



Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2026 – 12:27 AM UTC

PDB ID : 2L28 / pdb_00002l28
BMRB ID : 17125
Title : Solution structure of lactobacillus casei dihydrofolate reductase apo-form, 25 conformers
Authors : Polshakov, V.I.; Birdsall, B.; Feeney, J.
Deposited on : 2010-08-13

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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

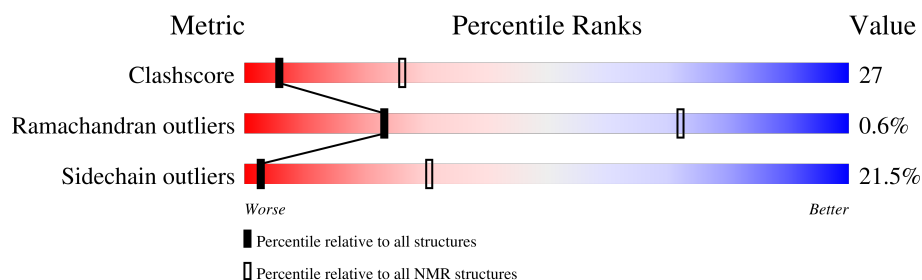
1 Overall quality at a glance

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	162	41% 40% • 14%

2 Ensemble composition and analysis

This entry contains 25 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:13, A:37-A:162 (139)	0.65	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 5 clusters and 1 single-model cluster was found.

Cluster number	Models
1	1, 4, 5, 6, 9, 10, 11, 12, 16, 19, 20, 21, 24
2	14, 18, 22
3	2, 8, 13
4	3, 17, 23
5	15, 25
Single-model clusters	7

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 2564 atoms, of which 1267 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Dihydrofolate reductase.

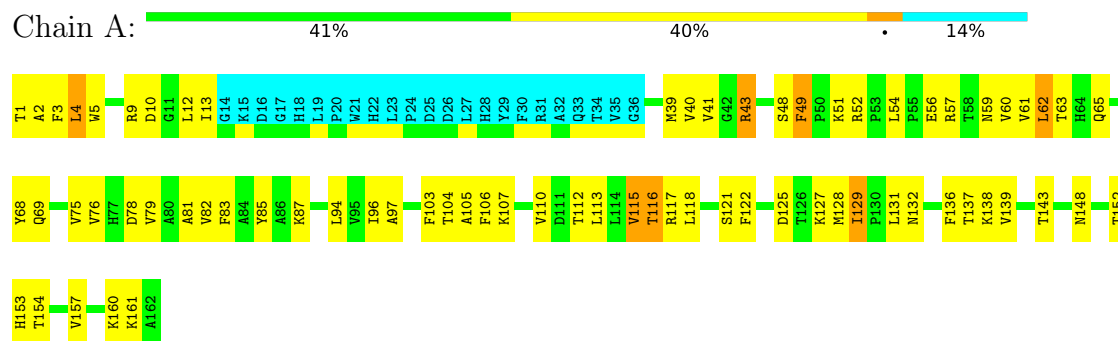
Mol	Chain	Residues	Atoms						Trace
1	A	162	Total	C	H	N	O	S	0
			2564	828	1267	225	242	2	

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: Dihydrofolate reductase

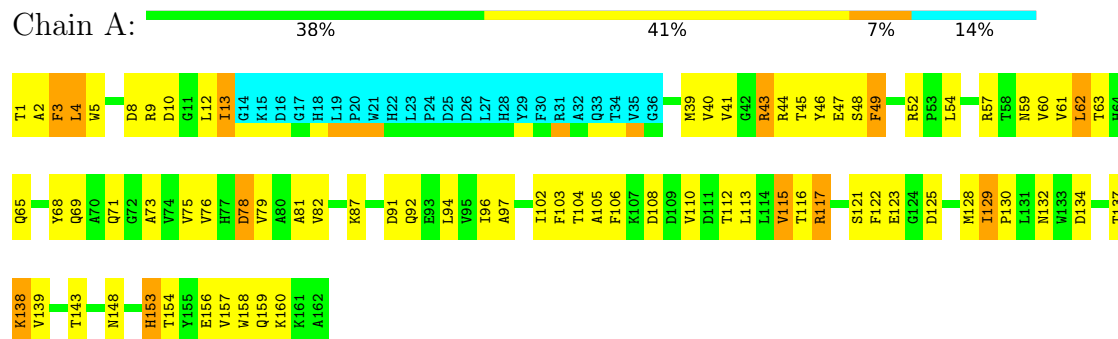


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

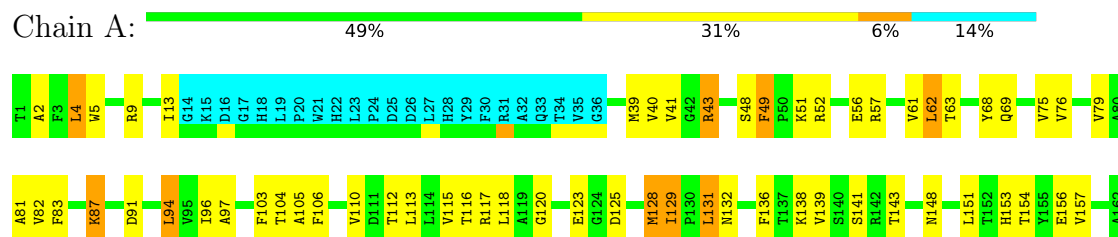
4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Dihydrofolate reductase

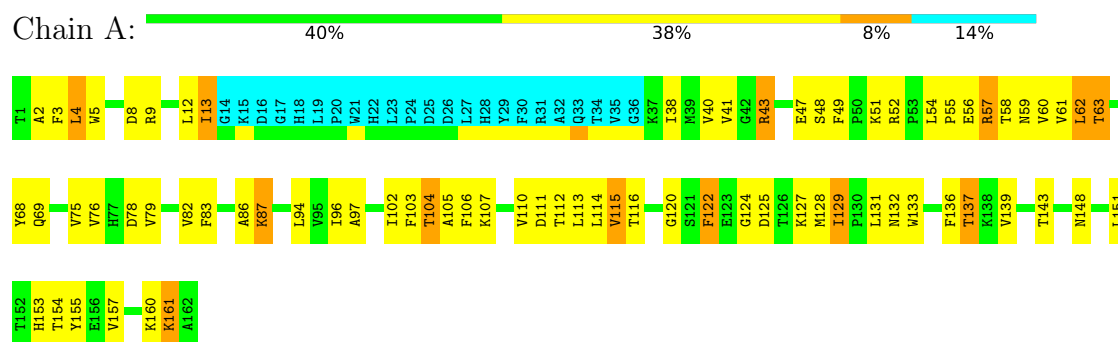


4.2.2 Score per residue for model 2

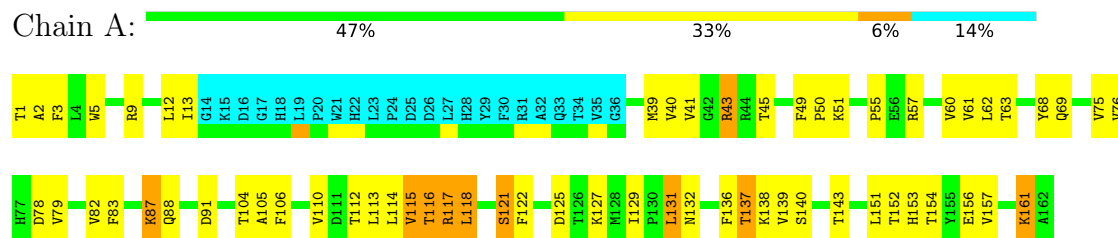
- Molecule 1: Dihydrofolate reductase



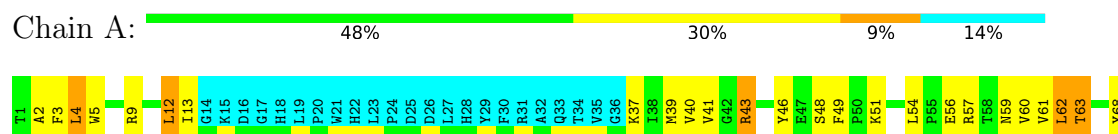
- Molecule 1: Dihydrofolate reductase



- Molecule 1: Dihydrofolate reductase



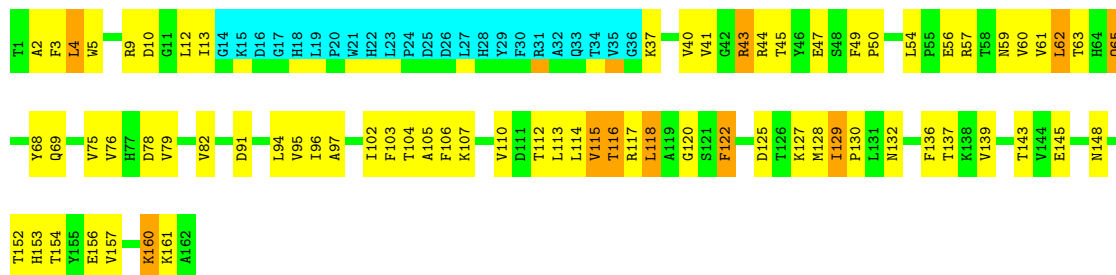
- Molecule 1: Dihydrofolate reductase





4.2.6 Score per residue for model 6

- Molecule 1: Dihydrofolate reductase



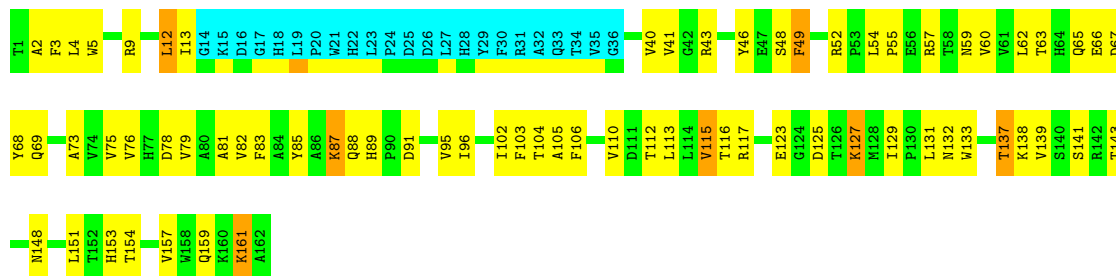
4.2.7 Score per residue for model 7

- Molecule 1: Dihydrofolate reductase



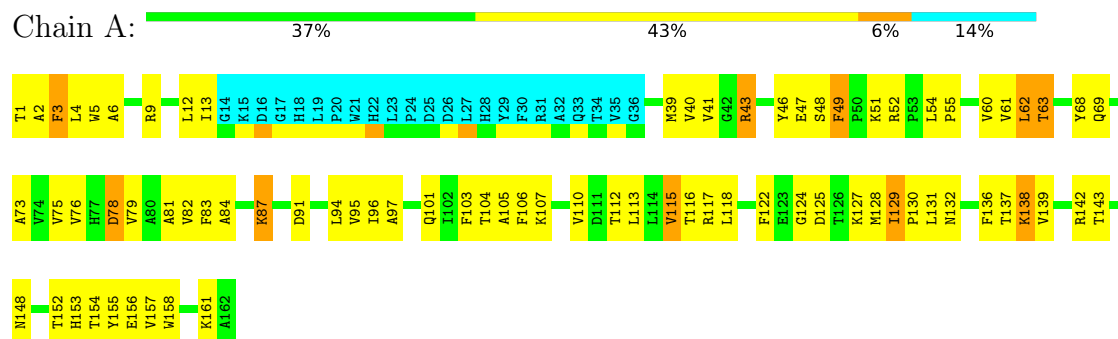
4.2.8 Score per residue for model 8

- 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



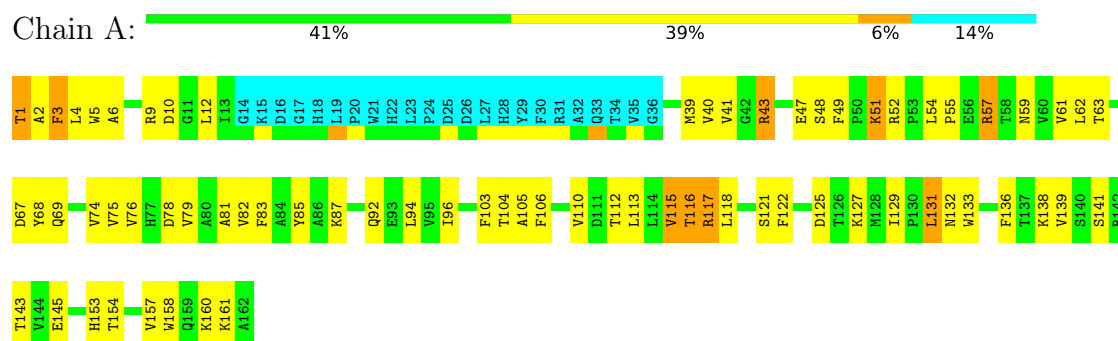
4.2.11 Score per residue for model 11

- Molecule 1: Dihydrofolate reductase



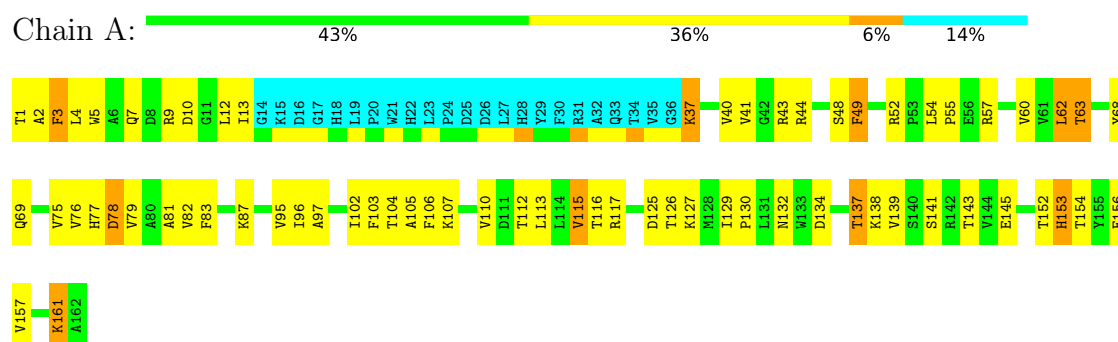
4.2.12 Score per residue for model 12

- Molecule 1: Dihydrofolate reductase



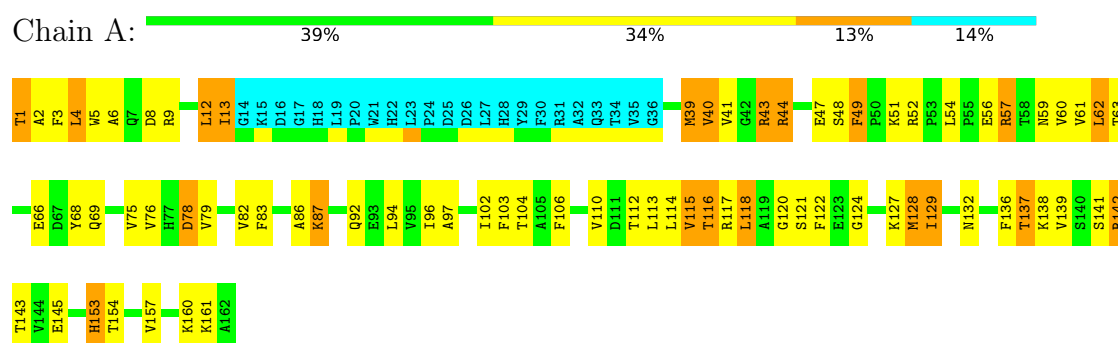
4.2.13 Score per residue for model 13

- Molecule 1: Dihydrofolate reductase



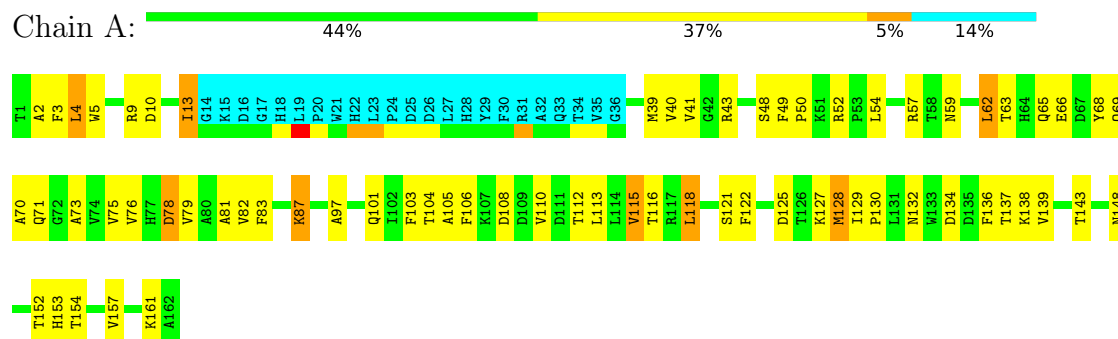
4.2.14 Score per residue for model 14

- Molecule 1: Dihydrofolate reductase



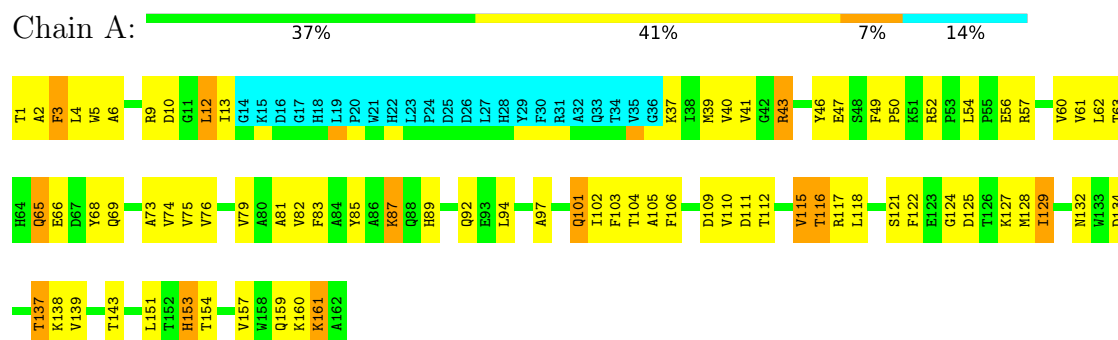
4.2.15 Score per residue for model 15

- Molecule 1: Dihydrofolate reductase



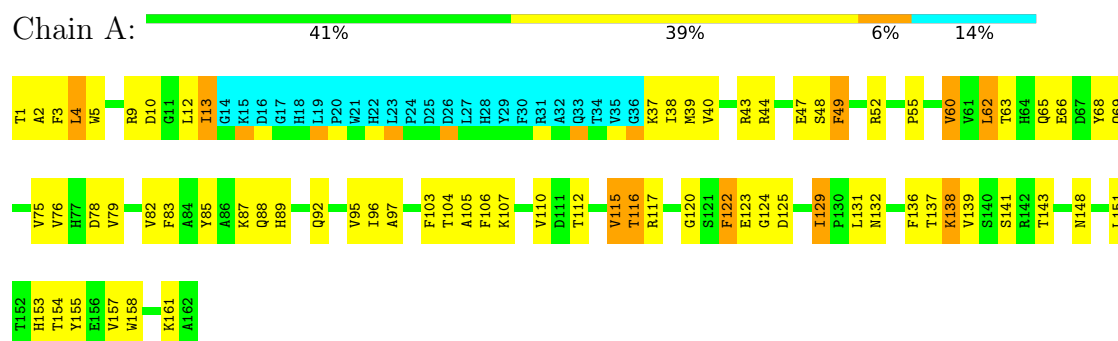
4.2.16 Score per residue for model 16

- Molecule 1: Dihydrofolate reductase



4.2.17 Score per residue for model 17

- Molecule 1: Dihydrofolate reductase



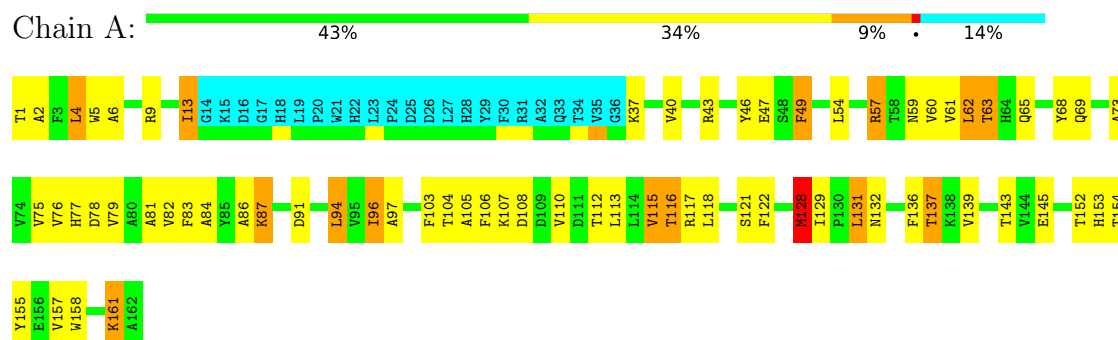
4.2.18 Score per residue for model 18

- Molecule 1: Dihydrofolate reductase



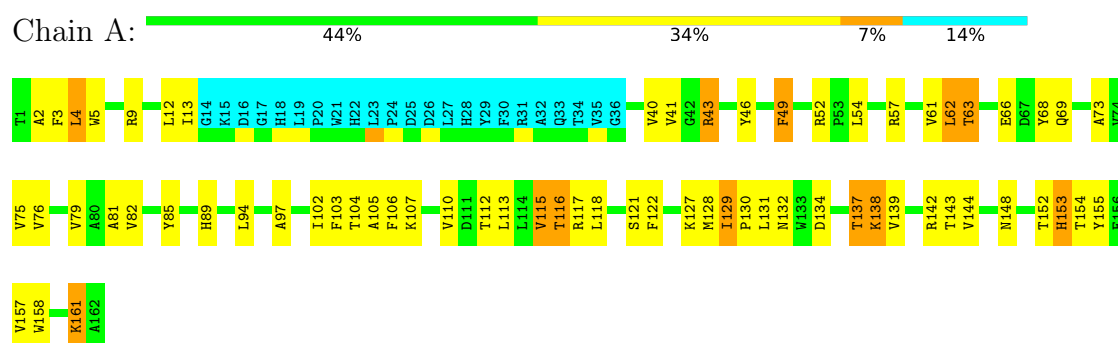
4.2.19 Score per residue for model 19

- Molecule 1: Dihydrofolate reductase



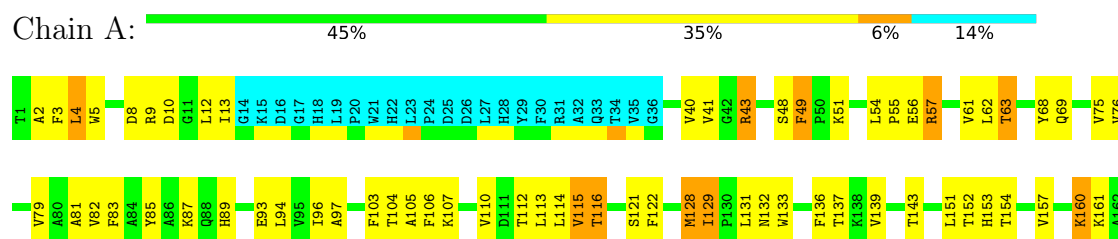
4.2.20 Score per residue for model 20

- Molecule 1: Dihydrofolate reductase



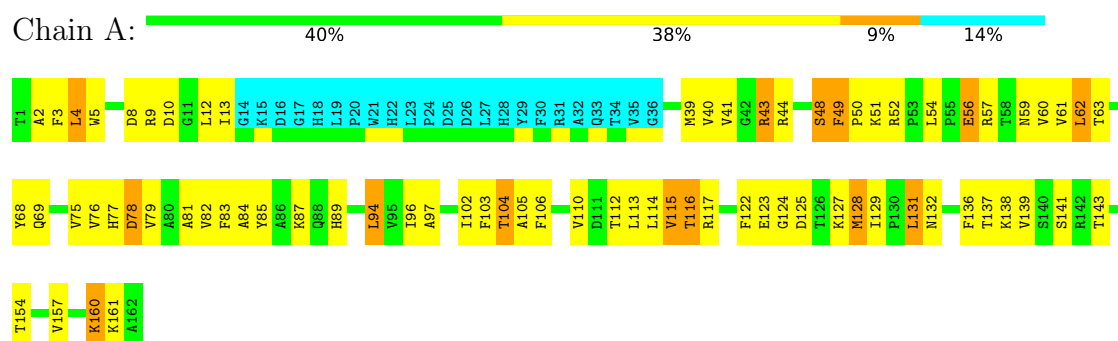
4.2.21 Score per residue for model 21

- Molecule 1: Dihydrofolate reductase



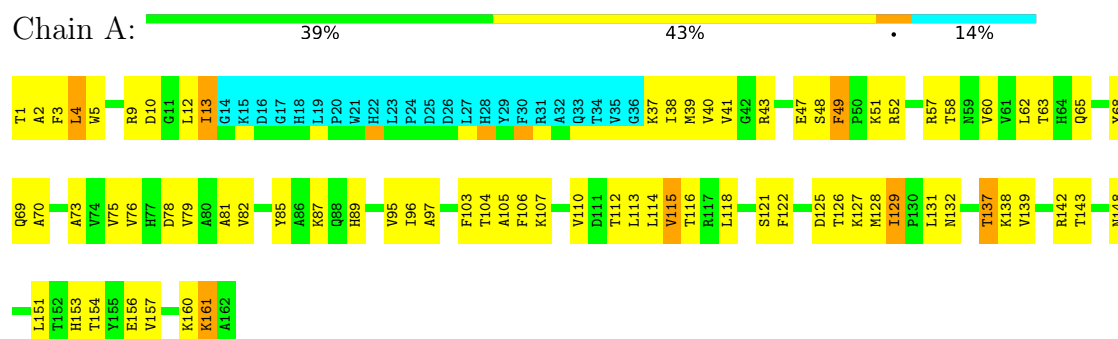
4.2.22 Score per residue for model 22

- Molecule 1: Dihydrofolate reductase



4.2.23 Score per residue for model 23

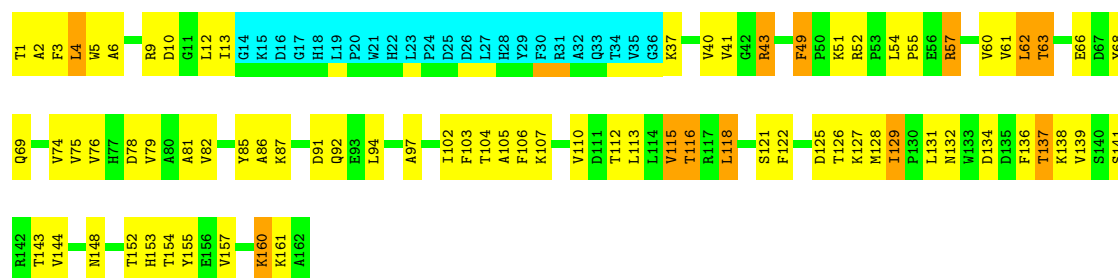
- Molecule 1: Dihydrofolate reductase



4.2.24 Score per residue for model 24

- Molecule 1: Dihydrofolate reductase

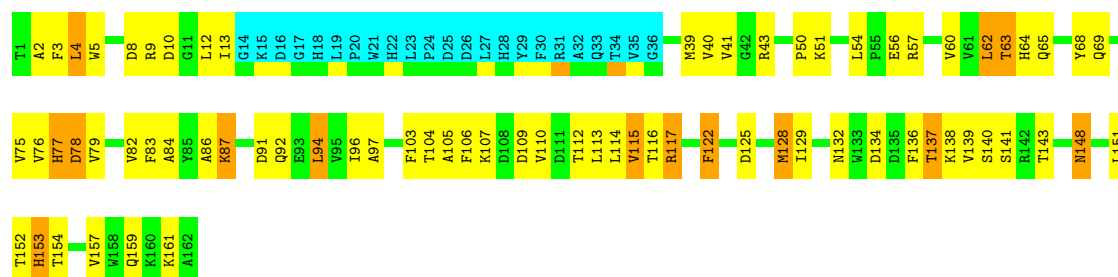




4.2.25 Score per residue for model 25

- Molecule 1: Dihydrofolate reductase

Chain A: 40% 37% 9% 14%



5 Refinement protocol and experimental data overview

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

Of the 50 calculated structures, 25 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
Anglesearch	geometry optimization	
CNS	structure solution	1.2
CNS	refinement	1.2

No chemical shift data was provided.

6 Model quality ⓘ

6.1 Standard geometry ⓘ

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1108	1092	1088	60±7
All	All	27700	27300	27200	1490

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:82:VAL:HG12	1:A:94:LEU:HD11	0.91	1.39	11	9
1:A:4:LEU:HD11	1:A:95:VAL:HG13	0.90	1.40	6	2
1:A:4:LEU:HD12	1:A:114:LEU:HD12	0.89	1.44	6	2
1:A:63:THR:HG21	1:A:68:TYR:CD2	0.88	2.02	11	25
1:A:79:VAL:HG13	1:A:106:PHE:CD2	0.86	2.05	13	25
1:A:49:PHE:CE1	1:A:54:LEU:HD11	0.86	2.05	9	8
1:A:63:THR:HG21	1:A:68:TYR:CG	0.85	2.06	21	23
1:A:76:VAL:HG21	1:A:82:VAL:HG22	0.83	1.48	18	25
1:A:68:TYR:O	1:A:75:VAL:HG11	0.81	1.74	6	23
1:A:139:VAL:HG22	1:A:157:VAL:O	0.80	1.76	8	25
1:A:86:ALA:HB2	1:A:94:LEU:HD12	0.80	1.54	25	3
1:A:4:LEU:HD11	1:A:95:VAL:CG1	0.79	2.07	23	2
1:A:4:LEU:HD22	1:A:4:LEU:O	0.79	1.78	24	12
1:A:69:GLN:HA	1:A:75:VAL:HG21	0.78	1.54	11	25

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:4:LEU:HD21	1:A:95:VAL:HG12	0.78	1.55	23	2
1:A:106:PHE:O	1:A:110:VAL:HG23	0.78	1.79	13	24
1:A:110:VAL:HG11	1:A:113:LEU:HD23	0.77	1.56	20	15
1:A:5:TRP:CH2	1:A:115:VAL:HG12	0.77	2.14	6	25
1:A:4:LEU:HD13	1:A:4:LEU:N	0.75	1.96	23	2
1:A:79:VAL:HG22	1:A:106:PHE:CD1	0.75	2.16	11	22
1:A:128:MET:HE3	1:A:129:ILE:HG13	0.75	1.56	20	7
1:A:76:VAL:HG21	1:A:82:VAL:CG2	0.74	2.12	19	13
1:A:3:PHE:CE2	1:A:110:VAL:HG21	0.74	2.17	23	1
1:A:110:VAL:HG11	1:A:113:LEU:CD2	0.74	2.11	20	10
1:A:79:VAL:HG21	1:A:105:ALA:O	0.74	1.82	17	24
1:A:143:THR:HG23	1:A:154:THR:OG1	0.74	1.83	20	25
1:A:62:LEU:HD13	1:A:102:ILE:HD12	0.73	1.59	11	2
1:A:62:LEU:HD12	1:A:76:VAL:HG23	0.73	1.58	13	3
1:A:118:LEU:HD23	1:A:152:THR:O	0.73	1.84	6	3
1:A:40:VAL:HG21	1:A:82:VAL:HG11	0.72	1.60	14	18
1:A:12:LEU:HD11	1:A:124:GLY:HA3	0.72	1.60	7	3
1:A:104:THR:CA	1:A:129:ILE:HD13	0.71	2.16	14	19
1:A:46:TYR:OH	1:A:73:ALA:HB2	0.71	1.84	5	7
1:A:12:LEU:HD13	1:A:124:GLY:HA3	0.71	1.63	3	2
1:A:86:ALA:HB2	1:A:94:LEU:HD13	0.71	1.63	14	4
1:A:142:ARG:C	1:A:154:THR:HG23	0.70	2.12	7	6
1:A:2:ALA:HA	1:A:112:THR:O	0.69	1.86	22	25
1:A:104:THR:HA	1:A:129:ILE:HD13	0.69	1.64	6	18
1:A:8:ASP:OD2	1:A:12:LEU:HD12	0.69	1.86	3	2
1:A:62:LEU:HD22	1:A:102:ILE:HD12	0.69	1.65	22	3
1:A:39:MET:HE3	1:A:41:VAL:CG1	0.68	2.19	12	10
1:A:62:LEU:HD21	1:A:78:ASP:HA	0.68	1.65	25	7
1:A:12:LEU:HD23	1:A:13:ILE:N	0.67	2.03	1	2
1:A:113:LEU:HD13	1:A:133:TRP:CZ3	0.67	2.25	12	4
1:A:49:PHE:CE2	1:A:54:LEU:HD11	0.66	2.25	10	1
1:A:79:VAL:HG22	1:A:106:PHE:CE1	0.65	2.26	16	13
1:A:54:LEU:HD13	1:A:57:ARG:HD2	0.65	1.66	12	6
1:A:59:ASN:O	1:A:73:ALA:HB1	0.65	1.92	19	3
1:A:60:VAL:HG12	1:A:76:VAL:HG22	0.65	1.69	3	17
1:A:4:LEU:O	1:A:4:LEU:HD13	0.65	1.92	15	9
1:A:118:LEU:HD13	1:A:122:PHE:CZ	0.64	2.27	4	4
1:A:65:GLN:HB3	1:A:68:TYR:HB2	0.64	1.68	25	8
1:A:137:THR:OG1	1:A:161:LYS:HE2	0.63	1.93	4	3
1:A:74:VAL:HG21	1:A:85:TYR:CE2	0.63	2.29	16	1
1:A:39:MET:HE3	1:A:41:VAL:HG13	0.63	1.71	14	13

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:4:LEU:HD13	1:A:4:LEU:O	0.63	1.93	2	3
1:A:79:VAL:HG11	1:A:109:ASP:OD2	0.62	1.94	16	1
1:A:40:VAL:HG13	1:A:60:VAL:HB	0.62	1.71	10	6
1:A:43:ARG:HA	1:A:61:VAL:HG13	0.62	1.70	16	17
1:A:145:GLU:HA	1:A:152:THR:HG23	0.62	1.71	19	4
1:A:137:THR:OG1	1:A:161:LYS:HE3	0.62	1.94	8	7
1:A:79:VAL:HG13	1:A:106:PHE:CE2	0.62	2.28	16	9
1:A:116:THR:HA	1:A:154:THR:O	0.62	1.93	24	12
1:A:4:LEU:HD22	1:A:4:LEU:C	0.61	2.20	18	12
1:A:62:LEU:HD11	1:A:78:ASP:CA	0.61	2.24	8	2
1:A:128:MET:HE2	1:A:129:ILE:HG13	0.61	1.71	25	5
1:A:62:LEU:HD22	1:A:102:ILE:CD1	0.61	2.26	24	6
1:A:78:ASP:O	1:A:82:VAL:HG23	0.61	1.96	25	14
1:A:1:THR:HG23	1:A:94:LEU:HD23	0.61	1.71	12	3
1:A:45:THR:HG22	1:A:49:PHE:CE2	0.60	2.32	4	3
1:A:131:LEU:HD13	1:A:133:TRP:CZ2	0.60	2.32	3	1
1:A:79:VAL:HG21	1:A:105:ALA:C	0.60	2.22	7	10
1:A:143:THR:HA	1:A:154:THR:HA	0.60	1.73	19	11
1:A:128:MET:HE3	1:A:129:ILE:CG1	0.59	2.26	20	3
1:A:76:VAL:HB	1:A:81:ALA:HB3	0.59	1.74	20	17
1:A:5:TRP:CD1	1:A:13:ILE:HG22	0.59	2.32	5	3
1:A:83:PHE:O	1:A:87:LYS:HG2	0.59	1.98	13	5
1:A:54:LEU:HB3	1:A:57:ARG:HD3	0.59	1.74	13	4
1:A:51:LYS:HB3	1:A:54:LEU:HD23	0.59	1.74	7	3
1:A:49:PHE:CZ	1:A:54:LEU:HD11	0.59	2.32	24	2
1:A:128:MET:HE1	1:A:131:LEU:CD1	0.58	2.28	2	4
1:A:113:LEU:HD11	1:A:136:PHE:CD1	0.58	2.33	19	6
1:A:113:LEU:O	1:A:114:LEU:HD23	0.58	1.98	23	4
1:A:62:LEU:HD12	1:A:76:VAL:CG2	0.58	2.28	13	2
1:A:3:PHE:CD1	1:A:110:VAL:HG21	0.58	2.33	16	3
1:A:41:VAL:HG11	1:A:49:PHE:CE2	0.58	2.33	22	5
1:A:82:VAL:HG21	1:A:106:PHE:CZ	0.58	2.34	8	15
1:A:3:PHE:CD2	1:A:110:VAL:HG21	0.58	2.33	23	1
1:A:82:VAL:CG1	1:A:94:LEU:HD11	0.58	2.28	20	8
1:A:113:LEU:HD11	1:A:136:PHE:CD2	0.58	2.33	3	3
1:A:54:LEU:HD12	1:A:59:ASN:HD21	0.57	1.58	12	11
1:A:62:LEU:HD11	1:A:78:ASP:C	0.57	2.24	13	2
1:A:4:LEU:HD22	1:A:4:LEU:H	0.57	1.59	23	2
1:A:39:MET:HA	1:A:95:VAL:O	0.57	1.99	23	2
1:A:40:VAL:CG2	1:A:94:LEU:HD21	0.57	2.30	5	1
1:A:1:THR:CG2	1:A:94:LEU:HD23	0.57	2.29	12	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:82:VAL:CG1	1:A:94:LEU:HD21	0.57	2.29	18	4
1:A:152:THR:O	1:A:152:THR:HG22	0.57	1.99	19	2
1:A:46:TYR:CZ	1:A:73:ALA:HB2	0.56	2.35	1	4
1:A:83:PHE:O	1:A:87:LYS:HB3	0.56	2.01	19	7
1:A:117:ARG:O	1:A:153:HIS:HA	0.56	2.00	19	14
1:A:40:VAL:CG2	1:A:82:VAL:HG11	0.56	2.30	7	9
1:A:5:TRP:CZ2	1:A:115:VAL:HG12	0.56	2.36	17	14
1:A:54:LEU:HD22	1:A:57:ARG:CZ	0.56	2.31	18	1
1:A:79:VAL:HG11	1:A:109:ASP:CB	0.55	2.30	25	1
1:A:49:PHE:HE1	1:A:54:LEU:HD11	0.55	1.62	14	1
1:A:13:ILE:H	1:A:13:ILE:HD13	0.55	1.62	23	2
1:A:54:LEU:HB2	1:A:57:ARG:HB2	0.55	1.77	13	3
1:A:3:PHE:C	1:A:4:LEU:HD13	0.55	2.26	23	2
1:A:86:ALA:HB2	1:A:94:LEU:CD1	0.55	2.30	25	2
1:A:4:LEU:N	1:A:4:LEU:CD1	0.54	2.68	6	2
1:A:13:ILE:HG21	1:A:128:MET:HG3	0.54	1.79	15	2
1:A:70:ALA:HB1	1:A:73:ALA:HB3	0.54	1.80	23	2
1:A:6:ALA:HB1	1:A:118:LEU:HD11	0.54	1.79	12	3
1:A:82:VAL:HG12	1:A:94:LEU:HD21	0.54	1.80	18	5
1:A:104:THR:HA	1:A:107:LYS:HD3	0.54	1.80	5	3
1:A:5:TRP:CH2	1:A:115:VAL:CG1	0.53	2.92	11	23
1:A:115:VAL:HG22	1:A:156:GLU:HB2	0.53	1.80	1	7
1:A:113:LEU:HD11	1:A:136:PHE:CG	0.53	2.39	4	5
1:A:3:PHE:CE1	1:A:110:VAL:HG22	0.53	2.38	20	9
1:A:3:PHE:CE1	1:A:110:VAL:CG2	0.53	2.92	18	15
1:A:129:ILE:HB	1:A:130:PRO:HD2	0.52	1.81	13	6
1:A:54:LEU:HD12	1:A:59:ASN:ND2	0.52	2.20	6	5
1:A:40:VAL:O	1:A:41:VAL:HG13	0.52	2.04	3	10
1:A:85:TYR:CZ	1:A:89:HIS:CD2	0.51	2.99	8	4
1:A:122:PHE:CD1	1:A:122:PHE:N	0.51	2.79	25	13
1:A:6:ALA:HB2	1:A:116:THR:OG1	0.51	2.06	14	2
1:A:12:LEU:HG	1:A:13:ILE:N	0.51	2.20	7	1
1:A:118:LEU:HD13	1:A:122:PHE:CE1	0.51	2.41	7	1
1:A:139:VAL:HG11	1:A:159:GLN:CD	0.51	2.31	1	3
1:A:54:LEU:HB3	1:A:57:ARG:HG3	0.51	1.82	10	1
1:A:3:PHE:HB2	1:A:113:LEU:HD23	0.51	1.83	12	1
1:A:41:VAL:HG11	1:A:49:PHE:CZ	0.51	2.41	22	3
1:A:61:VAL:HG11	1:A:68:TYR:CE1	0.51	2.40	10	6
1:A:139:VAL:HG11	1:A:159:GLN:HE21	0.51	1.66	25	2
1:A:49:PHE:CD2	1:A:54:LEU:HD11	0.51	2.41	19	2
1:A:83:PHE:O	1:A:87:LYS:CG	0.51	2.59	11	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:40:VAL:O	1:A:41:VAL:CG1	0.51	2.59	21	13
1:A:48:SER:O	1:A:49:PHE:C	0.50	2.53	22	17
1:A:39:MET:HE1	1:A:59:ASN:OD1	0.50	2.06	11	4
1:A:4:LEU:HD21	1:A:95:VAL:CG1	0.50	2.32	6	1
1:A:4:LEU:C	1:A:4:LEU:HD22	0.50	2.31	2	1
1:A:41:VAL:HG22	1:A:60:VAL:O	0.50	2.07	11	7
1:A:12:LEU:HA	1:A:127:LYS:HA	0.50	1.82	5	2
1:A:41:VAL:HG11	1:A:49:PHE:HE2	0.50	1.65	24	1
1:A:40:VAL:CG2	1:A:94:LEU:HD11	0.50	2.37	22	1
1:A:68:TYR:C	1:A:75:VAL:HG11	0.50	2.32	11	4
1:A:143:THR:N	1:A:154:THR:HG23	0.49	2.22	11	8
1:A:3:PHE:CZ	1:A:110:VAL:CG2	0.49	2.94	23	2
1:A:13:ILE:HD13	1:A:13:ILE:N	0.49	2.21	19	1
1:A:4:LEU:O	1:A:4:LEU:HD22	0.49	2.07	2	3
1:A:148:ASN:HB3	1:A:151:LEU:HG	0.49	1.83	23	7
1:A:104:THR:N	1:A:129:ILE:HD13	0.49	2.23	9	2
1:A:83:PHE:O	1:A:87:LYS:HG3	0.49	2.08	18	2
1:A:139:VAL:HG11	1:A:159:GLN:OE1	0.49	2.07	1	1
1:A:112:THR:HG23	1:A:158:TRP:O	0.49	2.07	12	3
1:A:128:MET:HE2	1:A:129:ILE:CG1	0.49	2.38	19	1
1:A:106:PHE:C	1:A:110:VAL:HG23	0.49	2.32	13	3
1:A:85:TYR:CZ	1:A:89:HIS:NE2	0.49	2.81	23	7
1:A:104:THR:CB	1:A:129:ILE:HD13	0.49	2.38	22	8
1:A:1:THR:HG23	1:A:94:LEU:O	0.49	2.08	16	1
1:A:13:ILE:HD11	1:A:126:THR:HG22	0.49	1.84	23	1
1:A:4:LEU:HB3	1:A:114:LEU:HD12	0.48	1.83	3	1
1:A:137:THR:OG1	1:A:161:LYS:CE	0.48	2.61	24	5
1:A:3:PHE:CD1	1:A:110:VAL:CG2	0.48	2.96	16	3
1:A:12:LEU:HD21	1:A:124:GLY:HA3	0.48	1.83	17	4
1:A:40:VAL:HG21	1:A:96:ILE:CD1	0.48	2.39	11	3
1:A:82:VAL:HG21	1:A:106:PHE:HZ	0.48	1.68	18	16
1:A:43:ARG:CA	1:A:61:VAL:HG13	0.48	2.39	5	2
1:A:60:VAL:HG12	1:A:76:VAL:CG2	0.48	2.39	3	1
1:A:84:ALA:O	1:A:87:LYS:CG	0.48	2.61	9	3
1:A:77:HIS:CD2	1:A:77:HIS:N	0.48	2.80	25	1
1:A:97:ALA:O	1:A:103:PHE:CZ	0.48	2.67	24	21
1:A:57:ARG:N	1:A:57:ARG:HD2	0.48	2.23	13	1
1:A:69:GLN:CA	1:A:75:VAL:HG21	0.48	2.34	19	1
1:A:144:VAL:HG21	1:A:155:TYR:CE2	0.48	2.44	24	2
1:A:118:LEU:HG	1:A:153:HIS:HB3	0.47	1.84	15	1
1:A:79:VAL:HG22	1:A:106:PHE:CG	0.47	2.44	20	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:138:LYS:HD2	1:A:141:SER:HB3	0.47	1.86	14	8
1:A:85:TYR:CE2	1:A:89:HIS:CD2	0.47	3.02	5	1
1:A:5:TRP:CZ3	1:A:115:VAL:HG12	0.47	2.45	19	6
1:A:85:TYR:CE1	1:A:89:HIS:NE2	0.47	2.83	7	3
1:A:118:LEU:HD22	1:A:122:PHE:CZ	0.47	2.44	20	2
1:A:54:LEU:HD22	1:A:57:ARG:NH1	0.47	2.25	7	3
1:A:3:PHE:CZ	1:A:110:VAL:HG21	0.47	2.45	23	1
1:A:62:LEU:HA	1:A:76:VAL:O	0.46	2.10	10	4
1:A:128:MET:HE1	1:A:131:LEU:HD12	0.46	1.87	2	2
1:A:5:TRP:HD1	1:A:13:ILE:HG22	0.46	1.70	15	3
1:A:63:THR:HG21	1:A:68:TYR:CB	0.46	2.40	22	2
1:A:96:ILE:HD13	1:A:96:ILE:N	0.46	2.25	19	1
1:A:54:LEU:HB3	1:A:57:ARG:CD	0.46	2.41	3	4
1:A:74:VAL:HG11	1:A:85:TYR:CD1	0.46	2.46	24	2
1:A:62:LEU:HD13	1:A:102:ILE:HG23	0.46	1.88	20	1
1:A:121:SER:C	1:A:122:PHE:CD1	0.46	2.94	7	11
1:A:153:HIS:N	1:A:153:HIS:ND1	0.46	2.64	5	1
1:A:40:VAL:CG2	1:A:96:ILE:HD12	0.46	2.41	9	1
1:A:6:ALA:HB1	1:A:118:LEU:CD1	0.46	2.41	12	1
1:A:13:ILE:HG21	1:A:128:MET:SD	0.46	2.51	3	1
1:A:40:VAL:HG21	1:A:96:ILE:HD12	0.46	1.88	9	1
1:A:5:TRP:CZ2	1:A:115:VAL:CG1	0.45	2.99	2	2
1:A:46:TYR:O	1:A:49:PHE:HB2	0.45	2.11	5	1
1:A:118:LEU:HD22	1:A:122:PHE:HZ	0.45	1.71	14	1
1:A:60:VAL:CG1	1:A:76:VAL:HG13	0.45	2.41	3	1
1:A:62:LEU:HG	1:A:76:VAL:HG23	0.45	1.89	2	2
1:A:4:LEU:O	1:A:4:LEU:CD2	0.45	2.59	22	6
1:A:70:ALA:CB	1:A:73:ALA:HB3	0.45	2.40	23	1
1:A:152:THR:HG22	1:A:153:HIS:N	0.45	2.26	5	10
1:A:40:VAL:CG2	1:A:96:ILE:CD1	0.45	2.95	11	13
1:A:104:THR:OG1	1:A:107:LYS:HD3	0.45	2.11	17	9
1:A:38:ILE:HA	1:A:58:THR:HB	0.45	1.89	3	1
1:A:43:ARG:HG2	1:A:63:THR:HB	0.45	1.88	18	1
1:A:74:VAL:HG21	1:A:85:TYR:CZ	0.45	2.47	24	1
1:A:4:LEU:H	1:A:4:LEU:CD1	0.45	2.25	5	1
1:A:79:VAL:HG11	1:A:109:ASP:HB2	0.45	1.88	25	1
1:A:62:LEU:HB3	1:A:102:ILE:HD12	0.44	1.89	13	2
1:A:40:VAL:HG12	1:A:41:VAL:N	0.44	2.28	8	9
1:A:40:VAL:C	1:A:41:VAL:HG13	0.44	2.38	21	10
1:A:136:PHE:CE2	1:A:160:LYS:HB2	0.44	2.47	21	8
1:A:52:ARG:O	1:A:52:ARG:HG2	0.44	2.13	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:38:ILE:CG2	1:A:60:VAL:CG2	0.44	2.96	23	1
1:A:4:LEU:H	1:A:4:LEU:HD13	0.44	1.73	5	2
1:A:3:PHE:CE1	1:A:110:VAL:HG21	0.44	2.48	16	1
1:A:13:ILE:HD13	1:A:126:THR:O	0.44	2.13	23	1
1:A:3:PHE:CZ	1:A:103:PHE:O	0.44	2.70	23	13
1:A:3:PHE:CZ	1:A:103:PHE:HA	0.44	2.48	12	4
1:A:3:PHE:CE1	1:A:96:ILE:HB	0.44	2.47	1	5
1:A:76:VAL:HG11	1:A:82:VAL:HA	0.44	1.89	18	2
1:A:65:GLN:O	1:A:77:HIS:CD2	0.44	2.71	19	1
1:A:138:LYS:HD3	1:A:158:TRP:CZ2	0.43	2.48	17	5
1:A:54:LEU:HB3	1:A:57:ARG:HD2	0.43	1.90	7	3
1:A:103:PHE:HB3	1:A:129:ILE:HG12	0.43	1.90	6	1
1:A:79:VAL:HG12	1:A:83:PHE:CE2	0.43	2.47	12	2
1:A:43:ARG:HD3	1:A:44:ARG:N	0.43	2.29	7	3
1:A:104:THR:HB	1:A:129:ILE:HG21	0.43	1.89	6	2
1:A:5:TRP:CH2	1:A:131:LEU:HD11	0.43	2.48	3	1
1:A:51:LYS:CE	1:A:54:LEU:HD23	0.43	2.44	3	1
1:A:152:THR:CG2	1:A:153:HIS:N	0.43	2.82	24	3
1:A:113:LEU:HB2	1:A:158:TRP:HB2	0.43	1.90	12	1
1:A:49:PHE:CD1	1:A:54:LEU:HD21	0.43	2.49	18	1
1:A:5:TRP:CH2	1:A:131:LEU:CD1	0.43	3.02	19	1
1:A:12:LEU:HD23	1:A:126:THR:O	0.43	2.14	24	1
1:A:64:HIS:O	1:A:64:HIS:CG	0.43	2.72	25	1
1:A:40:VAL:HB	1:A:96:ILE:HD12	0.43	1.91	2	1
1:A:106:PHE:CD1	1:A:106:PHE:N	0.42	2.87	21	9
1:A:129:ILE:HD12	1:A:130:PRO:O	0.42	2.14	15	1
1:A:143:THR:CA	1:A:154:THR:HG23	0.42	2.44	16	1
1:A:4:LEU:HD22	1:A:96:ILE:O	0.42	2.13	6	2
1:A:2:ALA:HB3	1:A:95:VAL:HG13	0.42	1.91	13	1
1:A:1:THR:O	1:A:111:ASP:N	0.42	2.51	16	1
1:A:40:VAL:HA	1:A:60:VAL:HB	0.42	1.89	23	1
1:A:86:ALA:CB	1:A:94:LEU:HD12	0.42	2.44	5	1
1:A:68:TYR:CD1	1:A:69:GLN:N	0.42	2.88	8	2
1:A:68:TYR:CE1	1:A:69:GLN:O	0.42	2.73	8	2
1:A:139:VAL:CG2	1:A:157:VAL:O	0.42	2.67	25	1
1:A:3:PHE:HB3	1:A:5:TRP:CZ3	0.42	2.50	4	5
1:A:143:THR:CG2	1:A:154:THR:OG1	0.42	2.67	5	2
1:A:60:VAL:HA	1:A:74:VAL:O	0.42	2.15	11	1
1:A:74:VAL:HG21	1:A:85:TYR:CE1	0.42	2.49	12	1
1:A:12:LEU:HD13	1:A:126:THR:O	0.42	2.14	13	1
1:A:63:THR:O	1:A:77:HIS:HA	0.42	2.15	13	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:12:LEU:HD11	1:A:124:GLY:CA	0.42	2.40	7	1
1:A:8:ASP:CG	1:A:12:LEU:HD12	0.42	2.39	3	1
1:A:62:LEU:HD23	1:A:77:HIS:C	0.42	2.39	11	1
1:A:57:ARG:CD	1:A:57:ARG:N	0.42	2.83	21	1
1:A:38:ILE:HG12	1:A:58:THR:HG21	0.42	1.91	23	1
1:A:3:PHE:CE2	1:A:103:PHE:O	0.42	2.73	18	4
1:A:4:LEU:O	1:A:4:LEU:CD1	0.42	2.66	15	1
1:A:54:LEU:CB	1:A:57:ARG:HB2	0.42	2.45	24	1
1:A:5:TRP:CZ2	1:A:131:LEU:CD1	0.41	3.03	4	2
1:A:110:VAL:O	1:A:136:PHE:CZ	0.41	2.73	14	2
1:A:151:LEU:O	1:A:153:HIS:CE1	0.41	2.73	16	1
1:A:4:LEU:C	1:A:4:LEU:CD2	0.41	2.93	19	2
1:A:154:THR:HG22	1:A:155:TYR:N	0.41	2.30	19	1
1:A:3:PHE:CD1	1:A:110:VAL:HG22	0.41	2.49	20	1
1:A:52:ARG:O	1:A:52:ARG:CG	0.41	2.68	14	1
1:A:74:VAL:HG21	1:A:85:TYR:CD2	0.41	2.49	16	1
1:A:111:ASP:HA	1:A:160:LYS:HB2	0.41	1.91	3	1
1:A:104:THR:HB	1:A:129:ILE:HD13	0.41	1.91	8	1
1:A:151:LEU:O	1:A:153:HIS:CD2	0.41	2.74	4	1
1:A:152:THR:C	1:A:153:HIS:CG	0.41	2.98	5	1
1:A:57:ARG:O	1:A:59:ASN:ND2	0.41	2.54	12	2
1:A:136:PHE:CE1	1:A:160:LYS:HB2	0.41	2.51	3	1
1:A:12:LEU:HD21	1:A:124:GLY:CA	0.41	2.46	9	1
1:A:85:TYR:CE1	1:A:89:HIS:CD2	0.41	3.09	7	1
1:A:62:LEU:CD1	1:A:102:ILE:HD12	0.41	2.38	11	1
1:A:8:ASP:HB3	1:A:122:PHE:CD1	0.41	2.51	1	1
1:A:46:TYR:CZ	1:A:73:ALA:CB	0.41	3.04	1	1
1:A:60:VAL:CG1	1:A:76:VAL:CG1	0.41	2.99	3	1
1:A:110:VAL:CG1	1:A:113:LEU:HD23	0.41	2.43	13	1
1:A:120:GLY:O	1:A:122:PHE:CE1	0.41	2.74	17	1
1:A:94:LEU:HD23	1:A:96:ILE:HD11	0.41	1.92	19	1
1:A:153:HIS:N	1:A:153:HIS:CD2	0.41	2.86	20	1
1:A:68:TYR:CD1	1:A:69:GLN:O	0.41	2.73	23	1
1:A:79:VAL:HG11	1:A:109:ASP:CG	0.41	2.40	25	1
1:A:112:THR:HA	1:A:158:TRP:O	0.41	2.16	11	1
1:A:13:ILE:HG21	1:A:128:MET:CG	0.41	2.44	15	1
1:A:38:ILE:HD11	1:A:92:GLN:HB2	0.41	1.93	17	1
1:A:62:LEU:HD11	1:A:106:PHE:CE1	0.40	2.51	11	1
1:A:110:VAL:O	1:A:136:PHE:CE1	0.40	2.74	25	2
1:A:153:HIS:CE1	1:A:155:TYR:OH	0.40	2.74	17	1
1:A:5:TRP:CD1	1:A:13:ILE:CG2	0.40	3.04	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:110:VAL:CG1	1:A:112:THR:O	0.40	2.70	10	1
1:A:101:GLN:NE2	1:A:102:ILE:HD13	0.40	2.30	16	1
1:A:52:ARG:CD	1:A:52:ARG:N	0.40	2.85	11	1
1:A:7:GLN:HA	1:A:12:LEU:O	0.40	2.16	18	1
1:A:81:ALA:O	1:A:84:ALA:HB3	0.40	2.16	22	1
1:A:96:ILE:N	1:A:96:ILE:HD13	0.40	2.31	8	1
1:A:87:LYS:HG3	1:A:88:GLN:N	0.40	2.31	4	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	137/162 (85%)	127±2 (93±1%)	9±2 (7±1%)	1±1 (1±0%)	23	72
All	All	3425/4050 (85%)	3169 (93%)	234 (7%)	22 (1%)	23	72

