



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 24, 2020 – 03:51 PM BST

PDB ID : 4APZ  
Title : Structure of B. subtilis genomic dUTPase YncF in complex with dU, PPi and Mg in P1  
Authors : Garcia-Nafria, J.; Timm, J.; Harrison, C.; Turkenburg, J.P.; Wilson, K.S.  
Deposited on : 2012-04-11  
Resolution : 2.01 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13  
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) : 2.13

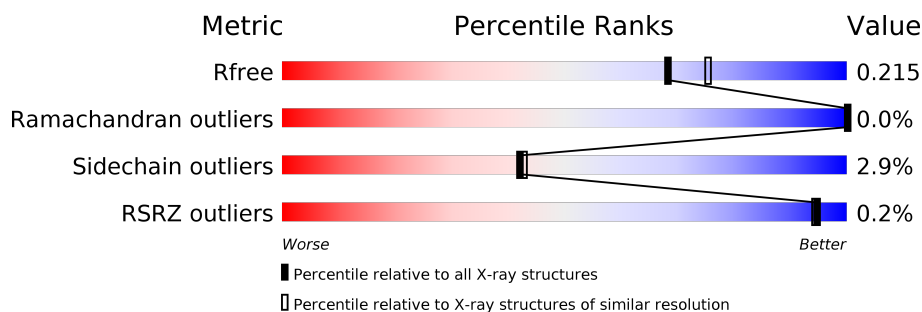
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.01 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.




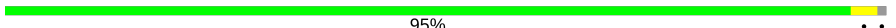
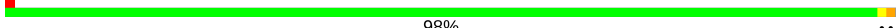
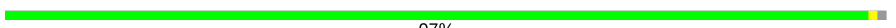











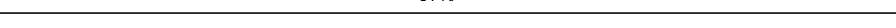
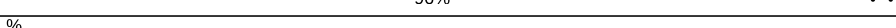
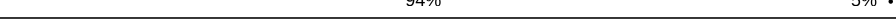
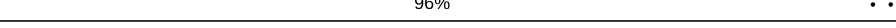
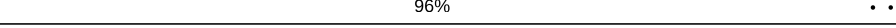
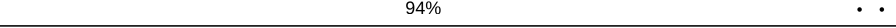

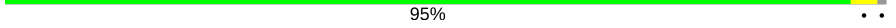
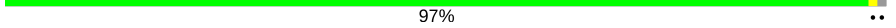
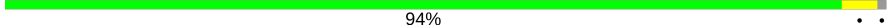
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	8085 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 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	1	144	 95% ..
1	2	144	 97% ..
1	3	144	 96% ...
1	4	144	 95% ..
1	5	144	 97% ...
1	6	144	 97% ..
1	7	144	 97% ..

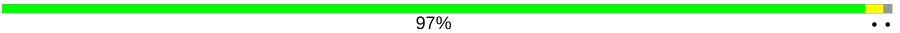



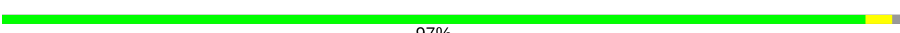








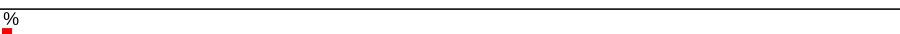

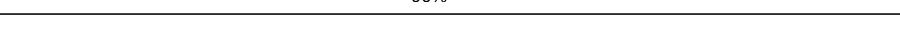
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Mol	Chain	Length	Quality of chain
1	8	144	 94% 5% .
1	9	144	 95% ..
1	A	144	 98% ...
1	B	144	 97% ..
1	C	144	 94% ..
1	D	144	 94% ..
1	E	144	 94% ..
1	F	144	 97% ..
1	G	144	 95% ..
1	H	144	 93% 6% .
1	I	144	 94% ..
1	J	144	 92% 6% .
1	K	144	 96% ..
1	L	144	 97% ..
1	M	144	 97% ..
1	N	144	 96% ..
1	O	144	 94% 5% .
1	P	144	 96% ..
1	Q	144	 96% ..
1	R	144	 94% ..
1	S	144	 92% 6% .
1	T	144	 95% ..
1	U	144	 97% ..
1	V	144	 94% ..
1	W	144	 94% ..

