Full wwPDB NMR Structure Validation Report (i)

Feb 23, 2022 – 02:36 PM EST

PDB ID	:	1YNX
Title	:	Solution structure of DNA binding domain A (DBD-A) of S.cerevisiae Replication Protein A (RPA)
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Deposited on	:	2005-01-26

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 (i)) were used in the production of this report:

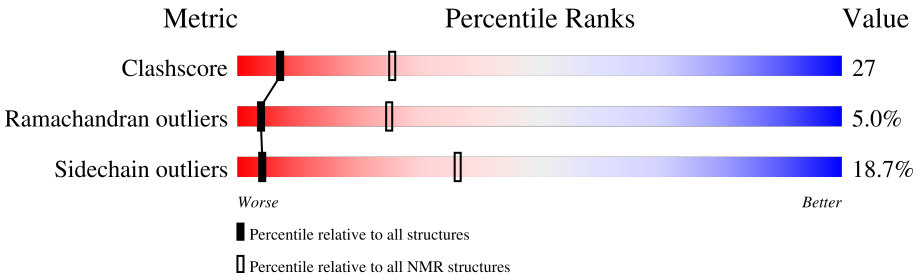
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

1 Overall quality at a glance (i)

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	114	45% 42% 8% 5%

2 Ensemble composition and analysis (i)

This entry contains 22 models. Model 1 is the overall representative, medoid model (most similar to other models). The authors have identified model 12 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:182-A:289 (108)	0.76	1

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

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

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

Cluster number	Models
1	1, 2, 3, 4, 7, 10, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22
2	8, 9, 11, 12
Single-model clusters	5; 6

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1851 atoms, of which 912 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Replication factor-A protein 1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	114	1851	600	912	159	179	1	0

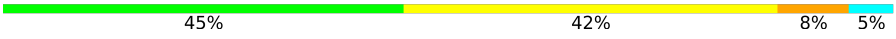
4 Residue-property plots

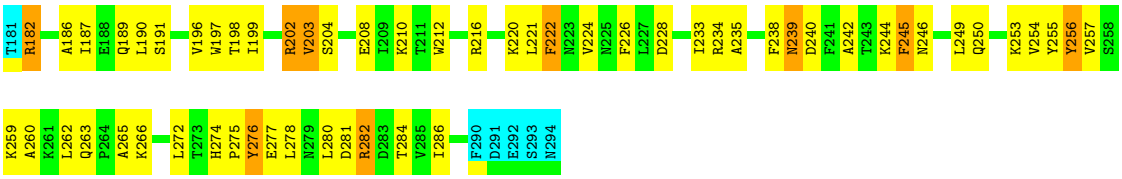
4.1 Average score per residue in the NMR ensemble

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: Replication factor-A protein 1

Chain A:





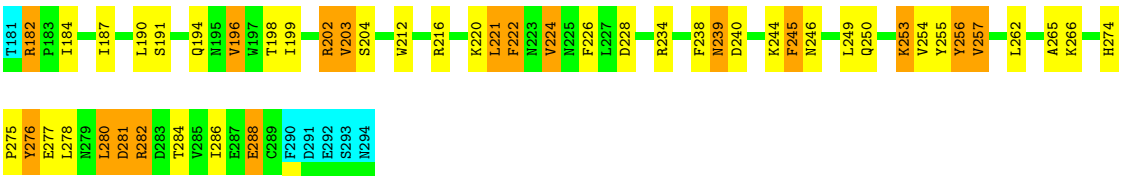
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

• Molecule 1: Replication factor-A protein 1

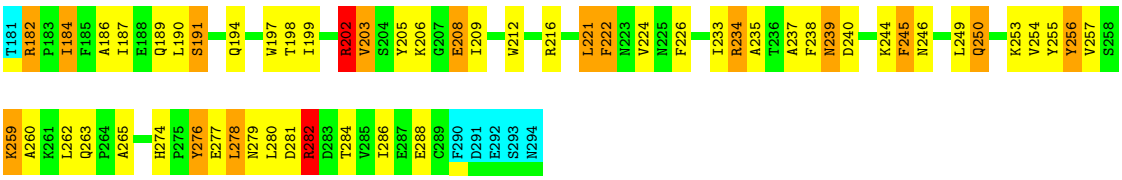
Chain A:



4.2.2 Score per residue for model 2

• Molecule 1: Replication factor-A protein 1

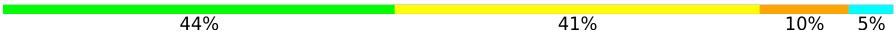
Chain A:

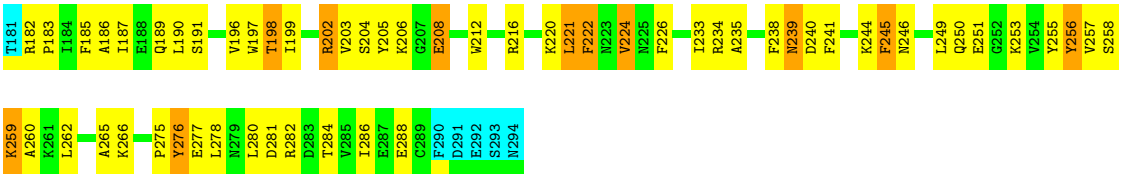


4.2.3 Score per residue for model 3

• Molecule 1: Replication factor-A protein 1

Chain A:

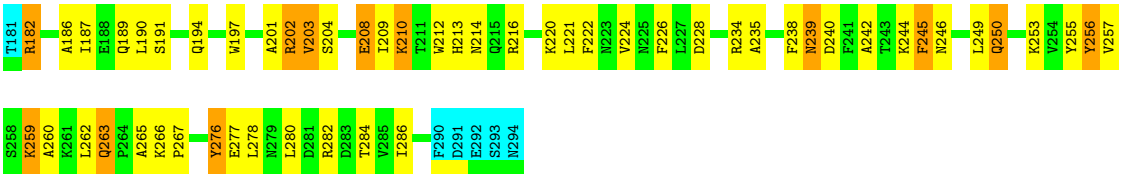




4.2.4 Score per residue for model 4

• Molecule 1: Replication factor-A protein 1

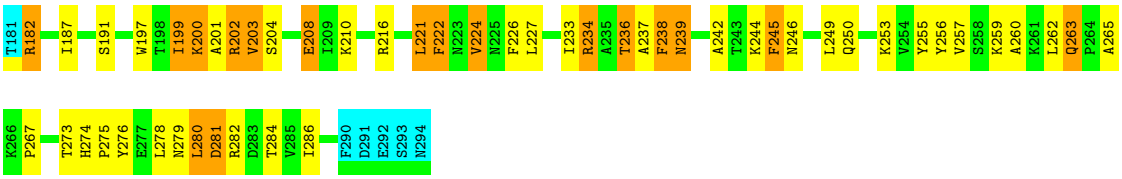
Chain A:



4.2.5 Score per residue for model 5

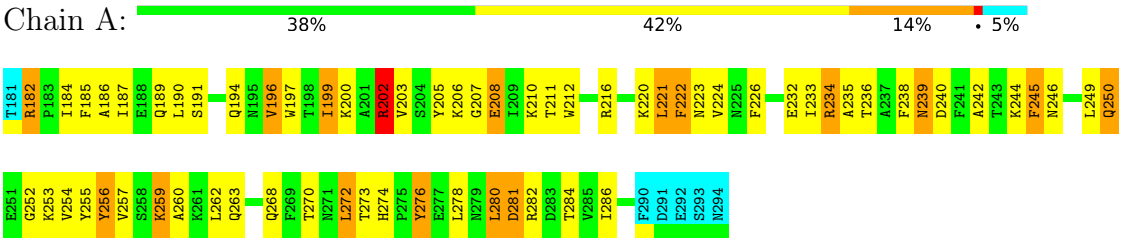
• Molecule 1: Replication factor-A protein 1

Chain A:



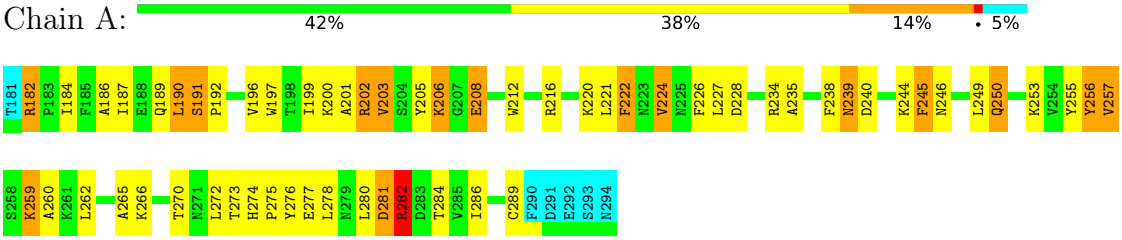
4.2.6 Score per residue for model 6

• Molecule 1: Replication factor-A protein 1



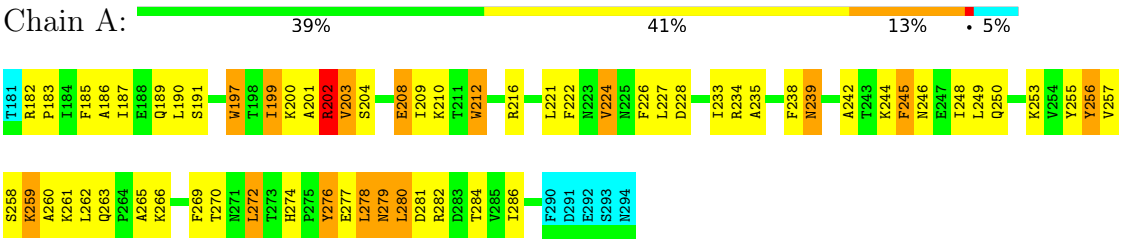
4.2.7 Score per residue for model 7

• Molecule 1: Replication factor-A protein 1



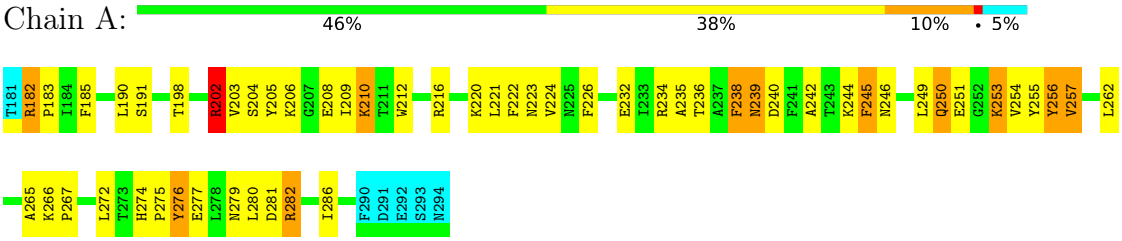
4.2.8 Score per residue for model 8

• Molecule 1: Replication factor-A protein 1



4.2.9 Score per residue for model 9

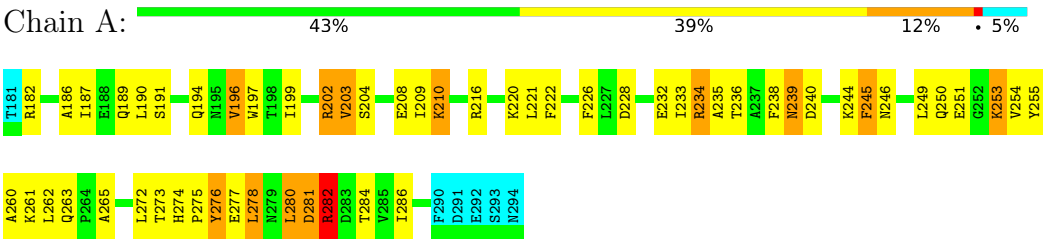
• Molecule 1: Replication factor-A protein 1



4.2.10 Score per residue for model 10

• Molecule 1: Replication factor-A protein 1

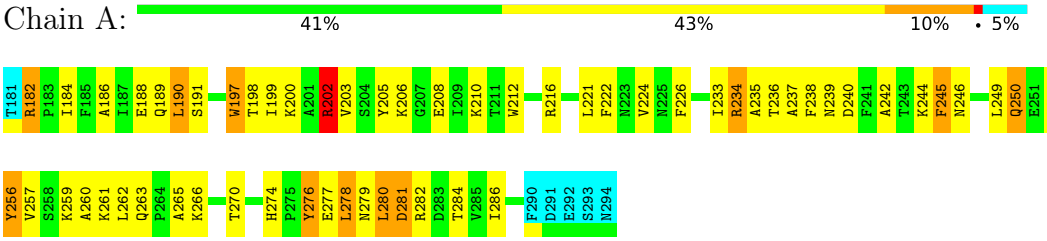
Chain A:



4.2.11 Score per residue for model 11

• Molecule 1: Replication factor-A protein 1

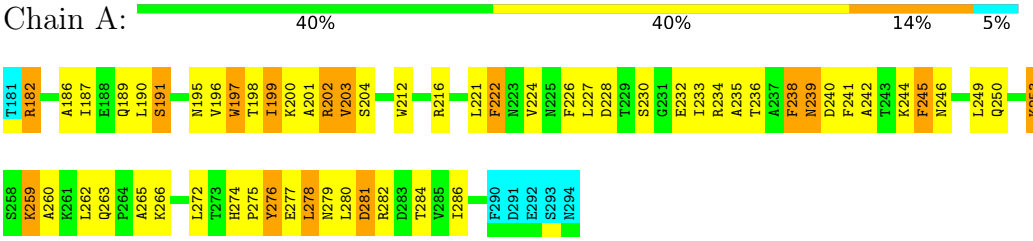
Chain A:



4.2.12 Score per residue for model 12

• Molecule 1: Replication factor-A protein 1

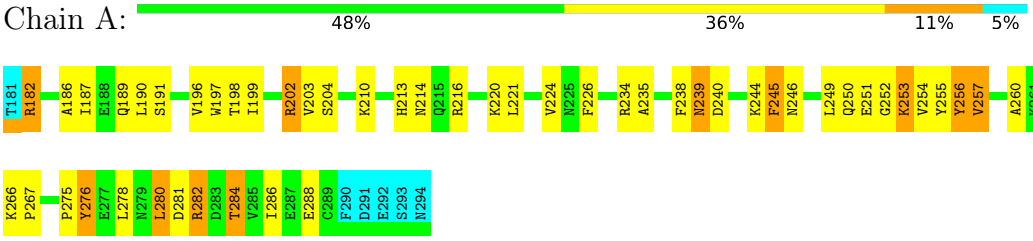
Chain A:



4.2.13 Score per residue for model 13

• Molecule 1: Replication factor-A protein 1

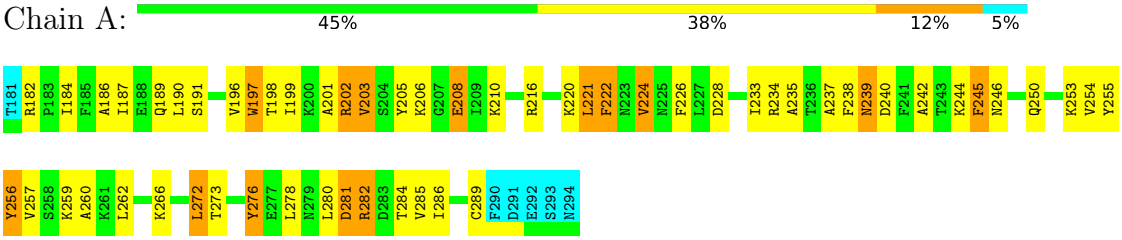
Chain A:



4.2.14 Score per residue for model 14

• Molecule 1: Replication factor-A protein 1

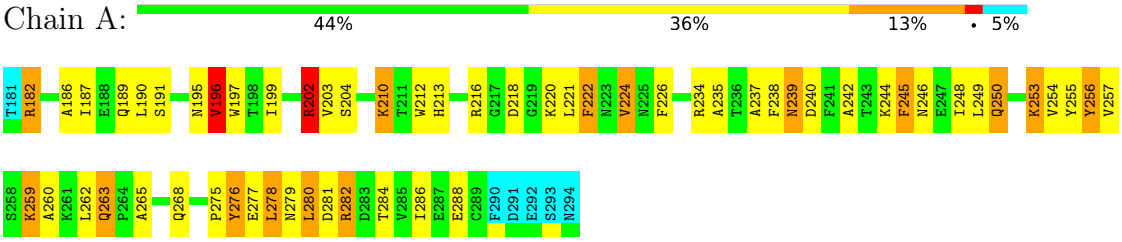
Chain A:



