



# Full wwPDB NMR Structure Validation Report ⓘ

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PDB ID : 1F5E  
Title : STRUCTURE OF TRANSCRIPTIONAL FACTOR ALCR IN COMPLEX  
WITH A TARGET DNA  
Authors : Cahuzac, B.; Cerdan, R.; Felenbok, B.; Guittet, E.  
Deposited on : 2000-06-14

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/NMRValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)  
NmrClust : Kelley et al. (1996)  
MolProbity : 4.02b-467  
Mogul : unknown  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : rb-20027457  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027457

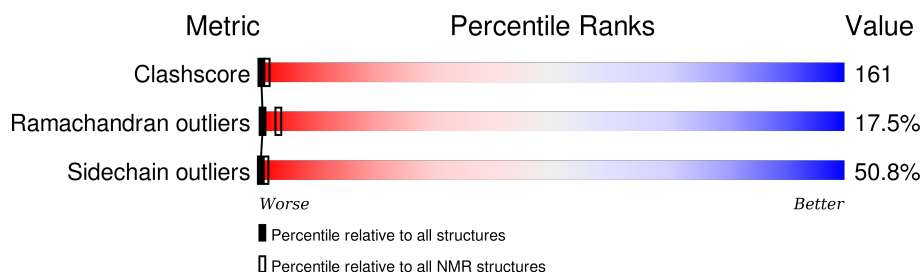
# 1 Overall quality at a glance

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	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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

Mol	Chain	Length	Quality of chain
1	A	10	 10% 90%
2	B	10	 50% 50%
3	P	65	 25% 32% 42%

## 2 Ensemble composition and analysis ⓘ

This entry contains 1 models. Identification of well-defined residues and clustering analysis are not possible.

### 3 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 1648 atoms, of which 710 are hydrogens and 0 are deuteriums.

- Molecule 1 is a DNA chain called DNA (5'-D(P\*CP\*GP\*TP\*GP\*CP\*GP\*GP\*AP\*TP\*C)-3').

Mol	Chain	Residues	Atoms						Trace
1	A	10	Total	C	H	N	O	P	0
			318	97	112	38	61	10	

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

Mol	Chain	Residues	Atoms						Trace
2	B	10	Total	C	H	N	O	P	0
			315	96	111	39	59	10	

- Molecule 3 is a protein called ETHANOL REGULON TRANSCRIPTIONAL FACTOR.

Mol	Chain	Residues	Atoms						Trace
3	P	65	Total	C	H	N	O	S	0
			1010	303	485	113	102	7	

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	-1	GLY	-	INSERTION	UNP P21228
P	0	SER	-	INSERTION	UNP P21228
P	61	ASN	ALA	engineered	UNP P21228
P	62	SER	LYS	engineered	UNP P21228
P	63	SER	GLY	engineered	UNP P21228

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
4	P	2	Total	Zn
			2	2

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		
5	B	1	Total	H	O
			3	2	1

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

These plots are provided for all protein, RNA and DNA 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: DNA (5'-D(P\*CP\*GP\*TP\*GP\*CP\*GP\*GP\*AP\*TP\*C)-3')

Chain A: 



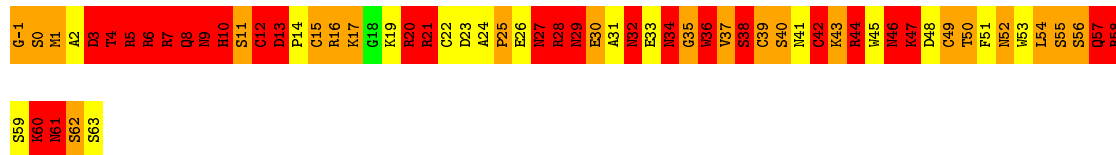
- Molecule 2: DNA (5'-D(P\*GP\*AP\*TP\*CP\*CP\*GP\*CP\*AP\*CP\*G)-3')

Chain B: 



- Molecule 3: ETHANOL REGULON TRANSCRIPTIONAL FACTOR

Chain P: 



## 5 Refinement protocol and experimental data overview ⓘ

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

Of the ? calculated structures, 1 were deposited, based on the following criterion: ?.

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

Software name	Classification	Version
DIANA	structure solution	
X-PLOR	refinement	3.1

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

## 6 Model quality ⓘ

### 6.1 Standard geometry ⓘ

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

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	9.27	49/230 (21.3%)	4.73	19/353 (5.4%)
2	B	5.88	33/228 (14.5%)	2.85	12/349 (3.4%)
3	P	18.97	205/534 (38.4%)	11.04	155/712 (21.8%)
All	All	14.89	287/992 (28.9%)	8.31	186/1414 (13.2%)