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Mol	Chain	Length	Quality of chain
1	X	144	 97% ..
1	Y	144	 95% ..
1	Z	144	 96% ..
1	a	144	 95% ..
1	b	144	 97% ..
1	c	144	 95% ..
1	d	144	 94% ..
1	e	144	 94% 5% .
1	f	144	 94% 5% .
1	g	144	 96% ..
1	h	144	 94% ..
1	i	144	 96% ..
1	j	144	 95% ..
1	k	144	 94% 5% .
1	l	144	 96% ..
1	m	144	 95% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	DUR	J	1145	X	-	-	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 60911 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 PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	142	Total	C	N	O	S	9	2	0
			1148	730	193	218	7			
1	2	142	Total	C	N	O	S	0	2	0
			1149	730	194	218	7			
1	3	142	Total	C	N	O	S	3	0	0
			1136	721	191	218	6			
1	4	142	Total	C	N	O	S	0	4	0
			1162	739	196	220	7			
1	5	142	Total	C	N	O	S	7	1	0
			1141	725	191	218	7			
1	6	142	Total	C	N	O	S	11	1	0
			1141	725	191	218	7			
1	7	142	Total	C	N	O	S	0	0	0
			1136	721	191	218	6			
1	8	142	Total	C	N	O	S	0	1	0
			1141	725	191	218	7			
1	9	142	Total	C	N	O	S	3	2	0
			1150	731	193	219	7			
1	A	143	Total	C	N	O	S	4	2	0
			1151	731	192	221	7			
1	B	142	Total	C	N	O	S	4	2	0
			1148	730	193	218	7			
1	C	142	Total	C	N	O	S	6	2	0
			1148	729	193	220	6			
1	D	142	Total	C	N	O	S	7	1	0
			1141	725	191	218	7			
1	E	142	Total	C	N	O	S	3	1	0
			1143	726	193	218	6			
1	F	143	Total	C	N	O	S	3	2	0
			1155	734	194	220	7			
1	G	142	Total	C	N	O	S	6	2	0
			1152	732	195	219	6			

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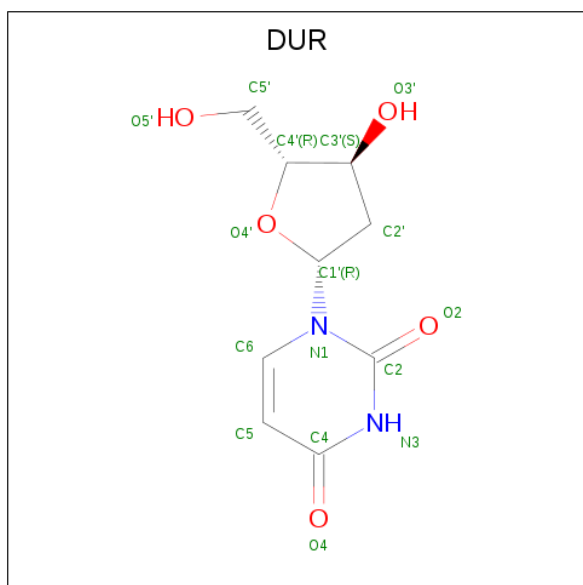
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	142	Total	C	N	O	S	3	0	0
			1136	721	191	218	6			
1	I	142	Total	C	N	O	S	7	1	0
			1141	725	191	218	7			
1	J	142	Total	C	N	O	S	2	1	0
			1143	726	193	218	6			
1	K	142	Total	C	N	O	S	11	1	0
			1142	725	191	220	6			
1	L	142	Total	C	N	O	S	0	0	0
			1136	721	191	218	6			
1	M	142	Total	C	N	O	S	2	1	0
			1139	723	191	219	6			
1	N	142	Total	C	N	O	S	3	0	0
			1136	721	191	218	6			
1	O	142	Total	C	N	O	S	0	0	0
			1136	721	191	218	6			
1	P	142	Total	C	N	O	S	2	2	0
			1150	731	193	219	7			
1	Q	143	Total	C	N	O	S	0	1	0
			1150	730	194	220	6			
1	R	142	Total	C	N	O	S	3	1	0
			1143	726	193	218	6			
1	S	142	Total	C	N	O	S	0	2	0
			1148	730	193	218	7			
1	T	142	Total	C	N	O	S	4	2	0
			1148	730	193	218	7			
1	U	142	Total	C	N	O	S	0	2	0
			1148	730	193	218	7			
1	V	142	Total	C	N	O	S	3	1	0
			1141	725	191	218	7			
1	W	142	Total	C	N	O	S	0	0	0
			1136	721	191	218	6			
1	X	142	Total	C	N	O	S	0	3	0
			1151	732	193	219	7			
1	Y	142	Total	C	N	O	S	3	1	0
			1141	725	191	218	7			
1	Z	142	Total	C	N	O	S	8	2	0
			1150	731	193	219	7			
1	a	143	Total	C	N	O	S	7	1	0
			1148	729	192	220	7			
1	b	143	Total	C	N	O	S	3	0	0
			1143	725	192	220	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	c	142	Total	C	N	O	S	8	2	0
			1148	730	193	218	7			
1	d	142	Total	C	N	O	S	0	1	0
			1141	725	191	218	7			
1	e	142	Total	C	N	O	S	0	1	0
			1141	725	191	218	7			
1	f	142	Total	C	N	O	S	0	1	0
			1141	725	191	218	7			
1	g	142	Total	C	N	O	S	3	2	0
			1153	732	194	220	7			
1	h	142	Total	C	N	O	S	4	0	0
			1136	721	191	218	6			
1	i	142	Total	C	N	O	S	4	1	0
			1141	725	191	218	7			
1	j	143	Total	C	N	O	S	2	1	0
			1148	729	192	220	7			
1	k	142	Total	C	N	O	S	4	1	0
			1141	725	191	218	7			
1	l	142	Total	C	N	O	S	0	2	0
			1148	730	193	218	7			
1	m	142	Total	C	N	O	S	0	1	0
			1141	725	191	218	7			

