



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 07:48 am BST

PDB ID : 5N9G
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

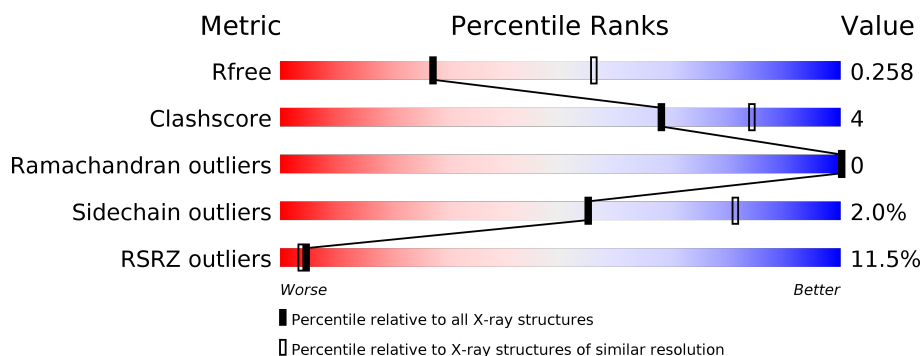
1 Overall quality at a glance

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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (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 on 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	<div> <div>10%</div> <div>75%</div> <div>7%</div> <div>19%</div> </div>
1	F	377	<div> <div>7%</div> <div>64%</div> <div>12%</div> <div>23%</div> </div>
2	B	200	<div> <div>9%</div> <div>81%</div> <div>8%</div> <div>11%</div> </div>
2	G	200	<div> <div>11%</div> <div>80%</div> <div>9%</div> <div>11%</div> </div>
3	C	175	<div> <div>13%</div> <div>51%</div> <div>5%</div> <div>45%</div> </div>
3	H	175	<div> <div>3%</div> <div>53%</div> <div>•</div> <div>44%</div> </div>

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Mol	Chain	Length	Quality of chain
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 (three-letter code: NA) (formula: Na).

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

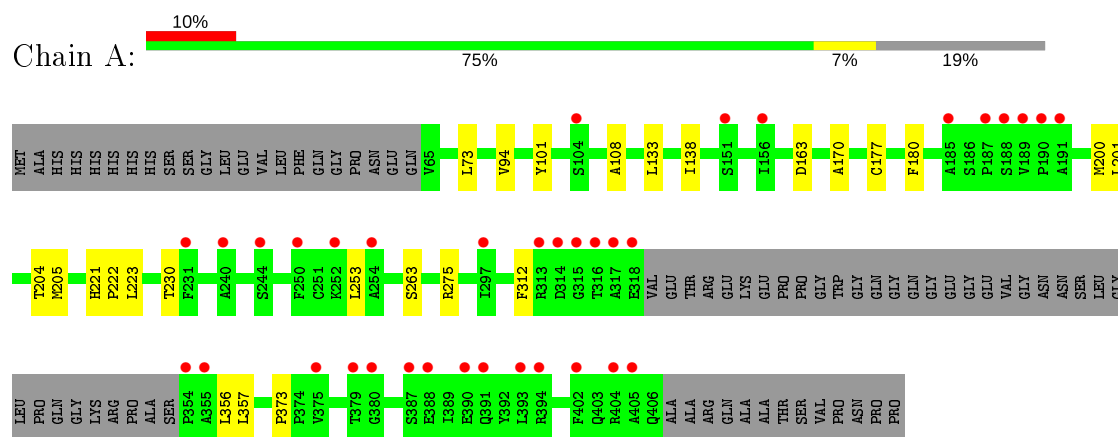
- Molecule 7 is water.

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		

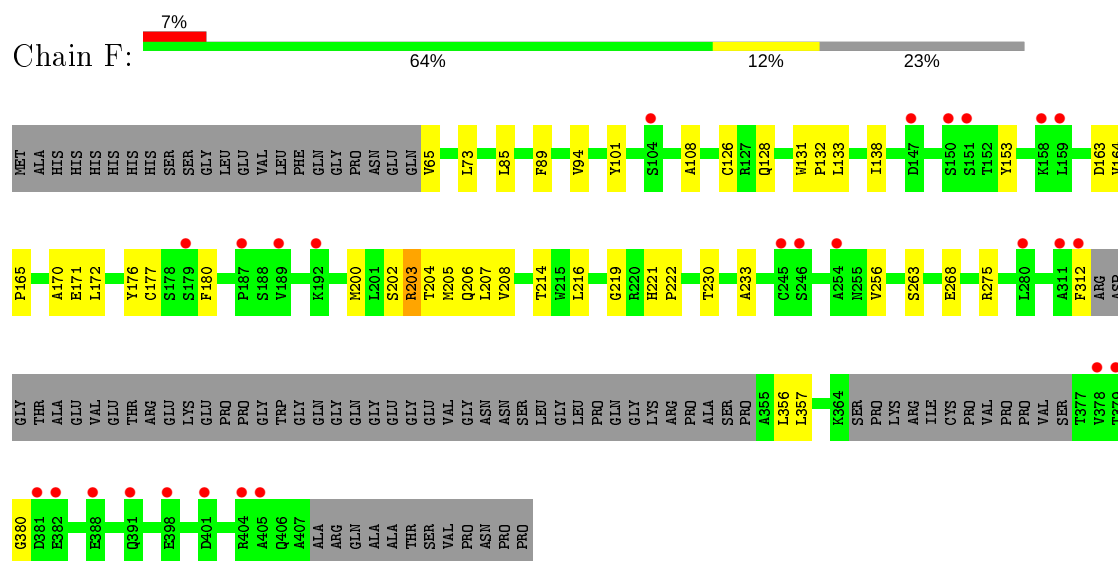
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

