



Full wwPDB NMR Structure Validation Report ⓘ

Mar 7, 2026 – 04:02 AM UTC

PDB ID : 2ITH / pdb_00002ith
BMRB ID : 6645
Title : NMR Structure of Haloferax volcanii DHFR
Authors : Binbuga, B.
Deposited on : 2006-10-19

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

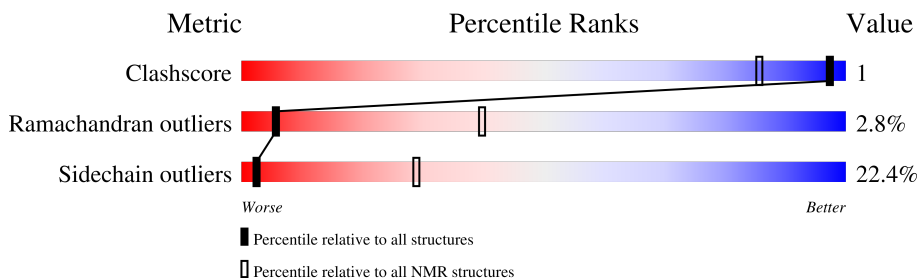
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 82%.

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	

2 Ensemble composition and analysis

This entry contains 20 models. The atoms present in the NMR models are not consistent. Some calculations may have failed as a result. All residues are included in the validation scores. Model 17 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:2-A:15, A:28-A:65, A:73-A:121, A:129-A:158 (131)	0.29	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 3 clusters and 3 single-model clusters were found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 2464 atoms, of which 1199 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Dihydrofolate reductase.

Mol	Chain	Residues	Atoms					Trace	
			Total	C	H	N	O		S
1	A	162	2464	788	1199	218	255	4	0

There is a discrepancy between the modelled and reference sequences:

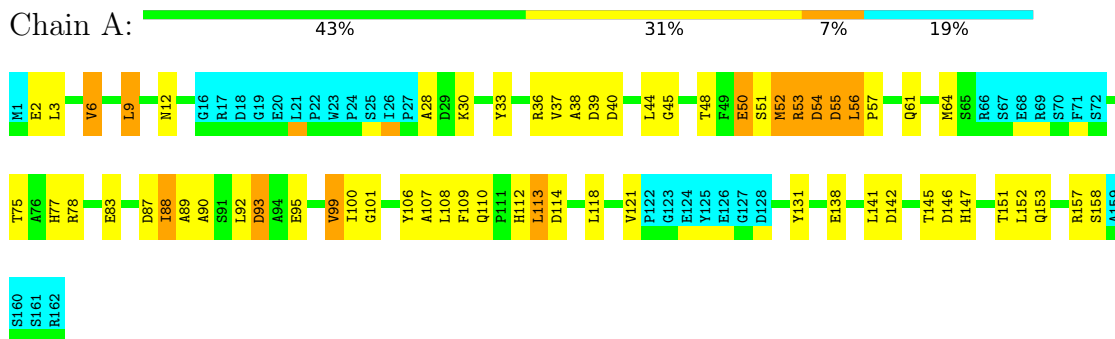
Chain	Residue	Modelled	Actual	Comment	Reference
A	37	VAL	ILE	SEE REMARK 999	UNP P15093

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

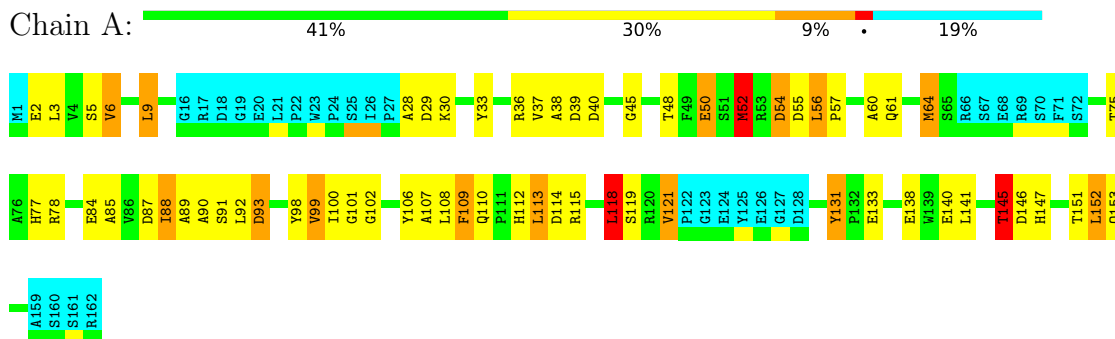


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

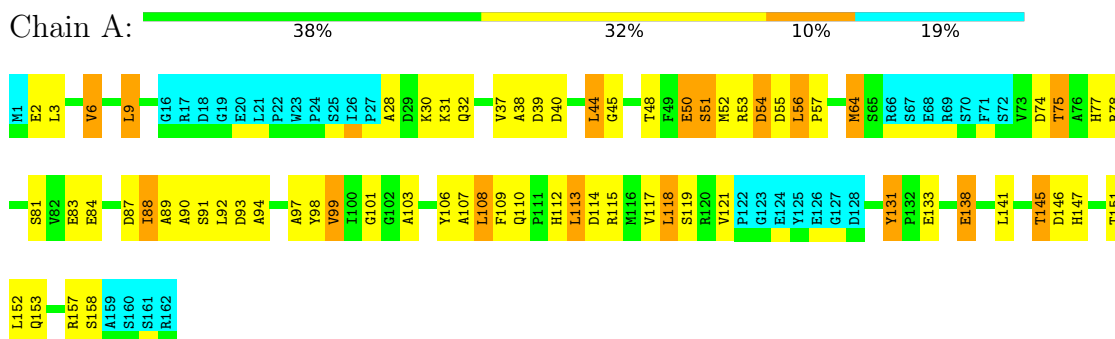
4.2.1 Score per residue for model 1

- Molecule 1: Dihydrofolate reductase



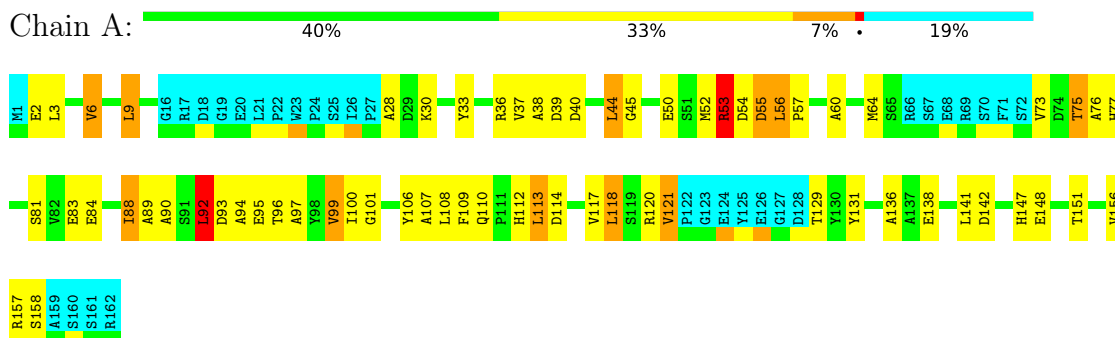
4.2.2 Score per residue for model 2

- Molecule 1: Dihydrofolate reductase



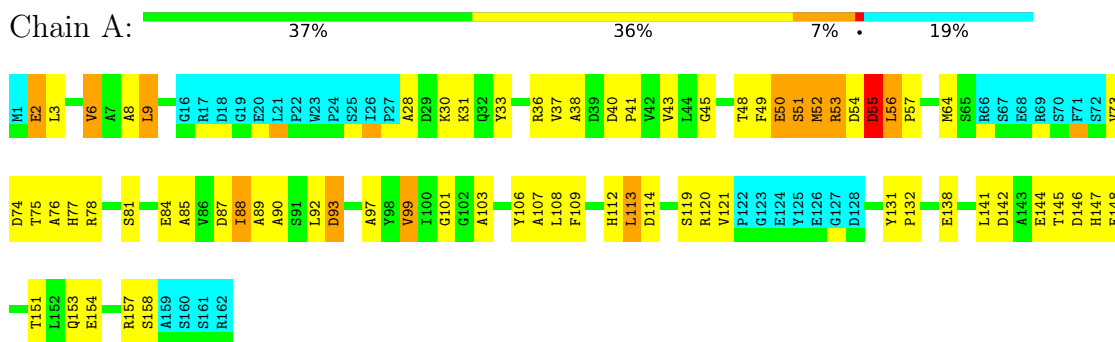
4.2.3 Score per residue for model 3

- Molecule 1: Dihydrofolate reductase



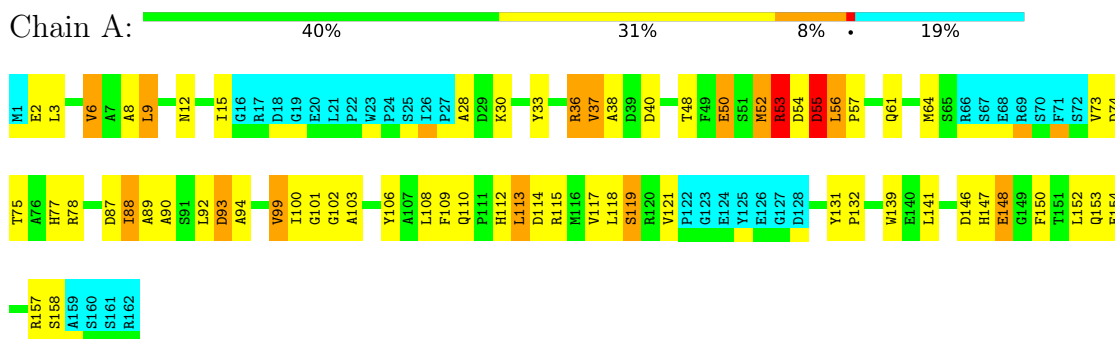
4.2.4 Score per residue for model 4

- Molecule 1: Dihydrofolate reductase



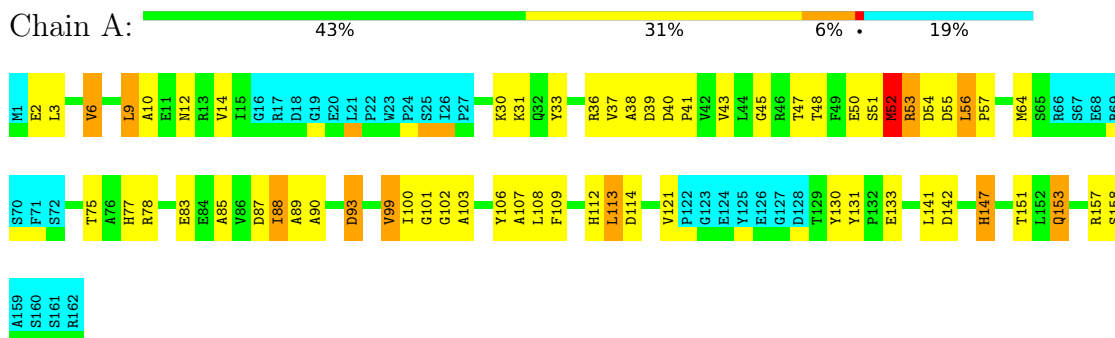
4.2.5 Score per residue for model 5

- Molecule 1: Dihydrofolate reductase



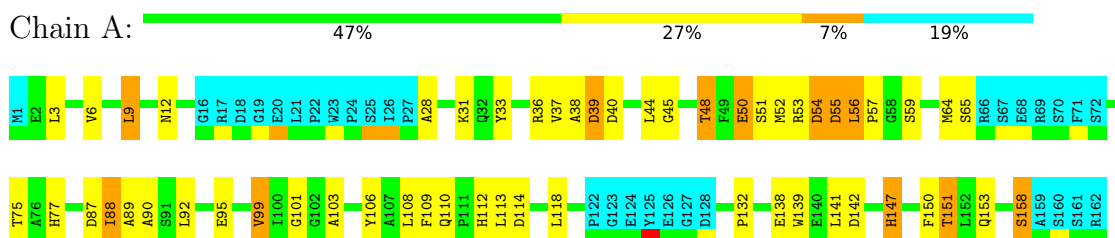
4.2.6 Score per residue for model 6

- Molecule 1: Dihydrofolate reductase



4.2.7 Score per residue for model 7

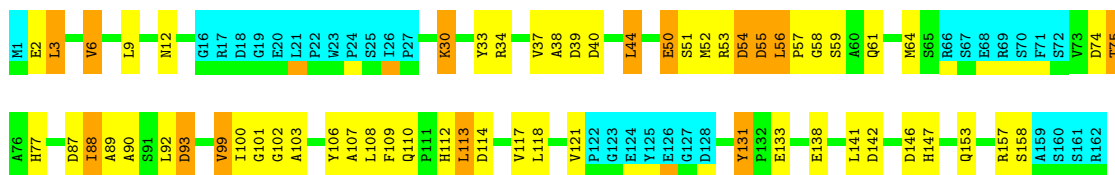
- Molecule 1: Dihydrofolate reductase



4.2.8 Score per residue for model 8

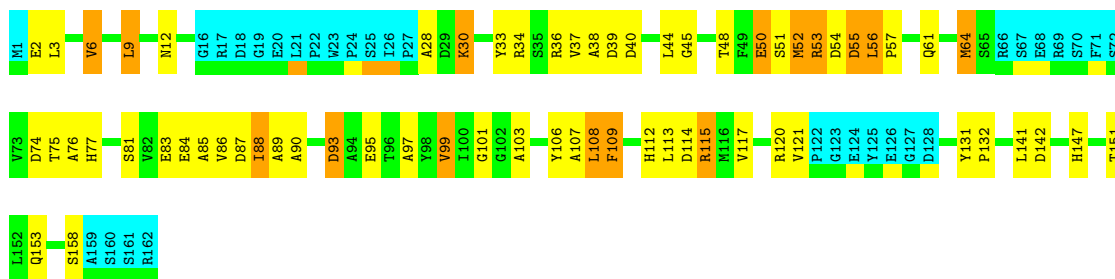
- Molecule 1: Dihydrofolate reductase





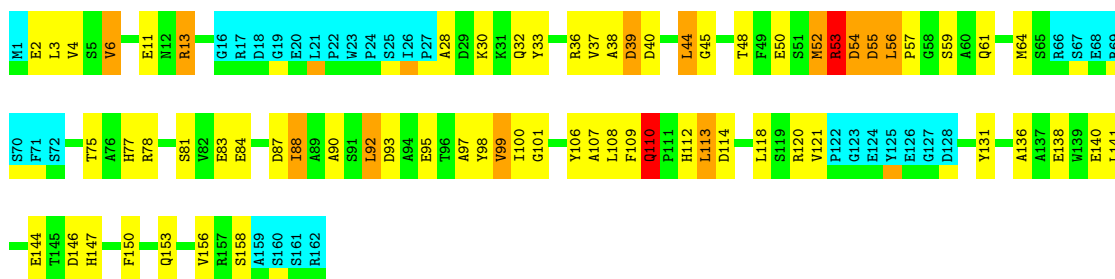
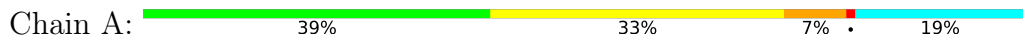
4.2.9 Score per residue for model 9

- Molecule 1: Dihydrofolate reductase



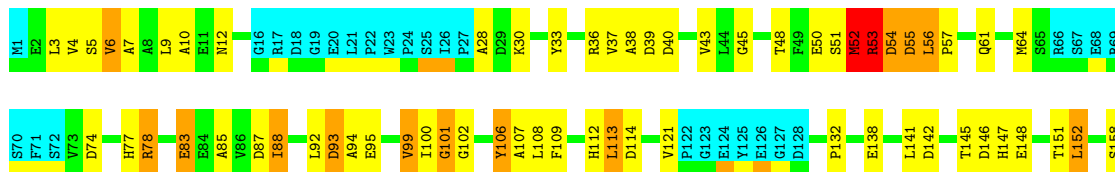
4.2.10 Score per residue for model 10

- Molecule 1: Dihydrofolate reductase



4.2.11 Score per residue for model 11

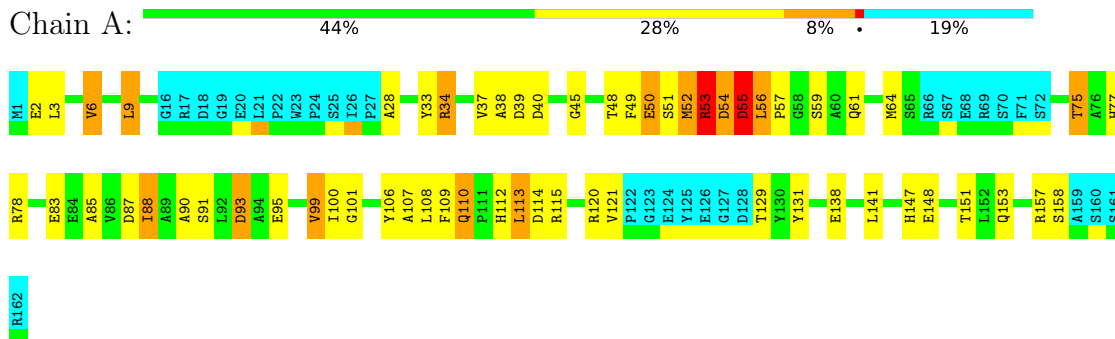
- Molecule 1: Dihydrofolate reductase





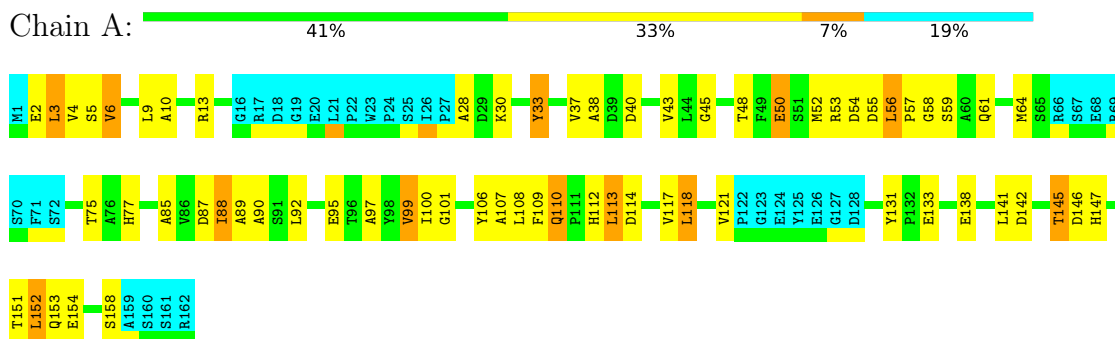
4.2.12 Score per residue for model 12

- Molecule 1: Dihydrofolate reductase



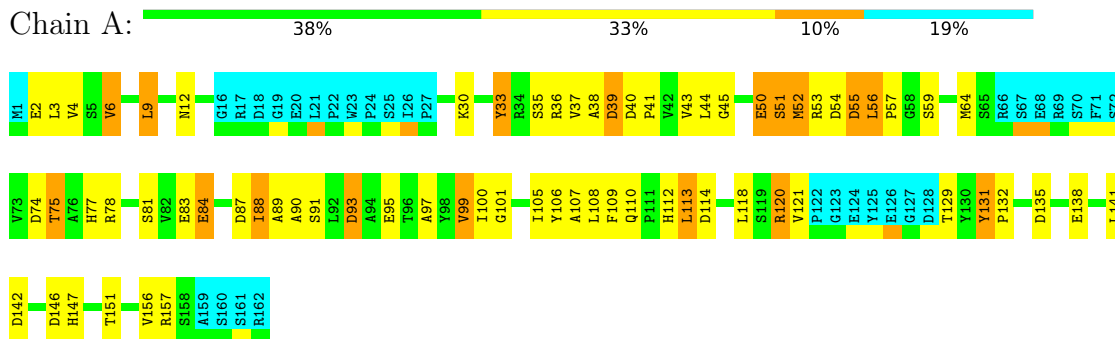
4.2.13 Score per residue for model 13

- Molecule 1: Dihydrofolate reductase



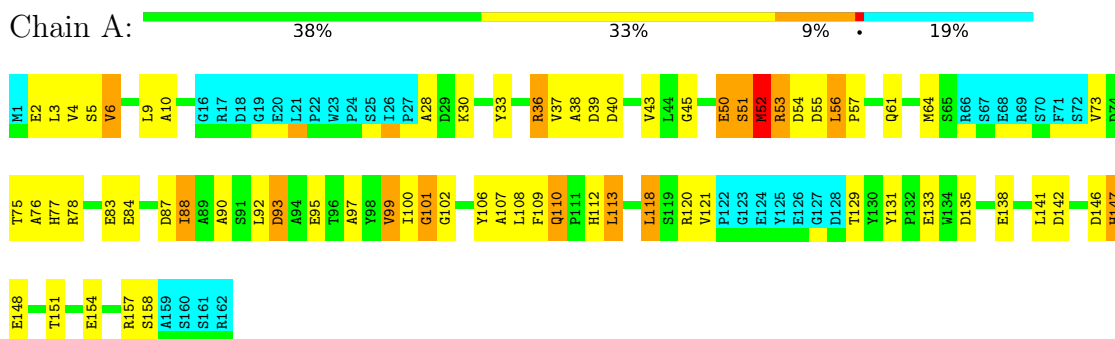
4.2.14 Score per residue for model 14

- Molecule 1: Dihydrofolate reductase



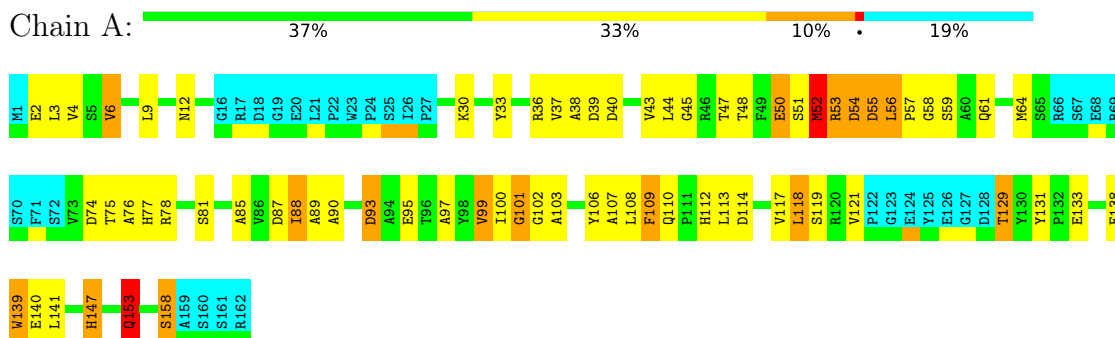
4.2.15 Score per residue for model 15

- Molecule 1: Dihydrofolate reductase



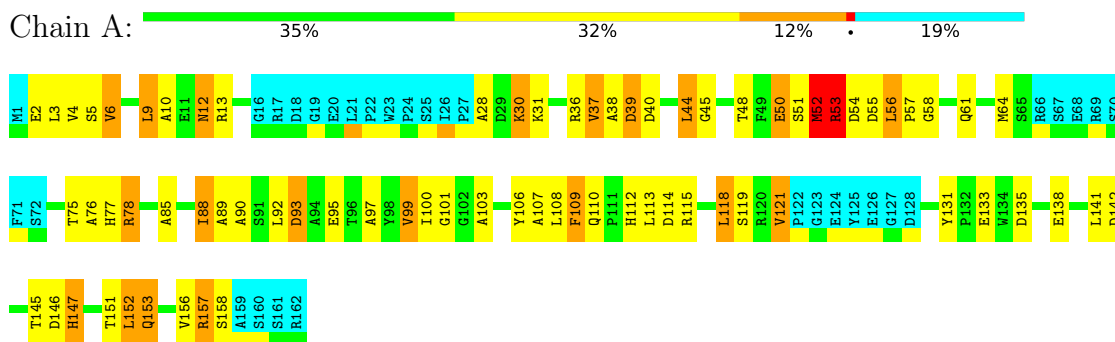
4.2.16 Score per residue for model 16

- Molecule 1: Dihydrofolate reductase



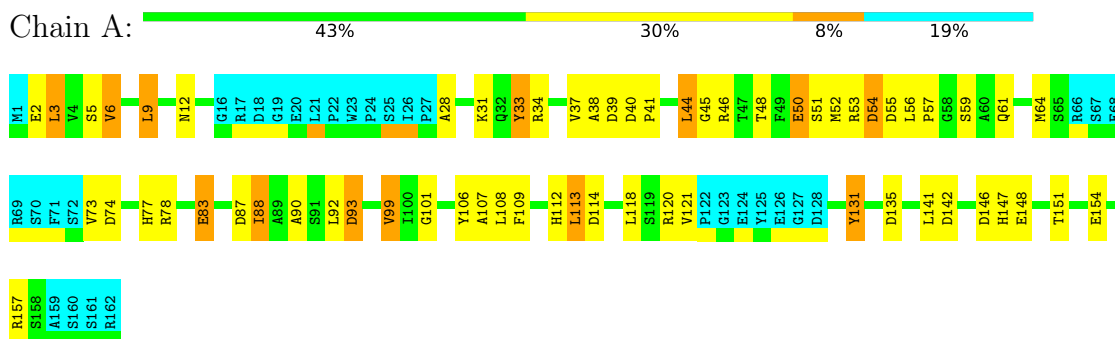
4.2.17 Score per residue for model 17 (medoid)

- Molecule 1: Dihydrofolate reductase



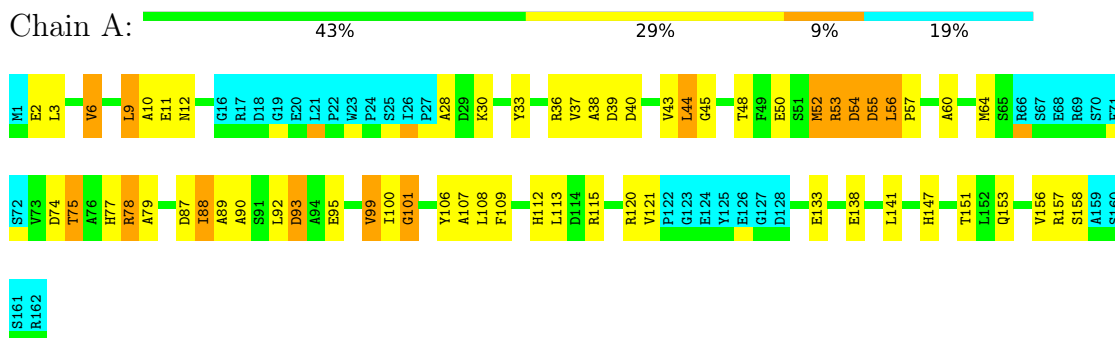
4.2.18 Score per residue for model 18

- Molecule 1: Dihydrofolate reductase



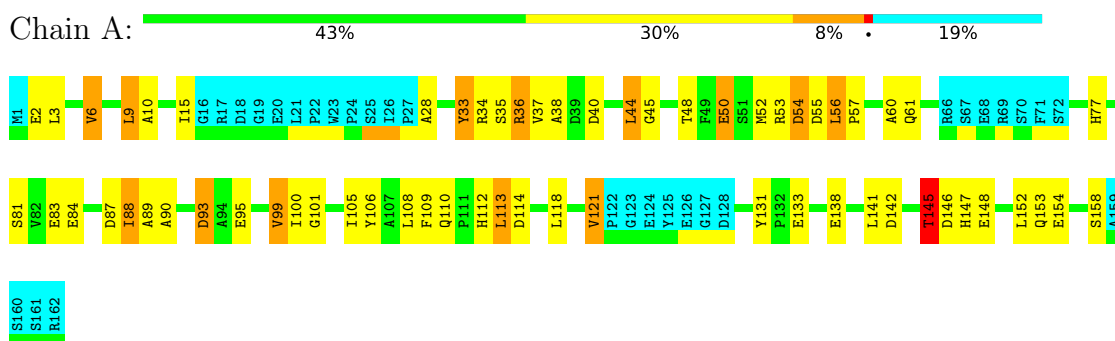
4.2.19 Score per residue for model 19

- Molecule 1: Dihydrofolate reductase



4.2.20 Score per residue for model 20

- Molecule 1: Dihydrofolate reductase



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 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
CNS	refinement	1.1

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1694
Number of shifts mapped to atoms	1694
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	82%

6 Model quality i

6.1 Standard geometry i

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	2.20±0.03	22±3/1044 (2.1± 0.3%)	2.18±0.03	43±3/1426 (3.0± 0.2%)
All	All	2.20	443/20880 (2.1%)	2.18	856/28520 (3.0%)

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	6.4±1.5
All	All	0	128

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
1	A	95	GLU	CA-C	9.32	1.59	1.52	19	13
1	A	6	VAL	CA-C	9.25	1.60	1.53	11	16
1	A	121	VAL	CA-C	8.90	1.60	1.53	18	19
1	A	54	ASP	CA-C	8.25	1.60	1.53	9	16
1	A	45	GLY	N-CA	7.63	1.50	1.44	14	18
1	A	6	VAL	CA-CB	7.35	1.61	1.53	11	6
1	A	147	HIS	CA-C	6.82	1.59	1.53	19	6
1	A	56	LEU	CA-C	6.55	1.61	1.53	16	19
1	A	30	LYS	CA-C	6.48	1.61	1.52	3	9
1	A	40	ASP	CA-C	6.34	1.60	1.53	15	20
1	A	110	GLN	CA-C	6.22	1.59	1.52	12	8
1	A	121	VAL	N-CA	6.21	1.51	1.46	10	7
1	A	58	GLY	N-CA	6.16	1.50	1.44	16	4
1	A	36	ARG	CA-C	5.98	1.58	1.53	10	5
1	A	55	ASP	CA-C	5.96	1.59	1.52	17	3
1	A	114	ASP	CA-C	5.91	1.60	1.52	14	17

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	131	TYR	CA-C	5.78	1.60	1.52	10	13
1	A	100	ILE	N-CA	5.77	1.53	1.46	3	5
1	A	39	ASP	CA-C	5.72	1.60	1.52	3	15
1	A	83	GLU	CA-C	5.71	1.60	1.52	14	10
1	A	147	HIS	CE1-NE2	5.69	1.38	1.32	15	18
1	A	53	ARG	CA-C	5.65	1.60	1.52	12	5
1	A	77	HIS	CA-C	5.65	1.59	1.52	12	6
1	A	77	HIS	CE1-NE2	5.61	1.38	1.32	2	17
1	A	156	VAL	CA-C	5.60	1.59	1.52	3	5
1	A	93	ASP	CA-CB	5.60	1.57	1.53	2	1
1	A	93	ASP	CA-C	5.60	1.59	1.53	2	1
1	A	81	SER	CA-C	5.60	1.58	1.53	2	2
1	A	112	HIS	ND1-CE1	5.59	1.38	1.32	11	18
1	A	99	VAL	CA-CB	5.57	1.62	1.54	20	8
1	A	117	VAL	CA-C	5.55	1.58	1.52	8	7
1	A	77	HIS	CG-CD2	5.53	1.42	1.35	12	1
1	A	97	ALA	CA-C	5.49	1.59	1.52	2	10
1	A	50	GLU	CA-C	5.47	1.60	1.52	18	3
1	A	75	THR	CA-C	5.46	1.60	1.52	19	7
1	A	9	LEU	CA-C	5.45	1.59	1.52	18	1
1	A	77	HIS	ND1-CE1	5.45	1.38	1.32	12	16
1	A	43	VAL	CA-C	5.45	1.59	1.52	16	8
1	A	103	ALA	N-CA	5.44	1.53	1.46	6	2
1	A	138	GLU	CA-C	5.43	1.59	1.52	2	15
1	A	65	SER	CA-C	5.39	1.58	1.53	7	1
1	A	73	VAL	CA-C	5.39	1.58	1.53	3	5
1	A	112	HIS	CE1-NE2	5.35	1.37	1.32	9	19
1	A	132	PRO	CA-C	5.31	1.58	1.53	7	1
1	A	139	TRP	CA-C	5.30	1.58	1.52	16	1
1	A	92	LEU	CA-C	5.28	1.57	1.53	17	1
1	A	147	HIS	CG-CD2	5.24	1.41	1.35	15	10
1	A	55	ASP	N-CA	5.23	1.52	1.46	17	1
1	A	112	HIS	CG-CD2	5.21	1.41	1.35	7	8
1	A	142	ASP	CA-C	5.20	1.59	1.52	9	2
1	A	51	SER	CA-C	5.20	1.59	1.52	4	2
1	A	8	ALA	CA-C	5.17	1.59	1.52	4	2
1	A	3	LEU	N-CA	5.14	1.52	1.45	8	2
1	A	4	VAL	CA-C	5.13	1.58	1.52	11	2
1	A	115	ARG	CA-C	5.08	1.58	1.52	9	1
1	A	119	SER	CA-C	5.06	1.58	1.52	5	1
1	A	7	ALA	CA-C	5.05	1.58	1.52	11	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	144	GLU	CA-C	5.04	1.58	1.52	10	1
1	A	153	GLN	CA-C	5.03	1.58	1.52	16	1
1	A	130	TYR	CA-C	5.03	1.58	1.52	6	1

All unique angle 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(°)	Ideal(°)	Models	
								Worst	Total
1	A	55	ASP	CA-CB-CG	14.99	127.59	112.60	17	13
1	A	39	ASP	CA-CB-CG	13.42	126.02	112.60	17	5
1	A	147	HIS	ND1-CE1-NE2	12.00	120.40	108.40	4	20
1	A	112	HIS	ND1-CE1-NE2	11.56	119.96	108.40	2	20
1	A	77	HIS	ND1-CE1-NE2	11.17	119.57	108.40	2	20
1	A	147	HIS	CE1-NE2-CD2	-10.91	98.09	109.00	6	20
1	A	112	HIS	CE1-NE2-CD2	-10.47	98.53	109.00	2	20
1	A	77	HIS	CE1-NE2-CD2	-10.38	98.62	109.00	2	20
1	A	77	HIS	CA-CB-CG	9.17	122.97	113.80	12	19
1	A	93	ASP	CA-CB-CG	9.00	121.60	112.60	3	17
1	A	52	MET	N-CA-C	8.19	122.98	112.34	9	19
1	A	158	SER	N-CA-C	8.09	120.80	109.15	3	12
1	A	50	GLU	CB-CG-CD	7.83	125.91	112.60	12	14
1	A	74	ASP	CA-CB-CG	7.73	120.33	112.60	18	4
1	A	154	GLU	CB-CG-CD	7.54	125.41	112.60	20	6
1	A	114	ASP	CA-CB-CG	7.49	120.09	112.60	4	9
1	A	109	PHE	N-CA-C	7.38	120.20	111.71	7	20
1	A	40	ASP	N-CA-C	7.33	120.18	110.36	17	20
1	A	88	ILE	N-CA-CB	7.29	121.51	110.58	17	20
1	A	53	ARG	N-CA-CB	-7.27	98.21	110.49	19	17
1	A	146	ASP	CA-CB-CG	7.18	119.78	112.60	5	13
1	A	100	ILE	N-CA-CB	7.09	118.84	110.55	13	13
1	A	2	GLU	CB-CA-C	7.06	124.47	110.42	8	18
1	A	142	ASP	CA-CB-CG	6.90	119.50	112.60	8	13
1	A	135	ASP	CA-CB-CG	6.87	119.47	112.60	14	2
1	A	38	ALA	N-CA-C	6.82	119.74	111.82	12	20
1	A	48	THR	N-CA-C	6.78	118.67	111.28	5	16
1	A	101	GLY	O-C-N	-6.77	116.08	123.05	15	4
1	A	91	SER	N-CA-C	6.69	119.41	111.71	12	4
1	A	88	ILE	N-CA-C	6.64	117.43	110.72	6	19
1	A	84	GLU	N-CA-C	6.62	119.32	111.71	3	8
1	A	6	VAL	CB-CA-C	6.60	117.89	111.23	8	6
1	A	87	ASP	CA-CB-CG	6.56	119.16	112.60	11	18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	153	GLN	OE1-CD-NE2	-6.55	116.05	122.60	10	12
1	A	54	ASP	CA-CB-CG	6.54	119.14	112.60	12	3
1	A	92	LEU	CB-CA-C	6.53	123.41	110.42	2	8
1	A	28	ALA	N-CA-C	6.52	118.39	111.28	1	16
1	A	107	ALA	N-CA-C	6.43	118.29	111.28	19	17
1	A	93	ASP	N-CA-C	6.42	117.98	110.41	3	1
1	A	36	ARG	N-CA-CB	-6.29	100.70	110.39	10	10
1	A	157	ARG	N-CA-C	6.23	118.83	110.35	3	12
1	A	40	ASP	CA-CB-CG	6.21	118.81	112.60	17	11
1	A	103	ALA	N-CA-CB	-6.18	100.05	110.49	6	9
1	A	90	ALA	N-CA-C	6.11	118.91	111.82	4	19
1	A	9	LEU	N-CA-C	6.11	118.13	108.79	19	14
1	A	112	HIS	CA-CB-CG	6.08	119.88	113.80	7	11
1	A	60	ALA	N-CA-C	6.05	117.97	108.96	19	4
1	A	6	VAL	CA-CB-CG2	6.02	120.64	110.40	9	18
1	A	118	LEU	N-CA-CB	-6.00	101.67	110.26	5	5
1	A	85	ALA	N-CA-C	5.98	117.60	111.14	1	9
1	A	138	GLU	CB-CG-CD	5.96	122.73	112.60	2	2
1	A	89	ALA	N-CA-C	5.89	117.38	111.07	17	15
1	A	55	ASP	CB-CA-C	5.88	119.44	109.75	12	2
1	A	31	LYS	N-CA-C	5.87	117.67	111.28	18	1
1	A	59	SER	N-CA-C	5.79	119.82	112.87	18	8
1	A	99	VAL	CA-CB-CG2	5.79	120.24	110.40	17	20
1	A	114	ASP	N-CA-CB	-5.77	101.64	110.01	9	2
1	A	44	LEU	N-CA-C	5.77	116.70	108.74	8	10
1	A	41	PRO	N-CA-C	5.75	120.10	111.14	4	4
1	A	132	PRO	N-CA-C	5.74	119.25	111.22	11	5
1	A	94	ALA	N-CA-C	5.72	118.10	109.23	2	4
1	A	29	ASP	CA-CB-CG	5.70	118.30	112.60	1	1
1	A	118	LEU	CB-CA-C	5.68	121.44	109.79	17	2
1	A	75	THR	CA-CB-CG2	5.67	120.15	110.50	17	5
1	A	49	PHE	CA-CB-CG	5.67	119.47	113.80	12	2
1	A	94	ALA	N-CA-CB	-5.66	102.45	111.62	3	1
1	A	51	SER	N-CA-C	5.66	117.31	111.03	16	2
1	A	79	ALA	N-CA-CB	-5.66	101.52	110.06	19	1
1	A	54	ASP	CB-CA-C	5.65	121.67	110.42	7	2
1	A	34	ARG	N-CA-C	5.65	120.02	113.18	9	3
1	A	100	ILE	N-CA-C	5.64	115.84	110.42	10	2
1	A	10	ALA	N-CA-CB	-5.64	100.96	110.49	19	7
1	A	131	TYR	N-CA-CB	-5.63	103.20	109.74	18	7
1	A	61	GLN	OE1-CD-NE2	-5.62	116.97	122.60	17	9

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	4	VAL	O-C-N	-5.61	117.34	123.18	17	5
1	A	133	GLU	N-CA-C	5.60	118.13	110.24	6	1
1	A	65	SER	O-C-N	-5.54	118.95	123.11	7	1
1	A	48	THR	CA-CB-CG2	5.50	119.84	110.50	5	2
1	A	5	SER	N-CA-C	5.49	117.67	108.73	18	4
1	A	99	VAL	CA-CB-CG1	5.46	119.68	110.40	1	2
1	A	156	VAL	N-CA-C	5.45	116.08	108.89	3	1
1	A	5	SER	N-CA-CB	-5.44	101.84	110.06	1	2
1	A	30	LYS	N-CA-C	5.43	119.40	112.34	17	2
1	A	37	VAL	CA-CB-CG1	5.43	119.63	110.40	17	2
1	A	148	GLU	N-CA-C	5.42	117.00	111.14	5	7
1	A	136	ALA	N-CA-CB	-5.38	103.84	111.00	10	2
1	A	13	ARG	N-CA-C	5.37	118.65	111.24	10	1
1	A	32	GLN	CB-CA-C	5.34	119.23	110.95	2	1
1	A	145	THR	CA-CB-CG2	5.32	119.54	110.50	1	5
1	A	86	VAL	CB-CA-C	5.31	118.98	112.02	9	1
1	A	53	ARG	N-CA-C	5.31	122.11	110.80	19	1
1	A	103	ALA	N-CA-C	5.30	117.47	111.11	7	1
1	A	112	HIS	CG-ND1-CE1	-5.28	100.33	109.30	14	18
1	A	50	GLU	CB-CA-C	5.26	121.30	110.31	18	2
1	A	87	ASP	N-CA-C	5.24	116.99	111.28	7	1
1	A	110	GLN	N-CA-C	5.23	121.38	109.81	16	2
1	A	147	HIS	CG-ND1-CE1	-5.21	100.44	109.30	4	7
1	A	78	ARG	CA-CB-CG	5.19	124.48	114.10	19	1
1	A	114	ASP	CB-CA-C	5.18	119.01	110.88	8	2
1	A	150	PHE	CA-CB-CG	5.14	118.94	113.80	5	3
1	A	77	HIS	CG-ND1-CE1	-5.14	100.56	109.30	5	3
1	A	2	GLU	CB-CG-CD	5.13	121.33	112.60	8	1
1	A	110	GLN	OE1-CD-NE2	-5.11	117.49	122.60	13	1
1	A	35	SER	N-CA-C	5.10	117.74	111.82	14	1
1	A	121	VAL	N-CA-C	5.08	112.58	107.55	17	1
1	A	3	LEU	N-CA-C	5.06	118.00	109.95	18	1
1	A	12	ASN	N-CA-C	5.06	118.74	112.47	17	1
1	A	150	PHE	N-CA-C	5.04	115.95	108.60	5	1
1	A	11	GLU	CB-CG-CD	5.04	121.16	112.60	19	1
1	A	119	SER	CB-CA-C	5.01	117.86	110.14	17	1
1	A	151	THR	CA-CB-CG2	5.01	119.01	110.50	7	1
1	A	61	GLN	CB-CG-CD	5.00	121.11	112.60	8	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	101	GLY	Peptide,Mainchain	20
1	A	50	GLU	Peptide	19
1	A	106	TYR	Sidechain	19
1	A	113	LEU	Peptide	16
1	A	52	MET	Peptide	9
1	A	102	GLY	Peptide	7
1	A	115	ARG	Sidechain	6
1	A	76	ALA	Peptide	6
1	A	33	TYR	Sidechain	5
1	A	98	TYR	Sidechain	3
1	A	53	ARG	Sidechain	3
1	A	120	ARG	Sidechain	3
1	A	78	ARG	Sidechain	2
1	A	34	ARG	Sidechain	1
1	A	13	ARG	Sidechain	1
1	A	157	ARG	Sidechain	1
1	A	46	ARG	Sidechain	1
1	A	35	SER	Peptide	1
1	A	36	ARG	Sidechain	1

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1023	979	979	1±1
All	All	20460	19580	19580	25

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 1.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:145:THR:HG22	1:A:152:LEU:HD12	0.56	1.74	1	6
1:A:47:THR:HG21	1:A:129:THR:OG1	0.54	2.03	16	1
1:A:52:MET:SD	1:A:55:ASP:O	0.47	2.73	4	5
1:A:64:MET:SD	1:A:108:LEU:HD11	0.47	2.50	9	2
1:A:118:LEU:HD12	1:A:131:TYR:CZ	0.46	2.45	8	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:118:LEU:HD23	1:A:153:GLN:HB3	0.45	1.86	16	1
1:A:64:MET:SD	1:A:109:PHE:CE2	0.41	3.13	1	3

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	131/162 (81%)	107±2 (82±2%)	20±3 (15±2%)	4±1 (3±1%)	6	40
All	All	2620/3240 (81%)	2148 (82%)	398 (15%)	74 (3%)	6	40

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

Mol	Chain	Res	Type	Models (Total)
1	A	57	PRO	20
1	A	93	ASP	14
1	A	53	ARG	11
1	A	75	THR	8
1	A	51	SER	6
1	A	158	SER	6
1	A	110	GLN	3
1	A	105	ILE	2
1	A	92	LEU	1
1	A	100	ILE	1
1	A	47	THR	1
1	A	52	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	106/132 (80%)	82±3 (78±2%)	24±3 (22±2%)	2	29
All	All	2120/2640 (80%)	1645 (78%)	475 (22%)	2	29

All 62 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	3	LEU	20
1	A	6	VAL	20
1	A	37	VAL	20
1	A	56	LEU	20
1	A	88	ILE	20
1	A	99	VAL	20
1	A	108	LEU	20
1	A	141	LEU	20
1	A	9	LEU	19
1	A	113	LEU	19
1	A	64	MET	18
1	A	33	TYR	17
1	A	55	ASP	17
1	A	151	THR	15
1	A	54	ASP	14
1	A	78	ARG	14
1	A	12	ASN	11
1	A	44	LEU	10
1	A	133	GLU	9
1	A	30	LYS	8
1	A	92	LEU	7
1	A	118	LEU	7
1	A	51	SER	7
1	A	120	ARG	7
1	A	110	GLN	6
1	A	74	ASP	6
1	A	53	ARG	6
1	A	81	SER	6
1	A	52	MET	5
1	A	119	SER	5
1	A	152	LEU	5
1	A	153	GLN	5
1	A	31	LYS	5
1	A	75	THR	5
1	A	129	THR	5
1	A	36	ARG	5

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Mol	Chain	Res	Type	Models (Total)
1	A	39	ASP	5
1	A	147	HIS	5
1	A	140	GLU	3
1	A	139	TRP	3
1	A	61	GLN	3
1	A	83	GLU	3
1	A	145	THR	2
1	A	138	GLU	2
1	A	15	ILE	2
1	A	93	ASP	2
1	A	148	GLU	2
1	A	106	TYR	2
1	A	13	ARG	2
1	A	84	GLU	2
1	A	135	ASP	2
1	A	34	ARG	2
1	A	96	THR	1
1	A	2	GLU	1
1	A	144	GLU	1
1	A	14	VAL	1
1	A	11	GLU	1
1	A	32	GLN	1
1	A	115	ARG	1
1	A	158	SER	1
1	A	109	PHE	1
1	A	121	VAL	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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 [i](#)

The completeness of assignment taking into account all chemical shift lists is 82% for the well-defined parts and 79% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping [i](#)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1694
Number of shifts mapped to atoms	1694
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	159	-0.25 ± 0.08	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	147	0.53 ± 0.13	Should be checked
$^{13}\text{C}'$	148	-0.15 ± 0.14	None needed (< 0.5 ppm)
^{15}N	147	0.25 ± 0.09	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 82%, i.e. 1427 atoms were assigned a chemical shift out of a possible 1743. 0 out of 24 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	634/652 (97%)	257/263 (98%)	253/262 (97%)	124/127 (98%)
Sidechain	793/959 (83%)	545/627 (87%)	248/298 (83%)	0/34 (0%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	0/132 (0%)	0/65 (0%)	0/61 (0%)	0/6 (0%)
Overall	1427/1743 (82%)	802/955 (84%)	501/621 (81%)	124/167 (74%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 79%, i.e. 1694 atoms were assigned a chemical shift out of a possible 2136. 0 out of 25 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	767/803 (96%)	313/325 (96%)	307/324 (95%)	147/154 (95%)
Sidechain	927/1170 (79%)	635/761 (83%)	292/363 (80%)	0/46 (0%)
Aromatic	0/163 (0%)	0/80 (0%)	0/76 (0%)	0/7 (0%)
Overall	1694/2136 (79%)	948/1166 (81%)	599/763 (79%)	147/207 (71%)

7.1.4 Statistically unusual chemical shifts [i](#)

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	22	PRO	CB	25.44	26.06 – 37.61	-5.5

7.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:

