



Full wwPDB NMR Structure Validation Report ⓘ

Mar 25, 2026 – 08:41 PM UTC

PDB ID : 2M2W / pdb_00002m2w
BMRB ID : 18935
Title : Ternary complex of ASFV Pol X with DNA and MgdGTP
Authors : Wu, W.; Su, M.; Tsai, M.
Deposited on : 2013-01-03

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

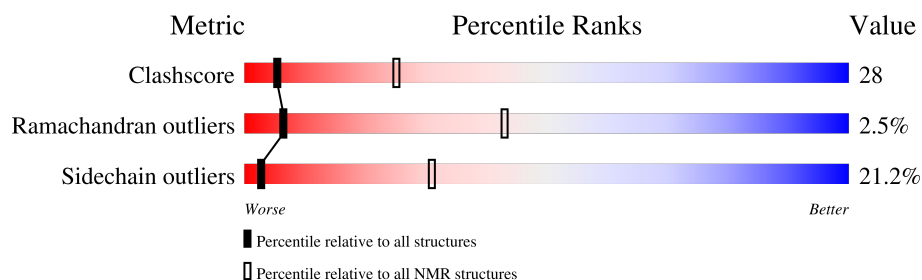
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 39%.

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	174	54% 39% 5% •
2	B	23	13% 70% 9% 9%

2 Ensemble composition and analysis

This entry contains 10 models. Model 1 is the overall representative, medoid model (most similar to other models).

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:1-A:80, A:85-A:174 (170)	0.81	1

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 3 clusters and 1 single-model cluster was found.

Cluster number	Models
1	1, 3, 7, 9, 10
2	2, 4
3	5, 6
Single-model clusters	8

3 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3774 atoms, of which 1829 are hydrogens and 0 are deuteriums.

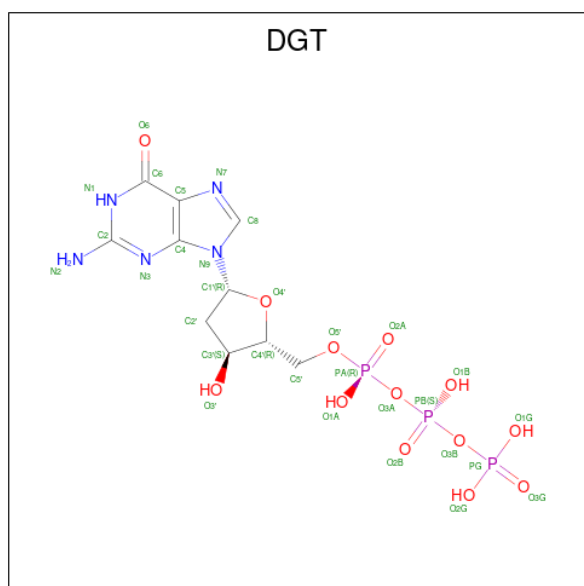
- Molecule 1 is a protein called Repair DNA polymerase X.

Mol	Chain	Residues	Atoms						Trace
1	A	174	Total	C	H	N	O	S	0
			3003	943	1569	248	239	4	

- Molecule 2 is a DNA chain called 5'-D(P*GP*GP*CP*GP*AP*AP*GP*CP*CP*GP*GP*GP*TP*GP*CP*GP*AP*AP*GP*CP*AP*CP*(DOC))-3'.

Mol	Chain	Residues	Atoms						Trace
2	B	23	Total	C	H	N	O	P	0
			734	223	256	98	134	23	

- Molecule 3 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (CCD ID: DGT) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					
3	A	1	Total	C	H	N	O	P
			35	10	4	5	13	3

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

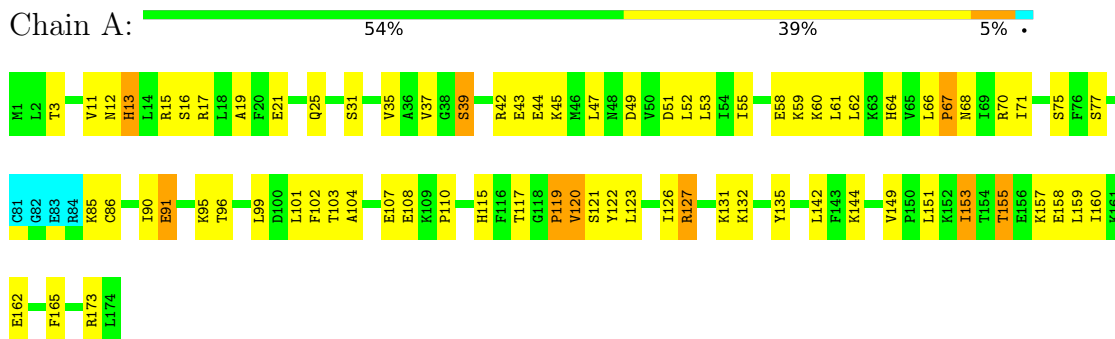
Mol	Chain	Residues	Atoms	
4	A	2	Total	Mg
			2	2

4 Residue-property plots

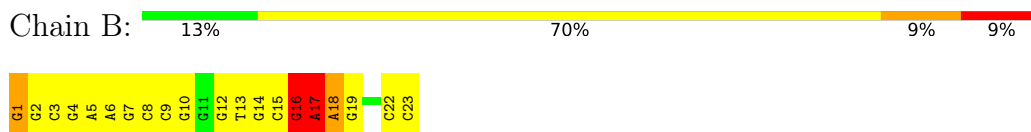
4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Repair DNA polymerase X



- Molecule 2: 5'-D(P*GP*GP*CP*GP*AP*AP*GP*CP*CP*GP*GP*GP*TP*GP*CP*GP*AP*AP*GP*CP*AP*CP*(DOC))-3'

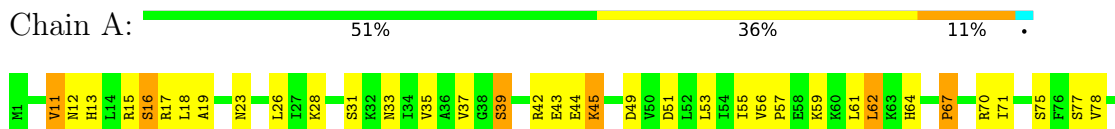


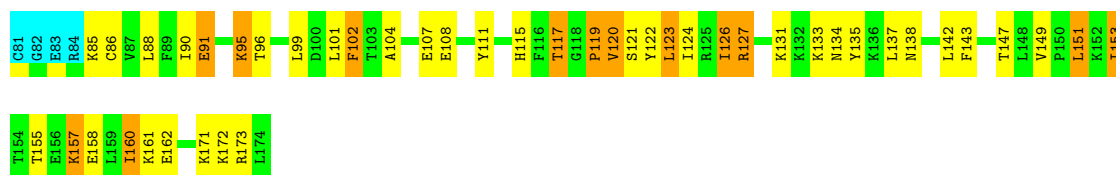
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

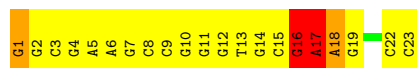
- Molecule 1: Repair DNA polymerase X





- Molecule 2: 5'-D(P*GP*GP*CP*GP*AP*AP*GP*CP*CP*GP*GP*GP*TP*GP*CP*GP*AP*AP*GP*CP*AP*CP*(DOC))-3'

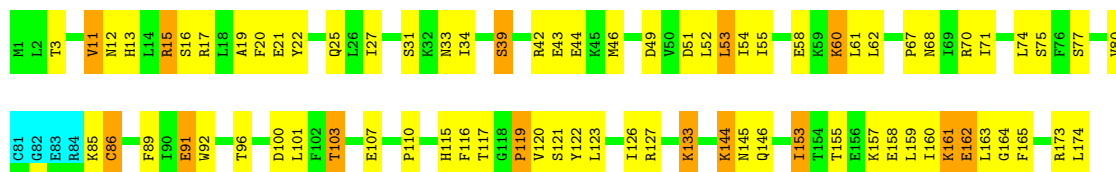
Chain B: 9% 74% 9% 9%



4.2.2 Score per residue for model 2

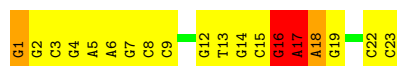
- Molecule 1: Repair DNA polymerase X

Chain A: 53% 36% 8%



- Molecule 2: 5'-D(P*GP*GP*CP*GP*AP*AP*GP*CP*CP*GP*GP*GP*TP*GP*CP*GP*AP*AP*GP*CP*AP*CP*(DOC))-3'

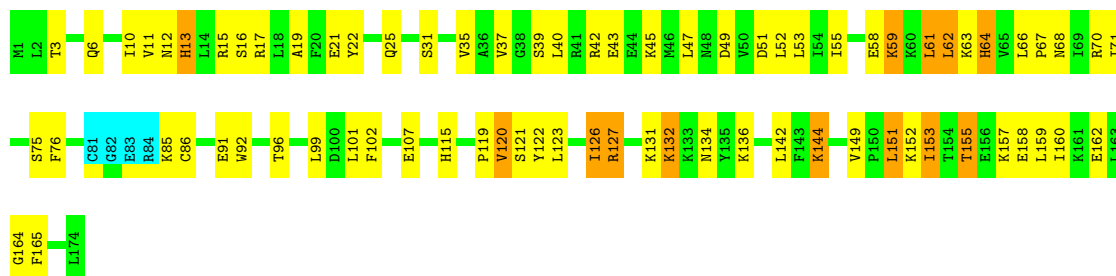
Chain B: 17% 65% 9% 9%



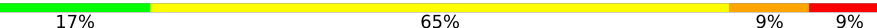
4.2.3 Score per residue for model 3

- Molecule 1: Repair DNA polymerase X

Chain A: 55% 36% 7%



- Molecule 2: 5'-D(P*GP*GP*CP*GP*AP*AP*GP*CP*CP*GP*GP*GP*TP*GP*CP*GP*AP*AP*GP*CP*AP*CP*(DOC))-3'

Chain B:  17% 65% 9% 9%



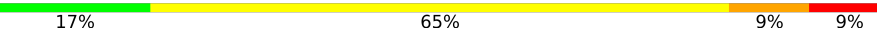
4.2.4 Score per residue for model 4

- Molecule 1: Repair DNA polymerase X

Chain A:  49% 37% 11% .



- Molecule 2: 5'-D(P*GP*GP*CP*GP*AP*AP*GP*CP*CP*GP*GP*GP*TP*GP*CP*GP*AP*AP*GP*CP*AP*CP*(DOC))-3'

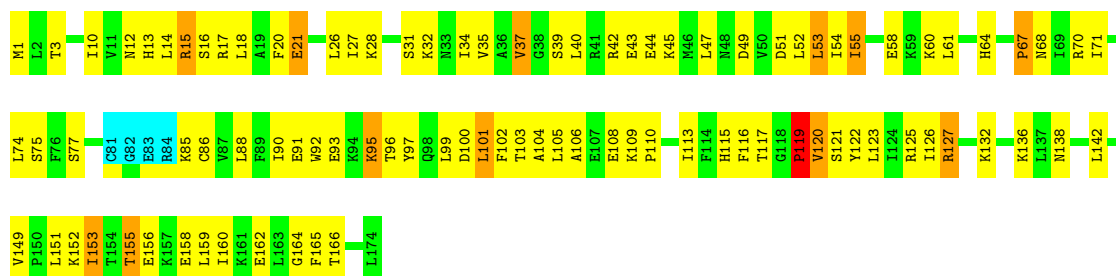
Chain B:  17% 65% 9% 9%



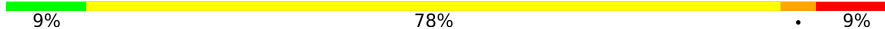
4.2.5 Score per residue for model 5

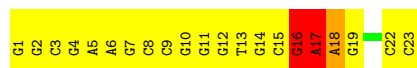
- Molecule 1: Repair DNA polymerase X

Chain A:  44% 47% 7% .



- Molecule 2: 5'-D(P*GP*GP*CP*GP*AP*AP*GP*CP*CP*GP*GP*GP*TP*GP*CP*GP*AP*AP*GP*CP*AP*CP*(DOC))-3'

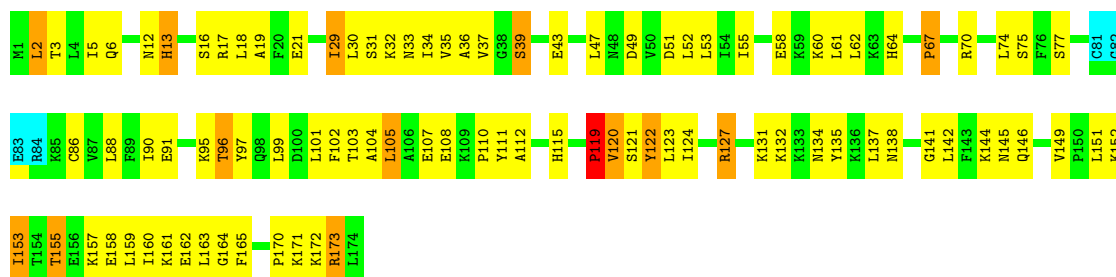
Chain B: 



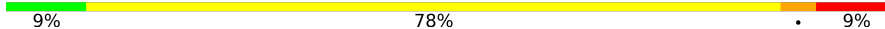
4.2.6 Score per residue for model 6

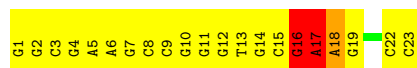
- Molecule 1: Repair DNA polymerase X

Chain A: 



- Molecule 2: 5'-D(P*GP*GP*CP*GP*AP*AP*GP*CP*CP*GP*GP*GP*TP*GP*CP*GP*AP*AP*GP*CP*AP*CP*(DOC))-3'

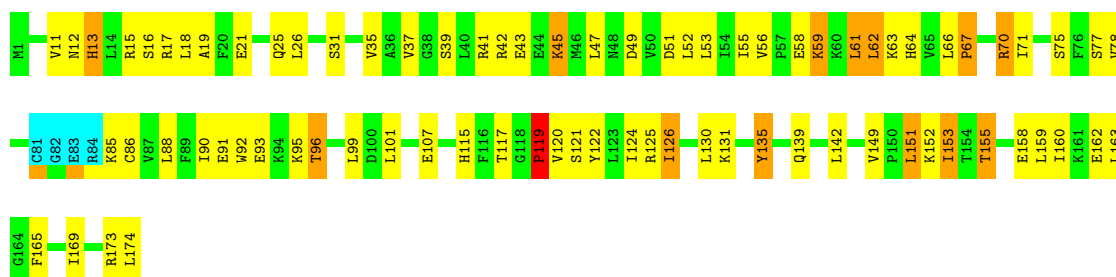
Chain B: 



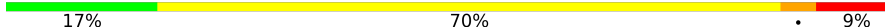
4.2.7 Score per residue for model 7

- Molecule 1: Repair DNA polymerase X

Chain A: 



- Molecule 2: 5'-D(P*GP*GP*CP*GP*AP*AP*GP*CP*CP*GP*GP*GP*TP*GP*CP*GP*AP*AP*GP*CP*AP*CP*(DOC))-3'

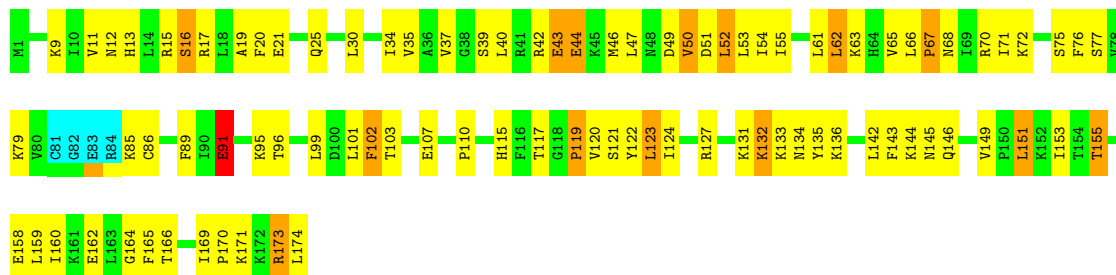
Chain B: 



4.2.8 Score per residue for model 8

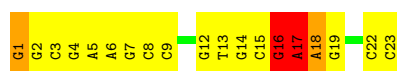
- Molecule 1: Repair DNA polymerase X

Chain A: 45% 44% 8% ..



- Molecule 2: 5'-D(P*GP*GP*CP*GP*AP*AP*GP*CP*CP*GP*GP*GP*TP*GP*CP*GP*AP*AP*GP*CP*AP*CP*(DOC))-3'

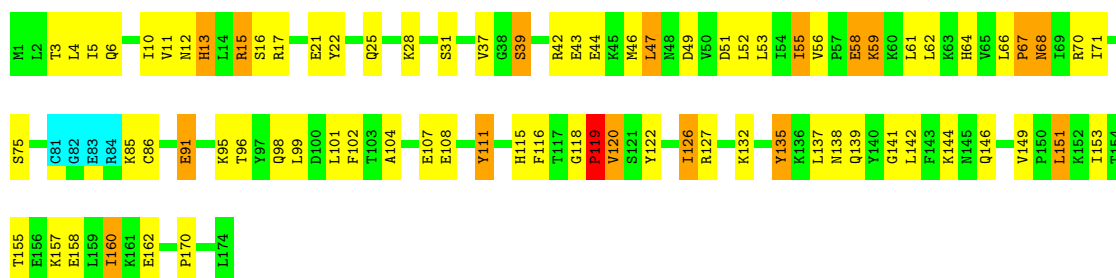
Chain B: 17% 65% 9% 9%



4.2.9 Score per residue for model 9

- Molecule 1: Repair DNA polymerase X

Chain A: 52% 36% 9% ..



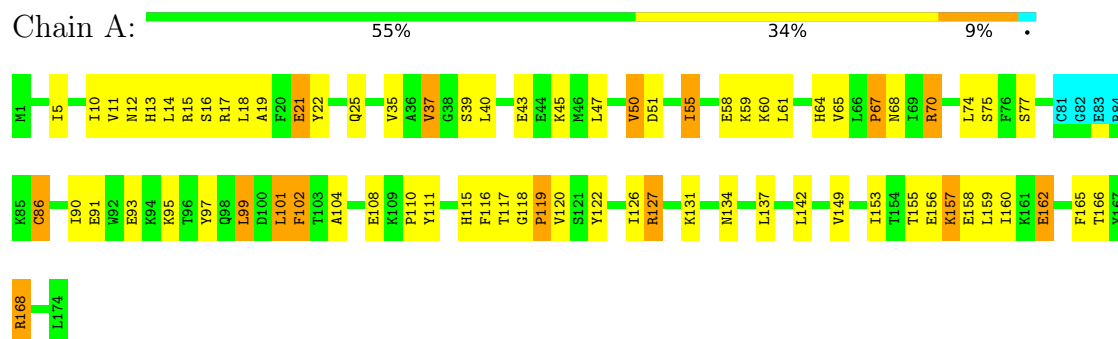
- Molecule 2: 5'-D(P*GP*GP*CP*GP*AP*AP*GP*CP*CP*GP*GP*GP*TP*GP*CP*GP*AP*AP*GP*CP*AP*CP*(DOC))-3'

Chain B: 17% 65% 9% 9%

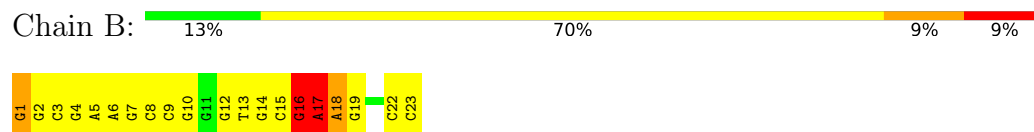


4.2.10 Score per residue for model 10

- Molecule 1: Repair DNA polymerase X



- Molecule 2: 5'-D(P*GP*GP*CP*GP*AP*AP*GP*CP*CP*GP*GP*GP*TP*GP*CP*GP*AP*AP*GP*CP*AP*CP*(DOC))-3'



5 Refinement protocol and experimental data overview

The models were refined using the following method: *distance geometry*.

Of the 2000 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
HADDOCK	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1212
Number of shifts mapped to atoms	1212
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	39%

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: MG, DOC, DGT

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	0.59±0.03	0±0/1429 (0.0± 0.0%)	0.94±0.03	2±1/1917 (0.1± 0.1%)
2	B	0.68±0.00	3±0/518 (0.6± 0.0%)	0.89±0.00	4±0/797 (0.5± 0.0%)
All	All	0.62	32/19470 (0.2%)	0.92	60/27140 (0.2%)

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
2	B	0.0±0.0	3.0±0.0
All	All	0	30

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	B	16	DG	C2-N3	-7.53	1.18	1.33	1	10
2	B	16	DG	N9-C4	-5.73	1.26	1.38	4	10
2	B	1	DG	OP3-P	5.60	1.59	1.48	9	10
1	A	29	ILE	C-O	5.32	1.29	1.24	6	1
1	A	91	GLU	C-O	5.12	1.29	1.24	8	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	B	16	DG	C4-N9-C1'	-8.29	114.56	127.00	3	10
1	A	119	PRO	N-CA-CB	-7.70	95.16	103.25	6	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	31	SER	N-CA-C	7.68	120.39	111.02	1	2
1	A	117	THR	N-CA-C	7.18	119.97	111.71	2	7
2	B	16	DG	C8-N9-C1'	6.89	137.34	127.00	9	10
2	B	17	DA	N9-C1'-C2'	5.82	122.23	113.50	4	10
1	A	117	THR	CA-C-N	-5.50	113.24	121.87	4	1
1	A	117	THR	C-N-CA	-5.50	113.24	121.87	4	1
2	B	16	DG	O4'-C1'-N9	-5.47	100.19	108.40	2	10
1	A	157	LYS	N-CA-C	-5.38	105.07	111.69	10	2
1	A	70	ARG	N-CA-C	5.25	115.17	108.24	7	3

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
2	B	16	DG	Sidechain	10
2	B	17	DA	Sidechain	10
2	B	18	DA	Sidechain	10

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1404	1542	1542	47±7
2	B	478	256	255	58±3
3	A	31	4	12	8±3
4	A	2	0	0	1±0
All	All	19150	18020	18090	1041

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 28.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:15:DC:H2'	2:B:16:DG:C6	1.16	1.76	4	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:16:DG:C2	2:B:18:DA:N6	1.03	2.27	3	10
2:B:16:DG:N2	2:B:18:DA:C6	0.97	2.32	2	10
2:B:15:DC:H2'	2:B:16:DG:C5	0.93	1.99	4	10
2:B:16:DG:N2	2:B:18:DA:N6	0.93	2.17	2	10
2:B:15:DC:C2'	2:B:16:DG:C5	0.90	2.55	9	10
2:B:5:DA:H2	2:B:6:DA:C5	0.89	1.86	7	10
2:B:17:DA:H1'	2:B:18:DA:OP2	0.88	1.68	10	10
2:B:5:DA:C2	2:B:6:DA:C5	0.84	2.66	3	10
3:A:201:DGT:H5'A	2:B:23:DOC:C3'	0.81	2.07	9	3
2:B:16:DG:H21	2:B:19:DG:N2	0.80	1.75	3	10
1:A:124:ILE:HG23	2:B:10:DG:H5'	0.77	1.57	6	3
2:B:15:DC:C2'	2:B:16:DG:C6	0.76	2.66	3	10
2:B:16:DG:N1	2:B:18:DA:N6	0.76	2.33	10	10
2:B:14:DG:H2''	2:B:15:DC:O4'	0.76	1.81	9	10
3:A:201:DGT:N3	2:B:23:DOC:H2'	0.76	1.95	4	5
2:B:17:DA:C2	2:B:18:DA:N6	0.76	2.54	5	10
2:B:17:DA:N3	2:B:18:DA:N7	0.73	2.36	9	10
2:B:16:DG:N2	2:B:19:DG:N2	0.73	2.36	3	10
1:A:138:ASN:HD21	2:B:11:DG:H5'	0.73	1.43	4	2
1:A:138:ASN:ND2	2:B:11:DG:H5'	0.72	1.97	4	4
1:A:115:HIS:NE2	3:A:201:DGT:H8	0.72	2.00	8	9
2:B:22:DC:H2''	2:B:23:DOC:H5''	0.71	1.61	10	2
1:A:127:ARG:NH2	2:B:10:DG:H1'	0.71	2.01	6	5
2:B:18:DA:H4'	2:B:19:DG:OP1	0.70	1.85	7	10
1:A:131:LYS:HA	1:A:135:TYR:O	0.70	1.86	8	4
3:A:201:DGT:O3G	4:A:203:MG:MG	0.70	1.33	1	10
3:A:201:DGT:H5'A	2:B:23:DOC:H3'1	0.70	1.62	9	2
2:B:2:DG:H2''	2:B:3:DC:O4'	0.70	1.87	3	10
3:A:201:DGT:H5'A	2:B:23:DOC:H3'2	0.69	1.63	7	1
1:A:115:HIS:CD2	3:A:201:DGT:H8	0.69	2.23	8	10
2:B:22:DC:H2''	2:B:23:DOC:H6	0.68	1.64	5	2
2:B:3:DC:H2'	2:B:4:DG:C6	0.68	2.24	2	10
2:B:23:DOC:H5'	2:B:23:DOC:H6	0.67	1.64	2	1
1:A:40:LEU:N	1:A:44:GLU:HG2	0.67	2.05	8	1
1:A:39:SER:C	1:A:44:GLU:HG2	0.66	2.14	8	1
2:B:4:DG:H2''	2:B:5:DA:OP2	0.66	1.89	8	10
2:B:5:DA:H2''	2:B:6:DA:OP2	0.65	1.89	3	10
1:A:160:ILE:HB	1:A:165:PHE:O	0.65	1.90	6	6
1:A:110:PRO:HB2	1:A:159:LEU:HD13	0.65	1.67	2	5
2:B:16:DG:C8	2:B:16:DG:OP2	0.65	2.50	6	10
3:A:201:DGT:H3'	3:A:201:DGT:O2B	0.65	1.91	2	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:13:DT:H2''	2:B:14:DG:C8	0.64	2.28	1	10
1:A:91:GLU:HA	1:A:95:LYS:O	0.64	1.92	1	7
1:A:91:GLU:HB2	1:A:96:THR:HG23	0.64	1.69	6	1
3:A:201:DGT:O2A	2:B:23:DOC:H3'2	0.64	1.91	7	1
3:A:201:DGT:C2	2:B:23:DOC:H2'	0.64	2.22	9	5
3:A:201:DGT:N2	2:B:23:DOC:H3'1	0.64	2.06	7	2
1:A:132:LYS:NZ	2:B:3:DC:H4'	0.64	2.07	8	1
1:A:62:LEU:HG	1:A:63:LYS:N	0.63	2.07	4	4
2:B:16:DG:N2	2:B:18:DA:C5	0.63	2.66	6	10
1:A:158:GLU:O	1:A:162:GLU:HB2	0.63	1.94	4	3
1:A:119:PRO:HD2	1:A:122:TYR:HB3	0.63	1.71	9	6
1:A:115:HIS:HA	1:A:123:LEU:HD21	0.62	1.70	1	2
1:A:91:GLU:HB3	1:A:96:THR:HG22	0.62	1.71	9	2
2:B:17:DA:C2	2:B:18:DA:N7	0.62	2.67	9	10
2:B:12:DG:H2'	2:B:13:DT:C6	0.62	2.30	7	10
2:B:17:DA:C1'	2:B:18:DA:OP2	0.62	2.48	4	10
3:A:201:DGT:H5'A	2:B:23:DOC:C2'	0.62	2.24	8	2
2:B:1:DG:H2''	2:B:2:DG:C8	0.61	2.30	3	5
1:A:157:LYS:O	1:A:160:ILE:HG13	0.61	1.95	6	5
1:A:63:LYS:O	1:A:66:LEU:HB2	0.60	1.96	3	3
3:A:201:DGT:O4'	2:B:23:DOC:H2''	0.60	1.96	4	1
1:A:105:LEU:O	1:A:108:GLU:HG2	0.59	1.98	6	2
1:A:21:GLU:HA	1:A:25:GLN:O	0.59	1.98	4	6
1:A:34:ILE:HA	1:A:53:LEU:O	0.59	1.97	4	3
1:A:42:ARG:HD2	1:A:44:GLU:OE1	0.59	1.98	9	1
2:B:5:DA:H2	2:B:6:DA:C4	0.59	2.16	10	10
2:B:13:DT:H2''	2:B:14:DG:N7	0.59	2.13	4	10
1:A:108:GLU:HG3	1:A:112:ALA:HB2	0.58	1.74	6	1
1:A:151:LEU:H	1:A:151:LEU:HD13	0.58	1.59	7	3
1:A:127:ARG:HH21	2:B:10:DG:H1'	0.58	1.57	5	1
1:A:137:LEU:H	1:A:137:LEU:HD23	0.58	1.57	10	1
1:A:75:SER:HB2	1:A:91:GLU:O	0.58	1.99	8	9
1:A:158:GLU:O	1:A:162:GLU:N	0.58	2.37	4	10
1:A:85:LYS:HD3	2:B:23:DOC:H1'	0.58	1.76	8	1
1:A:118:GLY:HA2	1:A:170:PRO:HG3	0.57	1.75	9	1
1:A:59:LYS:O	1:A:62:LEU:HD23	0.57	1.98	3	2
1:A:20:PHE:HA	1:A:68:ASN:O	0.57	1.99	4	2
2:B:16:DG:H1'	2:B:17:DA:C8	0.57	2.35	5	10
1:A:102:PHE:CE2	3:A:201:DGT:H4'	0.57	2.35	8	2
1:A:115:HIS:HE2	3:A:201:DGT:H8	0.56	1.59	7	2
1:A:151:LEU:H	1:A:151:LEU:HD23	0.56	1.60	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:4:DG:H22	2:B:7:DG:N2	0.56	1.99	2	10
2:B:8:DC:H4'	2:B:8:DC:OP1	0.56	2.00	2	10
2:B:22:DC:H2''	2:B:23:DOC:C6	0.56	2.31	5	2
1:A:44:GLU:OE2	1:A:47:LEU:HG	0.56	2.00	8	1
1:A:122:TYR:CD1	1:A:174:LEU:HG	0.56	2.36	2	1
2:B:15:DC:H2''	2:B:16:DG:C5	0.55	2.36	6	10
2:B:23:DOC:H6	2:B:23:DOC:C5'	0.55	2.32	2	1
1:A:157:LYS:HA	1:A:160:ILE:CG1	0.55	2.31	9	2
2:B:22:DC:H2''	2:B:23:DOC:C5'	0.55	2.32	6	2
1:A:11:VAL:O	1:A:15:ARG:HB2	0.55	2.01	2	3
1:A:15:ARG:N	1:A:15:ARG:HD2	0.55	2.15	5	1
1:A:104:ALA:HB1	1:A:108:GLU:OE2	0.54	2.03	10	2
1:A:132:LYS:HE3	2:B:3:DC:H2''	0.54	1.78	3	1
1:A:138:ASN:OD1	2:B:11:DG:H5'	0.54	2.01	5	2
1:A:91:GLU:HG2	1:A:96:THR:HG22	0.54	1.78	4	1
2:B:22:DC:H2''	2:B:23:DOC:OP1	0.54	2.02	2	1
1:A:108:GLU:OE1	1:A:139:GLN:HB3	0.54	2.03	9	1
2:B:16:DG:N2	2:B:19:DG:H22	0.54	2.01	8	10
1:A:75:SER:CB	1:A:91:GLU:HB2	0.54	2.33	8	3
3:A:201:DGT:N2	2:B:23:DOC:H2'	0.54	2.18	3	1
1:A:75:SER:HB2	1:A:91:GLU:HB2	0.53	1.80	9	3
2:B:16:DG:H2''	2:B:17:DA:C8	0.53	2.38	4	10
1:A:77:SER:O	1:A:88:LEU:HA	0.53	2.04	6	4
2:B:23:DOC:H5'	2:B:23:DOC:C6	0.53	2.34	2	1
2:B:1:DG:C2'	2:B:2:DG:C8	0.53	2.92	2	1
1:A:109:LYS:O	1:A:113:ILE:HG12	0.53	2.04	5	2
1:A:44:GLU:OE1	1:A:47:LEU:HA	0.53	2.04	8	1
1:A:85:LYS:HG3	2:B:23:DOC:H1'	0.53	1.79	5	1
2:B:6:DA:N7	2:B:7:DG:C2	0.53	2.77	5	10
1:A:153:ILE:HB	1:A:158:GLU:HB3	0.53	1.81	7	5
1:A:39:SER:O	1:A:43:GLU:N	0.52	2.42	8	10
3:A:201:DGT:H5'	2:B:23:DOC:H3'2	0.52	1.80	4	1
1:A:173:ARG:O	1:A:173:ARG:HD3	0.52	2.05	8	1
1:A:74:LEU:HD21	1:A:92:TRP:HB3	0.52	1.81	5	1
2:B:6:DA:N7	2:B:7:DG:N2	0.52	2.58	5	10
1:A:155:THR:HG22	1:A:156:GLU:OE1	0.52	2.04	5	1
2:B:5:DA:H2	2:B:6:DA:N7	0.52	2.03	8	10
1:A:75:SER:CB	1:A:91:GLU:HB3	0.52	2.35	10	5
1:A:138:ASN:CG	2:B:11:DG:H5'	0.52	2.29	9	2
1:A:47:LEU:HD22	1:A:50:VAL:HG22	0.52	1.82	8	1
1:A:14:LEU:O	1:A:18:LEU:HB2	0.52	2.05	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:37:VAL:O	1:A:51:ASP:N	0.52	2.43	10	8
1:A:42:ARG:O	1:A:43:GLU:HB3	0.51	2.04	8	1
1:A:120:VAL:HA	1:A:123:LEU:HD12	0.51	1.82	3	1
1:A:122:TYR:O	1:A:126:ILE:HB	0.51	2.05	3	5
1:A:119:PRO:HD2	1:A:122:TYR:CB	0.51	2.35	2	3
1:A:61:LEU:HA	1:A:64:HIS:HB2	0.51	1.81	3	4
1:A:135:TYR:HB3	1:A:142:LEU:HD12	0.51	1.81	1	1
1:A:116:PHE:HA	3:A:201:DGT:O3'	0.51	2.05	5	5
1:A:118:GLY:HA3	1:A:168:ARG:HH12	0.51	1.65	10	1
1:A:119:PRO:HG2	1:A:122:TYR:HB2	0.51	1.83	6	1
2:B:15:DC:H2''	2:B:16:DG:C4	0.51	2.41	4	10
1:A:35:VAL:O	1:A:53:LEU:N	0.51	2.42	5	4
1:A:90:ILE:O	1:A:97:TYR:N	0.51	2.44	6	3
1:A:13:HIS:O	1:A:17:ARG:N	0.51	2.44	3	10
1:A:37:VAL:HB	1:A:51:ASP:HB2	0.50	1.81	8	4
1:A:36:ALA:HA	1:A:52:LEU:HD12	0.50	1.84	6	1
3:A:201:DGT:N1	2:B:23:DOC:C5	0.50	2.75	8	1
1:A:137:LEU:O	1:A:137:LEU:HG	0.50	2.07	10	1
1:A:106:ALA:O	1:A:109:LYS:HB2	0.50	2.06	5	1
1:A:15:ARG:NE	1:A:34:ILE:HG21	0.50	2.21	5	1
1:A:75:SER:HB2	1:A:91:GLU:HB3	0.50	1.83	6	2
1:A:122:TYR:CE1	1:A:174:LEU:HA	0.50	2.42	8	1
1:A:10:ILE:O	1:A:14:LEU:HG	0.50	2.07	10	1
1:A:51:ASP:O	1:A:52:LEU:HG	0.50	2.06	5	2
1:A:37:VAL:HG22	1:A:51:ASP:HB2	0.49	1.84	4	1
2:B:5:DA:C2	2:B:6:DA:N7	0.49	2.81	8	10
1:A:104:ALA:HB1	1:A:108:GLU:OE1	0.49	2.07	6	2
1:A:21:GLU:O	1:A:67:PRO:HB2	0.49	2.08	7	1
1:A:90:ILE:O	1:A:96:THR:HA	0.48	2.08	1	3
1:A:20:PHE:CE1	1:A:27:ILE:HB	0.48	2.43	2	2
1:A:142:LEU:O	1:A:149:VAL:N	0.48	2.43	8	9
1:A:86:CYS:O	1:A:101:LEU:N	0.48	2.45	3	10
1:A:42:ARG:NH1	3:A:201:DGT:O1G	0.48	2.46	5	1
1:A:10:ILE:O	1:A:14:LEU:HB2	0.48	2.08	5	1
1:A:153:ILE:HD12	1:A:162:GLU:CD	0.48	2.34	1	1
1:A:19:ALA:N	1:A:70:ARG:O	0.47	2.47	3	7
2:B:8:DC:H2'	2:B:9:DC:C5	0.47	2.45	4	10
1:A:88:LEU:HD13	1:A:101:LEU:HD21	0.47	1.86	5	1
1:A:64:HIS:C	1:A:67:PRO:HD2	0.47	2.34	5	5
1:A:22:TYR:N	1:A:25:GLN:O	0.47	2.44	10	1
2:B:4:DG:H1	2:B:6:DA:H62	0.47	1.53	6	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:201:DGT:O2A	2:B:23:DOC:H3'1	0.47	2.09	3	2
2:B:5:DA:C2	2:B:6:DA:C4	0.47	3.01	6	10
1:A:125:ARG:HH22	2:B:3:DC:H4'	0.47	1.69	5	2
1:A:91:GLU:HG2	1:A:96:THR:HG23	0.47	1.87	1	1
1:A:159:LEU:O	1:A:163:LEU:HB2	0.46	2.09	2	1
1:A:39:SER:OG	1:A:47:LEU:HB3	0.46	2.09	3	1
1:A:151:LEU:H	1:A:151:LEU:CD1	0.46	2.22	7	1
1:A:170:PRO:O	1:A:173:ARG:HG3	0.46	2.10	8	1
1:A:60:LYS:N	1:A:60:LYS:HE3	0.46	2.26	4	1
1:A:12:ASN:O	1:A:16:SER:N	0.46	2.49	4	10
1:A:42:ARG:O	1:A:43:GLU:HB2	0.46	2.10	4	2
2:B:22:DC:H2''	2:B:23:DOC:H5'	0.46	1.87	1	1
2:B:4:DG:H22	2:B:7:DG:H21	0.46	1.54	9	10
3:A:201:DGT:PB	3:A:201:DGT:H3'	0.46	2.51	4	1
1:A:55:ILE:HG22	1:A:104:ALA:O	0.46	2.11	10	3
1:A:43:GLU:HG2	1:A:43:GLU:O	0.46	2.10	8	1
1:A:6:GLN:O	1:A:10:ILE:HG12	0.46	2.11	9	1
1:A:54:ILE:O	1:A:103:THR:HA	0.45	2.11	5	3
1:A:133:LYS:HA	1:A:133:LYS:HZ3	0.45	1.70	2	1
1:A:76:PHE:CD1	1:A:76:PHE:N	0.45	2.84	4	1
1:A:78:VAL:HG13	1:A:88:LEU:HG	0.45	1.87	1	1
1:A:124:ILE:O	1:A:127:ARG:HD2	0.45	2.11	4	1
1:A:5:ILE:HG13	1:A:6:GLN:N	0.45	2.27	6	1
1:A:45:LYS:HE2	1:A:45:LYS:N	0.45	2.27	1	2
1:A:111:TYR:N	1:A:111:TYR:CD1	0.45	2.84	9	2
1:A:145:ASN:O	1:A:146:GLN:HB2	0.45	2.12	6	3
1:A:2:LEU:O	1:A:47:LEU:HB2	0.45	2.11	6	1
1:A:11:VAL:O	1:A:15:ARG:N	0.45	2.48	2	7
1:A:131:LYS:O	1:A:134:ASN:N	0.45	2.48	3	5
2:B:5:DA:N1	2:B:6:DA:C6	0.45	2.85	3	10
1:A:17:ARG:HG3	1:A:17:ARG:O	0.45	2.11	10	1
1:A:136:LYS:O	1:A:143:PHE:N	0.45	2.45	8	1
1:A:75:SER:HB3	1:A:91:GLU:OE2	0.45	2.11	9	1
1:A:111:TYR:CE1	1:A:137:LEU:HB2	0.45	2.47	10	1
1:A:75:SER:HB2	1:A:91:GLU:CB	0.44	2.41	6	1
1:A:45:LYS:N	1:A:45:LYS:HD3	0.44	2.27	5	1
1:A:173:ARG:O	1:A:174:LEU:HB2	0.44	2.12	7	1
1:A:125:ARG:NH2	2:B:3:DC:H4'	0.44	2.28	5	1
1:A:170:PRO:O	1:A:173:ARG:HB3	0.44	2.13	6	1
2:B:12:DG:C2'	2:B:13:DT:C6	0.44	3.01	1	5
2:B:15:DC:H4'	2:B:15:DC:OP1	0.44	2.12	1	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:1:DG:H2'	2:B:2:DG:C8	0.44	2.47	10	2
1:A:56:VAL:HB	1:A:62:LEU:HA	0.44	1.89	7	2
2:B:17:DA:H8	2:B:17:DA:OP2	0.44	1.96	10	4
1:A:155:THR:O	1:A:159:LEU:N	0.44	2.48	6	4
1:A:138:ASN:N	1:A:141:GLY:O	0.44	2.48	4	1
1:A:78:VAL:HG22	1:A:88:LEU:HG	0.44	1.88	7	1
1:A:56:VAL:CB	1:A:62:LEU:HA	0.44	2.42	1	1
3:A:201:DGT:N3	3:A:201:DGT:H5'	0.44	2.28	7	2
1:A:89:PHE:CZ	1:A:96:THR:HB	0.44	2.48	2	1
1:A:160:ILE:O	1:A:164:GLY:N	0.44	2.49	5	5
1:A:6:GLN:O	1:A:10:ILE:HG23	0.44	2.13	3	1
1:A:64:HIS:O	1:A:67:PRO:HD2	0.44	2.13	6	2
1:A:88:LEU:HD13	1:A:101:LEU:CD2	0.44	2.41	5	1
1:A:158:GLU:HA	1:A:161:LYS:HD2	0.44	1.88	6	1
1:A:45:LYS:HE2	1:A:45:LYS:H	0.44	1.73	1	1
3:A:201:DGT:H3'	3:A:201:DGT:PB	0.44	2.53	2	1
1:A:115:HIS:HE2	3:A:201:DGT:C8	0.44	2.25	7	1
2:B:6:DA:H1'	2:B:7:DG:O5'	0.43	2.13	8	10
1:A:21:GLU:N	1:A:68:ASN:O	0.43	2.45	8	5
1:A:50:VAL:O	1:A:99:LEU:HD11	0.43	2.12	10	1
2:B:3:DC:H4'	2:B:3:DC:OP1	0.43	2.13	2	1
1:A:21:GLU:HB2	1:A:68:ASN:HB3	0.43	1.89	5	1
1:A:111:TYR:OH	1:A:151:LEU:HB3	0.43	2.13	9	1
1:A:111:TYR:CE1	1:A:137:LEU:HD11	0.43	2.48	6	1
3:A:201:DGT:C5'	2:B:23:DOC:H3'2	0.43	2.38	7	1
1:A:39:SER:HB2	1:A:44:GLU:CG	0.43	2.44	8	1
1:A:136:LYS:O	1:A:142:LEU:HA	0.43	2.13	8	1
1:A:101:LEU:N	1:A:101:LEU:HD13	0.43	2.29	5	1
1:A:153:ILE:HB	1:A:158:GLU:CB	0.43	2.43	5	1
1:A:143:PHE:HA	1:A:147:THR:O	0.43	2.14	1	1
1:A:157:LYS:O	1:A:161:LYS:HB2	0.43	2.13	1	1
1:A:37:VAL:HB	1:A:51:ASP:CB	0.43	2.43	3	1
1:A:15:ARG:NH1	1:A:52:LEU:HD22	0.43	2.28	4	1
1:A:35:VAL:O	1:A:52:LEU:HA	0.43	2.14	4	1
1:A:124:ILE:HG23	1:A:127:ARG:CZ	0.43	2.43	8	1
2:B:5:DA:H2	2:B:6:DA:C8	0.43	2.32	8	10
3:A:201:DGT:H5'	2:B:23:DOC:C3'	0.43	2.43	4	1
1:A:42:ARG:NH1	3:A:201:DGT:O2G	0.43	2.49	5	1
1:A:107:GLU:HB2	1:A:151:LEU:HD21	0.43	1.90	8	1
1:A:136:LYS:HB2	1:A:143:PHE:HB2	0.43	1.90	8	1
1:A:19:ALA:O	1:A:70:ARG:N	0.43	2.49	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:201:DGT:N3	2:B:23:DOC:C2'	0.43	2.77	4	1
1:A:115:HIS:HA	1:A:123:LEU:HD11	0.43	1.89	6	1
1:A:138:ASN:O	1:A:141:GLY:N	0.43	2.49	9	2
2:B:16:DG:H2''	2:B:17:DA:OP2	0.42	2.14	10	6
1:A:62:LEU:HG	1:A:63:LYS:H	0.42	1.73	3	1
1:A:158:GLU:HA	1:A:161:LYS:CD	0.42	2.44	6	1
1:A:2:LEU:HB3	1:A:97:TYR:CE1	0.42	2.48	6	1
1:A:61:LEU:O	1:A:65:VAL:HG23	0.42	2.13	8	2
1:A:33:ASN:O	1:A:54:ILE:HA	0.42	2.13	2	1
1:A:51:ASP:C	1:A:52:LEU:HG	0.42	2.39	5	1
1:A:21:GLU:HB3	1:A:68:ASN:CB	0.42	2.44	9	2
2:B:12:DG:H2'	2:B:13:DT:C5	0.42	2.48	1	2
1:A:153:ILE:CB	1:A:158:GLU:HB3	0.42	2.45	3	1
1:A:39:SER:HB3	1:A:47:LEU:HD12	0.42	1.91	9	1
1:A:134:ASN:O	1:A:144:LYS:HG2	0.42	2.14	3	1
2:B:16:DG:H1	2:B:18:DA:N6	0.42	2.12	10	1
1:A:17:ARG:HA	1:A:17:ARG:NE	0.42	2.30	3	1
1:A:21:GLU:HB2	1:A:68:ASN:CB	0.42	2.44	3	1
1:A:71:ILE:O	1:A:76:PHE:HZ	0.42	1.97	4	1
1:A:77:SER:N	1:A:89:PHE:O	0.42	2.50	4	1
1:A:110:PRO:HA	1:A:156:GLU:OE2	0.42	2.15	10	1
1:A:119:PRO:O	1:A:122:TYR:N	0.42	2.53	5	7
1:A:60:LYS:N	1:A:60:LYS:HD3	0.42	2.30	2	1
2:B:18:DA:C4'	2:B:19:DG:OP1	0.42	2.66	4	2
1:A:85:LYS:HZ3	3:A:201:DGT:H5'	0.42	1.75	5	1
1:A:18:LEU:HB3	1:A:29:ILE:HB	0.42	1.92	6	1
1:A:75:SER:O	1:A:91:GLU:N	0.42	2.45	10	2
1:A:33:ASN:HD21	1:A:57:PRO:HD3	0.42	1.75	1	1
1:A:157:LYS:O	1:A:161:LYS:HB3	0.42	2.13	2	1
1:A:108:GLU:HG2	1:A:139:GLN:O	0.42	2.14	9	1
2:B:17:DA:OP2	2:B:17:DA:H8	0.41	1.97	3	2
2:B:6:DA:H2''	2:B:7:DG:OP2	0.41	2.13	8	1
1:A:58:GLU:O	1:A:62:LEU:HB2	0.41	2.15	9	1
1:A:22:TYR:O	1:A:25:GLN:N	0.41	2.51	9	2
1:A:93:GLU:O	1:A:94:LYS:HB2	0.41	2.15	4	1
1:A:151:LEU:HD13	1:A:151:LEU:N	0.41	2.30	8	1
2:B:16:DG:H1	2:B:18:DA:H61	0.41	1.59	8	3
2:B:16:DG:N3	2:B:16:DG:O4'	0.41	2.48	3	1
1:A:153:ILE:HD12	1:A:162:GLU:HG2	0.41	1.92	5	1
1:A:159:LEU:O	1:A:163:LEU:N	0.41	2.52	6	2
2:B:15:DC:OP1	2:B:15:DC:H4'	0.41	2.16	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:VAL:O	1:A:15:ARG:HB3	0.41	2.16	9	1
1:A:127:ARG:HA	1:A:137:LEU:HD21	0.41	1.91	10	1
1:A:19:ALA:HA	1:A:28:LYS:HA	0.41	1.92	1	1
1:A:8:LYS:O	1:A:12:ASN:N	0.41	2.48	4	1
2:B:16:DG:O4'	2:B:16:DG:N3	0.41	2.49	7	2
1:A:44:GLU:HG3	1:A:46:MET:H	0.41	1.75	2	1
3:A:201:DGT:O1B	3:A:201:DGT:C2'	0.41	2.69	2	1
1:A:104:ALA:HB1	1:A:108:GLU:CD	0.41	2.40	4	1
1:A:34:ILE:CG2	1:A:52:LEU:HD11	0.41	2.46	8	1
1:A:66:LEU:O	1:A:67:PRO:C	0.41	2.64	9	1
1:A:61:LEU:HD12	1:A:61:LEU:H	0.41	1.76	10	1
1:A:42:ARG:NH1	1:A:117:THR:O	0.41	2.54	1	1
1:A:35:VAL:N	1:A:53:LEU:O	0.40	2.52	5	1
1:A:59:LYS:N	1:A:59:LYS:HD2	0.40	2.30	9	1
1:A:116:PHE:CA	3:A:201:DGT:O3'	0.40	2.70	10	1
1:A:101:LEU:HG	1:A:102:PHE:H	0.40	1.77	10	1
1:A:144:LYS:O	1:A:145:ASN:C	0.40	2.63	2	1
1:A:151:LEU:N	1:A:151:LEU:HD13	0.40	2.31	3	1
3:A:201:DGT:O2A	2:B:23:DOC:H5''	0.40	2.16	8	1
1:A:42:ARG:NH1	3:A:201:DGT:PG	0.40	2.95	5	1
1:A:66:LEU:N	1:A:67:PRO:HD2	0.40	2.32	8	1
1:A:76:PHE:HA	1:A:89:PHE:O	0.40	2.16	8	1
1:A:135:TYR:CE1	1:A:144:LYS:HB2	0.40	2.52	9	1

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	168/174 (97%)	152±2 (91±1%)	11±2 (7±1%)	4±1 (2±1%)	6	43
All	All	1680/1740 (97%)	1525 (91%)	113 (7%)	42 (2%)	6	43

All 7 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	67	PRO	10
1	A	119	PRO	10
1	A	120	VAL	10
1	A	61	LEU	7
1	A	173	ARG	2
1	A	43	GLU	2
1	A	132	LYS	1

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	156/159 (98%)	123±3 (79±2%)	33±3 (21±2%)	3	31
All	All	1560/1590 (98%)	1229 (79%)	331 (21%)	3	31

All 101 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	55	ILE	10
1	A	153	ILE	10
1	A	155	THR	10
1	A	99	LEU	9
1	A	49	ASP	8
1	A	121	SER	8
1	A	126	ILE	8
1	A	127	ARG	8
1	A	53	LEU	7
1	A	62	LEU	7
1	A	71	ILE	7
1	A	102	PHE	7
1	A	151	LEU	7
1	A	58	GLU	7
1	A	107	GLU	6
1	A	3	THR	6
1	A	31	SER	6
1	A	39	SER	5
1	A	45	LYS	5

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Mol	Chain	Res	Type	Models (Total)
1	A	59	LYS	5
1	A	123	LEU	5
1	A	60	LYS	5
1	A	13	HIS	5
1	A	35	VAL	4
1	A	91	GLU	4
1	A	120	VAL	4
1	A	133	LYS	4
1	A	15	ARG	4
1	A	52	LEU	4
1	A	144	LYS	4
1	A	96	THR	4
1	A	132	LYS	4
1	A	152	LYS	4
1	A	93	GLU	4
1	A	47	LEU	4
1	A	26	LEU	3
1	A	44	GLU	3
1	A	171	LYS	3
1	A	173	ARG	3
1	A	74	LEU	3
1	A	77	SER	3
1	A	92	TRP	3
1	A	103	THR	3
1	A	162	GLU	3
1	A	40	LEU	3
1	A	28	LYS	3
1	A	32	LYS	3
1	A	37	VAL	3
1	A	169	ILE	3
1	A	21	GLU	3
1	A	166	THR	3
1	A	11	VAL	2
1	A	16	SER	2
1	A	18	LEU	2
1	A	95	LYS	2
1	A	137	LEU	2
1	A	160	ILE	2
1	A	172	LYS	2
1	A	51	ASP	2
1	A	86	CYS	2
1	A	100	ASP	2

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Mol	Chain	Res	Type	Models (Total)
1	A	42	ARG	2
1	A	76	PHE	2
1	A	136	LYS	2
1	A	4	LEU	2
1	A	70	ARG	2
1	A	72	LYS	2
1	A	139	GLN	2
1	A	101	LEU	2
1	A	165	PHE	2
1	A	30	LEU	2
1	A	135	TYR	2
1	A	46	MET	2
1	A	50	VAL	2
1	A	5	ILE	2
1	A	23	ASN	1
1	A	80	VAL	1
1	A	85	LYS	1
1	A	161	LYS	1
1	A	22	TYR	1
1	A	64	HIS	1
1	A	8	LYS	1
1	A	66	LEU	1
1	A	69	ILE	1
1	A	1	MET	1
1	A	2	LEU	1
1	A	33	ASN	1
1	A	34	ILE	1
1	A	105	LEU	1
1	A	122	TYR	1
1	A	41	ARG	1
1	A	130	LEU	1
1	A	9	LYS	1
1	A	79	LYS	1
1	A	56	VAL	1
1	A	68	ASN	1
1	A	98	GLN	1
1	A	111	TYR	1
1	A	146	GLN	1
1	A	159	LEU	1
1	A	168	ARG	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue 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	DOC	B	23	2	16,19,20	0.34±0.02	0±0 (0±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	DOC	B	23	2	20,26,29	0.50±0.11	0±0 (0±0%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DOC	B	23	2	-	0±0,7,18,19	0±0,2,2,2

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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
3	DGT	A	201	4	32,33,33	1.32±0.01	2±1 (7±2%)

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
3	DGT	A	201	4	48,52,52	1.69±0.02	12±1 (24±1%)

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
3	DGT	A	201	4	-	0±0,22,34,34	0±0,3,3,3

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
3	A	201	DGT	PG-O3G	3.63	1.61	1.50	4	10
3	A	201	DGT	C5-N7	2.93	1.33	1.39	7	10
3	A	201	DGT	PB-O3A	2.22	1.61	1.59	3	4
3	A	201	DGT	PA-O3A	2.05	1.61	1.59	4	1

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

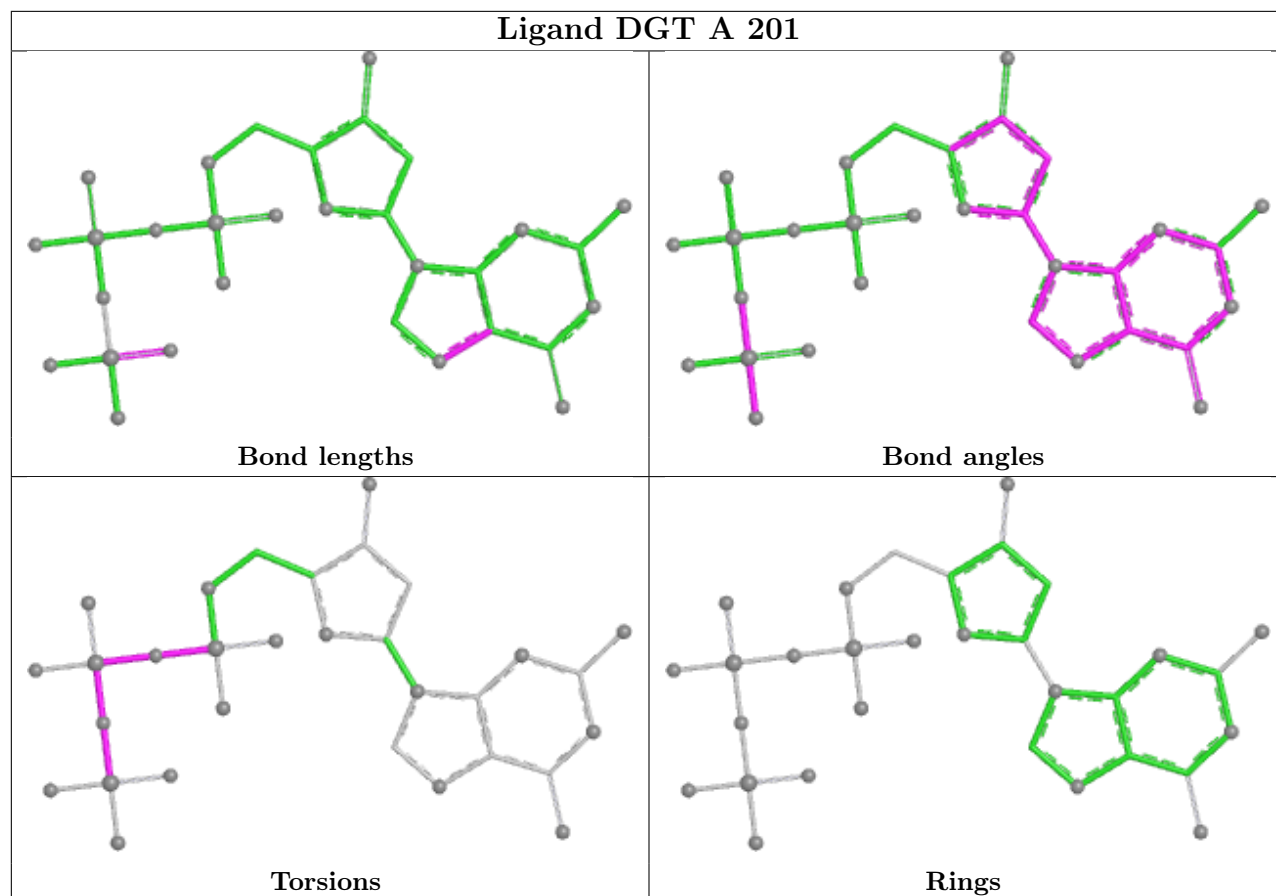
Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
3	A	201	DGT	C2-N3-C4	5.29	121.41	112.30	2	10
3	A	201	DGT	C5-C4-N3	4.84	120.68	128.39	10	10
3	A	201	DGT	C2-N1-C6	3.30	119.12	125.11	1	10
3	A	201	DGT	O4'-C1'-C2'	3.11	100.44	106.25	4	3
3	A	201	DGT	N9-C4-N3	3.09	132.13	125.95	7	10
3	A	201	DGT	O2G-PG-O3B	2.73	113.79	104.64	6	10
3	A	201	DGT	C2'-C3'-C4'	2.52	97.70	102.80	7	7
3	A	201	DGT	O4'-C1'-N9	2.40	112.12	107.86	7	3
3	A	201	DGT	N9-C8-N7	2.36	109.02	113.40	2	10
3	A	201	DGT	C4-C5-N7	2.29	107.04	110.67	10	10
3	A	201	DGT	C3'-C2'-C1'	2.26	97.06	102.60	10	6
3	A	201	DGT	C8-N7-C5	2.26	108.28	104.26	5	10
3	A	201	DGT	C5-C6-N1	2.23	118.92	113.25	1	9
3	A	201	DGT	O6-C6-C5	2.17	120.82	126.53	8	10

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](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 39% for the well-defined parts and 39% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	1212
Number of shifts mapped to atoms	1212
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	165	0.28 ± 0.15	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	157	1.09 ± 0.17	Should be checked
$^{13}\text{C}'$	161	0.12 ± 0.09	None needed (< 0.5 ppm)
^{15}N	165	1.36 ± 0.34	Should be applied

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 39%, i.e. 1193 atoms were assigned a chemical shift out of a possible 3035. 0 out of 38 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	640/845 (76%)	161/341 (47%)	318/340 (94%)	161/164 (98%)
Sidechain	528/1566 (34%)	286/1022 (28%)	242/480 (50%)	0/64 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	25/176 (14%)	25/86 (29%)	0/86 (0%)	0/4 (0%)
Sugar	0/264 (0%)	0/154 (0%)	0/110 (0%)	0/0 (—%)
Base	0/184 (0%)	0/118 (0%)	0/34 (0%)	0/32 (0%)
Overall	1193/3035 (39%)	472/1721 (27%)	560/1050 (53%)	161/264 (61%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 39%, i.e. 1212 atoms were assigned a chemical shift out of a possible 3084. 0 out of 38 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	656/866 (76%)	165/350 (47%)	326/348 (94%)	165/168 (98%)
Sidechain	531/1594 (33%)	286/1039 (28%)	245/488 (50%)	0/67 (0%)
Aromatic	25/176 (14%)	25/86 (29%)	0/86 (0%)	0/4 (0%)
Sugar	0/264 (0%)	0/154 (0%)	0/110 (0%)	0/0 (—%)
Base	0/184 (0%)	0/118 (0%)	0/34 (0%)	0/32 (0%)
Overall	1212/3084 (39%)	476/1747 (27%)	571/1066 (54%)	165/271 (61%)

7.1.4 Statistically unusual chemical shifts ⓘ

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots ⓘ

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

Random coil index (RCI) for chain A:

