



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:15 PM GMT

PDB ID : 3SN9  
Title : Fic protein from NEISSERIA MENINGITIDIS mutant S182A/E186A in complex with AMPPNP  
Authors : Goepfert, A.; Stanger, F.; Schirmer, T.  
Deposited on : 2011-06-29  
Resolution : 3.03 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

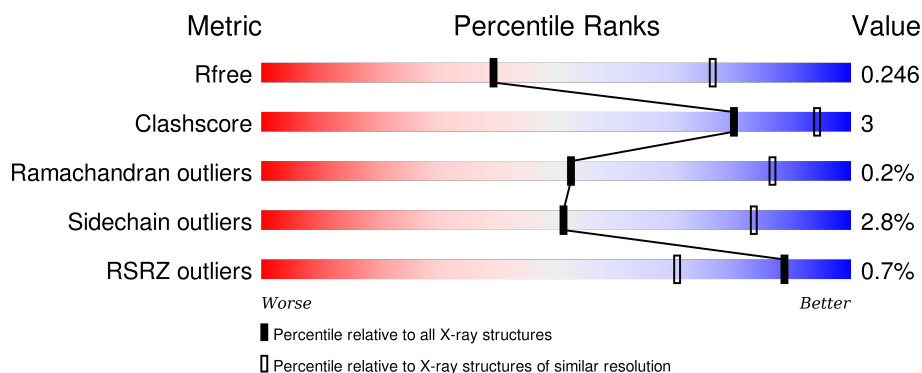
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.03 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))
$R_{free}$	91344	1995 (3.08-3.00)
Clashscore	102246	2351 (3.08-3.00)
Ramachandran outliers	100387	2272 (3.08-3.00)
Sidechain outliers	100360	2275 (3.08-3.00)
RSRZ outliers	91569	2013 (3.08-3.00)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	188	<div> <div>76%</div> <div>7% • 16%</div> </div>
1	B	188	<div> <div>77%</div> <div>7% • 16%</div> </div>
1	C	188	<div> <div>%</div> <div>78% • • 16%</div> </div>
1	D	188	<div> <div>74%</div> <div>9% • 16%</div> </div>
1	E	188	<div> <div>%</div> <div>74% 9% • 16%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	188	 74% 10% • 16%
1	G	188	 76% 7% • 16%
1	H	188	 77% 6% • 16%
1	I	188	 76% 7% • 16%
1	J	188	 76% 7% • 16%
1	K	188	 78% 5% • 16%
1	L	188	 78% 5% • 16%
1	M	188	 77% 6% • 16%
1	N	188	 78% 5% • 16%
1	O	188	 77% 6% • 16%
1	P	188	 80% • • 16%

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 21120 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 Cell filamentation protein Fic-related protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	158	Total	C	N	O	S	0	0	0
			1289	819	226	240	4			
1	B	158	Total	C	N	O	S	0	0	0
			1289	819	226	240	4			
1	C	158	Total	C	N	O	S	0	0	0
			1289	819	226	240	4			
1	D	158	Total	C	N	O	S	0	0	0
			1289	819	226	240	4			
1	E	158	Total	C	N	O	S	0	0	0
			1289	819	226	240	4			
1	F	158	Total	C	N	O	S	0	0	0
			1289	819	226	240	4			
1	G	158	Total	C	N	O	S	0	0	0
			1289	819	226	240	4			
1	H	158	Total	C	N	O	S	0	0	0
			1289	819	226	240	4			
1	I	158	Total	C	N	O	S	0	0	0
			1289	819	226	240	4			
1	J	158	Total	C	N	O	S	0	0	0
			1289	819	226	240	4			
1	K	158	Total	C	N	O	S	0	0	0
			1289	819	226	240	4			
1	L	158	Total	C	N	O	S	0	0	0
			1289	819	226	240	4			
1	M	158	Total	C	N	O	S	0	0	0
			1289	819	226	240	4			
1	N	158	Total	C	N	O	S	0	0	0
			1289	819	226	240	4			
1	O	158	Total	C	N	O	S	0	0	0
			1289	819	226	240	4			
1	P	158	Total	C	N	O	S	0	0	0
			1289	819	226	240	4			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	MET	-	EXPRESSION TAG	UNP Q7DDR9
A	5	HIS	-	EXPRESSION TAG	UNP Q7DDR9
A	6	HIS	-	EXPRESSION TAG	UNP Q7DDR9
A	7	HIS	-	EXPRESSION TAG	UNP Q7DDR9
A	8	HIS	-	EXPRESSION TAG	UNP Q7DDR9
A	9	HIS	-	EXPRESSION TAG	UNP Q7DDR9
A	10	HIS	-	EXPRESSION TAG	UNP Q7DDR9
A	182	ALA	SER	ENGINEERED MUTATION	UNP Q7DDR9
A	186	ALA	GLU	ENGINEERED MUTATION	UNP Q7DDR9
B	4	MET	-	EXPRESSION TAG	UNP Q7DDR9
B	5	HIS	-	EXPRESSION TAG	UNP Q7DDR9
B	6	HIS	-	EXPRESSION TAG	UNP Q7DDR9
B	7	HIS	-	EXPRESSION TAG	UNP Q7DDR9
B	8	HIS	-	EXPRESSION TAG	UNP Q7DDR9
B	9	HIS	-	EXPRESSION TAG	UNP Q7DDR9
B	10	HIS	-	EXPRESSION TAG	UNP Q7DDR9
B	182	ALA	SER	ENGINEERED MUTATION	UNP Q7DDR9
B	186	ALA	GLU	ENGINEERED MUTATION	UNP Q7DDR9
C	4	MET	-	EXPRESSION TAG	UNP Q7DDR9
C	5	HIS	-	EXPRESSION TAG	UNP Q7DDR9
C	6	HIS	-	EXPRESSION TAG	UNP Q7DDR9
C	7	HIS	-	EXPRESSION TAG	UNP Q7DDR9
C	8	HIS	-	EXPRESSION TAG	UNP Q7DDR9
C	9	HIS	-	EXPRESSION TAG	UNP Q7DDR9
C	10	HIS	-	EXPRESSION TAG	UNP Q7DDR9
C	182	ALA	SER	ENGINEERED MUTATION	UNP Q7DDR9
C	186	ALA	GLU	ENGINEERED MUTATION	UNP Q7DDR9
D	4	MET	-	EXPRESSION TAG	UNP Q7DDR9
D	5	HIS	-	EXPRESSION TAG	UNP Q7DDR9
D	6	HIS	-	EXPRESSION TAG	UNP Q7DDR9
D	7	HIS	-	EXPRESSION TAG	UNP Q7DDR9
D	8	HIS	-	EXPRESSION TAG	UNP Q7DDR9
D	9	HIS	-	EXPRESSION TAG	UNP Q7DDR9
D	10	HIS	-	EXPRESSION TAG	UNP Q7DDR9
D	182	ALA	SER	ENGINEERED MUTATION	UNP Q7DDR9
D	186	ALA	GLU	ENGINEERED MUTATION	UNP Q7DDR9
E	4	MET	-	EXPRESSION TAG	UNP Q7DDR9
E	5	HIS	-	EXPRESSION TAG	UNP Q7DDR9
E	6	HIS	-	EXPRESSION TAG	UNP Q7DDR9
E	7	HIS	-	EXPRESSION TAG	UNP Q7DDR9
E	8	HIS	-	EXPRESSION TAG	UNP Q7DDR9
E	9	HIS	-	EXPRESSION TAG	UNP Q7DDR9