4.2.15 Score per residue for model 15

• Molecule 1: Replication factor-A protein 1

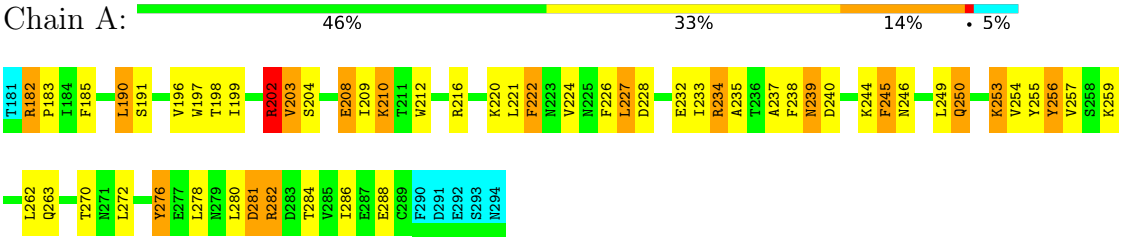
Chain A:



4.2.16 Score per residue for model 16

• Molecule 1: Replication factor-A protein 1

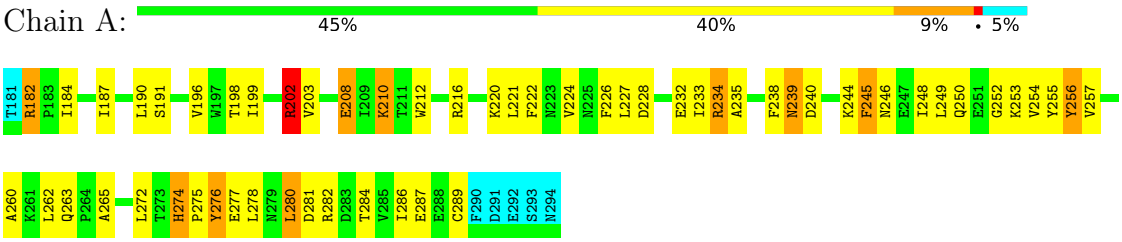
Chain A:



4.2.17 Score per residue for model 17

• Molecule 1: Replication factor-A protein 1

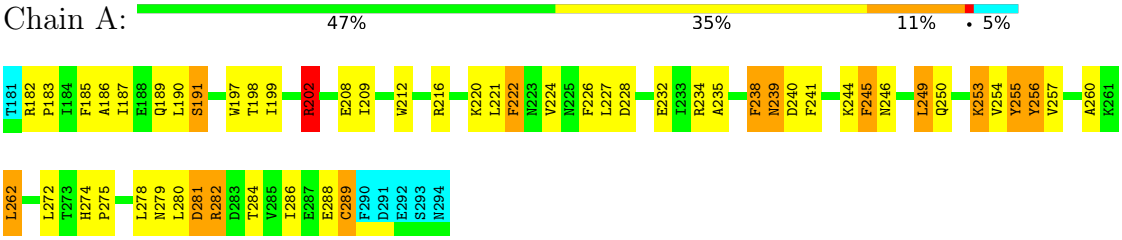
Chain A:



4.2.18 Score per residue for model 18

• Molecule 1: Replication factor-A protein 1

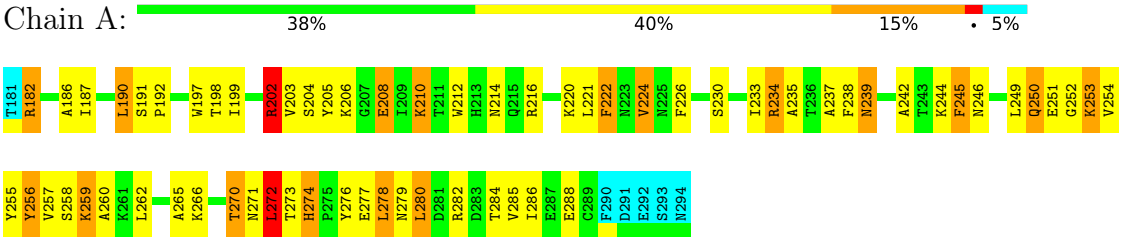
Chain A:



4.2.19 Score per residue for model 19

• Molecule 1: Replication factor-A protein 1

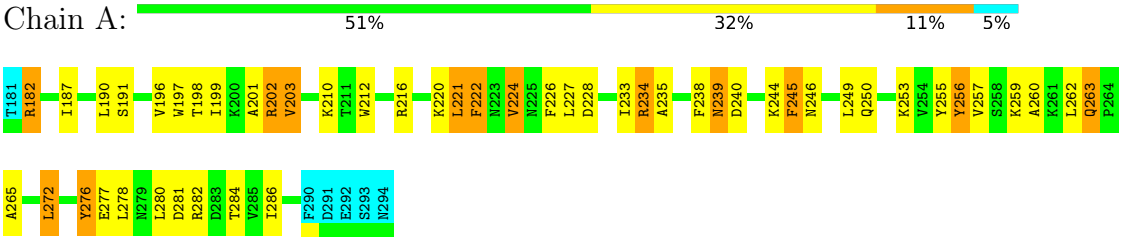
Chain A:



4.2.20 Score per residue for model 20

• Molecule 1: Replication factor-A protein 1

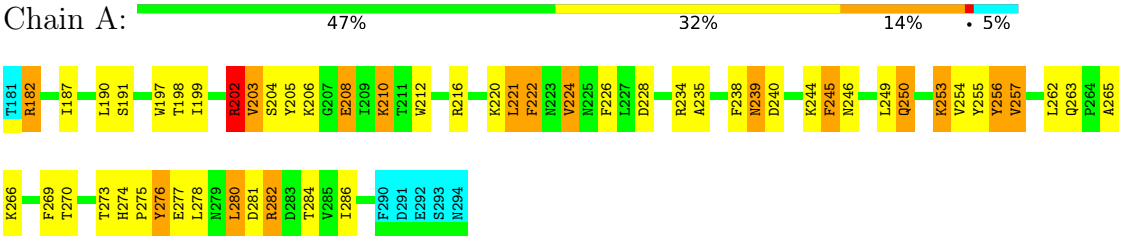
Chain A:



4.2.21 Score per residue for model 21

• Molecule 1: Replication factor-A protein 1

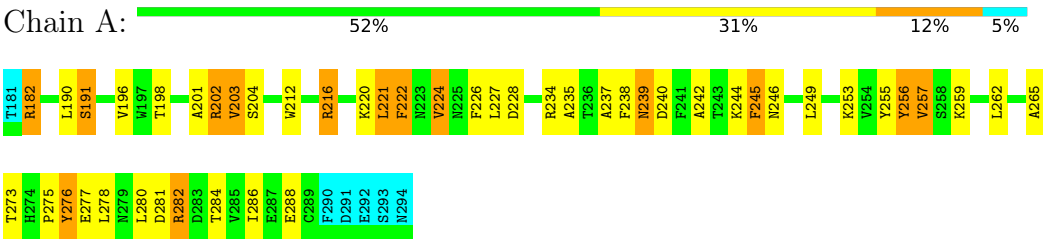
Chain A:



4.2.22 Score per residue for model 22

• Molecule 1: Replication factor-A protein 1

Chain A:



5 Refinement protocol and experimental data overview

The models were refined using the following method: *Torsional Angle Dynamics with Internal Variable Module*.

Of the 100 calculated structures, 22 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
X-PLOR	structure solution	NIH 2.9.6
X-PLOR	refinement	NIH 2.9.6

No chemical shift data was provided.

