



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:32 AM UTC

PDB ID : 1IGN / pdb\_00001ign  
Title : DNA-BINDING DOMAIN OF RAP1 IN COMPLEX WITH TELOMERIC DNA SITE  
Authors : Koenig, P.; Giraldo, R.; Chapman, L.; Rhodes, D.  
Deposited on : 1996-02-29  
Resolution : 2.25 Å(reported)

This is a Full wwPDB X-ray 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

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

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>.

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

MolProbity : 4-5-2 with Phenix2.0  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

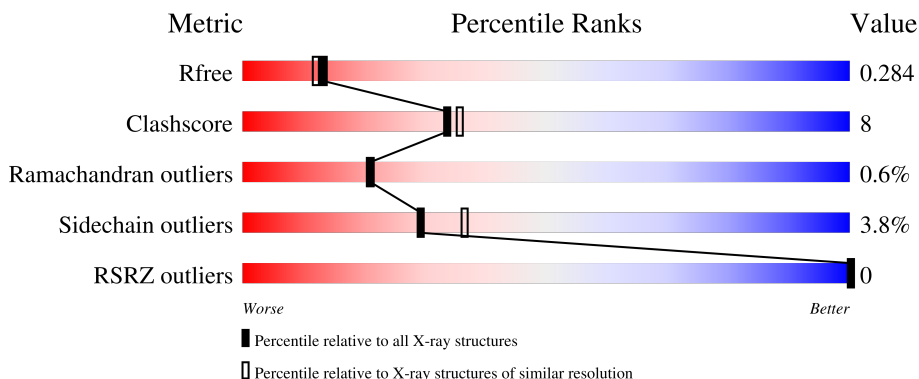
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 Å.

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)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	C	19	
1	E	19	
2	D	19	
2	F	19	
3	A	246	

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Mol	Chain	Length	Quality of chain
3	B	246	 55% 20% • 23%

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 4908 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	C	19	Total 376	C 179	N 73	O 106	P 18	0	0	0
1	E	18	Total 360	C 170	N 70	O 102	P 18	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	D	19	Total 394	C 187	N 71	O 118	P 18	0	0	0
2	F	19	Total 394	C 187	N 71	O 118	P 18	0	0	0

- Molecule 3 is a protein called PROTEIN (RAP1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	189	Total 1589	C 1010	N 283	O 295	S 1	0	0	0
3	B	189	Total 1589	C 1010	N 283	O 295	S 1	0	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	17	Total 17 O 17	0	0
4	D	16	Total 16 O 16	0	0
4	E	15	Total 15 O 15	0	0

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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
4	F	13	Total 13	O 13	0	0
4	A	71	Total 71	O 71	0	0
4	B	74	Total 74	O 74	0	0

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

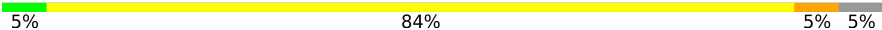
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: DNA (5'-D(\*CP\*CP\*GP\*CP\*AP\*CP\*AP\*CP\*CP\*CP\*AP\*CP\*AP\*CP\*AP\*CP\*CP\*AP\*G)-3')

Chain C: 

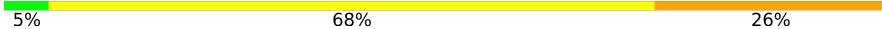


- Molecule 1: DNA (5'-D(\*CP\*CP\*GP\*CP\*AP\*CP\*AP\*CP\*CP\*CP\*AP\*CP\*AP\*CP\*AP\*CP\*CP\*AP\*G)-3')

Chain E: 

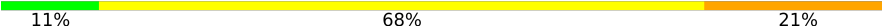


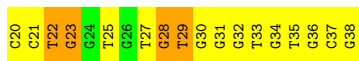
- Molecule 2: DNA (5'-D(\*CP\*CP\*TP\*GP\*GP\*TP\*GP\*TP\*GP\*TP\*GP\*GP\*GP\*TP\*GP\*TP\*G P\*CP\*G)-3')

Chain D: 



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

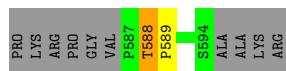
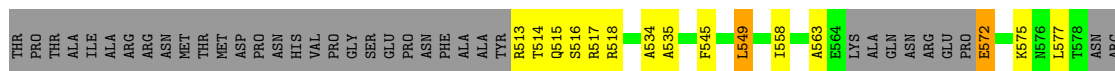
Chain F: 



- Molecule 3: PROTEIN (RAP1)

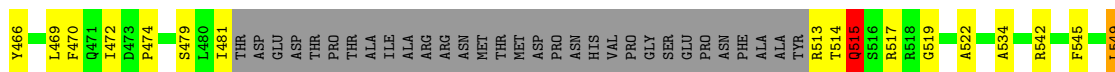
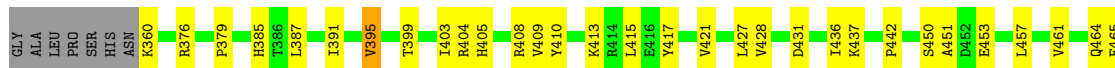
Chain A: 





- Molecule 3: PROTEIN (RAP1)

Chain B: 55% 20% 23%



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.61Å 90.61Å 80.36Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	16.00 – 2.25 16.00 – 2.26	Depositor EDS
% Data completeness (in resolution range)	95.9 (16.00-2.25) 96.3 (16.00-2.26)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.06 (at 2.25Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.219 , 0.294 0.211 , 0.284	Depositor DCC
$R_{free}$ test set	1652 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.8	Xtriage
Anisotropy	0.276	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 54.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l 0.036 for h,-h-k,-l 0.062 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	4908	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality i

### 5.1 Standard geometry i

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 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	C	1.30	1/421 (0.2%)	2.08	19/644 (3.0%)
1	E	1.33	1/403 (0.2%)	2.32	31/616 (5.0%)
2	D	1.30	2/441 (0.5%)	2.43	39/682 (5.7%)
2	F	1.25	0/441	2.18	32/682 (4.7%)
3	A	0.59	0/1627	0.99	11/2191 (0.5%)
3	B	0.58	0/1627	1.05	10/2191 (0.5%)
All	All	0.90	4/4960 (0.1%)	1.60	142/7006 (2.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	29	DT	O3'-P	-8.10	1.49	1.61
1	E	13	DA	O3'-P	-7.44	1.50	1.61
1	C	12	DC	P-O5'	-6.46	1.47	1.60
2	D	30	DG	P-O5'	-5.83	1.48	1.60

