD2	2:B:144:LEU:CD2	0.41	2.98	2	1
1:A:39:LEU:CD2	2:B:112:LYS:O	0.41	2.67	3	2
2:B:174:SER:O	2:B:178:ILE:CD1	0.41	2.67	5	1
1:A:13:THR:HG22	2:B:124:LEU:HD22	0.41	1.92	17	3
1:A:21:LEU:C	1:A:21:LEU:HD12	0.41	2.35	8	2
2:B:193:LEU:O	2:B:196:LYS:CG	0.41	2.68	3	2
2:B:115:LEU:HD12	2:B:118:GLN:OE1	0.41	2.16	11	1
2:B:157:MET:HG3	2:B:158:THR:N	0.41	2.30	17	1
1:A:11:ILE:HG23	1:A:13:THR:N	0.41	2.30	5	3
1:A:22:MET:O	1:A:26:ILE:CD1	0.41	2.68	5	2
1:A:13:THR:HG22	1:A:16:ILE:HG21	0.41	1.90	11	1
1:A:15:PHE:CD1	1:A:16:ILE:N	0.41	2.88	13	1
2:B:119:GLN:O	2:B:123:LEU:N	0.41	2.53	15	1
1:A:30:LEU:HD11	2:B:118:GLN:HB2	0.41	1.92	16	1
1:A:15:PHE:CE1	2:B:196:LYS:HB2	0.41	2.50	3	4
2:B:180:HIS:O	2:B:184:CYS:N	0.41	2.54	10	1
2:B:119:GLN:O	2:B:122:LEU:N	0.41	2.53	16	3
2:B:122:LEU:HA	2:B:122:LEU:HD22	0.41	1.81	10	1
1:A:36:LEU:HD12	1:A:37:PRO:CD	0.41	2.46	2	2
2:B:113:ARG:O	2:B:116:ILE:HB	0.41	2.14	10	1
2:B:125:HIS:CD2	2:B:147:CYS:SG	0.41	3.14	13	1
1:A:49:MET:CE	2:B:116:ILE:HG12	0.41	2.46	1	1
1:A:40:TRP:CD1	2:B:112:LYS:HE2	0.41	2.51	2	1
2:B:191:VAL:O	2:B:195:LEU:HD13	0.41	2.16	9	1
2:B:133:GLU:OE1	2:B:139:VAL:HG22	0.41	2.16	13	1
1:A:11:ILE:CG2	1:A:13:THR:CG2	0.41	2.94	16	1
2:B:121:VAL:HG23	2:B:195:LEU:HD21	0.41	1.93	4	1
1:A:37:PRO:CG	2:B:115:LEU:CD1	0.41	2.98	4	1
1:A:15:PHE:CD1	2:B:196:LYS:HG3	0.41	2.51	16	1
2:B:120:LEU:CD2	2:B:177:ILE:HG22	0.41	2.46	17	1
1:A:26:ILE:N	1:A:26:ILE:HD12	0.40	2.31	8	2
1:A:15:PHE:CZ	2:B:196:LYS:HG3	0.40	2.51	13	1
2:B:120:LEU:O	2:B:124:LEU:HB2	0.40	2.16	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:109:ASP:O	2:B:112:LYS:CD	0.40	2.70	9	1
1:A:21:LEU:HD12	1:A:22:MET:N	0.40	2.30	11	1
2:B:124:LEU:O	2:B:127:HIS:HB3	0.40	2.17	11	1
2:B:175:ARG:O	2:B:179:SER:CB	0.40	2.70	9	1
1:A:11:ILE:HD13	2:B:124:LEU:CD2	0.40	2.46	13	1
2:B:120:LEU:HA	2:B:120:LEU:HD13	0.40	1.82	14	1
2:B:130:GLN:NE2	2:B:154:LEU:CB	0.40	2.85	6	1
1:A:25:VAL:HG11	2:B:144:LEU:CD1	0.40	2.38	7	1
2:B:122:LEU:HD22	2:B:122:LEU:HA	0.40	1.82	7	1
2:B:124:LEU:CD1	2:B:195:LEU:HD12	0.40	2.47	7	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	40/52 (77%)	33±1 (82±3%)	4±1 (9±3%)	3±1 (9±2%)	1	12
2	B	85/101 (84%)	75±1 (88±1%)	8±1 (9±1%)	2±0 (3±1%)	8	43
All	All	2125/2601 (82%)	1838 (86%)	189 (9%)	98 (5%)	4	27