6 Model quality

6.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.03±0.00	0±0/912 (0.0± 0.0%)	1.26±0.00	0±0/1237 (0.0± 0.0%)
All	All	1.03	0/20064 (0.0%)	1.26	1/27214 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	5.0±0.0
All	All	0	110

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	256	TYR	N-CA-CB	-5.23	101.19	110.60	6	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	182	ARG	Sidechain	22
1	A	202	ARG	Sidechain	22
1	A	216	ARG	Sidechain	22
1	A	234	ARG	Sidechain	22
1	A	282	ARG	Sidechain	22

6.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	889	873	873	47±7
All	All	19558	19206	19206	1043

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 27.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:280:LEU:HD21	1:A:284:THR:HG21	1.13	1.19	5	12
1:A:249:LEU:HD12	1:A:286:ILE:HG21	1.03	1.29	19	1
1:A:280:LEU:HD11	1:A:284:THR:HG21	0.94	1.35	18	5
1:A:257:VAL:HG12	1:A:286:ILE:HG22	0.91	1.39	13	5
1:A:203:VAL:HG23	1:A:226:PHE:CE2	0.91	2.00	4	2
1:A:198:THR:HG23	1:A:256:TYR:CE1	0.91	2.01	20	8
1:A:212:TRP:CH2	1:A:221:LEU:HD13	0.88	2.03	12	4
1:A:203:VAL:HG23	1:A:226:PHE:CE1	0.88	2.03	1	11
1:A:197:TRP:CH2	1:A:260:ALA:HB3	0.87	2.04	8	12
1:A:280:LEU:HD11	1:A:286:ILE:HD11	0.87	1.44	20	2
1:A:260:ALA:HB1	1:A:278:LEU:HD21	0.86	1.45	17	3
1:A:190:LEU:HD11	1:A:199:ILE:HD12	0.82	1.48	15	1
1:A:245:PHE:CE1	1:A:286:ILE:HD12	0.82	2.07	16	2
1:A:190:LEU:HD22	1:A:276:TYR:CD2	0.82	2.10	9	1
1:A:273:THR:HG22	1:A:274:HIS:CD2	0.81	2.11	5	3
1:A:257:VAL:HG22	1:A:286:ILE:HD12	0.81	1.49	19	1
1:A:245:PHE:CD1	1:A:286:ILE:HD13	0.81	2.09	21	3
1:A:190:LEU:HD12	1:A:262:LEU:HD11	0.81	1.53	18	1
1:A:249:LEU:HD12	1:A:286:ILE:CG2	0.80	2.06	19	1
1:A:194:GLN:O	1:A:196:VAL:HG12	0.80	1.77	1	3
1:A:212:TRP:CZ2	1:A:221:LEU:HD13	0.79	2.12	9	1
1:A:197:TRP:CZ2	1:A:260:ALA:HB3	0.79	2.12	19	7
1:A:280:LEU:HD11	1:A:286:ILE:CD1	0.79	2.07	20	2
1:A:262:LEU:HD11	1:A:276:TYR:CE2	0.79	2.13	11	5
1:A:212:TRP:CZ3	1:A:221:LEU:HD22	0.79	2.12	12	2
1:A:245:PHE:CZ	1:A:249:LEU:HD22	0.78	2.13	22	3
1:A:220:LYS:O	1:A:221:LEU:HD12	0.77	1.79	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:232:GLU:OE1	1:A:272:LEU:HD22	0.76	1.81	16	4
1:A:257:VAL:HG13	1:A:286:ILE:CD1	0.76	2.10	19	2
1:A:190:LEU:HD22	1:A:276:TYR:CE2	0.76	2.15	9	1
1:A:260:ALA:HB1	1:A:278:LEU:HD11	0.76	1.58	19	2
1:A:280:LEU:CD2	1:A:284:THR:HG21	0.75	2.12	2	5
1:A:187:ILE:CD1	1:A:199:ILE:HD11	0.74	2.12	7	4
1:A:265:ALA:HB2	1:A:277:GLU:HG2	0.74	1.57	19	4
1:A:226:PHE:CE1	1:A:235:ALA:HB3	0.74	2.17	4	3
1:A:203:VAL:HG11	1:A:251:GLU:HA	0.74	1.60	3	2
1:A:221:LEU:HD11	1:A:236:THR:HG22	0.73	1.60	11	2
1:A:280:LEU:CD1	1:A:284:THR:HG21	0.73	2.11	18	5
1:A:222:PHE:CZ	1:A:224:VAL:HG13	0.73	2.19	8	1
1:A:190:LEU:HD22	1:A:262:LEU:HD23	0.73	1.61	21	2
1:A:262:LEU:HD13	1:A:263:GLN:N	0.73	1.97	4	9
1:A:265:ALA:HB2	1:A:277:GLU:HG3	0.72	1.60	17	12
1:A:265:ALA:HB3	1:A:275:PRO:HB2	0.72	1.61	5	4
1:A:262:LEU:HD21	1:A:276:TYR:CD2	0.72	2.19	15	2
1:A:269:PHE:CD2	1:A:270:THR:HG23	0.72	2.18	8	2
1:A:221:LEU:HD11	1:A:236:THR:CG2	0.71	2.13	11	2
1:A:186:ALA:HB3	1:A:189:GLN:HG2	0.71	1.60	12	8
1:A:280:LEU:CG	1:A:284:THR:HG21	0.71	2.14	2	5
1:A:197:TRP:CD1	1:A:262:LEU:HD12	0.71	2.20	18	1
1:A:187:ILE:HD13	1:A:199:ILE:HD11	0.71	1.63	2	3
1:A:273:THR:HG22	1:A:274:HIS:ND1	0.70	2.01	7	2
1:A:257:VAL:HG13	1:A:286:ILE:HD11	0.70	1.61	19	1
1:A:280:LEU:HD21	1:A:284:THR:CB	0.70	2.17	15	7
1:A:201:ALA:HB1	1:A:227:LEU:O	0.70	1.85	5	2
1:A:262:LEU:HD21	1:A:276:TYR:CE1	0.70	2.21	1	5
1:A:249:LEU:HD11	1:A:255:TYR:CE2	0.70	2.22	18	1
1:A:257:VAL:HG22	1:A:286:ILE:HG22	0.70	1.64	8	1
1:A:280:LEU:HD11	1:A:284:THR:CG2	0.69	2.17	16	6
1:A:262:LEU:HD11	1:A:276:TYR:CE1	0.69	2.22	12	5
1:A:280:LEU:HD21	1:A:284:THR:OG1	0.69	1.87	17	5
1:A:212:TRP:CZ3	1:A:221:LEU:HD13	0.69	2.22	8	1
1:A:202:ARG:HB2	1:A:254:VAL:HG22	0.68	1.64	6	6
1:A:280:LEU:HD13	1:A:281:ASP:N	0.68	2.04	11	10
1:A:255:TYR:CE2	1:A:257:VAL:HG22	0.68	2.24	14	9
1:A:245:PHE:CD1	1:A:286:ILE:HD12	0.67	2.24	9	5
1:A:190:LEU:HD22	1:A:197:TRP:CD2	0.67	2.24	15	1
1:A:245:PHE:CE1	1:A:249:LEU:HD12	0.67	2.25	8	1
1:A:260:ALA:CB	1:A:278:LEU:HD21	0.67	2.19	17	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:222:PHE:CE2	1:A:224:VAL:HG13	0.67	2.24	19	8
1:A:262:LEU:HD22	1:A:278:LEU:CD2	0.67	2.19	13	2
1:A:245:PHE:CE1	1:A:249:LEU:HD13	0.67	2.24	12	5
1:A:191:SER:C	1:A:262:LEU:HD22	0.66	2.11	18	1
1:A:187:ILE:HG22	1:A:199:ILE:HD11	0.65	1.67	21	2
1:A:249:LEU:HD21	1:A:286:ILE:CG2	0.65	2.21	5	1
1:A:265:ALA:HB2	1:A:277:GLU:CG	0.65	2.20	19	5
1:A:197:TRP:NE1	1:A:262:LEU:HD12	0.65	2.06	18	1
1:A:257:VAL:HG13	1:A:286:ILE:HG12	0.65	1.69	4	5
1:A:191:SER:O	1:A:262:LEU:HD13	0.65	1.92	18	1
1:A:221:LEU:HD12	1:A:238:PHE:HA	0.65	1.68	8	7
1:A:186:ALA:HB1	1:A:230:SER:CB	0.65	2.21	19	1
1:A:245:PHE:CE2	1:A:249:LEU:HD12	0.64	2.27	13	2
1:A:187:ILE:HG12	1:A:199:ILE:HD11	0.64	1.69	3	3
1:A:222:PHE:CE2	1:A:224:VAL:HG23	0.64	2.28	2	4
1:A:262:LEU:HD21	1:A:276:TYR:CE2	0.64	2.28	4	8
1:A:190:LEU:CD1	1:A:199:ILE:HD13	0.64	2.23	20	1
1:A:245:PHE:CE1	1:A:286:ILE:HG21	0.64	2.28	20	4
1:A:187:ILE:HG23	1:A:228:ASP:OD2	0.64	1.91	20	2
1:A:202:ARG:NH1	1:A:227:LEU:HD23	0.63	2.08	8	1
1:A:221:LEU:HD12	1:A:237:ALA:O	0.63	1.94	11	1
1:A:184:ILE:HG13	1:A:198:THR:HG22	0.63	1.70	2	1
1:A:262:LEU:HD22	1:A:278:LEU:HD21	0.63	1.71	13	2
1:A:260:ALA:HB2	1:A:284:THR:HG23	0.63	1.71	20	1
1:A:198:THR:HG22	1:A:258:SER:HA	0.62	1.70	19	1
1:A:202:ARG:HB2	1:A:254:VAL:HG12	0.62	1.71	15	4
1:A:186:ALA:HB3	1:A:189:GLN:CG	0.62	2.25	6	2
1:A:186:ALA:HB1	1:A:230:SER:OG	0.62	1.94	12	1
1:A:245:PHE:CD1	1:A:286:ILE:HG21	0.62	2.30	20	3
1:A:272:LEU:HD12	1:A:273:THR:O	0.62	1.95	22	1
1:A:257:VAL:HG13	1:A:286:ILE:CG1	0.62	2.24	2	3
1:A:245:PHE:CD2	1:A:286:ILE:HD13	0.62	2.30	10	4
1:A:190:LEU:HD12	1:A:262:LEU:CD1	0.62	2.25	18	2
1:A:226:PHE:CE2	1:A:235:ALA:HB3	0.61	2.30	11	16
1:A:232:GLU:CD	1:A:272:LEU:HD13	0.61	2.16	10	2
1:A:280:LEU:HD21	1:A:284:THR:CG2	0.61	2.25	11	10
1:A:238:PHE:O	1:A:242:ALA:HB2	0.61	1.95	5	9
1:A:190:LEU:HD12	1:A:262:LEU:HD13	0.61	1.72	16	1
1:A:232:GLU:OE2	1:A:272:LEU:HD13	0.61	1.94	10	2
1:A:248:ILE:HD12	1:A:286:ILE:HD11	0.61	1.73	8	1
1:A:192:PRO:N	1:A:262:LEU:HD12	0.60	2.11	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:260:ALA:HB1	1:A:278:LEU:CD2	0.60	2.25	17	2
1:A:272:LEU:HD22	1:A:273:THR:N	0.60	2.12	19	1
1:A:262:LEU:HD11	1:A:276:TYR:CZ	0.60	2.32	15	7
1:A:270:THR:HG22	1:A:272:LEU:HG	0.60	1.72	6	1
1:A:257:VAL:HG12	1:A:286:ILE:CG2	0.60	2.22	13	1
1:A:190:LEU:CG	1:A:262:LEU:HD11	0.59	2.27	9	1
1:A:212:TRP:CE3	1:A:221:LEU:HD22	0.59	2.32	11	2
1:A:270:THR:HG22	1:A:272:LEU:CG	0.59	2.27	6	1
1:A:190:LEU:HD21	1:A:197:TRP:CH2	0.59	2.33	19	1
1:A:199:ILE:HD12	1:A:233:ILE:CD1	0.59	2.27	8	2
1:A:190:LEU:HD22	1:A:262:LEU:CD2	0.59	2.26	21	3
1:A:221:LEU:CD2	1:A:236:THR:HG22	0.58	2.29	5	1
1:A:273:THR:HG22	1:A:274:HIS:CE1	0.58	2.33	7	1
1:A:238:PHE:O	1:A:239:ASN:O	0.58	2.21	2	20
1:A:265:ALA:HB3	1:A:275:PRO:O	0.58	1.98	9	4
1:A:249:LEU:HD22	1:A:255:TYR:CD2	0.58	2.34	1	2
1:A:257:VAL:HG12	1:A:286:ILE:HG23	0.58	1.76	20	1
1:A:245:PHE:CD1	1:A:246:ASN:N	0.58	2.72	15	6
1:A:222:PHE:CD1	1:A:237:ALA:HB3	0.57	2.34	15	4
1:A:187:ILE:HG21	1:A:232:GLU:O	0.57	1.99	18	1
1:A:249:LEU:HD23	1:A:250:GLN:N	0.57	2.13	9	4
1:A:191:SER:C	1:A:262:LEU:HD12	0.57	2.20	12	4
1:A:280:LEU:HG	1:A:284:THR:HG21	0.57	1.74	12	2
1:A:187:ILE:HD11	1:A:228:ASP:HB3	0.57	1.75	1	5
1:A:249:LEU:HD12	1:A:286:ILE:HD12	0.57	1.75	18	1
1:A:203:VAL:HG23	1:A:226:PHE:CD1	0.56	2.35	12	6
1:A:227:LEU:HD23	1:A:228:ASP:N	0.56	2.15	20	5
1:A:190:LEU:HD11	1:A:199:ILE:CD1	0.56	2.29	15	1
1:A:249:LEU:HD23	1:A:250:GLN:O	0.56	2.01	21	8
1:A:245:PHE:CZ	1:A:249:LEU:HD13	0.56	2.35	10	4
1:A:245:PHE:CD2	1:A:246:ASN:N	0.56	2.74	6	16
1:A:221:LEU:HD21	1:A:238:PHE:CE1	0.56	2.35	2	1
1:A:226:PHE:HE2	1:A:235:ALA:HB3	0.56	1.61	13	16
1:A:222:PHE:O	1:A:236:THR:HG23	0.56	2.01	12	1
1:A:187:ILE:HD13	1:A:232:GLU:O	0.56	2.01	6	1
1:A:245:PHE:O	1:A:286:ILE:HD11	0.56	2.01	15	3
1:A:262:LEU:HD21	1:A:276:TYR:CD1	0.56	2.36	14	2
1:A:262:LEU:CD2	1:A:278:LEU:HD21	0.56	2.31	21	1
1:A:245:PHE:HA	1:A:286:ILE:HD11	0.56	1.78	1	3
1:A:190:LEU:CD1	1:A:262:LEU:HD11	0.56	2.28	18	1
1:A:245:PHE:HD1	1:A:286:ILE:HD13	0.55	1.59	18	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:232:GLU:OE1	1:A:272:LEU:HD13	0.55	2.00	17	2
1:A:203:VAL:HG11	1:A:252:GLY:H	0.55	1.61	17	2
1:A:196:VAL:HG13	1:A:259:LYS:HA	0.55	1.78	16	1
1:A:265:ALA:HB3	1:A:275:PRO:CB	0.55	2.31	5	2
1:A:192:PRO:HD3	1:A:262:LEU:HD12	0.55	1.78	19	1
1:A:199:ILE:HD12	1:A:233:ILE:HD11	0.54	1.80	8	2
1:A:184:ILE:CD1	1:A:198:THR:HG22	0.54	2.32	11	1
1:A:190:LEU:HB3	1:A:262:LEU:HD21	0.54	1.79	18	1
1:A:191:SER:O	1:A:262:LEU:HD22	0.54	2.02	18	1
1:A:221:LEU:HD11	1:A:238:PHE:CD1	0.54	2.38	21	3
1:A:190:LEU:HD12	1:A:199:ILE:HD12	0.54	1.79	7	1
1:A:280:LEU:HD23	1:A:281:ASP:N	0.54	2.18	12	3
1:A:272:LEU:HD22	1:A:272:LEU:C	0.54	2.23	19	1
1:A:197:TRP:CH2	1:A:278:LEU:HD21	0.54	2.37	8	3
1:A:261:LYS:O	1:A:278:LEU:HD13	0.54	2.02	10	2
1:A:249:LEU:HD21	1:A:286:ILE:HG23	0.54	1.80	5	1
1:A:221:LEU:HD13	1:A:222:PHE:N	0.54	2.17	2	1
1:A:196:VAL:HG13	1:A:196:VAL:O	0.53	2.03	10	5
1:A:198:THR:HG23	1:A:256:TYR:CD1	0.53	2.37	16	4
1:A:270:THR:HG22	1:A:270:THR:O	0.53	2.04	16	2
1:A:259:LYS:O	1:A:260:ALA:HB2	0.53	2.04	8	10
1:A:197:TRP:CZ2	1:A:278:LEU:HD22	0.53	2.39	14	2
1:A:196:VAL:HG12	1:A:259:LYS:HA	0.52	1.79	14	2
1:A:190:LEU:HD13	1:A:262:LEU:CD2	0.52	2.34	14	3
1:A:184:ILE:HG12	1:A:198:THR:HG22	0.52	1.81	1	2
1:A:187:ILE:HD12	1:A:199:ILE:HD11	0.52	1.81	7	2
1:A:223:ASN:HB3	1:A:236:THR:HG22	0.52	1.82	9	1
1:A:186:ALA:HB3	1:A:189:GLN:HG3	0.52	1.80	11	5
1:A:222:PHE:CE1	1:A:245:PHE:CE2	0.52	2.98	17	2
1:A:222:PHE:CE1	1:A:245:PHE:CE1	0.52	2.98	15	1
1:A:203:VAL:HG11	1:A:252:GLY:N	0.52	2.20	19	5
1:A:198:THR:HG22	1:A:258:SER:CA	0.52	2.34	19	1
1:A:226:PHE:HE1	1:A:235:ALA:HB3	0.51	1.62	17	3
1:A:196:VAL:HG23	1:A:259:LYS:HA	0.51	1.81	22	1
1:A:199:ILE:HD13	1:A:233:ILE:HD12	0.51	1.82	6	2
1:A:210:LYS:O	1:A:221:LEU:N	0.51	2.44	4	6
1:A:222:PHE:CE2	1:A:224:VAL:CG2	0.51	2.93	2	5
1:A:200:LYS:O	1:A:201:ALA:HB2	0.51	2.06	8	3
1:A:280:LEU:C	1:A:280:LEU:HD23	0.51	2.26	22	9
1:A:190:LEU:HD21	1:A:197:TRP:CD2	0.51	2.40	3	3
1:A:262:LEU:C	1:A:262:LEU:HD13	0.51	2.26	7	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:222:PHE:CE1	1:A:224:VAL:HG13	0.51	2.41	8	1
1:A:224:VAL:HG13	1:A:226:PHE:CE2	0.51	2.41	13	1
1:A:272:LEU:HD12	1:A:273:THR:HG23	0.51	1.82	14	1
1:A:259:LYS:O	1:A:284:THR:HG23	0.50	2.06	19	3
1:A:222:PHE:CZ	1:A:224:VAL:CG2	0.50	2.94	16	5
1:A:190:LEU:HD11	1:A:199:ILE:HD13	0.50	1.82	20	1
1:A:272:LEU:HD11	1:A:275:PRO:HA	0.50	1.84	22	1
1:A:184:ILE:HD12	1:A:200:LYS:N	0.50	2.22	11	1
1:A:197:TRP:CH2	1:A:278:LEU:HD22	0.50	2.41	16	1
1:A:190:LEU:HD22	1:A:262:LEU:HG	0.50	1.82	11	7
1:A:199:ILE:CD1	1:A:233:ILE:HD11	0.50	2.37	12	1
1:A:249:LEU:HD11	1:A:255:TYR:CZ	0.50	2.42	7	2
1:A:249:LEU:HG	1:A:286:ILE:HD12	0.49	1.84	13	1
1:A:285:VAL:O	1:A:286:ILE:HD13	0.49	2.06	19	1
1:A:184:ILE:HD11	1:A:198:THR:HG22	0.49	1.84	11	1
1:A:197:TRP:HH2	1:A:278:LEU:HD11	0.49	1.66	12	1
1:A:262:LEU:HD13	1:A:262:LEU:C	0.49	2.27	15	8
1:A:196:VAL:HG21	1:A:259:LYS:NZ	0.49	2.22	22	1
1:A:187:ILE:CG1	1:A:199:ILE:HD11	0.49	2.38	13	1
1:A:248:ILE:HG22	1:A:287:GLU:HA	0.49	1.84	17	1
1:A:186:ALA:HB1	1:A:230:SER:HB3	0.49	1.82	19	1
1:A:272:LEU:CD1	1:A:272:LEU:N	0.49	2.75	19	1
1:A:257:VAL:CG1	1:A:286:ILE:HG22	0.49	2.33	21	1
1:A:226:PHE:CE1	1:A:255:TYR:CE1	0.48	3.01	1	2
1:A:280:LEU:HD23	1:A:280:LEU:C	0.48	2.28	7	2
1:A:187:ILE:HD13	1:A:232:GLU:C	0.48	2.29	6	1
1:A:203:VAL:HG11	1:A:251:GLU:C	0.48	2.29	13	1
1:A:222:PHE:CD1	1:A:222:PHE:C	0.48	2.87	15	7
1:A:187:ILE:HD11	1:A:228:ASP:OD2	0.48	2.08	10	1
1:A:257:VAL:HG22	1:A:286:ILE:HG23	0.48	1.85	12	1
1:A:255:TYR:CD1	1:A:255:TYR:N	0.48	2.82	12	16
1:A:186:ALA:HB1	1:A:230:SER:HB2	0.48	1.86	19	1
1:A:222:PHE:CZ	1:A:224:VAL:HG22	0.48	2.44	7	2
1:A:270:THR:O	1:A:271:ASN:CB	0.48	2.62	19	1
1:A:221:LEU:HD12	1:A:238:PHE:CD1	0.48	2.44	22	2
1:A:221:LEU:HD22	1:A:238:PHE:HA	0.48	1.83	2	1
1:A:261:LYS:O	1:A:278:LEU:HD23	0.48	2.08	8	1
1:A:212:TRP:CD1	1:A:212:TRP:N	0.47	2.82	3	13
1:A:190:LEU:CD1	1:A:199:ILE:HD12	0.47	2.29	15	3
1:A:212:TRP:CH2	1:A:238:PHE:CE1	0.47	3.02	12	2
1:A:203:VAL:HG13	1:A:203:VAL:O	0.47	2.09	11	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:220:LYS:O	1:A:239:ASN:N	0.47	2.48	19	15
1:A:209:ILE:HG22	1:A:220:LYS:CG	0.47	2.39	9	3
1:A:257:VAL:CG1	1:A:286:ILE:HG23	0.47	2.38	20	1
1:A:224:VAL:CG1	1:A:226:PHE:CZ	0.47	2.97	2	4
1:A:255:TYR:CE2	1:A:257:VAL:CG2	0.47	2.97	10	6
1:A:223:ASN:HB2	1:A:236:THR:HG22	0.47	1.86	6	1
1:A:278:LEU:HD13	1:A:279:ASN:N	0.47	2.24	2	3
1:A:198:THR:HG22	1:A:258:SER:CB	0.47	2.40	3	2
1:A:209:ILE:HG23	1:A:221:LEU:O	0.47	2.09	4	1
1:A:221:LEU:HD23	1:A:236:THR:HG22	0.47	1.86	5	1
1:A:187:ILE:HA	1:A:199:ILE:HD11	0.47	1.85	17	1
1:A:257:VAL:HG13	1:A:286:ILE:HG13	0.47	1.87	2	1
1:A:222:PHE:CD1	1:A:242:ALA:HB1	0.47	2.44	6	1
1:A:253:LYS:CE	1:A:255:TYR:CD1	0.47	2.98	21	6
1:A:197:TRP:HH2	1:A:260:ALA:HB3	0.47	1.65	11	1
1:A:187:ILE:HD11	1:A:233:ILE:HG22	0.47	1.86	19	1
1:A:203:VAL:HG23	1:A:226:PHE:CD2	0.47	2.44	4	1
1:A:197:TRP:CZ3	1:A:199:ILE:CG2	0.47	2.98	8	2
1:A:196:VAL:HG13	1:A:259:LYS:CA	0.47	2.39	16	1
1:A:224:VAL:HG11	1:A:226:PHE:CE2	0.46	2.45	5	1
1:A:245:PHE:HE1	1:A:286:ILE:HG21	0.46	1.69	12	1
1:A:256:TYR:CD1	1:A:257:VAL:N	0.46	2.84	20	2
1:A:222:PHE:HD1	1:A:237:ALA:HB3	0.46	1.71	15	1
1:A:187:ILE:HD13	1:A:233:ILE:CG2	0.46	2.41	3	1
1:A:245:PHE:CZ	1:A:249:LEU:HD12	0.46	2.45	5	2
1:A:190:LEU:HD21	1:A:199:ILE:HD12	0.46	1.86	16	1
1:A:190:LEU:CD1	1:A:197:TRP:CG	0.46	2.99	6	1
1:A:248:ILE:HG21	1:A:286:ILE:O	0.46	2.11	15	1
1:A:245:PHE:HB2	1:A:286:ILE:HD13	0.46	1.88	2	1
1:A:190:LEU:HD22	1:A:197:TRP:CE3	0.46	2.46	15	1
1:A:280:LEU:HD12	1:A:286:ILE:HD11	0.46	1.85	14	3
1:A:245:PHE:CE2	1:A:249:LEU:CD1	0.45	2.99	1	3
1:A:190:LEU:HB2	1:A:276:TYR:CE2	0.45	2.46	14	6
1:A:221:LEU:HD21	1:A:238:PHE:CD1	0.45	2.47	2	1
1:A:253:LYS:NZ	1:A:255:TYR:CD1	0.45	2.84	9	3
1:A:262:LEU:HD21	1:A:276:TYR:HE2	0.45	1.71	13	1
1:A:245:PHE:CE2	1:A:249:LEU:HD13	0.45	2.46	15	1
1:A:221:LEU:HD23	1:A:222:PHE:N	0.45	2.26	18	2
1:A:197:TRP:CH2	1:A:278:LEU:HD13	0.45	2.45	14	2
1:A:270:THR:OG1	1:A:272:LEU:HD21	0.45	2.12	8	1
1:A:197:TRP:HH2	1:A:278:LEU:HD21	0.45	1.71	15	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:245:PHE:CD1	1:A:280:LEU:CD1	0.45	2.99	9	1
1:A:265:ALA:HB3	1:A:275:PRO:C	0.45	2.32	9	1
1:A:280:LEU:HD11	1:A:284:THR:HB	0.45	1.88	21	1
1:A:257:VAL:HG13	1:A:286:ILE:HG22	0.45	1.88	10	1
1:A:190:LEU:HD12	1:A:199:ILE:HD13	0.45	1.88	20	1
1:A:224:VAL:CG1	1:A:226:PHE:CE2	0.45	2.99	1	3
1:A:187:ILE:HG23	1:A:233:ILE:HD12	0.45	1.89	3	1
1:A:196:VAL:HG23	1:A:259:LYS:HG2	0.45	1.88	7	2
1:A:190:LEU:HD13	1:A:262:LEU:HD23	0.45	1.89	14	1
1:A:221:LEU:CD1	1:A:238:PHE:CE1	0.45	3.00	22	1
1:A:245:PHE:HD2	1:A:286:ILE:HD13	0.45	1.72	7	3
1:A:190:LEU:HG	1:A:262:LEU:HD11	0.45	1.89	9	1
1:A:258:SER:O	1:A:284:THR:HG23	0.45	2.11	8	1
1:A:255:TYR:CE2	1:A:257:VAL:CG1	0.44	3.00	18	1
1:A:196:VAL:HG21	1:A:259:LYS:CE	0.44	2.42	22	1
1:A:245:PHE:CD1	1:A:286:ILE:CD1	0.44	3.00	3	1
1:A:199:ILE:CD1	1:A:233:ILE:HD13	0.44	2.42	10	1
1:A:190:LEU:HB3	1:A:262:LEU:HD11	0.44	1.88	18	1
1:A:197:TRP:CE3	1:A:199:ILE:HG12	0.44	2.47	11	1
1:A:249:LEU:HD21	1:A:286:ILE:HB	0.44	1.89	6	1
