



# Full wwPDB NMR Structure Validation Report ⓘ

Apr 27, 2016 – 06:04 AM BST

PDB ID : 3CYS  
Title : DETERMINATION OF THE NMR SOLUTION STRUCTURE OF THE CYCLOPHILIN A-CYCLOSPORIN A COMPLEX  
Authors : Spitzfaden, C.; Braun, W.; Wider, G.; Widmer, H.; Wuthrich, K.  
Deposited on : 1994-02-28

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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 : 1.7.1 (RC1), CSD as537be (2016)  
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

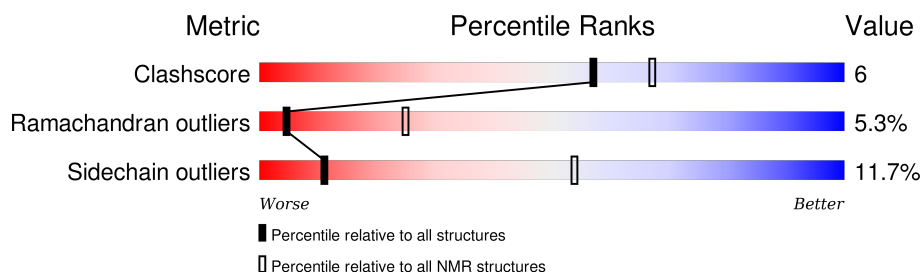
# 1 Overall quality at a glance

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  $\geq 3$ , 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	165	
2	B	11	

## 2 Ensemble composition and analysis

This entry contains 22 models. Model 17 is the overall representative, medoid model (most similar to other models).

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:3-A:66, A:77-A:165, B:209-B:209, B:211-B:211 (155)	0.68	17

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. No single-model clusters were found.

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

### 3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 2675 atoms, of which 1325 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called PEPTIDYL-PROLYL CIS-TRANS ISOMERASE A.

Mol	Chain	Residues	Atoms						Trace
1	A	165	Total	C	H	N	O	S	0
			2500	802	1235	218	236	9	

- Molecule 2 is a protein called CYCLOSPORIN A.

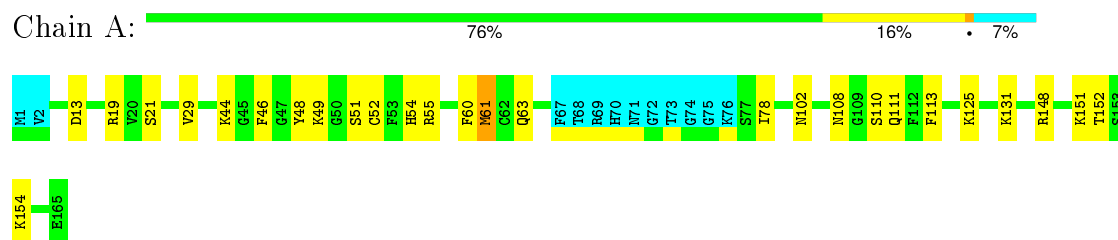
Mol	Chain	Residues	Atoms					Trace
2	B	11	Total	C	H	N	O	0
			175	62	90	11	12	

## 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: PEPTIDYL-PROLYL CIS-TRANS ISOMERASE A



- Molecule 2: CYCLOSPORIN A

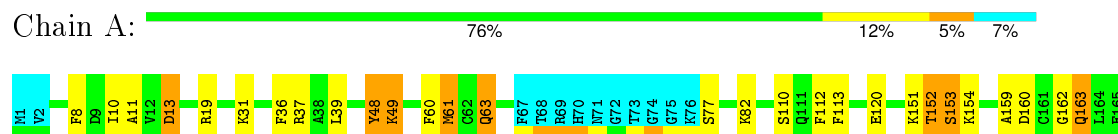


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

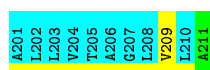
#### 4.2.1 Score per residue for model 1

- Molecule 1: PEPTIDYL-PROLYL CIS-TRANS ISOMERASE A



- Molecule 2: CYCLOSPORIN A

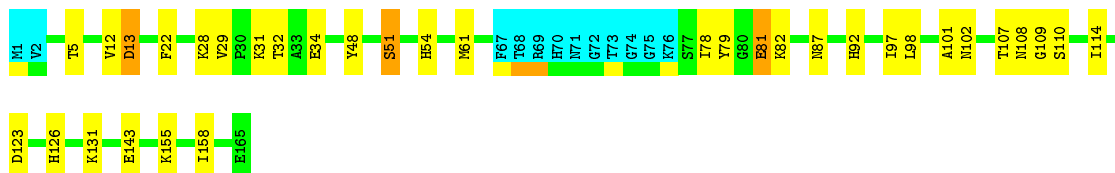




#### 4.2.2 Score per residue for model 2

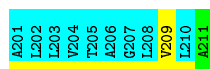
- Molecule 1: PEPTIDYL-PROLYL CIS-TRANS ISOMERASE A

Chain A: 72% 19% 7%



- Molecule 2: CYCLOSPORIN A

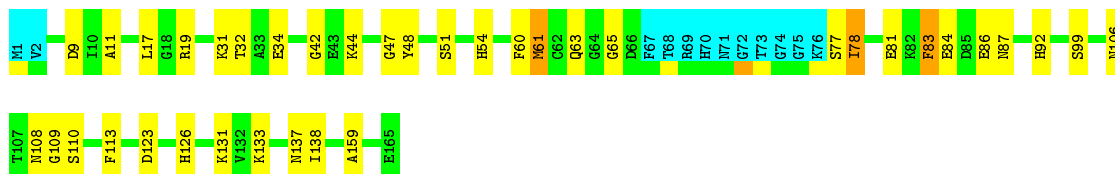
Chain B: 9% 9% 82%



#### 4.2.3 Score per residue for model 3

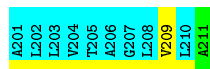
- Molecule 1: PEPTIDYL-PROLYL CIS-TRANS ISOMERASE A

Chain A: 70% 21% 7%



- Molecule 2: CYCLOSPORIN A

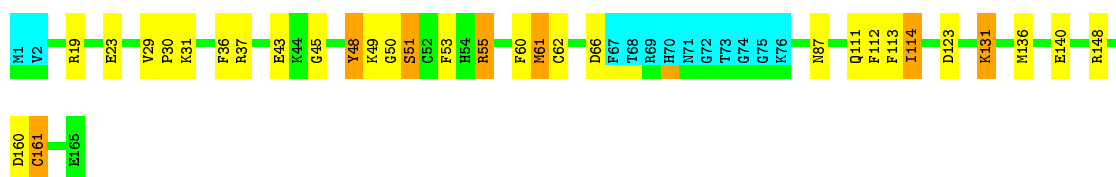
Chain B: 9% 9% 82%



#### 4.2.4 Score per residue for model 4

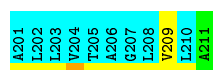
- Molecule 1: PEPTIDYL-PROLYL CIS-TRANS ISOMERASE A

Chain A: 74% 15% 7%



- Molecule 2: CYCLOSPORIN A

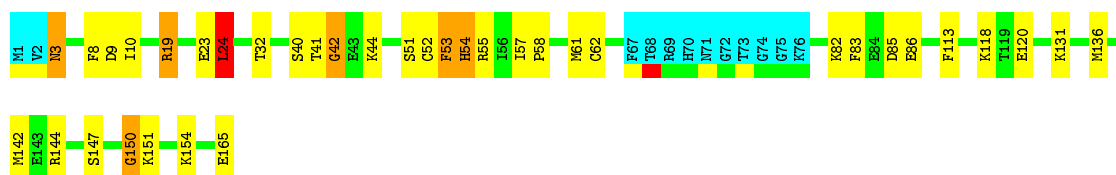
Chain B: 9% 9% 82%



#### 4.2.5 Score per residue for model 5

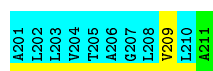
- Molecule 1: PEPTIDYL-PROLYL CIS-TRANS ISOMERASE A

Chain A: 70% 18% 7%



- Molecule 2: CYCLOSPORIN A

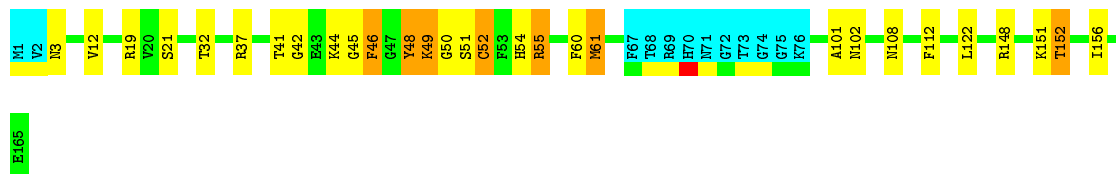
Chain B: 9% 9% 82%



#### 4.2.6 Score per residue for model 6

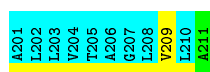
- Molecule 1: PEPTIDYL-PROLYL CIS-TRANS ISOMERASE A

Chain A: 75% 13% 7%



- Molecule 2: CYCLOSPORIN A

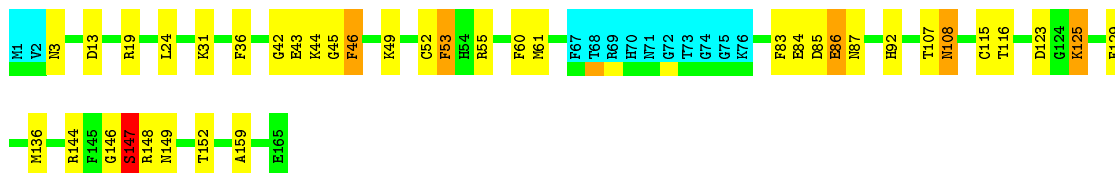
Chain B: 9% 9% 82%



#### 4.2.7 Score per residue for model 7

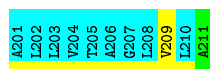
- Molecule 1: PEPTIDYL-PROLYL CIS-TRANS ISOMERASE A

Chain A: 70% 19% 7%



- Molecule 2: CYCLOSPORIN A

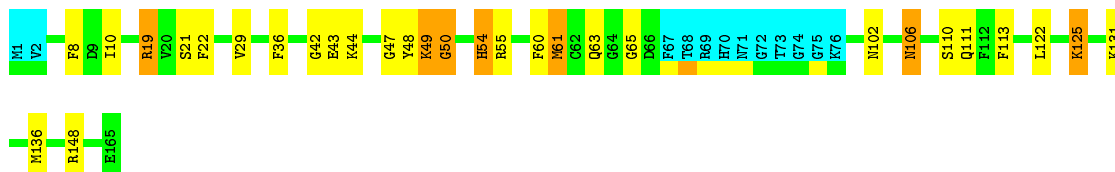
Chain B: 9% 9% 82%



#### 4.2.8 Score per residue for model 8

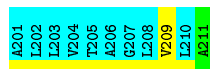
- Molecule 1: PEPTIDYL-PROLYL CIS-TRANS ISOMERASE A

Chain A: 75% 14% 7%



- Molecule 2: CYCLOSPORIN A

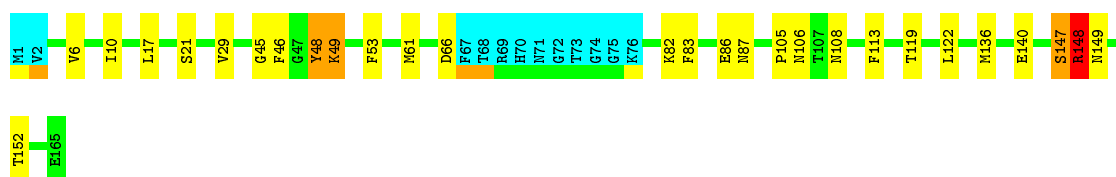
Chain B: 9% 9% 82%



#### 4.2.9 Score per residue for model 9

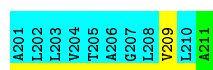
- Molecule 1: PEPTIDYL-PROLYL CIS-TRANS ISOMERASE A

Chain A: 76% 15% 7%



- Molecule 2: CYCLOSPORIN A

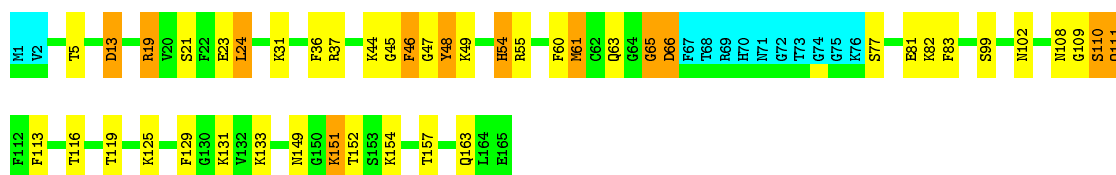
Chain B: 9% 9% 82%



#### 4.2.10 Score per residue for model 10

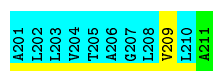
- Molecule 1: PEPTIDYL-PROLYL CIS-TRANS ISOMERASE A

Chain A: 65% 20% 7% 7%



- Molecule 2: CYCLOSPORIN A

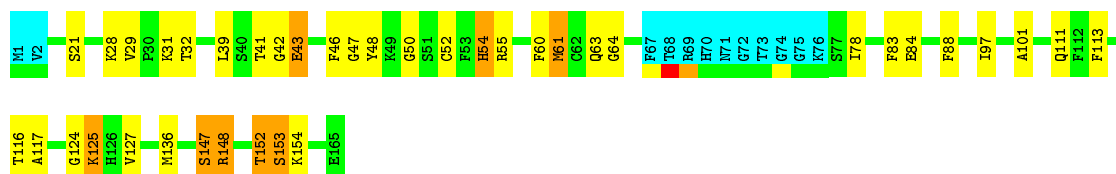
Chain B: 9% 9% 82%



#### 4.2.11 Score per residue for model 11

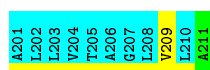
- Molecule 1: PEPTIDYL-PROLYL CIS-TRANS ISOMERASE A

Chain A: 69% 19% 5% 7%



- Molecule 2: CYCLOSPORIN A

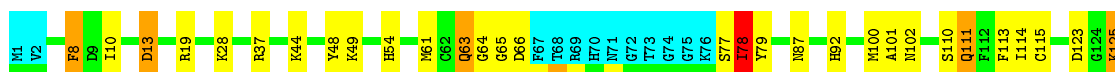
Chain B: 9% 9% 82%



#### 4.2.12 Score per residue for model 12

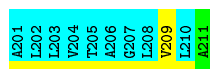
- Molecule 1: PEPTIDYL-PROLYL CIS-TRANS ISOMERASE A

Chain A: 69% 19% • • 7%



- Molecule 2: CYCLOSPORIN A

Chain B: 9% 9% 82%



#### 4.2.13 Score per residue for model 13

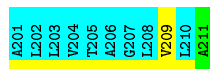
- Molecule 1: PEPTIDYL-PROLYL CIS-TRANS ISOMERASE A

Chain A: 71% 18% • 7%



- Molecule 2: CYCLOSPORIN A

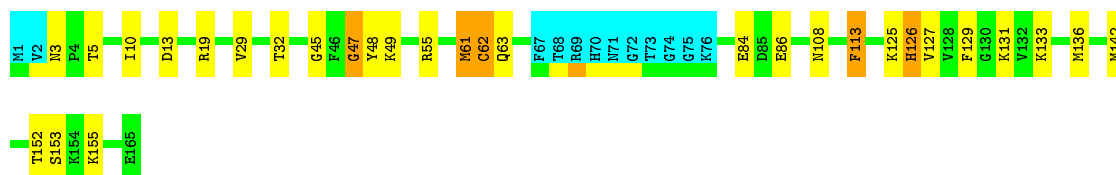
Chain B: 9% 9% 82%



#### 4.2.14 Score per residue for model 14

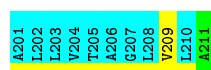
- Molecule 1: PEPTIDYL-PROLYL CIS-TRANS ISOMERASE A

Chain A: 75% 15% • 7%



- Molecule 2: CYCLOSPORIN A

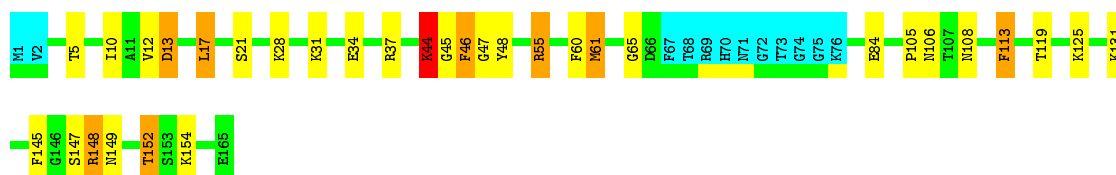
Chain B: 9% 9% 82%



#### 4.2.15 Score per residue for model 15

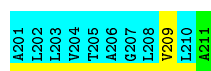
- Molecule 1: PEPTIDYL-PROLYL CIS-TRANS ISOMERASE A

Chain A: 73% 15% 5% 7%



- Molecule 2: CYCLOSPORIN A

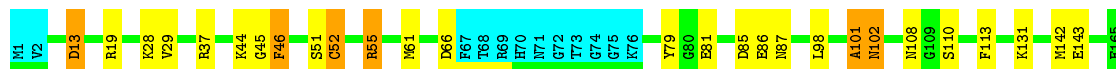
Chain B: 9% 9% 82%



#### 4.2.16 Score per residue for model 16

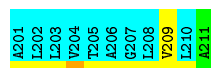
- Molecule 1: PEPTIDYL-PROLYL CIS-TRANS ISOMERASE A

Chain A: 76% 13% 7%



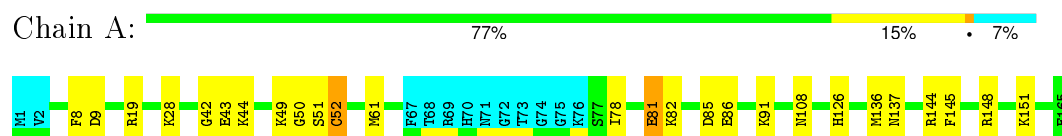
- Molecule 2: CYCLOSPORIN A

Chain B: 9% 9% 82%



### 4.2.17 Score per residue for model 17 (medoid)

- Molecule 1: PEPTIDYL-PROLYL CIS-TRANS ISOMERASE A

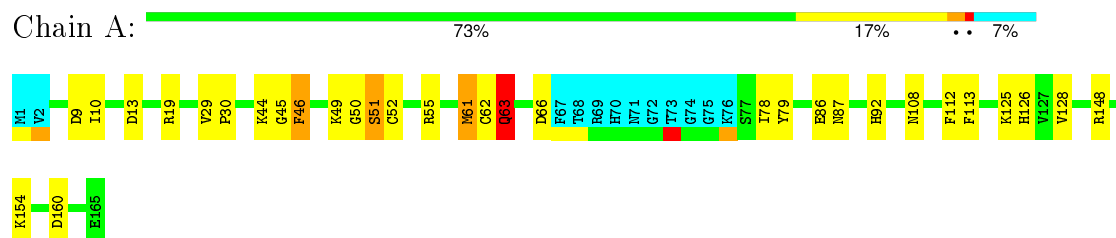


- Molecule 2: CYCLOSPORIN A



### 4.2.18 Score per residue for model 18

- Molecule 1: PEPTIDYL-PROLYL CIS-TRANS ISOMERASE A

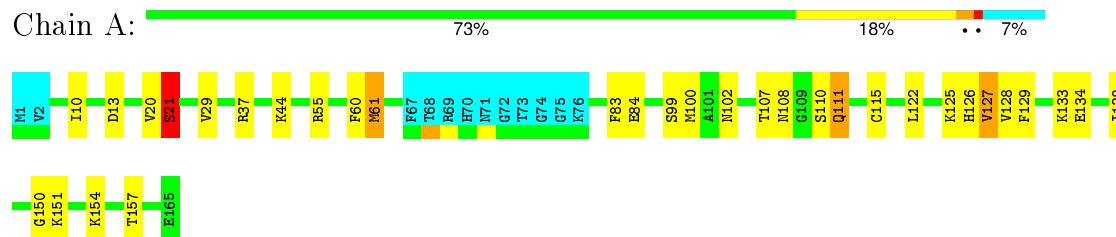


- Molecule 2: CYCLOSPORIN A



### 4.2.19 Score per residue for model 19

- Molecule 1: PEPTIDYL-PROLYL CIS-TRANS ISOMERASE A

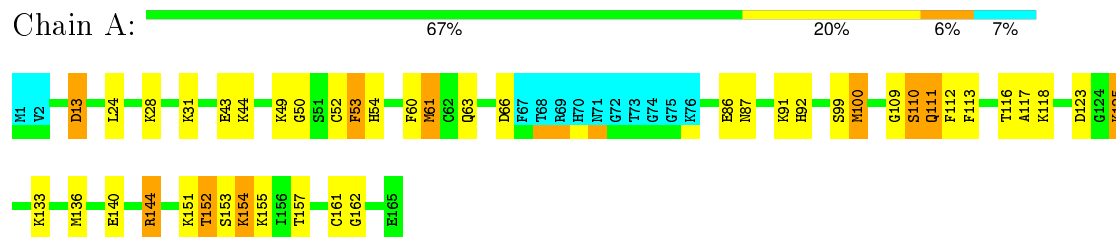


- Molecule 2: CYCLOSPORIN A



#### 4.2.20 Score per residue for model 20

- Molecule 1: PEPTIDYL-PROLYL CIS-TRANS ISOMERASE A

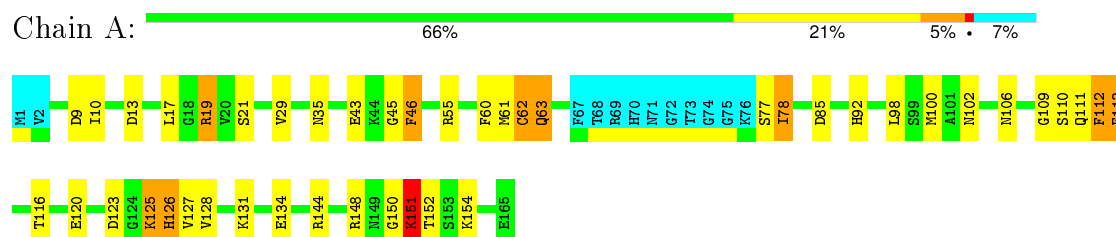


- Molecule 2: CYCLOSPORIN A



#### 4.2.21 Score per residue for model 21

- Molecule 1: PEPTIDYL-PROLYL CIS-TRANS ISOMERASE A

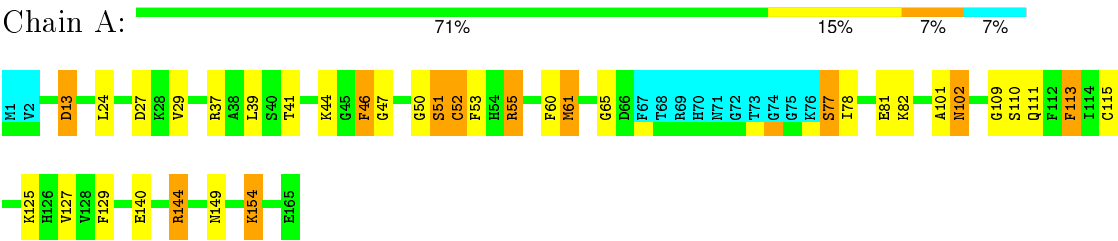


- Molecule 2: CYCLOSPORIN A



#### 4.2.22 Score per residue for model 22

- Molecule 1: PEPTIDYL-PROLYL CIS-TRANS ISOMERASE A



● Molecule 2: CYCLOSPORIN A



## 5 Refinement protocol and experimental data overview ⓘ

Of the ? calculated structures, 22 were deposited, based on the following criterion: ?.

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

Software name	Classification	Version
DIANA, FANTOM 3.1	refinement	

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: ABA, MLE, DAL, MVA, BMT, SAR

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

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	1.8±1.0
All	All	0	39

There are no bond-length outliers.

There are no bond-angle outliers.

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	19	ARG	Sidechain	13
1	A	55	ARG	Sidechain	12
1	A	37	ARG	Sidechain	6
1	A	148	ARG	Sidechain	4
1	A	144	ARG	Sidechain	4

### 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	1175	1146	1146	14±6
2	B	12	14	14	0±0
All	All	26114	25520	25520	319

