



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:22 AM UTC

PDB ID : 5N9G / pdb_00005n9g
Title : TFIIB -TBP/Brf2/DNA and SANT domain of Bdp1-
Authors : Gouge, J.; Vannini, A.; Guthertz, N.
Deposited on : 2017-02-24
Resolution : 2.70 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

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>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (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

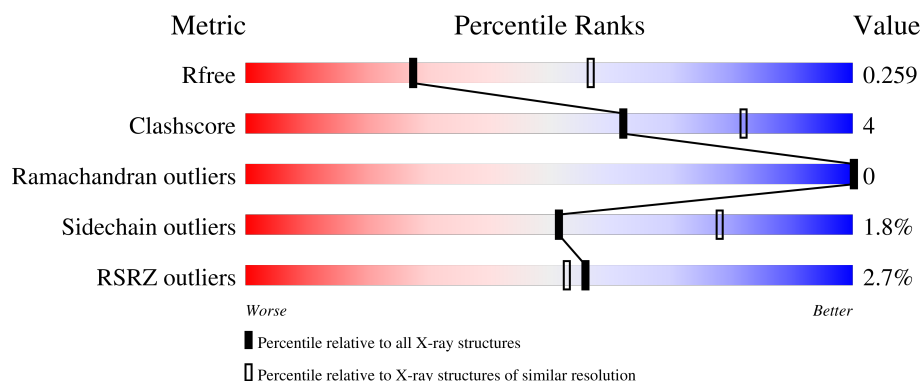
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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.



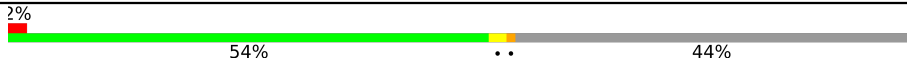
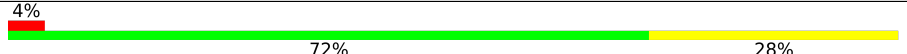
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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 ≥ 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	A	377	3% 74% 7% 19%
1	F	377	2% 63% 13% 23%
2	B	200	2% 79% 10% 11%
2	G	200	2% 79% 10% 11%
3	C	175	2% 50% 5% 45%

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Mol	Chain	Length	Quality of chain
3	H	175	
4	D	27	
4	I	27	
5	E	25	
5	J	25	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11643 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 protein called Transcription factor IIIB 50 kDa subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	307	Total	C	N	O	S	83	1	0
			2445	1553	439	436	17			
1	F	289	Total	C	N	O	S	0	1	0
			2311	1470	414	411	16			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	43	MET	-	initiating methionine	UNP Q9HAW0
A	44	ALA	-	expression tag	UNP Q9HAW0
A	45	HIS	-	expression tag	UNP Q9HAW0
A	46	HIS	-	expression tag	UNP Q9HAW0
A	47	HIS	-	expression tag	UNP Q9HAW0
A	48	HIS	-	expression tag	UNP Q9HAW0
A	49	HIS	-	expression tag	UNP Q9HAW0
A	50	HIS	-	expression tag	UNP Q9HAW0
A	51	SER	-	expression tag	UNP Q9HAW0
A	52	SER	-	expression tag	UNP Q9HAW0
A	53	GLY	-	expression tag	UNP Q9HAW0
A	54	LEU	-	expression tag	UNP Q9HAW0
A	55	GLU	-	expression tag	UNP Q9HAW0
A	56	VAL	-	expression tag	UNP Q9HAW0
A	57	LEU	-	expression tag	UNP Q9HAW0
A	58	PHE	-	expression tag	UNP Q9HAW0
A	59	GLN	-	expression tag	UNP Q9HAW0
A	60	GLY	-	expression tag	UNP Q9HAW0
A	61	PRO	-	expression tag	UNP Q9HAW0
F	43	MET	-	initiating methionine	UNP Q9HAW0
F	44	ALA	-	expression tag	UNP Q9HAW0
F	45	HIS	-	expression tag	UNP Q9HAW0
F	46	HIS	-	expression tag	UNP Q9HAW0
F	47	HIS	-	expression tag	UNP Q9HAW0
F	48	HIS	-	expression tag	UNP Q9HAW0

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Chain	Residue	Modelled	Actual	Comment	Reference
F	49	HIS	-	expression tag	UNP Q9HAW0
F	50	HIS	-	expression tag	UNP Q9HAW0
F	51	SER	-	expression tag	UNP Q9HAW0
F	52	SER	-	expression tag	UNP Q9HAW0
F	53	GLY	-	expression tag	UNP Q9HAW0
F	54	LEU	-	expression tag	UNP Q9HAW0
F	55	GLU	-	expression tag	UNP Q9HAW0
F	56	VAL	-	expression tag	UNP Q9HAW0
F	57	LEU	-	expression tag	UNP Q9HAW0
F	58	PHE	-	expression tag	UNP Q9HAW0
F	59	GLN	-	expression tag	UNP Q9HAW0
F	60	GLY	-	expression tag	UNP Q9HAW0
F	61	PRO	-	expression tag	UNP Q9HAW0

- Molecule 2 is a protein called TATA-box-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	178	Total	C	N	O	S	0	0	0
			1402	909	246	240	7			
2	G	178	Total	C	N	O	S	0	0	0
			1402	909	246	240	7			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	140	MET	-	initiating methionine	UNP P20226
B	141	ALA	-	expression tag	UNP P20226
B	142	HIS	-	expression tag	UNP P20226
B	143	HIS	-	expression tag	UNP P20226
B	144	HIS	-	expression tag	UNP P20226
B	145	HIS	-	expression tag	UNP P20226
B	146	HIS	-	expression tag	UNP P20226
B	147	HIS	-	expression tag	UNP P20226
B	148	SER	-	expression tag	UNP P20226
B	149	SER	-	expression tag	UNP P20226
B	150	GLY	-	expression tag	UNP P20226
B	151	LEU	-	expression tag	UNP P20226
B	152	GLU	-	expression tag	UNP P20226
B	153	VAL	-	expression tag	UNP P20226
B	154	LEU	-	expression tag	UNP P20226
B	155	PHE	-	expression tag	UNP P20226
B	156	GLN	-	expression tag	UNP P20226

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Chain	Residue	Modelled	Actual	Comment	Reference
B	157	GLY	-	expression tag	UNP P20226
B	158	PRO	-	expression tag	UNP P20226
G	140	MET	-	initiating methionine	UNP P20226
G	141	ALA	-	expression tag	UNP P20226
G	142	HIS	-	expression tag	UNP P20226
G	143	HIS	-	expression tag	UNP P20226
G	144	HIS	-	expression tag	UNP P20226
G	145	HIS	-	expression tag	UNP P20226
G	146	HIS	-	expression tag	UNP P20226
G	147	HIS	-	expression tag	UNP P20226
G	148	SER	-	expression tag	UNP P20226
G	149	SER	-	expression tag	UNP P20226
G	150	GLY	-	expression tag	UNP P20226
G	151	LEU	-	expression tag	UNP P20226
G	152	GLU	-	expression tag	UNP P20226
G	153	VAL	-	expression tag	UNP P20226
G	154	LEU	-	expression tag	UNP P20226
G	155	PHE	-	expression tag	UNP P20226
G	156	GLN	-	expression tag	UNP P20226
G	157	GLY	-	expression tag	UNP P20226
G	158	PRO	-	expression tag	UNP P20226

- Molecule 3 is a protein called Transcription factor TFIIB component B'' homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	97	Total	C	N	O	S	44	0	0
			825	533	143	146	3			
3	H	98	Total	C	N	O	S	43	0	0
			839	542	146	148	3			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	222	MET	-	initiating methionine	UNP A6H8Y1
C	223	ALA	-	expression tag	UNP A6H8Y1
C	224	HIS	-	expression tag	UNP A6H8Y1
C	225	HIS	-	expression tag	UNP A6H8Y1
C	226	HIS	-	expression tag	UNP A6H8Y1
C	227	HIS	-	expression tag	UNP A6H8Y1
C	228	HIS	-	expression tag	UNP A6H8Y1
C	229	HIS	-	expression tag	UNP A6H8Y1
C	230	SER	-	expression tag	UNP A6H8Y1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	231	SER	-	expression tag	UNP A6H8Y1
C	232	GLY	-	expression tag	UNP A6H8Y1
C	233	LEU	-	expression tag	UNP A6H8Y1
C	234	GLU	-	expression tag	UNP A6H8Y1
C	235	VAL	-	expression tag	UNP A6H8Y1
C	236	LEU	-	expression tag	UNP A6H8Y1
C	237	PHE	-	expression tag	UNP A6H8Y1
C	238	GLN	-	expression tag	UNP A6H8Y1
C	239	GLY	-	expression tag	UNP A6H8Y1
C	240	PRO	-	expression tag	UNP A6H8Y1
H	222	MET	-	initiating methionine	UNP A6H8Y1
H	223	ALA	-	expression tag	UNP A6H8Y1
H	224	HIS	-	expression tag	UNP A6H8Y1
H	225	HIS	-	expression tag	UNP A6H8Y1
H	226	HIS	-	expression tag	UNP A6H8Y1
H	227	HIS	-	expression tag	UNP A6H8Y1
H	228	HIS	-	expression tag	UNP A6H8Y1
H	229	HIS	-	expression tag	UNP A6H8Y1
H	230	SER	-	expression tag	UNP A6H8Y1
H	231	SER	-	expression tag	UNP A6H8Y1
H	232	GLY	-	expression tag	UNP A6H8Y1
H	233	LEU	-	expression tag	UNP A6H8Y1
H	234	GLU	-	expression tag	UNP A6H8Y1
H	235	VAL	-	expression tag	UNP A6H8Y1
H	236	LEU	-	expression tag	UNP A6H8Y1
H	237	PHE	-	expression tag	UNP A6H8Y1
H	238	GLN	-	expression tag	UNP A6H8Y1
H	239	GLY	-	expression tag	UNP A6H8Y1
H	240	PRO	-	expression tag	UNP A6H8Y1

- Molecule 4 is DNA/RNA hybrid called DNA/RNA (27-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	27	Total	C	N	O	P	0	0	0
			541	261	93	161	26			
4	I	27	Total	C	N	O	P	0	0	0
			541	261	93	161	26			

- Molecule 5 is DNA/RNA hybrid called DNA/RNA (25-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	25	Total	C	N	O	P	0	0	0
			519	248	100	147	24			
5	J	25	Total	C	N	O	P	0	0	0
			519	248	100	147	24			

- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	1	Total	Na	0	0
			1	1		

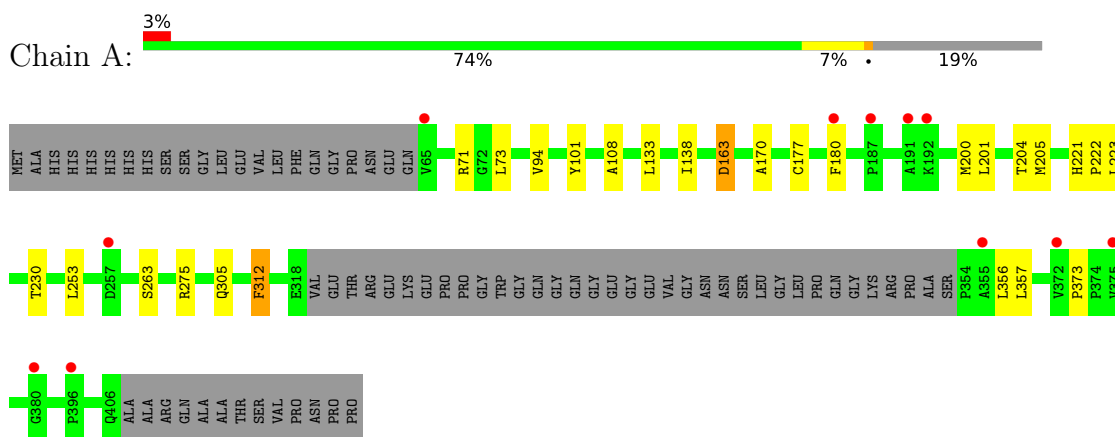
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	58	Total	O	0	0
			58	58		
7	B	30	Total	O	0	0
			30	30		
7	C	15	Total	O	0	0
			15	15		
7	D	9	Total	O	0	0
			9	9		
7	E	27	Total	O	0	0
			27	27		
7	F	80	Total	O	0	0
			80	80		
7	G	33	Total	O	0	0
			33	33		
7	H	12	Total	O	0	0
			12	12		
7	I	12	Total	O	0	0
			12	12		
7	J	22	Total	O	0	0
			22	22		

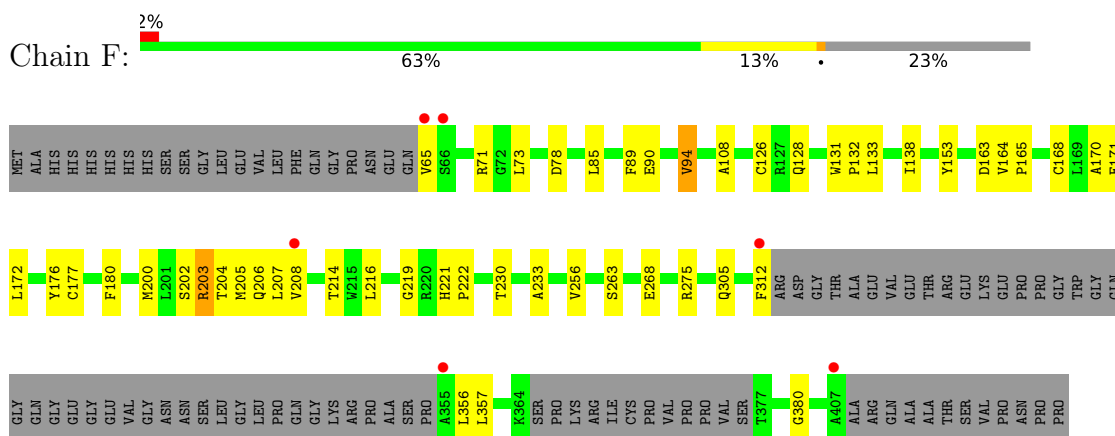
3 Residue-property plots [i](#)

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.

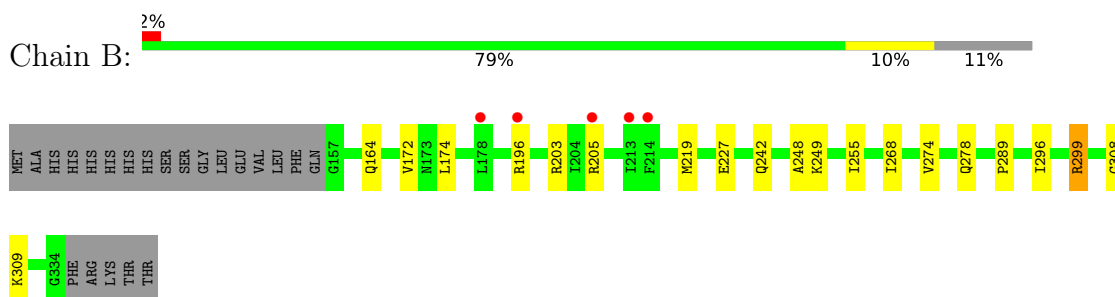
- Molecule 1: Transcription factor IIIB 50 kDa subunit



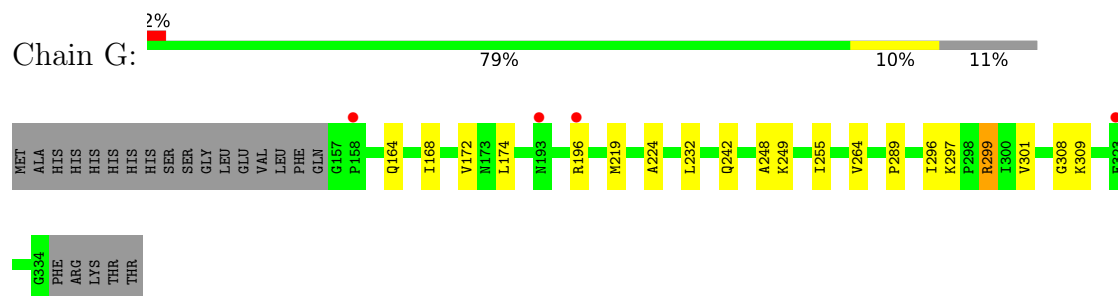
- Molecule 1: Transcription factor IIIB 50 kDa subunit