All (142) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	19	DG	N9-C1'-C2'	14.00	134.51	113.50
2	F	22	DT	O3'-P-O5'	-10.67	88.00	104.00
2	D	24	DG	C4'-C3'-O3'	-10.06	94.92	110.00
2	D	23	DG	P-O3'-C3'	9.78	134.87	120.20
2	D	25	DT	O4'-C1'-N1	9.58	122.77	108.40
3	A	385	HIS	N-CA-C	-9.18	101.98	113.55
1	E	18	DA	P-O3'-C3'	9.05	133.78	120.20
2	F	32	DG	N9-C1'-C2'	8.95	126.93	113.50
2	D	38	DG	N9-C1'-C2'	8.77	126.65	113.50
2	F	23	DG	P-O3'-C3'	8.68	133.22	120.20
1	C	14	DC	P-O3'-C3'	8.46	132.90	120.20
3	B	385	HIS	N-CA-C	-8.32	103.65	113.88
2	D	27	DT	O4'-C1'-C2'	-8.30	93.95	106.40
1	E	14	DC	C4'-C3'-O3'	-8.06	97.91	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	28	DG	O4'-C1'-C2'	-7.96	94.45	106.40
1	E	2	DC	P-O3'-C3'	7.88	132.02	120.20
2	D	38	DG	O5'-C5'-C4'	7.86	122.59	110.80
2	D	25	DT	C4'-C3'-O3'	-7.79	98.32	110.00
1	E	6	DC	P-O5'-C5'	7.75	131.62	120.00
2	D	29	DT	O4'-C1'-N1	-7.65	96.93	108.40
1	E	4	DC	P-O5'-C5'	7.60	131.41	120.00
3	B	572	GLU	CA-C-N	-7.41	112.69	120.03
3	B	572	GLU	C-N-CA	-7.41	112.69	120.03
1	C	16	DC	O3'-P-O5'	-7.34	92.98	104.00
2	D	32	DG	N9-C1'-C2'	7.34	124.50	113.50
1	C	7	DA	O4'-C1'-C2'	-7.32	95.42	106.40
2	D	32	DG	O3'-P-O5'	-7.31	93.03	104.00
3	B	395	VAL	CA-C-N	7.14	126.82	119.82
3	B	395	VAL	C-N-CA	7.14	126.82	119.82
2	F	33	DT	O4'-C1'-C2'	-7.11	95.73	106.40
2	D	22	DT	O3'-P-O5'	-7.08	93.38	104.00
2	F	37	DC	C4'-C3'-O3'	-6.96	99.56	110.00
2	F	32	DG	O3'-P-O5'	-6.94	93.59	104.00
2	D	26	DG	P-O5'-C5'	6.89	130.33	120.00
1	E	17	DC	O4'-C1'-C2'	-6.86	96.11	106.40
2	D	33	DT	C5-C4-O4	6.82	132.83	122.60
1	E	8	DC	C4'-C3'-O3'	-6.79	99.81	110.00
3	B	442	PRO	CA-C-N	-6.67	113.11	119.85
3	B	442	PRO	C-N-CA	-6.67	113.11	119.85
2	D	32	DG	P-O5'-C5'	6.58	129.87	120.00
1	C	6	DC	C1'-O4'-C4'	-6.55	99.88	109.70
2	F	37	DC	O3'-P-O5'	-6.52	94.23	104.00
1	C	8	DC	O4'-C1'-C2'	-6.50	96.65	106.40
1	C	5	DA	O4'-C1'-C2'	-6.49	96.67	106.40
2	F	28	DG	C2'-C3'-O3'	-6.48	101.78	111.50
2	D	25	DT	O3'-P-O5'	-6.46	94.31	104.00
1	C	14	DC	O4'-C1'-C2'	-6.46	96.71	106.40
2	D	35	DT	O3'-P-O5'	-6.43	94.35	104.00
1	E	15	DA	C4'-C3'-O3'	-6.41	100.38	110.00
1	E	18	DA	C5'-C4'-C3'	-6.40	105.30	114.90
2	D	34	DG	P-O3'-C3'	6.40	129.80	120.20
2	D	31	DG	P-O3'-C3'	6.39	129.79	120.20
2	D	31	DG	C4'-C3'-O3'	-6.37	100.45	110.00
2	F	25	DT	C4'-C3'-O3'	-6.36	100.46	110.00
2	D	37	DC	O4'-C1'-N1	-6.36	98.86	108.40
2	F	29	DT	O4'-C1'-N1	-6.35	98.88	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	11	DA	P-O3'-C3'	6.31	129.67	120.20
2	D	24	DG	P-O5'-C5'	-6.27	110.60	120.00
2	F	34	DG	O3'-P-O5'	-6.23	94.65	104.00
2	D	38	DG	P-O5'-C5'	6.16	129.25	120.00
1	E	7	DA	O4'-C1'-C2'	-6.16	97.16	106.40
1	E	14	DC	P-O3'-C3'	6.12	129.38	120.20
1	E	14	DC	O4'-C1'-N1	6.10	117.55	108.40
2	D	31	DG	O4'-C1'-N9	6.05	117.47	108.40
2	F	35	DT	C4'-C3'-O3'	-6.05	100.93	110.00
1	C	19	DG	N9-C1'-C2'	6.03	122.54	113.50
2	D	29	DT	N1-C1'-C2'	6.02	122.53	113.50
2	F	35	DT	C6-C5-C7	-6.02	114.97	124.00
1	E	18	DA	N9-C1'-C2'	-6.01	104.48	113.50
2	F	31	DG	O4'-C1'-C2'	-6.00	97.39	106.40
3	A	395	VAL	CA-C-N	5.99	127.33	119.84
3	A	395	VAL	C-N-CA	5.99	127.33	119.84
3	B	431	ASP	N-CA-C	5.99	118.59	111.71
1	C	12	DC	O4'-C1'-C2'	-5.98	97.43	106.40
1	E	5	DA	O3'-P-O5'	-5.96	95.06	104.00
2	F	20	DC	C2'-C3'-O3'	-5.95	102.58	111.50
2	F	36	DG	O4'-C1'-N9	5.89	117.23	108.40
3	A	469	LEU	N-CA-C	5.86	117.75	111.36
2	F	30	DG	O3'-P-O5'	-5.83	95.26	104.00
2	D	33	DT	C5'-C4'-O4'	5.80	118.10	109.40
1	E	10	DC	C4'-C3'-O3'	-5.79	101.31	110.00
2	D	36	DG	O4'-C1'-N9	5.75	117.02	108.40
1	C	5	DA	P-O3'-C3'	5.75	128.82	120.20
2	F	37	DC	P-O3'-C3'	5.74	128.80	120.20
2	F	20	DC	N1-C1'-C2'	-5.73	104.90	113.50
1	C	9	DC	O4'-C1'-C2'	-5.73	97.81	106.40
2	F	23	DG	P-O5'-C5'	5.67	128.51	120.00
2	D	34	DG	O3'-P-O5'	5.66	112.50	104.00
1	E	14	DC	O4'-C1'-C2'	-5.66	97.92	106.40
2	D	21	DC	P-O5'-C5'	5.64	128.46	120.00
1	C	6	DC	O3'-P-O5'	5.63	112.45	104.00
2	D	21	DC	N1-C1'-C2'	5.61	121.91	113.50
1	E	2	DC	C2'-C3'-O3'	-5.59	103.12	111.50
3	B	534	ALA	N-CA-C	5.59	119.63	113.21
1	E	3	DG	P-O5'-C5'	-5.58	111.63	120.00
2	F	20	DC	O4'-C1'-N1	5.58	116.77	108.40
2	D	28	DG	P-O3'-C3'	5.57	128.55	120.20
1	E	13	DA	P-O5'-C5'	5.55	128.33	120.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	8	DC	P-O3'-C3'	5.54	128.50	120.20
3	B	515	GLN	N-CA-C	5.50	116.34	108.74
2	F	32	DG	P-O3'-C3'	5.47	128.41	120.20
2	D	38	DG	C5'-C4'-O4'	5.47	117.61	109.40
1	E	16	DC	C4'-C3'-O3'	-5.47	101.80	110.00
2	F	27	DT	O4'-C1'-C2'	-5.46	98.20	106.40
2	F	34	DG	C5'-C4'-O4'	5.44	117.56	109.40
3	A	442	PRO	CA-C-N	-5.41	114.35	119.76
3	A	442	PRO	C-N-CA	-5.41	114.35	119.76
2	F	32	DG	C5'-C4'-O4'	-5.41	101.29	109.40
2	D	33	DT	P-O5'-C5'	5.40	128.10	120.00
1	E	12	DC	C4'-C3'-O3'	-5.39	101.91	110.00
3	A	534	ALA	N-CA-C	5.37	119.39	113.21
1	C	13	DA	C4'-C3'-O3'	-5.36	101.96	110.00
2	D	27	DT	C2'-C3'-O3'	5.36	119.54	111.50
2	F	21	DC	C3'-C2'-C1'	5.36	109.64	101.60
1	C	2	DC	C1'-O4'-C4'	-5.35	101.67	109.70
3	A	572	GLU	CA-C-N	-5.35	114.45	119.85
3	A	572	GLU	C-N-CA	-5.35	114.45	119.85
2	F	36	DG	C5'-C4'-C3'	-5.35	106.88	114.90
2	F	33	DT	C1'-O4'-C4'	5.32	117.69	109.70
2	D	33	DT	C4'-C3'-O3'	-5.32	102.03	110.00
1	E	17	DC	O3'-P-O5'	-5.28	96.08	104.00
2	D	33	DT	N3-C4-O4	-5.26	114.71	122.60
1	C	8	DC	O3'-P-O5'	-5.21	96.19	104.00
3	A	535	ALA	N-CA-C	-5.21	106.43	112.89
3	A	411	LEU	N-CA-C	5.20	118.78	112.23
1	E	11	DA	P-O3'-C3'	5.20	127.99	120.20
1	C	14	DC	N1-C2-O2	5.19	126.98	119.20
1	E	19	DG	C5'-C4'-C3'	-5.17	107.14	114.90
2	D	29	DT	O4'-C1'-C2'	-5.16	98.66	106.40
2	D	26	DG	O4'-C1'-C2'	-5.16	98.67	106.40
2	F	38	DG	N9-C1'-C2'	5.12	121.18	113.50
2	F	27	DT	C5-C4-O4	5.11	130.27	122.60
1	C	17	DC	N1-C1'-C2'	-5.11	105.84	113.50
1	E	4	DC	P-O3'-C3'	5.10	127.85	120.20
1	E	19	DG	O4'-C1'-C2'	-5.10	98.75	106.40
2	F	20	DC	C3'-C2'-C1'	5.10	109.25	101.60
2	D	22	DT	O4'-C1'-C2'	-5.08	98.79	106.40
1	E	2	DC	N1-C1'-C2'	5.06	121.09	113.50
1	E	2	DC	O5'-C5'-C4'	5.04	118.35	110.80
2	F	29	DT	P-O5'-C5'	5.02	127.53	120.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	6	DC	C4'-C3'-O3'	-5.02	102.48	110.00
1	E	17	DC	P-O3'-C3'	5.01	127.71	120.20

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 the 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 within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	376	0	211	3	0
1	E	360	0	199	1	0
2	D	394	0	217	8	0
2	F	394	0	217	3	0
3	A	1589	0	1542	27	0
3	B	1589	0	1542	32	0
4	A	71	0	0	0	0
4	B	74	0	0	0	0
4	C	17	0	0	1	0
4	D	16	0	0	0	0
4	E	15	0	0	1	0
4	F	13	0	0	1	0
All	All	4908	0	3928	66	0

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 8.

All (66) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:36:DG:H21	3:A:360:LYS:HE3	1.38	0.86
1:E:2:DC:P	1:E:2:DC:H2'	2.26	0.76
3:B:428:VAL:HG12	3:B:436:ILE:HD12	1.73	0.71
2:D:36:DG:N2	3:A:360:LYS:HE3	2.09	0.68
3:B:451:ALA:HB2	3:B:572:GLU:HB3	1.80	0.64
3:B:464:GLN:NE2	3:B:522:ALA:HB2	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:470:PHE:O	3:A:472:ILE:HG13	2.02	0.60
3:A:465:PHE:HD2	3:A:515:GLN:OE1	1.85	0.60
4:F:900:HOH:O	3:B:360:LYS:HE3	2.02	0.59
3:B:417:TYR:CE2	3:B:437:LYS:HD2	2.41	0.55
3:A:407:PHE:HA	3:A:411:LEU:HB2	1.89	0.54
3:A:451:ALA:HB2	3:A:572:GLU:HB3	1.89	0.54
3:B:457:LEU:O	3:B:461:VAL:HG23	2.08	0.54
3:A:465:PHE:HB3	3:A:513:ARG:NH2	2.22	0.54
3:A:466:TYR:CD1	3:A:474:PRO:HG3	2.42	0.54
3:B:421:VAL:HG12	3:B:427:LEU:HD23	1.89	0.54
3:B:465:PHE:HD2	3:B:515:GLN:OE1	1.91	0.53
3:B:428:VAL:CG1	3:B:436:ILE:HD12	2.38	0.52
4:E:879:HOH:O	3:B:588:THR:HB	2.09	0.52
3:A:514:THR:HG22	3:A:515:GLN:H	1.75	0.51
3:A:459:ILE:HD13	3:A:558:ILE:HD13	1.93	0.50
2:F:28:DG:H2''	2:F:29:DT:H71	1.94	0.50
3:A:514:THR:HG22	3:A:515:GLN:N	2.27	0.50
2:D:31:DG:N7	3:A:404:ARG:NH2	2.56	0.49
3:A:458:ALA:HA	3:A:549:LEU:HD11	1.93	0.49
3:B:395:VAL:O	3:B:395:VAL:HG23	2.12	0.49
2:D:23:DG:OP1	3:A:518:ARG:NH1	2.45	0.49
2:D:23:DG:P	3:A:518:ARG:NH1	2.86	0.48
4:C:888:HOH:O	3:A:575:LYS:HD2	2.12	0.48
1:C:5:DA:H5''	3:A:361:ALA:O	2.13	0.48
3:B:575:LYS:O	3:B:577:LEU:HD13	2.12	0.48
3:B:451:ALA:CB	3:B:572:GLU:HB3	2.43	0.48
3:B:479:SER:OG	3:B:481:ILE:HG12	2.13	0.48
3:B:465:PHE:HB3	3:B:513:ARG:HH22	1.78	0.47
3:B:545:PHE:HA	3:B:549:LEU:HB2	1.96	0.47
3:B:465:PHE:HB3	3:B:513:ARG:NH2	2.28	0.47
2:F:22:DT:H2''	2:F:23:DG:C8	2.50	0.47
3:A:545:PHE:HA	3:A:549:LEU:HB2	1.97	0.47
3:B:514:THR:HG23	3:B:555:ASP:CG	2.40	0.47
1:C:17:DC:H2''	1:C:18:DA:C8	2.50	0.47
3:B:465:PHE:CE1	3:B:519:GLY:HA2	2.50	0.46
3:B:470:PHE:O	3:B:472:ILE:HG13	2.16	0.46
2:F:23:DG:O6	3:B:542:ARG:NH2	2.49	0.46
3:A:465:PHE:HB3	3:A:513:ARG:HH22	1.81	0.46
3:A:413:LYS:NZ	3:A:413:LYS:HB2	2.31	0.46
3:B:514:THR:HG22	3:B:515:GLN:N	2.31	0.46
3:B:404:ARG:O	3:B:408:ARG:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:23:DG:P	3:A:518:ARG:HH12	2.39	0.44
3:A:465:PHE:CB	3:A:513:ARG:NH2	2.80	0.44
3:B:588:THR:HA	3:B:589:PRO:HD3	1.79	0.44
1:C:18:DA:H2''	1:C:19:DG:C8	2.53	0.43
2:D:28:DG:O5'	2:D:28:DG:H2'	2.19	0.43
3:B:405:HIS:CE1	3:B:409:VAL:HG21	2.53	0.43
3:A:470:PHE:HE2	3:A:513:ARG:HD3	1.83	0.43
3:B:399:THR:O	3:B:403:ILE:HG13	2.19	0.43
2:D:22:DT:H2''	2:D:23:DG:C8	2.54	0.42
3:B:410:TYR:HA	3:B:413:LYS:HE3	2.00	0.42
3:A:384:THR:HG22	3:A:445:ILE:HD12	2.02	0.42
3:B:376:ARG:O	3:B:379:PRO:HD3	2.19	0.42
3:A:430:ASP:OD2	3:A:434:ASN:HB2	2.20	0.42
3:B:450:SER:OG	3:B:453:GLU:HG3	2.20	0.41
3:A:376:ARG:HG2	3:A:417:TYR:O	2.20	0.41
3:B:469:LEU:HD12	3:B:513:ARG:NH1	2.34	0.41
3:B:466:TYR:CD2	3:B:474:PRO:HG3	2.55	0.41
3:B:387:LEU:O	3:B:391:ILE:HG13	2.20	0.41
3:A:588:THR:HA	3:A:589:PRO:HD3	1.92	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 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 X-ray entries followed by that with respect to entries of similar resolution.

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	A	181/246 (74%)	169 (93%)	10 (6%)	2 (1%)	11	8
3	B	181/246 (74%)	170 (94%)	11 (6%)	0	100	100
All	All	362/492 (74%)	339 (94%)	21 (6%)	2 (1%)	21	21

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	516	SER
3	A	563	ALA

### 5.3.2 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 X-ray entries followed by that with respect to entries of similar resolution.

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	A	171/217 (79%)	163 (95%)	8 (5%)	23	26
3	B	171/217 (79%)	166 (97%)	5 (3%)	37	47
All	All	342/434 (79%)	329 (96%)	13 (4%)	29	36

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	408	ARG
3	A	413	LYS
3	A	415	LEU
3	A	432	ASP
3	A	517	ARG
3	A	549	LEU
3	A	577	LEU
3	A	588	THR
3	B	415	LEU
3	B	515	GLN
3	B	517	ARG
3	B	549	LEU
3	B	577	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	B	576	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	C	19/19 (100%)	-2.00	0 100 100	16, 24, 50, 76	0
1	E	18/19 (94%)	-2.03	0 100 100	16, 24, 41, 56	0
2	D	19/19 (100%)	-2.02	0 100 100	16, 28, 42, 52	0
2	F	19/19 (100%)	-2.04	0 100 100	17, 28, 47, 49	0
3	A	189/246 (76%)	-1.63	0 100 100	9, 29, 53, 64	0
3	B	189/246 (76%)	-1.62	0 100 100	6, 30, 54, 72	0
All	All	453/568 (79%)	-1.69	0 100 100	6, 29, 53, 76	0

There are no RSRZ outliers to report.

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.