



# Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 09:15 PM BST

PDB ID : 2HM9  
Title : Solution structure of dihydrofolate reductase complexed with trimethoprim,  
33 structures  
Authors : Polshakov, V.I.; Birdsall, B.  
Deposited on : 2006-07-11

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

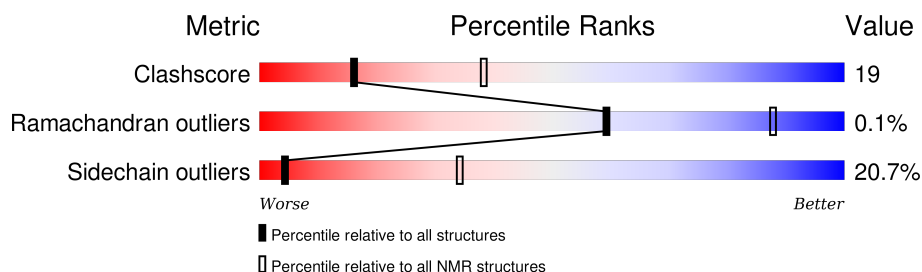
# 1 Overall quality at a glance

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	162	 59% 39% ..

## 2 Ensemble composition and analysis

This entry contains 33 models. Model 1 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:1-A:161 (161)	0.21	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 4 clusters and 2 single-model clusters were found.

Cluster number	Models
1	1, 3, 4, 6, 8, 9, 10, 12, 13, 14, 15, 24, 25, 26, 29
2	2, 7, 19, 21, 22, 30, 31, 32
3	5, 16, 17, 18, 20
4	27, 28, 33
Single-model clusters	11; 23

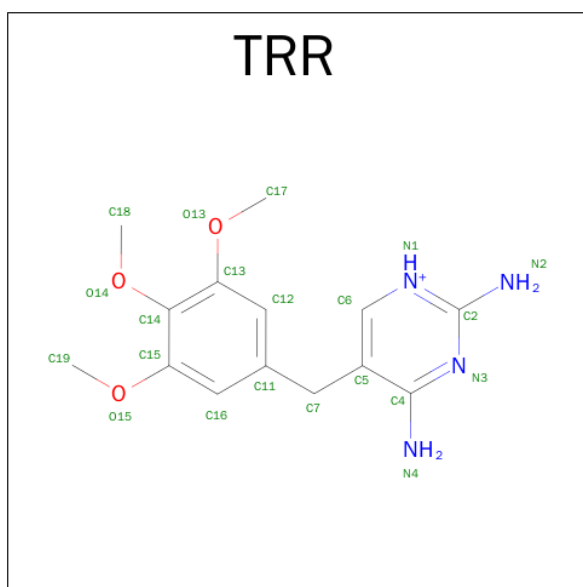
### 3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 2604 atoms, of which 1286 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Dihydrofolate reductase.

Mol	Chain	Residues	Atoms						Trace
1	A	162	Total	C	H	N	O	S	0
			2564	828	1267	225	242	2	

- Molecule 2 is 2,4-DIAMINO-5-(3,4,5-TRIMETHOXY-BENZYL)-PYRIMIDIN-1-IUM (three-letter code: TRR) (formula: C<sub>14</sub>H<sub>19</sub>N<sub>4</sub>O<sub>3</sub>).



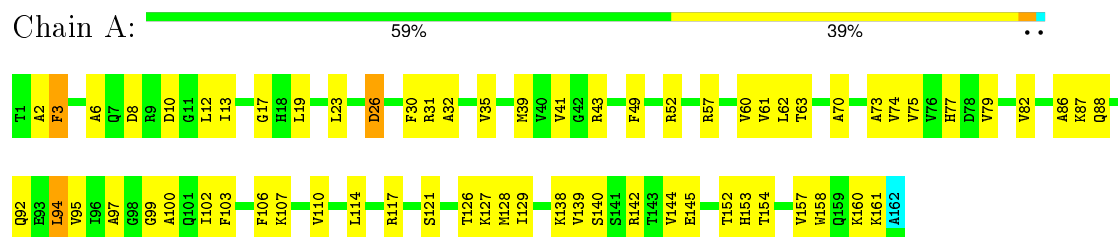
Mol	Chain	Residues	Atoms				
2	A	1	Total	C	H	N	O
			40	14	19	4	3

## 4 Residue-property plots

### 4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Dihydrofolate reductase

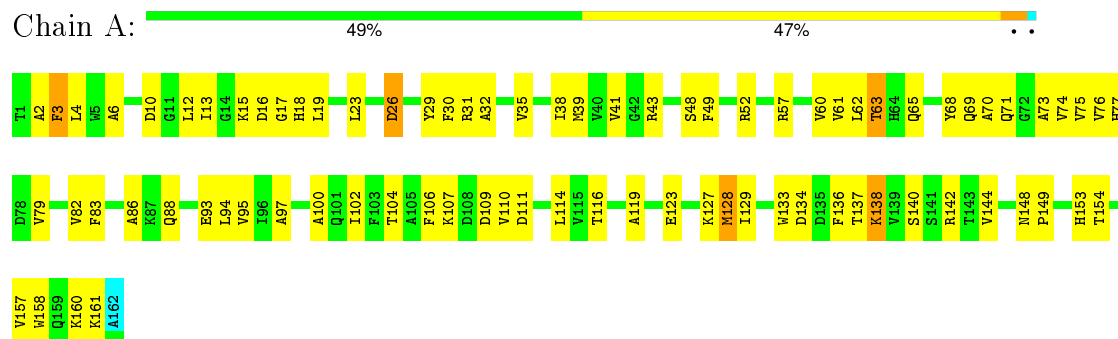


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

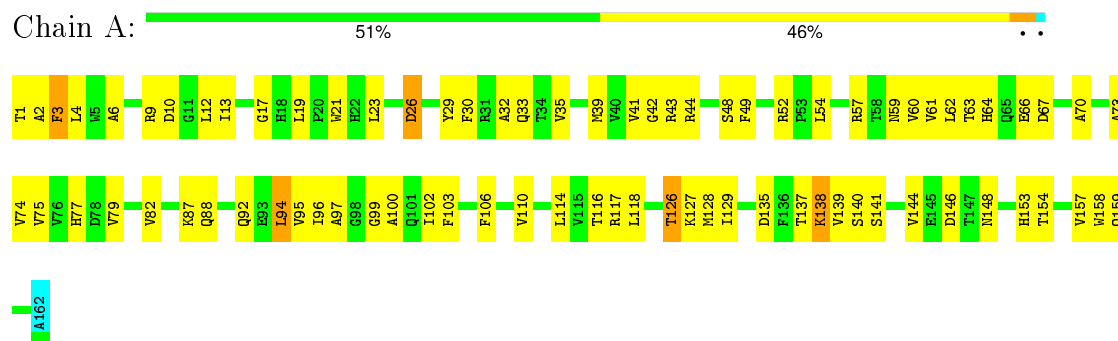
#### 4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Dihydrofolate reductase



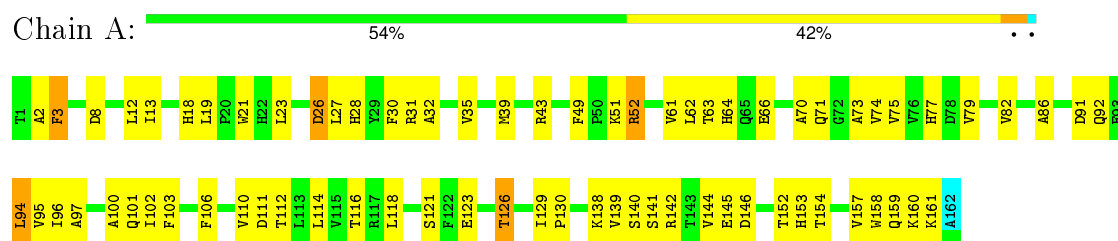
#### 4.2.2 Score per residue for model 2

- Molecule 1: Dihydrofolate reductase



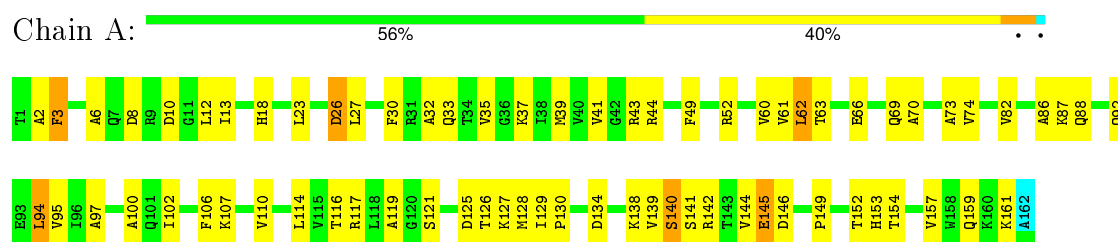
#### 4.2.3 Score per residue for model 3

- Molecule 1: Dihydrofolate reductase



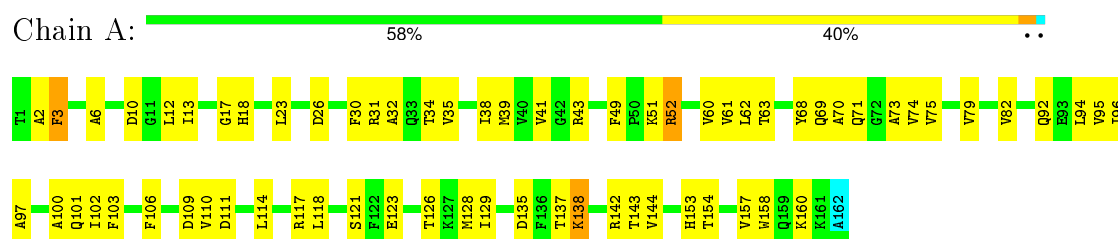
#### 4.2.4 Score per residue for model 4

- Molecule 1: Dihydrofolate reductase



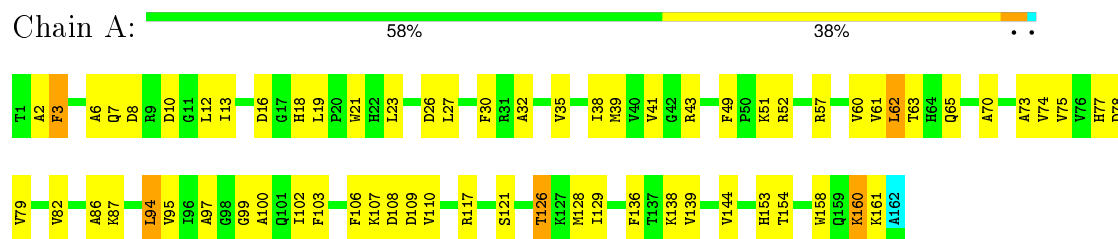
#### 4.2.5 Score per residue for model 5

- Molecule 1: Dihydrofolate reductase



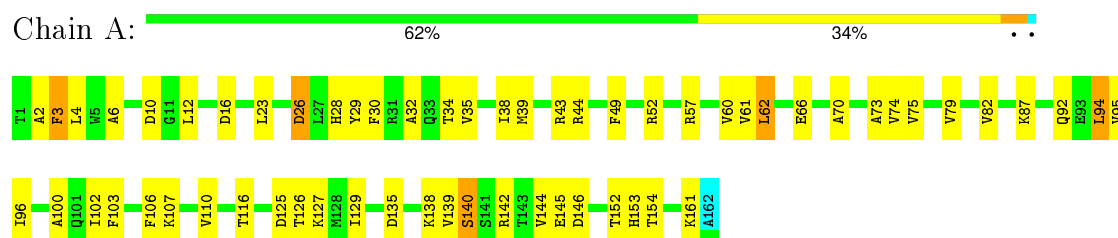
### 4.2.6 Score per residue for model 6

- Molecule 1: Dihydrofolate reductase



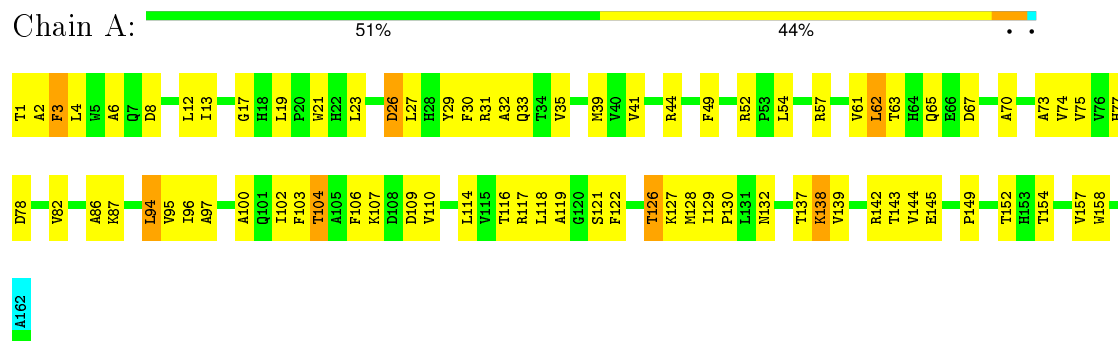
### 4.2.7 Score per residue for model 7

- Molecule 1: Dihydrofolate reductase



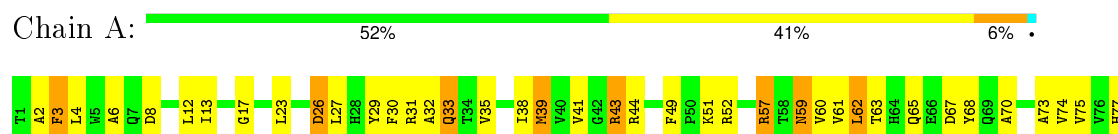
### 4.2.8 Score per residue for model 8

- Molecule 1: Dihydrofolate reductase



### 4.2.9 Score per residue for model 9

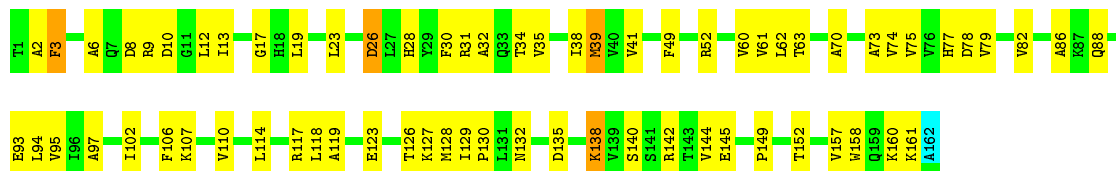
- Molecule 1: Dihydrofolate reductase





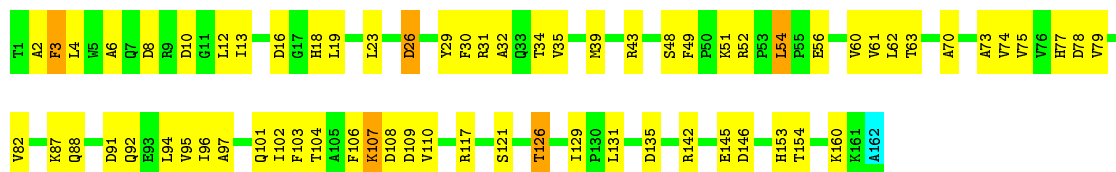
#### 4.2.10 Score per residue for model 10

- Molecule 1: Dihydrofolate reductase



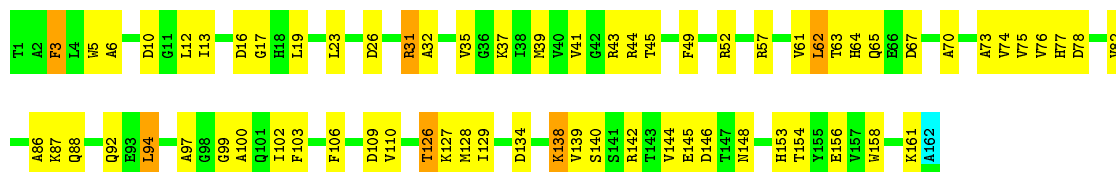
#### 4.2.11 Score per residue for model 11

- Molecule 1: Dihydrofolate reductase



#### 4.2.12 Score per residue for model 12

- Molecule 1: Dihydrofolate reductase

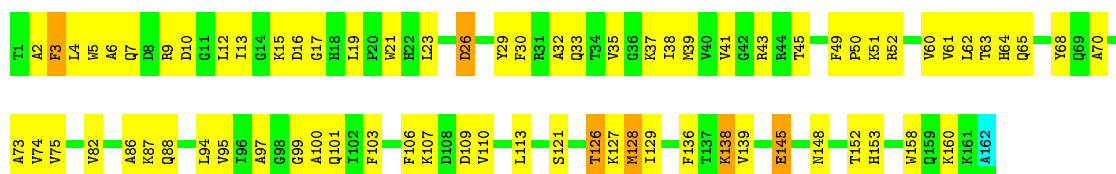


#### 4.2.13 Score per residue for model 13

- Molecule 1: Dihydrofolate reductase



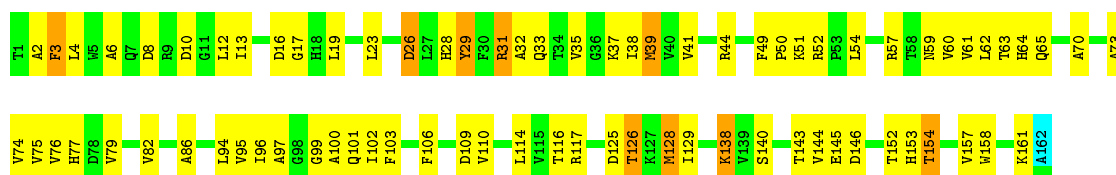




#### 4.2.14 Score per residue for model 14

- Molecule 1: Dihydrofolate reductase

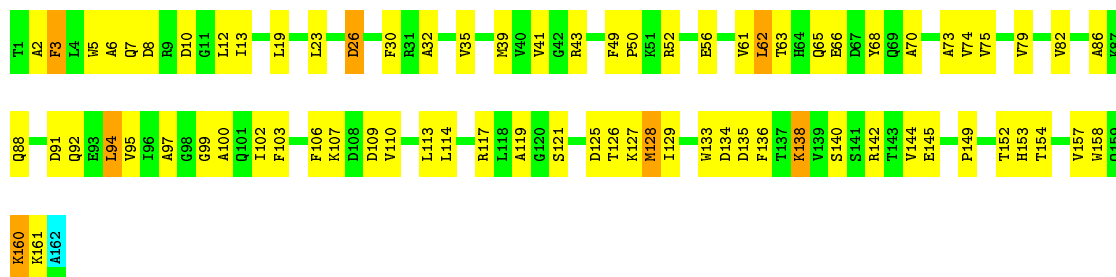
Chain A: 52% 42% 6% .



#### 4.2.15 Score per residue for model 15

- Molecule 1: Dihydrofolate reductase

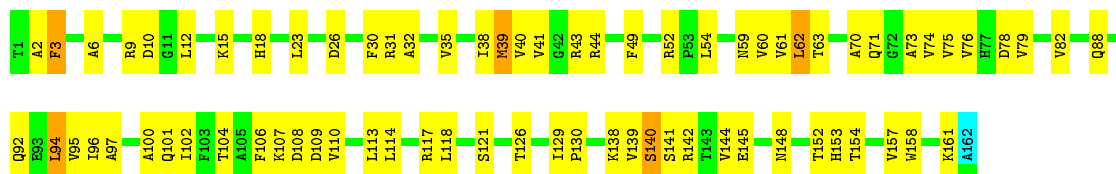
Chain A: 52% 43% . .



#### 4.2.16 Score per residue for model 16

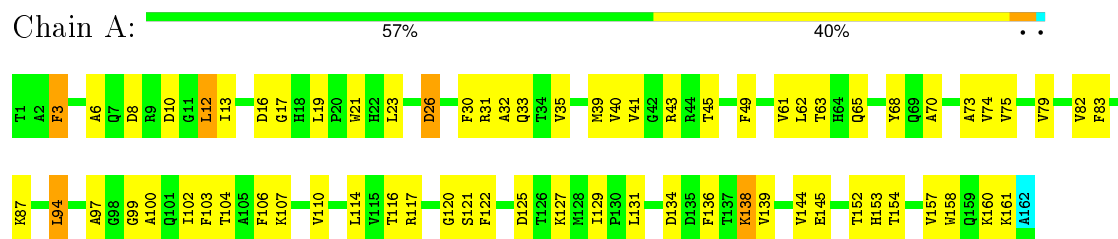
- Molecule 1: Dihydrofolate reductase

Chain A: 54% 43% . .



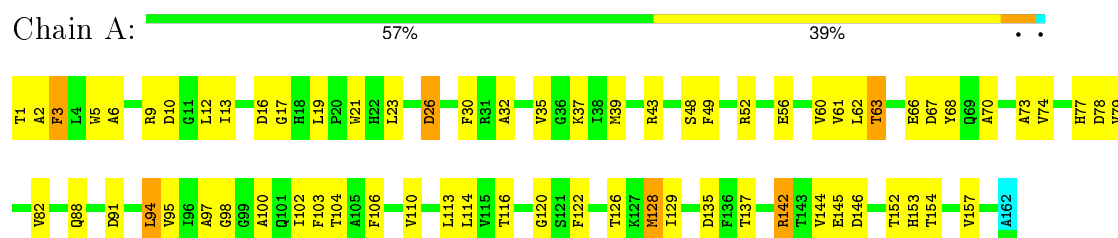
## 4.2.17 Score per residue for model 17

- Molecule 1: Dihydrofolate reductase



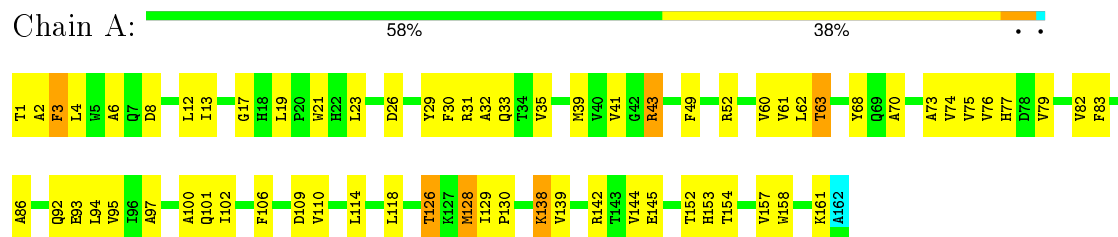
## 4.2.18 Score per residue for model 18

- Molecule 1: Dihydrofolate reductase



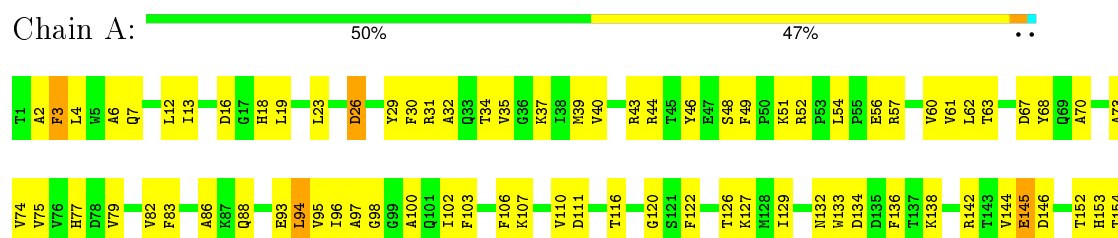
## 4.2.19 Score per residue for model 19

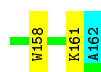
- Molecule 1: Dihydrofolate reductase



## 4.2.20 Score per residue for model 20

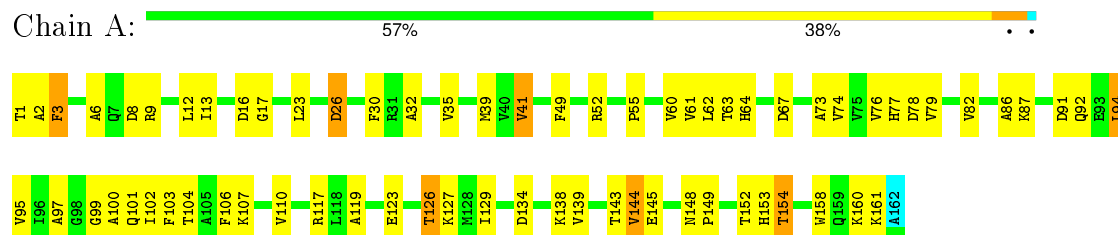
- Molecule 1: Dihydrofolate reductase





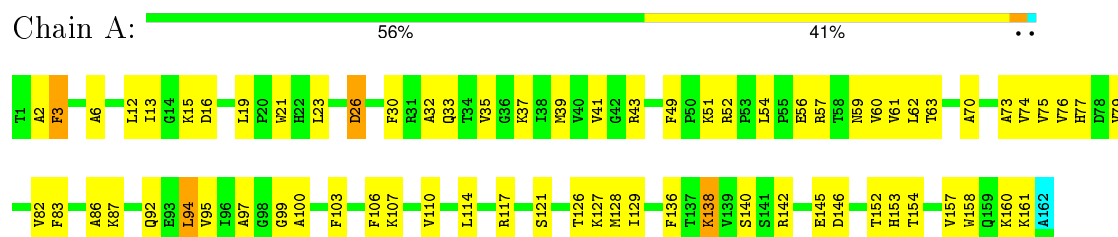
#### 4.2.21 Score per residue for model 21

- Molecule 1: Dihydrofolate reductase



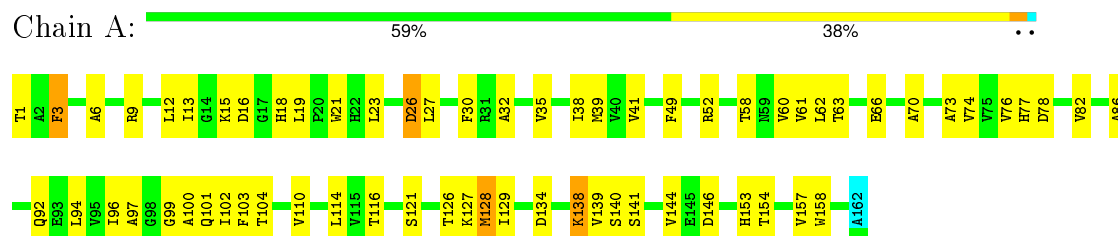
#### 4.2.22 Score per residue for model 22

- Molecule 1: Dihydrofolate reductase



#### 4.2.23 Score per residue for model 23

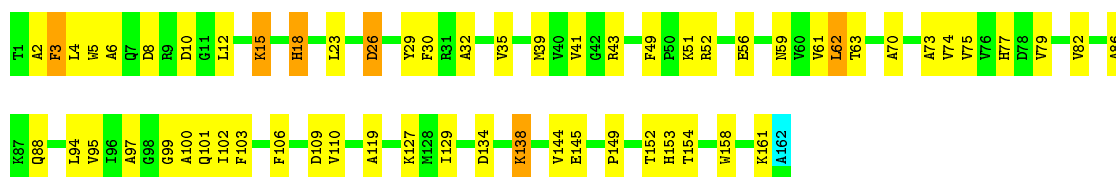
- Molecule 1: Dihydrofolate reductase



#### 4.2.24 Score per residue for model 24

- Molecule 1: Dihydrofolate reductase

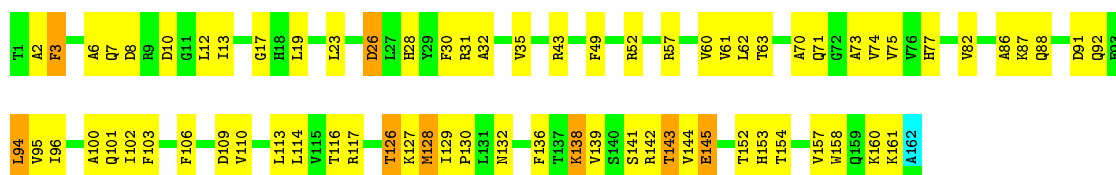




#### 4.2.25 Score per residue for model 25

- Molecule 1: Dihydrofolate reductase

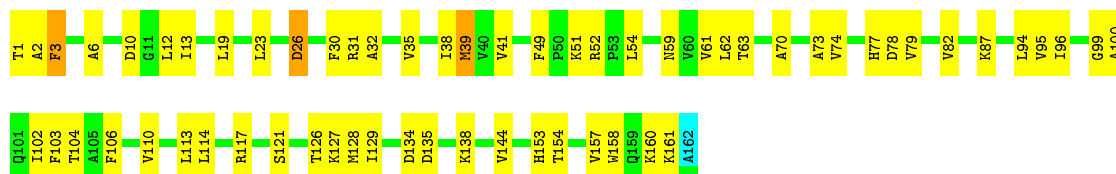
Chain A: 55% 40% 5% .



#### 4.2.26 Score per residue for model 26

- Molecule 1: Dihydrofolate reductase

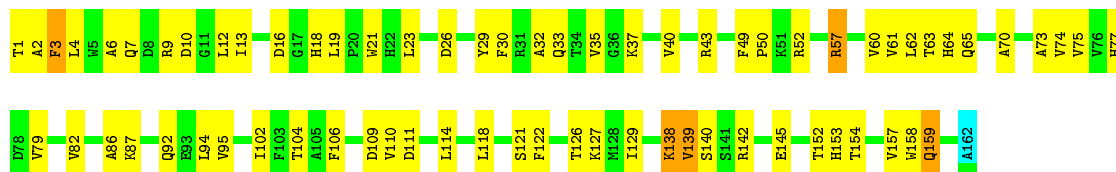
Chain A: 62% 36% . .



#### 4.2.27 Score per residue for model 27

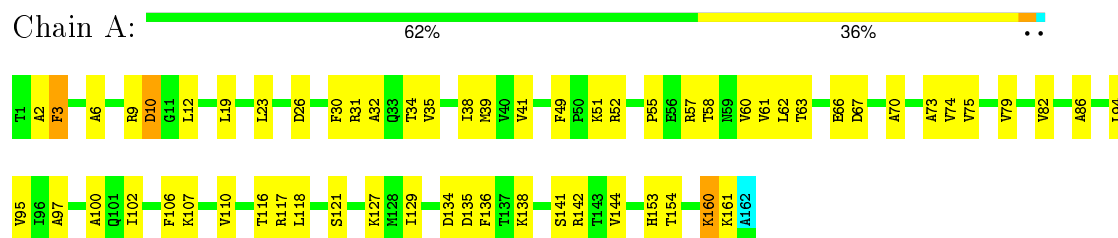
- Molecule 1: Dihydrofolate reductase

Chain A: 56% 40% . .



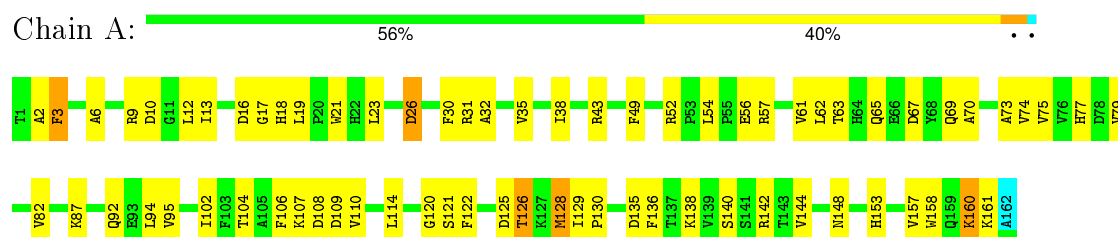
#### 4.2.28 Score per residue for model 28

- Molecule 1: Dihydrofolate reductase



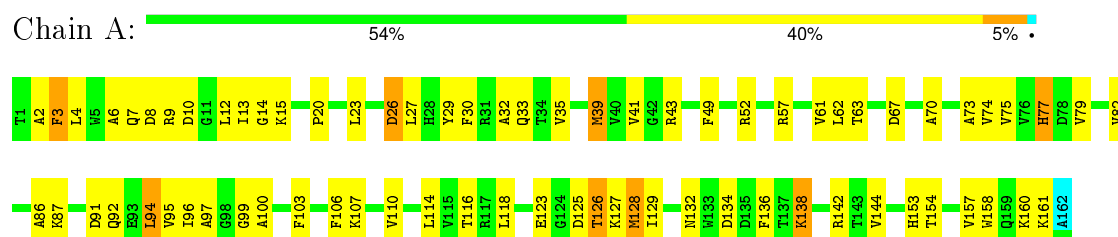
#### 4.2.29 Score per residue for model 29

- Molecule 1: Dihydrofolate reductase



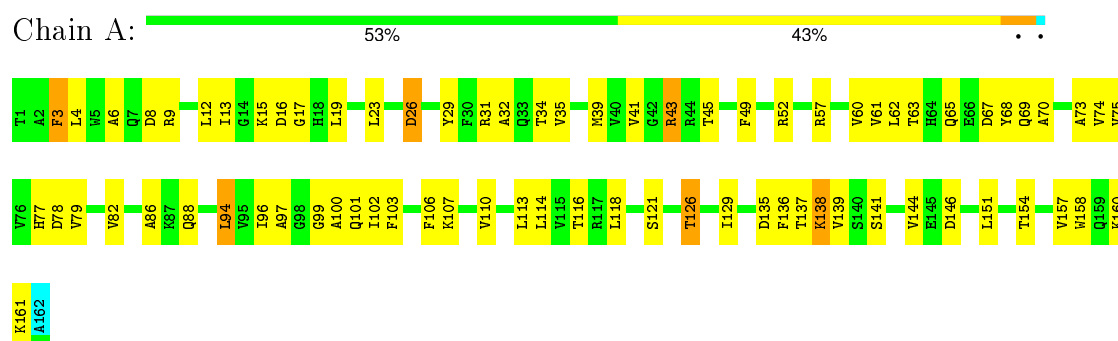
#### 4.2.30 Score per residue for model 30

- Molecule 1: Dihydrofolate reductase



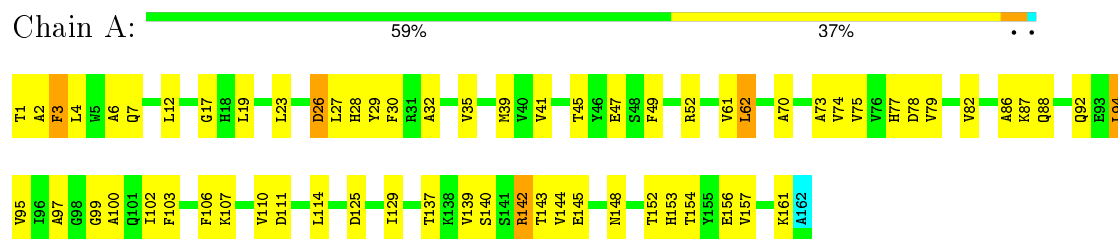
#### 4.2.31 Score per residue for model 31

- Molecule 1: Dihydrofolate reductase



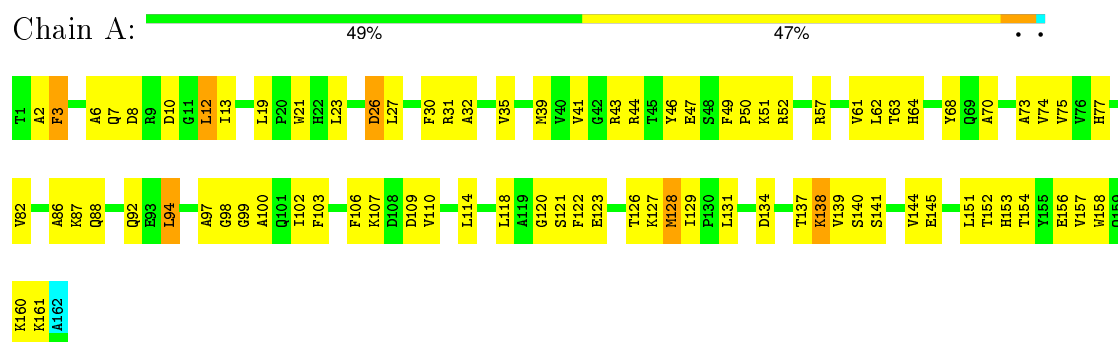
### 4.2.32 Score per residue for model 32

- Molecule 1: Dihydrofolate reductase



### 4.2.33 Score per residue for model 33

- Molecule 1: Dihydrofolate reductase



## 5 Refinement protocol and experimental data overview

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

Of the 33 calculated structures, 33 were deposited, based on the following criterion: *all calculated structures submitted*.

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

Software name	Classification	Version
XPLOR-NIH	refinement	3.11
CNS	refinement	1.0

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: TRR

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	1291	1262	1255	47±6
2	A	21	19	19	5±2
All	All	43296	42273	42042	1593

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 19.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:61:VAL:HG23	1:A:73:ALA:HB3	1.13	1.17	23	33
1:A:100:ALA:HB1	1:A:129:ILE:HG23	1.05	1.24	9	29
1:A:41:VAL:HG12	1:A:97:ALA:HB3	0.96	1.37	15	21
1:A:86:ALA:HB2	1:A:94:LEU:HD13	0.94	1.36	31	24
1:A:62:LEU:HD23	1:A:102:ILE:HD12	0.93	1.40	7	9
1:A:3:PHE:CE1	1:A:110:VAL:HG21	0.91	2.00	29	33
1:A:2:ALA:HB3	1:A:95:VAL:HG22	0.85	1.42	2	28
1:A:23:LEU:HD22	1:A:118:LEU:HD21	0.83	1.50	27	12
1:A:61:VAL:HG21	1:A:70:ALA:HB1	0.83	1.49	25	21
1:A:41:VAL:HG12	1:A:97:ALA:CB	0.83	2.03	2	18
1:A:61:VAL:CG2	1:A:73:ALA:HB3	0.82	2.03	18	33

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:13:ILE:HD11	1:A:126:THR:HG22	0.81	1.50	15	23
1:A:3:PHE:CD1	1:A:110:VAL:HG21	0.81	2.11	11	33
1:A:6:ALA:HB2	2:A:170:TRR:N2	0.80	1.92	7	32
1:A:61:VAL:HG23	1:A:73:ALA:CB	0.79	2.06	25	33
1:A:106:PHE:O	1:A:110:VAL:HG23	0.79	1.78	22	28
1:A:23:LEU:HD21	1:A:153:HIS:CE1	0.78	2.12	11	17
1:A:1:THR:HG23	1:A:94:LEU:HD23	0.77	1.56	27	3
1:A:32:ALA:O	1:A:35:VAL:HG22	0.77	1.79	7	33
1:A:62:LEU:CD2	1:A:102:ILE:HD12	0.75	2.12	28	12
1:A:62:LEU:HD13	1:A:82:VAL:HG21	0.75	1.57	4	6
1:A:100:ALA:HB1	1:A:129:ILE:CG2	0.74	2.10	9	16
1:A:61:VAL:HG11	1:A:70:ALA:CB	0.74	2.13	11	29
1:A:61:VAL:HG11	1:A:70:ALA:HB2	0.73	1.60	24	23
1:A:13:ILE:HD11	1:A:126:THR:CG2	0.73	2.13	23	23
1:A:23:LEU:HD23	1:A:26:ASP:HB3	0.73	1.59	20	23
1:A:19:LEU:HB2	2:A:170:TRR:H183	0.72	1.61	10	7
1:A:70:ALA:HB3	1:A:75:VAL:HG22	0.72	1.61	15	6
1:A:26:ASP:OD2	1:A:116:THR:HG21	0.72	1.85	20	14
1:A:114:LEU:HD23	1:A:157:VAL:HG13	0.71	1.60	2	14
1:A:39:MET:SD	1:A:97:ALA:HB2	0.69	2.27	5	21
1:A:23:LEU:HD23	1:A:26:ASP:CB	0.69	2.18	20	21
1:A:62:LEU:CD1	1:A:82:VAL:HG21	0.69	2.18	19	32
1:A:129:ILE:HD12	1:A:130:PRO:O	0.69	1.88	10	8
1:A:54:LEU:HD22	1:A:57:ARG:CZ	0.69	2.16	20	2
1:A:70:ALA:HB3	1:A:75:VAL:CG2	0.68	2.17	15	12
1:A:23:LEU:HD21	1:A:153:HIS:ND1	0.67	2.04	13	27
1:A:3:PHE:CE1	1:A:96:ILE:HD13	0.67	2.25	23	3
1:A:62:LEU:HD22	1:A:102:ILE:CD1	0.66	2.20	27	6
1:A:61:VAL:HG21	1:A:70:ALA:CB	0.66	2.20	26	19
1:A:62:LEU:HD12	1:A:82:VAL:HG21	0.65	1.68	19	11
1:A:107:LYS:HD2	1:A:131:LEU:HD23	0.65	1.67	11	2
1:A:1:THR:CG2	1:A:110:VAL:HG22	0.65	2.20	26	4
1:A:17:GLY:O	2:A:170:TRR:H191	0.65	1.92	12	17
1:A:62:LEU:HD22	1:A:102:ILE:HD12	0.65	1.69	26	12
1:A:104:THR:HG23	1:A:129:ILE:HG21	0.64	1.68	26	2
1:A:104:THR:CG2	1:A:129:ILE:HG21	0.63	2.23	26	2
1:A:76:VAL:HG21	1:A:82:VAL:HG22	0.63	1.71	1	8
1:A:19:LEU:HD12	2:A:170:TRR:C16	0.62	2.24	15	6
1:A:39:MET:SD	1:A:41:VAL:HG13	0.61	2.35	26	5
1:A:70:ALA:HB3	1:A:75:VAL:HG23	0.61	1.71	27	7
1:A:19:LEU:HD12	2:A:170:TRR:C13	0.61	2.25	3	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:26:ASP:OD1	1:A:116:THR:HG21	0.61	1.95	8	2
1:A:79:VAL:HG13	1:A:106:PHE:CE1	0.60	2.31	2	23
1:A:54:LEU:HD12	1:A:59:ASN:ND2	0.60	2.12	22	3
1:A:104:THR:OG1	1:A:129:ILE:HG21	0.59	1.97	11	5
1:A:142:ARG:O	1:A:154:THR:HG23	0.59	1.97	32	11
1:A:68:TYR:CE1	1:A:70:ALA:HB2	0.59	2.31	18	1
1:A:104:THR:HG22	1:A:129:ILE:HD13	0.59	1.73	26	1
1:A:23:LEU:HD11	1:A:151:LEU:O	0.59	1.96	31	2
1:A:13:ILE:HG23	1:A:128:MET:HB2	0.59	1.74	14	17
1:A:63:THR:HG23	1:A:77:HIS:ND1	0.59	2.13	10	21
1:A:79:VAL:HG13	1:A:106:PHE:CZ	0.58	2.34	19	19
1:A:62:LEU:HD13	1:A:82:VAL:CG2	0.57	2.29	7	3
1:A:19:LEU:HD12	2:A:170:TRR:C15	0.57	2.29	1	8
1:A:139:VAL:HG11	1:A:159:GLN:HG3	0.57	1.75	2	2
1:A:18:HIS:HA	2:A:170:TRR:H191	0.56	1.76	6	7
1:A:62:LEU:HD12	1:A:82:VAL:CG2	0.56	2.31	25	14
1:A:114:LEU:HD23	1:A:157:VAL:HG22	0.56	1.78	14	9
1:A:19:LEU:HD12	2:A:170:TRR:C14	0.56	2.31	28	6
1:A:19:LEU:HD22	1:A:21:TRP:NE1	0.55	2.15	6	4
1:A:4:LEU:HD11	1:A:29:TYR:CE2	0.55	2.35	1	13
1:A:3:PHE:HE1	1:A:96:ILE:HD13	0.55	1.62	11	3
1:A:102:ILE:HD13	1:A:102:ILE:N	0.55	2.16	9	5
1:A:38:ILE:CG2	1:A:94:LEU:HD12	0.55	2.31	13	13
1:A:35:VAL:HG12	1:A:57:ARG:NE	0.54	2.18	9	1
1:A:54:LEU:HD13	1:A:57:ARG:NH2	0.54	2.17	29	1
1:A:41:VAL:CG1	1:A:97:ALA:HB3	0.53	2.25	15	2
1:A:3:PHE:CE1	1:A:96:ILE:HD12	0.53	2.38	31	2
1:A:35:VAL:HG12	1:A:57:ARG:NH1	0.53	2.18	30	9
1:A:19:LEU:HD13	1:A:27:LEU:CD2	0.53	2.34	3	1
2:A:170:TRR:O13	2:A:170:TRR:H183	0.53	2.03	28	3
1:A:145:GLU:HA	1:A:152:THR:HG23	0.53	1.80	3	21
1:A:4:LEU:HD11	1:A:29:TYR:CE1	0.52	2.39	14	1
2:A:170:TRR:H183	2:A:170:TRR:O13	0.52	2.04	22	6
1:A:143:THR:HG23	1:A:154:THR:OG1	0.52	2.04	14	6
1:A:102:ILE:N	1:A:102:ILE:HD13	0.52	2.20	12	3
1:A:63:THR:HG21	1:A:68:TYR:HB3	0.52	1.82	13	5
1:A:100:ALA:CB	1:A:129:ILE:HG23	0.52	2.17	9	4
1:A:104:THR:HG23	1:A:129:ILE:HD13	0.52	1.81	8	1
1:A:70:ALA:N	1:A:75:VAL:HG21	0.51	2.20	27	6
2:A:170:TRR:H183	2:A:170:TRR:O15	0.51	2.04	26	3
1:A:23:LEU:HD21	1:A:153:HIS:CG	0.51	2.41	21	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:61:VAL:CG2	1:A:70:ALA:HB1	0.51	2.30	25	1
1:A:61:VAL:N	1:A:74:VAL:O	0.51	2.43	1	33
1:A:60:VAL:HG13	1:A:74:VAL:O	0.51	2.06	22	22
1:A:19:LEU:HD22	1:A:21:TRP:CZ2	0.51	2.41	23	3
2:A:170:TRR:H182	2:A:170:TRR:O13	0.50	2.06	25	2
1:A:3:PHE:HE1	1:A:96:ILE:HD12	0.50	1.66	31	1
1:A:30:PHE:CD1	2:A:170:TRR:C4	0.50	2.95	23	30
2:A:170:TRR:O15	2:A:170:TRR:H183	0.50	2.06	33	3
1:A:35:VAL:HG12	1:A:57:ARG:CZ	0.50	2.37	9	2
1:A:138:LYS:N	1:A:158:TRP:CE3	0.50	2.80	15	23
1:A:79:VAL:CG1	1:A:106:PHE:CE1	0.50	2.94	17	12
1:A:33:GLN:NE2	1:A:114:LEU:HD13	0.49	2.22	9	1
2:A:170:TRR:O13	2:A:170:TRR:H182	0.49	2.06	16	5
1:A:35:VAL:HG12	1:A:57:ARG:HD3	0.49	1.82	2	1
1:A:54:LEU:HD12	1:A:59:ASN:HD21	0.49	1.67	22	3
1:A:70:ALA:H	1:A:75:VAL:HG21	0.49	1.67	15	6
1:A:144:VAL:HG23	1:A:153:HIS:O	0.49	2.08	21	6
1:A:3:PHE:CE1	1:A:110:VAL:CG2	0.49	2.94	23	5
1:A:54:LEU:HD23	1:A:54:LEU:N	0.49	2.23	8	1
1:A:62:LEU:HD22	1:A:102:ILE:HG23	0.49	1.83	16	1
1:A:63:THR:HG23	1:A:77:HIS:HD1	0.48	1.68	14	3
1:A:2:ALA:HB3	1:A:95:VAL:CG2	0.48	2.35	16	3
1:A:63:THR:CG2	1:A:77:HIS:CE1	0.48	2.96	20	14
1:A:99:GLY:O	1:A:103:PHE:CD2	0.48	2.67	14	17
1:A:62:LEU:HD23	1:A:102:ILE:CD1	0.48	2.34	4	1
1:A:35:VAL:HG23	1:A:35:VAL:O	0.48	2.09	9	14
1:A:61:VAL:O	1:A:75:VAL:HA	0.47	2.09	14	24
1:A:54:LEU:N	1:A:54:LEU:HD23	0.47	2.24	11	1
1:A:75:VAL:CG1	1:A:77:HIS:CE1	0.47	2.98	32	4
1:A:30:PHE:CD1	2:A:170:TRR:C5	0.47	2.98	3	5
1:A:35:VAL:O	1:A:35:VAL:HG23	0.47	2.09	4	19
1:A:13:ILE:HG23	1:A:128:MET:CB	0.47	2.40	14	4
1:A:128:MET:CE	1:A:131:LEU:HD11	0.47	2.40	33	1
1:A:34:THR:HG21	1:A:39:MET:SD	0.47	2.50	28	5
1:A:136:PHE:CE2	1:A:160:LYS:CG	0.47	2.98	6	6
1:A:27:LEU:N	1:A:27:LEU:HD23	0.46	2.25	8	3
1:A:31:ARG:O	1:A:35:VAL:HG13	0.46	2.10	12	7
1:A:40:VAL:HB	1:A:96:ILE:HD13	0.46	1.86	20	2
1:A:139:VAL:HG23	1:A:140:SER:N	0.46	2.25	2	5
1:A:35:VAL:HG12	1:A:57:ARG:NH2	0.46	2.25	9	2
1:A:38:ILE:HG22	1:A:94:LEU:HD12	0.46	1.88	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:113:LEU:HD11	1:A:136:PHE:CD2	0.46	2.46	25	4
1:A:64:HIS:CD2	1:A:65:GLN:N	0.46	2.85	13	1
1:A:27:LEU:HD23	1:A:27:LEU:N	0.45	2.26	4	4
1:A:3:PHE:HB2	1:A:113:LEU:HD23	0.45	1.88	26	2
1:A:19:LEU:HD22	1:A:21:TRP:CE2	0.45	2.46	13	2
1:A:75:VAL:O	1:A:75:VAL:HG12	0.45	2.11	1	4
1:A:19:LEU:CD2	1:A:21:TRP:CZ2	0.45	2.99	23	5
1:A:23:LEU:HD23	1:A:26:ASP:HB2	0.45	1.89	1	1
1:A:77:HIS:N	1:A:77:HIS:CD2	0.45	2.85	26	1
1:A:27:LEU:HD22	2:A:170:TRR:C13	0.44	2.42	23	1
1:A:139:VAL:HG21	1:A:159:GLN:HG3	0.44	1.89	27	1
1:A:2:ALA:N	1:A:94:LEU:O	0.44	2.50	18	5
1:A:21:TRP:HB3	1:A:122:PHE:CE2	0.44	2.47	17	4
1:A:62:LEU:HD22	1:A:102:ILE:HD11	0.44	1.89	11	1
1:A:120:GLY:O	1:A:122:PHE:CE1	0.44	2.71	33	5
1:A:41:VAL:HG21	1:A:52:ARG:HH12	0.44	1.73	5	1
1:A:75:VAL:HG12	1:A:75:VAL:O	0.44	2.12	19	6
1:A:40:VAL:HG21	1:A:94:LEU:HD21	0.44	1.89	17	1
1:A:96:ILE:HG23	1:A:102:ILE:CG2	0.43	2.43	14	1
1:A:119:ALA:HB3	1:A:149:PRO:O	0.43	2.12	8	8
1:A:138:LYS:CD	1:A:158:TRP:CZ2	0.43	3.01	14	2
1:A:98:GLY:HA2	1:A:103:PHE:CE2	0.43	2.49	18	2
1:A:62:LEU:CD1	1:A:82:VAL:CG2	0.43	2.95	7	2
1:A:96:ILE:O	1:A:103:PHE:CE1	0.43	2.72	8	6
1:A:136:PHE:CD1	1:A:136:PHE:N	0.43	2.87	30	2
1:A:75:VAL:HG13	1:A:77:HIS:CE1	0.43	2.49	1	2
1:A:46:TYR:CD2	1:A:68:TYR:OH	0.43	2.70	33	2
1:A:68:TYR:HE1	1:A:70:ALA:HB2	0.43	1.72	18	1
1:A:15:LYS:O	1:A:18:HIS:CE1	0.43	2.71	16	1
2:A:170:TRR:C12	2:A:170:TRR:H6	0.42	2.44	9	4
1:A:2:ALA:CB	1:A:95:VAL:HG22	0.42	2.36	16	2
1:A:110:VAL:HG11	1:A:113:LEU:HD23	0.42	1.90	18	1
1:A:43:ARG:CG	1:A:68:TYR:CZ	0.42	3.02	31	2
1:A:139:VAL:HG11	1:A:159:GLN:CG	0.42	2.45	3	2
1:A:96:ILE:HG23	1:A:102:ILE:HG22	0.42	1.91	2	2
1:A:19:LEU:HD11	2:A:170:TRR:C6	0.42	2.45	27	3
1:A:104:THR:CG2	1:A:129:ILE:HD13	0.42	2.41	26	1
1:A:59:ASN:O	1:A:73:ALA:HA	0.42	2.15	9	1
1:A:113:LEU:CD1	1:A:136:PHE:CD2	0.42	3.03	25	2
1:A:15:LYS:O	1:A:18:HIS:CD2	0.42	2.73	24	2
1:A:83:PHE:CE2	1:A:106:PHE:CD1	0.41	3.08	1	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:170:TRR:H6	2:A:170:TRR:C12	0.41	2.45	22	4
1:A:133:TRP:O	1:A:136:PHE:O	0.41	2.39	20	3
1:A:63:THR:HG23	1:A:77:HIS:CE1	0.41	2.51	19	1
1:A:104:THR:HG1	1:A:129:ILE:HG21	0.41	1.74	16	1
1:A:3:PHE:CZ	1:A:103:PHE:O	0.41	2.73	11	1
1:A:43:ARG:CG	1:A:68:TYR:CE2	0.41	3.04	9	1
1:A:1:THR:O	1:A:110:VAL:HG13	0.41	2.15	23	1
1:A:18:HIS:O	1:A:18:HIS:CG	0.41	2.73	3	1
1:A:4:LEU:CD2	1:A:30:PHE:CD1	0.41	3.04	27	1
1:A:139:VAL:CG2	1:A:140:SER:N	0.41	2.84	4	1
1:A:9:ARG:CG	1:A:10:ASP:N	0.41	2.83	28	1
1:A:1:THR:OG1	1:A:83:PHE:CE1	0.41	2.74	19	1
1:A:98:GLY:HA3	1:A:103:PHE:CE2	0.41	2.51	33	1
1:A:42:GLY:CA	1:A:102:ILE:CG1	0.41	2.98	2	1
1:A:95:VAL:HG12	1:A:96:ILE:N	0.41	2.31	2	1
1:A:83:PHE:CE2	1:A:106:PHE:CE1	0.41	3.09	20	3
1:A:21:TRP:CB	1:A:122:PHE:CZ	0.41	3.03	8	1
1:A:61:VAL:CB	1:A:70:ALA:CB	0.41	2.99	27	1
1:A:52:ARG:CD	1:A:52:ARG:N	0.41	2.84	3	1
1:A:35:VAL:O	1:A:35:VAL:CG2	0.41	2.69	32	2
1:A:8:ASP:OD1	1:A:12:LEU:N	0.41	2.53	17	2
1:A:35:VAL:CG1	1:A:57:ARG:NH2	0.41	2.84	27	1
1:A:60:VAL:CG1	1:A:74:VAL:O	0.40	2.69	5	2
1:A:1:THR:HG21	1:A:110:VAL:HG22	0.40	1.92	26	1
1:A:103:PHE:O	1:A:107:LYS:N	0.40	2.55	30	1
1:A:14:GLY:CA	1:A:20:PRO:CD	0.40	3.00	30	1
1:A:55:PRO:O	1:A:57:ARG:NE	0.40	2.54	28	1
1:A:34:THR:HG21	1:A:39:MET:CE	0.40	2.46	10	1
1:A:58:THR:HG22	1:A:58:THR:O	0.40	2.16	28	1
1:A:13:ILE:O	1:A:21:TRP:CH2	0.40	2.74	22	2
1:A:138:LYS:HD3	1:A:158:TRP:CZ2	0.40	2.52	27	1
1:A:29:TYR:CE1	1:A:33:GLN:OE1	0.40	2.75	27	1
1:A:60:VAL:CA	1:A:73:ALA:HB1	0.40	2.46	7	1
1:A:82:VAL:HB	1:A:106:PHE:CZ	0.40	2.52	28	1
1:A:41:VAL:O	1:A:41:VAL:HG23	0.40	2.16	19	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	160/162 (99%)	157±1 (98±1%)	3±1 (2±1%)	0±0 (0±0%)	59	88
All	All	5280/5346 (99%)	5183 (98%)	91 (2%)	6 (0%)	59	88

All 2 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	50	PRO	5
1	A	55	PRO	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	137/137 (100%)	109±4 (79±3%)	28±4 (21±3%)	4	34
All	All	4521/4521 (100%)	3584 (79%)	937 (21%)	4	34

All 83 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	12	LEU	33
1	A	3	PHE	33
1	A	49	PHE	33
1	A	26	ASP	32
1	A	52	ARG	32
1	A	43	ARG	25
1	A	161	LYS	25
1	A	144	VAL	24

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Mol	Chain	Res	Type	Models (Total)
1	A	10	ASP	23
1	A	138	LYS	23
1	A	127	LYS	22
1	A	94	LEU	20
1	A	92	GLN	19
1	A	121	SER	19
1	A	154	THR	19
1	A	87	LYS	19
1	A	107	LYS	18
1	A	88	GLN	17
1	A	126	THR	17
1	A	160	LYS	17
1	A	117	ARG	17
1	A	128	MET	16
1	A	109	ASP	16
1	A	16	ASP	16
1	A	140	SER	15
1	A	8	ASP	15
1	A	31	ARG	14
1	A	134	ASP	13
1	A	51	LYS	13
1	A	78	ASP	13
1	A	139	VAL	13
1	A	146	ASP	12
1	A	101	GLN	12
1	A	142	ARG	12
1	A	65	GLN	11
1	A	135	ASP	11
1	A	67	ASP	11
1	A	9	ARG	11
1	A	62	LEU	10
1	A	44	ARG	10
1	A	33	GLN	10
1	A	141	SER	10
1	A	7	GLN	9
1	A	63	THR	8
1	A	66	GLU	8
1	A	148	ASN	8
1	A	37	LYS	8
1	A	125	ASP	8
1	A	39	MET	8
1	A	137	THR	8

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Mol	Chain	Res	Type	Models (Total)
1	A	123	GLU	7
1	A	91	ASP	7
1	A	56	GLU	7
1	A	64	HIS	7
1	A	111	ASP	7
1	A	145	GLU	7
1	A	28	HIS	6
1	A	15	LYS	6
1	A	69	GLN	5
1	A	71	GLN	5
1	A	5	TRP	5
1	A	45	THR	5
1	A	48	SER	5
1	A	132	ASN	5
1	A	57	ARG	4
1	A	108	ASP	4
1	A	93	GLU	4
1	A	104	THR	4
1	A	156	GLU	3
1	A	41	VAL	2
1	A	18	HIS	2
1	A	47	GLU	2
1	A	59	ASN	2
1	A	159	GLN	1
1	A	143	THR	1
1	A	29	TYR	1
1	A	1	THR	1
1	A	58	THR	1
1	A	112	THR	1
1	A	54	LEU	1
1	A	40	VAL	1
1	A	34	THR	1
1	A	77	HIS	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

1 ligand is 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	TRR	A	170	-	22,22,22	1.51±0.12	0±0 (0±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	TRR	A	170	-	30,30,30	1.52±0.07	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	TRR	A	170	-	-	0±0,10,10,10	0±0,2,2,2

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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