All 12 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	B	169	ALA	17
2	B	163	GLY	17
1	A	32	ARG	16
1	A	10	VAL	16
1	A	11	ILE	15
1	A	41	LEU	8
1	A	43	GLN	2
2	B	177	ILE	2
1	A	42	GLY	2
2	B	197	ASN	1
2	B	143	ASN	1

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Mol	Chain	Res	Type	Models (Total)
2	B	145	PRO	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	38/46 (83%)	27±2 (72±4%)	11±2 (28±4%)	2	18
2	B	79/89 (89%)	52±4 (65±5%)	27±4 (35±5%)	1	10
All	All	1989/2295 (87%)	1340 (67%)	649 (33%)	1	12

All 88 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	B	162	SER	17
2	B	158	THR	17
2	B	120	LEU	17
2	B	181	TRP	17
2	B	122	LEU	17
2	B	154	LEU	16
2	B	191	VAL	15
2	B	161	GLN	15
1	A	46	PHE	15
1	A	12	ASP	15
2	B	109	ASP	14
1	A	16	ILE	14
2	B	178	ILE	14
2	B	144	LEU	14
1	A	14	ASP	13
2	B	142	CYS	13
2	B	174	SER	13
2	B	150	MET	12
1	A	47	ASP	11
2	B	164	LYS	11
2	B	116	ILE	11
2	B	195	LEU	11
1	A	45	GLU	11

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Mol	Chain	Res	Type	Models (Total)
1	A	28	MET	10
2	B	112	LYS	10
2	B	184	CYS	10
2	B	196	LYS	10
2	B	193	LEU	9
1	A	10	VAL	9
2	B	175	ARG	9
2	B	157	MET	8
2	B	146	HIS	8
2	B	159	HIS	8
2	B	140	ARG	8
2	B	165	SER	8
2	B	136	ASN	8
2	B	182	LYS	8
2	B	131	ARG	8
2	B	128	LYS	8
2	B	192	CYS	8
2	B	133	GLU	7
1	A	22	MET	7
2	B	151	LYS	7
2	B	123	LEU	7
1	A	11	ILE	7
1	A	32	ARG	6
2	B	180	HIS	6
2	B	114	LYS	6
2	B	148	ARG	6
1	A	17	ASP	6
2	B	130	GLN	6
1	A	43	GLN	6
1	A	35	GLU	6
1	A	41	LEU	6
1	A	21	LEU	5
2	B	143	ASN	5
1	A	15	PHE	4
2	B	134	GLN	4
2	B	113	ARG	4
2	B	119	GLN	4
1	A	23	SER	4
2	B	176	GLN	4
1	A	49	MET	4
2	B	132	ARG	4
1	A	27	GLU	4

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Mol	Chain	Res	Type	Models (Total)
1	A	18	GLU	3
2	B	183	ASN	3
1	A	34	LYS	3
1	A	19	GLU	3
2	B	118	GLN	3
1	A	48	PHE	3
1	A	36	LEU	2
2	B	127	HIS	2
1	A	39	LEU	2
1	A	44	ASN	2
2	B	179	SER	2
2	B	149	THR	2
2	B	189	CYS	2
2	B	138	GLU	2
2	B	111	GLU	2
1	A	33	ILE	1
1	A	38	GLU	1
2	B	173	SER	1
2	B	117	GLN	1
1	A	13	THR	1
2	B	167	GLN	1
2	B	155	ASN	1
2	B	152	ASN	1

6.3.3 RNA

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains

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

6.5 Carbohydrates

There are no carbohydrates in this entry.

6.6 Ligand geometry

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided