



Full wwPDB NMR Structure Validation Report ⓘ

Mar 1, 2026 – 08:39 AM UTC

PDB ID : 1F5E / pdb_00001f5e
Title : STRUCTURE OF TRANSCRIPTIONAL FACTOR ALCR IN COMPLEX
WITH A TARGET DNA
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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

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

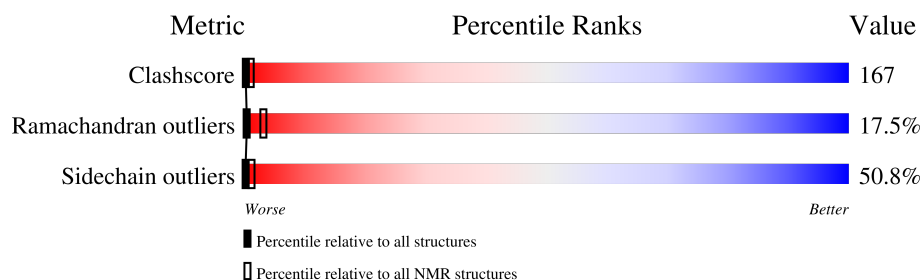
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment 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	10	 10% 10% 80%
2	B	10	 50% 50%
3	P	65	 . 25% 29% 45%

2 Ensemble composition and analysis ⓘ

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

3 Entry composition

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 mutation	UNP P21228
P	62	SER	LYS	engineered mutation	UNP P21228
P	63	SER	GLY	engineered mutation	UNP P21228

- Molecule 4 is ZINC ION (CCD ID: 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, 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: DNA (5'-D(P*CP*GP*TP*GP*CP*GP*GP*AP*TP*C)-3')

Chain A: 



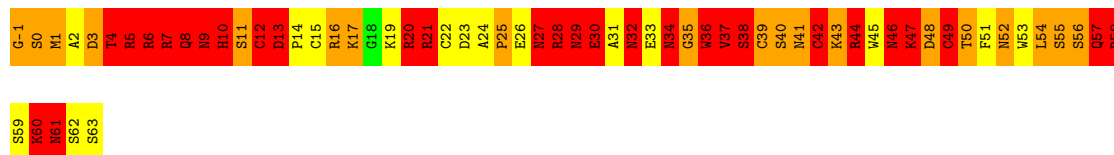
- Molecule 2: DNA (5'-D(P*GP*AP*TP*CP*CP*GP*CP*AP*CP*G)-3')

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.

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: 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	6.78	27/230 (11.7%)	2.91	18/353 (5.1%)
2	B	4.27	18/228 (7.9%)	1.70	9/349 (2.6%)
3	P	19.99	214/534 (40.1%)	8.97	165/712 (23.2%)
All	All	15.17	259/992 (26.1%)	6.59	192/1414 (13.6%)

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

Mol	Chain	Chirality	Planarity
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	1	MET	N-CA	-87.10	0.67	1.46
3	P	0	SER	CA-CB	-84.85	0.10	1.53
3	P	62	SER	CA-C	-82.45	0.51	1.52
3	P	61	ASN	C-O	-73.49	0.31	1.24
3	P	62	SER	C-O	-73.43	0.43	1.23
3	P	62	SER	CA-CB	-73.20	0.39	1.53
3	P	7	ARG	CZ-NH1	-68.25	0.37	1.32
3	P	0	SER	N-CA	-67.19	0.59	1.46
3	P	61	ASN	CA-CB	-64.25	0.44	1.53
3	P	0	SER	CA-C	-63.39	0.67	1.52
3	P	7	ARG	NE-CZ	-60.60	0.66	1.33
3	P	1	MET	SD-CE	-60.02	0.29	1.79
3	P	-1	GLY	N-CA	-59.71	0.50	1.45
3	P	63	SER	C-OXT	-55.84	0.11	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	13	ASP	CG-OD1	-53.27	0.24	1.25
3	P	-1	GLY	CA-C	-53.21	0.56	1.52
3	P	63	SER	CA-C	-52.31	0.43	1.52
3	P	33	GLU	CD-OE2	-51.53	0.27	1.25
3	P	62	SER	N-CA	-51.38	0.84	1.46
3	P	61	ASN	CA-C	-50.19	0.85	1.52
1	A	1	DC	P-OP1	-49.43	0.49	1.48
3	P	62	SER	CB-OG	-49.03	0.44	1.42
3	P	63	SER	N-CA	-48.98	0.53	1.46
3	P	63	SER	C-O	-48.24	0.27	1.23
3	P	1	MET	CA-C	-48.14	0.94	1.53
3	P	48	ASP	CG-OD2	-47.29	0.35	1.25
3	P	26	GLU	CD-OE1	-47.24	0.35	1.25
3	P	63	SER	CA-CB	-47.08	0.59	1.53
3	P	61	ASN	C-N	-46.10	0.74	1.33
3	P	2	ALA	N-CA	-45.66	0.91	1.46
3	P	59	SER	CA-CB	-45.55	0.84	1.54
3	P	48	ASP	CG-OD1	-45.53	0.38	1.25
3	P	-1	GLY	C-O	-45.28	0.33	1.23
3	P	0	SER	CB-OG	-44.95	0.52	1.42
3	P	56	SER	CB-OG	-44.94	0.52	1.42
3	P	40	SER	CB-OG	-44.62	0.53	1.42
3	P	61	ASN	CG-OD1	-42.97	0.41	1.23
1	A	10	DC	P-OP2	-42.53	0.63	1.48
3	P	2	ALA	C-N	-41.85	0.85	1.33
3	P	27	ASN	CG-ND2	-41.63	0.45	1.33
3	P	1	MET	CB-CG	-41.59	0.27	1.52
3	P	60	LYS	CA-C	-41.49	0.97	1.52
3	P	6	ARG	NE-CZ	-41.17	0.87	1.33
3	P	61	ASN	N-CA	-40.76	0.93	1.46
3	P	62	SER	C-N	-40.41	0.76	1.33
3	P	54	LEU	CB-CG	-40.27	0.72	1.53
3	P	60	LYS	C-O	-39.88	0.73	1.24
3	P	28	ARG	CZ-NH1	-39.83	0.77	1.32
3	P	1	MET	CG-SD	-39.76	0.81	1.80
3	P	3	ASP	CG-OD1	-39.53	0.50	1.25
3	P	63	SER	CB-OG	-38.80	0.64	1.42
3	P	0	SER	C-O	-38.79	0.75	1.24
3	P	3	ASP	CG-OD2	-38.64	0.52	1.25
2	B	1	DG	P-OP1	-38.17	0.72	1.48
3	P	13	ASP	CG-OD2	-37.90	0.53	1.25
3	P	4	THR	CB-OG1	-37.89	0.83	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	DC	P-OP2	-37.85	0.72	1.48
3	P	3	ASP	N-CA	-37.39	1.01	1.46
3	P	2	ALA	C-O	-37.24	0.80	1.24
3	P	2	ALA	CA-C	-36.86	1.06	1.52
3	P	33	GLU	CD-OE1	-36.68	0.55	1.25
3	P	61	ASN	CB-CG	-36.66	0.60	1.52
3	P	-1	GLY	C-N	-35.65	0.83	1.33
3	P	46	ASN	CB-CG	-35.63	0.62	1.52
3	P	20	ARG	NE-CZ	-35.14	0.94	1.33
3	P	59	SER	CA-C	-35.08	1.07	1.52
1	A	10	DC	P-OP1	-34.64	0.79	1.48
3	P	4	THR	C-O	-34.61	0.78	1.24
3	P	46	ASN	CG-OD1	-34.48	0.58	1.23
3	P	61	ASN	CG-ND2	-34.28	0.61	1.33
3	P	60	LYS	N-CA	-33.61	1.02	1.46
3	P	29	ASN	CG-OD1	-33.34	0.60	1.23
3	P	32	ASN	CG-OD1	-32.78	0.61	1.23
3	P	30	GLU	CD-OE2	-32.52	0.63	1.25
3	P	28	ARG	CZ-NH2	-32.32	0.91	1.33
3	P	17	LYS	CD-CE	-32.28	0.55	1.52
3	P	30	GLU	CD-OE1	-32.08	0.64	1.25
3	P	4	THR	CA-CB	-31.53	1.05	1.53
2	B	1	DG	P-OP2	-30.83	0.86	1.48
3	P	60	LYS	C-N	-30.71	0.90	1.33
3	P	44	ARG	NE-CZ	-30.43	0.99	1.33
3	P	10	HIS	CD2-NE2	-30.34	1.04	1.37
3	P	10	HIS	ND1-CE1	-30.05	1.02	1.32
3	P	27	ASN	CG-OD1	-29.98	0.66	1.23
3	P	7	ARG	CZ-NH2	-29.70	0.94	1.33
3	P	10	HIS	CB-CG	-29.43	1.08	1.50
3	P	4	THR	C-N	-29.36	0.99	1.33
3	P	60	LYS	CD-CE	-28.95	0.65	1.52
3	P	1	MET	CA-CB	-28.76	0.74	1.54
3	P	59	SER	CB-OG	-28.74	0.84	1.42
3	P	7	ARG	CD-NE	-28.68	1.06	1.46
1	A	10	DC	O5'-C5'	-28.43	0.57	1.42
3	P	28	ARG	CD-NE	-27.20	1.08	1.46
3	P	3	ASP	CB-CG	-27.09	0.84	1.52
3	P	1	MET	C-O	-26.98	0.94	1.24
3	P	38	SER	CB-OG	-25.99	0.90	1.42
3	P	43	LYS	CB-CG	-25.64	0.75	1.52
1	A	10	DC	P-O5'	-25.44	1.09	1.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	8	GLN	C-O	-25.24	0.92	1.24
3	P	4	THR	N-CA	-25.06	1.14	1.46
3	P	21	ARG	CZ-NH2	-24.55	1.01	1.33
3	P	7	ARG	CG-CD	-24.50	0.79	1.52
3	P	46	ASN	CG-ND2	-24.47	0.81	1.33
3	P	5	ARG	CG-CD	-24.45	0.79	1.52
3	P	32	ASN	CB-CG	-24.44	0.91	1.52
3	P	3	ASP	C-N	-24.11	1.00	1.33
3	P	26	GLU	CD-OE2	-24.09	0.79	1.25
3	P	3	ASP	CA-C	-24.05	1.19	1.52
3	P	21	ARG	CD-NE	-23.85	1.12	1.46
3	P	13	ASP	CB-CG	-23.71	0.92	1.52
3	P	7	ARG	CB-CG	-23.67	0.81	1.52
3	P	5	ARG	NE-CZ	-23.35	1.07	1.33
3	P	0	SER	C-N	-22.60	0.95	1.34
3	P	57	GLN	CD-OE1	-22.59	0.80	1.23
3	P	3	ASP	CA-CB	-22.59	1.18	1.52
3	P	3	ASP	C-O	-22.19	0.85	1.23
3	P	44	ARG	CZ-NH2	-22.02	1.04	1.33
3	P	60	LYS	CG-CD	-21.77	0.87	1.52
3	P	60	LYS	CE-NZ	-21.66	0.84	1.49
3	P	48	ASP	CB-CG	-21.65	0.97	1.52
3	P	7	ARG	CA-CB	-21.60	1.17	1.53
3	P	33	GLU	CG-CD	-20.70	1.00	1.52
3	P	42	CYS	CB-SG	-20.56	1.13	1.81
3	P	44	ARG	CD-NE	-20.28	1.17	1.46
3	P	1	MET	C-N	-20.28	1.07	1.33
3	P	8	GLN	CD-OE1	-19.98	0.85	1.23
3	P	28	ARG	NE-CZ	-19.53	1.11	1.33
3	P	54	LEU	CG-CD2	-19.17	0.89	1.52
3	P	17	LYS	CB-CG	-18.70	0.96	1.52
3	P	30	GLU	CB-CG	-17.46	1.00	1.52
3	P	27	ASN	CB-CG	-17.21	1.09	1.52
3	P	55	SER	CB-OG	-17.16	1.07	1.42
3	P	9	ASN	CG-OD1	-17.02	0.91	1.23
3	P	21	ARG	CB-CG	-16.79	1.02	1.52
3	P	36	TRP	NE1-CE2	-16.72	1.19	1.37
3	P	17	LYS	CG-CD	-16.63	1.02	1.52
3	P	20	ARG	CZ-NH1	-16.54	1.09	1.32
3	P	34	ASN	CB-CG	-16.34	1.11	1.52
3	P	58	ARG	C-O	-16.07	1.07	1.23
3	P	5	ARG	CZ-NH1	-15.82	1.10	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	34	ASN	CG-OD1	-15.76	0.93	1.23
3	P	12	CYS	CB-SG	-15.35	1.30	1.81
1	A	9	DT	O3'-P	-15.20	1.38	1.61
3	P	59	SER	C-N	-15.18	1.12	1.33
3	P	59	SER	C-O	-14.97	1.04	1.24
2	B	6	DG	O3'-P	-14.92	1.38	1.61
3	P	6	ARG	CZ-NH2	-14.91	1.14	1.33
3	P	43	LYS	CE-NZ	-14.80	1.04	1.49
3	P	54	LEU	CG-CD1	-14.65	1.04	1.52
3	P	60	LYS	CA-CB	-14.52	1.28	1.53
3	P	6	ARG	CG-CD	-14.39	1.09	1.52
3	P	60	LYS	CB-CG	-14.30	1.09	1.52
3	P	50	THR	CB-OG1	-14.26	1.21	1.43
3	P	25	PRO	C-O	-14.22	1.05	1.24
3	P	17	LYS	CE-NZ	-14.16	1.06	1.49
3	P	6	ARG	CZ-NH1	-14.04	1.13	1.32
2	B	7	DC	P-OP1	-14.01	1.20	1.48
3	P	6	ARG	CD-NE	-13.98	1.26	1.46
3	P	2	ALA	CA-CB	-13.94	1.31	1.53
3	P	10	HIS	CG-ND1	-13.94	1.23	1.38
1	A	6	DG	P-OP2	-13.06	1.22	1.48
3	P	47	LYS	CD-CE	-12.61	1.14	1.52
3	P	28	ARG	CB-CG	-12.57	1.14	1.52
3	P	10	HIS	CG-CD2	-12.34	1.22	1.35
1	A	6	DG	P-OP1	-12.32	1.23	1.48
2	B	7	DC	P-OP2	-12.18	1.24	1.48
2	B	1	DG	O3'-P	-12.09	1.43	1.61
3	P	5	ARG	CA-CB	-11.87	1.38	1.53
1	A	9	DT	C3'-O3'	-11.80	1.07	1.42
3	P	4	THR	CB-CG2	-11.77	1.13	1.52
3	P	26	GLU	CB-CG	-11.74	1.17	1.52
3	P	26	GLU	CG-CD	-11.71	1.22	1.52
3	P	29	ASN	CB-CG	-11.66	1.23	1.52
3	P	29	ASN	CG-ND2	-11.39	1.09	1.33
3	P	22	CYS	CA-CB	-11.37	1.35	1.53
2	B	1	DG	C3'-C2'	-11.31	1.30	1.52
1	A	10	DC	C4'-O4'	-11.24	1.23	1.45
3	P	21	ARG	NE-CZ	-11.16	1.20	1.33
3	P	25	PRO	C-N	-11.08	1.18	1.33
3	P	44	ARG	CB-CG	-10.74	1.20	1.52
3	P	36	TRP	CD2-CE3	-10.69	1.23	1.40
3	P	5	ARG	CZ-NH2	-10.07	1.20	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	11	SER	CB-OG	-9.91	1.22	1.42
3	P	57	GLN	CD-NE2	-9.88	1.12	1.33
3	P	16	ARG	CZ-NH1	-9.71	1.19	1.32
1	A	10	DC	C5'-C4'	-9.67	1.32	1.52
3	P	16	ARG	CG-CD	-9.54	1.23	1.52
3	P	58	ARG	CG-CD	-9.53	1.23	1.52
1	A	6	DG	O5'-C5'	-9.51	1.14	1.42
3	P	7	ARG	C-O	-9.50	1.12	1.24
3	P	5	ARG	CD-NE	-9.38	1.33	1.46
3	P	58	ARG	C-N	-9.24	1.20	1.33
3	P	43	LYS	CD-CE	-9.09	1.25	1.52
3	P	22	CYS	CB-SG	-9.06	1.51	1.81
3	P	4	THR	CA-C	-8.98	1.38	1.52
3	P	50	THR	CB-CG2	-8.92	1.23	1.52
3	P	7	ARG	C-N	-8.91	1.21	1.33
1	A	10	DC	C3'-O3'	-8.91	1.16	1.42
3	P	8	GLN	CD-NE2	-8.84	1.14	1.33
2	B	1	DG	C4'-C3'	-8.81	1.35	1.52
3	P	5	ARG	N-CA	-8.74	1.32	1.46
3	P	6	ARG	C-O	-8.70	1.13	1.24
3	P	6	ARG	C-N	-8.45	1.21	1.33
1	A	9	DT	C4'-C3'	-8.40	1.35	1.52
3	P	7	ARG	CA-C	-8.34	1.41	1.52
3	P	44	ARG	CZ-NH1	-8.30	1.21	1.32
3	P	58	ARG	CZ-NH2	-8.24	1.22	1.33
3	P	9	ASN	CB-CG	-8.15	1.31	1.52
3	P	47	LYS	CE-NZ	-8.03	1.25	1.49
2	B	1	DG	O4'-C1'	-8.00	1.25	1.41
3	P	36	TRP	CZ2-CH2	-7.74	1.22	1.37
1	A	6	DG	P-O5'	-7.67	1.45	1.60
1	A	2	DG	O3'-P	-7.63	1.49	1.61
1	A	3	DT	P-OP2	-7.51	1.33	1.48
3	P	8	GLN	C-N	-7.50	1.16	1.33
3	P	8	GLN	CG-CD	-7.36	1.33	1.52
3	P	8	GLN	CB-CG	-7.35	1.30	1.52
3	P	6	ARG	CB-CG	-7.27	1.30	1.52
2	B	2	DA	P-OP1	-7.17	1.34	1.48
1	A	2	DG	C3'-C2'	-7.16	1.38	1.52
1	A	10	DC	C3'-C2'	-7.05	1.38	1.52
3	P	21	ARG	CZ-NH1	-7.05	1.22	1.32
1	A	3	DT	P-OP1	-7.04	1.34	1.48
2	B	5	DC	C3'-C2'	-6.95	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	8	GLN	N-CA	-6.88	1.37	1.46
3	P	36	TRP	CG-CD2	-6.79	1.31	1.43
3	P	7	ARG	N-CA	-6.66	1.37	1.46
3	P	28	ARG	CG-CD	-6.59	1.32	1.52
3	P	16	ARG	NE-CZ	-6.53	1.25	1.33
3	P	58	ARG	CA-C	-6.49	1.46	1.53
2	B	7	DC	P-O5'	-6.47	1.47	1.60
1	A	3	DT	P-O5'	-6.42	1.47	1.60
3	P	6	ARG	N-CA	-6.35	1.38	1.46
3	P	5	ARG	CA-C	-6.32	1.45	1.52
2	B	1	DG	C4'-O4'	-6.31	1.32	1.45
1	A	10	DC	C2'-C1'	-6.27	1.40	1.52
3	P	16	ARG	CB-CG	-6.23	1.33	1.52
3	P	5	ARG	C-O	-5.98	1.17	1.23
1	A	7	DG	P-O5'	-5.93	1.48	1.60
3	P	20	ARG	CZ-NH2	-5.91	1.25	1.33
2	B	1	DG	C5'-C4'	-5.89	1.40	1.52
2	B	7	DC	C5'-C4'	-5.78	1.40	1.52
2	B	1	DG	C2'-C1'	-5.78	1.41	1.52
2	B	7	DC	O4'-C1'	-5.77	1.30	1.41
3	P	33	GLU	CB-CG	-5.72	1.35	1.52
3	P	58	ARG	CD-NE	-5.65	1.38	1.46
3	P	5	ARG	CB-CG	-5.65	1.35	1.52
1	A	9	DT	C5'-C4'	-5.55	1.41	1.52
1	A	7	DG	P-OP1	-5.53	1.37	1.48
3	P	58	ARG	CZ-NH1	-5.46	1.25	1.32
3	P	58	ARG	NE-CZ	-5.44	1.27	1.33
3	P	57	GLN	C-O	-5.28	1.17	1.24
1	A	7	DG	P-OP2	-5.25	1.38	1.48
3	P	21	ARG	CG-CD	-5.20	1.36	1.52
3	P	44	ARG	CG-CD	-5.20	1.36	1.52
3	P	43	LYS	CG-CD	-5.18	1.36	1.52
3	P	6	ARG	CA-CB	-5.12	1.44	1.53
3	P	41	ASN	CG-OD1	-5.11	1.13	1.23
2	B	6	DG	P-O5'	-5.04	1.50	1.60

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	-75.96	45.54	121.50
3	P	-1	GLY	CA-C-O	-51.18	13.33	120.80
3	P	62	SER	CA-C-O	-51.15	66.58	121.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	7	ARG	NE-CZ-NH2	49.66	163.90	119.20
3	P	27	ASN	OD1-CG-ND2	-46.77	75.83	122.60
3	P	48	ASP	OD1-CG-OD2	-45.99	12.52	122.90
3	P	3	ASP	CA-CB-CG	35.76	148.36	112.60
3	P	32	ASN	CB-CG-OD1	-33.59	53.62	120.80
3	P	1	MET	CA-CB-CG	-33.45	47.20	114.10
3	P	61	ASN	CA-CB-CG	32.72	145.32	112.60
3	P	-1	GLY	O-C-N	30.96	172.53	123.00
3	P	62	SER	N-CA-C	29.77	148.56	108.38
3	P	33	GLU	OE1-CD-OE2	-29.13	52.98	122.90
3	P	0	SER	N-CA-C	28.98	172.52	110.80
3	P	13	ASP	OD1-CG-OD2	-28.97	53.37	122.90
3	P	7	ARG	CD-NE-CZ	28.34	164.07	124.40
3	P	32	ASN	OD1-CG-ND2	28.25	150.85	122.60
3	P	-1	GLY	CA-C-N	27.93	174.89	121.54
3	P	-1	GLY	C-N-CA	27.93	174.89	121.54
1	A	9	DT	O3'-P-O5'	26.86	144.29	104.00
3	P	46	ASN	CA-CB-CG	26.77	139.37	112.60
3	P	32	ASN	CB-CG-ND2	26.09	155.53	116.40
3	P	30	GLU	OE1-CD-OE2	-24.78	63.43	122.90
3	P	48	ASP	CB-CG-OD1	24.22	174.10	118.40
3	P	7	ARG	CG-CD-NE	24.21	165.27	112.00
3	P	62	SER	O-C-N	24.09	148.77	122.99
3	P	7	ARG	NH1-CZ-NH2	24.05	150.57	119.30
3	P	32	ASN	CA-CB-CG	23.99	136.59	112.60
3	P	48	ASP	CB-CG-OD2	23.91	173.38	118.40
3	P	62	SER	CB-CA-C	-23.84	62.81	111.91
3	P	0	SER	CB-CA-C	-23.55	63.57	110.42
3	P	5	ARG	CG-CD-NE	23.33	163.33	112.00
3	P	43	LYS	CA-CB-CG	20.96	156.03	114.10
3	P	40	SER	CA-CB-OG	20.21	151.52	111.10
3	P	56	SER	CA-CB-OG	19.97	151.05	111.10
3	P	13	ASP	CB-CG-OD2	19.89	164.15	118.40
3	P	61	ASN	CA-C-N	19.71	154.82	122.10
3	P	61	ASN	C-N-CA	19.71	154.82	122.10
3	P	33	GLU	CG-CD-OE1	19.49	163.23	118.40
3	P	29	ASN	CB-CG-ND2	19.15	145.12	116.40
3	P	30	GLU	CB-CG-CD	18.38	143.84	112.60
3	P	60	LYS	CG-CD-CE	-18.22	69.38	111.30
1	A	1	DC	OP1-P-OP2	-18.09	65.72	120.00
3	P	28	ARG	NE-CZ-NH2	17.66	135.09	119.20
3	P	26	GLU	OE1-CD-OE2	-17.59	80.68	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	57	GLN	OE1-CD-NE2	-17.36	105.24	122.60
3	P	26	GLU	CG-CD-OE2	17.08	157.68	118.40
3	P	20	ARG	NE-CZ-NH1	-17.07	104.43	121.50
3	P	-1	GLY	N-CA-C	16.94	162.44	113.30
1	A	10	DC	O5'-P-OP1	-16.88	58.37	109.00
3	P	59	SER	N-CA-C	16.69	135.42	113.72
2	B	1	DG	OP1-P-OP2	-16.45	70.66	120.00
3	P	3	ASP	N-CA-CB	-16.29	88.10	110.42
3	P	28	ARG	NH1-CZ-NH2	-16.17	98.28	119.30
3	P	46	ASN	OD1-CG-ND2	16.09	138.69	122.60
3	P	0	SER	CA-C-O	-15.63	98.16	120.51
3	P	0	SER	O-C-N	15.54	143.26	122.59
3	P	27	ASN	CB-CG-OD1	15.47	151.74	120.80
3	P	62	SER	CA-C-N	15.43	149.47	121.70
3	P	62	SER	C-N-CA	15.43	149.47	121.70
3	P	61	ASN	N-CA-C	15.31	143.42	110.80
3	P	1	MET	CG-SD-CE	-15.09	67.70	100.90
3	P	4	THR	O-C-N	-14.97	103.20	122.37
3	P	46	ASN	CB-CG-OD1	-14.95	90.90	120.80
3	P	5	ARG	CB-CG-CD	14.63	144.96	111.30
3	P	10	HIS	ND1-CG-CD2	14.63	120.73	106.10
3	P	21	ARG	CB-CG-CD	14.55	144.77	111.30
1	A	1	DC	O5'-P-OP2	14.50	151.50	108.00
3	P	61	ASN	CA-C-O	-14.37	99.95	120.51
3	P	13	ASP	CA-CB-CG	14.16	126.76	112.60
3	P	54	LEU	CD1-CG-CD2	-14.06	79.88	110.80
1	A	10	DC	P-O5'-C5'	13.99	140.99	120.00
3	P	44	ARG	NE-CZ-NH2	-13.99	106.61	119.20
3	P	59	SER	CA-CB-OG	13.98	139.06	111.10
3	P	57	GLN	CG-CD-NE2	13.86	137.19	116.40
3	P	62	SER	N-CA-CB	13.63	132.77	111.24
3	P	27	ASN	CA-CB-CG	13.20	125.80	112.60
3	P	30	GLU	CG-CD-OE1	13.09	148.51	118.40
3	P	28	ARG	CG-CD-NE	13.04	140.68	112.00
3	P	17	LYS	CG-CD-CE	12.93	141.04	111.30
3	P	63	SER	CA-C-O	12.91	159.74	121.00
3	P	30	GLU	CG-CD-OE2	12.89	148.06	118.40
1	A	9	DT	OP2-P-O3'	-12.76	69.72	108.00
3	P	34	ASN	CA-CB-CG	12.74	125.34	112.60
3	P	7	ARG	CA-CB-CG	-12.62	88.86	114.10
3	P	63	SER	CB-CA-C	-12.57	86.22	110.10
3	P	1	MET	O-C-N	12.10	135.97	122.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	60	LYS	CD-CE-NZ	-12.04	73.36	111.90
3	P	6	ARG	NH1-CZ-NH2	11.97	134.86	119.30
3	P	29	ASN	OD1-CG-ND2	-11.97	110.63	122.60
3	P	61	ASN	CB-CG-ND2	11.90	134.25	116.40
3	P	44	ARG	CD-NE-CZ	-11.78	107.90	124.40
3	P	59	SER	CB-CA-C	-11.74	89.83	109.55
3	P	61	ASN	O-C-N	-11.38	107.45	122.59
3	P	22	CYS	CA-CB-SG	11.16	140.06	114.40
1	A	1	DC	O5'-P-OP1	11.13	142.39	109.00
3	P	33	GLU	CG-CD-OE2	11.04	143.79	118.40
2	B	1	DG	O5'-P-OP1	11.02	142.06	109.00
3	P	34	ASN	CB-CG-OD1	-10.98	98.83	120.80
3	P	4	THR	N-CA-C	10.86	125.10	112.93
3	P	8	GLN	CG-CD-NE2	10.86	132.69	116.40
3	P	10	HIS	CA-CB-CG	10.80	124.60	113.80
3	P	20	ARG	NH1-CZ-NH2	10.80	133.34	119.30
3	P	9	ASN	CB-CG-ND2	10.78	132.56	116.40
3	P	27	ASN	CB-CG-ND2	10.68	132.42	116.40
3	P	13	ASP	CB-CG-OD1	10.47	142.47	118.40
3	P	3	ASP	CB-CA-C	10.18	124.53	111.40
3	P	33	GLU	CB-CG-CD	10.17	129.88	112.60
3	P	61	ASN	CB-CA-C	-10.16	90.21	110.42
3	P	63	SER	N-CA-C	9.94	138.84	111.00
3	P	10	HIS	CG-CD2-NE2	-9.94	97.27	107.20
3	P	43	LYS	CD-CE-NZ	9.88	143.51	111.90
3	P	34	ASN	OD1-CG-ND2	9.83	132.43	122.60
3	P	60	LYS	CB-CG-CD	-9.64	89.14	111.30
1	A	9	DT	OP1-P-O3'	9.63	136.89	108.00
3	P	6	ARG	NE-CZ-NH1	-9.55	111.94	121.50
3	P	61	ASN	CB-CG-OD1	-9.49	101.82	120.80
3	P	1	MET	N-CA-CB	9.42	131.55	111.10
3	P	1	MET	CB-CG-SD	-9.40	84.50	112.70
3	P	46	ASN	CB-CG-ND2	9.34	130.41	116.40
3	P	8	GLN	OE1-CD-NE2	-9.16	113.44	122.60
1	A	10	DC	C5'-C4'-C3'	9.15	128.63	114.90
3	P	47	LYS	CG-CD-CE	9.09	132.20	111.30
3	P	8	GLN	O-C-N	-8.95	110.68	122.59
3	P	5	ARG	NE-CZ-NH1	-8.89	112.61	121.50
3	P	21	ARG	NE-CZ-NH1	8.82	130.32	121.50
3	P	44	ARG	CB-CG-CD	8.82	131.58	111.30
3	P	10	HIS	CG-ND1-CE1	-8.80	94.33	109.30
3	P	63	SER	CA-CB-OG	-8.65	93.81	111.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	4	THR	N-CA-CB	-8.62	98.67	110.56
3	P	59	SER	O-C-N	8.56	132.88	122.35
3	P	63	SER	N-CA-CB	8.54	125.02	110.50
3	P	10	HIS	ND1-CE1-NE2	8.51	116.91	108.40
3	P	3	ASP	N-CA-C	8.33	122.97	111.55
3	P	28	ARG	CB-CG-CD	8.31	130.41	111.30
3	P	4	THR	CA-C-N	8.28	136.45	122.20
3	P	4	THR	C-N-CA	8.28	136.45	122.20
3	P	29	ASN	CB-CG-OD1	-8.28	104.25	120.80
1	A	10	DC	C4'-C3'-C2'	8.22	114.74	102.40
3	P	34	ASN	CB-CG-ND2	8.22	128.73	116.40
3	P	22	CYS	N-CA-C	8.19	119.44	108.38
1	A	9	DT	P-O3'-C3'	8.18	132.47	120.20
3	P	7	ARG	N-CA-C	8.18	128.22	110.80
3	P	3	ASP	OD1-CG-OD2	-8.12	103.42	122.90
3	P	1	MET	CB-CA-C	-8.05	87.84	110.14
1	A	9	DT	C4'-C3'-C2'	7.94	114.31	102.40
3	P	0	SER	N-CA-CB	7.85	123.76	110.49
3	P	7	ARG	CB-CG-CD	-7.52	94.01	111.30
3	P	42	CYS	CA-CB-SG	7.42	131.46	114.40
3	P	6	ARG	CD-NE-CZ	-7.39	114.05	124.40
3	P	5	ARG	CA-CB-CG	7.37	128.84	114.10
3	P	9	ASN	CB-CG-OD1	-7.36	106.08	120.80
3	P	8	GLN	CA-C-N	7.31	132.61	120.70
3	P	8	GLN	C-N-CA	7.31	132.61	120.70
3	P	1	MET	CA-C-O	-7.28	111.44	119.08
3	P	44	ARG	CG-CD-NE	7.27	127.99	112.00
3	P	44	ARG	NH1-CZ-NH2	7.14	128.58	119.30
3	P	43	LYS	CB-CG-CD	-6.99	95.23	111.30
3	P	21	ARG	NE-CZ-NH2	-6.98	112.92	119.20
3	P	2	ALA	N-CA-C	-6.96	102.26	111.24
3	P	60	LYS	CA-CB-CG	-6.90	100.30	114.10
1	A	10	DC	O5'-P-OP2	6.89	128.66	108.00
2	B	5	DC	P-O3'-C3'	6.88	130.52	120.20
2	B	1	DG	C3'-C2'-C1'	6.84	111.86	101.60
1	A	10	DC	O4'-C4'-C3'	-6.73	95.31	105.40
1	A	10	DC	C1'-O4'-C4'	6.72	119.78	109.70
3	P	6	ARG	NE-CZ-NH2	-6.68	113.19	119.20
3	P	21	ARG	CD-NE-CZ	-6.63	115.11	124.40
3	P	10	HIS	CB-CG-ND1	-6.62	112.77	122.70
2	B	5	DC	C3'-C2'-C1'	6.50	111.34	101.60
3	P	28	ARG	CD-NE-CZ	6.45	133.43	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	6	DG	O3'-P-O5'	6.41	113.61	104.00
1	A	5	DC	O3'-P-O5'	6.36	113.54	104.00
1	A	2	DG	P-O3'-C3'	6.24	129.56	120.20
3	P	36	TRP	CG-CD2-CE3	-6.16	127.74	133.90
3	P	12	CYS	CA-CB-SG	6.04	128.30	114.40
1	A	10	DC	O5'-C5'-C4'	5.75	119.42	110.80
3	P	25	PRO	O-C-N	-5.68	114.97	122.64
3	P	41	ASN	OD1-CG-ND2	-5.60	117.00	122.60
2	B	1	DG	P-O3'-C3'	5.50	128.45	120.20
3	P	50	THR	CA-CB-OG1	5.40	117.70	109.60
3	P	48	ASP	CA-CB-CG	5.33	117.93	112.60
3	P	26	GLU	CB-CG-CD	5.31	121.63	112.60
3	P	36	TRP	CD2-CE2-CZ2	5.30	127.70	122.40
3	P	30	GLU	CA-CB-CG	5.19	124.48	114.10
3	P	36	TRP	CE2-CD2-CG	5.19	113.43	107.20
3	P	17	LYS	CB-CG-CD	5.16	123.16	111.30
2	B	1	DG	O5'-C5'-C4'	5.14	118.51	110.80
3	P	16	ARG	CB-CG-CD	5.14	123.12	111.30
3	P	28	ARG	NE-CZ-NH1	5.13	126.63	121.50
2	B	1	DG	O5'-P-OP2	5.02	123.06	108.00
3	P	5	ARG	NH1-CZ-NH2	5.00	125.80	119.30