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Chain	Residue	Modelled	Actual	Comment	Reference
E	10	HIS	-	EXPRESSION TAG	UNP Q7DDR9
E	182	ALA	SER	ENGINEERED MUTATION	UNP Q7DDR9
E	186	ALA	GLU	ENGINEERED MUTATION	UNP Q7DDR9
F	4	MET	-	EXPRESSION TAG	UNP Q7DDR9
F	5	HIS	-	EXPRESSION TAG	UNP Q7DDR9
F	6	HIS	-	EXPRESSION TAG	UNP Q7DDR9
F	7	HIS	-	EXPRESSION TAG	UNP Q7DDR9
F	8	HIS	-	EXPRESSION TAG	UNP Q7DDR9
F	9	HIS	-	EXPRESSION TAG	UNP Q7DDR9
F	10	HIS	-	EXPRESSION TAG	UNP Q7DDR9
F	182	ALA	SER	ENGINEERED MUTATION	UNP Q7DDR9
F	186	ALA	GLU	ENGINEERED MUTATION	UNP Q7DDR9
G	4	MET	-	EXPRESSION TAG	UNP Q7DDR9
G	5	HIS	-	EXPRESSION TAG	UNP Q7DDR9
G	6	HIS	-	EXPRESSION TAG	UNP Q7DDR9
G	7	HIS	-	EXPRESSION TAG	UNP Q7DDR9
G	8	HIS	-	EXPRESSION TAG	UNP Q7DDR9
G	9	HIS	-	EXPRESSION TAG	UNP Q7DDR9
G	10	HIS	-	EXPRESSION TAG	UNP Q7DDR9
G	182	ALA	SER	ENGINEERED MUTATION	UNP Q7DDR9
G	186	ALA	GLU	ENGINEERED MUTATION	UNP Q7DDR9
H	4	MET	-	EXPRESSION TAG	UNP Q7DDR9
H	5	HIS	-	EXPRESSION TAG	UNP Q7DDR9
H	6	HIS	-	EXPRESSION TAG	UNP Q7DDR9
H	7	HIS	-	EXPRESSION TAG	UNP Q7DDR9
H	8	HIS	-	EXPRESSION TAG	UNP Q7DDR9
H	9	HIS	-	EXPRESSION TAG	UNP Q7DDR9
H	10	HIS	-	EXPRESSION TAG	UNP Q7DDR9
H	182	ALA	SER	ENGINEERED MUTATION	UNP Q7DDR9
H	186	ALA	GLU	ENGINEERED MUTATION	UNP Q7DDR9
I	4	MET	-	EXPRESSION TAG	UNP Q7DDR9
I	5	HIS	-	EXPRESSION TAG	UNP Q7DDR9
I	6	HIS	-	EXPRESSION TAG	UNP Q7DDR9
I	7	HIS	-	EXPRESSION TAG	UNP Q7DDR9
I	8	HIS	-	EXPRESSION TAG	UNP Q7DDR9
I	9	HIS	-	EXPRESSION TAG	UNP Q7DDR9
I	10	HIS	-	EXPRESSION TAG	UNP Q7DDR9
I	182	ALA	SER	ENGINEERED MUTATION	UNP Q7DDR9
I	186	ALA	GLU	ENGINEERED MUTATION	UNP Q7DDR9
J	4	MET	-	EXPRESSION TAG	UNP Q7DDR9
J	5	HIS	-	EXPRESSION TAG	UNP Q7DDR9
J	6	HIS	-	EXPRESSION TAG	UNP Q7DDR9

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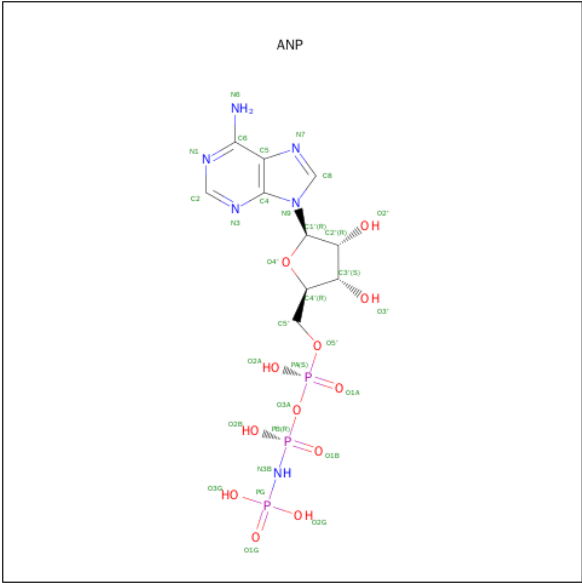
Chain	Residue	Modelled	Actual	Comment	Reference
J	7	HIS	-	EXPRESSION TAG	UNP Q7DDR9
J	8	HIS	-	EXPRESSION TAG	UNP Q7DDR9
J	9	HIS	-	EXPRESSION TAG	UNP Q7DDR9
J	10	HIS	-	EXPRESSION TAG	UNP Q7DDR9
J	182	ALA	SER	ENGINEERED MUTATION	UNP Q7DDR9
J	186	ALA	GLU	ENGINEERED MUTATION	UNP Q7DDR9
K	4	MET	-	EXPRESSION TAG	UNP Q7DDR9
K	5	HIS	-	EXPRESSION TAG	UNP Q7DDR9
K	6	HIS	-	EXPRESSION TAG	UNP Q7DDR9
K	7	HIS	-	EXPRESSION TAG	UNP Q7DDR9
K	8	HIS	-	EXPRESSION TAG	UNP Q7DDR9
K	9	HIS	-	EXPRESSION TAG	UNP Q7DDR9
K	10	HIS	-	EXPRESSION TAG	UNP Q7DDR9
K	182	ALA	SER	ENGINEERED MUTATION	UNP Q7DDR9
K	186	ALA	GLU	ENGINEERED MUTATION	UNP Q7DDR9
L	4	MET	-	EXPRESSION TAG	UNP Q7DDR9
L	5	HIS	-	EXPRESSION TAG	UNP Q7DDR9
L	6	HIS	-	EXPRESSION TAG	UNP Q7DDR9
L	7	HIS	-	EXPRESSION TAG	UNP Q7DDR9
L	8	HIS	-	EXPRESSION TAG	UNP Q7DDR9
L	9	HIS	-	EXPRESSION TAG	UNP Q7DDR9
L	10	HIS	-	EXPRESSION TAG	UNP Q7DDR9
L	182	ALA	SER	ENGINEERED MUTATION	UNP Q7DDR9
L	186	ALA	GLU	ENGINEERED MUTATION	UNP Q7DDR9
M	4	MET	-	EXPRESSION TAG	UNP Q7DDR9
M	5	HIS	-	EXPRESSION TAG	UNP Q7DDR9
M	6	HIS	-	EXPRESSION TAG	UNP Q7DDR9
M	7	HIS	-	EXPRESSION TAG	UNP Q7DDR9
M	8	HIS	-	EXPRESSION TAG	UNP Q7DDR9
M	9	HIS	-	EXPRESSION TAG	UNP Q7DDR9
M	10	HIS	-	EXPRESSION TAG	UNP Q7DDR9
M	182	ALA	SER	ENGINEERED MUTATION	UNP Q7DDR9
M	186	ALA	GLU	ENGINEERED MUTATION	UNP Q7DDR9
N	4	MET	-	EXPRESSION TAG	UNP Q7DDR9
N	5	HIS	-	EXPRESSION TAG	UNP Q7DDR9
N	6	HIS	-	EXPRESSION TAG	UNP Q7DDR9
N	7	HIS	-	EXPRESSION TAG	UNP Q7DDR9
N	8	HIS	-	EXPRESSION TAG	UNP Q7DDR9
N	9	HIS	-	EXPRESSION TAG	UNP Q7DDR9
N	10	HIS	-	EXPRESSION TAG	UNP Q7DDR9
N	182	ALA	SER	ENGINEERED MUTATION	UNP Q7DDR9
N	186	ALA	GLU	ENGINEERED MUTATION	UNP Q7DDR9

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Chain	Residue	Modelled	Actual	Comment	Reference
O	4	MET	-	EXPRESSION TAG	UNP Q7DDR9
O	5	HIS	-	EXPRESSION TAG	UNP Q7DDR9
O	6	HIS	-	EXPRESSION TAG	UNP Q7DDR9
O	7	HIS	-	EXPRESSION TAG	UNP Q7DDR9
O	8	HIS	-	EXPRESSION TAG	UNP Q7DDR9
O	9	HIS	-	EXPRESSION TAG	UNP Q7DDR9
O	10	HIS	-	EXPRESSION TAG	UNP Q7DDR9
O	182	ALA	SER	ENGINEERED MUTATION	UNP Q7DDR9
O	186	ALA	GLU	ENGINEERED MUTATION	UNP Q7DDR9
P	4	MET	-	EXPRESSION TAG	UNP Q7DDR9
P	5	HIS	-	EXPRESSION TAG	UNP Q7DDR9
P	6	HIS	-	EXPRESSION TAG	UNP Q7DDR9
P	7	HIS	-	EXPRESSION TAG	UNP Q7DDR9
P	8	HIS	-	EXPRESSION TAG	UNP Q7DDR9
P	9	HIS	-	EXPRESSION TAG	UNP Q7DDR9
P	10	HIS	-	EXPRESSION TAG	UNP Q7DDR9
P	182	ALA	SER	ENGINEERED MUTATION	UNP Q7DDR9
P	186	ALA	GLU	ENGINEERED MUTATION	UNP Q7DDR9

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>12</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