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:29:VAL:HG11	1:A:129:PHE:CE1	0.87	2.04	13	3
1:A:62:CYS:SG	1:A:142:MET:SD	0.82	2.77	14	2
1:A:129:PHE:O	1:A:129:PHE:CG	0.80	2.34	14	1
1:A:29:VAL:HG21	1:A:129:PHE:CG	0.77	2.13	19	2
1:A:29:VAL:HG11	1:A:129:PHE:CZ	0.72	2.20	19	1
1:A:111:GLN:O	1:A:112:PHE:CG	0.71	2.43	21	1
1:A:12:VAL:HG12	1:A:13:ASP:OD1	0.68	1.88	2	1
1:A:147:SER:O	1:A:148:ARG:CB	0.68	2.41	11	1
1:A:45:GLY:O	1:A:46:PHE:CG	0.67	2.47	18	7
1:A:62:CYS:O	1:A:63:GLN:CB	0.66	2.44	13	1
1:A:52:CYS:O	1:A:53:PHE:CG	0.66	2.48	7	3
1:A:77:SER:O	1:A:79:TYR:N	0.66	2.27	12	1
1:A:101:ALA:O	1:A:102:ASN:CB	0.66	2.43	22	4
1:A:47:GLY:C	1:A:48:TYR:CD1	0.65	2.70	11	2
1:A:127:VAL:CG1	1:A:129:PHE:CE2	0.61	2.83	13	2
1:A:29:VAL:HG23	1:A:29:VAL:O	0.60	1.96	13	1
1:A:45:GLY:C	1:A:46:PHE:CG	0.60	2.75	16	7
1:A:61:MET:SD	1:A:113:PHE:CE2	0.60	2.95	14	1
1:A:111:GLN:C	1:A:112:PHE:CG	0.60	2.74	21	1
1:A:152:THR:O	1:A:153:SER:C	0.59	2.38	11	3
1:A:29:VAL:HG11	1:A:129:PHE:CE2	0.59	2.33	19	1
1:A:50:GLY:O	1:A:51:SER:C	0.58	2.42	4	3
1:A:41:THR:O	1:A:41:THR:HG23	0.58	1.98	6	2
1:A:46:PHE:CD1	1:A:46:PHE:C	0.58	2.73	22	1
1:A:108:ASN:ND2	1:A:108:ASN:C	0.58	2.55	7	1
1:A:113:PHE:O	1:A:113:PHE:CG	0.58	2.57	13	3
1:A:61:MET:SD	1:A:113:PHE:CE1	0.58	2.97	4	1
1:A:111:GLN:O	1:A:112:PHE:CD1	0.58	2.57	21	1
1:A:110:SER:O	1:A:111:GLN:C	0.58	2.41	10	4
1:A:46:PHE:CG	1:A:47:GLY:N	0.57	2.71	22	1
1:A:42:GLY:O	1:A:46:PHE:N	0.57	2.37	6	1
1:A:47:GLY:O	1:A:49:LYS:N	0.57	2.37	8	1
1:A:62:CYS:O	1:A:114:ILE:N	0.57	2.38	13	1
1:A:60:PHE:CD2	1:A:61:MET:SD	0.57	2.98	3	8
1:A:47:GLY:C	1:A:48:TYR:CG	0.57	2.78	3	2
1:A:45:GLY:O	1:A:46:PHE:CD1	0.57	2.58	18	5
1:A:8:PHE:CE2	1:A:22:PHE:CE1	0.56	2.94	8	1
1:A:50:GLY:O	1:A:52:CYS:N	0.56	2.39	18	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:88:PHE:CD1	1:A:124:GLY:O	0.55	2.59	11	1
1:A:111:GLN:C	1:A:112:PHE:CD2	0.55	2.80	21	1
1:A:128:VAL:O	1:A:129:PHE:CD1	0.55	2.60	19	2
1:A:23:GLU:O	1:A:24:LEU:C	0.55	2.45	10	2
1:A:112:PHE:O	1:A:113:PHE:CD1	0.55	2.59	1	3
1:A:61:MET:C	1:A:61:MET:SD	0.54	2.85	10	5
1:A:113:PHE:CD1	1:A:113:PHE:C	0.54	2.81	15	1
1:A:83:PHE:CD2	1:A:84:GLU:O	0.54	2.61	7	1
1:A:77:SER:OG	1:A:78:ILE:N	0.53	2.42	13	4
1:A:57:ILE:HG23	1:A:58:PRO:HD2	0.53	1.81	5	1
1:A:42:GLY:O	1:A:43:GLU:C	0.53	2.48	7	2
1:A:111:GLN:O	1:A:112:PHE:O	0.53	2.26	21	1
1:A:127:VAL:HG13	1:A:129:PHE:CE2	0.52	2.39	19	1
1:A:41:THR:HG23	1:A:41:THR:O	0.52	2.03	22	1
1:A:60:PHE:CG	1:A:61:MET:HG3	0.52	2.40	19	2
1:A:112:PHE:O	1:A:113:PHE:CG	0.52	2.62	21	1
1:A:83:PHE:CE2	1:A:84:GLU:O	0.52	2.62	3	2
1:A:45:GLY:C	1:A:46:PHE:CD2	0.52	2.82	15	7
1:A:42:GLY:O	1:A:44:LYS:N	0.52	2.42	17	1
1:A:112:PHE:O	1:A:113:PHE:CD2	0.52	2.63	21	1
1:A:113:PHE:CD2	1:A:113:PHE:O	0.52	2.63	13	1
1:A:8:PHE:CE2	1:A:10:ILE:HD11	0.51	2.40	12	2
1:A:150:GLY:O	1:A:151:LYS:CB	0.51	2.58	21	2
1:A:10:ILE:HD12	1:A:10:ILE:N	0.51	2.21	21	5
1:A:129:PHE:O	1:A:129:PHE:CD1	0.51	2.63	14	1
1:A:47:GLY:O	1:A:48:TYR:C	0.51	2.48	10	3
1:A:10:ILE:N	1:A:10:ILE:HD12	0.51	2.21	15	5
1:A:48:TYR:O	1:A:49:LYS:C	0.51	2.49	6	2
1:A:8:PHE:C	1:A:8:PHE:CD1	0.51	2.83	12	1
1:A:36:PHE:CD2	1:A:129:PHE:CE2	0.51	2.98	7	2
1:A:43:GLU:O	1:A:46:PHE:CD2	0.50	2.64	11	1
1:A:92:HIS:CD2	1:A:123:ASP:HA	0.50	2.41	21	6
1:A:48:TYR:CZ	1:A:112:PHE:CZ	0.50	3.00	1	1
1:A:116:THR:O	1:A:117:ALA:HB2	0.50	2.07	20	2
1:A:11:ALA:HB2	1:A:159:ALA:HB2	0.50	1.82	1	2
1:A:99:SER:OG	1:A:100:MET:N	0.49	2.45	19	2
1:A:41:THR:O	1:A:42:GLY:C	0.49	2.50	5	1
1:A:36:PHE:CD2	1:A:129:PHE:CZ	0.49	3.01	7	1
1:A:3:ASN:C	1:A:3:ASN:OD1	0.49	2.50	5	1
1:A:52:CYS:O	1:A:53:PHE:O	0.49	2.31	7	3
1:A:22:PHE:CD2	1:A:98:LEU:HD13	0.49	2.43	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:62:CYS:O	1:A:63:GLN:HB2	0.49	2.07	21	2
1:A:77:SER:OG	1:A:78:ILE:HG23	0.49	2.08	22	1
1:A:108:ASN:C	1:A:108:ASN:OD1	0.48	2.52	2	1
1:A:47:GLY:O	1:A:48:TYR:CG	0.48	2.66	3	2
1:A:49:LYS:NZ	1:A:160:ASP:OD2	0.48	2.46	18	1
1:A:63:GLN:CG	1:A:113:PHE:HA	0.48	2.39	12	2
1:A:147:SER:O	1:A:149:ASN:N	0.48	2.47	9	3
1:A:45:GLY:O	1:A:46:PHE:O	0.48	2.32	6	7
1:A:52:CYS:O	1:A:53:PHE:CD2	0.48	2.67	7	2
1:A:90:LEU:HD22	1:A:90:LEU:N	0.48	2.23	13	1
1:A:52:CYS:C	1:A:53:PHE:CG	0.48	2.87	5	3
1:A:127:VAL:CG1	1:A:129:PHE:CD2	0.47	2.97	19	1
1:A:63:GLN:HB2	1:A:113:PHE:CD2	0.47	2.44	1	1
1:A:62:CYS:SG	1:A:114:ILE:HD12	0.47	2.49	4	1
1:A:147:SER:O	1:A:148:ARG:HB3	0.47	2.09	11	1
1:A:8:PHE:CE1	1:A:10:ILE:HD11	0.47	2.44	1	1
1:A:47:GLY:O	1:A:48:TYR:CD2	0.47	2.68	3	1
1:A:113:PHE:C	1:A:113:PHE:CD1	0.47	2.88	22	1
1:A:152:THR:OG1	1:A:153:SER:N	0.47	2.48	14	1
1:A:29:VAL:HG11	1:A:129:PHE:CD1	0.47	2.45	22	2
1:A:49:LYS:NZ	1:A:160:ASP:OD1	0.47	2.48	1	1
1:A:101:ALA:HB3	1:A:113:PHE:CE1	0.47	2.45	11	1
1:A:32:THR:HG23	1:A:83:PHE:CE2	0.47	2.44	3	1
1:A:107:THR:O	1:A:107:THR:CG2	0.47	2.63	13	1
1:A:118:LYS:NZ	1:A:120:GLU:OE1	0.47	2.44	5	1
1:A:47:GLY:O	1:A:48:TYR:CD1	0.46	2.68	11	1
1:A:36:PHE:CE2	1:A:112:PHE:CZ	0.46	3.04	1	1
1:A:127:VAL:HG11	1:A:129:PHE:CE2	0.45	2.46	22	1
1:A:61:MET:SD	1:A:61:MET:C	0.45	2.95	21	2
1:A:156:ILE:O	1:A:157:THR:HG23	0.45	2.11	12	1
1:A:77:SER:O	1:A:78:ILE:C	0.45	2.55	12	1
1:A:60:PHE:CD2	1:A:61:MET:HG3	0.45	2.46	4	2
1:A:19:ARG:NH2	1:A:21:SER:OG	0.45	2.49	21	1
1:A:99:SER:OG	1:A:113:PHE:CZ	0.45	2.65	10	2
1:A:45:GLY:O	1:A:46:PHE:CD2	0.45	2.70	10	2
1:A:108:ASN:OD1	1:A:108:ASN:C	0.45	2.56	6	1
1:A:63:GLN:CB	1:A:113:PHE:CD2	0.45	3.00	1	1
1:A:65:GLY:O	1:A:66:ASP:C	0.45	2.56	10	2
1:A:63:GLN:O	1:A:113:PHE:CE1	0.45	2.70	21	1
1:A:61:MET:HG2	1:A:113:PHE:CE2	0.44	2.47	4	1
1:A:54:HIS:CG	1:A:54:HIS:O	0.44	2.69	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:63:GLN:HB2	1:A:113:PHE:HA	0.44	1.89	18	3
1:A:110:SER:OG	1:A:111:GLN:N	0.44	2.51	10	3
1:A:106:ASN:O	1:A:106:ASN:CG	0.44	2.54	8	1
1:A:147:SER:O	1:A:148:ARG:C	0.44	2.55	9	1
1:A:66:ASP:N	1:A:66:ASP:OD1	0.44	2.50	9	1
1:A:61:MET:SD	1:A:113:PHE:CZ	0.44	3.10	14	2
1:A:29:VAL:HG21	1:A:129:PHE:CB	0.44	2.42	19	1
1:A:146:GLY:O	1:A:147:SER:CB	0.44	2.66	7	1
1:A:47:GLY:O	1:A:48:TYR:HB2	0.44	2.13	8	1
1:A:112:PHE:CD1	1:A:112:PHE:N	0.44	2.86	4	1
1:A:138:ILE:HD12	1:A:138:ILE:N	0.44	2.27	3	2
1:A:52:CYS:C	1:A:53:PHE:CD2	0.44	2.91	7	2
1:A:41:THR:HA	1:A:48:TYR:CE1	0.44	2.47	11	1
1:A:85:ASP:O	1:A:86:GLU:CB	0.44	2.66	16	1
1:A:112:PHE:C	1:A:113:PHE:CD1	0.44	2.91	20	1
1:A:101:ALA:O	1:A:102:ASN:HB3	0.44	2.13	22	1
1:A:105:PRO:O	1:A:106:ASN:C	0.43	2.56	15	2
1:A:51:SER:O	1:A:52:CYS:SG	0.43	2.75	16	1
1:A:51:SER:O	1:A:52:CYS:CB	0.43	2.64	18	1
1:A:63:GLN:CB	1:A:113:PHE:HA	0.43	2.43	18	1
1:A:138:ILE:N	1:A:138:ILE:HD12	0.43	2.27	19	1
1:A:133:LYS:NZ	1:A:134:GLU:OE1	0.43	2.52	19	1
1:A:31:LYS:NZ	1:A:84:GLU:OE1	0.43	2.51	11	1
1:A:48:TYR:CZ	1:A:161:CYS:HB2	0.43	2.49	4	1
1:A:52:CYS:SG	1:A:52:CYS:O	0.43	2.76	11	1
1:A:48:TYR:O	1:A:158:ILE:HG21	0.43	2.14	2	1
1:A:34:GLU:OE1	1:A:44:LYS:NZ	0.43	2.51	3	1
1:A:43:GLU:CG	1:A:43:GLU:O	0.43	2.66	21	1
1:A:83:PHE:CZ	1:A:108:ASN:OD1	0.43	2.71	10	2
1:A:113:PHE:CZ	1:A:115:CYS:SG	0.43	3.08	22	1
1:A:43:GLU:O	1:A:44:LYS:HB3	0.43	2.12	7	1
1:A:162:GLY:O	1:A:163:GLN:CB	0.42	2.65	1	1
1:A:43:GLU:O	1:A:46:PHE:CE2	0.42	2.72	11	1
1:A:12:VAL:HG22	1:A:156:ILE:CD1	0.42	2.44	6	1
1:A:39:LEU:HD23	1:A:46:PHE:CE2	0.42	2.49	22	1
1:A:62:CYS:SG	1:A:62:CYS:O	0.42	2.76	5	1
1:A:63:GLN:OE1	1:A:64:GLY:N	0.42	2.53	12	1
1:A:39:LEU:HD23	1:A:43:GLU:CG	0.42	2.43	11	1
1:A:110:SER:O	1:A:112:PHE:N	0.42	2.51	21	1
1:A:41:THR:O	1:A:41:THR:CG2	0.42	2.66	6	1
1:A:109:GLY:O	1:A:110:SER:CB	0.42	2.67	22	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:GLU:OE2	1:A:131:LYS:NZ	0.42	2.52	4	1
1:A:39:LEU:CD2	1:A:46:PHE:CE2	0.42	3.03	22	1
1:A:151:LYS:O	1:A:152:THR:C	0.42	2.58	6	1
1:A:92:HIS:CD2	1:A:92:HIS:N	0.42	2.88	2	1
1:A:85:ASP:CG	1:A:86:GLU:N	0.42	2.71	7	1
1:A:81:GLU:OE2	1:A:82:LYS:NZ	0.42	2.53	10	1
1:A:107:THR:O	1:A:108:ASN:C	0.42	2.59	7	2
1:A:36:PHE:CE2	1:A:112:PHE:CE1	0.42	3.07	1	1
1:A:30:PRO:O	1:A:31:LYS:CB	0.41	2.68	4	1
1:A:92:HIS:CE1	1:A:128:VAL:CG2	0.41	3.03	18	1
1:A:13:ASP:OD2	1:A:155:LYS:NZ	0.41	2.52	20	1
1:A:9:ASP:C	1:A:10:ILE:HD12	0.41	2.35	21	1
1:A:61:MET:SD	1:A:61:MET:O	0.41	2.79	18	1
1:A:108:ASN:ND2	1:A:108:ASN:H	0.41	2.13	18	1
1:A:124:GLY:O	1:A:125:LYS:C	0.41	2.59	11	1
1:A:102:ASN:OD1	1:A:125:LYS:NZ	0.41	2.53	8	1
1:A:111:GLN:C	1:A:112:PHE:O	0.41	2.59	21	1
1:A:9:ASP:OD2	1:A:19:ARG:NH1	0.41	2.53	5	1
1:A:150:GLY:O	1:A:151:LYS:CG	0.41	2.68	21	1
1:A:54:HIS:N	1:A:54:HIS:CD2	0.41	2.89	10	1
1:A:61:MET:HG2	1:A:113:PHE:CZ	0.41	2.50	4	1
1:A:51:SER:OG	1:A:52:CYS:N	0.41	2.52	22	1
1:A:81:GLU:CG	1:A:81:GLU:O	0.41	2.69	22	1
1:A:49:LYS:NZ	1:A:159:ALA:O	0.41	2.52	7	1
1:A:48:TYR:O	1:A:50:GLY:N	0.41	2.54	8	1
1:A:8:PHE:CZ	1:A:10:ILE:HD11	0.41	2.50	5	1
1:A:81:GLU:OE1	1:A:82:LYS:NZ	0.40	2.53	17	1
1:A:101:ALA:O	1:A:102:ASN:HB2	0.40	2.16	2	2
1:A:12:VAL:CG2	1:A:17:LEU:HD23	0.40	2.47	15	1
1:A:62:CYS:O	1:A:63:GLN:OE1	0.40	2.39	21	1
1:A:43:GLU:C	1:A:43:GLU:CD	0.40	2.80	11	1
1:A:61:MET:HG3	1:A:113:PHE:CD2	0.40	2.51	5	1
1:A:20:VAL:O	1:A:21:SER:CB	0.40	2.69	19	1
1:A:127:VAL:HG13	1:A:129:PHE:CE1	0.40	2.52	22	1
1:A:52:CYS:O	1:A:53:PHE:HB2	0.40	2.16	22	1
1:A:34:GLU:OE2	1:A:44:LYS:NZ	0.40	2.54	15	1
1:A:92:HIS:NE2	1:A:128:VAL:CG2	0.40	2.85	21	1

## 6.3 Torsion angles

### 6.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	152/165 (92%)	122±5 (80±3%)	22±4 (14±3%)	8±3 (5±2%)	4	25
2	B	1/11 (9%)	1±0 (95±21%)	0±0 (5±21%)	0±0 (0±0%)	100	100
All	All	3366/3872 (87%)	2704 (80%)	484 (14%)	178 (5%)	4	25

All 52 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	13	ASP	12
1	A	148	ARG	10
1	A	110	SER	9
1	A	125	LYS	8
1	A	154	LYS	8
1	A	44	LYS	7
1	A	46	PHE	7
1	A	63	GLN	6
1	A	54	HIS	6
1	A	51	SER	6
1	A	65	GLY	5
1	A	109	GLY	5
1	A	152	THR	5
1	A	111	GLN	5
1	A	24	LEU	4
1	A	50	GLY	4
1	A	127	VAL	4
1	A	28	LYS	4
1	A	114	ILE	3
1	A	53	PHE	3
1	A	31	LYS	3
1	A	45	GLY	3
1	A	86	GLU	3
1	A	49	LYS	3
1	A	36	PHE	3
1	A	66	ASP	3

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Mol	Chain	Res	Type	Models (Total)
1	A	147	SER	3
1	A	42	GLY	3
1	A	52	CYS	2
1	A	21	SER	2
1	A	60	PHE	2
1	A	150	GLY	2
1	A	48	TYR	2
1	A	151	LYS	2
1	A	81	GLU	2
1	A	3	ASN	2
1	A	102	ASN	2
1	A	47	GLY	1
1	A	133	LYS	1
1	A	153	SER	1
1	A	64	GLY	1
1	A	77	SER	1
1	A	112	PHE	1
1	A	30	PRO	1
1	A	155	LYS	1
1	A	162	GLY	1
1	A	43	GLU	1
1	A	113	PHE	1
1	A	78	ILE	1
1	A	55	ARG	1
1	A	101	ALA	1
1	A	134	GLU	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	124/133 (93%)	109±3 (88±2%)	15±3 (12±2%)	11	53
2	B	1/1 (100%)	1±0 (100±0%)	0±0 (0±0%)	100	100
All	All	2750/2948 (93%)	2428 (88%)	322 (12%)	11	54

All 85 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	61	MET	19
1	A	131	LYS	11
1	A	136	MET	9
1	A	29	VAL	9
1	A	87	ASN	9
1	A	125	LYS	9
1	A	13	ASP	8
1	A	21	SER	8
1	A	49	LYS	8
1	A	55	ARG	7
1	A	78	ILE	7
1	A	63	GLN	6
1	A	144	ARG	6
1	A	44	LYS	6
1	A	108	ASN	6
1	A	140	GLU	6
1	A	151	LYS	6
1	A	48	TYR	5
1	A	152	THR	5
1	A	54	HIS	5
1	A	86	GLU	5
1	A	82	LYS	5
1	A	102	ASN	5
1	A	154	LYS	5
1	A	32	THR	5
1	A	19	ARG	5
1	A	28	LYS	5
1	A	133	LYS	4
1	A	111	GLN	4
1	A	157	THR	4
1	A	17	LEU	4
1	A	31	LYS	4
1	A	5	THR	4
1	A	62	CYS	4
1	A	116	THR	3
1	A	79	TYR	3
1	A	100	MET	3
1	A	85	ASP	3
1	A	9	ASP	3
1	A	143	GLU	3
1	A	83	PHE	3
1	A	113	PHE	3
1	A	115	CYS	3

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Mol	Chain	Res	Type	Models (Total)
1	A	106	ASN	3
1	A	126	HIS	3
1	A	43	GLU	3
1	A	119	THR	3
1	A	52	CYS	3
1	A	37	ARG	3
1	A	8	PHE	2
1	A	91	LYS	2
1	A	77	SER	2
1	A	165	GLU	2
1	A	120	GLU	2
1	A	98	LEU	2
1	A	97	ILE	2
1	A	53	PHE	2
1	A	24	LEU	2
1	A	163	GLN	2
1	A	84	GLU	2
1	A	145	PHE	2
1	A	137	ASN	2
1	A	147	SER	2
1	A	149	ASN	2
1	A	66	ASP	2
1	A	155	LYS	2
1	A	3	ASN	2
1	A	81	GLU	2
1	A	46	PHE	2
1	A	107	THR	2
1	A	51	SER	2
1	A	161	CYS	2
1	A	153	SER	1
1	A	160	ASP	1
1	A	27	ASP	1
1	A	39	LEU	1
1	A	148	ARG	1
1	A	112	PHE	1
1	A	123	ASP	1
1	A	40	SER	1
1	A	35	ASN	1
1	A	142	MET	1
1	A	34	GLU	1
1	A	6	VAL	1
1	A	118	LYS	1

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

9 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	DAL	B	201	2	1,4,5	0.81±0.01	0±0 (0±0%)
2	MLE	B	202	2	7,8,9	4.68±0.01	1±0 (14±0%)
2	MLE	B	203	2	7,8,9	4.68±0.01	1±0 (14±0%)
2	MVA	B	204	2	6,7,8	5.08±0.01	1±0 (16±0%)
2	BMT	B	205	2	11,12,13	3.95±0.01	1±0 (9±0%)
2	ABA	B	206	2	3,5,6	0.54±0.01	0±0 (0±0%)
2	SAR	B	207	2	4,4,5	8.73±0.01	1±0 (25±0%)
2	MLE	B	208	2	7,8,9	4.68±0.01	1±0 (14±0%)
2	MLE	B	210	2	7,8,9	4.69±0.01	1±0 (14±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	DAL	B	201	2	1,4,6	0.58±0.00	0±0 (0±0%)
2	MLE	B	202	2	7,9,11	0.74±0.00	0±0 (0±0%)
2	MLE	B	203	2	7,9,11	0.75±0.00	0±0 (0±0%)
2	MVA	B	204	2	6,8,10	0.77±0.01	0±0 (0±0%)
2	BMT	B	205	2	11,14,16	1.81±0.00	0±0 (0±0%)
2	ABA	B	206	2	3,5,7	1.26±0.01	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	SAR	B	207	2	2,3,5	1.52±0.01	0±0 (0±0%)
2	MLE	B	208	2	7,9,11	0.75±0.01	0±0 (0±0%)
2	MLE	B	210	2	7,9,11	0.75±0.01	0±0 (0±0%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DAL	B	201	2	-	0±0,0,2,4	0±0,0,0,0
2	MLE	B	202	2	-	0±0,4,8,10	0±0,0,0,0
2	MLE	B	203	2	-	0±0,4,8,10	0±0,0,0,0
2	MVA	B	204	2	-	0±0,5,8,10	0±0,0,0,0
2	BMT	B	205	2	-	0±0,13,16,18	0±0,0,0,0
2	ABA	B	206	2	-	0±0,2,4,6	0±0,0,0,0
2	SAR	B	207	2	-	0±0,1,2,3	0±0,0,0,0
2	MLE	B	208	2	-	0±0,4,8,10	0±0,0,0,0
2	MLE	B	210	2	-	0±0,4,8,10	0±0,0,0,0

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	207	SAR	CN-N	17.41	1.84	1.47	20	22
2	B	210	MLE	CN-N	12.33	1.81	1.46	19	22
2	B	208	MLE	CN-N	12.32	1.81	1.46	19	22
2	B	202	MLE	CN-N	12.32	1.81	1.46	12	22
2	B	205	BMT	CN-N	12.32	1.81	1.46	17	22
2	B	203	MLE	CN-N	12.31	1.81	1.46	16	22
2	B	204	MVA	CN-N	12.31	1.81	1.46	20	22

There are no bond-angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 6.5 Carbohydrates

There are no carbohydrates 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