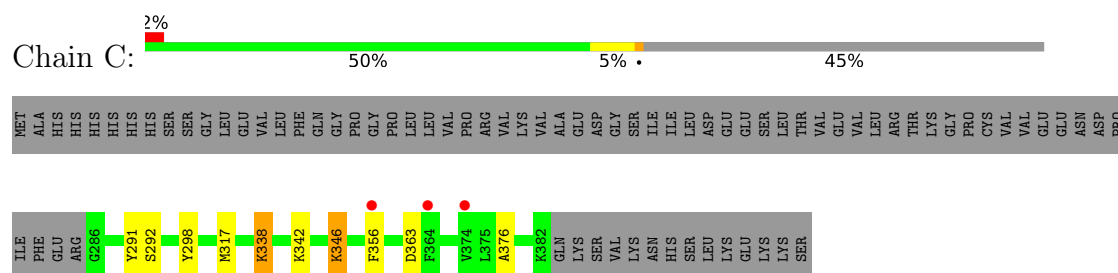
- Molecule 2: TATA-box-binding protein



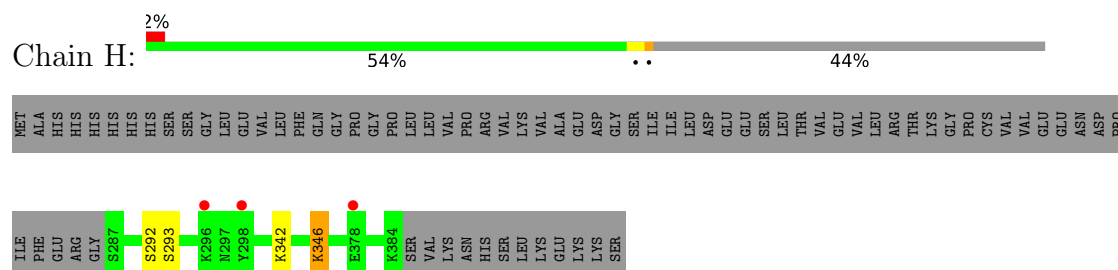
- Molecule 2: TATA-box-binding protein



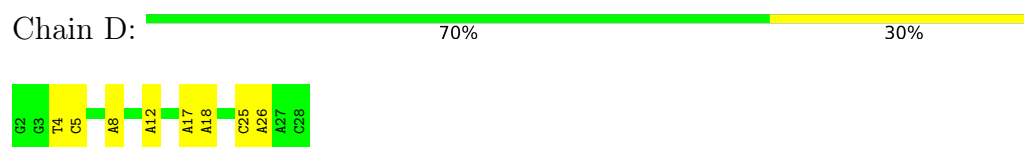
- Molecule 3: Transcription factor TFIIB component B'' homolog



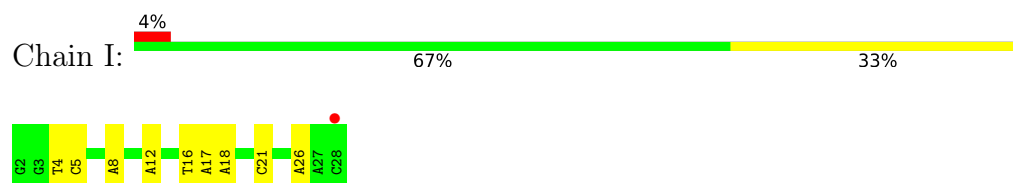
- Molecule 3: Transcription factor TFIIB component B'' homolog



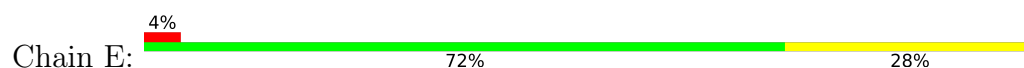
- Molecule 4: DNA/RNA (27-MER)

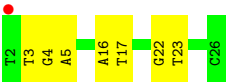


- Molecule 4: DNA/RNA (27-MER)



- Molecule 5: DNA/RNA (25-MER)





● Molecule 5: DNA/RNA (25-MER)



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.19Å 124.08Å 88.61Å 90.00° 99.51° 90.00°	Depositor
Resolution (Å)	49.04 – 2.70 49.04 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.0 (49.04-2.70) 99.0 (49.04-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 2.69Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.194 , 0.234 0.214 , 0.259	Depositor DCC
R_{free} test set	2369 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	61.8	Xtriage
Anisotropy	0.568	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 89.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11643	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.44% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

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

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	A	0.87	0/2493	1.32	7/3384 (0.2%)
1	F	0.90	0/2353	1.35	9/3190 (0.3%)
2	B	0.79	0/1428	1.17	0/1924
2	G	0.83	0/1428	1.20	0/1924
3	C	0.90	1/847 (0.1%)	1.44	6/1131 (0.5%)
3	H	0.83	0/861	1.40	2/1149 (0.2%)
4	D	0.54	0/604	0.64	0/928
4	I	0.55	0/604	0.65	0/928
5	E	0.50	0/584	0.68	0/902
5	J	0.50	0/584	0.69	0/902
All	All	0.80	1/11786 (0.0%)	1.19	24/16362 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	338	LYS	CA-C	5.91	1.60	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	312	PHE	CA-C-N	6.22	128.62	120.28
1	A	312	PHE	C-N-CA	6.22	128.62	120.28
3	C	298	TYR	CA-C-N	6.07	129.49	120.87
3	C	298	TYR	C-N-CA	6.07	129.49	120.87
3	C	376	ALA	CA-C-N	5.88	128.08	120.44
3	C	376	ALA	C-N-CA	5.88	128.08	120.44
1	A	163	ASP	N-CA-C	-5.66	99.50	108.73
1	F	305	GLN	CA-C-N	5.65	127.79	120.44
1	F	305	GLN	C-N-CA	5.65	127.79	120.44
1	F	168	CYS	CA-C-N	5.48	127.56	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	168	CYS	C-N-CA	5.48	127.56	120.44
1	A	305	GLN	CA-C-N	5.31	127.34	120.44
1	A	305	GLN	C-N-CA	5.31	127.34	120.44
1	A	71	ARG	CA-C-N	5.17	125.57	119.94
1	A	71	ARG	C-N-CA	5.17	125.57	119.94
3	H	346	LYS	CA-C-N	5.11	127.54	120.29
3	H	346	LYS	C-N-CA	5.11	127.54	120.29
1	F	78	ASP	CB-CA-C	-5.09	102.89	110.88
3	C	346	LYS	CA-C-N	5.08	127.50	120.29
3	C	346	LYS	C-N-CA	5.08	127.50	120.29
1	F	71	ARG	CA-C-N	5.08	125.59	120.00
1	F	71	ARG	C-N-CA	5.08	125.59	120.00
1	F	90	GLU	CA-C-N	5.05	127.05	120.28
1	F	90	GLU	C-N-CA	5.05	127.05	120.28

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	A	2445	0	2525	15	0
1	F	2311	0	2385	27	0
2	B	1402	0	1489	18	0
2	G	1402	0	1489	14	0
3	C	825	0	812	9	0
3	H	839	0	830	3	0
4	D	541	0	307	8	0
4	I	541	0	307	8	0
5	E	519	0	284	6	0
5	J	519	0	284	5	0
6	H	1	0	0	0	0
7	A	58	0	0	0	0
7	B	30	0	0	1	0
7	C	15	0	0	0	0
7	D	9	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	E	27	0	0	0	0
7	F	80	0	0	2	0
7	G	33	0	0	1	0
7	H	12	0	0	0	0
7	I	12	0	0	1	0
7	J	22	0	0	0	0
All	All	11643	0	10712	88	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 4.

All (88) 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:B:203:ARG:HH12	3:C:338:LYS:HZ2	1.10	0.96
1:A:373:PRO:HD2	2:B:164:GLN:HG2	1.49	0.92
1:A:133:LEU:HD21	1:A:138:ILE:HD11	1.54	0.89
1:F:133:LEU:HD21	1:F:138:ILE:HD11	1.62	0.81
2:B:299:ARG:HD3	2:G:299:ARG:HD3	1.67	0.76
4:I:4:DT:H2''	4:I:5:DC:O5'	1.87	0.75
2:B:203:ARG:HH12	3:C:338:LYS:NZ	1.86	0.73
1:A:221[B]:HIS:HE2	3:C:292:SER:H	1.37	0.72
1:F:200:MET:O	1:F:204:THR:HG22	1.93	0.68
2:B:203:ARG:NH1	3:C:338:LYS:HZ2	1.88	0.67
1:F:221[B]:HIS:HE2	3:H:292:SER:H	1.45	0.64
4:D:26:A:H2	5:E:3:DT:H3	1.43	0.64
1:F:132:PRO:HD3	1:F:171:GLU:HB3	1.80	0.63
1:F:204:THR:O	1:F:208:VAL:HG23	1.99	0.62
2:G:309:LYS:HD3	4:I:17:A:H5''	1.84	0.58
1:A:223:LEU:HD23	3:C:291:TYR:HB2	1.85	0.57
2:G:242:GLN:HG3	2:G:248:ALA:HB3	1.85	0.57
2:B:309:LYS:HD3	4:D:17:A:H5''	1.86	0.57
2:B:242:GLN:HG3	2:B:248:ALA:HB3	1.87	0.57
2:G:264:VAL:HG22	2:G:308:GLY:O	2.04	0.57
1:A:108:ALA:HB3	4:D:8:DA:H5'	1.87	0.56
1:F:221[B]:HIS:ND1	1:F:222:PRO:HD2	2.21	0.56
1:A:73:LEU:HD22	1:A:94:VAL:HG13	1.89	0.55
2:B:203:ARG:NH1	3:C:338:LYS:NZ	2.51	0.55
1:A:200:MET:O	1:A:204:THR:HG22	2.06	0.55
1:F:204:THR:HB	1:F:230:THR:HA	1.89	0.54
5:E:4:G:H2'	5:E:5:A:C8	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:219:GLY:HA3	7:F:522:HOH:O	2.11	0.51
1:F:216:LEU:HD22	1:F:268:GLU:HB3	1.92	0.49
5:E:22:DG:H2''	5:E:23:DT:OP2	2.11	0.49
4:D:4:DT:H2''	4:D:5:DC:O5'	2.13	0.49
1:F:85:LEU:HD22	1:F:89:PHE:CD2	2.48	0.48
4:I:26:A:H2	5:J:3:DT:H3	1.61	0.48
2:B:274:VAL:O	2:B:278:GLN:HG2	2.14	0.48
1:F:275:ARG:HD2	1:F:312:PHE:CE1	2.49	0.48
1:A:221[B]:HIS:ND1	1:A:222:PRO:HD2	2.28	0.48
1:A:373:PRO:CD	2:B:164:GLN:HG2	2.34	0.48
1:A:275:ARG:HD2	1:A:312:PHE:CE1	2.49	0.47
1:F:73:LEU:HD22	1:F:94:VAL:HG13	1.95	0.47
3:H:293:SER:HB2	4:I:21:C:H5''	1.96	0.47
2:G:289:PRO:HG2	4:I:18:A:N3	2.31	0.46
3:C:317:MET:HE2	3:C:363:ASP:H	1.79	0.46
1:A:180:PHE:CZ	1:A:230:THR:HG21	2.51	0.45
2:G:301:VAL:HG11	5:J:13:A:H4'	1.98	0.45
2:B:296:ILE:O	2:B:299:ARG:HG2	2.17	0.45
7:B:405:HOH:O	2:G:297:LYS:HG2	2.16	0.45
1:F:126:CYS:HB3	1:F:131:TRP:HB3	1.98	0.45
2:B:289:PRO:HG2	4:D:18:A:N3	2.32	0.44
4:D:25:C:H42	5:E:4:G:H1	1.63	0.44
1:A:177:CYS:HA	1:A:180:PHE:CD1	2.52	0.44
2:B:205:ARG:NH1	3:C:356:PHE:CD1	2.85	0.44
1:F:65:VAL:HA	7:F:507:HOH:O	2.16	0.44
2:G:296:ILE:O	2:G:299:ARG:HG2	2.18	0.44
1:F:128:GLN:HA	1:F:165:PRO:HG2	1.99	0.44
1:F:170:ALA:HA	1:F:205:MET:SD	2.58	0.44
1:F:214:THR:HA	1:F:357:LEU:HD11	1.98	0.44
3:H:342:LYS:O	3:H:346:LYS:HG2	2.18	0.44
1:A:312:PHE:CB	1:A:357:LEU:HB2	2.47	0.44
1:A:201:LEU:HA	1:A:204:THR:HG22	2.00	0.43
2:G:168:ILE:HG12	2:G:224:ALA:O	2.18	0.43
5:J:22:DG:H2''	5:J:23:DT:OP2	2.17	0.43
1:F:108:ALA:HB3	4:I:8:DA:H5'	1.99	0.43
1:F:177:CYS:HA	1:F:180:PHE:CD1	2.53	0.43
4:I:16:DT:H71	7:I:106:HOH:O	2.17	0.43
2:B:196:ARG:HD3	4:D:12:A:OP1	2.18	0.43
1:F:312:PHE:HB3	1:F:357:LEU:HB2	2.00	0.43
5:J:3:DT:H2'	5:J:4:G:C8	2.54	0.42
3:C:342:LYS:O	3:C:346:LYS:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:268:ILE:CD1	2:B:308:GLY:HA2	2.49	0.42
5:E:16:A:H2''	5:E:17:DT:H5'	2.02	0.42
1:F:202:SER:O	1:F:206:GLN:HG3	2.19	0.42
1:F:312:PHE:CB	1:F:357:LEU:HB2	2.49	0.42
2:G:196:ARG:HD3	4:I:12:A:OP1	2.19	0.42
1:A:170:ALA:HA	1:A:205:MET:SD	2.60	0.42
2:B:174:LEU:HA	2:B:249:LYS:O	2.20	0.42
1:F:153:TYR:OH	1:F:164:VAL:HG11	2.20	0.42
5:E:3:DT:H2'	5:E:4:G:C8	2.55	0.42
2:G:172:VAL:CG1	2:G:219:MET:HE2	2.50	0.41
5:J:16:A:H2''	5:J:17:DT:H5'	2.03	0.41
1:F:172:LEU:O	1:F:176:TYR:HB3	2.21	0.41
2:G:174:LEU:HA	2:G:249:LYS:O	2.21	0.41
1:F:85:LEU:HD21	1:F:126:CYS:SG	2.61	0.41
2:G:172:VAL:HG12	2:G:219:MET:HE2	2.02	0.41
2:B:299:ARG:HG3	7:G:428:HOH:O	2.21	0.41
4:D:4:DT:H4'	4:D:5:DC:OP1	2.21	0.40
1:F:203:ARG:HB3	1:F:233:ALA:HB1	2.02	0.40
1:F:380:GLY:HA2	2:G:232:LEU:HB2	2.03	0.40
2:B:172:VAL:CG1	2:B:219:MET:HE2	2.51	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	
1	A	304/377 (81%)	302 (99%)	2 (1%)	0	100	100
1	F	284/377 (75%)	280 (99%)	4 (1%)	0	100	100
2	B	176/200 (88%)	174 (99%)	2 (1%)	0	100	100
2	G	176/200 (88%)	171 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	95/175 (54%)	92 (97%)	3 (3%)	0	100	100
3	H	96/175 (55%)	91 (95%)	5 (5%)	0	100	100
All	All	1131/1504 (75%)	1110 (98%)	21 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 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 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	
1	A	274/327 (84%)	269 (98%)	5 (2%)	51	78
1	F	257/327 (79%)	250 (97%)	7 (3%)	39	69
2	B	152/172 (88%)	149 (98%)	3 (2%)	48	76
2	G	152/172 (88%)	149 (98%)	3 (2%)	48	76
3	C	88/159 (55%)	88 (100%)	0	100	100
3	H	90/159 (57%)	90 (100%)	0	100	100
All	All	1013/1316 (77%)	995 (98%)	18 (2%)	51	78