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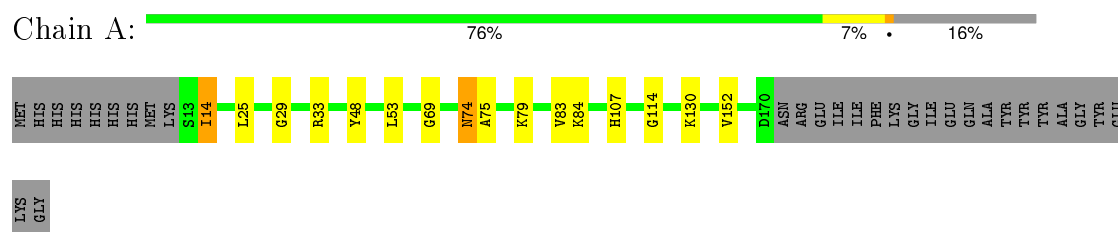
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total 31	C 10	N 6	O 12	P 3	0	0
2	D	1	Total 31	C 10	N 6	O 12	P 3	0	0
2	E	1	Total 31	C 10	N 6	O 12	P 3	0	0
2	F	1	Total 31	C 10	N 6	O 12	P 3	0	0
2	G	1	Total 31	C 10	N 6	O 12	P 3	0	0
2	H	1	Total 31	C 10	N 6	O 12	P 3	0	0
2	I	1	Total 31	C 10	N 6	O 12	P 3	0	0
2	J	1	Total 31	C 10	N 6	O 12	P 3	0	0
2	K	1	Total 31	C 10	N 6	O 12	P 3	0	0
2	L	1	Total 31	C 10	N 6	O 12	P 3	0	0
2	M	1	Total 31	C 10	N 6	O 12	P 3	0	0
2	N	1	Total 31	C 10	N 6	O 12	P 3	0	0
2	O	1	Total 31	C 10	N 6	O 12	P 3	0	0
2	P	1	Total 31	C 10	N 6	O 12	P 3	0	0

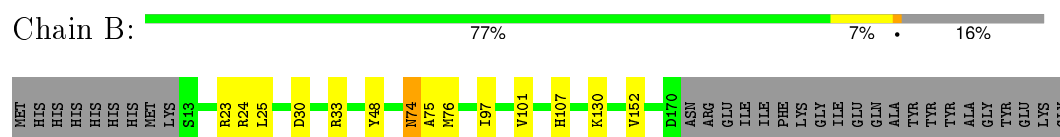
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

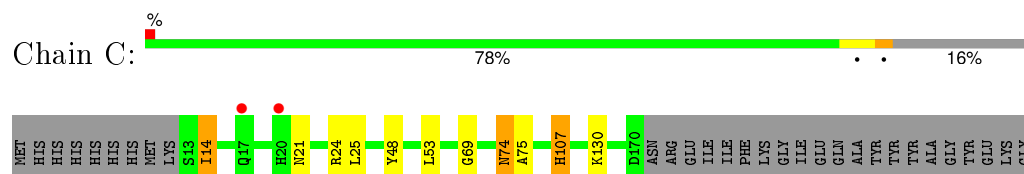
- Molecule 1: Cell filamentation protein Fic-related protein



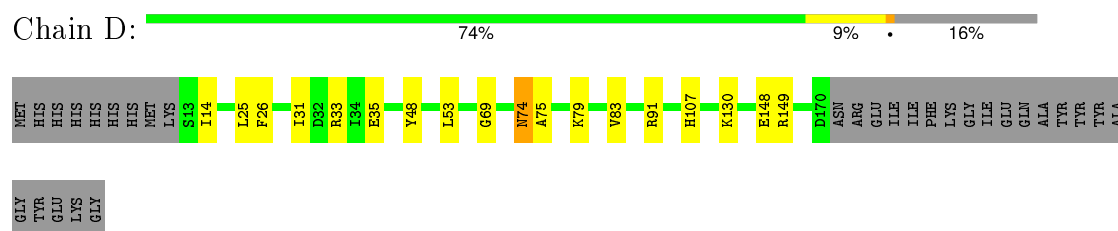
- Molecule 1: Cell filamentation protein Fic-related protein



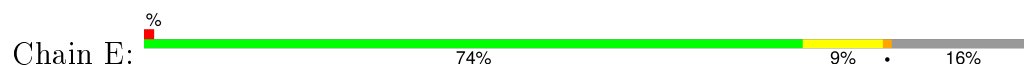
- Molecule 1: Cell filamentation protein Fic-related protein

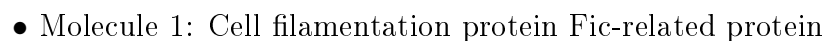
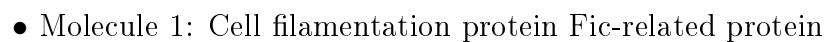
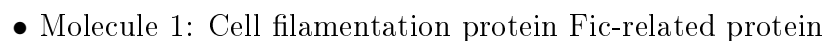


- Molecule 1: Cell filamentation protein Fic-related protein

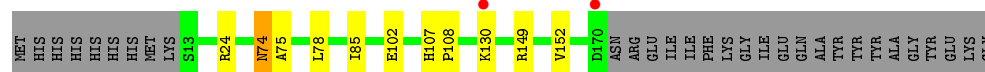
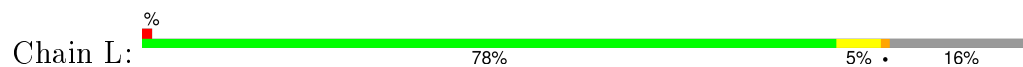


- Molecule 1: Cell filamentation protein Fic-related protein

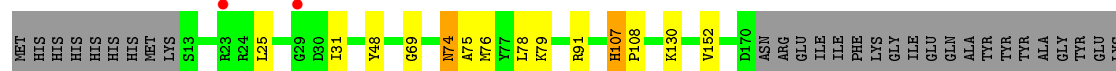
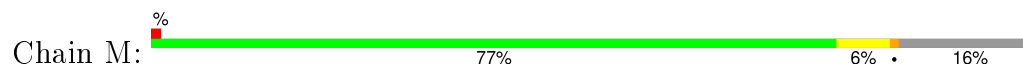




- Molecule 1: Cell filamentation protein Fic-related protein

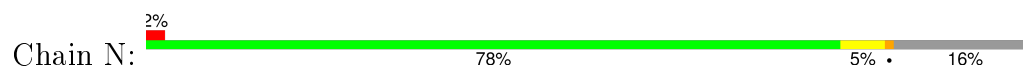


- Molecule 1: Cell filamentation protein Fic-related protein

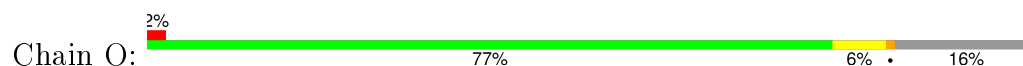


GLY

- Molecule 1: Cell filamentation protein Fic-related protein

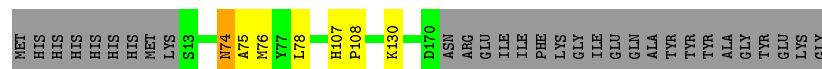
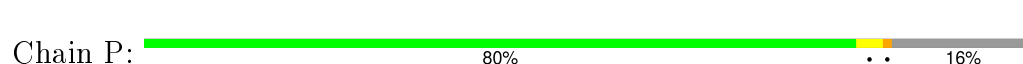


- Molecule 1: Cell filamentation protein Fic-related protein



GLU  
LYS  
GLY

- Molecule 1: Cell filamentation protein Fic-related protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	110.31Å 136.92Å 114.66Å 90.00° 100.26° 90.00°	Depositor
Resolution (Å)	15.00 – 3.03 87.07 – 3.03	Depositor EDS
% Data completeness (in resolution range)	89.9 (15.00-3.03) 90.0 (87.07-3.03)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.98 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.222 , 0.248 0.225 , 0.246	Depositor DCC
$R_{free}$ test set	2943 reflections (5.36%)	DCC
Wilson B-factor (Å <sup>2</sup> )	61.7	Xtriage
Anisotropy	0.220	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 41.5	EDS
Estimated twinning fraction	0.035 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 58464 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	21120	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.06% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: ANP