- Molecule 2 is 2'-DEOXYURIDINE (three-letter code: DUR) (formula: C<sub>9</sub>H<sub>12</sub>N<sub>2</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	1	1	Total 16	C 9	N 2	O 5	0	0
2	2	1	Total 16	C 9	N 2	O 5	0	0
2	3	1	Total 16	C 9	N 2	O 5	0	0
2	4	1	Total 16	C 9	N 2	O 5	0	0
2	5	1	Total 16	C 9	N 2	O 5	0	0
2	6	1	Total 16	C 9	N 2	O 5	0	0
2	7	1	Total 16	C 9	N 2	O 5	0	0
2	8	1	Total 16	C 9	N 2	O 5	0	0
2	9	1	Total 16	C 9	N 2	O 5	0	0
2	A	1	Total 16	C 9	N 2	O 5	0	0
2	B	1	Total 16	C 9	N 2	O 5	0	0
2	C	1	Total 16	C 9	N 2	O 5	0	0
2	D	1	Total 16	C 9	N 2	O 5	0	0
2	E	1	Total 16	C 9	N 2	O 5	0	0
2	F	1	Total 16	C 9	N 2	O 5	0	0
2	G	1	Total 16	C 9	N 2	O 5	0	0
2	H	1	Total 16	C 9	N 2	O 5	0	0
2	I	1	Total 16	C 9	N 2	O 5	0	0
2	J	1	Total 16	C 9	N 2	O 5	0	0
2	K	1	Total 16	C 9	N 2	O 5	0	0
2	L	1	Total 16	C 9	N 2	O 5	0	0
2	M	1	Total 16	C 9	N 2	O 5	0	0

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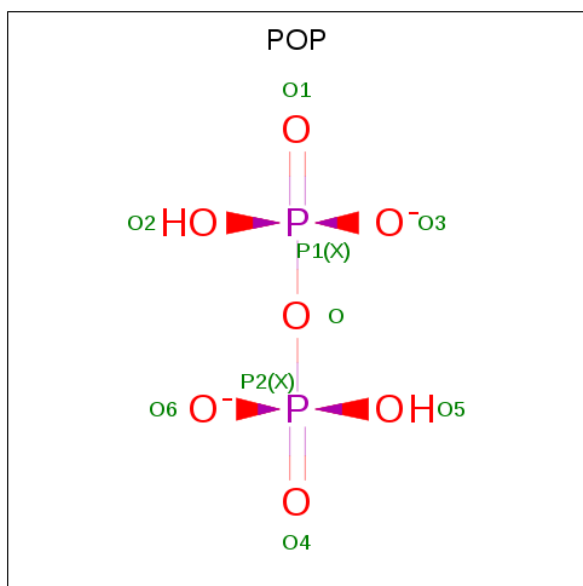
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	N	1	Total 16	C 9	N 2	O 5	0	0
2	O	1	Total 16	C 9	N 2	O 5	0	0
2	P	1	Total 16	C 9	N 2	O 5	0	0
2	Q	1	Total 16	C 9	N 2	O 5	0	0
2	R	1	Total 16	C 9	N 2	O 5	0	0
2	S	1	Total 16	C 9	N 2	O 5	0	0
2	T	1	Total 16	C 9	N 2	O 5	0	0
2	U	1	Total 16	C 9	N 2	O 5	0	0
2	V	1	Total 16	C 9	N 2	O 5	0	0
2	W	1	Total 16	C 9	N 2	O 5	0	0
2	X	1	Total 16	C 9	N 2	O 5	0	0
2	Y	1	Total 16	C 9	N 2	O 5	0	0
2	Z	1	Total 16	C 9	N 2	O 5	0	0
2	a	1	Total 16	C 9	N 2	O 5	0	0
2	b	1	Total 16	C 9	N 2	O 5	0	0
2	c	1	Total 16	C 9	N 2	O 5	0	0
2	d	1	Total 16	C 9	N 2	O 5	0	0
2	e	1	Total 16	C 9	N 2	O 5	0	0
2	f	1	Total 16	C 9	N 2	O 5	0	0
2	g	1	Total 16	C 9	N 2	O 5	0	0
2	h	1	Total 16	C 9	N 2	O 5	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	i	1	Total	C	N	O	0	0
			16	9	2	5		
2	j	1	Total	C	N	O	0	0
			16	9	2	5		
2	k	1	Total	C	N	O	0	0
			16	9	2	5		
2	l	1	Total	C	N	O	0	0
			16	9	2	5		
2	m	1	Total	C	N	O	0	0
			16	9	2	5		