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	101	TYR
1	A	163	ASP
1	A	253	LEU
1	A	263	SER
1	A	356	LEU
2	B	227	GLU
2	B	255	ILE
2	B	299	ARG
1	F	94	VAL
1	F	163	ASP
1	F	203	ARG
1	F	207	LEU

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Mol	Chain	Res	Type
1	F	256	VAL
1	F	263	SER
1	F	356	LEU
2	G	164	GLN
2	G	255	ILE
2	G	299	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	GLN
1	A	99	GLN
2	B	166	GLN
2	B	278	GLN
3	C	348	ASN
1	F	70	GLN
1	F	99	GLN
1	F	130	ASN
2	G	166	GLN
3	H	348	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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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, 95th 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 ²)	Q<0.9
1	A	296/377 (78%)	0.50	11 (3%) 45 41	24, 75, 137, 163	1 (0%)
1	F	289/377 (76%)	0.33	6 (2%) 63 61	24, 72, 138, 149	1 (0%)
2	B	178/200 (89%)	0.33	5 (2%) 55 51	49, 75, 110, 123	0
2	G	178/200 (89%)	0.36	4 (2%) 62 59	46, 77, 110, 130	0
3	C	97/175 (55%)	0.50	3 (3%) 51 48	59, 95, 130, 144	11 (11%)
3	H	98/175 (56%)	0.54	3 (3%) 51 48	54, 88, 125, 134	11 (11%)
4	D	27/27 (100%)	0.05	0 100 100	62, 75, 148, 169	0
4	I	27/27 (100%)	0.05	1 (3%) 45 41	62, 77, 146, 160	0
5	E	25/25 (100%)	0.09	1 (4%) 42 38	62, 83, 128, 148	0
5	J	25/25 (100%)	0.17	0 100 100	60, 85, 126, 153	0
All	All	1240/1608 (77%)	0.39	34 (2%) 56 53	24, 78, 133, 169	24 (1%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	375	VAL	4.6
1	A	65	VAL	4.2
2	G	323	GLU	3.6
2	B	196	ARG	3.5
1	A	372	VAL	3.2
1	F	407	ALA	3.0
1	A	380	GLY	3.0
2	G	158	PRO	2.9
1	F	355	ALA	2.8
2	B	178	LEU	2.7
2	G	196	ARG	2.7
3	H	298	TYR	2.6
1	A	191	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	257	ASP	2.5
2	B	205	ARG	2.4
2	G	193	ASN	2.4
1	A	187	PRO	2.4
3	H	296	LYS	2.4
1	A	396	PRO	2.3
5	E	2	DT	2.3
3	H	378	GLU	2.2
1	F	66	SER	2.2
3	C	356	PHE	2.2
3	C	364	PHE	2.2
1	A	355	ALA	2.1
1	A	192	LYS	2.1
1	F	312	PHE	2.1
1	F	208	VAL	2.1
2	B	213	ILE	2.1
3	C	374	VAL	2.1
4	I	28	DC	2.1
1	A	180	PHE	2.1
2	B	214	PHE	2.1
1	F	65	VAL	2.0

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	NA	H	401	1/1	0.90	0.14	83,83,83,83	0

6.5 Other polymers [i](#)

There are no such residues in this entry.