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
3	P	7	0
All	All	7	0

All bond outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	0	SER	CA-CB	-95.25	0.10	1.52
3	P	33	GLU	CD-OE2	-89.28	0.27	1.25
3	P	26	GLU	CD-OE1	-81.88	0.35	1.25
3	P	62	SER	CA-CB	-75.69	0.39	1.52
3	P	62	SER	CB-OG	-75.50	0.44	1.42
3	P	7	ARG	CZ-NH1	-73.74	0.37	1.33
3	P	0	SER	CB-OG	-69.23	0.52	1.42
3	P	56	SER	CB-OG	-69.21	0.52	1.42
3	P	40	SER	CB-OG	-68.72	0.53	1.42
3	P	-1	GLY	N-CA	-64.02	0.50	1.46
3	P	33	GLU	CD-OE1	-63.64	0.55	1.25
3	P	63	SER	CA-CB	-62.45	0.59	1.52
3	P	63	SER	CB-OG	-59.77	0.64	1.42
3	P	-1	GLY	CA-C	-59.73	0.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	63	SER	C-OXT	-58.68	0.11	1.23
1	A	1	DC	P-OP1	-58.45	0.49	1.49
3	P	-1	GLY	C-O	-56.66	0.33	1.23
3	P	30	GLU	CD-OE2	-56.44	0.63	1.25
3	P	30	GLU	CD-OE1	-55.69	0.64	1.25
3	P	7	ARG	NE-CZ	-51.27	0.66	1.33
3	P	63	SER	C-O	-50.68	0.27	1.23
1	A	10	DC	P-OP2	-50.34	0.63	1.49
1	A	10	DC	P-O5'	-50.18	1.09	1.59
3	P	61	ASN	C-O	-48.40	0.31	1.23
3	P	63	SER	N-CA	-46.58	0.53	1.46
3	P	59	SER	CA-CB	-45.74	0.84	1.52
2	B	1	DG	P-OP1	-45.20	0.72	1.49
1	A	1	DC	P-OP2	-44.82	0.72	1.49
3	P	59	SER	CB-OG	-44.29	0.84	1.42
3	P	13	ASP	CG-OD1	-44.01	0.24	1.25
3	P	0	SER	N-CA	-43.41	0.59	1.46
3	P	28	ARG	CZ-NH1	-43.13	0.77	1.33
3	P	63	SER	CA-C	-42.25	0.43	1.52
3	P	62	SER	C-O	-42.24	0.43	1.23
3	P	26	GLU	CD-OE2	-41.88	0.79	1.25
3	P	61	ASN	CA-CB	-41.64	0.44	1.53
1	A	10	DC	P-OP1	-41.05	0.79	1.49
3	P	42	CYS	CB-SG	-40.51	1.13	1.82
3	P	38	SER	CB-OG	-40.06	0.90	1.42
3	P	1	MET	N-CA	-39.62	0.67	1.46
3	P	61	ASN	CB-CG	-39.41	0.60	1.51
3	P	48	ASP	CG-OD2	-39.06	0.35	1.25
3	P	62	SER	CA-C	-39.06	0.51	1.52
3	P	1	MET	CB-CG	-38.64	0.27	1.51
3	P	1	MET	CG-SD	-38.38	0.81	1.81
3	P	46	ASN	CB-CG	-38.29	0.62	1.51
3	P	17	LYS	CD-CE	-38.25	0.55	1.51
3	P	48	ASP	CG-OD1	-37.62	0.38	1.25
3	P	61	ASN	CG-OD1	-37.30	0.41	1.24
2	B	1	DG	P-OP2	-36.57	0.86	1.49
3	P	1	MET	CA-CB	-35.94	0.74	1.53
3	P	6	ARG	NE-CZ	-34.83	0.87	1.33
3	P	27	ASN	CG-ND2	-34.81	0.45	1.32
3	P	33	GLU	CG-CD	-34.43	1.00	1.51
3	P	60	LYS	CD-CE	-34.26	0.65	1.51
1	A	10	DC	O5'-C5'	-33.92	0.57	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	0	SER	CA-C	-32.74	0.67	1.52
3	P	3	ASP	CG-OD1	-32.66	0.50	1.25
3	P	3	ASP	CB-CG	-32.10	0.84	1.51
3	P	28	ARG	CZ-NH2	-32.01	0.91	1.33
3	P	3	ASP	CG-OD2	-31.92	0.52	1.25
3	P	13	ASP	CG-OD2	-31.31	0.53	1.25
3	P	62	SER	N-CA	-30.93	0.84	1.46
3	P	12	CYS	CB-SG	-30.39	1.30	1.82
3	P	4	THR	CB-OG1	-30.06	0.83	1.43
3	P	46	ASN	CG-OD1	-29.96	0.58	1.24
3	P	20	ARG	NE-CZ	-29.74	0.94	1.33
3	P	7	ARG	CZ-NH2	-29.39	0.94	1.33
3	P	7	ARG	CG-CD	-29.20	0.79	1.51
3	P	5	ARG	CG-CD	-29.13	0.79	1.51
3	P	29	ASN	CG-OD1	-28.98	0.60	1.24
3	P	61	ASN	CG-ND2	-28.64	0.61	1.32
3	P	43	LYS	CB-CG	-28.53	0.75	1.52
3	P	32	ASN	CG-OD1	-28.50	0.61	1.24
1	A	9	DT	C3'-O3'	-28.24	1.07	1.44
3	P	13	ASP	CB-CG	-28.08	0.92	1.51
3	P	54	LEU	CB-CG	-27.46	0.72	1.52
3	P	30	GLU	CB-CG	-27.42	1.00	1.52
3	P	2	ALA	N-CA	-27.38	0.91	1.46
3	P	1	MET	SD-CE	-26.49	0.29	1.77
3	P	55	SER	CB-OG	-26.48	1.07	1.42
3	P	61	ASN	N-CA	-26.37	0.93	1.46
3	P	7	ARG	CB-CG	-26.34	0.81	1.52
3	P	32	ASN	CB-CG	-26.13	0.91	1.51
3	P	60	LYS	C-O	-26.11	0.73	1.23
3	P	27	ASN	CG-OD1	-26.07	0.66	1.24
3	P	61	ASN	CA-C	-25.94	0.85	1.52
3	P	60	LYS	CE-NZ	-25.88	0.84	1.49
3	P	44	ARG	NE-CZ	-25.75	0.99	1.33
3	P	61	ASN	C-N	-25.74	0.74	1.34
3	P	48	ASP	CB-CG	-25.63	0.97	1.51
3	P	0	SER	C-O	-25.39	0.75	1.23
3	P	62	SER	C-N	-24.90	0.76	1.34
3	P	21	ARG	CZ-NH2	-24.24	1.01	1.33
3	P	4	THR	C-O	-23.83	0.78	1.23
3	P	7	ARG	CD-NE	-23.74	1.06	1.46
3	P	10	HIS	CB-CG	-22.83	1.08	1.50
3	P	2	ALA	C-O	-22.58	0.80	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	28	ARG	CD-NE	-22.52	1.08	1.46
3	P	1	MET	CA-C	-22.34	0.94	1.52
3	P	3	ASP	N-CA	-22.19	1.01	1.46
1	A	10	DC	C4'-O4'	-22.08	1.23	1.45
3	P	-1	GLY	C-N	-21.86	0.83	1.34
3	P	60	LYS	N-CA	-21.76	1.02	1.46
3	P	44	ARG	CZ-NH2	-21.72	1.04	1.33
1	A	10	DC	C3'-O3'	-21.56	1.16	1.44
3	P	60	LYS	CA-C	-21.45	0.97	1.52
3	P	2	ALA	C-N	-20.92	0.85	1.34
3	P	17	LYS	CB-CG	-20.82	0.96	1.52
3	P	46	ASN	CG-ND2	-20.39	0.81	1.32
3	P	3	ASP	C-O	-19.88	0.85	1.23
3	P	5	ARG	NE-CZ	-19.76	1.07	1.33
3	P	21	ARG	CD-NE	-19.76	1.12	1.46
3	P	57	GLN	CD-OE1	-19.70	0.80	1.24
3	P	26	GLU	CG-CD	-19.45	1.22	1.51
3	P	60	LYS	CG-CD	-19.21	0.87	1.52
1	A	9	DT	O3'-P	-19.00	1.38	1.61
3	P	60	LYS	C-N	-18.85	0.90	1.34
3	P	21	ARG	CB-CG	-18.69	1.02	1.52
2	B	6	DG	O3'-P	-18.64	1.38	1.61
3	P	26	GLU	CB-CG	-18.38	1.17	1.52
3	P	4	THR	CA-CB	-18.27	1.05	1.53
2	B	1	DG	C3'-C2'	-18.27	1.30	1.52
3	P	27	ASN	CB-CG	-18.27	1.09	1.51
3	P	22	CYS	CB-SG	-18.18	1.51	1.82
3	P	20	ARG	CZ-NH1	-18.04	1.09	1.33
3	P	2	ALA	CA-C	-17.72	1.06	1.52
3	P	43	LYS	CE-NZ	-17.64	1.04	1.49
3	P	59	SER	CA-C	-17.55	1.07	1.52
3	P	8	GLN	CD-OE1	-17.43	0.85	1.24
2	B	1	DG	C4'-C3'	-17.42	1.35	1.52
3	P	34	ASN	CB-CG	-17.33	1.11	1.51
3	P	5	ARG	CZ-NH1	-17.27	1.10	1.33
3	P	6	ARG	CG-CD	-17.07	1.09	1.51
3	P	54	LEU	CG-CD2	-16.91	0.89	1.51
3	P	17	LYS	CE-NZ	-16.87	1.06	1.49
3	P	0	SER	C-N	-16.83	0.95	1.34
3	P	44	ARG	CD-NE	-16.82	1.17	1.46
3	P	7	ARG	CA-CB	-16.81	1.17	1.53