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

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	468	238
5	B	1	2	0	3
All	All	938	710	693	272

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 167.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)
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:3:ASP:CG	3:P:3:ASP:CA	1.37	1.95
3:P:13:ASP:HB2	3:P:53:TRP:CH2	1.35	1.56
3:P:5:ARG:CD	3:P:5:ARG:CB	1.32	2.05
3:P:46:ASN:CG	3:P:46:ASN:CA	1.29	2.04
2:B:2:DA:N3	3:P:6:ARG:NH2	1.25	1.81
3:P:55:SER:O	3:P:60:LYS:HG3	1.25	1.17
3:P:42:CYS:CB	3:P:42:CYS:SG	1.22	1.13
3:P:13:ASP:CG	3:P:13:ASP:CA	1.14	2.20
3:P:5:ARG:CG	3:P:5:ARG:NE	1.13	2.09
1:A:1:DC:OP2	1:A:1:DC:P	1.12	0.72
3:P:56:SER:OG	3:P:56:SER:CA	1.11	1.98
3:P:13:ASP:CB	3:P:53:TRP:HZ2	1.11	1.40
3:P:40:SER:OG	3:P:40:SER:CA	1.11	1.99
3:P:13:ASP:CG	3:P:53:TRP:CH2	1.11	2.28
3:P:13:ASP:CG	3:P:53:TRP:CZ2	1.10	2.29
3:P:32:ASN:OD1	3:P:32:ASN:ND2	1.10	1.84
3:P:32:ASN:CG	3:P:32:ASN:CA	1.09	2.25
2:B:1:DG:OP1	2:B:1:DG:P	1.09	0.72
3:P:32:ASN:ND2	3:P:32:ASN:CB	1.09	2.14
3:P:30:GLU:OE1	3:P:30:GLU:CG	1.08	2.02
3:P:20:ARG:HG3	3:P:20:ARG:NH1	1.08	1.61
3:P:30:GLU:CG	3:P:30:GLU:OE2	1.07	2.01
3:P:42:CYS:SG	3:P:42:CYS:CA	1.07	2.42
3:P:11:SER:O	3:P:16:ARG:NH1	1.06	1.87
2:B:1:DG:P	2:B:1:DG:OP2	1.05	0.86
3:P:55:SER:O	3:P:60:LYS:CG	1.04	2.06
3:P:3:ASP:CG	3:P:3:ASP:N	1.03	2.16
3:P:32:ASN:OD1	3:P:32:ASN:CB	1.03	0.73
3:P:32:ASN:OD1	3:P:32:ASN:HB3	1.03	1.47

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
3:P:13:ASP:HB2	3:P:13:ASP:CG	1.02	1.51
3:P:13:ASP:CG	3:P:13:ASP:HB3	1.01	1.51
3:P:42:CYS:SG	3:P:42:CYS:HB2	1.01	1.66
3:P:42:CYS:SG	3:P:42:CYS:HB3	0.99	1.66
3:P:13:ASP:CB	3:P:53:TRP:CH2	0.99	2.32
3:P:32:ASN:OD1	3:P:32:ASN:CA	0.98	2.11
2:B:3:DT:OP2	3:P:16:ARG:CZ	0.98	2.11
3:P:13:ASP:CB	3:P:13:ASP:CG	0.97	0.92
3:P:32:ASN:CG	3:P:32:ASN:CB	0.95	0.91
3:P:32:ASN:CG	3:P:32:ASN:HB3	0.95	1.46
3:P:32:ASN:CG	3:P:32:ASN:HB2	0.95	1.47
3:P:56:SER:OG	3:P:56:SER:HB2	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
3:P:20:ARG:CG	3:P:20:ARG:HH11	0.91	1.51
3:P:56:SER:OG	3:P:56:SER:HB3	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:P	1:A:1:DC:OP1	0.89	0.49
3:P:30:GLU:OE1	3:P:30:GLU:CD	0.89	0.64
3:P:3:ASP:CG	3:P:3:ASP:HB3	0.88	1.38
3:P:30:GLU:OE2	3:P:30:GLU:CD	0.88	0.63
3:P:3:ASP:CG	3:P:3:ASP:HB2	0.88	1.38
3:P:36:TRP:CE3	3:P:37:VAL:HG12	0.87	2.05
3:P:27:ASN:OD1	3:P:27:ASN:CG	0.87	0.66
1:A:1:DC:OP1	1:A:1:DC:O5'	0.85	1.94
3:P:32:ASN:OD1	3:P:32:ASN:CG	0.85	0.61
3:P:3:ASP:CG	3:P:3:ASP:CB	0.85	0.84
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
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:40:SER:OG	3:P:40:SER:CB	0.82	0.52
3:P:56:SER:OG	3:P:56:SER:CB	0.82	0.52
2:B:3:DT:P	3:P:16:ARG:HH21	0.82	1.97
1:A:2:DG:C5'	3:P:44:ARG:O	0.81	2.29
3:P:5:ARG:CD	3:P:5:ARG:HG3	0.81	1.35
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:42:CYS:CB	3:P:42:CYS:HG	0.78	1.90
3:P:5:ARG:CD	3:P:5:ARG:CG	0.78	0.79
3:P:46:ASN:CG	3:P:46:ASN:HB3	0.78	1.26

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
2:B:4:DC:N4	2:B:5:DC:N4	0.77	2.33
3:P:46:ASN:CG	3:P:46:ASN:HB2	0.77	1.26
3:P:46:ASN:CG	3:P:46:ASN:HD22	0.77	1.45
3:P:5:ARG:CG	3:P:5:ARG:HD2	0.77	1.30
2:B:6:DG:N7	3:P:20:ARG:NH2	0.76	2.33
3:P:13:ASP:HB3	3:P:53:TRP:HZ2	0.76	1.35
3:P:28:ARG:HH21	3:P:50:THR:HA	0.76	1.40
3:P:13:ASP:HB3	3:P:53:TRP:CZ2	0.76	2.12
3:P:46:ASN:CG	3:P:46:ASN:HD21	0.76	1.45
2:B:3:DT:P	3:P:16:ARG:NH2	0.75	2.58
3:P:5:ARG:CG	3:P:5:ARG:HD3	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
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:20:ARG:HB3	3:P:41:ASN:OD1	0.71	1.85
3:P:46:ASN:CG	3:P:46:ASN:ND2	0.71	0.81
2:B:7:DC:H2''	2:B:8:DA:C8	0.70	2.21
3:P:4:THR:O	3:P:4:THR:HG23	0.70	1.65
3:P:36:TRP:CG	3:P:37:VAL:H	0.69	2.05
3:P:13:ASP:CG	3:P:53:TRP:HH2	0.69	1.94
1:A:1:DC:OP2	1:A:1:DC:OP1	0.69	0.69
1:A:4:DG:N7	3:P:45:TRP:CZ2	0.69	2.60
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:56:SER:HA	3:P:60:LYS:HB2	0.67	1.65
3:P:46:ASN:CG	3:P:46:ASN:CB	0.67	0.63
3:P:-1:GLY:N	3:P:-1:GLY:HA3	0.67	1.13
3:P:30:GLU:OE1	3:P:30:GLU:OE2	0.66	0.67
3:P:-1:GLY:C	3:P:-1:GLY:HA2	0.66	1.16
3:P:-1:GLY:HA3	3:P:-1:GLY:C	0.66	1.16
3:P:9:ASN:C	3:P:10:HIS:CD2	0.66	2.73
3:P:32:ASN:OD1	3:P:32:ASN:HB2	0.66	0.89
3:P:28:ARG:O	3:P:31:ALA:HB3	0.65	1.91
3:P:53:TRP:N	3:P:53:TRP:CD1	0.65	2.63
3:P:36:TRP:CE3	3:P:36:TRP:C	0.65	2.74
3:P:44:ARG:HG2	3:P:44:ARG:HH11	0.65	1.48

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
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:36:TRP:C	3:P:37:VAL:HG12	0.64	2.16
3:P:52:ASN:C	3:P:54:LEU:N	0.64	2.50
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:NH1	3:P:20:ARG:CG	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:13:ASP:CG	3:P:13:ASP:C	0.63	2.66
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:45:TRP:O	3:P:46:ASN:C	0.62	2.43
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
2:B:5:DC:N4	3:P:19:LYS:O	0.61	2.33
3:P:6:ARG:O	3:P:7:ARG:CB	0.61	2.36
3:P:13:ASP:N	3:P:14:PRO:HD2	0.61	2.10
3:P:5:ARG:HG2	3:P:5:ARG:HD3	0.61	1.12
3:P:36:TRP:CE3	3:P:36:TRP:CA	0.61	2.84
3:P:31:ALA:O	3:P:35:GLY:N	0.60	2.34
3:P:28:ARG:HD3	3:P:51:PHE:CD1	0.60	2.31
3:P:36:TRP:CG	3:P:37:VAL:N	0.60	2.64
1:A:4:DG:N7	3:P:45:TRP:CH2	0.60	2.70
3:P:52:ASN:O	3:P:55:SER:N	0.59	2.35
3:P:15:CYS:SG	3:P:41:ASN:CG	0.59	2.85
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
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
3:P:-1:GLY:N	3:P:-1:GLY:HA2	0.57	1.13
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:52:ASN:O	3:P:53:TRP:C	0.56	2.45
3:P:36:TRP:CD2	3:P:37:VAL:N	0.56	2.73

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
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:31:ALA:CB	3:P:36:TRP:HB2	0.54	2.32
2:B:1:DG:P	2:B:1:DG:C8	0.54	3.01
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:N	3:P:52:ASN:ND2	0.52	2.57
3:P:13:ASP:N	3:P:14:PRO:CD	0.52	2.72
3:P:23:ASP:O	3:P:24:ALA:C	0.52	2.52
3:P:41:ASN:C	3:P:43:LYS:N	0.52	2.65
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:42:CYS:SG	3:P:42:CYS:N	0.51	2.83
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:54:LEU:C	3:P:56:SER:N	0.50	2.64
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
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:53:TRP:CD1	3:P:53:TRP:H	0.48	2.25
3:P:36:TRP:CA	3:P:36:TRP:HE3	0.48	2.21
3:P:4:THR:C	3:P:5:ARG:HG2	0.48	2.31
3:P:36:TRP:O	3:P:37:VAL:HB	0.48	2.08

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
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
3:P:41:ASN:O	3:P:42:CYS:C	0.47	2.53
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:51:PHE:HA	3:P:54:LEU:HD12	0.47	1.85
3:P:54:LEU:O	3:P:55:SER:C	0.47	2.56
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:20:ARG:HB3	3:P:41:ASN:CG	0.47	2.35
2:B:8:DA:C4	2:B:9:DC:C4	0.47	3.02
3:P:37:VAL:HG13	3:P:38:SER:N	0.47	2.22
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:11:SER:HB3	3:P:15:CYS:CB	0.46	2.41
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
3:P:-1:GLY:CA	3:P:-1:GLY:H3	0.45	1.15
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:-1:GLY:CA	3:P:-1:GLY:H1	0.45	1.15
3:P:29:ASN:HA	3:P:32:ASN:ND2	0.45	2.26
3:P:52:ASN:C	3:P:54:LEU:H	0.45	2.19
2:B:3:DT:H5''	3:P:10:HIS:HA	0.45	1.88
1:A:6:DG:H2''	1:A:7:DG:OP2	0.45	2.05
3:P:45:TRP:C	3:P:47:LYS:N	0.45	2.75
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
1:A:9:DT:C2	1:A:10:DC:C4	0.44	3.05
3:P:42:CYS:O	3:P:46:ASN:CA	0.44	2.66
3:P:-1:GLY:CA	3:P:-1:GLY:H2	0.44	1.15
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:3:DT:OP1	3:P:10:HIS:HB3	0.43	2.13

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
2:B:4:DC:H5''	3:P:8:GLN:HE21	0.43	1.72
3:P:36:TRP:O	3:P:37:VAL:HG12	0.43	2.12
3:P:36:TRP:C	3:P:37:VAL:CG1	0.43	2.84
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
3:P:12:CYS:C	3:P:14:PRO:HD2	0.43	2.38
1:A:3:DT:H6	3:P:45:TRP:NE1	0.43	2.11
3:P:48:ASP:O	3:P:49:CYS:C	0.43	2.61
2:B:6:DG:O6	3:P:20:ARG:NE	0.42	2.52
3:P:40:SER:CB	3:P:40:SER:HG	0.42	1.13
1:A:9:DT:C2'	1:A:10:DC:C5	0.42	3.03
3:P:56:SER:CB	3:P:56:SER:HG	0.42	1.13
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
3:P:25:PRO:C	3:P:27:ASN:H	0.42	2.21
3:P:50:THR:C	3:P:51:PHE:HD1	0.42	2.23
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:32:ASN:CG	3:P:32:ASN:N	0.41	2.78
3:P:20:ARG:HD2	3:P:20:ARG:HA	0.41	1.58
3:P:36:TRP:O	3:P:37:VAL:CG1	0.41	2.69
3:P:25:PRO:C	3:P:27:ASN:N	0.40	2.74
2:B:6:DG:N7	3:P:20:ARG:CZ	0.40	2.84
3:P:36:TRP:CE3	3:P:36:TRP:HA	0.40	2.47
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 ⓘ

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
3	P	63/65 (97%)	36 (57%)	16 (25%)	11 (17%)	0 3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
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	6	ARG
3	P	7	ARG
3	P	10	HIS
3	P	35	GLY
3	P	37	VAL
3	P	39	CYS
3	P	46	ASN
3	P	47	LYS
3	P	49	CYS
3	P	60	LYS
3	P	61	ASN

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
3	P	59/59 (100%)	29 (49%)	30 (51%)	0 1
All	All	59/59 (100%)	29 (49%)	30 (51%)	0 1

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	0	SER
3	P	1	MET
3	P	4	THR
3	P	5	ARG
3	P	6	ARG
3	P	8	GLN
3	P	9	ASN
3	P	12	CYS

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Mol	Chain	Res	Type
3	P	13	ASP
3	P	17	LYS
3	P	20	ARG
3	P	21	ARG
3	P	27	ASN
3	P	28	ARG
3	P	29	ASN
3	P	30	GLU
3	P	32	ASN
3	P	34	ASN
3	P	36	TRP
3	P	37	VAL
3	P	38	SER
3	P	42	CYS
3	P	44	ARG
3	P	46	ASN
3	P	49	CYS
3	P	52	ASN
3	P	57	GLN
3	P	58	ARG
3	P	60	LYS
3	P	61	ASN

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](#)

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	P	13
1	A	1
2	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	9:DT	O3'	10:DC	P	1.38
1	B	6:DG	O3'	7:DC	P	1.38
1	P	58:ARG	C	59:SER	N	1.20
1	P	25:PRO	C	26:GLU	N	1.18
1	P	8:GLN	C	9:ASN	N	1.16
1	P	59:SER	C	60:LYS	N	1.12
1	P	1:MET	C	2:ALA	N	1.07
1	P	3:ASP	C	4:THR	N	1.00
1	P	4:THR	C	5:ARG	N	0.99
1	P	0:SER	C	1:MET	N	0.95
1	P	60:LYS	C	61:ASN	N	0.90
1	P	2:ALA	C	3:ASP	N	0.85
1	P	-1:GLY	C	0:SER	N	0.83
1	P	62:SER	C	63:SER	N	0.76
1	P	61:ASN	C	62:SER	N	0.74

7 Chemical shift validation

No chemical shift data were provided