1:A:262:LEU:CD1	1:A:276:TYR:CE1	0.44	3.00	14	1
1:A:190:LEU:HD22	1:A:262:LEU:CG	0.44	2.43	1	1
1:A:196:VAL:HG13	1:A:259:LYS:HG2	0.44	1.90	16	1
1:A:221:LEU:HD11	1:A:238:PHE:CE1	0.44	2.48	20	1
1:A:210:LYS:N	1:A:210:LYS:HD2	0.43	2.28	15	5
1:A:198:THR:CG2	1:A:256:TYR:CE1	0.43	3.00	11	1
1:A:195:ASN:OD1	1:A:196:VAL:HG13	0.43	2.13	12	1
1:A:270:THR:HG21	1:A:272:LEU:CD2	0.43	2.43	22	1
1:A:222:PHE:CZ	1:A:224:VAL:HG23	0.43	2.48	5	2
1:A:227:LEU:HD13	1:A:228:ASP:N	0.43	2.28	16	1
1:A:222:PHE:CE1	1:A:245:PHE:CZ	0.43	3.06	17	1
1:A:272:LEU:N	1:A:272:LEU:CD2	0.43	2.80	20	1
1:A:256:TYR:O	1:A:256:TYR:CD1	0.43	2.72	15	12
1:A:221:LEU:HD13	1:A:222:PHE:H	0.43	1.73	2	1
1:A:278:LEU:HD23	1:A:279:ASN:N	0.43	2.28	18	2
1:A:205:TYR:CE2	1:A:206:LYS:O	0.43	2.71	3	6
1:A:237:ALA:CB	1:A:242:ALA:HB2	0.43	2.44	22	2
1:A:222:PHE:CE2	1:A:224:VAL:CG1	0.43	2.99	19	2
1:A:256:TYR:CD1	1:A:256:TYR:C	0.43	2.92	20	2
1:A:238:PHE:CE1	1:A:279:ASN:OD1	0.43	2.72	9	4
1:A:199:ILE:HD13	1:A:233:ILE:CD1	0.43	2.43	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:226:PHE:CZ	1:A:255:TYR:OH	0.43	2.72	14	3
1:A:286:ILE:C	1:A:286:ILE:HD12	0.43	2.34	22	1
1:A:273:THR:CG2	1:A:274:HIS:CE1	0.43	3.02	7	1
1:A:199:ILE:HD11	1:A:233:ILE:HD13	0.43	1.90	10	1
1:A:190:LEU:HD21	1:A:197:TRP:CZ3	0.43	2.49	19	1
1:A:187:ILE:HG22	1:A:199:ILE:CD1	0.43	2.41	21	1
1:A:222:PHE:CZ	1:A:224:VAL:CG1	0.42	3.02	18	1
1:A:260:ALA:HB2	1:A:284:THR:CG2	0.42	2.43	20	1
1:A:245:PHE:HD1	1:A:286:ILE:HG21	0.42	1.74	21	1
1:A:270:THR:HG22	1:A:272:LEU:CD2	0.42	2.44	6	1
1:A:221:LEU:HD21	1:A:236:THR:CG2	0.42	2.44	10	1
1:A:255:TYR:CG	1:A:256:TYR:N	0.42	2.84	18	1
1:A:273:THR:O	1:A:274:HIS:CG	0.42	2.72	19	1
1:A:238:PHE:CZ	1:A:279:ASN:OD1	0.42	2.72	8	1
1:A:190:LEU:CB	1:A:276:TYR:CZ	0.42	3.03	10	1
1:A:190:LEU:HD23	1:A:262:LEU:HD11	0.42	1.92	9	1
1:A:241:PHE:CG	1:A:281:ASP:O	0.42	2.72	3	1
1:A:201:ALA:O	1:A:255:TYR:CD1	0.42	2.72	8	8
1:A:205:TYR:CE1	1:A:206:LYS:O	0.42	2.73	11	3
1:A:226:PHE:CD1	1:A:226:PHE:N	0.42	2.87	16	2
1:A:190:LEU:N	1:A:190:LEU:CD2	0.42	2.83	6	4
1:A:253:LYS:HG2	1:A:254:VAL:N	0.42	2.30	13	3
1:A:286:ILE:HD12	1:A:286:ILE:N	0.42	2.30	2	1
1:A:183:PRO:O	1:A:185:PHE:CD2	0.42	2.73	18	3
1:A:222:PHE:CE2	1:A:246:ASN:ND2	0.42	2.88	11	1
1:A:210:LYS:HE2	1:A:221:LEU:HD23	0.42	1.91	16	1
1:A:209:ILE:CG2	1:A:220:LYS:CD	0.42	2.97	18	1
1:A:233:ILE:CG1	1:A:234:ARG:N	0.42	2.83	20	9
1:A:224:VAL:HG11	1:A:226:PHE:CZ	0.42	2.49	5	1
1:A:184:ILE:HD13	1:A:200:LYS:HE3	0.42	1.90	7	1
1:A:270:THR:HG23	1:A:272:LEU:HG	0.42	1.90	7	1
1:A:226:PHE:CE1	1:A:255:TYR:CZ	0.42	3.08	1	1
1:A:226:PHE:CG	1:A:255:TYR:OH	0.42	2.72	6	2
1:A:198:THR:HG23	1:A:256:TYR:CE2	0.42	2.50	12	2
1:A:197:TRP:CZ2	1:A:260:ALA:O	0.42	2.73	5	2
1:A:190:LEU:CD1	1:A:262:LEU:CD1	0.42	2.98	16	1
1:A:197:TRP:HZ3	1:A:257:VAL:HG23	0.42	1.75	18	1
1:A:274:HIS:N	1:A:275:PRO:CD	0.41	2.82	17	6
1:A:258:SER:O	1:A:259:LYS:O	0.41	2.39	19	1
1:A:280:LEU:CD2	1:A:284:THR:CG2	0.41	2.97	19	1
1:A:190:LEU:HD12	1:A:190:LEU:N	0.41	2.31	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:249:LEU:CD2	1:A:255:TYR:CD2	0.41	3.03	1	1
1:A:226:PHE:CD2	1:A:255:TYR:OH	0.41	2.73	13	1
1:A:208:GLU:CG	1:A:209:ILE:N	0.41	2.84	8	1
1:A:190:LEU:CD2	1:A:262:LEU:HD11	0.41	2.45	9	1
1:A:222:PHE:CE2	1:A:224:VAL:HG21	0.41	2.51	17	1
1:A:239:ASN:OD1	1:A:241:PHE:CD2	0.41	2.73	3	1
1:A:262:LEU:HD23	1:A:278:LEU:HD21	0.41	1.92	7	1
1:A:222:PHE:CZ	1:A:246:ASN:OD1	0.41	2.74	22	2
1:A:213:HIS:CD2	1:A:218:ASP:OD1	0.41	2.74	15	1
1:A:226:PHE:CE2	1:A:255:TYR:OH	0.41	2.74	13	2
1:A:196:VAL:O	1:A:196:VAL:HG22	0.41	2.16	6	1
1:A:223:ASN:CB	1:A:236:THR:HG22	0.41	2.45	6	1
1:A:190:LEU:HB2	1:A:276:TYR:CZ	0.41	2.51	10	1
1:A:197:TRP:CE3	1:A:199:ILE:CG1	0.41	3.04	11	1
1:A:195:ASN:C	1:A:196:VAL:HG12	0.41	2.34	15	1
1:A:241:PHE:CD2	1:A:281:ASP:O	0.40	2.75	3	1
1:A:222:PHE:CD1	1:A:222:PHE:O	0.40	2.74	5	1
1:A:187:ILE:CD1	1:A:199:ILE:CD1	0.40	2.99	10	1
1:A:188:GLU:OE2	1:A:274:HIS:CE1	0.40	2.74	11	1
1:A:238:PHE:CD2	1:A:281:ASP:OD2	0.40	2.74	16	2
1:A:197:TRP:CZ2	1:A:278:LEU:HD21	0.40	2.51	2	1
1:A:261:LYS:CE	1:A:282:ARG:NE	0.40	2.84	10	1
1:A:226:PHE:CE1	1:A:255:TYR:OH	0.40	2.72	11	1
1:A:187:ILE:O	1:A:276:TYR:CE2	0.40	2.74	15	1
1:A:209:ILE:HA	1:A:222:PHE:HB2	0.40	1.93	2	1
1:A:209:ILE:CG2	1:A:220:LYS:CG	0.40	3.00	4	1
1:A:208:GLU:O	1:A:222:PHE:HA	0.40	2.16	5	1
1:A:237:ALA:HB2	1:A:245:PHE:CE2	0.40	2.51	5	1
1:A:209:ILE:CG2	1:A:220:LYS:HG2	0.40	2.46	10	1
1:A:198:THR:HG23	1:A:256:TYR:HE2	0.40	1.76	12	1
1:A:241:PHE:CD2	1:A:281:ASP:OD1	0.40	2.74	18	1
1:A:187:ILE:O	1:A:276:TYR:CZ	0.40	2.75	6	2
1:A:207:GLY:O	1:A:208:GLU:HG2	0.40	2.17	6	1
1:A:245:PHE:CE1	1:A:249:LEU:CD1	0.40	3.01	8	1
1:A:183:PRO:O	1:A:185:PHE:CE1	0.40	2.74	9	1
1:A:239:ASN:O	1:A:241:PHE:N	0.40	2.54	12	1
1:A:183:PRO:O	1:A:185:PHE:CE2	0.40	2.74	16	1
1:A:210:LYS:HD2	1:A:210:LYS:N	0.40	2.30	19	1
1:A:245:PHE:CD1	1:A:245:PHE:C	0.40	2.94	1	1
1:A:256:TYR:OH	1:A:285:VAL:HG12	0.40	2.15	14	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	108/114 (95%)	94±3 (88±2%)	8±2 (8±2%)	5±1 (5±1%)	4 25
All	All	2376/2508 (95%)	2079 (88%)	179 (8%)	118 (5%)	4 25