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	0.45	0/1311	0.55	0/1765
1	B	0.46	0/1311	0.55	0/1765
1	C	0.49	0/1311	0.56	0/1765
1	D	0.49	0/1311	0.57	1/1765 (0.1%)
1	E	0.51	0/1311	0.57	0/1765
1	F	0.47	0/1311	0.53	0/1765
1	G	0.46	0/1311	0.53	0/1765
1	H	0.48	0/1311	0.56	0/1765
1	I	0.45	0/1311	0.55	0/1765
1	J	0.44	0/1311	0.56	0/1765
1	K	0.43	0/1311	0.55	0/1765
1	L	0.40	0/1311	0.52	0/1765
1	M	0.42	0/1311	0.54	0/1765
1	N	0.42	0/1311	0.55	0/1765
1	O	0.38	0/1311	0.51	0/1765
1	P	0.40	0/1311	0.53	0/1765
All	All	0.45	0/20976	0.55	1/28240 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	91	ARG	NE-CZ-NH1	5.07	122.84	120.30

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	1289	0	1285	13	0
1	B	1289	0	1285	9	0
1	C	1289	0	1285	8	0
1	D	1289	0	1285	17	0
1	E	1289	0	1285	19	0
1	F	1289	0	1285	20	0
1	G	1289	0	1285	11	0
1	H	1289	0	1285	15	0
1	I	1289	0	1285	16	0
1	J	1289	0	1285	12	0
1	K	1289	0	1285	4	0
1	L	1289	0	1285	8	0
1	M	1289	0	1285	19	0
1	N	1289	0	1285	6	0
1	O	1289	0	1285	8	0
1	P	1289	0	1285	3	0
2	A	31	0	13	1	0
2	B	31	0	13	0	0
2	C	31	0	13	1	0
2	D	31	0	13	1	0
2	E	31	0	13	0	0
2	F	31	0	13	1	0
2	G	31	0	13	0	0
2	H	31	0	13	1	0
2	I	31	0	13	0	0
2	J	31	0	13	1	0
2	K	31	0	13	0	0
2	L	31	0	13	0	0
2	M	31	0	13	1	0
2	N	31	0	13	1	0
2	O	31	0	13	0	0
2	P	31	0	13	0	0
All	All	21120	0	20768	141	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 3.

All (141) 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:D:35:GLU:HB2	1:F:44:GLN:HE21	1.36	0.91
1:E:14:ILE:HD12	1:E:53:LEU:HD22	1.57	0.86
1:A:84:LYS:NZ	1:H:167:ASP:HB2	1.95	0.81
1:A:84:LYS:HZ3	1:H:167:ASP:HB2	1.45	0.81
1:E:14:ILE:HG23	1:E:53:LEU:HD13	1.64	0.80
1:C:14:ILE:HD13	1:C:53:LEU:HB3	1.69	0.73
1:G:69:GLY:HA2	1:L:152:VAL:HG21	1.71	0.71
1:D:35:GLU:HB2	1:F:44:GLN:NE2	2.04	0.71
1:I:30:ASP:HA	1:I:33:ARG:HH11	1.55	0.71
1:C:69:GLY:HA2	1:E:152:VAL:HG21	1.73	0.69
1:E:79:LYS:HZ3	1:M:91:ARG:NH2	1.89	0.69
1:D:35:GLU:CB	1:F:44:GLN:HE21	2.06	0.69
1:B:152:VAL:HG21	1:D:69:GLY:HA2	1.76	0.67
1:E:79:LYS:NZ	1:M:91:ARG:CZ	2.59	0.66
1:D:79:LYS:HD3	1:F:79:LYS:HE2	1.79	0.64
1:E:74:ASN:HD22	1:E:75:ALA:N	1.94	0.64
1:E:79:LYS:NZ	1:M:91:ARG:NH2	2.45	0.64
1:B:30:ASP:HA	1:B:33:ARG:NH1	2.13	0.64
1:F:30:ASP:HA	1:F:33:ARG:HH11	1.63	0.64
1:I:30:ASP:HA	1:I:33:ARG:NH1	2.13	0.63
1:D:14:ILE:CD1	1:D:53:LEU:HB3	2.28	0.63
1:E:79:LYS:HZ3	1:M:91:ARG:CZ	2.12	0.63
1:H:168:ASP:OD1	1:M:79:LYS:HE2	1.99	0.62
1:E:14:ILE:O	1:E:16:GLU:N	2.33	0.62
1:G:14:ILE:HD12	1:G:53:LEU:HB3	1.82	0.62
1:C:24:ARG:NH1	1:J:29:GLY:HA3	2.15	0.61
1:P:74:ASN:HD22	1:P:75:ALA:N	1.99	0.61
1:B:30:ASP:HA	1:B:33:ARG:HH11	1.65	0.61
1:G:74:ASN:HD22	1:G:75:ALA:N	1.99	0.61
1:H:167:ASP:OD2	1:M:76:MET:HA	2.01	0.60
1:J:74:ASN:HD22	1:J:75:ALA:N	1.99	0.60
1:M:74:ASN:HD22	1:M:75:ALA:N	2.00	0.59
1:B:74:ASN:HD22	1:B:75:ALA:N	1.99	0.59
1:O:74:ASN:HD22	1:O:75:ALA:N	2.00	0.59
1:A:74:ASN:HD22	1:A:75:ALA:N	1.99	0.59
1:C:107:HIS:HE1	2:C:300:ANP:O4'	1.85	0.59
1:F:74:ASN:HD22	1:F:75:ALA:N	2.01	0.58
1:K:74:ASN:HD22	1:K:75:ALA:N	2.01	0.58
1:I:74:ASN:HD22	1:I:75:ALA:N	2.00	0.58
1:N:74:ASN:HD22	1:N:75:ALA:N	1.99	0.58
1:E:62:GLU:OE1	1:M:91:ARG:NH2	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:74:ASN:HD22	1:L:75:ALA:N	2.02	0.57
1:C:24:ARG:HH12	1:J:29:GLY:HA3	1.69	0.57
1:D:74:ASN:HD22	1:D:75:ALA:N	2.03	0.57
1:C:74:ASN:HD22	1:C:75:ALA:N	2.03	0.56
1:H:74:ASN:HD22	1:H:75:ALA:N	2.03	0.56
1:D:35:GLU:OE1	1:F:47:ARG:NH1	2.39	0.56
1:D:14:ILE:HD12	1:D:53:LEU:HB3	1.86	0.56
1:A:84:LYS:NZ	1:H:167:ASP:CB	2.66	0.55
1:I:24:ARG:CZ	1:J:32:ASP:HB2	2.36	0.55
1:C:21:ASN:ND2	1:I:33:ARG:HH21	2.04	0.55
1:I:102:GLU:OE2	1:O:71:ARG:NH1	2.36	0.55
1:G:25:LEU:HD13	1:G:48:TYR:CD2	2.41	0.54
1:H:25:LEU:HD13	1:H:48:TYR:CG	2.43	0.53
1:N:107:HIS:HE1	2:N:300:ANP:O4'	1.91	0.53
1:A:14:ILE:HD13	1:A:53:LEU:HB3	1.90	0.53
1:A:84:LYS:HZ3	1:H:167:ASP:CB	2.20	0.52
1:E:60:ILE:O	1:M:91:ARG:NH1	2.42	0.52
1:F:30:ASP:HA	1:F:33:ARG:NH1	2.26	0.51
1:I:24:ARG:NH1	1:I:28:SER:HB3	2.26	0.51
1:J:14:ILE:HD13	1:J:53:LEU:HB3	1.92	0.51
1:I:24:ARG:NH1	1:J:32:ASP:CB	2.74	0.50
1:H:25:LEU:HD13	1:H:48:TYR:CD2	2.45	0.50
1:F:25:LEU:HD13	1:F:48:TYR:CD2	2.47	0.50
1:A:69:GLY:HA2	1:M:152:VAL:HG21	1.94	0.50
1:A:152:VAL:HG21	1:M:69:GLY:HA2	1.93	0.50
1:J:25:LEU:HD13	1:J:48:TYR:CD2	2.47	0.49
1:M:25:LEU:HD13	1:M:48:TYR:CD2	2.47	0.49
1:F:69:GLY:HA2	1:H:152:VAL:HG21	1.94	0.49
1:B:24:ARG:O	1:B:25:LEU:C	2.51	0.49
1:E:14:ILE:HD12	1:E:53:LEU:CD2	2.38	0.49
1:F:25:LEU:HD13	1:F:48:TYR:CG	2.47	0.49
1:D:83:VAL:HG13	1:F:59:GLN:NE2	2.27	0.48
1:G:76:MET:HE1	1:L:85:ILE:HA	1.96	0.48
1:G:71:ARG:NH1	1:L:102:GLU:OE2	2.38	0.48
1:B:25:LEU:HD13	1:B:48:TYR:CG	2.47	0.48
1:B:74:ASN:HD22	1:B:76:MET:H	1.62	0.47
1:F:152:VAL:HG21	1:H:69:GLY:HA2	1.95	0.47
1:G:25:LEU:HD13	1:G:48:TYR:CG	2.50	0.47
1:E:14:ILE:O	1:E:17:GLN:N	2.48	0.47
1:I:24:ARG:HH12	1:I:28:SER:HB3	1.78	0.46
1:J:14:ILE:HG22	1:J:15:ASP:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:152:VAL:HG21	1:O:69:GLY:HA2	1.97	0.46
1:P:78:LEU:HD21	1:P:108:PRO:HA	1.98	0.46
1:M:25:LEU:HD13	1:M:48:TYR:CG	2.51	0.46
1:H:168:ASP:HA	1:M:79:LYS:HZ3	1.81	0.45
1:A:29:GLY:O	1:A:33:ARG:NH1	2.49	0.45
1:F:74:ASN:HD22	1:F:76:MET:H	1.64	0.45
1:A:114:GLY:HA3	2:A:300:ANP:O3G	2.16	0.45
1:M:74:ASN:HD22	1:M:76:MET:H	1.64	0.45
1:D:149:ARG:NH2	1:L:149:ARG:HB2	2.31	0.45
1:E:13:SER:O	1:E:14:ILE:C	2.56	0.44
1:J:74:ASN:HD22	1:J:76:MET:H	1.66	0.44
1:I:78:LEU:HD21	1:I:108:PRO:HA	2.00	0.44
1:C:25:LEU:HD13	1:C:48:TYR:CG	2.52	0.44
1:I:71:ARG:HD3	1:O:151:PRO:O	2.17	0.44
1:K:78:LEU:HD21	1:K:108:PRO:HA	2.00	0.44
1:H:74:ASN:HD22	1:H:76:MET:H	1.64	0.43
1:B:97:ILE:O	1:B:101:VAL:HG23	2.18	0.43
1:E:14:ILE:C	1:E:16:GLU:H	2.22	0.43
1:E:14:ILE:CD1	1:E:53:LEU:HD22	2.41	0.43
1:D:35:GLU:CA	1:F:44:GLN:HE21	2.30	0.43
1:A:84:LYS:HZ2	1:H:167:ASP:HB2	1.78	0.43
1:F:113:ASN:HB2	2:F:300:ANP:O1A	2.19	0.43
1:J:114:GLY:HA3	2:J:300:ANP:O3G	2.19	0.43
1:A:25:LEU:HD13	1:A:48:TYR:CG	2.53	0.43
1:I:69:GLY:HA2	1:O:152:VAL:HG21	2.01	0.43
1:N:97:ILE:O	1:N:101:VAL:HG23	2.19	0.43
1:F:78:LEU:HD21	1:F:108:PRO:HA	2.01	0.42
1:D:35:GLU:HB2	1:F:44:GLN:HG2	2.01	0.42
1:K:29:GLY:O	1:K:33:ARG:NH1	2.52	0.42
1:E:149:ARG:NH2	1:N:149:ARG:HB2	2.34	0.42
1:I:76:MET:HE1	1:O:85:ILE:HA	2.01	0.42
1:G:13:SER:O	1:G:16:GLU:N	2.52	0.42
1:L:78:LEU:HD21	1:L:108:PRO:HA	2.00	0.42
1:N:25:LEU:HD13	1:N:48:TYR:CD2	2.54	0.42
1:E:74:ASN:C	1:E:74:ASN:HD22	2.22	0.42
1:O:78:LEU:HD21	1:O:108:PRO:HA	2.01	0.42
1:M:25:LEU:HD23	1:M:31:ILE:HD13	2.01	0.42
1:O:80:GLU:OE1	1:O:80:GLU:N	2.49	0.42
1:F:79:LYS:O	1:F:83:VAL:HG23	2.20	0.41
1:I:74:ASN:HD22	1:I:76:MET:H	1.69	0.41
1:M:78:LEU:HD21	1:M:108:PRO:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:25:LEU:HD13	1:D:48:TYR:CG	2.55	0.41
1:G:69:GLY:CA	1:L:152:VAL:HG21	2.47	0.41
1:I:24:ARG:CZ	1:J:32:ASP:CB	2.98	0.41
1:E:97:ILE:O	1:E:101:VAL:HG23	2.21	0.41
1:P:74:ASN:HD22	1:P:76:MET:H	1.67	0.41
1:B:25:LEU:HD13	1:B:48:TYR:CD2	2.56	0.41
1:N:74:ASN:HD22	1:N:76:MET:H	1.68	0.41
1:G:76:MET:CE	1:L:85:ILE:HA	2.51	0.41
1:D:26:PHE:CE1	1:D:31:ILE:HG12	2.55	0.41
1:G:78:LEU:HD21	1:G:108:PRO:HA	2.02	0.41
1:J:13:SER:CB	1:J:17:GLN:HE21	2.33	0.41
1:M:107:HIS:HE1	2:M:300:ANP:O4'	2.04	0.41
1:M:74:ASN:ND2	1:M:76:MET:H	2.19	0.40
1:H:114:GLY:HA3	2:H:300:ANP:O3G	2.21	0.40
1:D:35:GLU:OE2	1:F:44:GLN:HA	2.22	0.40
1:A:79:LYS:O	1:A:83:VAL:HG23	2.21	0.40
1:D:148:GLU:HA	2:D:300:ANP:N1	2.37	0.40
1:K:74:ASN:HD22	1:K:76:MET:H	1.68	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	156/188 (83%)	155 (99%)	0	1 (1%)	30	70
1	B	156/188 (83%)	155 (99%)	1 (1%)	0	100	100
1	C	156/188 (83%)	155 (99%)	1 (1%)	0	100	100
1	D	156/188 (83%)	155 (99%)	1 (1%)	0	100	100
1	E	156/188 (83%)	153 (98%)	1 (1%)	2 (1%)	15	51
1	F	156/188 (83%)	154 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	156/188 (83%)	154 (99%)	2 (1%)	0	100	100
1	H	156/188 (83%)	155 (99%)	1 (1%)	0	100	100
1	I	156/188 (83%)	155 (99%)	1 (1%)	0	100	100
1	J	156/188 (83%)	154 (99%)	1 (1%)	1 (1%)	30	70
1	K	156/188 (83%)	155 (99%)	1 (1%)	0	100	100
1	L	156/188 (83%)	154 (99%)	2 (1%)	0	100	100
1	M	156/188 (83%)	155 (99%)	1 (1%)	0	100	100
1	N	156/188 (83%)	154 (99%)	2 (1%)	0	100	100
1	O	156/188 (83%)	154 (99%)	2 (1%)	0	100	100
1	P	156/188 (83%)	156 (100%)	0	0	100	100
All	All	2496/3008 (83%)	2473 (99%)	19 (1%)	4 (0%)	52	87

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	14	ILE
1	E	15	ASP
1	J	14	ILE
1	A	14	ILE

### 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	
1	A	138/164 (84%)	135 (98%)	3 (2%)	60	87
1	B	138/164 (84%)	134 (97%)	4 (3%)	50	83
1	C	138/164 (84%)	134 (97%)	4 (3%)	50	83
1	D	138/164 (84%)	134 (97%)	4 (3%)	50	83
1	E	138/164 (84%)	133 (96%)	5 (4%)	42	78
1	F	138/164 (84%)	135 (98%)	3 (2%)	60	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	138/164 (84%)	135 (98%)	3 (2%)	60	87
1	H	138/164 (84%)	134 (97%)	4 (3%)	50	83
1	I	138/164 (84%)	134 (97%)	4 (3%)	50	83
1	J	138/164 (84%)	135 (98%)	3 (2%)	60	87
1	K	138/164 (84%)	133 (96%)	5 (4%)	42	78
1	L	138/164 (84%)	134 (97%)	4 (3%)	50	83
1	M	138/164 (84%)	135 (98%)	3 (2%)	60	87
1	N	138/164 (84%)	133 (96%)	5 (4%)	42	78
1	O	138/164 (84%)	134 (97%)	4 (3%)	50	83
1	P	138/164 (84%)	135 (98%)	3 (2%)	60	87
All	All	2208/2624 (84%)	2147 (97%)	61 (3%)	51	83

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
1	A	107	HIS
1	A	130	LYS
1	B	23	ARG
1	B	74	ASN
1	B	107	HIS
1	B	130	LYS
1	C	14	ILE
1	C	74	ASN
1	C	107	HIS
1	C	130	LYS
1	D	33	ARG
1	D	74	ASN
1	D	107	HIS
1	D	130	LYS
1	E	23	ARG
1	E	33	ARG
1	E	74	ASN
1	E	107	HIS
1	E	130	LYS
1	F	74	ASN
1	F	107	HIS
1	F	130	LYS

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Mol	Chain	Res	Type
1	G	74	ASN
1	G	107	HIS
1	G	130	LYS
1	H	24	ARG
1	H	74	ASN
1	H	107	HIS
1	H	130	LYS
1	I	24	ARG
1	I	74	ASN
1	I	107	HIS
1	I	130	LYS
1	J	74	ASN
1	J	107	HIS
1	J	130	LYS
1	K	23	ARG
1	K	24	ARG
1	K	74	ASN
1	K	107	HIS
1	K	130	LYS
1	L	24	ARG
1	L	74	ASN
1	L	107	HIS
1	L	130	LYS
1	M	74	ASN
1	M	107	HIS
1	M	130	LYS
1	N	15	ASP
1	N	62	GLU
1	N	74	ASN
1	N	107	HIS
1	N	130	LYS
1	O	62	GLU
1	O	74	ASN
1	O	107	HIS
1	O	130	LYS
1	P	74	ASN
1	P	107	HIS
1	P	130	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
1	B	21	ASN
1	B	43	GLN
1	B	74	ASN
1	C	17	GLN
1	C	21	ASN
1	C	43	GLN
1	C	74	ASN
1	C	107	HIS
1	D	21	ASN
1	D	43	GLN
1	D	74	ASN
1	E	21	ASN
1	E	74	ASN
1	F	21	ASN
1	F	43	GLN
1	F	74	ASN
1	G	17	GLN
1	G	21	ASN
1	G	43	GLN
1	G	74	ASN
1	H	20	HIS
1	H	21	ASN
1	H	43	GLN
1	H	74	ASN
1	I	21	ASN
1	I	43	GLN
1	I	74	ASN
1	J	17	GLN
1	J	21	ASN
1	J	74	ASN
1	K	17	GLN
1	K	21	ASN
1	K	43	GLN
1	K	74	ASN
1	L	21	ASN
1	L	43	GLN
1	L	74	ASN
1	M	21	ASN
1	M	74	ASN
1	N	17	GLN
1	N	21	ASN
1	N	43	GLN

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Mol	Chain	Res	Type
1	N	74	ASN
1	O	21	ASN
1	O	74	ASN
1	P	21	ASN
1	P	74	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

16 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	ANP	A	300	-	27,33,33	2.48	6 (22%)	30,52,52	2.26	7 (23%)
2	ANP	B	300	-	27,33,33	2.64	6 (22%)	30,52,52	2.29	7 (23%)
2	ANP	C	300	-	27,33,33	2.52	6 (22%)	30,52,52	2.38	8 (26%)
2	ANP	D	300	-	27,33,33	2.62	6 (22%)	30,52,52	2.13	6 (20%)
2	ANP	E	300	-	27,33,33	2.51	7 (25%)	30,52,52	2.29	9 (30%)
2	ANP	F	300	-	27,33,33	2.40	7 (25%)	30,52,52	1.95	6 (20%)
2	ANP	G	300	-	27,33,33	2.45	6 (22%)	30,52,52	2.41	7 (23%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	ANP	H	300	-	27,33,33	2.42	6 (22%)	30,52,52	2.04	7 (23%)
2	ANP	I	300	-	27,33,33	2.50	6 (22%)	30,52,52	2.29	10 (33%)
2	ANP	J	300	-	27,33,33	2.53	6 (22%)	30,52,52	2.14	7 (23%)
2	ANP	K	300	-	27,33,33	2.35	7 (25%)	30,52,52	2.21	8 (26%)
2	ANP	L	300	-	27,33,33	2.36	6 (22%)	30,52,52	2.30	6 (20%)
2	ANP	M	300	-	27,33,33	2.34	7 (25%)	30,52,52	2.27	7 (23%)
2	ANP	N	300	-	27,33,33	2.45	6 (22%)	30,52,52	2.39	6 (20%)
2	ANP	O	300	-	27,33,33	2.46	6 (22%)	30,52,52	2.47	7 (23%)
2	ANP	P	300	-	27,33,33	2.46	6 (22%)	30,52,52	2.18	7 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ANP	A	300	-	-	0/12/38/38	0/3/3/3
2	ANP	B	300	-	-	0/12/38/38	0/3/3/3
2	ANP	C	300	-	-	0/12/38/38	0/3/3/3
2	ANP	D	300	-	-	0/12/38/38	0/3/3/3
2	ANP	E	300	-	-	0/12/38/38	0/3/3/3
2	ANP	F	300	-	-	0/12/38/38	0/3/3/3
2	ANP	G	300	-	-	0/12/38/38	0/3/3/3
2	ANP	H	300	-	-	0/12/38/38	0/3/3/3
2	ANP	I	300	-	-	0/12/38/38	0/3/3/3
2	ANP	J	300	-	-	0/12/38/38	0/3/3/3
2	ANP	K	300	-	-	0/12/38/38	0/3/3/3
2	ANP	L	300	-	-	0/12/38/38	0/3/3/3
2	ANP	M	300	-	-	0/12/38/38	0/3/3/3
2	ANP	N	300	-	-	0/12/38/38	0/3/3/3
2	ANP	O	300	-	-	0/12/38/38	0/3/3/3
2	ANP	P	300	-	-	0/12/38/38	0/3/3/3

All (100) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	300	ANP	C5-N7	-2.05	1.32	1.39
2	K	300	ANP	PG-O3G	-2.03	1.51	1.56
2	M	300	ANP	PG-O3G	-2.02	1.51	1.56
2	F	300	ANP	PG-O3G	-2.00	1.51	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	300	ANP	C5-C4	2.11	1.45	1.40
2	H	300	ANP	C5-C4	2.39	1.45	1.40
2	C	300	ANP	C5-C4	2.44	1.46	1.40
2	M	300	ANP	C5-C4	2.49	1.46	1.40
2	P	300	ANP	C5-C4	2.52	1.46	1.40
2	B	300	ANP	C5-C4	2.53	1.46	1.40
2	G	300	ANP	C5-C4	2.57	1.46	1.40
2	L	300	ANP	C5-C4	2.66	1.46	1.40
2	O	300	ANP	C5-C4	2.68	1.46	1.40
2	D	300	ANP	C5-C4	2.69	1.46	1.40
2	A	300	ANP	C5-C4	2.72	1.46	1.40
2	J	300	ANP	C5-C4	2.86	1.46	1.40
2	F	300	ANP	C5-C4	2.86	1.47	1.40
2	K	300	ANP	C5-C4	2.93	1.47	1.40
2	I	300	ANP	C5-C4	2.94	1.47	1.40
2	M	300	ANP	PB-O3A	3.04	1.62	1.59
2	N	300	ANP	C5-C4	3.05	1.47	1.40
2	F	300	ANP	PB-O3A	3.34	1.63	1.59
2	N	300	ANP	PB-O3A	3.34	1.63	1.59
2	I	300	ANP	PB-O3A	3.49	1.63	1.59
2	E	300	ANP	PB-O3A	3.58	1.63	1.59
2	H	300	ANP	PB-O3A	4.13	1.64	1.59
2	G	300	ANP	PB-O3A	4.21	1.64	1.59
2	L	300	ANP	PB-O3A	4.25	1.64	1.59
2	O	300	ANP	PB-O3A	4.31	1.64	1.59
2	A	300	ANP	PB-O3A	4.33	1.64	1.59
2	D	300	ANP	PB-O3A	4.37	1.64	1.59
2	J	300	ANP	PG-O1G	4.43	1.51	1.46
2	P	300	ANP	PB-N3B	4.49	1.75	1.63
2	B	300	ANP	PB-O3A	4.52	1.64	1.59
2	K	300	ANP	PB-N3B	4.55	1.75	1.63
2	K	300	ANP	PB-O3A	4.58	1.64	1.59
2	P	300	ANP	PG-N3B	4.67	1.75	1.63
2	K	300	ANP	PB-O1B	4.73	1.51	1.46
2	F	300	ANP	PG-O1G	4.73	1.51	1.46
2	K	300	ANP	PG-N3B	4.75	1.75	1.63
2	H	300	ANP	PG-O1G	4.75	1.51	1.46
2	A	300	ANP	PG-O1G	4.78	1.51	1.46
2	L	300	ANP	PB-N3B	4.80	1.76	1.63
2	E	300	ANP	PG-N3B	4.80	1.76	1.63
2	M	300	ANP	PG-O1G	4.84	1.51	1.46
2	F	300	ANP	PG-N3B	4.96	1.76	1.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	300	ANP	PB-N3B	5.03	1.76	1.63
2	F	300	ANP	PB-N3B	5.05	1.76	1.63
2	L	300	ANP	PG-N3B	5.08	1.76	1.63
2	C	300	ANP	PB-O3A	5.09	1.65	1.59
2	G	300	ANP	PG-O1G	5.09	1.52	1.46
2	H	300	ANP	PB-N3B	5.14	1.77	1.63
2	L	300	ANP	PB-O1B	5.16	1.52	1.46
2	A	300	ANP	PB-N3B	5.22	1.77	1.63
2	M	300	ANP	PB-N3B	5.28	1.77	1.63
2	H	300	ANP	PG-N3B	5.30	1.77	1.63
2	N	300	ANP	PG-O1G	5.31	1.52	1.46
2	I	300	ANP	PB-O1B	5.32	1.52	1.46
2	C	300	ANP	PG-O1G	5.34	1.52	1.46
2	P	300	ANP	PB-O1B	5.36	1.52	1.46
2	E	300	ANP	PG-O1G	5.38	1.52	1.46
2	O	300	ANP	PB-N3B	5.40	1.77	1.63
2	G	300	ANP	PB-N3B	5.40	1.77	1.63
2	P	300	ANP	PG-O1G	5.41	1.52	1.46
2	O	300	ANP	PG-O1G	5.43	1.52	1.46
2	J	300	ANP	PG-N3B	5.43	1.77	1.63
2	O	300	ANP	PG-N3B	5.44	1.77	1.63
2	C	300	ANP	PB-N3B	5.45	1.77	1.63
2	M	300	ANP	PG-N3B	5.47	1.77	1.63
2	N	300	ANP	PB-O1B	5.47	1.52	1.46
2	O	300	ANP	PB-O1B	5.48	1.52	1.46
2	A	300	ANP	PG-N3B	5.52	1.77	1.63
2	N	300	ANP	PB-N3B	5.52	1.78	1.63
2	C	300	ANP	PB-O1B	5.54	1.52	1.46
2	J	300	ANP	PB-N3B	5.57	1.78	1.63
2	I	300	ANP	PG-O1G	5.57	1.52	1.46
2	M	300	ANP	PB-O1B	5.60	1.52	1.46
2	B	300	ANP	PG-O1G	5.61	1.52	1.46
2	G	300	ANP	PB-O1B	5.62	1.52	1.46
2	J	300	ANP	PB-O3A	5.62	1.66	1.59
2	L	300	ANP	PG-O1G	5.64	1.52	1.46
2	G	300	ANP	PG-N3B	5.65	1.78	1.63
2	N	300	ANP	PG-N3B	5.69	1.78	1.63
2	C	300	ANP	PG-N3B	5.71	1.78	1.63
2	D	300	ANP	PG-O1G	5.71	1.52	1.46
2	B	300	ANP	PG-N3B	5.76	1.78	1.63
2	I	300	ANP	PB-N3B	5.79	1.78	1.63
2	J	300	ANP	PB-O1B	5.81	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	300	ANP	PB-N3B	5.81	1.78	1.63
2	K	300	ANP	PG-O1G	5.82	1.52	1.46
2	B	300	ANP	PB-N3B	5.87	1.78	1.63
2	D	300	ANP	PG-N3B	5.91	1.79	1.63
2	I	300	ANP	PG-N3B	6.10	1.79	1.63
2	H	300	ANP	PB-O1B	6.12	1.53	1.46
2	D	300	ANP	PB-O1B	6.12	1.53	1.46
2	A	300	ANP	PB-O1B	6.14	1.53	1.46
2	P	300	ANP	PB-O3A	6.15	1.66	1.59
2	F	300	ANP	PB-O1B	6.32	1.53	1.46
2	B	300	ANP	PB-O1B	6.60	1.53	1.46
2	E	300	ANP	PB-O1B	7.29	1.54	1.46

All (115) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	300	ANP	N3-C2-N1	-8.96	122.03	128.89
2	O	300	ANP	N3-C2-N1	-8.53	122.36	128.89
2	N	300	ANP	N3-C2-N1	-8.30	122.54	128.89
2	C	300	ANP	N3-C2-N1	-8.21	122.61	128.89
2	B	300	ANP	N3-C2-N1	-7.82	122.91	128.89
2	L	300	ANP	N3-C2-N1	-7.74	122.97	128.89
2	G	300	ANP	N3-C2-N1	-7.70	123.00	128.89
2	P	300	ANP	N3-C2-N1	-7.63	123.05	128.89
2	A	300	ANP	N3-C2-N1	-7.39	123.24	128.89
2	M	300	ANP	N3-C2-N1	-7.25	123.34	128.89
2	K	300	ANP	N3-C2-N1	-7.19	123.39	128.89
2	I	300	ANP	N3-C2-N1	-6.81	123.68	128.89
2	H	300	ANP	N3-C2-N1	-6.60	123.84	128.89
2	L	300	ANP	O1G-PG-N3B	-6.12	102.51	111.90
2	E	300	ANP	O1G-PG-N3B	-5.94	102.78	111.90
2	D	300	ANP	N3-C2-N1	-5.84	124.43	128.89
2	N	300	ANP	O1G-PG-N3B	-5.79	103.02	111.90
2	E	300	ANP	N3-C2-N1	-5.76	124.48	128.89
2	F	300	ANP	N3-C2-N1	-5.70	124.53	128.89
2	G	300	ANP	O1G-PG-N3B	-5.64	103.25	111.90
2	O	300	ANP	O1G-PG-N3B	-4.93	104.34	111.90
2	O	300	ANP	O1B-PB-N3B	-4.78	104.56	111.90
2	A	300	ANP	O1B-PB-N3B	-4.78	104.56	111.90
2	I	300	ANP	O1B-PB-N3B	-4.75	104.62	111.90
2	B	300	ANP	O1G-PG-N3B	-4.72	104.65	111.90
2	M	300	ANP	O1G-PG-N3B	-4.39	105.16	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	300	ANP	O1G-PG-N3B	-4.38	105.19	111.90
2	C	300	ANP	O1B-PB-N3B	-4.30	105.30	111.90
2	H	300	ANP	O1B-PB-N3B	-4.28	105.33	111.90
2	K	300	ANP	O1G-PG-N3B	-4.26	105.36	111.90
2	P	300	ANP	O1B-PB-N3B	-4.17	105.50	111.90
2	G	300	ANP	O1B-PB-N3B	-4.16	105.52	111.90
2	D	300	ANP	O1B-PB-N3B	-4.04	105.70	111.90
2	I	300	ANP	C4-C5-N7	-3.86	105.93	109.48
2	I	300	ANP	O1G-PG-N3B	-3.85	106.00	111.90
2	B	300	ANP	O1B-PB-N3B	-3.77	106.11	111.90
2	A	300	ANP	O1G-PG-N3B	-3.75	106.14	111.90
2	E	300	ANP	C4-C5-N7	-3.75	106.03	109.48
2	K	300	ANP	O1B-PB-N3B	-3.66	106.29	111.90
2	D	300	ANP	C4-C5-N7	-3.62	106.15	109.48
2	M	300	ANP	C4-C5-N7	-3.61	106.16	109.48
2	N	300	ANP	O1B-PB-N3B	-3.54	106.47	111.90
2	O	300	ANP	C4-C5-N7	-3.53	106.24	109.48
2	C	300	ANP	O1G-PG-N3B	-3.48	106.56	111.90
2	F	300	ANP	C4-C5-N7	-3.48	106.28	109.48
2	C	300	ANP	C4-C5-N7	-3.45	106.30	109.48
2	F	300	ANP	O1B-PB-N3B	-3.45	106.60	111.90
2	L	300	ANP	O1B-PB-N3B	-3.35	106.76	111.90
2	F	300	ANP	O1G-PG-N3B	-3.31	106.82	111.90
2	D	300	ANP	O1G-PG-N3B	-3.26	106.89	111.90
2	H	300	ANP	C4-C5-N7	-3.11	106.62	109.48
2	M	300	ANP	O1B-PB-N3B	-3.09	107.17	111.90
2	M	300	ANP	C2'-C1'-N9	-3.06	109.61	114.29
2	K	300	ANP	C4-C5-N7	-3.06	106.67	109.48
2	J	300	ANP	O1G-PG-N3B	-2.96	107.36	111.90
2	E	300	ANP	O1B-PB-N3B	-2.94	107.40	111.90
2	P	300	ANP	C4-C5-N7	-2.76	106.94	109.48
2	M	300	ANP	PA-O3A-PB	-2.71	123.59	132.67
2	H	300	ANP	O1G-PG-N3B	-2.58	107.94	111.90
2	B	300	ANP	PA-O3A-PB	-2.57	124.05	132.67
2	E	300	ANP	O3A-PA-O5'	-2.55	96.18	102.94
2	G	300	ANP	C4-C5-N7	-2.54	107.14	109.48
2	L	300	ANP	C4-C5-N7	-2.50	107.17	109.48
2	I	300	ANP	O3A-PA-O5'	-2.37	96.65	102.94
2	A	300	ANP	C4-C5-N7	-2.37	107.30	109.48
2	N	300	ANP	C4-C5-N7	-2.33	107.34	109.48
2	E	300	ANP	O2'-C2'-C3'	-2.32	104.27	111.83
2	I	300	ANP	C2'-C1'-N9	-2.31	110.76	114.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	300	ANP	C4-C5-N7	-2.16	107.50	109.48
2	H	300	ANP	PA-O3A-PB	-2.13	125.54	132.67
2	I	300	ANP	C1'-N9-C4	-2.11	123.75	126.94
2	J	300	ANP	O3G-PG-O1G	-2.05	108.03	113.49
2	J	300	ANP	C1'-N9-C4	-2.02	123.89	126.94
2	K	300	ANP	O3A-PB-N3B	2.00	111.94	106.44
2	H	300	ANP	O3G-PG-O2G	2.08	113.75	107.58
2	A	300	ANP	O3G-PG-O2G	2.11	113.84	107.58
2	J	300	ANP	C2-N1-C6	2.14	122.60	118.77
2	E	300	ANP	O3A-PB-N3B	2.18	112.43	106.44
2	O	300	ANP	C4'-O4'-C1'	2.20	112.14	109.72
2	L	300	ANP	O3G-PG-O2G	2.22	114.17	107.58
2	O	300	ANP	O3A-PB-N3B	2.25	112.64	106.44
2	I	300	ANP	O3G-PG-O2G	2.26	114.27	107.58
2	P	300	ANP	C4'-O4'-C1'	2.26	112.20	109.72
2	G	300	ANP	O3A-PB-N3B	2.27	112.69	106.44
2	B	300	ANP	O3A-PB-N3B	2.31	112.80	106.44
2	F	300	ANP	O3G-PG-O2G	2.33	114.50	107.58
2	D	300	ANP	O3G-PG-O2G	2.35	114.55	107.58
2	I	300	ANP	O3A-PB-N3B	2.39	113.02	106.44
2	C	300	ANP	O3G-PG-O2G	2.42	114.75	107.58
2	C	300	ANP	O4'-C1'-N9	2.43	113.19	108.10
2	K	300	ANP	O2A-PA-O3A	2.53	116.58	105.09
2	G	300	ANP	O2A-PA-O3A	2.59	116.86	105.09
2	A	300	ANP	O3A-PB-N3B	2.63	113.68	106.44
2	P	300	ANP	O3A-PB-N3B	2.64	113.70	106.44
2	J	300	ANP	O3G-PG-O2G	2.64	115.42	107.58
2	C	300	ANP	O3A-PB-N3B	2.66	113.74	106.44
2	P	300	ANP	O2B-PB-O1B	2.66	115.55	110.00
2	K	300	ANP	C4'-O4'-C1'	2.87	112.87	109.72
2	J	300	ANP	O2B-PB-O1B	2.93	116.12	110.00
2	E	300	ANP	O2A-PA-O3A	3.03	118.83	105.09
2	N	300	ANP	C4'-O4'-C1'	3.09	113.11	109.72
2	C	300	ANP	O2B-PB-O1B	4.02	118.39	110.00
2	F	300	ANP	O2B-PB-O1B	4.15	118.65	110.00
2	I	300	ANP	O2B-PB-O1B	4.22	118.81	110.00
2	M	300	ANP	O2B-PB-O1B	4.35	119.08	110.00
2	O	300	ANP	O2B-PB-O1B	4.35	119.08	110.00
2	K	300	ANP	O2B-PB-O1B	4.36	119.10	110.00
2	L	300	ANP	O2B-PB-O1B	4.41	119.21	110.00
2	N	300	ANP	O2B-PB-O1B	4.42	119.22	110.00
2	A	300	ANP	O2B-PB-O1B	4.49	119.36	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	300	ANP	O2B-PB-O1B	4.64	119.69	110.00
2	E	300	ANP	O2B-PB-O1B	4.79	119.99	110.00
2	G	300	ANP	O2B-PB-O1B	4.89	120.21	110.00
2	B	300	ANP	O2B-PB-O1B	5.03	120.50	110.00
2	D	300	ANP	O2B-PB-O1B	5.23	120.91	110.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	300	ANP	1	0
2	C	300	ANP	1	0
2	D	300	ANP	1	0
2	F	300	ANP	1	0
2	H	300	ANP	1	0
2	J	300	ANP	1	0
2	M	300	ANP	1	0
2	N	300	ANP	1	0

## 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, 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	A	158/188 (84%)	-0.08	0 100 100	34, 54, 81, 99	0
1	B	158/188 (84%)	-0.19	0 100 100	34, 53, 84, 99	0
1	C	158/188 (84%)	-0.08	2 (1%) 79 53	31, 52, 90, 100	0
1	D	158/188 (84%)	-0.11	0 100 100	31, 51, 98, 108	0
1	E	158/188 (84%)	-0.10	1 (0%) 90 74	30, 49, 79, 94	0
1	F	158/188 (84%)	-0.09	1 (0%) 90 74	33, 51, 82, 95	0
1	G	158/188 (84%)	-0.07	0 100 100	37, 55, 83, 94	0
1	H	158/188 (84%)	-0.11	0 100 100	33, 54, 101, 120	0
1	I	158/188 (84%)	-0.09	0 100 100	37, 60, 89, 102	0
1	J	158/188 (84%)	-0.04	2 (1%) 79 53	42, 63, 90, 100	0
1	K	158/188 (84%)	-0.13	0 100 100	41, 61, 90, 106	0
1	L	158/188 (84%)	-0.00	2 (1%) 79 53	42, 71, 122, 134	0
1	M	158/188 (84%)	0.17	2 (1%) 79 53	40, 79, 145, 163	0
1	N	158/188 (84%)	0.14	3 (1%) 70 41	48, 80, 134, 145	0
1	O	158/188 (84%)	0.22	4 (2%) 61 30	52, 84, 140, 149	0
1	P	158/188 (84%)	-0.08	0 100 100	43, 76, 133, 147	0
All	All	2528/3008 (84%)	-0.04	17 (0%) 89 70	30, 62, 115, 163	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	19	LEU	3.5
1	L	170	ASP	3.2
1	F	163	ASP	2.8
1	N	170	ASP	2.8
1	O	165	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	M	29	GLY	2.5
1	L	130	LYS	2.5
1	O	166	THR	2.4
1	N	33	ARG	2.4
1	J	136	GLN	2.4
1	C	17	GLN	2.3
1	M	23	ARG	2.3
1	J	170	ASP	2.1
1	O	115	ARG	2.1
1	O	26	PHE	2.1
1	C	20	HIS	2.1
1	N	22	ALA	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	ANP	P	300	31/31	0.94	0.19	-0.48	29,35,50,51	0
2	ANP	B	300	31/31	0.96	0.18	-0.59	30,33,51,51	0
2	ANP	M	300	31/31	0.93	0.20	-0.69	26,32,57,58	0
2	ANP	N	300	31/31	0.92	0.19	-0.72	33,40,56,57	0
2	ANP	K	300	31/31	0.95	0.15	-0.82	29,32,47,48	0
2	ANP	L	300	31/31	0.95	0.16	-0.92	25,28,46,46	0
2	ANP	D	300	31/31	0.92	0.19	-0.99	30,34,60,60	0
2	ANP	I	300	31/31	0.95	0.16	-1.01	24,32,51,52	0
2	ANP	H	300	31/31	0.93	0.16	-1.03	22,27,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ANP	O	300	31/31	0.93	0.16	-1.07	22,28,39,39	0
2	ANP	A	300	31/31	0.95	0.17	-1.21	25,28,46,46	0
2	ANP	E	300	31/31	0.95	0.17	-1.21	27,30,50,51	0
2	ANP	C	300	31/31	0.94	0.16	-1.28	32,37,59,60	0
2	ANP	F	300	31/31	0.95	0.16	-1.48	26,30,44,44	0
2	ANP	G	300	31/31	0.95	0.16	-1.62	32,38,54,54	0
2	ANP	J	300	31/31	0.96	0.15	-1.68	21,23,44,44	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.