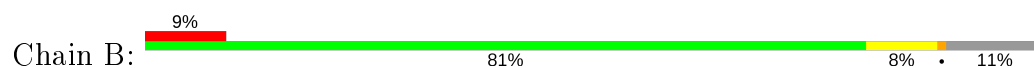
- Molecule 1: Transcription factor IIIB 50 kDa subunit

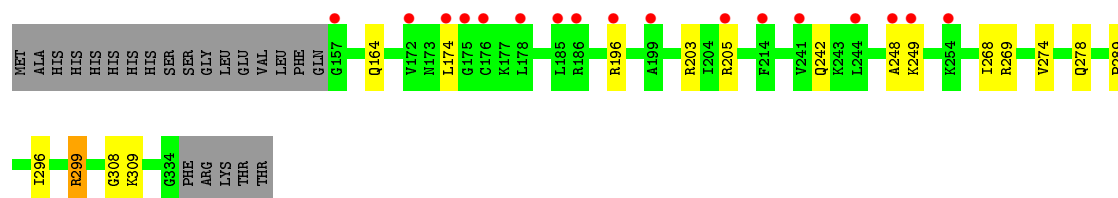


- Molecule 1: Transcription factor IIIB 50 kDa subunit

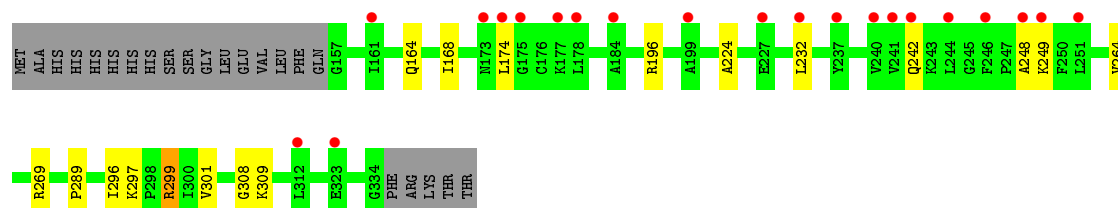
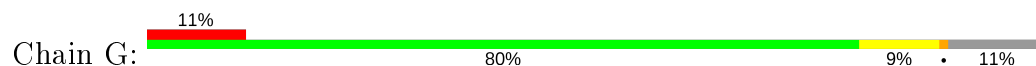


- Molecule 2: TATA-box-binding protein

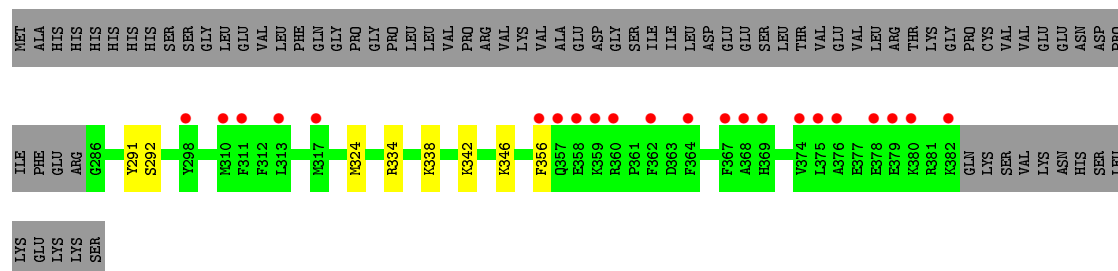




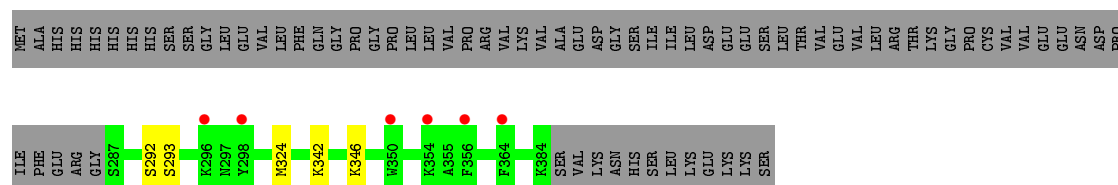
- Molecule 2: TATA-box-binding protein



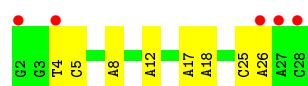
- Molecule 3: Transcription factor TFIIB component B' homolog



- Molecule 3: Transcription factor TFIIB component B' homolog



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

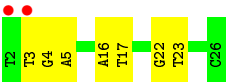


- Molecule 4: DNA/RNA (27-MER)

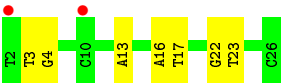




● Molecule 5: DNA/RNA (25-MER)



● 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	81.19 Å 124.08 Å 88.61 Å 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 2.69 Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.194 , 0.234 0.216 , 0.258	Depositor DCC
R_{free} test set	2369 reflections (5.03%)	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)	0.32 , 65.0	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 [i](#)

5.1 Standard geometry [i](#)

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	0.51	0/2493	0.66	0/3384
1	F	0.53	0/2353	0.66	0/3190
2	B	0.45	0/1428	0.68	0/1924
2	G	0.47	0/1428	0.67	0/1924
3	C	0.52	0/847	0.64	0/1131
3	H	0.48	0/861	0.61	0/1149
4	D	1.11	0/604	0.98	0/928
4	I	1.12	0/604	0.99	0/928
5	E	1.06	0/584	1.01	0/902
5	J	1.09	0/584	1.01	0/902
All	All	0.66	0/11786	0.75	0/16362

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 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	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	1402	0	1489	12	0
3	C	825	0	812	7	0
3	H	839	0	830	3	0
4	D	541	0	307	8	0
4	I	541	0	307	7	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
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	0	0
7	J	22	0	0	0	0
All	All	11643	0	10712	82	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 (82) 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)
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
2:B:203:ARG:HH12	3:C:338:LYS:HZ2	1.25	0.84
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
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
2:B:203:ARG:NH1	3:C:338:LYS:NZ	2.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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: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

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 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 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
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%)	59	83
1	F	257/327 (79%)	250 (97%)	7 (3%)	44	74
2	B	152/172 (88%)	150 (99%)	2 (1%)	69	87
2	G	152/172 (88%)	149 (98%)	3 (2%)	55	81
3	C	88/159 (55%)	86 (98%)	2 (2%)	50	78
3	H	90/159 (57%)	89 (99%)	1 (1%)	73	90
All	All	1013/1316 (77%)	993 (98%)	20 (2%)	55	81

All (20) 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	269	ARG
2	B	299	ARG

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Mol	Chain	Res	Type
3	C	324	MET
3	C	334	ARG
1	F	101	TYR
1	F	163	ASP
1	F	203	ARG
1	F	207	LEU
1	F	256	VAL
1	F	263	SER
1	F	356	LEU
2	G	164	GLN
2	G	269	ARG
2	G	299	ARG
3	H	324	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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 [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 ⓘ

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%)	0.81	36 (12%) 4 3	49, 75, 137, 163	0
1	F	289/377 (76%)	0.59	26 (8%) 9 7	47, 72, 138, 149	0
2	B	178/200 (89%)	0.66	17 (9%) 8 6	49, 75, 110, 123	0
2	G	178/200 (89%)	0.76	21 (11%) 4 3	46, 77, 110, 130	0
3	C	97/175 (55%)	1.21	22 (22%) 0 0	68, 100, 134, 149	11 (11%)
3	H	98/175 (56%)	0.44	6 (6%) 21 20	63, 92, 125, 134	11 (11%)
4	D	27/27 (100%)	0.88	5 (18%) 1 1	62, 75, 148, 169	0
4	I	27/27 (100%)	1.05	6 (22%) 0 0	62, 77, 146, 160	0
5	E	25/25 (100%)	0.69	2 (8%) 12 10	62, 83, 128, 148	0
5	J	25/25 (100%)	0.52	2 (8%) 12 10	60, 85, 126, 153	0
All	All	1240/1608 (77%)	0.73	143 (11%) 4 4	46, 79, 133, 169	22 (1%)

All (143) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	248	ALA	7.1
1	A	188	SER	6.9
1	A	187	PRO	6.9
1	A	380	GLY	6.2
2	G	241	VAL	5.9
4	D	27	A	5.8
2	B	178	LEU	5.6
2	B	248	ALA	5.5
4	I	27	A	5.5
1	A	402	PHE	5.4
3	C	375	LEU	5.2
1	F	404	ARG	5.1
2	B	205	ARG	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	355	ALA	5.0
4	I	2	DG	5.0
5	E	2	DT	4.9
2	B	174	LEU	4.6
3	C	369	HIS	4.6
1	F	312	PHE	4.6
1	A	189	VAL	4.5
1	A	387	SER	4.5
3	H	298	TYR	4.5
2	B	175	GLY	4.5
3	C	356	PHE	4.5
1	A	191	ALA	4.4
2	G	175	GLY	4.3
2	B	196	ARG	4.2
2	B	244	LEU	4.2
3	C	379	GLU	4.2
1	A	313	ARG	4.2
1	F	245	CYS	4.2
1	A	316	THR	4.2
1	F	391	GLN	4.2
3	C	374	VAL	4.2
3	C	380	LYS	4.1
1	A	244	SER	4.1
3	H	364	PHE	4.0
3	C	362	PHE	4.0
2	G	242	GLN	4.0
1	F	246	SER	4.0
3	C	382	LYS	3.9
1	F	151	SER	3.8
1	A	375	VAL	3.8
2	G	244	LEU	3.7
4	D	28	DC	3.7
3	C	311	PHE	3.7
4	D	26	A	3.6
1	F	378	VAL	3.6
2	G	323	GLU	3.6
2	B	241	VAL	3.6
1	F	254	ALA	3.5
3	H	354	LYS	3.5
1	A	393	LEU	3.5
2	G	237	TYR	3.4
3	C	298	TYR	3.4

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Mol	Chain	Res	Type	RSRZ
4	I	28	DC	3.4
3	C	317	MET	3.4
3	H	296	LYS	3.3
1	A	190	PRO	3.3
3	C	357	GLN	3.2
2	G	246	PHE	3.2
1	A	297	ILE	3.2
1	F	388	GLU	3.2
4	I	26	A	3.1
2	G	240	VAL	3.1
1	A	379	THR	3.1
1	F	405	ALA	3.1
1	A	315	GLY	3.0
1	A	151	SER	3.0
1	A	314	ASP	3.0
3	C	364	PHE	3.0
3	H	356	PHE	3.0
3	C	376	ALA	3.0
1	A	390	GLU	3.0
2	G	184	ALA	3.0
2	B	199	ALA	2.9
2	G	251	LEU	2.9
2	G	161	ILE	2.9
1	F	381	ASP	2.9
1	A	185	ALA	2.9
3	H	350	TRP	2.8
4	D	2	DG	2.8
1	A	404	ARG	2.8
3	C	378	GLU	2.8
3	C	313	LEU	2.8
1	A	354	PRO	2.8
2	G	174	LEU	2.8
1	A	405	ALA	2.8
1	A	317	ALA	2.7
1	F	187	PRO	2.7
1	A	388	GLU	2.7
4	D	4	DT	2.7
1	A	240	ALA	2.7
4	I	25	C	2.7
2	B	185	LEU	2.7
2	G	249	LYS	2.7
1	F	401	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
4	I	3	DG	2.6
3	C	367	PHE	2.6
1	F	382	GLU	2.6
3	C	310	MET	2.6
5	J	2	DT	2.6
1	F	379	THR	2.5
1	A	318	GLU	2.5
1	F	179	SER	2.5
1	F	104	SER	2.5
2	G	227	GLU	2.4
1	F	189	VAL	2.4
5	E	3	DT	2.3
1	A	231	PHE	2.3
2	G	312	LEU	2.3
1	F	311	ALA	2.3
2	G	173	ASN	2.3
2	G	178	LEU	2.3
1	A	104	SER	2.3
1	A	391	GLN	2.3
2	B	176	CYS	2.3
3	C	358	GLU	2.2
2	B	254	LYS	2.2
2	B	186	ARG	2.2
1	F	398	GLU	2.2
1	F	150	SER	2.2
1	F	159	LEU	2.2
1	A	252	LYS	2.2
2	G	177	LYS	2.2
3	C	360	ARG	2.2
1	F	280	LEU	2.2
1	F	147	ASP	2.2
5	J	10	C	2.2
2	B	249	LYS	2.2
1	A	250	PHE	2.2
2	B	157	GLY	2.1
2	G	199	ALA	2.1
1	A	156	ILE	2.1
3	C	359	LYS	2.1
2	B	214	PHE	2.1
2	B	172	VAL	2.1
1	A	254	ALA	2.1
1	F	192	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
2	G	232	LEU	2.1
1	A	394	ARG	2.1
3	C	368	ALA	2.0
1	F	158	LYS	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 carbohydrates 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(\AA^2)	Q<0.9
6	NA	H	401	1/1	0.87	0.18	83,83,83,83	0

6.5 Other polymers [i](#)

There are no such residues in this entry.