All 18 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	239	ASN	22
1	A	240	ASP	19
1	A	208	GLU	15
1	A	281	ASP	13
1	A	282	ARG	12
1	A	259	LYS	10
1	A	196	VAL	4
1	A	267	PRO	4
1	A	289	CYS	4
1	A	238	PHE	3
1	A	194	GLN	2
1	A	214	ASN	2
1	A	272	LEU	2
1	A	190	LEU	2
1	A	184	ILE	1
1	A	212	TRP	1
1	A	213	HIS	1
1	A	270	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	96/102 (94%)	78±2 (81±2%)	18±2 (19±2%)	4 36
All	All	2112/2244 (94%)	1718 (81%)	394 (19%)	4 36

All 52 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	191	SER	22
1	A	202	ARG	22
1	A	244	LYS	22
1	A	245	PHE	22
1	A	253	LYS	22
1	A	256	TYR	22
1	A	250	GLN	21
1	A	276	TYR	21
1	A	182	ARG	17
1	A	222	PHE	16
1	A	204	SER	14
1	A	224	VAL	14
1	A	203	VAL	13
1	A	278	LEU	13
1	A	210	LYS	13
1	A	266	LYS	12
1	A	280	LEU	11
1	A	208	GLU	10
1	A	221	LEU	9
1	A	263	GLN	9
1	A	257	VAL	7
1	A	288	GLU	6
1	A	274	HIS	5
1	A	197	TRP	5
1	A	199	ILE	4
1	A	272	LEU	4
1	A	184	ILE	2
1	A	282	ARG	2
1	A	198	THR	2
1	A	200	LYS	2
1	A	259	LYS	2
1	A	268	GLN	2
1	A	284	THR	2
1	A	190	LEU	2
1	A	251	GLU	2
1	A	254	VAL	2

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Mol	Chain	Res	Type	Models (Total)
1	A	238	PHE	2
1	A	262	LEU	2
1	A	213	HIS	1
1	A	236	THR	1
1	A	185	PHE	1
1	A	211	THR	1
1	A	212	TRP	1
1	A	206	LYS	1
1	A	279	ASN	1
1	A	196	VAL	1
1	A	227	LEU	1
1	A	249	LEU	1
1	A	255	TYR	1
1	A	289	CYS	1
1	A	214	ASN	1
1	A	216	ARG	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 monosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

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