



# Full wwPDB NMR Structure Validation Report ⓘ

Feb 9, 2022 – 08:22 AM EST

PDB ID : 1DIU  
Title : DIHYDROFOLATE REDUCTASE (E.C.1.5.1.3) COMPLEX WITH BRODI  
MOPRIM-4,6-DICARBOXYLATE  
Authors : Morgan, W.D.; Birdsall, B.; Polshakov, V.I.; Sali, D.; Kompis, I.; Feeney, J.  
Deposited on : 1995-08-01

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We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : 2.26  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.26

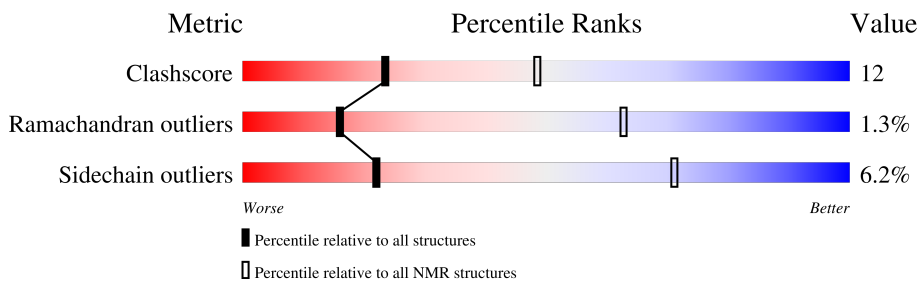
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment was not calculated.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	

## 2 Ensemble composition and analysis

This entry contains 18 models. Model 15 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:28, A:34-A:162 (157)	0.02	15

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. No single-model clusters were found.

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

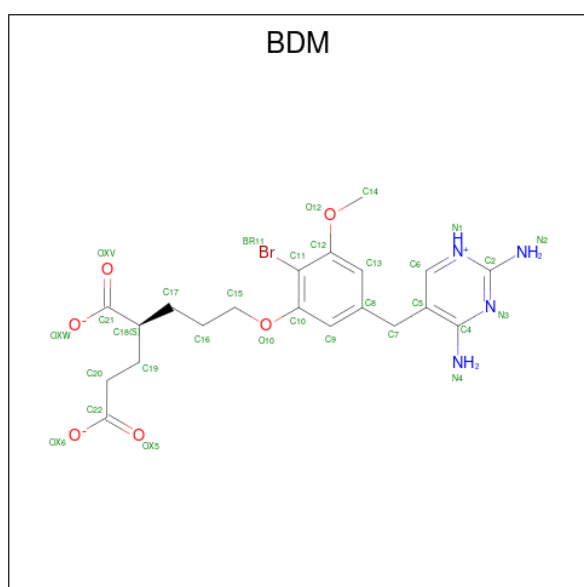
### 3 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 2618 atoms, of which 1290 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	2563	828	1266	225	242	2	0

- Molecule 2 is BRODIMOPRIM-4,6-DICARBOXYLATE (three-letter code: BDM) (formula:  $C_{20}H_{24}BrN_4O_6$ ).



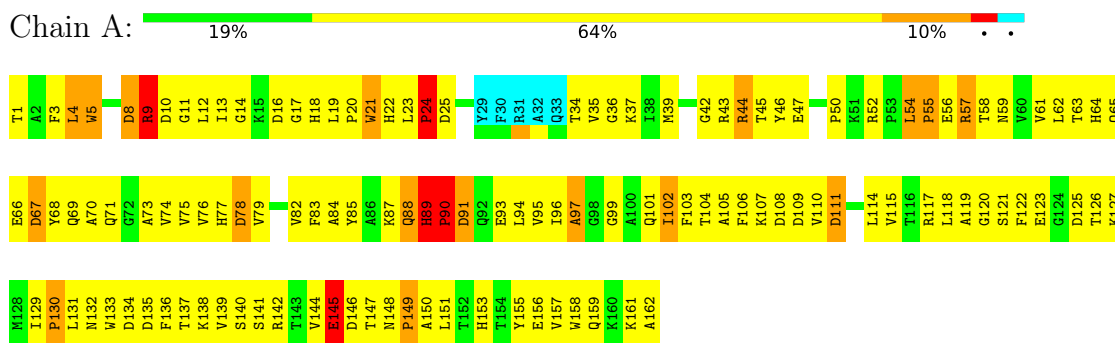
Mol	Chain	Residues	Atoms					
			Total	Br	C	H	N	O
2	A	1	55	1	20	24	4	6

## 4 Residue-property plots [i](#)

### 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.

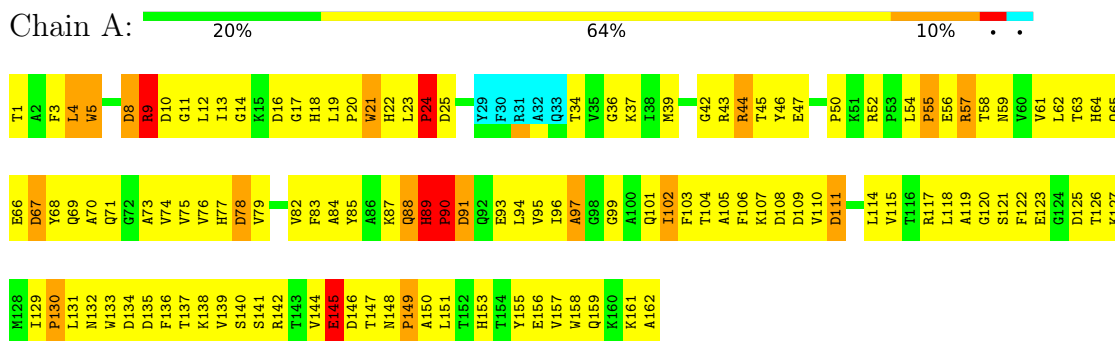
#### 4.2.1 Score per residue for model 1

- Molecule 1: DIHYDROFOLATE REDUCTASE



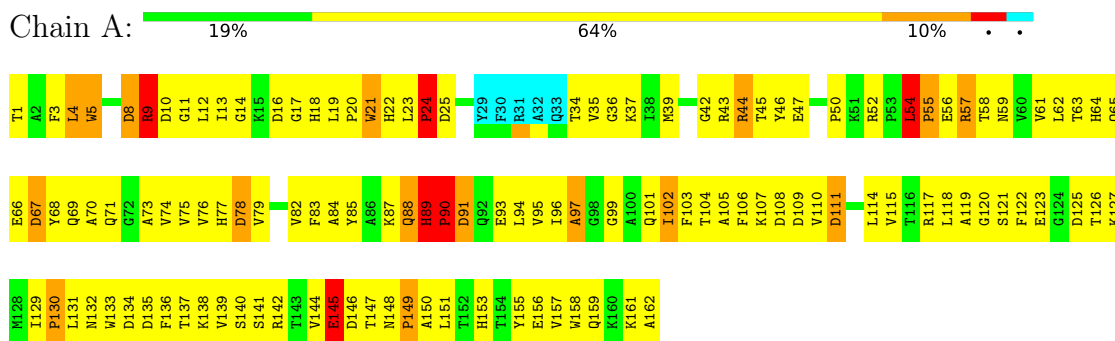
### 4.2.2 Score per residue for model 2

- Molecule 1: DIHYDROFOLATE REDUCTASE



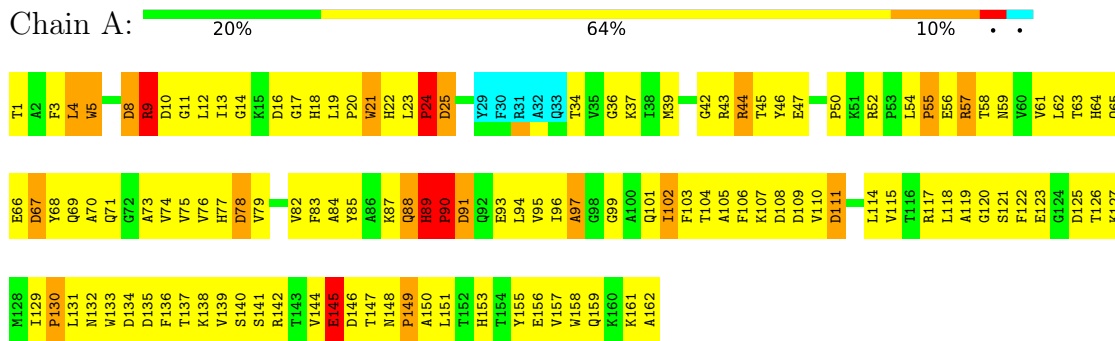
### 4.2.3 Score per residue for model 3

- Molecule 1: DIHYDROFOLATE REDUCTASE



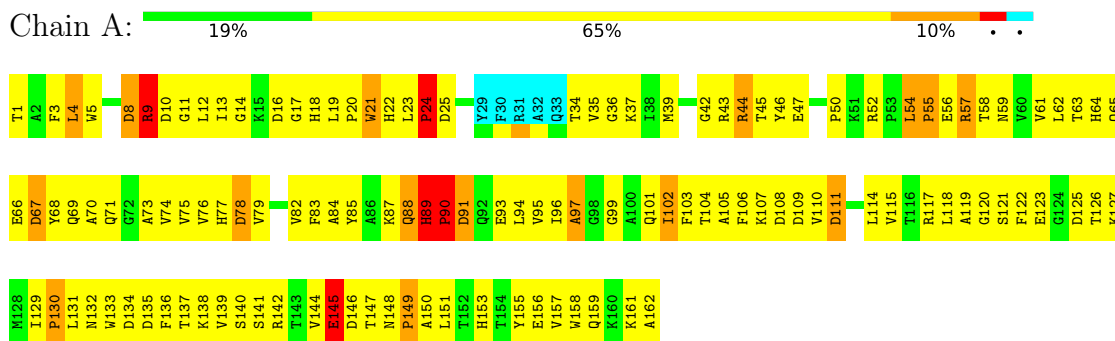
### 4.2.4 Score per residue for model 4

- Molecule 1: DIHYDROFOLATE REDUCTASE



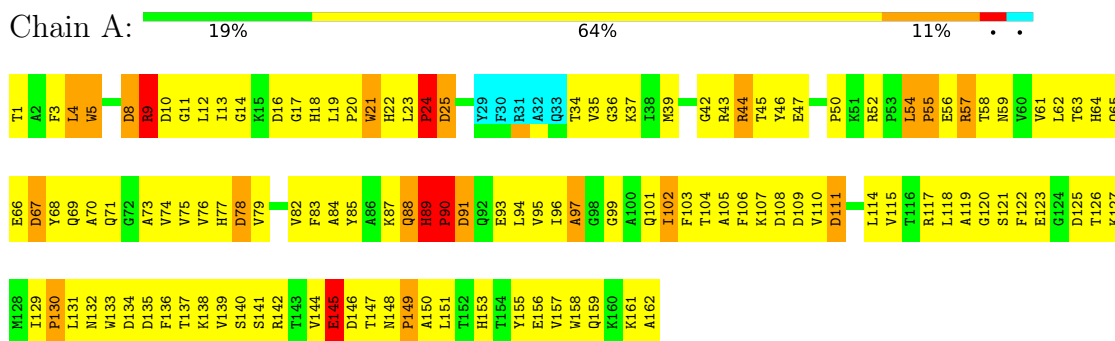
### 4.2.5 Score per residue for model 5

#### • Molecule 1: DIHYDROFOLATE REDUCTASE



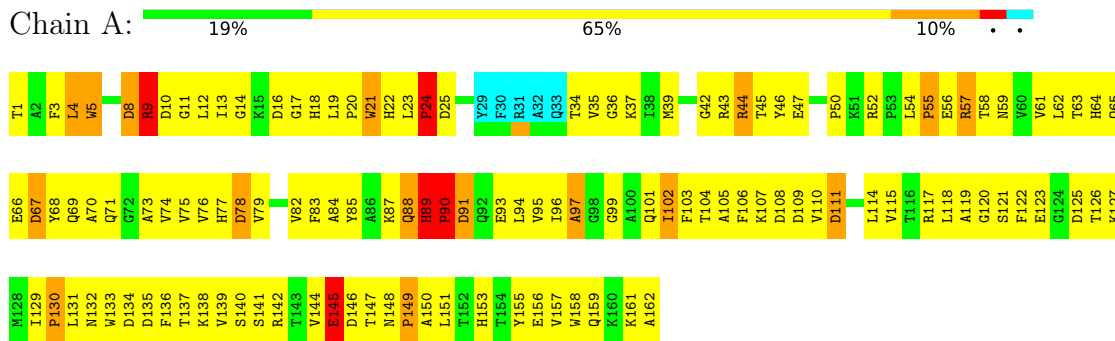
### 4.2.6 Score per residue for model 6

#### • Molecule 1: DIHYDROFOLATE REDUCTASE



### 4.2.7 Score per residue for model 7

#### • Molecule 1: DIHYDROFOLATE REDUCTASE

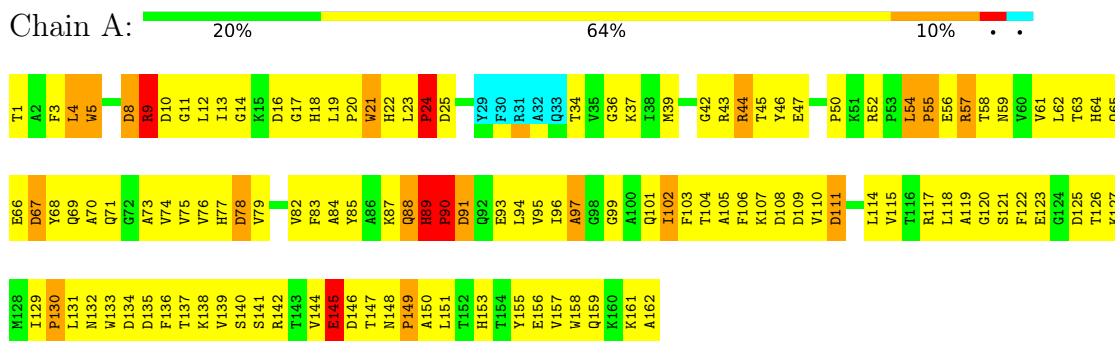






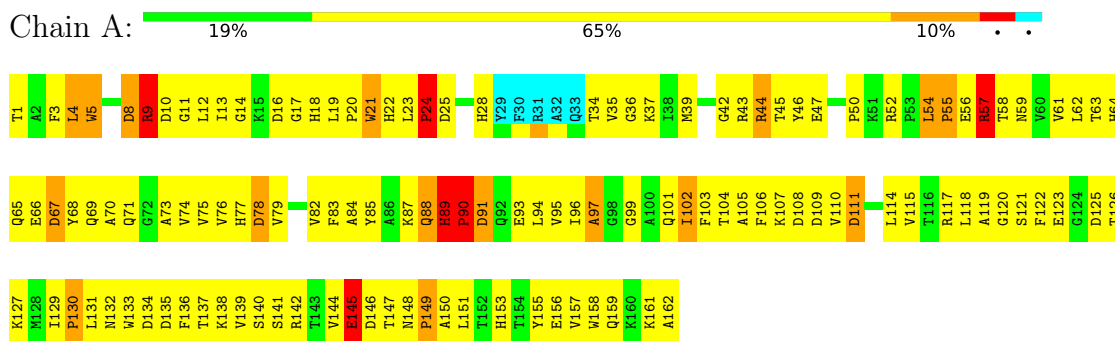
### 4.2.11 Score per residue for model 11

#### • Molecule 1: DIHYDROFOLATE REDUCTASE



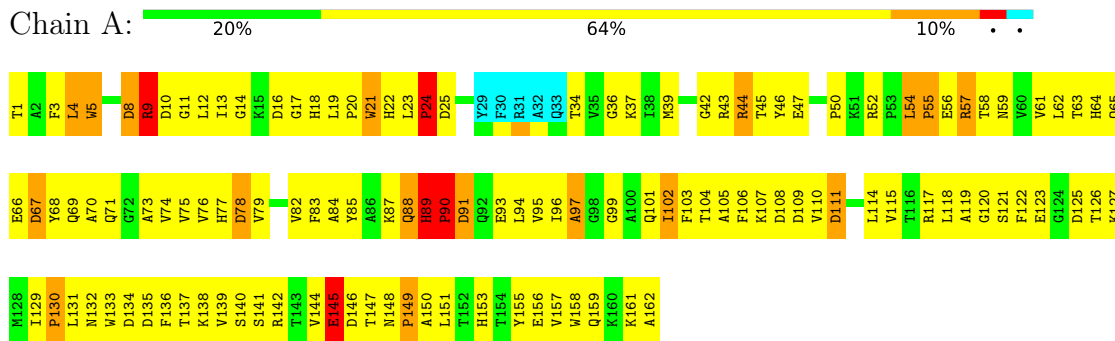
### 4.2.12 Score per residue for model 12

#### • Molecule 1: DIHYDROFOLATE REDUCTASE



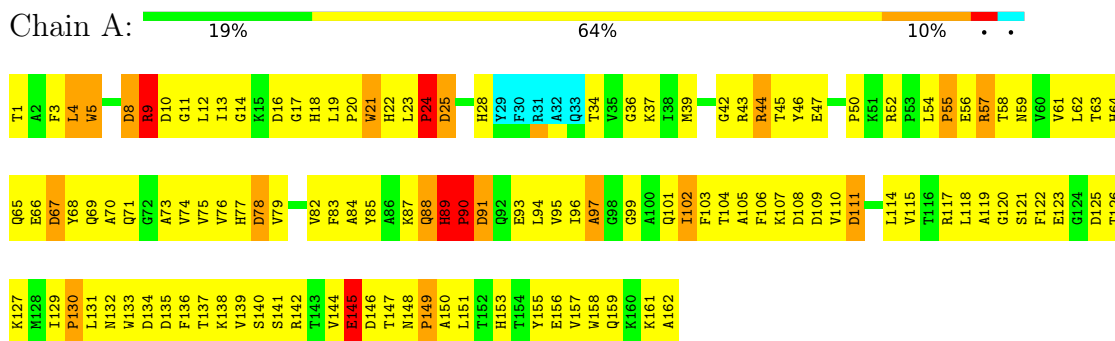
### 4.2.13 Score per residue for model 13

#### • Molecule 1: DIHYDROFOLATE REDUCTASE



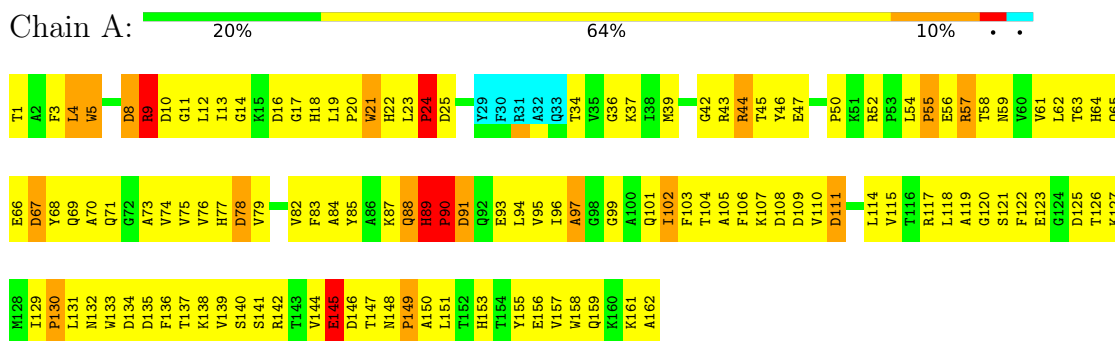
## 4.2.14 Score per residue for model 14

## • Molecule 1: DIHYDROFOLATE REDUCTASE



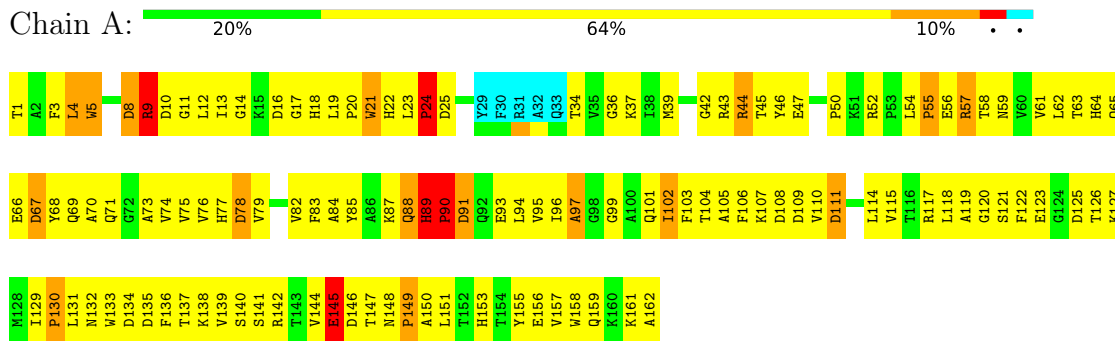
## 4.2.15 Score per residue for model 15 (medoid)

## • Molecule 1: DIHYDROFOLATE REDUCTASE



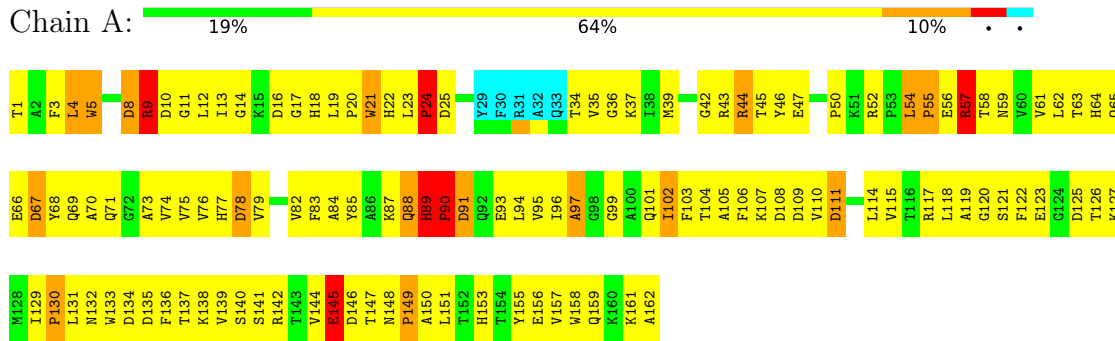
## 4.2.16 Score per residue for model 16

## • Molecule 1: DIHYDROFOLATE REDUCTASE



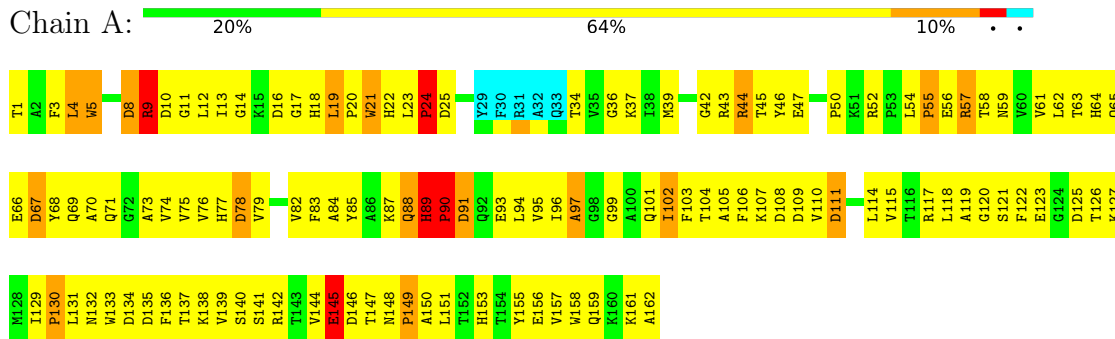
### 4.2.17 Score per residue for model 17

- Molecule 1: DIHYDROFOLATE REDUCTASE



### 4.2.18 Score per residue for model 18

- Molecule 1: DIHYDROFOLATE REDUCTASE



## 5 Refinement protocol and experimental data overview

Of the ? calculated structures, 18 were deposited, based on the following criterion: ?.

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

Software name	Classification	Version
Discover	refinement	

No chemical shift data was provided.

## 6 Model quality i

### 6.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: BDM

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	3.96±0.00	136±0/1282 ( 10.6± 0.0%)	5.23±0.00	307±1/1747 ( 17.6± 0.0%)
All	All	3.96	2448/23076 ( 10.6%)	5.23	5534/31446 ( 17.6%)

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	1.0±0.0	5.5±0.6
All	All	18	99

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	90	PRO	N-CD	73.02	2.50	1.47	1	18
1	A	145	GLU	CD-OE2	22.01	1.49	1.25	1	18
1	A	24	PRO	N-CD	21.82	1.78	1.47	1	18
1	A	89	HIS	C-N	-19.65	0.96	1.34	1	18
1	A	130	PRO	N-CD	18.06	1.73	1.47	1	18
1	A	89	HIS	C-O	18.04	1.57	1.23	1	18
1	A	142	ARG	NE-CZ	16.83	1.54	1.33	1	18
1	A	149	PRO	N-CD	16.21	1.70	1.47	1	18
1	A	55	PRO	N-CD	15.24	1.69	1.47	1	18
1	A	67	ASP	CA-CB	15.22	1.87	1.53	1	18
1	A	145	GLU	CD-OE1	14.48	1.41	1.25	1	18
1	A	145	GLU	CB-CG	13.38	1.77	1.52	1	18
1	A	117	ARG	NE-CZ	-13.30	1.15	1.33	1	18
1	A	20	PRO	N-CD	12.98	1.66	1.47	1	18

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	140	SER	CA-CB	11.89	1.70	1.52	1	18
1	A	117	ARG	CZ-NH1	11.59	1.48	1.33	1	18
1	A	19	LEU	C-N	11.41	1.55	1.34	1	18
1	A	121	SER	CB-OG	-10.90	1.28	1.42	1	18
1	A	67	ASP	CG-OD1	10.82	1.50	1.25	1	18
1	A	129	ILE	C-N	10.79	1.54	1.34	1	18
1	A	108	ASP	CB-CG	10.54	1.73	1.51	1	18
1	A	90	PRO	N-CA	10.29	1.64	1.47	1	18
1	A	123	GLU	CD-OE1	9.80	1.36	1.25	1	18
1	A	105	ALA	C-O	9.77	1.42	1.23	1	18
1	A	67	ASP	CG-OD2	9.76	1.47	1.25	1	18
1	A	44	ARG	CZ-NH1	9.48	1.45	1.33	1	18
1	A	18	HIS	CD2-NE2	9.46	1.61	1.42	1	18
1	A	145	GLU	CG-CD	9.42	1.66	1.51	1	18
1	A	109	ASP	CB-CG	9.15	1.71	1.51	1	18
1	A	93	GLU	CD-OE1	9.12	1.35	1.25	1	18
1	A	140	SER	CB-OG	-9.06	1.30	1.42	1	18
1	A	142	ARG	CZ-NH1	8.97	1.44	1.33	1	18
1	A	148	ASN	C-N	8.88	1.51	1.34	1	18
1	A	23	LEU	C-N	8.77	1.50	1.34	1	18
1	A	162	ALA	C-O	8.45	1.39	1.23	1	18
1	A	44	ARG	CD-NE	-8.44	1.32	1.46	1	18
1	A	56	GLU	CB-CG	8.17	1.67	1.52	1	18
1	A	134	ASP	CG-OD1	8.15	1.44	1.25	1	18
1	A	78	ASP	C-O	8.08	1.38	1.23	1	18
1	A	133	TRP	CD2-CE2	7.84	1.50	1.41	1	18
1	A	78	ASP	CG-OD2	7.83	1.43	1.25	1	18
1	A	91	ASP	CA-CB	7.78	1.71	1.53	1	18
1	A	134	ASP	CG-OD2	7.74	1.43	1.25	1	18
1	A	158	TRP	CZ3-CH2	7.73	1.52	1.40	1	18
1	A	99	GLY	CA-C	-7.63	1.39	1.51	1	18
1	A	3	PHE	CG-CD1	7.63	1.50	1.38	1	18
1	A	106	PHE	CE2-CZ	7.50	1.51	1.37	1	18
1	A	17	GLY	N-CA	7.50	1.57	1.46	1	18
1	A	23	LEU	C-O	-7.41	1.09	1.23	1	18
1	A	162	ALA	C-OXT	7.40	1.37	1.23	1	18
1	A	14	GLY	CA-C	7.31	1.63	1.51	1	18
1	A	85	TYR	CG-CD2	7.24	1.48	1.39	1	18
1	A	87	LYS	CD-CE	7.22	1.69	1.51	1	18
1	A	56	GLU	CD-OE1	7.16	1.33	1.25	1	18
1	A	9	ARG	CZ-NH2	7.15	1.42	1.33	1	18