All 5 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	55	PRO	9
1	A	50	PRO	6
1	A	120	GLY	4
1	A	49	PHE	2
1	A	128	MET	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	118/137 (86%)	93±3 (78±3%)	25±3 (22±3%)	3	30
All	All	2950/3425 (86%)	2315 (78%)	635 (22%)	3	30

All 68 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	43	ARG	25
1	A	116	THR	25
1	A	132	ASN	25
1	A	9	ARG	24
1	A	115	VAL	24
1	A	62	LEU	23
1	A	137	THR	23
1	A	13	ILE	21
1	A	87	LYS	18
1	A	125	ASP	18
1	A	127	LYS	18
1	A	161	LYS	18
1	A	4	LEU	17
1	A	52	ARG	16
1	A	129	ILE	16
1	A	10	ASP	14
1	A	49	PHE	14
1	A	51	LYS	14
1	A	131	LEU	14
1	A	78	ASP	13
1	A	138	LYS	12
1	A	12	LEU	12
1	A	47	GLU	11
1	A	91	ASP	11
1	A	148	ASN	11
1	A	153	HIS	11
1	A	160	LYS	11
1	A	128	MET	11
1	A	63	THR	11
1	A	1	THR	10
1	A	57	ARG	9
1	A	117	ARG	9
1	A	92	GLN	8
1	A	134	ASP	8
1	A	3	PHE	7
1	A	123	GLU	7

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Mol	Chain	Res	Type	Models (Total)
1	A	118	LEU	7
1	A	56	GLU	7
1	A	66	GLU	7
1	A	44	ARG	6
1	A	94	LEU	6
1	A	37	LYS	6
1	A	122	PHE	5
1	A	65	GLN	4
1	A	141	SER	4
1	A	71	GLN	3
1	A	108	ASP	3
1	A	48	SER	3
1	A	104	THR	3
1	A	107	LYS	3
1	A	101	GLN	3
1	A	8	ASP	3
1	A	121	SER	2
1	A	140	SER	2
1	A	67	ASP	2
1	A	88	GLN	2
1	A	142	ARG	2
1	A	145	GLU	2
1	A	77	HIS	2
1	A	135	ASP	1
1	A	7	GLN	1
1	A	39	MET	1
1	A	40	VAL	1
1	A	60	VAL	1
1	A	126	THR	1
1	A	156	GLU	1
1	A	96	ILE	1
1	A	93	GLU	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 [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided