



Full wwPDB NMR Structure Validation Report ⓘ

Mar 1, 2026 – 05:45 AM UTC

PDB ID : 1DIU / pdb_00001diu
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

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
Mogul	:	2022.3.0, CSD as543be (2022)
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

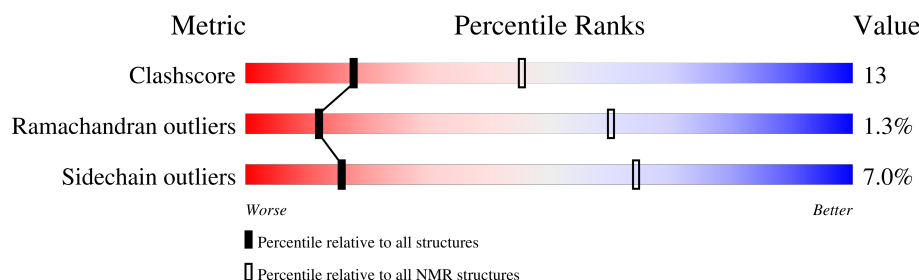
1 Overall quality at a glance

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	 7% 75% 11% . .

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)	0.04	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

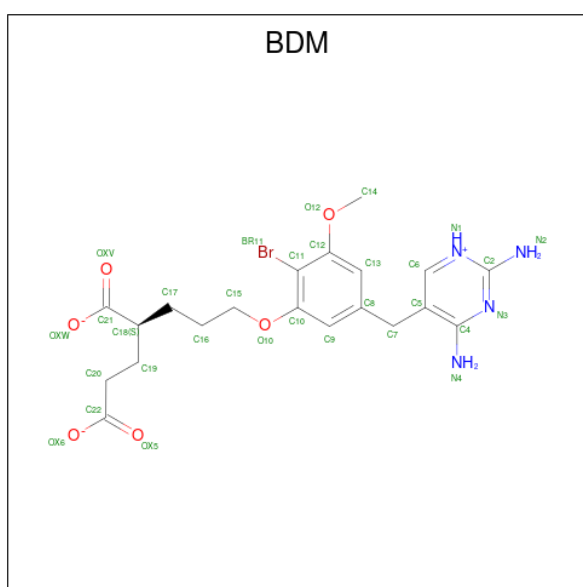
3 Entry composition [i](#)

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
1	A	162	Total	C	H	N	O	S	0
			2563	828	1266	225	242	2	

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



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

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

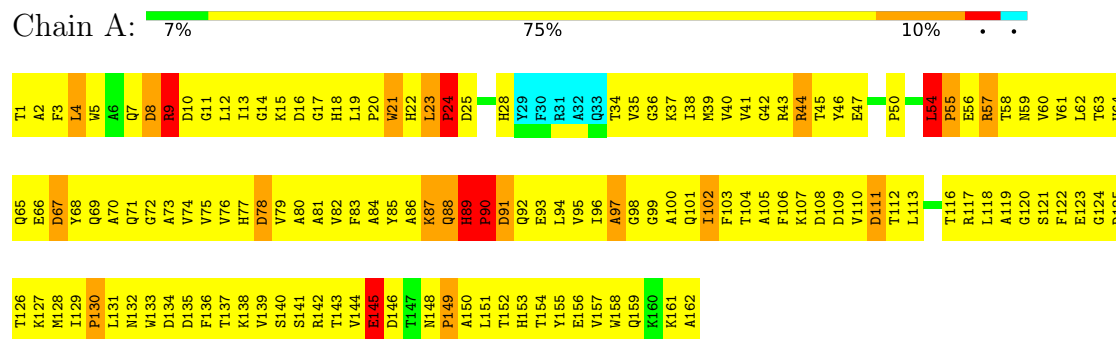


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

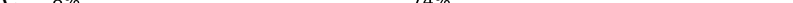
4.2.1 Score per residue for model 1

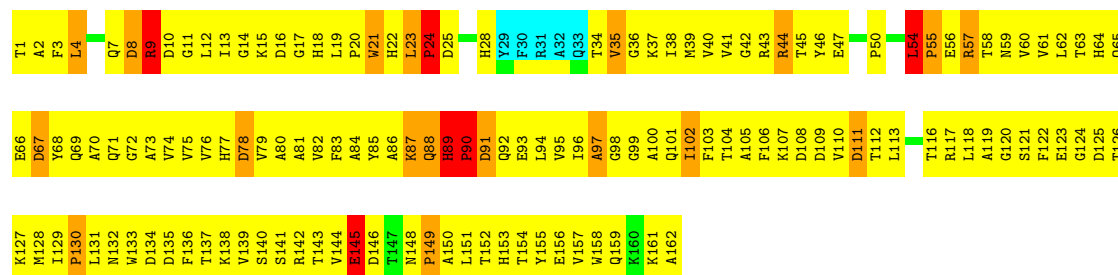
• Molecule 1: DIHYDROFOLATE REDUCTASE



4.2.5 Score per residue for model 5

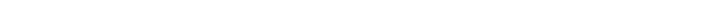
• Molecule 1: DIHYDROFOLATE REDUCTASE

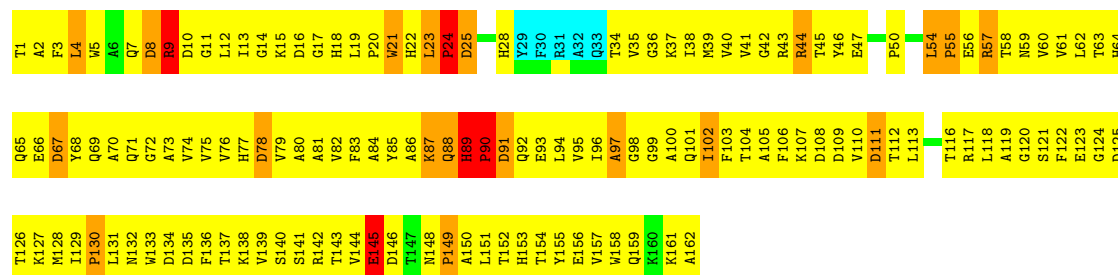
Chain A:  8% 74% 11% . .



4.2.6 Score per residue for model 6

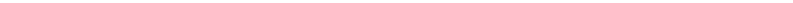
- Molecule 1: DIHYDROFOLATE REDUCTASE

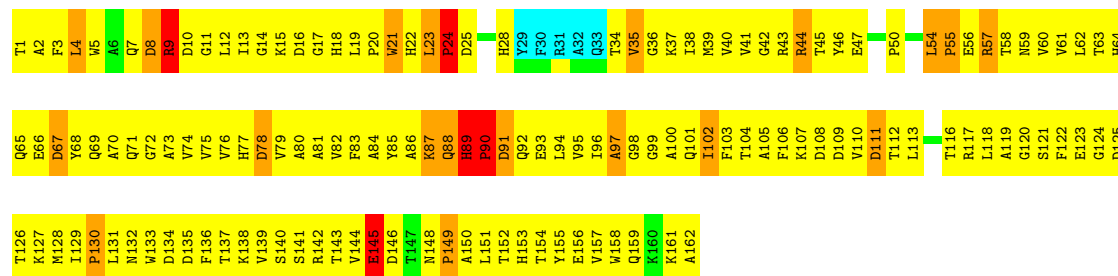
Chain A:  7% 75% 12% . .



4.2.7 Score per residue for model 7

- Molecule 1: DIHYDROFOLATE REDUCTASE

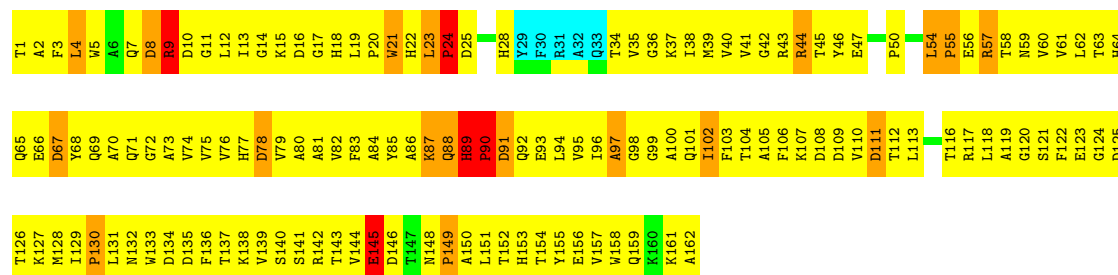
Chain A:  7% 75% 12% . .



4.2.8 Score per residue for model 8

• Molecule 1: DIHYDROFOLATE REDUCTASE

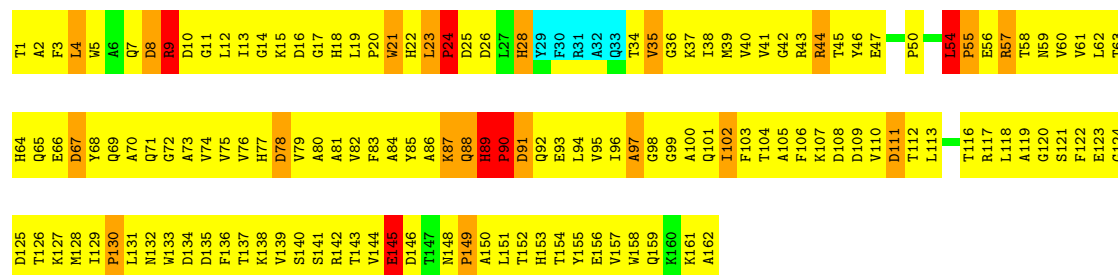
Chain A: 7% 75% 11% . .



4.2.9 Score per residue for model 9

• Molecule 1: DIHYDROFOLATE REDUCTASE

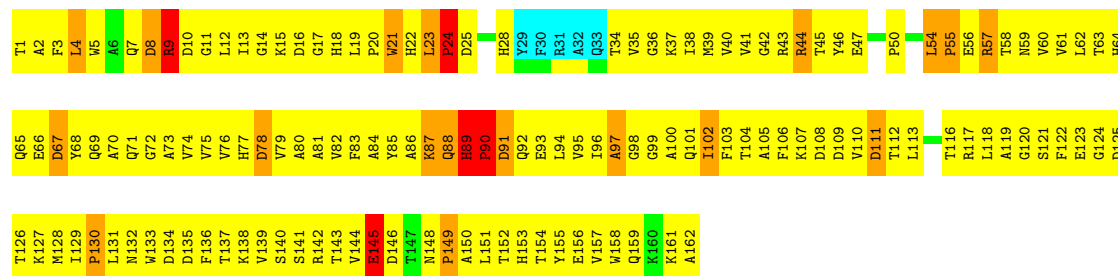
Chain A: 7% 75% 12% . .



4.2.10 Score per residue for model 10

• Molecule 1: DIHYDROFOLATE REDUCTASE

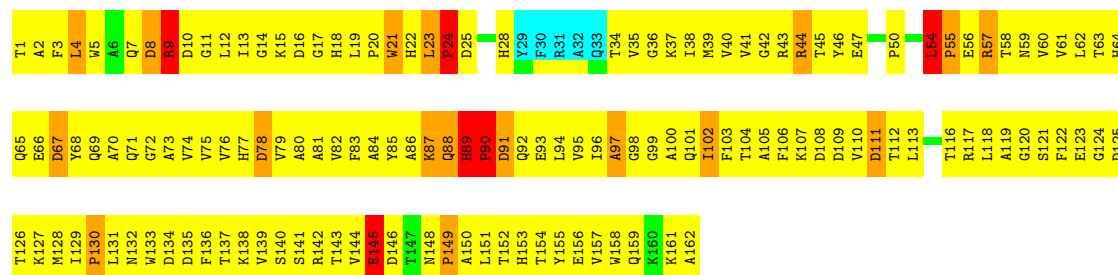
Chain A: 7% 75% 11% . .



4.2.11 Score per residue for model 11

• Molecule 1: DIHYDROFOLATE REDUCTASE

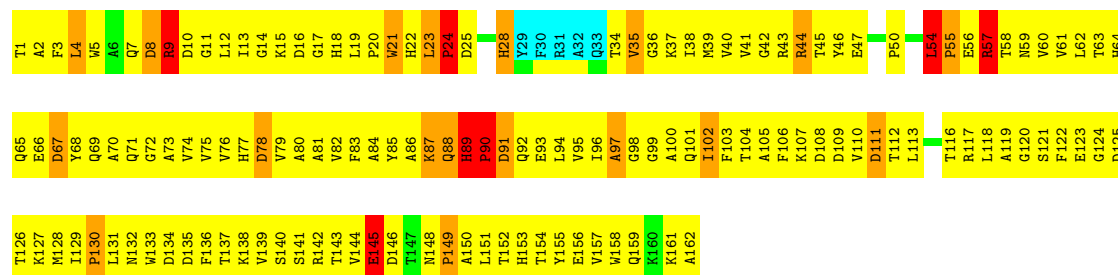
Chain A: 7% 75% 10%



4.2.12 Score per residue for model 12

• Molecule 1: DIHYDROFOLATE REDUCTASE

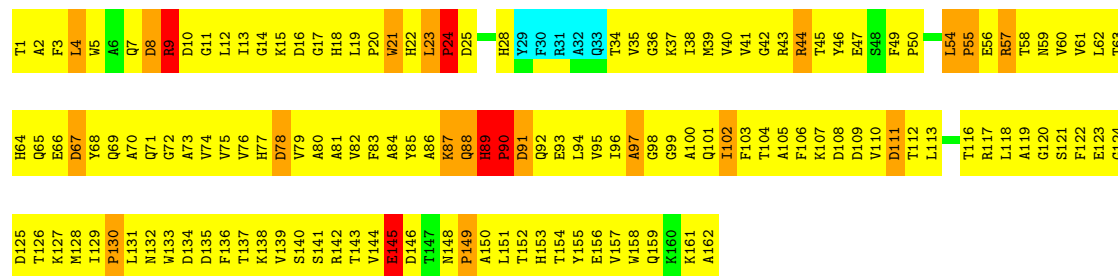
Chain A: 7% 74% 11%



4.2.13 Score per residue for model 13

• Molecule 1: DIHYDROFOLATE REDUCTASE

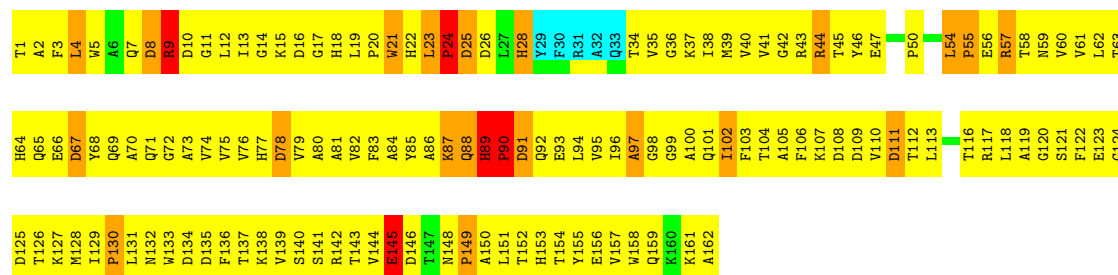
Chain A: 7% 76% 11%



4.2.14 Score per residue for model 14

• Molecule 1: DIHYDROFOLATE REDUCTASE

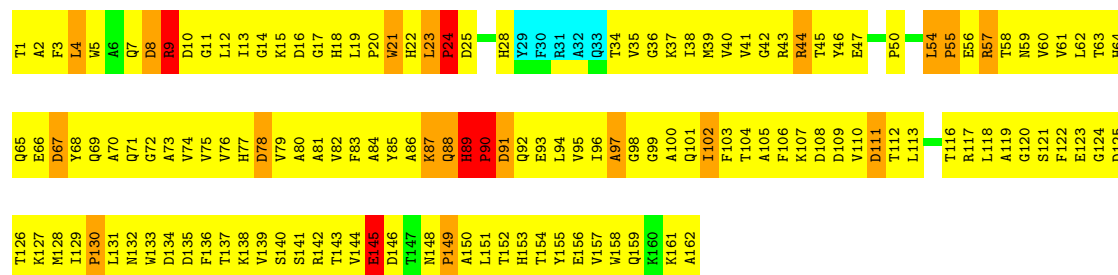
Chain A: 7% 75% 12%



4.2.15 Score per residue for model 15 (medoid)

• Molecule 1: DIHYDROFOLATE REDUCTASE

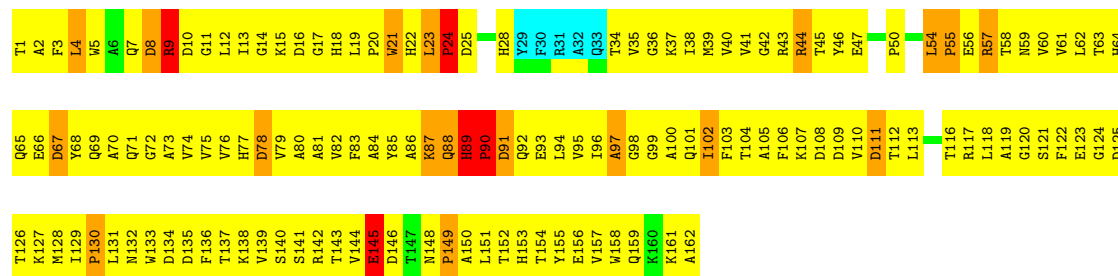
Chain A: 7% 75% 11%



4.2.16 Score per residue for model 16

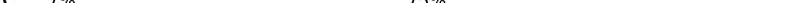
• Molecule 1: DIHYDROFOLATE REDUCTASE

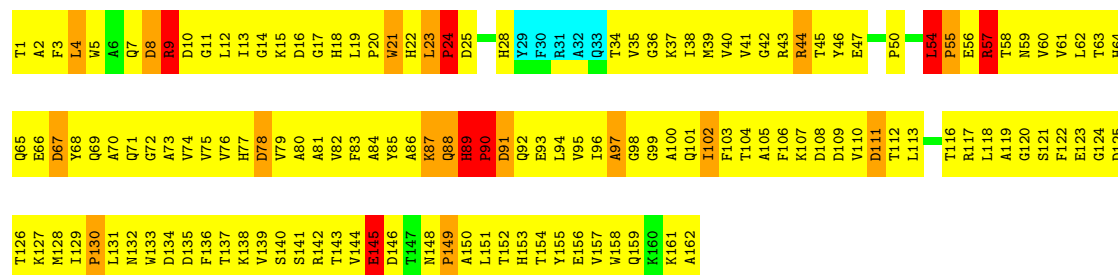
Chain A: 7% 75% 11%



4.2.17 Score per residue for model 17

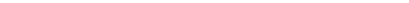
- Molecule 1: DIHYDROFOLATE REDUCTASE

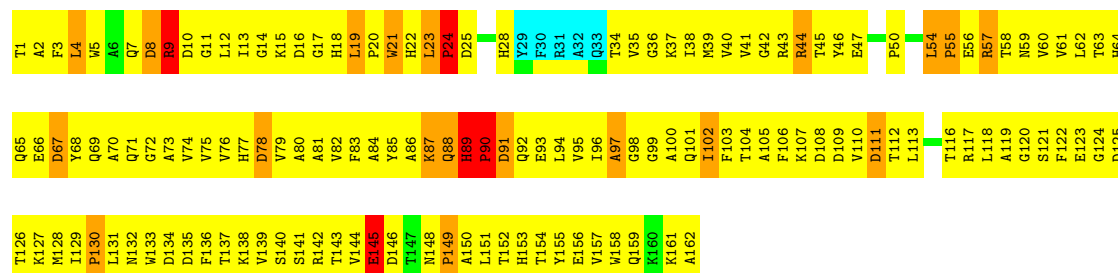
Chain A:  7% 75% 10% . .



4.2.18 Score per residue for model 18

- Molecule 1: DIHYDROFOLATE REDUCTASE

Chain A:  7% 75% 12% 2% 2%



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	4.75±0.00	233±1/1282 (18.2± 0.1%)	5.08±0.00	446±2/1747 (25.5± 0.1%)
All	All	4.75	4202/23076 (18.2%)	5.08	8024/31446 (25.5%)

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	73.09	2.50	1.47	1	18
1	A	89	HIS	C-O	26.09	1.57	1.24	1	18
1	A	19	LEU	C-N	23.38	1.55	1.33	1	18
1	A	24	PRO	N-CD	21.89	1.78	1.47	1	18
1	A	18	HIS	CD2-NE2	21.79	1.61	1.37	1	18
1	A	142	ARG	NE-CZ	19.89	1.54	1.33	1	18
1	A	67	ASP	CA-CB	19.71	1.87	1.53	1	18
1	A	130	PRO	N-CD	18.13	1.73	1.47	1	18
1	A	129	ILE	C-N	17.98	1.54	1.33	1	18
1	A	149	PRO	N-CD	16.29	1.70	1.47	1	18
1	A	89	HIS	C-N	-15.78	0.96	1.33	1	18
1	A	117	ARG	NE-CZ	-15.72	1.15	1.33	1	18
1	A	148	ASN	C-N	15.34	1.51	1.34	1	18
1	A	55	PRO	N-CD	15.31	1.69	1.47	1	18

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	105	ALA	C-O	14.16	1.42	1.24	1	18
1	A	90	PRO	N-CA	13.62	1.64	1.47	1	18
1	A	23	LEU	C-O	-13.43	1.09	1.24	1	18
1	A	135	ASP	CA-C	13.17	1.71	1.52	1	18
1	A	67	ASP	CG-OD1	13.10	1.50	1.25	1	18
1	A	18	HIS	CG-ND1	13.06	1.52	1.38	1	18
1	A	20	PRO	N-CD	13.05	1.66	1.47	1	18
1	A	145	GLU	CD-OE2	12.90	1.49	1.25	1	18
1	A	18	HIS	ND1-CE1	12.85	1.45	1.32	1	18
1	A	78	ASP	C-O	12.75	1.38	1.23	1	18
1	A	23	LEU	C-N	12.45	1.50	1.34	1	18
1	A	67	ASP	CG-OD2	11.81	1.47	1.25	1	18
1	A	95	VAL	CA-C	11.74	1.68	1.52	1	18
1	A	77	HIS	CE1-NE2	11.71	1.44	1.32	1	18
1	A	148	ASN	CA-C	11.67	1.66	1.52	1	18
1	A	67	ASP	C-N	11.26	1.48	1.33	1	18
1	A	146	ASP	CA-C	11.25	1.66	1.52	1	18
1	A	117	ARG	CZ-NH1	10.97	1.48	1.32	1	18
1	A	14	GLY	CA-C	10.84	1.63	1.51	1	18
1	A	19	LEU	C-O	-10.71	1.10	1.23	1	18
1	A	142	ARG	CA-C	10.61	1.65	1.52	1	18
1	A	22	HIS	CG-CD2	10.56	1.47	1.35	1	18
1	A	64	HIS	CG-ND1	-10.55	1.26	1.38	1	18
1	A	94	LEU	CA-C	10.43	1.65	1.52	1	18
1	A	16	ASP	CA-CB	10.37	1.69	1.53	1	18
1	A	148	ASN	C-O	-10.37	1.11	1.24	1	18
1	A	20	PRO	N-CA	10.36	1.59	1.47	1	18
1	A	132	ASN	N-CA	10.31	1.59	1.46	1	18
1	A	44	ARG	CD-NE	-10.11	1.32	1.46	1	18
1	A	58	THR	CA-CB	10.08	1.66	1.53	1	18
1	A	134	ASP	CG-OD1	9.86	1.44	1.25	1	18
1	A	91	ASP	CA-CB	9.71	1.71	1.53	1	18
1	A	23	LEU	CA-C	9.70	1.64	1.52	1	18
1	A	55	PRO	N-CA	9.66	1.55	1.46	1	18
1	A	134	ASP	CA-CB	9.59	1.69	1.53	1	18
1	A	152	THR	CA-C	9.51	1.65	1.52	1	18
1	A	78	ASP	CG-OD2	9.48	1.43	1.25	1	18
1	A	8	ASP	N-CA	9.40	1.57	1.45	1	18
1	A	134	ASP	CG-OD2	9.38	1.43	1.25	1	18
1	A	91	ASP	C-N	9.34	1.45	1.33	1	18
1	A	11	GLY	C-N	9.26	1.45	1.33	1	18

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	123	GLU	CA-CB	9.12	1.67	1.53	1	18
1	A	25	ASP	C-O	-9.10	1.13	1.24	1	18
1	A	44	ARG	CZ-NH1	9.02	1.45	1.32	1	18
1	A	137	THR	C-O	8.95	1.34	1.24	1	18
1	A	77	HIS	CA-CB	8.94	1.67	1.53	1	18
1	A	83	PHE	C-N	-8.93	1.22	1.33	1	18
1	A	86	ALA	CA-C	8.85	1.64	1.52	1	18
1	A	70	ALA	C-O	8.75	1.33	1.23	1	18
1	A	108	ASP	CB-CG	8.73	1.73	1.52	1	18
1	A	139	VAL	CA-CB	8.68	1.66	1.54	1	18
1	A	142	ARG	CZ-NH1	8.54	1.44	1.32	1	18
1	A	145	GLU	CD-OE1	8.54	1.41	1.25	1	18
1	A	75	VAL	C-N	8.50	1.44	1.33	1	18
1	A	81	ALA	CA-C	-8.47	1.41	1.52	1	18
1	A	79	VAL	CA-CB	8.41	1.66	1.54	1	18
1	A	145	GLU	CB-CG	8.38	1.77	1.52	1	18
1	A	144	VAL	CA-C	8.35	1.63	1.52	1	18
1	A	129	ILE	C-O	-8.34	1.14	1.24	1	18
1	A	60	VAL	C-N	-8.21	1.23	1.33	1	18
1	A	63	THR	C-O	8.18	1.33	1.23	1	18
1	A	13	ILE	C-N	8.17	1.45	1.33	1	18
1	A	64	HIS	ND1-CE1	8.10	1.40	1.32	1	18
1	A	39	MET	N-CA	-8.08	1.36	1.46	1	18
1	A	161	LYS	C-N	8.07	1.44	1.33	1	18
1	A	140	SER	CA-CB	8.04	1.70	1.54	1	18
1	A	65	GLN	CD-NE2	8.03	1.50	1.33	1	18
1	A	17	GLY	N-CA	8.01	1.57	1.45	1	18
1	A	131	LEU	C-O	7.95	1.33	1.23	1	18
1	A	162	ALA	C-O	7.92	1.39	1.23	1	18
1	A	92	GLN	CA-C	7.92	1.62	1.52	1	18
1	A	91	ASP	C-O	7.86	1.34	1.24	1	18
1	A	24	PRO	CA-CB	7.84	1.65	1.53	1	18
1	A	82	VAL	N-CA	-7.82	1.37	1.46	1	18
1	A	111	ASP	N-CA	7.80	1.55	1.45	1	18
1	A	91	ASP	CA-C	7.78	1.63	1.52	1	18
1	A	70	ALA	CA-CB	7.76	1.62	1.52	1	18
1	A	123	GLU	CA-C	-7.75	1.43	1.52	1	18
1	A	132	ASN	C-O	7.72	1.34	1.23	1	18
1	A	149	PRO	C-O	7.71	1.34	1.24	1	18
1	A	141	SER	C-O	7.66	1.32	1.23	1	18
1	A	142	ARG	N-CA	7.63	1.55	1.46	1	18

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	109	ASP	CB-CG	7.57	1.71	1.52	1	18
1	A	25	ASP	N-CA	-7.56	1.37	1.46	1	18
1	A	98	GLY	C-O	-7.54	1.16	1.24	1	18
1	A	108	ASP	CG-OD2	7.46	1.39	1.25	1	18
1	A	44	ARG	CA-C	-7.28	1.43	1.52	1	18
1	A	125	ASP	CG-OD1	7.28	1.39	1.25	1	18
1	A	76	VAL	C-N	7.22	1.44	1.33	1	18
1	A	22	HIS	C-O	-7.17	1.14	1.23	1	18
1	A	118	LEU	CB-CG	7.17	1.67	1.53	1	18
1	A	162	ALA	CA-C	7.16	1.68	1.52	1	18
1	A	22	HIS	CE1-NE2	7.10	1.39	1.32	1	18
1	A	91	ASP	CG-OD1	7.08	1.38	1.25	1	18
1	A	69	GLN	C-O	-7.07	1.15	1.24	1	18
1	A	121	SER	CB-OG	-7.04	1.28	1.42	1	18
1	A	45	THR	CA-C	6.99	1.61	1.52	1	18
1	A	162	ALA	C-OXT	6.93	1.37	1.23	1	18
1	A	111	ASP	CG-OD1	6.91	1.38	1.25	1	18
1	A	99	GLY	CA-C	-6.90	1.39	1.52	1	18
1	A	130	PRO	C-O	6.90	1.31	1.23	1	18
1	A	97	ALA	CA-C	6.89	1.61	1.52	1	18
1	A	43	ARG	C-N	6.88	1.43	1.33	1	18
1	A	82	VAL	CA-CB	6.87	1.62	1.54	1	18
1	A	9	ARG	CZ-NH2	6.85	1.42	1.33	1	18
1	A	65	GLN	CA-CB	-6.84	1.44	1.52	1	18
1	A	46	TYR	C-O	6.83	1.32	1.24	1	18
1	A	94	LEU	CB-CG	-6.82	1.39	1.53	1	18
1	A	92	GLN	N-CA	6.78	1.54	1.46	1	18
1	A	2	ALA	CA-C	6.77	1.61	1.52	1	18
1	A	107	LYS	N-CA	6.75	1.54	1.46	1	18
1	A	155	TYR	N-CA	6.75	1.54	1.46	1	18
1	A	107	LYS	CA-CB	6.73	1.65	1.53	1	18
1	A	84	ALA	N-CA	6.73	1.54	1.46	1	18
1	A	137	THR	CA-CB	6.68	1.65	1.53	1	18
1	A	65	GLN	C-O	6.59	1.31	1.23	1	18
1	A	128	MET	CA-C	6.59	1.61	1.52	1	18
1	A	59	ASN	CA-C	-6.57	1.44	1.52	1	18
1	A	43	ARG	NE-CZ	6.55	1.40	1.33	1	18
1	A	89	HIS	CA-C	-6.54	1.44	1.52	1	18
1	A	138	LYS	N-CA	-6.48	1.38	1.46	1	18
1	A	9	ARG	CZ-NH1	6.48	1.41	1.32	1	18
1	A	161	LYS	C-O	6.46	1.31	1.23	1	18

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	64	HIS	CD2-NE2	6.44	1.45	1.37	1	18
1	A	159	GLN	CB-CG	6.44	1.71	1.52	1	18
1	A	129	ILE	CA-C	6.43	1.59	1.52	1	18
1	A	108	ASP	CG-OD1	6.43	1.37	1.25	1	18
1	A	103	PHE	C-N	6.38	1.42	1.33	1	18
1	A	8	ASP	C-N	6.36	1.42	1.33	1	18
1	A	38	ILE	CA-CB	6.35	1.60	1.53	1	18
1	A	104	THR	N-CA	6.33	1.54	1.46	1	18
1	A	105	ALA	CA-C	-6.32	1.44	1.52	1	18
1	A	89	HIS	ND1-CE1	6.30	1.38	1.32	1	18
1	A	109	ASP	CG-OD2	6.28	1.37	1.25	1	18
1	A	24	PRO	C-N	-6.28	1.26	1.33	1	18
1	A	123	GLU	C-O	6.27	1.31	1.23	1	18
1	A	43	ARG	CA-C	6.25	1.61	1.52	1	18
1	A	55	PRO	CA-C	-6.23	1.47	1.53	1	18
1	A	121	SER	C-O	6.22	1.31	1.24	1	18
1	A	8	ASP	CG-OD1	6.20	1.37	1.25	1	18
1	A	95	VAL	C-O	-6.20	1.17	1.24	1	18
1	A	10	ASP	CG-OD1	6.19	1.37	1.25	1	18
1	A	127	LYS	CA-C	6.12	1.60	1.52	1	18
1	A	153	HIS	N-CA	6.11	1.53	1.45	1	18
1	A	109	ASP	CA-CB	6.11	1.62	1.53	1	18
1	A	22	HIS	ND1-CE1	6.09	1.38	1.32	1	18
1	A	87	LYS	CA-C	6.09	1.60	1.52	1	18
1	A	78	ASP	CA-C	-6.09	1.45	1.52	1	18
1	A	146	ASP	CG-OD1	6.06	1.36	1.25	1	18
1	A	120	GLY	N-CA	-6.05	1.38	1.45	1	18
1	A	36	GLY	CA-C	-6.05	1.43	1.51	1	18
1	A	68	TYR	CA-CB	6.05	1.63	1.53	1	18
1	A	9	ARG	CA-C	-6.05	1.44	1.52	1	18
1	A	88	GLN	C-N	6.04	1.46	1.33	1	18
1	A	13	ILE	CA-CB	6.03	1.62	1.54	1	18
1	A	98	GLY	C-N	5.99	1.41	1.33	1	18
1	A	119	ALA	N-CA	5.99	1.54	1.46	1	18
1	A	157	VAL	N-CA	5.93	1.54	1.46	1	18
1	A	148	ASN	N-CA	5.91	1.54	1.46	1	18
1	A	23	LEU	CB-CG	-5.90	1.41	1.53	1	18
1	A	91	ASP	CG-OD2	5.89	1.36	1.25	1	18
1	A	7	GLN	C-O	-5.86	1.16	1.23	1	18
1	A	69	GLN	CD-NE2	5.86	1.45	1.33	1	18
1	A	140	SER	CB-OG	-5.84	1.30	1.42	1	18

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	118	LEU	N-CA	5.83	1.53	1.45	1	18
1	A	123	GLU	CD-OE1	5.83	1.36	1.25	1	18
1	A	35	VAL	CA-C	5.83	1.59	1.52	1	6
1	A	106	PHE	CA-CB	5.81	1.62	1.53	1	18
1	A	77	HIS	CD2-NE2	-5.81	1.31	1.37	1	18
1	A	102	ILE	CA-CB	5.80	1.62	1.54	1	18
1	A	44	ARG	CZ-NH2	5.79	1.41	1.33	1	18
1	A	83	PHE	CA-C	5.75	1.60	1.52	1	18
1	A	4	LEU	CA-CB	5.75	1.61	1.53	3	18
1	A	18	HIS	CA-CB	5.75	1.62	1.53	1	18
1	A	45	THR	N-CA	5.69	1.53	1.46	1	18
1	A	154	THR	CA-C	5.62	1.59	1.52	1	18
1	A	87	LYS	CD-CE	5.62	1.69	1.52	1	18
1	A	145	GLU	CG-CD	5.61	1.66	1.52	1	18
1	A	9	ARG	CA-CB	5.58	1.63	1.53	1	18
1	A	131	LEU	N-CA	5.57	1.53	1.45	1	18
1	A	145	GLU	CA-CB	5.54	1.62	1.53	1	18
1	A	133	TRP	CD2-CE2	5.54	1.50	1.41	1	18
1	A	106	PHE	N-CA	5.53	1.52	1.46	1	18
1	A	152	THR	C-N	-5.51	1.26	1.33	1	18
1	A	9	ARG	NE-CZ	5.49	1.39	1.33	1	18
1	A	113	LEU	C-O	5.49	1.30	1.24	1	18
1	A	23	LEU	N-CA	5.46	1.52	1.46	1	18
1	A	64	HIS	CG-CD2	5.46	1.41	1.35	1	18
1	A	110	VAL	N-CA	5.45	1.52	1.46	1	18
1	A	93	GLU	CD-OE1	5.44	1.35	1.25	1	18
1	A	78	ASP	CG-OD1	5.42	1.35	1.25	1	18
1	A	3	PHE	CG-CD1	5.41	1.50	1.38	1	18
1	A	9	ARG	CG-CD	5.41	1.68	1.52	1	18
1	A	22	HIS	CD2-NE2	-5.36	1.31	1.37	1	18
1	A	96	ILE	C-O	-5.36	1.18	1.24	1	18
1	A	117	ARG	CB-CG	-5.35	1.36	1.52	1	18
1	A	116	THR	CA-C	5.34	1.59	1.52	1	18
1	A	117	ARG	CA-C	5.32	1.59	1.52	1	18
1	A	15	LYS	C-O	5.32	1.30	1.23	1	18
1	A	128	MET	N-CA	5.31	1.52	1.46	1	18
1	A	78	ASP	N-CA	5.30	1.52	1.46	1	18
1	A	28	HIS	CE1-NE2	5.29	1.37	1.32	12	16
1	A	132	ASN	CB-CG	5.27	1.65	1.52	1	18
1	A	105	ALA	N-CA	5.27	1.53	1.46	1	18
1	A	107	LYS	CD-CE	5.27	1.68	1.52	1	18

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	116	THR	C-N	-5.22	1.25	1.33	1	18
1	A	153	HIS	CD2-NE2	-5.22	1.32	1.37	1	18
1	A	135	ASP	CG-OD2	5.21	1.35	1.25	1	18
1	A	61	VAL	CA-C	-5.21	1.46	1.52	1	18
1	A	93	GLU	N-CA	5.20	1.52	1.46	1	18
1	A	64	HIS	C-N	5.19	1.40	1.33	1	18
1	A	100	ALA	CA-C	5.19	1.59	1.52	1	18
1	A	36	GLY	C-O	-5.17	1.17	1.24	2	18
1	A	28	HIS	CG-CD2	5.16	1.41	1.35	13	4
1	A	135	ASP	CB-CG	5.15	1.65	1.52	1	18
1	A	126	THR	CA-CB	5.14	1.62	1.53	1	18
1	A	102	ILE	N-CA	5.11	1.53	1.46	1	18
1	A	63	THR	C-N	-5.10	1.25	1.33	1	18
1	A	56	GLU	CB-CG	5.08	1.67	1.52	1	18
1	A	14	GLY	N-CA	5.05	1.50	1.45	1	18
1	A	77	HIS	CG-CD2	5.01	1.41	1.35	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	47.11	161.60	119.20	1	18
1	A	90	PRO	N-CA-CB	32.03	136.88	103.25	1	18
1	A	90	PRO	CA-N-CD	-31.42	68.02	112.00	1	18
1	A	9	ARG	CD-NE-CZ	29.54	165.75	124.40	1	18
1	A	148	ASN	CA-C-O	23.86	136.98	119.32	1	18
1	A	117	ARG	NE-CZ-NH1	-23.14	98.36	121.50	1	18
1	A	78	ASP	CA-CB-CG	22.82	135.42	112.60	1	18
1	A	117	ARG	CD-NE-CZ	22.21	155.49	124.40	1	18
1	A	67	ASP	OD1-CG-OD2	19.23	169.06	122.90	1	18
1	A	89	HIS	C-N-CD	-19.09	46.75	125.00	1	18
1	A	19	LEU	CA-C-O	18.61	139.81	120.64	1	18
1	A	142	ARG	NE-CZ-NH2	-16.27	104.56	119.20	1	18
1	A	148	ASN	CA-C-N	-15.89	103.34	119.87	1	18
1	A	148	ASN	C-N-CA	-15.89	103.34	119.87	1	18
1	A	88	GLN	CA-C-O	15.88	138.91	119.38	1	18
1	A	89	HIS	CA-C-O	-15.80	98.51	120.16	1	18
1	A	71	GLN	OE1-CD-NE2	-15.65	106.95	122.60	1	18
1	A	111	ASP	OD1-CG-OD2	15.57	160.26	122.90	1	18
1	A	56	GLU	OE1-CD-OE2	15.43	159.94	122.90	1	18
1	A	69	GLN	OE1-CD-NE2	-15.41	107.19	122.60	1	18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	131	LEU	CD1-CG-CD2	15.30	144.46	110.80	1	18
1	A	117	ARG	NH1-CZ-NH2	-14.85	99.99	119.30	1	18
1	A	19	LEU	CA-C-N	-14.82	104.00	120.45	1	18
1	A	19	LEU	C-N-CA	-14.82	104.00	120.45	1	18
1	A	140	SER	CA-CB-OG	-14.58	81.94	111.10	1	18
1	A	142	ARG	CD-NE-CZ	-14.54	104.05	124.40	1	18
1	A	105	ALA	O-C-N	-14.26	104.73	122.27	1	18
1	A	111	ASP	CB-CG-OD1	-14.07	86.04	118.40	1	18
1	A	64	HIS	CB-CG-CD2	-13.99	113.02	131.20	1	18
1	A	62	LEU	O-C-N	-13.86	107.42	123.22	1	18
1	A	137	THR	CA-C-O	-13.51	106.39	120.71	1	18
1	A	132	ASN	CA-C-N	13.45	138.30	120.28	1	18
1	A	132	ASN	C-N-CA	13.45	138.30	120.28	1	18
1	A	76	VAL	CA-C-O	13.45	135.39	121.67	1	18
1	A	123	GLU	O-C-N	-13.34	107.59	123.19	1	18
1	A	159	GLN	OE1-CD-NE2	-13.13	109.47	122.60	1	18
1	A	110	VAL	CA-C-O	13.06	137.61	121.02	1	18
1	A	157	VAL	CA-C-O	-12.93	106.94	120.39	1	18
1	A	132	ASN	CA-CB-CG	-12.88	99.72	112.60	1	18
1	A	22	HIS	CA-C-O	12.65	137.48	120.15	1	18
1	A	3	PHE	CG-CD2-CE2	12.63	142.17	120.70	1	18
1	A	66	GLU	CG-CD-OE2	-12.63	89.36	118.40	1	18
1	A	110	VAL	O-C-N	-12.29	108.57	122.83	1	18
1	A	78	ASP	O-C-N	-12.18	110.48	123.26	1	18
1	A	44	ARG	N-CA-CB	-12.13	92.28	110.12	1	18
1	A	132	ASN	CA-C-O	-11.93	107.70	121.66	1	18
1	A	65	GLN	CG-CD-NE2	-11.81	98.69	116.40	1	18
1	A	129	ILE	CA-C-O	11.79	135.76	119.95	1	18
1	A	83	PHE	CA-C-O	-11.60	108.25	120.55	1	18
1	A	67	ASP	CB-CA-C	-11.60	88.07	110.11	1	18
1	A	73	ALA	O-C-N	-11.54	106.94	122.97	1	18
1	A	23	LEU	CA-C-O	11.39	134.44	121.22	1	18
1	A	66	GLU	OE1-CD-OE2	11.38	150.21	122.90	1	18
1	A	125	ASP	CA-CB-CG	11.38	123.98	112.60	1	18
1	A	89	HIS	CG-CD2-NE2	11.36	118.56	107.20	1	18
1	A	58	THR	CA-CB-OG1	-11.33	92.61	109.60	1	18
1	A	45	THR	N-CA-C	-11.25	98.99	111.14	1	18
1	A	59	ASN	O-C-N	-11.18	110.48	123.22	1	18
1	A	158	TRP	CE2-CD2-CE3	11.12	129.92	118.80	1	18
1	A	129	ILE	CA-C-N	-11.03	108.32	119.90	1	18
1	A	129	ILE	C-N-CA	-11.03	108.32	119.90	1	18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	8	ASP	CA-C-O	11.02	134.33	121.88	1	18
1	A	88	GLN	CA-CB-CG	11.02	136.14	114.10	1	18
1	A	108	ASP	O-C-N	10.92	135.99	122.34	1	18
1	A	63	THR	CA-C-O	-10.71	107.75	120.60	1	18
1	A	23	LEU	CA-C-N	-10.71	107.16	119.05	1	18
1	A	23	LEU	C-N-CA	-10.71	107.16	119.05	1	18
1	A	44	ARG	NE-CZ-NH2	-10.64	109.62	119.20	1	18
1	A	45	THR	CA-C-O	-10.58	109.80	120.70	1	18
1	A	159	GLN	CB-CG-CD	-10.50	94.75	112.60	1	18
1	A	80	ALA	N-CA-C	-10.49	99.84	111.28	1	18
1	A	91	ASP	CA-CB-CG	-10.44	102.16	112.60	1	18
1	A	108	ASP	CA-C-N	-10.43	106.30	122.37	1	18
1	A	108	ASP	C-N-CA	-10.43	106.30	122.37	1	18
1	A	161	LYS	CA-C-O	-10.38	110.55	121.55	1	18
1	A	28	HIS	ND1-CE1-NE2	10.38	118.78	108.40	9	18
1	A	149	PRO	CA-C-N	10.35	135.19	120.28	1	18
1	A	149	PRO	C-N-CA	10.35	135.19	120.28	1	18
1	A	162	ALA	CB-CA-C	-10.26	95.11	110.50	1	18
1	A	44	ARG	CG-CD-NE	10.24	134.53	112.00	1	18
1	A	65	GLN	OE1-CD-NE2	10.21	132.81	122.60	1	18
1	A	45	THR	CA-CB-OG1	-10.19	94.32	109.60	1	18
1	A	65	GLN	O-C-N	-10.19	108.62	122.48	1	18
1	A	149	PRO	N-CA-CB	10.18	112.98	103.41	1	18
1	A	148	ASN	CB-CG-ND2	-10.14	101.19	116.40	1	18
1	A	89	HIS	ND1-CG-CD2	-10.12	95.98	106.10	1	18
1	A	88	GLN	CA-C-N	10.09	146.41	121.80	1	18
1	A	88	GLN	C-N-CA	10.09	146.41	121.80	1	18
1	A	56	GLU	CG-CD-OE2	-10.06	95.25	118.40	1	18
1	A	67	ASP	CB-CG-OD2	-10.06	95.26	118.40	1	18
1	A	67	ASP	N-CA-C	9.98	125.27	113.20	1	18
1	A	158	TRP	NE1-CE2-CD2	9.95	120.33	107.40	1	18
1	A	153	HIS	CG-CD2-NE2	9.94	117.14	107.20	1	18
1	A	67	ASP	CB-CG-OD1	-9.88	95.67	118.40	1	18
1	A	77	HIS	ND1-CE1-NE2	-9.76	98.64	108.40	1	18
1	A	148	ASN	N-CA-C	-9.73	95.72	109.24	1	18
1	A	123	GLU	OE1-CD-OE2	9.64	146.04	122.90	1	18
1	A	157	VAL	O-C-N	9.59	133.37	123.20	1	18
1	A	3	PHE	CD1-CG-CD2	-9.58	104.23	118.60	1	18
1	A	90	PRO	CA-C-N	9.57	139.87	122.06	1	18
1	A	90	PRO	C-N-CA	9.57	139.87	122.06	1	18
1	A	24	PRO	CA-N-CD	-9.55	98.62	112.00	1	18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	35	VAL	N-CA-CB	9.54	121.46	110.49	8	18
1	A	107	LYS	CB-CG-CD	9.54	133.25	111.30	1	18
1	A	73	ALA	CA-C-N	9.54	136.09	123.11	1	18
1	A	73	ALA	C-N-CA	9.54	136.09	123.11	1	18
1	A	13	ILE	CA-C-O	9.48	128.75	118.98	1	18
1	A	87	LYS	N-CA-CB	9.46	124.03	110.12	1	18
1	A	101	GLN	OE1-CD-NE2	-9.41	113.19	122.60	1	18
1	A	109	ASP	N-CA-CB	-9.39	95.49	110.98	1	18
1	A	21	TRP	CB-CG-CD1	9.38	140.98	126.90	1	18
1	A	9	ARG	CG-CD-NE	-9.31	91.53	112.00	1	18
1	A	161	LYS	CD-CE-NZ	9.30	141.66	111.90	1	18
1	A	123	GLU	N-CA-CB	-9.24	95.27	110.52	1	18
1	A	25	ASP	CA-C-O	9.22	130.76	120.90	1	18
1	A	105	ALA	N-CA-C	-9.22	101.13	111.82	1	18
1	A	22	HIS	CA-CB-CG	-9.21	104.59	113.80	1	18
1	A	21	TRP	CB-CG-CD2	-9.20	113.92	126.80	1	18
1	A	61	VAL	O-C-N	-9.17	113.56	123.18	1	18
1	A	8	ASP	N-CA-C	-9.12	97.77	110.35	1	18
1	A	28	HIS	CE1-NE2-CD2	-9.11	99.89	109.00	10	18
1	A	20	PRO	CB-CA-C	-9.10	98.05	110.88	1	18
1	A	88	GLN	O-C-N	-9.02	110.34	122.43	1	18
1	A	62	LEU	CD1-CG-CD2	-9.01	90.98	110.80	1	18
1	A	132	ASN	CB-CA-C	8.98	126.23	111.41	1	18
1	A	59	ASN	CB-CG-ND2	8.94	129.80	116.40	1	18
1	A	44	ARG	O-C-N	-8.93	112.65	122.12	1	18
1	A	150	ALA	O-C-N	-8.93	111.77	122.22	1	18
1	A	64	HIS	CG-CD2-NE2	-8.91	98.29	107.20	1	18
1	A	118	LEU	CB-CG-CD2	-8.90	84.00	110.70	1	18
1	A	149	PRO	N-CD-CG	-8.79	90.01	103.20	1	18
1	A	43	ARG	CA-C-N	-8.78	108.52	120.28	1	18
1	A	43	ARG	C-N-CA	-8.78	108.52	120.28	1	18
1	A	67	ASP	N-CA-CB	-8.72	96.29	110.42	1	18
1	A	97	ALA	CA-C-O	-8.70	109.33	119.59	1	18
1	A	127	LYS	CB-CG-CD	-8.65	91.41	111.30	1	18
1	A	141	SER	O-C-N	-8.64	112.81	123.44	1	18
1	A	64	HIS	ND1-CE1-NE2	-8.63	99.77	108.40	1	18
1	A	89	HIS	CB-CG-CD2	8.62	142.41	131.20	1	18
1	A	90	PRO	O-C-N	-8.61	111.02	122.64	1	18
1	A	148	ASN	CB-CG-OD1	8.54	137.87	120.80	1	18
1	A	161	LYS	CG-CD-CE	-8.53	91.69	111.30	1	18
1	A	141	SER	CA-CB-OG	-8.52	94.05	111.10	1	18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	46	TYR	O-C-N	-8.52	113.09	122.12	1	18
1	A	69	GLN	CG-CD-OE1	8.44	137.68	120.80	1	18
1	A	64	HIS	CB-CG-ND1	8.40	135.31	122.70	1	18
1	A	108	ASP	OD1-CG-OD2	8.40	143.07	122.90	1	18
1	A	108	ASP	CA-CB-CG	8.38	120.98	112.60	1	18
1	A	88	GLN	N-CA-C	8.37	122.75	112.54	1	18
1	A	79	VAL	CA-C-N	8.35	131.47	120.28	1	18
1	A	79	VAL	C-N-CA	8.35	131.47	120.28	1	18
1	A	90	PRO	CA-C-O	8.35	135.79	120.60	1	18
1	A	55	PRO	CA-N-CD	-8.34	100.33	112.00	1	18
1	A	88	GLN	OE1-CD-NE2	-8.33	114.27	122.60	1	18
1	A	89	HIS	N-CA-CB	8.32	125.18	110.37	1	18
1	A	25	ASP	O-C-N	-8.30	113.45	122.09	5	18
1	A	153	HIS	ND1-CG-CD2	-8.30	97.80	106.10	1	18
1	A	101	GLN	CA-CB-CG	-8.28	97.54	114.10	1	18
1	A	62	LEU	N-CA-CB	8.26	123.89	110.42	1	18
1	A	57	ARG	N-CA-C	-8.23	96.20	108.79	1	18
1	A	78	ASP	OD1-CG-OD2	8.16	142.48	122.90	1	18
1	A	123	GLU	CA-C-O	8.14	129.83	120.80	1	18
1	A	66	GLU	CA-CB-CG	-8.13	97.84	114.10	1	18
1	A	88	GLN	CG-CD-OE1	8.12	137.04	120.80	1	18
1	A	91	ASP	OD1-CG-OD2	-8.11	103.43	122.90	1	18
1	A	145	GLU	CB-CG-CD	-8.10	98.83	112.60	1	18
1	A	113	LEU	CA-C-O	-8.03	111.48	120.32	1	18
1	A	144	VAL	CA-C-N	-8.03	110.68	122.65	1	18
1	A	144	VAL	C-N-CA	-8.03	110.68	122.65	1	18
1	A	137	THR	CA-CB-OG1	-7.98	97.63	109.60	1	18
1	A	82	VAL	O-C-N	-7.96	113.42	121.94	1	18
1	A	89	HIS	CB-CA-C	7.94	125.82	110.17	1	18
1	A	97	ALA	O-C-N	7.94	131.70	122.25	1	18
1	A	126	THR	CA-CB-OG1	-7.94	97.69	109.60	1	18
1	A	117	ARG	CA-C-O	-7.94	111.87	120.36	1	18
1	A	47	GLU	CA-CB-CG	-7.91	98.28	114.10	1	18
1	A	88	GLN	CB-CG-CD	7.85	125.94	112.60	1	18
1	A	42	GLY	CA-C-O	7.83	130.35	121.90	1	18
1	A	54	LEU	CA-C-N	7.78	128.22	120.52	8	17
1	A	54	LEU	C-N-CA	7.78	128.22	120.52	8	17
1	A	92	GLN	CA-C-O	7.77	128.85	120.38	1	18
1	A	142	ARG	NH1-CZ-NH2	7.76	129.40	119.30	1	18
1	A	74	VAL	CA-C-O	7.67	129.64	120.66	1	18
1	A	161	LYS	CB-CG-CD	-7.66	93.69	111.30	1	18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	149	PRO	CA-CB-CG	-7.63	90.00	104.50	1	18
1	A	82	VAL	CA-C-O	7.61	130.01	121.18	1	18
1	A	123	GLU	CG-CD-OE2	-7.58	100.98	118.40	1	18
1	A	69	GLN	CA-C-O	7.57	128.53	120.36	1	18
1	A	122	PHE	CA-CB-CG	-7.55	106.25	113.80	1	18
1	A	124	GLY	CA-C-O	7.53	129.27	121.21	1	18
1	A	135	ASP	N-CA-CB	7.51	122.59	110.42	1	18
1	A	98	GLY	CA-C-O	-7.49	114.85	122.56	1	18
1	A	89	HIS	CE1-NE2-CD2	-7.44	101.56	109.00	1	18
1	A	35	VAL	CA-C-O	-7.41	111.52	120.78	6	15
1	A	68	TYR	CB-CG-CD1	-7.38	109.73	120.80	1	18
1	A	74	VAL	O-C-N	-7.32	113.29	122.88	1	18
1	A	135	ASP	OD1-CG-OD2	7.28	140.38	122.90	1	18
1	A	91	ASP	CB-CG-OD2	7.27	135.11	118.40	1	18
1	A	20	PRO	CA-N-CD	-7.25	101.85	112.00	1	18
1	A	64	HIS	CA-CB-CG	-7.23	106.57	113.80	1	18
1	A	62	LEU	CB-CG-CD2	-7.23	89.02	110.70	1	18
1	A	155	TYR	CB-CG-CD1	-7.15	110.07	120.80	1	18
1	A	109	ASP	CB-CG-OD2	-7.14	101.97	118.40	1	18
1	A	118	LEU	CB-CA-C	7.14	121.72	109.51	1	18
1	A	134	ASP	CB-CG-OD2	-7.13	102.00	118.40	1	18
1	A	125	ASP	CB-CG-OD2	7.13	134.79	118.40	1	18
1	A	84	ALA	O-C-N	-7.09	114.60	122.12	1	18
1	A	135	ASP	CB-CG-OD2	-7.09	102.09	118.40	1	18
1	A	87	LYS	O-C-N	-7.09	114.60	122.12	1	18
1	A	128	MET	CA-C-O	7.07	129.08	121.16	1	18
1	A	92	GLN	CB-CG-CD	-7.07	100.58	112.60	1	18
1	A	107	LYS	N-CA-C	-7.07	103.76	112.38	1	18
1	A	142	ARG	N-CA-C	-7.04	96.22	108.69	1	18
1	A	23	LEU	C-N-CD	7.04	153.88	125.00	1	18
1	A	83	PHE	CB-CG-CD2	-7.04	108.73	120.70	1	18
1	A	145	GLU	CA-C-O	7.01	128.58	120.80	1	18
1	A	117	ARG	O-C-N	6.99	131.19	123.22	1	18
1	A	150	ALA	CA-C-N	6.98	133.94	121.66	1	18
1	A	150	ALA	C-N-CA	6.98	133.94	121.66	1	18
1	A	82	VAL	N-CA-C	-6.94	103.90	110.42	1	18
1	A	78	ASP	N-CA-CB	-6.93	100.79	111.46	1	18
1	A	18	HIS	CA-CB-CG	6.92	120.72	113.80	1	18
1	A	24	PRO	CA-C-O	-6.91	109.09	119.86	1	18
1	A	105	ALA	CA-C-N	6.86	133.31	122.60	1	18
1	A	105	ALA	C-N-CA	6.86	133.31	122.60	1	18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	47	GLU	O-C-N	-6.83	114.22	122.22	18	18
1	A	55	PRO	CB-CA-C	-6.83	100.64	110.75	3	18
1	A	125	ASP	N-CA-CB	-6.83	100.35	111.01	1	18
1	A	105	ALA	CA-C-O	-6.83	112.12	119.97	1	18
1	A	153	HIS	CE1-NE2-CD2	-6.83	102.17	109.00	1	18
1	A	145	GLU	O-C-N	-6.81	115.22	123.19	1	18
1	A	132	ASN	CB-CG-ND2	-6.80	106.20	116.40	1	18
1	A	41	VAL	CA-C-N	6.80	126.80	120.34	1	18
1	A	41	VAL	C-N-CA	6.80	126.80	120.34	1	18
1	A	109	ASP	N-CA-C	-6.79	103.36	112.94	1	18
1	A	89	HIS	CA-C-N	-6.77	111.37	119.84	1	18
1	A	89	HIS	C-N-CA	-6.77	111.37	119.84	1	18
1	A	158	TRP	CE2-CD2-CG	-6.77	99.08	107.20	1	18
1	A	159	GLN	CG-CD-OE1	6.74	134.28	120.80	1	18
1	A	13	ILE	CA-C-N	-6.74	110.08	121.47	1	18
1	A	13	ILE	C-N-CA	-6.74	110.08	121.47	1	18
1	A	64	HIS	O-C-N	6.74	131.98	122.41	1	18
1	A	42	GLY	O-C-N	-6.72	114.22	122.76	1	18
1	A	134	ASP	O-C-N	-6.72	114.00	122.27	1	18
1	A	102	ILE	CA-CB-CG2	6.72	121.92	110.50	1	18
1	A	19	LEU	C-N-CD	6.71	152.50	125.00	1	18
1	A	109	ASP	OD1-CG-OD2	6.68	138.94	122.90	1	18
1	A	150	ALA	CA-C-O	6.68	127.65	120.10	1	18
1	A	104	THR	N-CA-CB	-6.68	100.31	110.12	1	18
1	A	121	SER	N-CA-CB	-6.67	99.48	110.68	1	18
1	A	54	LEU	N-CA-CB	6.66	120.54	110.02	13	17
1	A	95	VAL	O-C-N	6.63	130.23	123.20	1	18
1	A	7	GLN	CA-C-O	6.62	128.74	121.06	1	18
1	A	130	PRO	N-CA-CB	6.61	109.17	103.36	1	18
1	A	151	LEU	N-CA-CB	6.59	120.73	110.44	1	18
1	A	13	ILE	N-CA-C	6.59	119.99	113.53	1	18
1	A	80	ALA	CA-C-O	-6.58	113.57	120.55	1	18
1	A	20	PRO	CA-C-N	6.58	133.12	122.53	1	18
1	A	20	PRO	C-N-CA	6.58	133.12	122.53	1	18
1	A	99	GLY	O-C-N	-6.57	112.50	123.00	1	18
1	A	19	LEU	N-CA-C	-6.56	100.66	110.24	1	18
1	A	96	ILE	CA-CB-CG1	6.54	121.52	110.40	1	18
1	A	44	ARG	N-CA-C	6.54	118.41	111.28	1	18
1	A	148	ASN	C-N-CD	6.53	151.75	125.00	1	18
1	A	109	ASP	CA-CB-CG	-6.52	106.08	112.60	1	18
1	A	135	ASP	O-C-N	6.52	132.03	122.39	1	18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	23	LEU	N-CA-CB	6.50	119.15	111.09	1	18
1	A	78	ASP	CB-CA-C	6.49	123.90	111.17	1	18
1	A	93	GLU	CG-CD-OE1	-6.49	103.48	118.40	1	18
1	A	67	ASP	CA-C-O	6.48	127.61	119.12	1	18
1	A	63	THR	OG1-CB-CG2	6.47	122.23	109.30	1	18
1	A	134	ASP	N-CA-C	-6.43	104.36	111.82	1	18
1	A	64	HIS	CE1-NE2-CD2	6.41	115.41	109.00	1	18
1	A	1	THR	CA-CB-CG2	6.39	121.36	110.50	1	18
1	A	83	PHE	CE1-CZ-CE2	6.39	131.50	120.00	1	18
1	A	119	ALA	N-CA-CB	-6.38	99.99	110.40	1	18
1	A	161	LYS	O-C-N	-6.38	114.97	122.81	1	18
1	A	25	ASP	OD1-CG-OD2	-6.37	107.61	122.90	1	18
1	A	1	THR	OG1-CB-CG2	-6.35	96.59	109.30	1	18
1	A	106	PHE	N-CA-C	-6.35	104.68	112.88	1	18
1	A	142	ARG	CG-CD-NE	6.32	125.91	112.00	1	18
1	A	91	ASP	N-CA-C	-6.32	105.57	113.28	1	18
1	A	111	ASP	CB-CA-C	6.32	119.69	109.07	1	18
1	A	44	ARG	CB-CG-CD	-6.31	96.79	111.30	1	18
1	A	153	HIS	ND1-CE1-NE2	6.30	114.70	108.40	1	18
1	A	159	GLN	CA-C-O	6.29	127.90	120.66	1	18
1	A	18	HIS	CE1-NE2-CD2	-6.29	102.71	109.00	1	18
1	A	96	ILE	CA-CB-CG2	-6.27	99.83	110.50	1	18
1	A	158	TRP	CD2-CE2-CZ2	-6.26	116.14	122.40	1	18
1	A	145	GLU	CG-CD-OE1	-6.25	104.01	118.40	1	18
1	A	71	GLN	CA-CB-CG	-6.25	101.59	114.10	1	18
1	A	144	VAL	CA-CB-CG2	-6.25	99.78	110.40	1	18
1	A	75	VAL	N-CA-CB	6.25	119.22	111.41	1	18
1	A	12	LEU	O-C-N	-6.24	115.19	122.87	1	18
1	A	119	ALA	O-C-N	-6.24	113.85	122.46	1	18
1	A	26	ASP	N-CA-CB	-6.23	100.62	110.28	9	2
1	A	83	PHE	CD1-CE1-CZ	-6.23	108.78	120.00	1	18
1	A	106	PHE	CB-CG-CD2	6.23	131.29	120.70	1	18
1	A	108	ASP	CB-CG-OD2	-6.22	104.09	118.40	1	18
1	A	118	LEU	CD1-CG-CD2	-6.22	97.11	110.80	1	18
1	A	25	ASP	CB-CG-OD1	6.22	132.70	118.40	1	18
1	A	56	GLU	CG-CD-OE1	-6.18	104.18	118.40	1	18
1	A	141	SER	N-CA-CB	-6.16	100.48	110.71	1	18
1	A	59	ASN	OD1-CG-ND2	-6.15	116.45	122.60	1	18
1	A	93	GLU	CA-CB-CG	6.11	126.31	114.10	1	18
1	A	15	LYS	CB-CA-C	-6.10	101.33	110.24	1	18
1	A	136	PHE	CA-CB-CG	-6.09	107.71	113.80	1	18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	58	THR	O-C-N	6.09	130.13	123.13	1	18
1	A	11	GLY	CA-C-N	-6.07	112.10	120.71	1	18
1	A	11	GLY	C-N-CA	-6.07	112.10	120.71	1	18
1	A	37	LYS	N-CA-CB	-6.05	101.41	110.60	1	18
1	A	3	PHE	CA-C-N	6.04	132.08	123.14	7	18
1	A	3	PHE	C-N-CA	6.04	132.08	123.14	7	18
1	A	38	ILE	O-C-N	-6.03	115.29	122.77	1	18
1	A	20	PRO	O-C-N	-6.03	112.48	122.36	1	18
1	A	123	GLU	CA-C-N	6.02	128.94	120.57	1	18
1	A	123	GLU	C-N-CA	6.02	128.94	120.57	1	18
1	A	99	GLY	CA-C-N	6.01	128.62	120.38	1	18
1	A	99	GLY	C-N-CA	6.01	128.62	120.38	1	18
1	A	119	ALA	N-CA-C	-6.01	105.43	112.89	1	18
1	A	134	ASP	CA-C-N	5.96	133.86	121.94	1	18
1	A	134	ASP	C-N-CA	5.96	133.86	121.94	1	18
1	A	9	ARG	NE-CZ-NH2	5.94	124.55	119.20	1	18
1	A	28	HIS	CA-CB-CG	5.93	119.73	113.80	4	4
1	A	130	PRO	CA-N-CD	-5.91	103.72	112.00	1	18
1	A	15	LYS	O-C-N	-5.90	115.26	123.34	1	18
1	A	67	ASP	CA-CB-CG	-5.90	106.70	112.60	1	18
1	A	85	TYR	O-C-N	-5.88	115.74	122.09	1	18
1	A	107	LYS	CA-C-O	-5.87	112.39	119.49	1	18
1	A	108	ASP	CA-C-O	-5.87	112.48	119.35	1	18
1	A	9	ARG	N-CA-C	5.86	119.53	112.38	1	18
1	A	59	ASN	CA-C-O	5.86	126.63	120.36	1	18
1	A	65	GLN	CA-C-N	5.86	132.73	121.54	1	18
1	A	65	GLN	C-N-CA	5.86	132.73	121.54	1	18
1	A	74	VAL	N-CA-C	-5.82	98.76	107.37	1	18
1	A	39	MET	CA-C-O	-5.82	114.36	120.58	1	18
1	A	3	PHE	CB-CG-CD1	5.81	130.58	120.70	1	18
1	A	109	ASP	O-C-N	-5.79	115.18	122.19	1	18
1	A	142	ARG	CA-CB-CG	-5.79	102.52	114.10	1	18
1	A	143	THR	O-C-N	-5.75	116.50	123.29	1	18
1	A	40	VAL	O-C-N	5.71	129.37	123.03	1	18
1	A	86	ALA	CA-C-N	5.70	127.92	120.28	1	18
1	A	86	ALA	C-N-CA	5.70	127.92	120.28	1	18
1	A	38	ILE	CB-CG1-CD1	-5.69	101.86	113.80	1	18
1	A	121	SER	O-C-N	-5.68	116.54	123.30	1	18
1	A	92	GLN	CA-CB-CG	-5.67	102.77	114.10	1	18
1	A	71	GLN	CB-CG-CD	-5.66	102.98	112.60	1	18
1	A	77	HIS	ND1-CG-CD2	-5.66	100.44	106.10	1	18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	21	TRP	CA-C-O	5.64	127.66	121.40	1	18
1	A	66	GLU	CA-C-O	5.63	128.56	120.51	1	18
1	A	154	THR	CA-CB-OG1	-5.62	101.18	109.60	1	18
1	A	22	HIS	CB-CG-ND1	5.61	131.12	122.70	1	18
1	A	83	PHE	CD1-CG-CD2	5.61	127.01	118.60	1	18
1	A	149	PRO	CB-CA-C	-5.61	102.97	111.44	1	18
1	A	130	PRO	CA-C-O	-5.59	114.66	121.03	1	18
1	A	91	ASP	CA-C-N	-5.59	115.29	123.00	1	18
1	A	91	ASP	C-N-CA	-5.59	115.29	123.00	1	18
1	A	78	ASP	CB-CG-OD2	-5.58	105.56	118.40	1	18
1	A	75	VAL	O-C-N	-5.58	114.55	122.76	1	18
1	A	135	ASP	CB-CA-C	-5.58	99.50	110.11	1	18
1	A	96	ILE	CB-CA-C	5.57	118.61	110.98	1	18
1	A	106	PHE	CG-CD2-CE2	5.56	130.15	120.70	1	18
1	A	106	PHE	CZ-CE2-CD2	-5.55	110.01	120.00	1	18
1	A	23	LEU	O-C-N	5.55	125.89	121.17	1	18
1	A	75	VAL	CA-C-N	5.54	130.90	122.92	1	18
1	A	75	VAL	C-N-CA	5.54	130.90	122.92	1	18
1	A	72	GLY	CA-C-O	-5.54	113.17	119.04	1	18
1	A	64	HIS	ND1-CG-CD2	5.54	111.64	106.10	1	18
1	A	85	TYR	CA-C-N	5.54	127.96	120.38	1	18
1	A	85	TYR	C-N-CA	5.54	127.96	120.38	1	18
1	A	107	LYS	CD-CE-NZ	-5.54	94.19	111.90	1	18
1	A	61	VAL	CA-C-O	5.53	126.34	120.48	1	18
1	A	130	PRO	N-CA-C	5.51	119.12	110.80	1	18
1	A	55	PRO	N-CA-C	5.50	119.32	111.13	3	3
1	A	37	LYS	CA-CB-CG	-5.49	103.11	114.10	1	18
1	A	104	THR	OG1-CB-CG2	-5.46	98.38	109.30	1	18
1	A	129	ILE	C-N-CD	5.46	147.40	125.00	1	18
1	A	60	VAL	N-CA-CB	-5.46	104.59	111.46	1	18
1	A	101	GLN	CB-CA-C	-5.43	101.61	110.85	1	18
1	A	106	PHE	CA-CB-CG	-5.43	108.37	113.80	1	18
1	A	78	ASP	CA-C-N	5.43	129.21	120.30	1	18
1	A	78	ASP	C-N-CA	5.43	129.21	120.30	1	18
1	A	159	GLN	CA-C-N	5.42	129.04	121.02	1	18
1	A	159	GLN	C-N-CA	5.42	129.04	121.02	1	18
1	A	91	ASP	CB-CA-C	5.42	120.12	109.72	1	18
1	A	37	LYS	CD-CE-NZ	5.41	129.22	111.90	1	18
1	A	133	TRP	N-CA-C	-5.41	105.38	111.28	1	18
1	A	102	ILE	CG1-CB-CG2	-5.39	94.53	110.70	1	18
1	A	24	PRO	CA-CB-CG	-5.38	94.27	104.50	1	18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	144	VAL	N-CA-CB	5.38	118.64	111.64	1	18
1	A	83	PHE	O-C-N	5.38	127.83	122.12	1	18
1	A	98	GLY	N-CA-C	5.38	119.70	112.17	1	18
1	A	112	THR	N-CA-CB	-5.38	101.51	111.13	1	18
1	A	125	ASP	OD1-CG-OD2	-5.38	110.00	122.90	1	18
1	A	22	HIS	ND1-CE1-NE2	-5.36	103.04	108.40	1	18
1	A	103	PHE	CG-CD1-CE1	-5.36	111.59	120.70	1	18
1	A	94	LEU	CA-C-O	5.36	126.09	120.36	1	18
1	A	11	GLY	CA-C-O	5.35	124.95	119.01	1	18
1	A	36	GLY	O-C-N	-5.35	116.33	122.42	2	14
1	A	118	LEU	N-CA-C	-5.34	101.83	110.32	1	18
1	A	21	TRP	O-C-N	-5.34	115.68	122.78	1	18
1	A	66	GLU	O-C-N	-5.33	115.50	122.59	1	18
1	A	63	THR	O-C-N	-5.31	116.91	123.33	1	18
1	A	102	ILE	CA-CB-CG1	5.30	119.41	110.40	1	18
1	A	82	VAL	N-CA-CB	5.30	116.64	110.65	1	18
1	A	151	LEU	CA-C-O	5.30	125.47	119.27	1	18
1	A	92	GLN	N-CA-C	-5.29	100.54	109.07	1	18
1	A	47	GLU	CB-CG-CD	-5.29	103.61	112.60	1	18
1	A	84	ALA	N-CA-C	-5.29	105.52	111.28	1	18
1	A	131	LEU	N-CA-C	-5.28	101.33	109.52	1	18
1	A	146	ASP	CA-C-O	-5.28	115.14	121.11	1	18
1	A	16	ASP	CA-CB-CG	5.28	117.88	112.60	1	18
1	A	102	ILE	O-C-N	5.27	127.76	121.80	1	18
1	A	10	ASP	CA-C-O	-5.27	113.19	119.35	1	18
1	A	150	ALA	N-CA-C	-5.27	105.66	111.71	1	18
1	A	63	THR	CA-CB-OG1	-5.24	101.73	109.60	1	18
1	A	92	GLN	O-C-N	-5.24	117.10	123.29	1	18
1	A	46	TYR	CA-C-N	5.24	127.82	120.28	1	18
1	A	46	TYR	C-N-CA	5.24	127.82	120.28	1	18
1	A	151	LEU	CD1-CG-CD2	5.23	122.31	110.80	1	18
1	A	58	THR	CA-C-O	-5.22	114.58	120.43	1	18
1	A	24	PRO	CA-C-N	5.22	127.58	120.54	1	18
1	A	24	PRO	C-N-CA	5.22	127.58	120.54	1	18
1	A	103	PHE	CD1-CG-CD2	5.22	126.42	118.60	1	18
1	A	71	GLN	CG-CD-OE1	5.21	131.22	120.80	1	18
1	A	93	GLU	O-C-N	-5.21	116.54	122.89	1	18
1	A	43	ARG	O-C-N	5.21	127.50	122.09	1	18
1	A	156	GLU	CB-CG-CD	-5.18	103.79	112.60	1	18
1	A	93	GLU	CB-CG-CD	-5.17	103.80	112.60	1	18
1	A	36	GLY	N-CA-C	5.16	121.63	114.92	1	11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	88	GLN	CG-CD-NE2	-5.14	108.69	116.40	1	18
1	A	149	PRO	CA-N-CD	-5.13	104.81	112.00	1	18
1	A	130	PRO	CA-C-N	-5.12	114.55	122.59	1	18
1	A	130	PRO	C-N-CA	-5.12	114.55	122.59	1	18
1	A	28	HIS	CB-CG-CD2	-5.11	124.56	131.20	13	2
1	A	135	ASP	CA-C-N	-5.10	114.58	122.59	1	18
1	A	135	ASP	C-N-CA	-5.10	114.58	122.59	1	18
1	A	57	ARG	NE-CZ-NH2	-5.09	114.62	119.20	16	1
1	A	161	LYS	N-CA-CB	-5.08	102.57	110.04	1	18
1	A	134	ASP	CB-CG-OD1	5.08	130.07	118.40	1	18
1	A	43	ARG	NH1-CZ-NH2	5.07	125.89	119.30	1	18
1	A	146	ASP	CB-CG-OD2	5.06	130.05	118.40	1	18
1	A	100	ALA	N-CA-C	5.06	117.45	111.33	1	18
1	A	83	PHE	CA-CB-CG	-5.05	108.75	113.80	1	18
1	A	3	PHE	CE1-CZ-CE2	-5.05	110.90	120.00	1	18
1	A	38	ILE	CA-C-N	5.05	129.14	122.42	1	18
1	A	38	ILE	C-N-CA	5.05	129.14	122.42	1	18
1	A	49	PHE	CA-CB-CG	5.02	118.82	113.80	13	1
1	A	42	GLY	N-CA-C	-5.01	105.68	112.14	1	18
1	A	77	HIS	CG-ND1-CE1	5.01	117.82	109.30	1	18
1	A	44	ARG	CA-C-N	5.01	127.25	120.44	1	18
1	A	44	ARG	C-N-CA	5.01	127.25	120.44	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	1216	34±1
2	A	31	24	24	4±1
All	All	23040	22428	22320	607

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 13.

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:89:HIS:C	1:A:90:PRO:CD	1.38	1.97	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: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:67:ASP:CB	1:A:67:ASP:C	0.99	2.34	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: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	0.74	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:67:ASP:CA	1:A:67:ASP:CG	0.63	2.69	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:8:ASP:OD1	1:A:8:ASP:C	0.56	2.48	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: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:23:LEU:O	1:A:24:PRO:C	0.44	2.60	1	18
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:67:ASP:N	1:A:67:ASP:CG	0.41	2.78	1	18
1:A:19:LEU:HD11	2:A:163:BDM:C13	0.41	2.46	18	1
1:A:67:ASP:CG	1:A:67:ASP:H	0.41	2.24	1	18
2:A:163:BDM:H172	2:A:163:BDM:H201	0.40	1.49	1	2

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	155/162 (96%)	152±0 (98±0%)	1±0 (1±0%)	2±0 (1±0%)	12	60
All	All	2790/2916 (96%)	2739 (98%)	15 (1%)	36 (1%)	12	60

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 ⓘ

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%)	124±0 (93±0%)	9±0 (7±0%)	16	64
All	All	2394/2466 (97%)	2227 (93%)	167 (7%)	16	64

All 10 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	87	LYS	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 oligosaccharides 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	-	31,32,32	1.14±0.05	2±1 (5±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	-	35,43,43	2.32±0.18	8±1 (23±3%)

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±0,22,22,22	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	C18-C21	3.29	1.57	1.51	18	18
2	A	163	BDM	C20-C22	2.53	1.56	1.50	9	4
2	A	163	BDM	OXW-C21	2.28	1.23	1.30	12	6
2	A	163	BDM	BR11-C11	2.02	1.94	1.89	10	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
2	A	163	BDM	C7-C8-C13	8.31	107.78	120.38	10	18
2	A	163	BDM	C7-C8-C9	8.01	132.54	120.38	10	18

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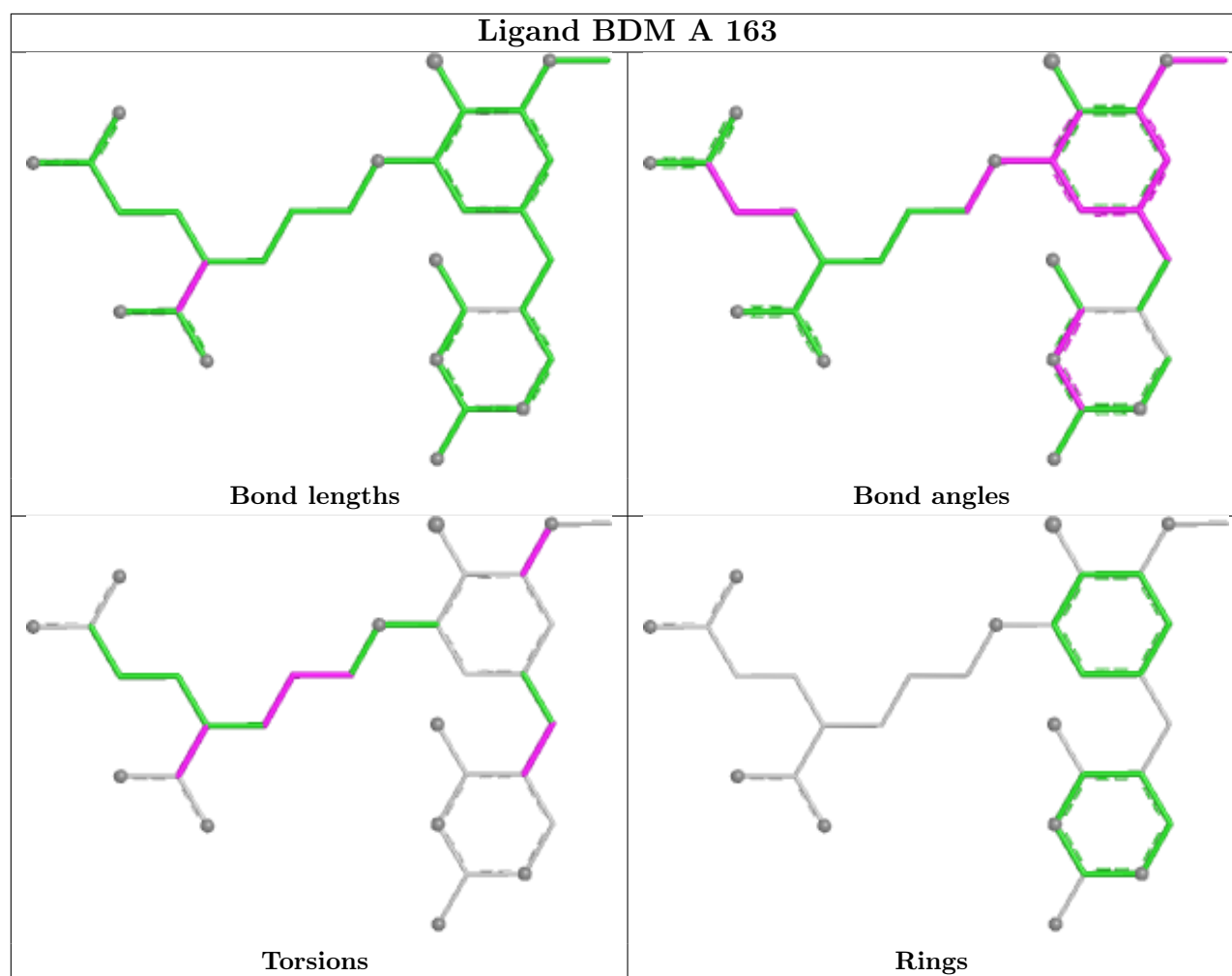
Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	A	163	BDM	O10-C10-C11	5.52	110.97	116.32	10	14
2	A	163	BDM	C20-C19-C18	5.37	122.97	113.45	9	6
2	A	163	BDM	C15-O10-C10	4.92	129.56	117.69	9	15
2	A	163	BDM	C14-O12-C12	4.83	110.43	117.51	10	18
2	A	163	BDM	C2-N3-C4	3.45	117.82	112.41	5	18
2	A	163	BDM	C19-C18-C17	3.31	95.09	115.13	18	5
2	A	163	BDM	OXW-C21-C18	3.19	122.44	114.16	4	4
2	A	163	BDM	O10-C10-C9	2.64	129.20	123.49	10	3
2	A	163	BDM	O12-C12-C13	2.51	119.76	124.08	16	17
2	A	163	BDM	OX6-C22-C20	2.44	121.71	114.00	9	2
2	A	163	BDM	OXV-C21-C18	2.23	116.94	122.86	4	1
2	A	163	BDM	C19-C20-C22	2.12	118.15	112.49	1	3
2	A	163	BDM	O12-C12-C11	2.08	120.03	116.22	16	5

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