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	159	GLN	CB-CG	7.12	1.71	1.52	1	18
1	A	68	TYR	CE1-CZ	7.09	1.47	1.38	1	18
1	A	20	PRO	N-CA	7.09	1.59	1.47	1	18
1	A	135	ASP	CA-C	7.05	1.71	1.52	1	18
1	A	134	ASP	CA-CB	6.93	1.69	1.53	1	18
1	A	65	GLN	CD-NE2	6.91	1.50	1.32	1	18
1	A	22	HIS	CG-CD2	6.89	1.47	1.35	1	18
1	A	19	LEU	C-O	-6.84	1.10	1.23	1	18
1	A	16	ASP	CA-CB	6.83	1.69	1.53	1	18
1	A	107	LYS	CD-CE	6.80	1.68	1.51	1	18
1	A	132	ASN	N-CA	6.77	1.59	1.46	1	18
1	A	13	ILE	C-N	6.76	1.45	1.33	1	18
1	A	9	ARG	CZ-NH1	6.75	1.41	1.33	1	18
1	A	66	GLU	CD-OE2	6.69	1.33	1.25	1	18
1	A	9	ARG	CG-CD	6.69	1.68	1.51	1	18
1	A	66	GLU	CB-CG	6.61	1.64	1.52	1	18
1	A	148	ASN	C-O	-6.43	1.11	1.23	1	18
1	A	18	HIS	CG-ND1	6.30	1.52	1.38	1	18
1	A	135	ASP	CB-CG	6.28	1.65	1.51	1	18
1	A	123	GLU	CA-CB	6.21	1.67	1.53	1	18
1	A	46	TYR	CG-CD1	6.18	1.47	1.39	1	18
1	A	67	ASP	C-N	6.18	1.48	1.34	1	18
1	A	108	ASP	CG-OD2	6.17	1.39	1.25	1	18
1	A	132	ASN	CB-CG	6.17	1.65	1.51	1	18
1	A	77	HIS	CA-CB	6.12	1.67	1.53	1	18
1	A	137	THR	C-O	6.12	1.34	1.23	1	18
1	A	44	ARG	CZ-NH2	6.10	1.41	1.33	1	18
1	A	125	ASP	CG-OD1	6.01	1.39	1.25	1	18
1	A	24	PRO	CA-CB	5.99	1.65	1.53	1	18
1	A	117	ARG	CB-CG	-5.98	1.36	1.52	1	18
1	A	47	GLU	CD-OE1	-5.96	1.19	1.25	1	18
1	A	144	VAL	CB-CG2	-5.92	1.40	1.52	1	18
1	A	95	VAL	CA-C	5.86	1.68	1.52	1	18
1	A	91	ASP	CG-OD1	5.85	1.38	1.25	1	18
1	A	91	ASP	C-O	5.82	1.34	1.23	1	18
1	A	149	PRO	C-O	5.78	1.34	1.23	1	18
1	A	162	ALA	CA-C	5.78	1.68	1.52	1	18
1	A	132	ASN	C-O	5.73	1.34	1.23	1	18
1	A	158	TRP	CG-CD1	5.71	1.44	1.36	1	18
1	A	111	ASP	CG-OD1	5.71	1.38	1.25	1	18
1	A	8	ASP	N-CA	5.69	1.57	1.46	1	18

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	83	PHE	CE1-CZ	5.65	1.48	1.37	1	18
1	A	122	PHE	CG-CD1	5.57	1.47	1.38	1	18
1	A	106	PHE	CB-CG	-5.56	1.42	1.51	1	18
1	A	43	ARG	NE-CZ	5.54	1.40	1.33	1	18
1	A	131	LEU	C-O	5.52	1.33	1.23	1	18
1	A	64	HIS	CG-ND1	-5.50	1.26	1.38	1	18
1	A	139	VAL	CA-CB	5.50	1.66	1.54	1	18
1	A	79	VAL	CB-CG1	-5.48	1.41	1.52	1	18
1	A	156	GLU	CB-CG	5.45	1.62	1.52	1	18
1	A	25	ASP	CB-CG	-5.44	1.40	1.51	1	18
1	A	46	TYR	CG-CD2	5.42	1.46	1.39	1	18
1	A	79	VAL	CA-CB	5.42	1.66	1.54	1	18
1	A	70	ALA	C-O	5.36	1.33	1.23	1	18
1	A	123	GLU	CD-OE2	5.35	1.31	1.25	1	18
1	A	63	THR	C-O	5.35	1.33	1.23	1	18
1	A	68	TYR	CE2-CZ	5.35	1.45	1.38	1	18
1	A	108	ASP	CG-OD1	5.31	1.37	1.25	1	18
1	A	36	GLY	CA-C	-5.28	1.43	1.51	1	18
1	A	118	LEU	CB-CG	5.26	1.67	1.52	1	18
1	A	88	GLN	C-N	5.21	1.46	1.34	1	18
1	A	120	GLY	N-CA	-5.21	1.38	1.46	1	18
1	A	58	THR	CA-CB	5.20	1.66	1.53	1	18
1	A	107	LYS	CA-CB	5.19	1.65	1.53	1	18
1	A	109	ASP	CG-OD2	5.19	1.37	1.25	1	18
1	A	83	PHE	C-N	-5.14	1.22	1.34	1	18
1	A	11	GLY	C-N	5.13	1.45	1.34	1	18
1	A	46	TYR	CE2-CZ	-5.13	1.31	1.38	1	18
1	A	25	ASP	C-O	-5.13	1.13	1.23	1	18
1	A	8	ASP	CG-OD1	5.12	1.37	1.25	1	18
1	A	10	ASP	CG-OD1	5.11	1.37	1.25	1	18
1	A	138	LYS	CE-NZ	5.11	1.61	1.49	1	18
1	A	146	ASP	CA-C	5.10	1.66	1.52	1	18
1	A	91	ASP	C-N	5.08	1.45	1.34	1	18
1	A	69	GLN	CD-NE2	5.08	1.45	1.32	1	18
1	A	77	HIS	CE1-NE2	5.05	1.44	1.32	1	18
1	A	46	TYR	CD2-CE2	5.02	1.46	1.39	1	18
1	A	55	PRO	N-CA	5.02	1.55	1.47	1	18
1	A	148	ASN	CA-C	5.01	1.66	1.52	1	18
1	A	115	VAL	CB-CG1	-5.01	1.42	1.52	1	18
1	A	146	ASP	CG-OD1	5.01	1.36	1.25	1	18