2	B	7	DC	P-OP1	-16.77	1.20	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	10	DC	C5'-C4'	-16.76	1.32	1.51
1	A	9	DT	C4'-C3'	-16.60	1.35	1.52
3	P	28	ARG	NE-CZ	-16.52	1.11	1.33
3	P	8	GLN	C-O	-16.41	0.92	1.23
3	P	3	ASP	CA-CB	-16.02	1.18	1.53
3	P	60	LYS	CB-CG	-15.92	1.09	1.52
3	P	4	THR	N-CA	-15.85	1.14	1.46
1	A	6	DG	P-OP2	-15.66	1.22	1.49
3	P	6	ARG	CZ-NH1	-15.36	1.13	1.33
3	P	11	SER	CB-OG	-15.33	1.22	1.42
3	P	10	HIS	CD2-NE2	-15.22	1.04	1.38
3	P	1	MET	C-O	-15.21	0.94	1.23
2	B	1	DG	O3'-P	-15.11	1.43	1.61
3	P	4	THR	C-N	-14.96	0.99	1.34
3	P	9	ASN	CG-OD1	-14.88	0.91	1.24
1	A	6	DG	P-OP1	-14.79	1.23	1.49
3	P	17	LYS	CG-CD	-14.67	1.02	1.52
3	P	47	LYS	CD-CE	-14.66	1.14	1.51
1	A	6	DG	P-O5'	-14.63	1.45	1.59
2	B	7	DC	P-OP2	-14.62	1.24	1.49
3	P	6	ARG	CZ-NH2	-14.61	1.14	1.33
3	P	3	ASP	C-N	-14.40	1.00	1.34
3	P	36	TRP	NE1-CE2	-14.22	1.19	1.37
3	P	28	ARG	CB-CG	-14.01	1.14	1.52
3	P	34	ASN	CG-OD1	-13.79	0.93	1.24
2	B	1	DG	O4'-C1'	-13.66	1.25	1.42
3	P	10	HIS	ND1-CE1	-12.90	1.02	1.34
3	P	54	LEU	CG-CD1	-12.88	1.04	1.51
3	P	3	ASP	CA-C	-12.82	1.19	1.52
3	P	29	ASN	CB-CG	-12.23	1.23	1.51
2	B	7	DC	P-O5'	-12.23	1.47	1.59
2	B	1	DG	C4'-O4'	-12.22	1.32	1.45
1	A	3	DT	P-O5'	-12.14	1.47	1.59
3	P	44	ARG	CB-CG	-11.97	1.20	1.52
1	A	10	DC	C2'-C1'	-11.84	1.40	1.52
3	P	4	THR	CB-CG2	-11.71	1.13	1.52
3	P	6	ARG	CD-NE	-11.63	1.26	1.46
3	P	1	MET	C-N	-11.56	1.07	1.34
3	P	36	TRP	CD2-CE3	-11.46	1.23	1.40
2	B	1	DG	N9-C8	-11.43	1.29	1.37
3	P	60	LYS	CA-CB	-11.37	1.28	1.53
1	A	2	DG	C3'-C2'	-11.36	1.38	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	16	ARG	CG-CD	-11.24	1.23	1.51
3	P	58	ARG	CG-CD	-11.24	1.23	1.51
1	A	6	DG	O5'-C5'	-11.21	1.14	1.42
1	A	10	DC	C3'-C2'	-11.17	1.38	1.52
1	A	7	DG	P-O5'	-11.16	1.48	1.59
3	P	50	THR	CB-OG1	-11.16	1.21	1.43
2	B	5	DC	C3'-C2'	-10.99	1.39	1.52
2	B	1	DG	C2'-C1'	-10.86	1.41	1.52
3	P	16	ARG	CZ-NH1	-10.68	1.19	1.33
3	P	43	LYS	CD-CE	-10.43	1.25	1.51
1	A	6	DG	C3'-O3'	-10.23	1.30	1.44
3	P	59	SER	C-O	-10.03	1.04	1.23
2	B	7	DC	O4'-C1'	-9.95	1.30	1.42
2	B	1	DG	C5'-C4'	-9.89	1.40	1.51
3	P	2	ALA	CA-CB	-9.89	1.31	1.52
3	P	5	ARG	CZ-NH2	-9.77	1.20	1.33
2	B	7	DC	C5'-C4'	-9.70	1.40	1.51
2	B	7	DC	C4'-C3'	-9.54	1.43	1.52
1	A	2	DG	O3'-P	-9.54	1.49	1.61
3	P	47	LYS	CE-NZ	-9.52	1.25	1.49
3	P	21	ARG	NE-CZ	-9.44	1.20	1.33
3	P	29	ASN	CG-ND2	-9.41	1.09	1.32
3	P	59	SER	C-N	-9.40	1.12	1.34
2	B	6	DG	P-O5'	-9.38	1.50	1.59
1	A	9	DT	C5'-C4'	-9.28	1.41	1.51
3	P	44	ARG	CZ-NH1	-9.17	1.21	1.33
1	A	3	DT	P-OP2	-9.13	1.33	1.49
1	A	10	DC	C4'-C3'	-9.13	1.43	1.52
3	P	25	PRO	C-O	-8.89	1.05	1.23
3	P	33	GLU	CB-CG	-8.87	1.35	1.52
3	P	50	THR	CB-CG2	-8.86	1.23	1.52
2	B	2	DA	P-OP1	-8.73	1.34	1.49
1	A	3	DT	P-OP1	-8.58	1.34	1.49
3	P	9	ASN	CB-CG	-8.42	1.31	1.51
3	P	58	ARG	C-O	-8.41	1.07	1.23
1	A	10	DC	N1-C6	-8.36	1.32	1.37
2	B	5	DC	C3'-O3'	-8.35	1.33	1.44
3	P	22	CYS	CA-CB	-8.21	1.35	1.53
3	P	8	GLN	CB-CG	-8.20	1.30	1.52
3	P	57	GLN	CD-NE2	-8.14	1.12	1.32
3	P	6	ARG	CB-CG	-8.12	1.30	1.52
2	B	1	DG	C6-N1	-8.09	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	58	ARG	CZ-NH2	-7.94	1.22	1.33
3	P	10	HIS	CG-CD2	-7.92	1.22	1.35
2	B	5	DC	O4'-C1'	-7.91	1.32	1.42
3	P	5	ARG	CD-NE	-7.84	1.33	1.46
3	P	21	ARG	CZ-NH1	-7.82	1.22	1.33
3	P	36	TRP	CZ2-CH2	-7.79	1.22	1.37
3	P	28	ARG	CG-CD	-7.71	1.32	1.51
2	B	1	DG	N3-C4	-7.61	1.30	1.35
3	P	8	GLN	CG-CD	-7.56	1.33	1.51
2	B	1	DG	N7-C5	-7.47	1.34	1.39
3	P	8	GLN	C-N	-7.47	1.16	1.34
3	P	36	TRP	CG-CD1	-7.30	1.26	1.36
3	P	5	ARG	CA-CB	-7.26	1.38	1.53
3	P	8	GLN	CD-NE2	-7.26	1.14	1.32
3	P	10	HIS	CG-ND1	-7.20	1.23	1.38
3	P	36	TRP	CG-CD2	-7.13	1.31	1.43
1	A	2	DG	C2'-C1'	-7.04	1.45	1.52
2	B	7	DC	C3'-O3'	-7.01	1.34	1.44
2	B	1	DG	C5-C4	-6.99	1.33	1.38
3	P	16	ARG	CB-CG	-6.96	1.33	1.52
3	P	25	PRO	C-N	-6.90	1.18	1.34
2	B	7	DC	C2'-C1'	-6.89	1.45	1.52
3	P	5	ARG	N-CA	-6.84	1.32	1.46
1	A	7	DG	P-OP1	-6.80	1.37	1.49
1	A	8	DA	P-O5'	-6.73	1.53	1.59
3	P	15	CYS	CB-SG	-6.52	1.71	1.82
1	A	5	DC	C3'-O3'	-6.51	1.35	1.44
1	A	7	DG	P-OP2	-6.48	1.38	1.49
1	A	3	DT	N1-C6	-6.43	1.33	1.38
3	P	5	ARG	CB-CG	-6.31	1.35	1.52
1	A	1	DC	P-O5'	-6.19	1.53	1.59
1	A	2	DG	C4'-O4'	-6.17	1.38	1.45
1	A	6	DG	C3'-C2'	-6.13	1.44	1.52
3	P	58	ARG	CZ-NH1	-6.11	1.25	1.33
3	P	58	ARG	C-N	-6.10	1.20	1.34
3	P	36	TRP	CE2-CZ2	-6.09	1.29	1.39
1	A	6	DG	C4'-C3'	-6.06	1.46	1.52
3	P	21	ARG	CG-CD	-6.04	1.36	1.51
3	P	44	ARG	CG-CD	-6.04	1.36	1.51
2	B	1	DG	N1-C2	-6.01	1.32	1.37
1	A	10	DC	N3-C4	-6.01	1.29	1.33
2	B	1	DG	P-O5'	-5.98	1.53	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	7	ARG	C-O	-5.97	1.12	1.23
1	A	4	DG	O3'-P	-5.88	1.54	1.61
1	A	2	DG	C4'-C3'	-5.86	1.46	1.52
1	A	5	DC	P-O5'	-5.76	1.53	1.59
3	P	4	THR	CA-C	-5.76	1.38	1.52
2	B	7	DC	N1-C6	-5.73	1.33	1.37
1	A	5	DC	O3'-P	-5.72	1.54	1.61
1	A	9	DT	P-O5'	-5.62	1.54	1.59
2	B	6	DG	P-OP2	-5.60	1.39	1.49
3	P	20	ARG	CZ-NH2	-5.60	1.25	1.33
3	P	7	ARG	C-N	-5.58	1.21	1.34
3	P	16	ARG	NE-CZ	-5.52	1.25	1.33
1	A	6	DG	C4'-O4'	-5.52	1.39	1.45
3	P	6	ARG	C-O	-5.44	1.13	1.23
1	A	9	DT	C3'-C2'	-5.43	1.45	1.52
1	A	5	DC	C4'-O4'	-5.41	1.39	1.45
1	A	5	DC	C5'-C4'	-5.35	1.45	1.51
3	P	6	ARG	C-N	-5.30	1.21	1.34
3	P	20	ARG	CG-CD	-5.26	1.38	1.51
2	B	2	DA	P-O5'	-5.23	1.54	1.59
1	A	2	DG	C3'-O3'	-5.02	1.37	1.44

All angle outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	7	ARG	NE-CZ-NH1	-149.53	45.54	120.30
3	P	7	ARG	NE-CZ-NH2	87.19	163.90	120.30
3	P	48	ASP	CB-CG-OD1	62.00	174.10	118.30
3	P	48	ASP	CB-CG-OD2	61.20	173.38	118.30
3	P	-1	GLY	CA-C-O	-59.60	13.33	120.60
3	P	33	GLU	OE1-CD-OE2	-58.60	52.98	123.30
3	P	48	ASP	OD1-CG-OD2	-58.31	12.52	123.30
3	P	13	ASP	CB-CG-OD2	50.95	164.15	118.30
3	P	30	GLU	OE1-CD-OE2	-49.89	63.43	123.30
1	A	10	DC	O5'-P-OP1	-43.61	58.37	110.70
3	P	1	MET	CA-CB-CG	-38.88	47.20	113.30
3	P	13	ASP	OD1-CG-OD2	-36.81	53.37	123.30
1	A	1	DC	OP1-P-OP2	-35.92	65.72	119.60
3	P	26	GLU	OE1-CD-OE2	-35.52	80.68	123.30
1	A	1	DC	O5'-P-OP2	34.00	151.50	110.70
3	P	32	ASN	CB-CG-OD1	-33.99	53.62	121.60
2	B	1	DG	OP1-P-OP2	-32.63	70.66	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	20	ARG	NE-CZ-NH1	-31.75	104.43	120.30
3	P	-1	GLY	O-C-N	31.15	172.53	122.70
3	P	28	ARG	NE-CZ-NH2	29.58	135.09	120.30
3	P	7	ARG	CD-NE-CZ	28.91	164.07	123.60
3	P	7	ARG	NH1-CZ-NH2	28.33	150.57	119.40
3	P	44	ARG	NE-CZ-NH2	-27.38	106.61	120.30
3	P	13	ASP	CB-CG-OD1	26.86	142.47	118.30
1	A	1	DC	O5'-P-OP1	26.41	142.39	110.70
2	B	1	DG	O5'-P-OP1	26.13	142.06	110.70
3	P	-1	GLY	CA-C-N	25.88	174.14	117.20
3	P	62	SER	CA-C-O	-25.48	66.58	120.10
3	P	7	ARG	CG-CD-NE	25.46	165.27	111.80
3	P	62	SER	CB-CA-C	-24.89	62.81	110.10
3	P	5	ARG	CG-CD-NE	24.54	163.33	111.80
3	P	0	SER	CB-CA-C	-24.49	63.57	110.10
3	P	0	SER	N-CA-C	22.79	172.52	111.00
3	P	33	GLU	CG-CD-OE1	22.46	163.23	118.30
3	P	-1	GLY	C-N-CA	21.28	174.89	121.70
1	A	9	DT	O3'-P-O5'	21.20	144.29	104.00
3	P	1	MET	CG-SD-CE	-20.32	67.70	100.20
3	P	21	ARG	NE-CZ-NH1	20.04	130.32	120.30
3	P	27	ASN	OD1-CG-ND2	-20.03	75.83	121.90
3	P	-1	GLY	N-CA-C	19.73	162.44	113.10
3	P	26	GLU	CG-CD-OE2	19.69	157.68	118.30
3	P	43	LYS	CA-CB-CG	19.38	156.03	113.40
3	P	28	ARG	NH1-CZ-NH2	-19.20	98.28	119.40
3	P	63	SER	CA-C-O	18.87	159.74	120.10
1	A	10	DC	O4'-C4'-C3'	-17.82	95.31	106.00
3	P	6	ARG	NE-CZ-NH1	-16.71	111.94	120.30
3	P	60	LYS	CD-CE-NZ	-16.67	73.36	111.70
3	P	62	SER	O-C-N	16.29	148.77	122.70
3	P	32	ASN	CB-CG-ND2	16.18	155.53	116.70
1	A	9	DT	OP2-P-O3'	-16.13	69.72	105.20
3	P	61	ASN	CA-C-N	16.09	152.59	117.20
3	P	3	ASP	CA-CB-CG	15.89	148.36	113.40
3	P	5	ARG	NE-CZ-NH1	-15.39	112.61	120.30
3	P	46	ASN	CB-CG-OD1	-15.35	90.90	121.60
3	P	30	GLU	CG-CD-OE1	15.11	148.51	118.30
3	P	27	ASN	CB-CG-OD1	15.07	151.74	121.60
1	A	10	DC	O5'-P-OP2	14.97	128.66	110.70
3	P	40	SER	CA-CB-OG	14.93	151.52	111.20
3	P	30	GLU	CG-CD-OE2	14.88	148.06	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	62	SER	N-CA-CB	14.85	132.77	110.50
3	P	21	ARG	NE-CZ-NH2	-14.76	112.92	120.30
3	P	56	SER	CA-CB-OG	14.76	151.05	111.20
3	P	61	ASN	CA-CB-CG	14.51	145.32	113.40
3	P	22	CYS	CA-CB-SG	14.48	140.06	114.00
1	A	9	DT	OP1-P-O3'	14.40	136.89	105.20
3	P	6	ARG	NE-CZ-NH2	-14.22	113.19	120.30
3	P	60	LYS	CG-CD-CE	-14.17	69.38	111.90
3	P	6	ARG	NH1-CZ-NH2	14.06	134.86	119.40
3	P	62	SER	N-CA-C	13.91	148.56	111.00
3	P	43	LYS	CD-CE-NZ	13.83	143.51	111.70
3	P	28	ARG	CG-CD-NE	13.75	140.68	111.80
3	P	61	ASN	C-N-CA	13.25	154.82	121.70
1	A	10	DC	C4'-C3'-C2'	12.93	114.74	103.10
3	P	0	SER	O-C-N	12.85	143.26	122.70
3	P	5	ARG	CB-CG-CD	12.83	144.96	111.60
3	P	21	ARG	CB-CG-CD	12.76	144.77	111.60
3	P	33	GLU	CG-CD-OE2	12.75	143.79	118.30
3	P	20	ARG	NH1-CZ-NH2	12.68	133.34	119.40
3	P	28	ARG	NE-CZ-NH1	12.66	126.63	120.30
3	P	32	ASN	OD1-CG-ND2	12.59	150.85	121.90
3	P	3	ASP	CB-CG-OD2	12.57	129.61	118.30
3	P	63	SER	CB-CA-C	-12.57	86.22	110.10
1	A	10	DC	P-O5'-C5'	12.56	140.99	120.90
3	P	3	ASP	N-CA-CB	-12.50	88.10	110.60
3	P	62	SER	CA-C-N	12.48	144.65	117.20
1	A	9	DT	C4'-C3'-C2'	12.45	114.31	103.10
3	P	4	THR	O-C-N	-12.19	103.20	122.70
3	P	61	ASN	N-CA-C	12.01	143.42	111.00
3	P	29	ASN	CB-CG-ND2	11.84	145.12	116.70
3	P	46	ASN	CA-CB-CG	11.80	139.37	113.40
3	P	1	MET	N-CA-CB	11.64	131.55	110.60
3	P	34	ASN	CB-CG-OD1	-11.38	98.83	121.60
3	P	1	MET	CB-CA-C	-11.28	87.84	110.40
3	P	44	ARG	CD-NE-CZ	-11.21	107.90	123.60
3	P	7	ARG	CA-CB-CG	-11.15	88.86	113.40
3	P	62	SER	C-N-CA	11.11	149.47	121.70
3	P	30	GLU	CB-CG-CD	10.98	143.84	114.20
3	P	59	SER	CB-CA-C	-10.67	89.83	110.10
1	A	9	DT	P-O3'-C3'	10.64	132.47	119.70
3	P	32	ASN	CA-CB-CG	10.54	136.59	113.40
3	P	3	ASP	OD1-CG-OD2	-10.46	103.42	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	0	SER	CA-C-O	-10.45	98.16	120.10
3	P	59	SER	CA-CB-OG	10.32	139.06	111.20
3	P	63	SER	N-CA-C	10.31	138.84	111.00
2	B	1	DG	O5'-P-OP2	10.30	123.06	110.70
3	P	54	LEU	CD1-CG-CD2	-10.21	79.88	110.50
3	P	61	ASN	CB-CA-C	-10.10	90.21	110.40
3	P	61	ASN	CB-CG-OD1	-9.89	101.82	121.60
3	P	36	TRP	CD1-CG-CD2	-9.87	98.40	106.30
3	P	17	LYS	CG-CD-CE	9.71	141.04	111.90
3	P	42	CYS	CA-CB-SG	9.70	131.46	114.00
1	A	10	DC	C1'-O4'-C4'	9.69	119.78	110.10
3	P	63	SER	N-CA-CB	9.68	125.02	110.50
3	P	3	ASP	CB-CG-OD1	9.63	126.97	118.30
3	P	61	ASN	CA-C-O	-9.59	99.95	120.10
3	P	61	ASN	O-C-N	-9.53	107.45	122.70
3	P	1	MET	CB-CG-SD	-9.30	84.50	112.40
3	P	59	SER	N-CA-C	9.04	135.42	111.00
2	B	5	DC	P-O3'-C3'	9.02	130.52	119.70
3	P	44	ARG	NE-CZ-NH1	8.96	124.78	120.30
3	P	0	SER	N-CA-CB	8.84	123.76	110.50
3	P	10	HIS	CG-ND1-CE1	-8.74	94.33	105.70
3	P	29	ASN	CB-CG-OD1	-8.68	104.25	121.60
3	P	60	LYS	CB-CG-CD	-8.64	89.14	111.60
1	A	10	DC	OP1-P-OP2	8.63	132.55	119.60
3	P	57	GLN	CG-CD-NE2	8.54	137.19	116.70
3	P	10	HIS	ND1-CG-CD2	8.52	120.73	108.80
3	P	44	ARG	NH1-CZ-NH2	8.35	128.58	119.40
3	P	1	MET	O-C-N	8.29	135.97	122.70
1	A	2	DG	P-O3'-C3'	8.22	129.56	119.70
1	A	10	DC	C5'-C4'-C3'	8.07	128.63	114.10
3	P	12	CYS	CA-CB-SG	7.94	128.30	114.00
2	B	1	DG	C3'-C2'-C1'	7.80	111.86	102.50
3	P	9	ASN	CB-CG-OD1	-7.76	106.08	121.60
2	B	7	DC	O5'-P-OP1	-7.75	98.73	105.70
3	P	44	ARG	CG-CD-NE	7.71	127.99	111.80
3	P	44	ARG	CB-CG-CD	7.69	131.58	111.60
3	P	36	TRP	CE2-CD2-CG	7.66	113.43	107.30
3	P	8	GLN	O-C-N	-7.51	110.68	122.70
2	B	5	DC	C3'-C2'-C1'	7.37	111.34	102.50
3	P	61	ASN	CB-CG-ND2	7.31	134.25	116.70
3	P	46	ASN	OD1-CG-ND2	7.30	138.69	121.90
2	B	1	DG	P-O3'-C3'	7.29	128.45	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	57	GLN	OE1-CD-NE2	-7.24	105.24	121.90
3	P	28	ARG	CB-CG-CD	7.24	130.41	111.60
3	P	4	THR	CA-C-N	7.10	132.82	117.20
3	P	3	ASP	CB-CA-C	7.07	124.53	110.40
3	P	28	ARG	CD-NE-CZ	7.02	133.43	123.60
3	P	54	LEU	CA-CB-CG	7.02	131.45	115.30
3	P	5	ARG	CA-CB-CG	7.02	128.84	113.40
3	P	16	ARG	NE-CZ-NH1	-6.85	116.88	120.30
3	P	36	TRP	CG-CD2-CE3	-6.84	127.74	133.90
3	P	6	ARG	CD-NE-CZ	-6.82	114.05	123.60
3	P	47	LYS	CG-CD-CE	6.77	132.20	111.90
3	P	7	ARG	CB-CG-CD	-6.76	94.01	111.60
3	P	8	GLN	CG-CD-NE2	6.66	132.69	116.70
3	P	9	ASN	CB-CG-ND2	6.61	132.56	116.70
3	P	16	ARG	NE-CZ-NH2	6.56	123.58	120.30
3	P	27	ASN	CB-CG-ND2	6.55	132.42	116.70
3	P	10	HIS	CA-CB-CG	6.47	124.60	113.60
2	B	1	DG	C4-C5-N7	-6.45	108.22	110.80
3	P	63	SER	CA-CB-OG	-6.44	93.81	111.20
3	P	7	ARG	N-CA-C	6.38	128.22	111.00
3	P	59	SER	O-C-N	6.36	132.88	122.70
3	P	43	LYS	CB-CG-CD	-6.30	95.23	111.60
3	P	10	HIS	CG-CD2-NE2	-6.28	97.27	109.20
1	A	6	DG	C4'-C3'-C2'	6.17	108.65	103.10
3	P	4	THR	N-CA-CB	-6.12	98.67	110.30
3	P	13	ASP	CA-CB-CG	6.07	126.76	113.40
3	P	21	ARG	CD-NE-CZ	-6.06	115.11	123.60
3	P	8	GLN	CA-C-N	6.05	130.52	117.20
3	P	60	LYS	CA-CB-CG	-5.95	100.30	113.40
3	P	4	THR	C-N-CA	5.90	136.45	121.70
3	P	36	TRP	CG-CD1-NE1	5.86	115.96	110.10
3	P	5	ARG	NH1-CZ-NH2	5.82	125.80	119.40
3	P	33	GLU	CB-CG-CD	5.81	129.88	114.20
3	P	46	ASN	CB-CG-ND2	5.71	130.41	116.70
3	P	27	ASN	CA-CB-CG	5.64	125.80	113.40
2	B	1	DG	O4'-C1'-C2'	-5.43	101.56	105.90
3	P	34	ASN	CA-CB-CG	5.43	125.34	113.40
3	P	4	THR	N-CA-C	5.22	125.10	111.00
2	B	6	DG	P-O3'-C3'	5.09	125.81	119.70
2	B	6	DG	O3'-P-O5'	5.06	113.61	104.00
3	P	30	GLU	CA-CB-CG	5.04	124.48	113.40
1	A	5	DC	O3'-P-O5'	5.02	113.54	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
3	P	34	ASN	CB-CG-ND2	5.01	128.73	116.70

All chiral outliers are listed below.

Mol	Chain	Res	Type	Atoms
3	P	0	SER	CA
3	P	1	MET	CA
3	P	4	THR	CB
3	P	59	SER	CA
3	P	61	ASN	CA
3	P	62	SER	CA
3	P	63	SER	CA

There are no planarity outliers.

## 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	206	112	113	30
2	B	204	111	112	42
3	P	525	485	466	229
5	B	1	2	0	3
All	All	938	710	691	263

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 161.

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

Atom-1	Atom-2	Clash( $\text{\AA}$ )	Distance( $\text{\AA}$ )
3:P:13:ASP:HB2	3:P:53:TRP:CZ2	1.64	1.23
3:P:13:ASP:CB	3:P:53:TRP:CZ2	1.42	1.99
3:P:27:ASN:OD1	3:P:27:ASN:CB	1.39	1.70
3:P:13:ASP:HB2	3:P:53:TRP:CH2	1.35	1.56
3:P:3:ASP:CA	3:P:3:ASP:CG	1.34	1.95
3:P:5:ARG:CD	3:P:5:ARG:CB	1.32	2.05
3:P:55:SER:O	3:P:60:LYS:HG3	1.25	1.17

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
2:B:2:DA:N3	3:P:6:ARG:NH2	1.25	1.81
3:P:46:ASN:CA	3:P:46:ASN:CG	1.25	2.04
3:P:42:CYS:SG	3:P:42:CYS:CB	1.22	1.13
3:P:5:ARG:NE	3:P:5:ARG:CG	1.13	2.09
1:A:1:DC:P	1:A:1:DC:OP2	1.12	0.72
3:P:56:SER:CA	3:P:56:SER:OG	1.11	1.98
3:P:13:ASP:CB	3:P:53:TRP:HZ2	1.11	1.40
3:P:40:SER:CA	3:P:40:SER:OG	1.11	1.99
3:P:13:ASP:CA	3:P:13:ASP:CG	1.10	2.20
3:P:32:ASN:OD1	3:P:32:ASN:ND2	1.10	1.84
2:B:1:DG:OP1	2:B:1:DG:P	1.09	0.72
3:P:32:ASN:CB	3:P:32:ASN:ND2	1.09	2.14
3:P:30:GLU:CG	3:P:30:GLU:OE1	1.08	2.02
3:P:20:ARG:HG3	3:P:20:ARG:NH1	1.08	1.61
3:P:30:GLU:OE2	3:P:30:GLU:CG	1.07	2.01
3:P:13:ASP:HB2	3:P:13:ASP:CG	1.07	1.51
3:P:42:CYS:SG	3:P:42:CYS:CA	1.07	2.42
3:P:13:ASP:CG	3:P:53:TRP:CH2	1.06	2.28
3:P:11:SER:O	3:P:16:ARG:NH1	1.06	1.87
3:P:13:ASP:CG	3:P:53:TRP:CZ2	1.06	2.29
3:P:13:ASP:HB3	3:P:13:ASP:CG	1.06	1.51
2:B:1:DG:OP2	2:B:1:DG:P	1.05	0.86
3:P:32:ASN:CA	3:P:32:ASN:CG	1.04	2.25
3:P:55:SER:O	3:P:60:LYS:CG	1.04	2.06
3:P:32:ASN:CG	3:P:32:ASN:HB2	1.03	1.47
3:P:32:ASN:CB	3:P:32:ASN:OD1	1.03	0.73
3:P:32:ASN:HB3	3:P:32:ASN:OD1	1.03	1.47
3:P:13:ASP:CB	3:P:13:ASP:CG	1.02	0.92
3:P:42:CYS:HB2	3:P:42:CYS:SG	1.01	1.66
3:P:32:ASN:CB	3:P:32:ASN:CG	1.00	0.91
3:P:32:ASN:HB3	3:P:32:ASN:CG	0.99	1.46
3:P:42:CYS:HB3	3:P:42:CYS:SG	0.99	1.66
3:P:13:ASP:CB	3:P:53:TRP:CH2	0.99	2.32
3:P:32:ASN:CA	3:P:32:ASN:OD1	0.98	2.11
2:B:3:DT:OP2	3:P:16:ARG:CZ	0.98	2.11
3:P:3:ASP:N	3:P:3:ASP:CG	0.97	2.16
3:P:3:ASP:CB	3:P:3:ASP:CG	0.93	0.84
3:P:3:ASP:HB3	3:P:3:ASP:CG	0.93	1.38
3:P:3:ASP:HB2	3:P:3:ASP:CG	0.92	1.38
3:P:56:SER:HB2	3:P:56:SER:OG	0.92	1.17
3:P:40:SER:OG	3:P:40:SER:HB3	0.92	1.17
2:B:3:DT:OP2	3:P:16:ARG:NH2	0.91	2.03

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
3:P:20:ARG:CG	3:P:20:ARG:HH11	0.91	1.51
3:P:56:SER:HB3	3:P:56:SER:OG	0.91	1.17
3:P:40:SER:OG	3:P:40:SER:HB2	0.91	1.17
2:B:3:DT:OP2	3:P:16:ARG:NE	0.90	2.05
1:A:1:DC:OP1	1:A:1:DC:P	0.89	0.49
3:P:36:TRP:CE3	3:P:37:VAL:HG12	0.87	2.05
1:A:1:DC:OP1	1:A:1:DC:O5'	0.85	1.94
3:P:27:ASN:OD1	3:P:27:ASN:ND2	0.85	0.70
3:P:13:ASP:OD1	3:P:53:TRP:CH2	0.84	2.24
3:P:30:GLU:CD	3:P:30:GLU:OE1	0.84	0.64
1:A:2:DG:H5''	3:P:44:ARG:O	0.84	1.73
3:P:36:TRP:CZ3	3:P:37:VAL:CG1	0.84	2.61
3:P:30:GLU:OE2	3:P:30:GLU:CD	0.83	0.63
3:P:27:ASN:OD1	3:P:27:ASN:CG	0.82	0.66
3:P:46:ASN:HB3	3:P:46:ASN:CG	0.82	1.26
3:P:40:SER:OG	3:P:40:SER:CB	0.82	0.52
3:P:56:SER:CB	3:P:56:SER:OG	0.82	0.52
2:B:3:DT:P	3:P:16:ARG:HH21	0.82	1.97
3:P:46:ASN:CG	3:P:46:ASN:HB2	0.81	1.26
3:P:4:THR:O	3:P:4:THR:HG23	0.81	1.65
1:A:2:DG:C5'	3:P:44:ARG:O	0.81	2.29
3:P:46:ASN:HD22	3:P:46:ASN:CG	0.81	1.45
3:P:5:ARG:CD	3:P:5:ARG:HG3	0.81	1.35
3:P:32:ASN:CG	3:P:32:ASN:OD1	0.81	0.61
2:B:1:DG:O5'	2:B:1:DG:C8	0.80	2.34
3:P:5:ARG:CD	3:P:5:ARG:HG2	0.80	1.35
3:P:46:ASN:HD21	3:P:46:ASN:CG	0.79	1.45
3:P:5:ARG:CD	3:P:5:ARG:CG	0.78	0.79
2:B:4:DC:N4	2:B:5:DC:N4	0.77	2.33
3:P:42:CYS:CB	3:P:42:CYS:HG	0.77	1.90
3:P:5:ARG:HD2	3:P:5:ARG:CG	0.77	1.30
2:B:6:DG:N7	3:P:20:ARG:NH2	0.76	2.33
3:P:28:ARG:HH21	3:P:50:THR:HA	0.76	1.40
3:P:13:ASP:HB3	3:P:53:TRP:HZ2	0.76	1.35
3:P:13:ASP:HB3	3:P:53:TRP:CZ2	0.76	2.12
3:P:46:ASN:CG	3:P:46:ASN:ND2	0.76	0.81
2:B:3:DT:P	3:P:16:ARG:NH2	0.75	2.58
3:P:5:ARG:HD3	3:P:5:ARG:CG	0.75	1.30
1:A:9:DT:H2''	1:A:10:DC:C6	0.75	2.16
2:B:4:DC:C4	2:B:5:DC:N4	0.75	2.55
3:P:36:TRP:CZ3	3:P:37:VAL:HG13	0.75	2.17
3:P:37:VAL:HG22	3:P:38:SER:N	0.74	1.94

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
3:P:36:TRP:CE3	3:P:37:VAL:CG1	0.74	2.70
2:B:8:DA:C4	2:B:9:DC:C5	0.74	2.76
3:P:39:CYS:O	3:P:43:LYS:CG	0.74	2.36
2:B:4:DC:N4	2:B:5:DC:H41	0.72	1.82
3:P:20:ARG:CB	3:P:41:ASN:OD1	0.72	2.37
3:P:46:ASN:CB	3:P:46:ASN:CG	0.72	0.63
3:P:20:ARG:HB3	3:P:41:ASN:OD1	0.71	1.85
2:B:7:DC:H2"	2:B:8:DA:C8	0.70	2.21
1:A:4:DG:N7	3:P:45:TRP:CZ2	0.69	2.60
1:A:1:DC:OP1	1:A:1:DC:OP2	0.69	0.69
3:P:-1:GLY:C	3:P:-1:GLY:HA3	0.69	1.16
3:P:37:VAL:HG13	3:P:38:SER:H	0.68	1.47
3:P:12:CYS:HB2	3:P:14:PRO:HD2	0.67	1.66
3:P:-1:GLY:N	3:P:-1:GLY:HA2	0.67	1.13
3:P:56:SER:HA	3:P:60:LYS:HB2	0.67	1.65
3:P:-1:GLY:N	3:P:-1:GLY:HA3	0.67	1.13
3:P:30:GLU:OE2	3:P:30:GLU:OE1	0.66	0.67
3:P:32:ASN:HB2	3:P:32:ASN:OD1	0.66	0.89
3:P:28:ARG:O	3:P:31:ALA:HB3	0.65	1.91
3:P:53:TRP:CD1	3:P:53:TRP:N	0.65	2.63
3:P:44:ARG:HG2	3:P:44:ARG:HH11	0.65	1.48
3:P:54:LEU:HD22	3:P:58:ARG:NH2	0.65	2.07
1:A:7:DG:N7	3:P:19:LYS:NZ	0.65	2.44
3:P:13:ASP:CG	3:P:53:TRP:HH2	0.64	1.94
3:P:36:TRP:CG	3:P:37:VAL:N	0.64	2.64
3:P:54:LEU:CD2	3:P:58:ARG:HH21	0.64	2.05
1:A:3:DT:C7	3:P:45:TRP:CZ2	0.64	2.80
3:P:20:ARG:CG	3:P:20:ARG:NH1	0.64	2.17
1:A:3:DT:C2'	1:A:4:DG:C8	0.64	2.81
3:P:39:CYS:O	3:P:43:LYS:HG2	0.63	1.92
3:P:54:LEU:CD2	3:P:58:ARG:NH2	0.63	2.62
3:P:11:SER:O	3:P:16:ARG:CZ	0.62	2.45
3:P:44:ARG:HG2	3:P:44:ARG:NH1	0.62	2.09
1:A:5:DC:N4	3:P:19:LYS:O	0.62	2.33
2:B:2:DA:OP1	3:P:58:ARG:NH1	0.62	2.33
3:P:9:ASN:C	3:P:10:HIS:CD2	0.61	2.73
3:P:28:ARG:NH2	3:P:50:THR:HA	0.61	2.08
3:P:56:SER:HA	3:P:60:LYS:CB	0.61	2.25
3:P:-1:GLY:C	3:P:-1:GLY:HA2	0.61	1.16
2:B:5:DC:N4	3:P:19:LYS:O	0.61	2.33
3:P:13:ASP:N	3:P:14:PRO:HD2	0.61	2.10
3:P:6:ARG:O	3:P:7:ARG:CB	0.61	2.36

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
3:P:36:TRP:CA	3:P:36:TRP:CE3	0.61	2.84
3:P:5:ARG:HD3	3:P:5:ARG:HG2	0.61	1.12
3:P:52:ASN:C	3:P:54:LEU:N	0.61	2.50
3:P:31:ALA:O	3:P:35:GLY:N	0.60	2.34
3:P:36:TRP:C	3:P:36:TRP:CE3	0.60	2.74
3:P:28:ARG:HD3	3:P:51:PHE:CD1	0.60	2.31
1:A:4:DG:N7	3:P:45:TRP:CH2	0.60	2.70
3:P:36:TRP:C	3:P:37:VAL:HG12	0.59	2.16
3:P:52:ASN:O	3:P:55:SER:N	0.59	2.35
3:P:36:TRP:O	3:P:37:VAL:CB	0.58	2.51
3:P:54:LEU:HD22	3:P:58:ARG:CZ	0.58	2.28
1:A:3:DT:C6	3:P:45:TRP:CZ2	0.58	2.91
1:A:3:DT:H2''	1:A:4:DG:C8	0.58	2.34
3:P:37:VAL:CG2	3:P:38:SER:N	0.57	2.66
3:P:45:TRP:O	3:P:46:ASN:C	0.57	2.43
2:B:1:DG:H2''	2:B:2:DA:O5'	0.57	1.98
3:P:42:CYS:HA	3:P:47:LYS:HB2	0.57	1.75
1:A:3:DT:H72	3:P:45:TRP:CZ2	0.57	2.34
3:P:11:SER:HB3	3:P:15:CYS:HB3	0.56	1.76
2:B:5:DC:OP2	3:P:21:ARG:NH2	0.56	2.33
3:P:36:TRP:CD2	3:P:37:VAL:N	0.56	2.73
2:B:8:DA:H2''	2:B:9:DC:OP2	0.55	1.99
3:P:52:ASN:O	3:P:54:LEU:N	0.55	2.40
1:A:3:DT:H71	3:P:45:TRP:NE1	0.55	2.16
3:P:15:CYS:SG	3:P:41:ASN:CG	0.55	2.85
3:P:31:ALA:CB	3:P:36:TRP:HB2	0.54	2.32
2:B:1:DG:C8	2:B:1:DG:P	0.54	3.01
3:P:13:ASP:C	3:P:13:ASP:CG	0.53	2.66
2:B:4:DC:OP1	3:P:9:ASN:ND2	0.53	2.41
3:P:4:THR:CG2	3:P:5:ARG:HG2	0.53	2.33
3:P:6:ARG:O	3:P:7:ARG:HB3	0.53	2.02
1:A:3:DT:C6	3:P:45:TRP:HZ2	0.53	2.21
3:P:9:ASN:O	3:P:10:HIS:CD2	0.53	2.62
3:P:51:PHE:HA	3:P:54:LEU:CD1	0.53	2.34
1:A:9:DT:C2'	1:A:10:DC:C6	0.53	2.90
3:P:52:ASN:ND2	3:P:52:ASN:N	0.52	2.57
3:P:13:ASP:N	3:P:14:PRO:CD	0.52	2.72
3:P:45:TRP:O	3:P:47:LYS:N	0.52	2.43
3:P:5:ARG:O	3:P:6:ARG:HB2	0.52	2.05
3:P:15:CYS:SG	3:P:41:ASN:CB	0.51	2.98
3:P:52:ASN:O	3:P:53:TRP:C	0.51	2.45
3:P:42:CYS:N	3:P:42:CYS:SG	0.51	2.83

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
2:B:4:DC:C4	2:B:5:DC:C4	0.51	2.98
2:B:4:DC:OP1	3:P:8:GLN:HB3	0.50	2.06
3:P:42:CYS:O	3:P:46:ASN:N	0.50	2.45
3:P:54:LEU:HD22	3:P:58:ARG:NE	0.50	2.21
3:P:36:TRP:CE3	3:P:37:VAL:N	0.50	2.80
3:P:13:ASP:CB	3:P:53:TRP:HH2	0.50	2.06
2:B:4:DC:H5''	3:P:8:GLN:HB2	0.49	1.84
3:P:41:ASN:C	3:P:43:LYS:N	0.49	2.65
1:A:3:DT:H71	3:P:45:TRP:CE2	0.49	2.41
3:P:36:TRP:CZ3	3:P:37:VAL:HG12	0.49	2.32
3:P:40:SER:O	3:P:44:ARG:CG	0.49	2.60
2:B:4:DC:C5	2:B:5:DC:C5	0.49	3.00
3:P:40:SER:O	3:P:44:ARG:HG3	0.49	2.07
2:B:2:DA:H3'	3:P:16:ARG:HE	0.48	1.66
2:B:5:DC:H2''	2:B:6:DG:C8	0.48	2.43
3:P:53:TRP:CG	3:P:54:LEU:N	0.48	2.82
2:B:4:DC:OP1	3:P:8:GLN:CB	0.48	2.62
3:P:5:ARG:O	3:P:6:ARG:CB	0.48	2.59
3:P:36:TRP:HE3	3:P:36:TRP:CA	0.48	2.21
3:P:36:TRP:O	3:P:37:VAL:HB	0.48	2.08
1:A:3:DT:H2'	1:A:4:DG:C8	0.48	2.43
3:P:15:CYS:SG	3:P:41:ASN:ND2	0.48	2.87
2:B:8:DA:H1'	2:B:9:DC:H5'	0.47	1.86
2:B:4:DC:H3'	3:P:8:GLN:NE2	0.47	2.23
2:B:3:DT:C7	5:B:70:HOH:O	0.47	2.62
3:P:23:ASP:O	3:P:24:ALA:C	0.47	2.52
3:P:51:PHE:HA	3:P:54:LEU:HD12	0.47	1.85
1:A:3:DT:C7	3:P:45:TRP:CE2	0.47	2.98
1:A:5:DC:H2''	1:A:6:DG:C8	0.47	2.44
2:B:2:DA:C2	3:P:6:ARG:NH2	0.47	2.71
3:P:37:VAL:HG13	3:P:38:SER:N	0.47	2.22
2:B:8:DA:C4	2:B:9:DC:C4	0.47	3.02
3:P:13:ASP:OD1	3:P:53:TRP:HH2	0.47	1.85
3:P:31:ALA:HA	3:P:34:ASN:ND2	0.46	2.24
3:P:54:LEU:C	3:P:56:SER:N	0.46	2.64
3:P:11:SER:HB3	3:P:15:CYS:CB	0.46	2.41
3:P:41:ASN:O	3:P:42:CYS:C	0.46	2.53
5:B:70:HOH:O	3:P:19:LYS:HA	0.46	2.10
3:P:4:THR:CG2	3:P:5:ARG:HH11	0.46	2.24
1:A:2:DG:O5'	3:P:44:ARG:O	0.46	2.34
3:P:12:CYS:HA	3:P:51:PHE:CE1	0.46	2.46
3:P:20:ARG:HB3	3:P:41:ASN:ND2	0.46	2.25

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
3:P:39:CYS:O	3:P:43:LYS:CB	0.45	2.59
3:P:41:ASN:O	3:P:43:LYS:N	0.45	2.50
3:P:29:ASN:HA	3:P:32:ASN:ND2	0.45	2.26
3:P:-1:GLY:H2	3:P:-1:GLY:CA	0.45	1.15
2:B:3:DT:H5"	3:P:10:HIS:HA	0.45	1.88
3:P:-1:GLY:H1	3:P:-1:GLY:CA	0.45	1.15
3:P:-1:GLY:CA	3:P:-1:GLY:H3	0.45	1.15
1:A:6:DG:H2"	1:A:7:DG:OP2	0.45	2.05
1:A:9:DT:C4	1:A:10:DC:N4	0.45	2.85
3:P:53:TRP:O	3:P:57:GLN:N	0.44	2.50
3:P:5:ARG:CB	3:P:5:ARG:HD2	0.44	2.08
3:P:42:CYS:O	3:P:46:ASN:CA	0.44	2.66
1:A:9:DT:C2	1:A:10:DC:C4	0.44	3.05
3:P:23:ASP:O	3:P:25:PRO:N	0.44	2.51
3:P:36:TRP:HE3	3:P:36:TRP:HA	0.44	1.71
2:B:9:DC:H2"	2:B:10:DG:C8	0.44	2.47
3:P:31:ALA:HB1	3:P:36:TRP:HB2	0.44	1.90
2:B:4:DC:H5"	3:P:8:GLN:HE21	0.43	1.72
2:B:3:DT:OP1	3:P:10:HIS:HB3	0.43	2.13
3:P:36:TRP:O	3:P:37:VAL:HG12	0.43	2.12
3:P:4:THR:C	3:P:5:ARG:HG2	0.43	2.31
3:P:54:LEU:O	3:P:56:SER:N	0.43	2.51
3:P:56:SER:HA	3:P:60:LYS:CG	0.43	2.44
1:A:2:DG:H2'	3:P:45:TRP:CD1	0.43	2.48
2:B:3:DT:H73	5:B:70:HOH:O	0.43	2.13
3:P:15:CYS:SG	3:P:41:ASN:HB2	0.43	2.53
1:A:3:DT:H6	3:P:45:TRP:NE1	0.43	2.11
2:B:6:DG:O6	3:P:20:ARG:NE	0.42	2.52
3:P:54:LEU:O	3:P:55:SER:C	0.42	2.56
3:P:20:ARG:HB3	3:P:41:ASN:CG	0.42	2.35
3:P:40:SER:CB	3:P:40:SER:HG	0.42	1.13
3:P:56:SER:CB	3:P:56:SER:HG	0.42	1.13
1:A:9:DT:C2'	1:A:10:DC:C5	0.42	3.03
3:P:27:ASN:O	3:P:31:ALA:N	0.42	2.52
3:P:20:ARG:HB3	3:P:41:ASN:HD21	0.42	1.75
3:P:4:THR:HG23	3:P:5:ARG:HG2	0.42	1.91
2:B:4:DC:C4	2:B:5:DC:C5	0.41	3.08
3:P:9:ASN:O	3:P:10:HIS:CB	0.41	2.66
3:P:36:TRP:O	3:P:37:VAL:CG1	0.41	2.69
3:P:20:ARG:HD2	3:P:20:ARG:HA	0.41	1.58
2:B:6:DG:N7	3:P:20:ARG:CZ	0.40	2.84
3:P:25:PRO:C	3:P:27:ASN:N	0.40	2.74

*Continued on next page...*

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
3:P:36:TRP:CE3	3:P:36:TRP:HA	0.40	2.47
3:P:45:TRP:C	3:P:47:LYS:N	0.40	2.75
3:P:56:SER:HA	3:P:60:LYS:HG3	0.40	1.93
3:P:9:ASN:O	3:P:10:HIS:HD2	0.40	1.99

## 6.3 Torsion angles [i](#)

### 6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	P	63/65 (97%)	36 (57%)	16 (25%)	11 (17%)	0	3
All	All	63/65 (97%)	36 (57%)	16 (25%)	11 (17%)	0	3

All 11 Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
3	P	39	CYS
3	P	60	LYS
3	P	7	ARG
3	P	37	VAL
3	P	10	HIS
3	P	47	LYS
3	P	35	GLY
3	P	6	ARG
3	P	61	ASN
3	P	49	CYS
3	P	46	ASN

### 6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	P	59/59 (100%)	29 (49%)	30 (51%)	<b>0</b> <b>1</b>
All	All	59/59 (100%)	29 (49%)	30 (51%)	<b>0</b> <b>1</b>

All 30 residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
3	P	32	ASN
3	P	38	SER
3	P	20	ARG
3	P	62	SER
3	P	52	ASN
3	P	6	ARG
3	P	34	ASN
3	P	57	GLN
3	P	36	TRP
3	P	1	MET
3	P	13	ASP
3	P	5	ARG
3	P	21	ARG
3	P	12	CYS
3	P	17	LYS
3	P	29	ASN
3	P	4	THR
3	P	28	ARG
3	P	9	ASN
3	P	49	CYS
3	P	46	ASN
3	P	0	SER
3	P	7	ARG
3	P	44	ARG
3	P	42	CYS
3	P	8	GLN
3	P	58	ARG
3	P	61	ASN
3	P	27	ASN
3	P	3	ASP

### 6.3.3 RNA ⓘ

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 carbohydrates in this entry.

## 6.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

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

There are no chain breaks in this entry.

## 7 Chemical shift validation

No chemical shift data were provided