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	117	ARG	NE-CZ-NH2	82.60	161.60	120.30	1	18
1	A	117	ARG	NE-CZ-NH1	-43.88	98.36	120.30	1	18
1	A	111	ASP	CB-CG-OD1	-35.84	86.04	118.30	1	18
1	A	89	HIS	C-N-CD	-33.57	46.75	120.60	1	18
1	A	142	ARG	NE-CZ-NH2	-31.48	104.56	120.30	1	18
1	A	90	PRO	CA-N-CD	-31.06	68.02	111.50	1	18
1	A	56	GLU	OE1-CD-OE2	30.53	159.94	123.30	1	18
1	A	9	ARG	CD-NE-CZ	30.11	165.75	123.60	1	18
1	A	90	PRO	N-CA-CB	27.98	136.88	103.30	1	18
1	A	67	ASP	CB-CG-OD2	-25.60	95.26	118.30	1	18
1	A	67	ASP	CB-CG-OD1	-25.14	95.67	118.30	1	18
1	A	67	ASP	OD1-CG-OD2	24.09	169.06	123.30	1	18
1	A	117	ARG	CD-NE-CZ	22.78	155.49	123.60	1	18
1	A	66	GLU	OE1-CD-OE2	22.43	150.21	123.30	1	18
1	A	44	ARG	NE-CZ-NH2	-21.35	109.62	120.30	1	18
1	A	111	ASP	OD1-CG-OD2	19.45	160.26	123.30	1	18
1	A	3	PHE	CG-CD2-CE2	19.43	142.17	120.80	1	18
1	A	123	GLU	OE1-CD-OE2	18.95	146.04	123.30	1	18
1	A	68	TYR	CB-CG-CD1	-18.78	109.73	121.00	1	18
1	A	91	ASP	CB-CG-OD2	18.68	135.11	118.30	1	18
1	A	125	ASP	CB-CG-OD2	18.33	134.79	118.30	1	18
1	A	155	TYR	CB-CG-CD1	-18.21	110.07	121.00	1	18
1	A	109	ASP	CB-CG-OD2	-18.15	101.97	118.30	1	18
1	A	134	ASP	CB-CG-OD2	-18.11	102.00	118.30	1	18
1	A	135	ASP	CB-CG-OD2	-18.02	102.09	118.30	1	18
1	A	117	ARG	NH1-CZ-NH2	-17.64	99.99	119.40	1	18
1	A	83	PHE	CB-CG-CD2	-17.23	108.73	120.80	1	18
1	A	25	ASP	CB-CG-OD1	16.00	132.70	118.30	1	18
1	A	118	LEU	CB-CG-CD2	-15.88	84.00	111.00	1	18
1	A	108	ASP	CB-CG-OD2	-15.79	104.09	118.30	1	18
1	A	106	PHE	CB-CG-CD2	14.98	131.29	120.80	1	18
1	A	66	GLU	CG-CD-OE2	-14.47	89.36	118.30	1	18
1	A	78	ASP	CB-CG-OD2	-14.16	105.56	118.30	1	18
1	A	3	PHE	CB-CG-CD1	13.97	130.58	120.80	1	18
1	A	142	ARG	CD-NE-CZ	-13.96	104.05	123.60	1	18
1	A	134	ASP	CB-CG-OD1	13.08	130.07	118.30	1	18
1	A	146	ASP	CB-CG-OD2	13.05	130.05	118.30	1	18
1	A	158	TRP	NE1-CE2-CD2	13.03	120.33	107.30	1	18
1	A	161	LYS	CD-CE-NZ	13.03	141.66	111.70	1	18
1	A	62	LEU	CB-CG-CD2	-12.93	89.02	111.00	1	18
1	A	23	LEU	C-N-CD	12.13	153.88	128.40	1	18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	44	ARG	NE-CZ-NH1	11.93	126.26	120.30	1	18
1	A	103	PHE	CB-CG-CD1	-11.79	112.55	120.80	1	18
1	A	105	ALA	CA-C-N	11.78	143.10	117.20	1	18
1	A	56	GLU	CG-CD-OE2	-11.52	95.25	118.30	1	18
1	A	142	ARG	NE-CZ-NH1	11.49	126.04	120.30	1	18
1	A	19	LEU	C-N-CD	11.47	152.50	128.40	1	18
1	A	57	ARG	NE-CZ-NH2	-11.36	114.62	120.30	16	18
1	A	131	LEU	CD1-CG-CD2	11.32	144.46	110.50	1	18
1	A	68	TYR	CB-CG-CD2	11.25	127.75	121.00	1	18
1	A	105	ALA	O-C-N	-11.23	104.73	122.70	1	18
1	A	67	ASP	CB-CA-C	-11.16	88.07	110.40	1	18
1	A	148	ASN	C-N-CD	11.12	151.75	128.40	1	18
1	A	140	SER	CA-CB-OG	-10.84	81.94	111.20	1	18
1	A	3	PHE	CD1-CG-CD2	-10.82	104.23	118.30	1	18
1	A	44	ARG	CG-CD-NE	10.82	134.53	111.80	1	18
1	A	21	TRP	CB-CG-CD1	10.75	140.98	127.00	1	18
1	A	91	ASP	OD1-CG-OD2	-10.46	103.43	123.30	1	18
1	A	108	ASP	OD1-CG-OD2	10.40	143.07	123.30	1	18
1	A	88	GLN	CA-CB-CG	10.34	136.14	113.40	1	18
1	A	57	ARG	NE-CZ-NH1	10.29	125.45	120.30	6	18
1	A	89	HIS	CA-C-O	-10.28	98.51	120.10	1	18
1	A	158	TRP	CE2-CD2-CG	-10.28	99.08	107.30	1	18
1	A	44	ARG	N-CA-CB	-10.18	92.28	110.60	1	18
1	A	16	ASP	CB-CG-OD1	10.17	127.46	118.30	1	18
1	A	78	ASP	OD1-CG-OD2	10.09	142.48	123.30	1	18
1	A	78	ASP	CA-CB-CG	10.01	135.42	113.40	1	18
1	A	162	ALA	CB-CA-C	-9.99	95.11	110.10	1	18
1	A	88	GLN	C-N-CA	9.88	146.41	121.70	1	18
1	A	73	ALA	O-C-N	-9.85	106.94	122.70	1	18
1	A	21	TRP	CB-CG-CD2	-9.75	113.92	126.60	1	18
1	A	9	ARG	CG-CD-NE	-9.65	91.53	111.80	1	18
1	A	62	LEU	O-C-N	-9.55	107.42	122.70	1	18
1	A	83	PHE	CD1-CE1-CZ	-9.43	108.78	120.10	1	18
1	A	158	TRP	CD1-NE1-CE2	-9.43	100.52	109.00	1	18
1	A	136	PHE	CB-CG-CD1	9.42	127.39	120.80	1	18
1	A	19	LEU	CA-C-O	9.38	139.81	120.10	1	18
1	A	158	TRP	CE2-CD2-CE3	9.35	129.92	118.70	1	18
1	A	24	PRO	CA-N-CD	-9.20	98.62	111.50	1	18
1	A	123	GLU	O-C-N	-9.19	107.59	123.20	1	18
1	A	142	ARG	NH1-CZ-NH2	9.09	129.40	119.40	1	18
1	A	129	ILE	C-N-CD	9.04	147.40	128.40	1	18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	135	ASP	OD1-CG-OD2	8.99	140.38	123.30	1	18
1	A	43	ARG	NE-CZ-NH2	-8.98	115.81	120.30	1	18
1	A	88	GLN	CA-C-O	8.96	138.91	120.10	1	18
1	A	110	VAL	O-C-N	-8.83	108.57	122.70	1	18
1	A	65	GLN	O-C-N	-8.80	108.62	122.70	1	18
1	A	149	PRO	N-CD-CG	-8.79	90.01	103.20	1	18
1	A	123	GLU	CG-CD-OE2	-8.66	100.98	118.30	1	18
1	A	78	ASP	CB-CG-OD1	-8.54	110.61	118.30	1	18
1	A	106	PHE	CB-CG-CD1	-8.52	114.84	120.80	1	18
1	A	123	GLU	N-CA-CB	-8.52	95.27	110.60	1	18
1	A	106	PHE	CG-CD2-CE2	8.50	130.15	120.80	1	18
1	A	9	ARG	NE-CZ-NH2	8.49	124.55	120.30	1	18
1	A	106	PHE	CZ-CE2-CD2	-8.41	110.01	120.10	1	18
1	A	109	ASP	N-CA-CB	-8.39	95.49	110.60	1	18
1	A	103	PHE	CG-CD1-CE1	-8.38	111.59	120.80	1	18
1	A	131	LEU	CB-CG-CD1	-8.35	96.80	111.00	1	18
1	A	110	VAL	CA-C-O	8.34	137.61	120.10	1	18
1	A	107	LYS	CB-CG-CD	8.32	133.25	111.60	1	18
1	A	108	ASP	O-C-N	8.31	135.99	122.70	1	18
1	A	22	HIS	CA-C-O	8.28	137.48	120.10	1	18
1	A	25	ASP	OD1-CG-OD2	-8.26	107.61	123.30	1	18
1	A	109	ASP	OD1-CG-OD2	8.23	138.94	123.30	1	18
1	A	85	TYR	CB-CG-CD2	8.14	125.89	121.00	1	18
1	A	148	ASN	CB-CG-OD1	8.14	137.87	121.60	1	18
1	A	89	HIS	N-CA-CB	8.10	125.18	110.60	1	18
1	A	149	PRO	N-CA-CB	8.07	112.98	103.30	1	18
1	A	63	THR	CA-C-N	8.06	134.94	117.20	1	18
1	A	69	GLN	CG-CD-OE1	8.04	137.68	121.60	1	18
1	A	148	ASN	CA-C-O	8.04	136.98	120.10	1	18
1	A	132	ASN	CA-C-N	8.03	134.87	117.20	1	18
1	A	55	PRO	CA-N-CD	-7.98	100.33	111.50	1	18
1	A	67	ASP	N-CA-CB	-7.95	96.29	110.60	1	18
1	A	52	ARG	NE-CZ-NH1	7.94	124.27	120.30	17	18
1	A	132	ASN	CB-CA-C	7.91	126.23	110.40	1	18
1	A	161	LYS	CA-C-N	7.81	134.39	117.20	1	18
1	A	58	THR	CA-CB-OG1	-7.80	92.61	109.00	1	18
1	A	127	LYS	CB-CG-CD	-7.76	91.41	111.60	1	18
1	A	46	TYR	CG-CD2-CE2	-7.76	115.09	121.30	1	18
1	A	88	GLN	O-C-N	-7.72	110.34	122.70	1	18
1	A	88	GLN	CG-CD-OE1	7.72	137.04	121.60	1	18
1	A	89	HIS	CB-CA-C	7.71	125.82	110.40	1	18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	102	ILE	CG1-CB-CG2	-7.67	94.53	111.40	1	18
1	A	78	ASP	O-C-N	-7.64	110.48	122.70	1	18
1	A	59	ASN	O-C-N	-7.64	110.48	122.70	1	18
1	A	37	LYS	CD-CE-NZ	7.62	129.22	111.70	1	18
1	A	107	LYS	CD-CE-NZ	-7.61	94.19	111.70	1	18
1	A	94	LEU	CB-CG-CD2	7.54	123.81	111.00	1	18
1	A	65	GLN	CG-CD-NE2	-7.50	98.69	116.70	1	18
1	A	87	LYS	N-CA-CB	7.46	124.03	110.60	1	18
1	A	129	ILE	CA-C-O	7.46	135.76	120.10	1	18
1	A	137	THR	CA-C-N	7.43	133.54	117.20	1	18
1	A	144	VAL	CA-CB-CG2	-7.42	99.78	110.90	1	18
1	A	46	TYR	CB-CG-CD1	-7.41	116.56	121.00	1	18
1	A	93	GLU	CG-CD-OE1	-7.41	103.48	118.30	1	18
1	A	149	PRO	CA-CB-CG	-7.37	90.00	104.00	1	18
1	A	121	SER	N-CA-CB	-7.34	99.48	110.50	1	18
1	A	3	PHE	CD1-CE1-CZ	7.30	128.87	120.10	1	18
1	A	90	PRO	O-C-N	-7.30	111.02	122.70	1	18
1	A	76	VAL	CA-C-O	7.28	135.39	120.10	1	18
1	A	90	PRO	C-N-CA	7.27	139.87	121.70	1	18
1	A	119	ALA	N-CA-CB	-7.22	99.99	110.10	1	18
1	A	101	GLN	CA-CB-CG	-7.21	97.54	113.40	1	18
1	A	89	HIS	ND1-CG-CD2	-7.16	95.98	106.00	1	18
1	A	145	GLU	CG-CD-OE1	-7.14	104.01	118.30	1	18
1	A	122	PHE	CG-CD2-CE2	-7.12	112.97	120.80	1	18
1	A	24	PRO	CA-C-N	7.10	132.82	117.20	1	18
1	A	43	ARG	NE-CZ-NH1	-7.09	116.75	120.30	1	18
1	A	66	GLU	CA-CB-CG	-7.07	97.84	113.40	1	18
1	A	56	GLU	CG-CD-OE1	-7.06	104.18	118.30	1	18
1	A	147	THR	CA-CB-CG2	-7.01	102.59	112.40	1	18
1	A	125	ASP	OD1-CG-OD2	-7.00	110.00	123.30	1	18
1	A	45	THR	CA-CB-OG1	-6.99	94.32	109.00	1	18
1	A	20	PRO	CA-N-CD	-6.90	101.85	111.50	1	18
1	A	136	PHE	CG-CD1-CE1	6.89	128.38	120.80	1	18
1	A	161	LYS	CB-CG-CD	-6.89	93.69	111.60	1	18
1	A	23	LEU	CA-C-N	-6.88	97.84	117.10	1	18
1	A	47	GLU	CA-CB-CG	-6.88	98.28	113.40	1	18
1	A	77	HIS	CG-ND1-CE1	6.87	117.82	108.20	1	18
1	A	119	ALA	CA-C-N	6.85	129.91	116.20	1	18
1	A	114	LEU	CB-CG-CD1	-6.85	99.36	111.00	1	18
1	A	150	ALA	O-C-N	-6.83	111.77	122.70	1	18
1	A	65	GLN	CA-C-N	6.83	132.22	117.20	1	18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	23	LEU	CA-C-O	6.83	134.44	120.10	1	18
1	A	133	TRP	CE2-CD2-CG	-6.82	101.85	107.30	1	18
1	A	89	HIS	CA-C-N	6.80	136.14	117.10	1	18
1	A	8	ASP	CA-C-O	6.78	134.33	120.10	1	18
1	A	78	ASP	CB-CA-C	6.75	123.90	110.40	1	18
1	A	62	LEU	N-CA-CB	6.74	123.89	110.40	1	18
1	A	161	LYS	CG-CD-CE	-6.74	91.69	111.90	1	18
1	A	12	LEU	CB-CG-CD1	-6.72	99.57	111.00	1	18
1	A	142	ARG	CG-CD-NE	6.72	125.91	111.80	1	18
1	A	83	PHE	CD1-CG-CD2	6.70	127.01	118.30	1	18
1	A	141	SER	N-CA-CB	-6.68	100.48	110.50	1	18
1	A	157	VAL	O-C-N	6.67	133.37	122.70	1	18
1	A	135	ASP	N-CA-CB	6.66	122.59	110.60	1	18
1	A	132	ASN	C-N-CA	6.64	138.30	121.70	1	18
1	A	137	THR	CA-C-O	-6.53	106.39	120.10	1	18
1	A	155	TYR	CB-CG-CD2	6.52	124.91	121.00	1	18
1	A	62	LEU	CD1-CG-CD2	-6.51	90.98	110.50	1	18
1	A	71	GLN	OE1-CD-NE2	-6.50	106.95	121.90	1	18
1	A	90	PRO	CA-C-O	6.50	135.79	120.20	1	18
1	A	159	GLN	CB-CG-CD	-6.48	94.75	111.60	1	18
1	A	148	ASN	CB-CG-ND2	-6.46	101.19	116.70	1	18
1	A	1	THR	CA-CB-CG2	6.40	121.36	112.40	1	18
1	A	69	GLN	OE1-CD-NE2	-6.39	107.19	121.90	1	18
1	A	83	PHE	CE1-CZ-CE2	6.39	131.50	120.00	1	18
1	A	20	PRO	O-C-N	-6.39	112.48	122.70	1	18
1	A	99	GLY	O-C-N	-6.38	112.50	122.70	1	18
1	A	131	LEU	CB-CG-CD2	-6.37	100.17	111.00	1	18
1	A	22	HIS	CA-C-N	-6.36	103.22	117.20	1	18
1	A	141	SER	CA-CB-OG	-6.35	94.05	111.20	1	18
1	A	159	GLN	CG-CD-OE1	6.34	134.28	121.60	1	18
1	A	155	TYR	CG-CD1-CE1	-6.30	116.26	121.30	1	18
1	A	44	ARG	O-C-N	-6.28	112.65	122.70	1	18
1	A	158	TRP	NE1-CE2-CZ2	-6.28	123.49	130.40	1	18
1	A	157	VAL	CA-C-O	-6.27	106.94	120.10	1	18
1	A	157	VAL	CG1-CB-CG2	6.26	120.92	110.90	1	18
1	A	103	PHE	CD1-CG-CD2	6.25	126.42	118.30	1	18
1	A	132	ASN	CA-CB-CG	-6.22	99.72	113.40	1	18
1	A	141	SER	O-C-N	-6.18	112.81	122.70	1	18
1	A	3	PHE	CB-CG-CD2	6.18	125.13	120.80	1	18
1	A	108	ASP	C-N-CA	-6.16	106.30	121.70	1	18
1	A	10	ASP	CB-CG-OD1	-6.12	112.80	118.30	1	18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	19	LEU	CA-C-N	-6.11	99.98	117.10	1	18
1	A	108	ASP	CB-CG-OD1	-6.11	112.80	118.30	1	18
1	A	155	TYR	CD1-CG-CD2	6.08	124.59	117.90	1	18
1	A	8	ASP	CB-CG-OD1	-6.08	112.83	118.30	1	18
1	A	118	LEU	CB-CA-C	6.07	121.72	110.20	1	18
1	A	73	ALA	CA-C-N	6.05	130.51	117.20	1	18
1	A	129	ILE	CA-C-N	-6.01	100.27	117.10	1	18
1	A	46	TYR	O-C-N	-6.00	113.09	122.70	1	18
1	A	136	PHE	CD1-CE1-CZ	-5.94	112.97	120.10	1	18
1	A	132	ASN	CA-C-O	-5.90	107.70	120.10	1	18
1	A	43	ARG	NH1-CZ-NH2	5.90	125.89	119.40	1	18
1	A	63	THR	CA-C-O	-5.88	107.75	120.10	1	18
1	A	74	VAL	O-C-N	-5.88	113.29	122.70	1	18
1	A	4	LEU	CA-CB-CG	5.88	128.82	115.30	9	18
1	A	9	ARG	NE-CZ-NH1	-5.88	117.36	120.30	1	18
1	A	93	GLU	CA-CB-CG	5.87	126.31	113.40	1	18
1	A	153	HIS	ND1-CG-CD2	-5.86	97.80	106.00	1	18
1	A	140	SER	CB-CA-C	-5.85	98.98	110.10	1	18
1	A	135	ASP	O-C-N	5.83	132.03	122.70	1	18
1	A	1	THR	OG1-CB-CG2	-5.83	96.59	110.00	1	18
1	A	13	ILE	C-N-CA	-5.82	110.08	122.30	1	18
1	A	64	HIS	O-C-N	5.80	131.98	122.70	1	18
1	A	82	VAL	O-C-N	-5.80	113.42	122.70	1	18
1	A	85	TYR	CD1-CE1-CZ	5.79	125.01	119.80	1	18
1	A	8	ASP	CA-C-N	-5.79	104.46	117.20	1	18
1	A	25	ASP	O-C-N	-5.78	113.45	122.70	5	18
1	A	73	ALA	C-N-CA	5.75	136.09	121.70	1	18
1	A	64	HIS	CG-CD2-NE2	-5.74	98.29	109.20	1	18
1	A	64	HIS	CB-CG-CD2	-5.74	113.02	130.80	1	18
1	A	61	VAL	O-C-N	-5.71	113.56	122.70	1	18
1	A	44	ARG	CB-CG-CD	-5.70	96.79	111.60	1	18
1	A	151	LEU	CB-CG-CD1	-5.70	101.32	111.00	1	18
1	A	125	ASP	N-CA-CB	-5.69	100.35	110.60	1	18
1	A	145	GLU	CB-CG-CD	-5.69	98.83	114.20	1	18
1	A	148	ASN	N-CA-C	-5.66	95.72	111.00	1	18
1	A	111	ASP	CB-CG-OD2	-5.65	113.21	118.30	1	18
1	A	83	PHE	CA-C-O	-5.64	108.25	120.10	1	18
1	A	76	VAL	CA-C-N	-5.62	104.84	117.20	1	18
1	A	20	PRO	CB-CA-C	-5.58	98.05	112.00	1	18
1	A	148	ASN	CA-C-N	-5.56	101.52	117.10	1	18
1	A	130	PRO	CA-N-CD	-5.56	103.72	111.50	1	18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	26	ASP	N-CA-CB	-5.54	100.62	110.60	9	1
1	A	96	ILE	CA-CB-CG1	5.54	121.52	111.00	1	18
1	A	4	LEU	CB-CG-CD2	5.53	120.41	111.00	1	18
1	A	96	ILE	CA-CB-CG2	-5.53	99.83	110.90	1	18
1	A	107	LYS	CA-C-N	5.52	129.35	117.20	1	18
1	A	88	GLN	CB-CG-CD	5.52	125.94	111.60	1	18
1	A	35	VAL	CA-C-N	5.52	127.23	116.20	1	4
1	A	102	ILE	CA-CB-CG2	5.51	121.92	110.90	1	18
1	A	119	ALA	O-C-N	-5.50	113.85	123.20	1	18
1	A	57	ARG	N-CA-C	-5.48	96.20	111.00	1	18
1	A	142	ARG	N-CA-C	-5.47	96.22	111.00	1	18
1	A	59	ASN	CB-CG-ND2	5.46	129.80	116.70	1	18
1	A	78	ASP	N-CA-CB	-5.45	100.79	110.60	1	18
1	A	135	ASP	CB-CA-C	-5.45	99.50	110.40	1	18
1	A	5	TRP	CD1-NE1-CE2	-5.44	104.10	109.00	12	18
1	A	122	PHE	CB-CG-CD1	-5.44	116.99	120.80	1	18
1	A	134	ASP	O-C-N	-5.44	114.00	122.70	1	18
1	A	61	VAL	CG1-CB-CG2	5.42	119.58	110.90	1	18
1	A	70	ALA	CB-CA-C	5.42	118.23	110.10	1	18
1	A	42	GLY	CA-C-O	5.42	130.35	120.60	1	18
1	A	137	THR	CA-CB-OG1	-5.41	97.63	109.00	1	18
1	A	159	GLN	OE1-CD-NE2	-5.41	109.47	121.90	1	18
1	A	149	PRO	C-N-CA	5.39	135.19	121.70	1	18
1	A	126	THR	CA-CB-OG1	-5.39	97.69	109.00	1	18
1	A	144	VAL	CG1-CB-CG2	5.38	119.51	110.90	1	18
1	A	71	GLN	CA-CB-CG	-5.37	101.59	113.40	1	18
1	A	122	PHE	CD1-CG-CD2	5.35	125.26	118.30	1	18
1	A	63	THR	OG1-CB-CG2	5.32	122.23	110.00	1	18
1	A	117	ARG	O-C-N	5.30	131.19	122.70	1	18
1	A	22	HIS	CA-CB-CG	-5.30	104.59	113.60	1	18
1	A	10	ASP	CB-CG-OD2	5.30	123.07	118.30	1	18
1	A	42	GLY	O-C-N	-5.30	114.22	122.70	1	18
1	A	139	VAL	CG1-CB-CG2	-5.30	102.42	110.90	1	18
1	A	47	GLU	O-C-N	-5.30	114.22	122.70	18	18
1	A	67	ASP	N-CA-C	5.29	125.27	111.00	1	18
1	A	43	ARG	C-N-CA	-5.27	108.52	121.70	1	18
1	A	127	LYS	CA-C-N	-5.27	105.61	117.20	1	18
1	A	104	THR	N-CA-CB	-5.26	100.31	110.30	1	18
1	A	122	PHE	CG-CD1-CE1	-5.26	115.01	120.80	1	18
1	A	8	ASP	CB-CG-OD2	5.26	123.03	118.30	1	18
1	A	122	PHE	CZ-CE2-CD2	5.22	126.36	120.10	1	18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	39	MET	CG-SD-CE	5.19	108.51	100.20	1	18
1	A	151	LEU	N-CA-CB	5.16	120.73	110.40	1	18
1	A	114	LEU	CA-CB-CG	-5.16	103.44	115.30	1	18
1	A	99	GLY	CA-C-O	5.15	129.87	120.60	1	18
1	A	158	TRP	CD2-CE2-CZ2	-5.13	116.14	122.30	1	18
1	A	97	ALA	CA-C-O	-5.13	109.33	120.10	1	18
1	A	24	PRO	CA-CB-CG	-5.12	94.27	104.00	1	18
1	A	77	HIS	ND1-CE1-NE2	-5.12	98.64	109.90	1	18
1	A	39	MET	CA-C-N	5.11	128.44	117.20	1	18
1	A	75	VAL	CG1-CB-CG2	5.11	119.08	110.90	1	18
1	A	54	LEU	N-CA-CB	5.11	120.62	110.40	3	3
1	A	37	LYS	N-CA-CB	-5.11	101.41	110.60	1	18
1	A	91	ASP	CA-CB-CG	-5.11	102.16	113.40	1	18
1	A	95	VAL	CA-CB-CG1	-5.11	103.24	110.90	1	18
1	A	75	VAL	O-C-N	-5.09	114.55	122.70	1	18
1	A	25	ASP	CA-C-O	5.08	130.76	120.10	1	18
1	A	84	ALA	O-C-N	-5.06	114.60	122.70	1	18
1	A	87	LYS	O-C-N	-5.06	114.60	122.70	1	18
1	A	104	THR	OG1-CB-CG2	-5.05	98.38	110.00	1	18
1	A	3	PHE	CE1-CZ-CE2	-5.05	110.90	120.00	1	18
1	A	134	ASP	CA-C-N	5.02	128.24	117.20	1	18
1	A	93	GLU	CG-CD-OE2	5.00	128.31	118.30	1	18
1	A	97	ALA	O-C-N	5.00	131.70	123.20	1	18

All unique chiral outliers are listed below.

Mol	Chain	Res	Type	Atoms	Models (Total)
1	A	89	HIS	CA	18

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	9	ARG	Sidechain	18
1	A	21	TRP	Mainchain	18
1	A	44	ARG	Sidechain	18
1	A	78	ASP	Mainchain	18
1	A	145	GLU	Mainchain	18
1	A	34	THR	Peptide	4
1	A	25	ASP	Mainchain	3
1	A	57	ARG	Sidechain	2



## 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	1249	1222	1214	30±1
2	A	31	24	24	4±1
All	All	23040	22428	22284	553

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 12.

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:GLU:CB	1:A:145:GLU:CG	1.58	1.77	1	18
1:A:67:ASP:CA	1:A:67:ASP:CB	1.48	1.87	1	18
1:A:149:PRO:N	1:A:149:PRO:CD	1.37	1.70	1	18
1:A:55:PRO:N	1:A:55:PRO:CD	1.35	1.69	1	18
1:A:89:HIS:C	1:A:90:PRO:CD	1.33	1.97	1	18
1:A:130:PRO:N	1:A:130:PRO:CD	1.33	1.73	1	18
1:A:24:PRO:CD	1:A:24:PRO:N	1.29	1.78	1	18
1:A:89:HIS:O	1:A:90:PRO:CD	1.09	0.79	1	18
1:A:89:HIS:O	1:A:90:PRO:CG	1.03	2.06	1	18
1:A:90:PRO:HD2	1:A:91:ASP:OD1	0.99	1.58	1	18
1:A:89:HIS:O	1:A:90:PRO:HD2	0.97	1.58	1	18
1:A:67:ASP:CB	1:A:67:ASP:C	0.95	2.34	1	18
1:A:4:LEU:HD23	1:A:97:ALA:HB2	0.77	1.55	9	18
1:A:67:ASP:CB	1:A:67:ASP:N	0.76	2.49	1	18
1:A:145:GLU:CB	1:A:145:GLU:CD	0.69	2.60	1	18
1:A:50:PRO:HD3	2:A:163:BDM:BR11	0.69	2.43	16	17
1:A:50:PRO:CD	2:A:163:BDM:BR11	0.68	2.97	16	18
1:A:90:PRO:CD	1:A:91:ASP:OD1	0.66	2.39	1	18
1:A:4:LEU:HD23	1:A:97:ALA:CB	0.61	2.25	18	18
1:A:50:PRO:HD2	2:A:163:BDM:BR11	0.60	2.51	18	16
1:A:67:ASP:CA	1:A:67:ASP:CG	0.56	2.69	1	18
1:A:89:HIS:CA	1:A:90:PRO:CD	0.55	2.82	1	18
1:A:145:GLU:CG	1:A:145:GLU:CA	0.52	2.83	1	18
1:A:8:ASP:OD1	1:A:8:ASP:C	0.51	2.48	1	18
1:A:5:TRP:HA	2:A:163:BDM:HN41	0.48	1.68	15	17
1:A:89:HIS:O	1:A:90:PRO:HD3	0.48	0.72	1	18

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:4:LEU:HD22	1:A:34:THR:CG2	0.48	2.39	18	14
1:A:67:ASP:CA	1:A:67:ASP:OD1	0.46	2.62	1	18
1:A:54:LEU:H	1:A:54:LEU:HD23	0.46	1.70	12	7
1:A:89:HIS:O	1:A:90:PRO:CB	0.45	2.56	1	18
1:A:57:ARG:NH2	2:A:163:BDM:OXW	0.44	2.50	12	4
1:A:67:ASP:CB	1:A:67:ASP:H	0.44	2.23	1	18
1:A:4:LEU:HD22	1:A:34:THR:HG23	0.43	1.89	10	4
1:A:57:ARG:NH1	2:A:163:BDM:OXW	0.42	2.52	10	1
2:A:163:BDM:H201	2:A:163:BDM:H172	0.42	1.56	15	2
1:A:19:LEU:HD11	2:A:163:BDM:C13	0.41	2.46	18	1
2:A:163:BDM:H172	2:A:163:BDM:H201	0.40	1.49	1	2

## 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	155/162 (96%)	152±0 (98±0%)	1±0 (1±0%)	2±0 (1±0%)	16	63
All	All	2790/2916 (96%)	2739 (98%)	15 (1%)	36 (1%)	16	63

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	89	HIS	18
1	A	90	PRO	18

### 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	133/137 (97%)	125±0 (94±0%)	8±0 (6±0%)	22 71
All	All	2394/2466 (97%)	2245 (94%)	149 (6%)	22 71

All 9 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	9	ARG	18
1	A	24	PRO	18
1	A	54	LEU	18
1	A	88	GLN	18
1	A	89	HIS	18
1	A	90	PRO	18
1	A	102	ILE	18
1	A	111	ASP	18
1	A	35	VAL	5

### 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 monosaccharides in this entry.

## 6.6 Ligand geometry [i](#)

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	BDM	A	163	-	26,32,32	1.02±0.03	2±0 (6±1%)

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	BDM	A	163	-	36,43,43	1.88±0.16	6±1 (17±2%)

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	BDM	A	163	-	-	0±0,16,22,22	0±0,2,2,2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	A	163	BDM	C6-C5	2.33	1.42	1.37	5	18
2	A	163	BDM	BR11-C11	2.25	1.94	1.89	10	3
2	A	163	BDM	C2-N1	2.15	1.32	1.35	5	9

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
2	A	163	BDM	C7-C8-C13	6.65	107.78	120.69	10	18
2	A	163	BDM	C7-C8-C9	6.10	132.54	120.69	10	18
2	A	163	BDM	O10-C10-C11	5.52	110.97	116.32	10	14
2	A	163	BDM	C15-O10-C10	4.85	129.56	117.69	9	15
2	A	163	BDM	C14-O12-C12	4.70	110.43	117.53	10	17
2	A	163	BDM	C19-C18-C21	4.37	119.04	112.53	6	4

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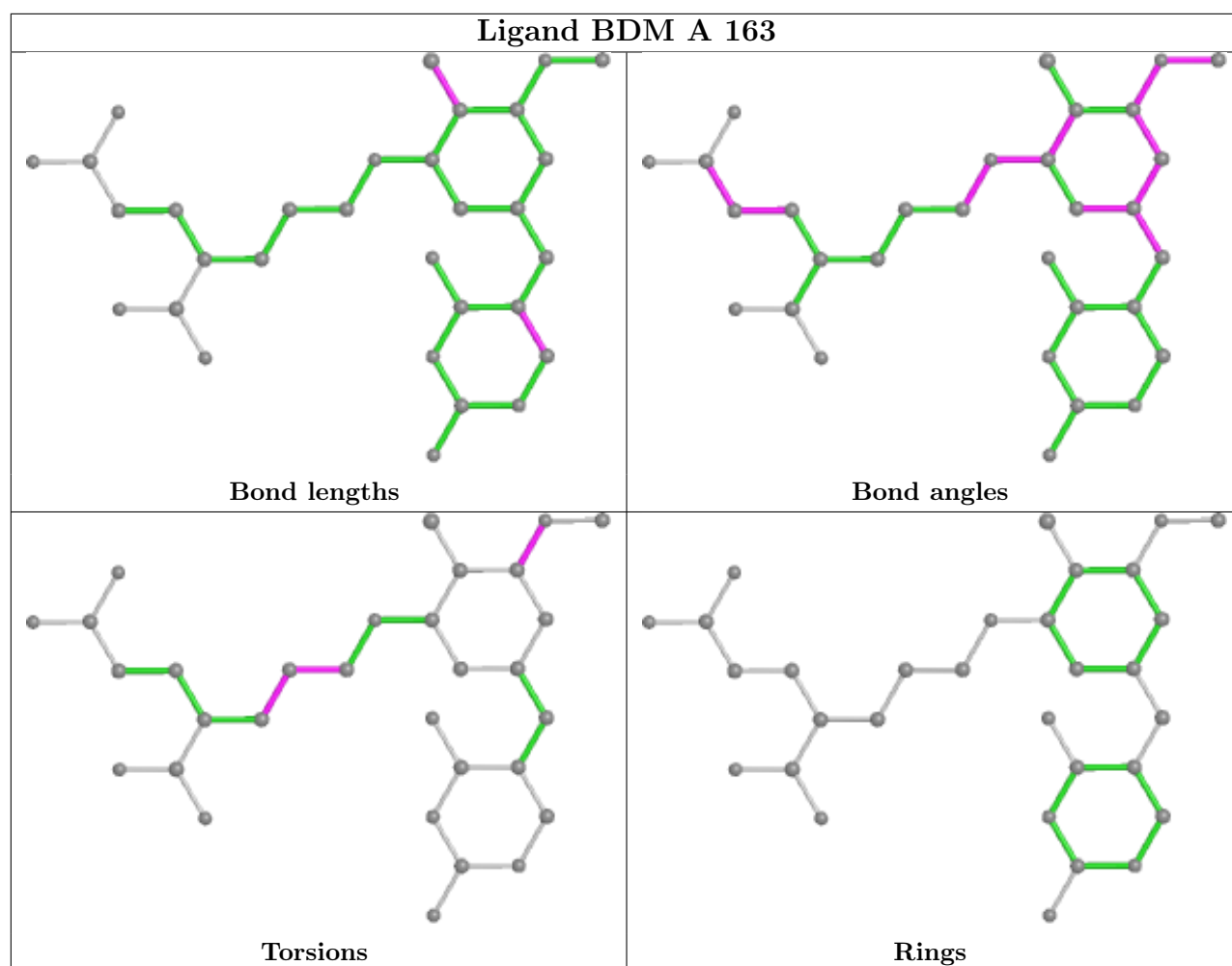
Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	A	163	BDM	C19-C18-C17	2.83	95.09	115.09	18	1
2	A	163	BDM	C17-C18-C21	2.76	116.65	112.53	16	3
2	A	163	BDM	O12-C12-C13	2.53	119.76	124.12	16	17
2	A	163	BDM	O10-C10-C9	2.45	129.20	123.58	10	1
2	A	163	BDM	C5-C6-N1	2.13	120.28	123.82	9	5
2	A	163	BDM	C19-C20-C22	2.12	118.15	113.59	1	2

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

## 6.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	1-A	1
1	2-A	1
1	3-A	1
1	4-A	1
1	5-A	1
1	6-A	1
1	7-A	1
1	8-A	1

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Mol	Chain	Number of breaks
1	9-A	1
1	10-A	1
1	11-A	1
1	12-A	1
1	13-A	1
1	14-A	1
1	15-A	1
1	16-A	1
1	17-A	1
1	18-A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	89:HIS	C	90:PRO	N	0.96
2	A	89:HIS	C	90:PRO	N	0.96
3	A	89:HIS	C	90:PRO	N	0.96
4	A	89:HIS	C	90:PRO	N	0.96
5	A	89:HIS	C	90:PRO	N	0.96
6	A	89:HIS	C	90:PRO	N	0.96
7	A	89:HIS	C	90:PRO	N	0.96
8	A	89:HIS	C	90:PRO	N	0.96
9	A	89:HIS	C	90:PRO	N	0.96
10	A	89:HIS	C	90:PRO	N	0.96
11	A	89:HIS	C	90:PRO	N	0.96
12	A	89:HIS	C	90:PRO	N	0.96
13	A	89:HIS	C	90:PRO	N	0.96
14	A	89:HIS	C	90:PRO	N	0.96
15	A	89:HIS	C	90:PRO	N	0.96
16	A	89:HIS	C	90:PRO	N	0.96
17	A	89:HIS	C	90:PRO	N	0.96
18	A	89:HIS	C	90:PRO	N	0.96

## 7 Chemical shift validation

No chemical shift data were provided