- Molecule 3 is PYROPHOSPHATE 2- (three-letter code: POP) (formula:  $\text{H}_2\text{O}_7\text{P}_2$ ).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	1	1	Total	O P	0	0
			9	7 2		
3	2	1	Total	O P	0	0
			9	7 2		
3	3	1	Total	O P	0	0
			9	7 2		
3	4	1	Total	O P	0	0
			9	7 2		
3	5	1	Total	O P	0	0
			9	7 2		
3	6	1	Total	O P	0	0
			9	7 2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	7	1	Total 9	O 7	P 2	0	0
3	8	1	Total 9	O 7	P 2	0	0
3	9	1	Total 9	O 7	P 2	0	0
3	A	1	Total 9	O 7	P 2	0	0
3	B	1	Total 9	O 7	P 2	0	0
3	C	1	Total 9	O 7	P 2	0	0
3	D	1	Total 9	O 7	P 2	0	0
3	E	1	Total 9	O 7	P 2	0	0
3	F	1	Total 9	O 7	P 2	0	0
3	G	1	Total 9	O 7	P 2	0	0
3	H	1	Total 9	O 7	P 2	0	0
3	I	1	Total 9	O 7	P 2	0	0
3	J	1	Total 9	O 7	P 2	0	0
3	K	1	Total 9	O 7	P 2	0	0
3	L	1	Total 9	O 7	P 2	0	0
3	M	1	Total 9	O 7	P 2	0	0
3	N	1	Total 9	O 7	P 2	0	0
3	O	1	Total 9	O 7	P 2	0	0
3	P	1	Total 9	O 7	P 2	0	0
3	Q	1	Total 9	O 7	P 2	0	0
3	R	1	Total 9	O 7	P 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	S	1	Total	O	P	0	0
			9	7	2		
3	T	1	Total	O	P	0	0
			9	7	2		
3	U	1	Total	O	P	0	0
			9	7	2		
3	V	1	Total	O	P	0	0
			9	7	2		
3	W	1	Total	O	P	0	0
			9	7	2		
3	X	1	Total	O	P	0	0
			9	7	2		
3	Y	1	Total	O	P	0	0
			9	7	2		
3	Z	1	Total	O	P	0	0
			9	7	2		
3	a	1	Total	O	P	0	0
			9	7	2		
3	b	1	Total	O	P	0	0
			9	7	2		
3	c	1	Total	O	P	0	0
			9	7	2		
3	d	1	Total	O	P	0	0
			9	7	2		
3	e	1	Total	O	P	0	0
			9	7	2		
3	f	1	Total	O	P	0	0
			9	7	2		
3	g	1	Total	O	P	0	0
			9	7	2		
3	h	1	Total	O	P	0	0
			9	7	2		
3	i	1	Total	O	P	0	0
			9	7	2		
3	j	1	Total	O	P	0	0
			9	7	2		
3	k	1	Total	O	P	0	0
			9	7	2		
3	l	1	Total	O	P	0	0
			9	7	2		
3	m	1	Total	O	P	0	0
			9	7	2		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	P	1	Total 1	Mg 1	0	0
4	g	1	Total 1	Mg 1	0	0
4	K	1	Total 1	Mg 1	0	0
4	h	1	Total 1	Mg 1	0	0
4	B	1	Total 1	Mg 1	0	0
4	c	1	Total 1	Mg 1	0	0
4	6	1	Total 1	Mg 1	0	0
4	W	1	Total 1	Mg 1	0	0
4	N	1	Total 1	Mg 1	0	0
4	X	1	Total 1	Mg 1	0	0
4	2	1	Total 1	Mg 1	0	0
4	S	1	Total 1	Mg 1	0	0
4	f	1	Total 1	Mg 1	0	0
4	J	1	Total 1	Mg 1	0	0
4	k	1	Total 1	Mg 1	0	0
4	E	1	Total 1	Mg 1	0	0
4	b	1	Total 1	Mg 1	0	0
4	V	1	Total 1	Mg 1	0	0
4	A	1	Total 1	Mg 1	0	0
4	5	1	Total 1	Mg 1	0	0
4	R	1	Total 1	Mg 1	0	0

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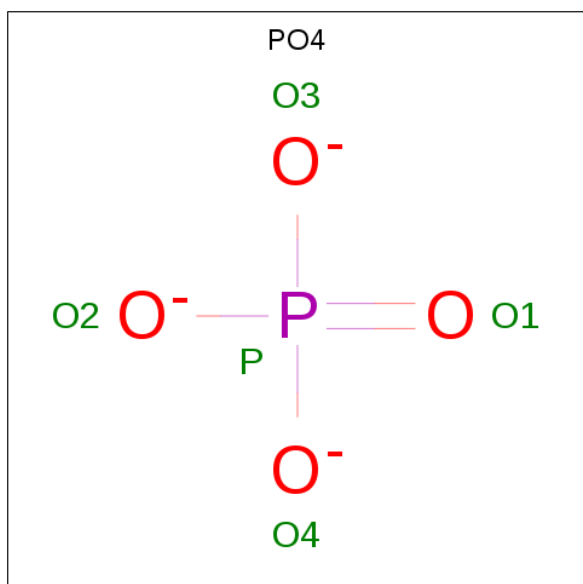
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	M	1	Total 1	Mg 1	0	0
4	j	1	Total 1	Mg 1	0	0
4	1	1	Total 1	Mg 1	0	0
4	D	1	Total 1	Mg 1	0	0
4	e	1	Total 1	Mg 1	0	0
4	I	1	Total 1	Mg 1	0	0
4	Z	1	Total 1	Mg 1	0	0
4	a	1	Total 1	Mg 1	0	0
4	4	1	Total 1	Mg 1	0	0
4	U	1	Total 1	Mg 1	0	0
4	9	1	Total 1	Mg 1	0	0
4	L	1	Total 1	Mg 1	0	0
4	m	1	Total 1	Mg 1	0	0
4	G	1	Total 1	Mg 1	0	0
4	Q	1	Total 1	Mg 1	0	0
4	d	1	Total 1	Mg 1	0	0
4	H	1	Total 1	Mg 1	0	0
4	i	1	Total 1	Mg 1	0	0
4	C	1	Total 1	Mg 1	0	0
4	7	1	Total 1	Mg 1	0	0
4	T	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	8	1	Total	Mg	0	0
			1	1		
4	O	1	Total	Mg	0	0
			1	1		
4	Y	1	Total	Mg	0	0
			1	1		
4	l	1	Total	Mg	0	0
			1	1		
4	3	1	Total	Mg	0	0
			1	1		
4	F	1	Total	Mg	0	0
			1	1		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	e	1	Total	O	P	0	0
			5	4	1		
5	l	1	Total	O	P	0	0
			5	4	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	1	120	Total	O	0	0
			120	120		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	2	139	Total 139	O 139	0	0
6	3	102	Total 102	O 102	0	0
6	4	85	Total 85	O 85	0	0
6	5	109	Total 109	O 109	0	0
6	6	93	Total 93	O 93	0	0
6	7	69	Total 69	O 69	0	0
6	8	136	Total 136	O 136	0	0
6	9	101	Total 101	O 101	0	0
6	A	122	Total 122	O 122	0	0
6	A	3	Total 3	O 3	0	0
6	B	96	Total 96	O 96	0	0
6	C	67	Total 67	O 67	0	0
6	D	133	Total 133	O 133	0	0
6	E	111	Total 111	O 111	0	0
6	F	86	Total 86	O 86	0	0
6	G	141	Total 141	O 141	0	0
6	H	123	Total 123	O 123	0	0
6	I	84	Total 84	O 84	0	0
6	J	116	Total 116	O 116	0	0
6	K	95	Total 95	O 95	0	0
6	L	70	Total 70	O 70	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	M	124	Total 124	O 124	0	0
6	N	98	Total 98	O 98	0	0
6	O	68	Total 68	O 68	0	0
6	P	142	Total 142	O 142	0	0
6	Q	103	Total 103	O 103	0	0
6	R	75	Total 75	O 75	0	0
6	S	133	Total 133	O 133	0	0
6	T	90	Total 90	O 90	0	0
6	U	62	Total 62	O 62	0	0
6	V	118	Total 118	O 118	0	0
6	W	97	Total 97	O 97	0	0
6	X	70	Total 70	O 70	0	0
6	Y	94	Total 94	O 94	0	0
6	Z	60	Total 60	O 60	0	0
6	a	1	Total 1	O 1	0	0
6	a	69	Total 69	O 69	0	0
6	b	127	Total 127	O 127	0	0
6	c	105	Total 105	O 105	0	0
6	d	63	Total 63	O 63	0	0
6	e	128	Total 128	O 128	0	0
6	f	92	Total 92	O 92	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	g	74	Total 74	O 74	0	0
6	h	143	Total 143	O 143	0	0
6	i	99	Total 99	O 99	0	0
6	j	63	Total 63	O 63	0	0
6	k	109	Total 109	O 109	0	0
6	l	69	Total 69	O 69	0	0
6	m	49	Total 49	O 49	0	0

### 3 Residue-property plots

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: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF

Chain 1:  95% ..



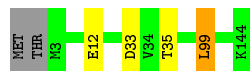
- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF

Chain 2:  97% ..



- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF

Chain 3:  96% ...



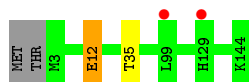
- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF

Chain 4:  95% ..



- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF

Chain 5:  97% ...



- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF

Chain 6: 97% ..



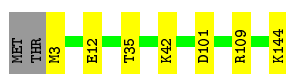
- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF

Chain 7: 97% ..



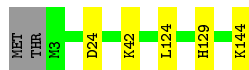
- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF

Chain 8: 94% 5% .



- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF

Chain 9: 95% ..



- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF

Chain A: 98% ...

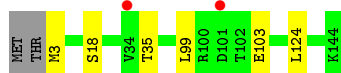


- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF

Chain B: 97% ..



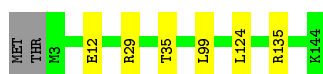
- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF



- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF



- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF



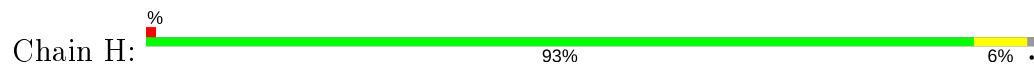
- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF

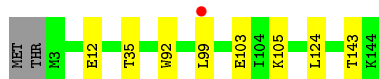


- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF



- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF





- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF

Chain I: 94% ..



- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF

Chain J: 92% 6% ..



- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF

Chain K: 96% ..



- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF

Chain L: 97% ..



- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF

Chain M: 97% ..



- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF

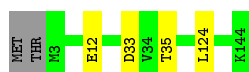
Chain N: 96% ..



- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF



- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF



- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF



- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF



- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF



- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF





- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF

Chain U: 97% ..



- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF

Chain V: 94% ..



- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF

Chain W: 94% ..



- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF

Chain X: 97% ..



- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF

Chain Y: 95% ..



- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF

Chain Z: 96% ..





- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF

Chain a:  95% ..



- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF

Chain b:  97% ..



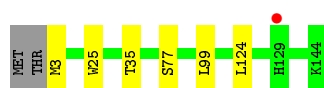
- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF

Chain c:  95% ..



- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF

Chain d:  94% ..



- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF

Chain e:  94% 5% .

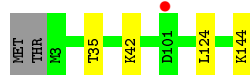


- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF

Chain f:  94% 5% .



- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF



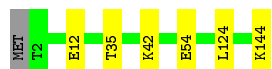
- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF



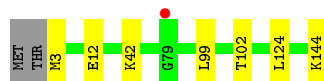
- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF



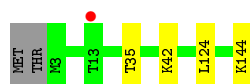
- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF



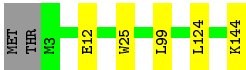
- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF



- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF



- Molecule 1: PROBABLE DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YNCF



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.06Å 97.07Å 193.85Å 89.72° 88.47° 90.11°	Depositor
Resolution (Å)	36.44 – 2.01 36.44 – 2.01	Depositor EDS
% Data completeness (in resolution range)	96.7 (36.44-2.01) 96.8 (36.44-2.01)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.29 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.6.0119	Depositor
R, $R_{free}$	0.169 , 0.212 0.174 , 0.215	Depositor DCC
$R_{free}$ test set	22967 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.3	Xtriage
Anisotropy	0.284	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 48.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.044 for k,-h,l 0.044 for -k,h,l 0.046 for h,-k,-l 0.048 for -h,k,-l 0.044 for -h,-k,l 0.039 for k,h,-l 0.115 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	60911	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.99% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, DUR, PO4, POP

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	1	0.81	0/1176	0.82	1/1582 (0.1%)
1	2	0.88	0/1176	0.85	0/1581
1	3	0.94	0/1157	0.89	2/1556 (0.1%)
1	4	0.96	1/1196 (0.1%)	0.90	3/1608 (0.2%)
1	5	0.85	0/1165	0.85	1/1567 (0.1%)
1	6	0.87	0/1165	0.86	1/1567 (0.1%)
1	7	0.82	0/1157	0.83	1/1556 (0.1%)
1	8	0.88	0/1165	0.86	2/1567 (0.1%)
1	9	0.90	0/1173	0.85	1/1575 (0.1%)
1	A	0.83	0/1178	0.82	1/1585 (0.1%)
1	B	0.86	0/1176	0.84	0/1582
1	C	0.80	0/1171	0.82	0/1572
1	D	0.90	1/1165 (0.1%)	0.88	1/1567 (0.1%)
1	E	0.90	0/1168	0.91	2/1571 (0.1%)
1	F	0.92	1/1183 (0.1%)	0.88	0/1592
1	G	0.92	0/1176	0.89	1/1579 (0.1%)
1	H	0.99	1/1157 (0.1%)	0.91	1/1556 (0.1%)
1	I	0.94	2/1165 (0.2%)	0.92	1/1567 (0.1%)
1	J	0.90	0/1168	0.92	5/1571 (0.3%)
1	K	0.86	0/1166	0.88	1/1568 (0.1%)
1	L	0.89	1/1157 (0.1%)	0.87	0/1556
1	M	0.90	0/1163	0.85	1/1564 (0.1%)
1	N	0.83	0/1157	0.86	2/1556 (0.1%)
1	O	0.90	0/1157	0.85	1/1556 (0.1%)
1	P	0.98	0/1173	0.88	1/1575 (0.1%)
1	Q	0.93	0/1175	0.91	2/1581 (0.1%)
1	R	0.94	0/1168	0.87	2/1571 (0.1%)
1	S	0.87	0/1176	0.86	3/1582 (0.2%)
1	T	0.86	0/1176	0.85	1/1582 (0.1%)
1	U	0.87	0/1176	0.86	0/1582
1	V	0.96	2/1165 (0.2%)	0.91	0/1567
1	W	0.92	2/1157 (0.2%)	0.85	2/1556 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	X	0.90	0/1182	0.91	1/1590 (0.1%)
1	Y	0.87	0/1165	0.88	0/1567
1	Z	0.85	0/1173	0.84	1/1575 (0.1%)
1	a	0.88	0/1172	0.89	2/1577 (0.1%)
1	b	0.87	0/1164	0.86	0/1566
1	c	0.89	1/1176 (0.1%)	0.87	1/1582 (0.1%)
1	d	0.89	1/1165 (0.1%)	0.88	1/1567 (0.1%)
1	e	0.92	2/1165 (0.2%)	0.86	0/1567
1	f	0.93	1/1165 (0.1%)	0.89	2/1567 (0.1%)
1	g	0.89	0/1173	0.85	0/1575
1	h	0.94	1/1157 (0.1%)	0.88	1/1556 (0.1%)
1	i	0.94	1/1165 (0.1%)	0.87	0/1567
1	j	0.93	0/1172	0.88	0/1577
1	k	0.92	0/1165	0.99	0/1567
1	l	0.81	0/1176	0.82	0/1582
1	m	0.81	1/1165 (0.1%)	0.85	1/1567 (0.1%)
All	All	0.89	19/56103 (0.0%)	0.87	50/75446 (0.1%)

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	W	25	TRP	CD2-CE2	5.90	1.48	1.41
1	m	25	TRP	CD2-CE2	5.78	1.48	1.41
1	F	25	TRP	CD2-CE2	5.77	1.48	1.41
1	c	37	LYS	CB-CG	-5.76	1.36	1.52
1	I	12	GLU	CG-CD	5.75	1.60	1.51

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	134	ASP	CB-CG-OD2	-6.00	112.90	118.30
1	K	109	ARG	NE-CZ-NH1	5.93	123.26	120.30
1	J	100	ARG	NE-CZ-NH2	-5.89	117.36	120.30
1	f	40	GLU	CA-CB-CG	5.88	126.33	113.40
1	J	134	ASP	CB-CG-OD1	5.87	123.58	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 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	1	142/144 (99%)	140 (99%)	1 (1%)	1 (1%)	22	16
1	2	142/144 (99%)	139 (98%)	3 (2%)	0	100	100
1	3	140/144 (97%)	138 (99%)	2 (1%)	0	100	100
1	4	144/144 (100%)	142 (99%)	2 (1%)	0	100	100
1	5	141/144 (98%)	140 (99%)	1 (1%)	0	100	100
1	6	141/144 (98%)	139 (99%)	2 (1%)	0	100	100
1	7	140/144 (97%)	138 (99%)	2 (1%)	0	100	100
1	8	141/144 (98%)	139 (99%)	2 (1%)	0	100	100
1	9	141/144 (98%)	139 (99%)	2 (1%)	0	100	100
1	A	143/144 (99%)	141 (99%)	2 (1%)	0	100	100
1	B	142/144 (99%)	141 (99%)	1 (1%)	0	100	100
1	C	141/144 (98%)	140 (99%)	1 (1%)	0	100	100
1	D	141/144 (98%)	139 (99%)	2 (1%)	0	100	100
1	E	141/144 (98%)	139 (99%)	2 (1%)	0	100	100
1	F	143/144 (99%)	141 (99%)	2 (1%)	0	100	100
1	G	141/144 (98%)	138 (98%)	3 (2%)	0	100	100
1	H	140/144 (97%)	139 (99%)	1 (1%)	0	100	100
1	I	141/144 (98%)	139 (99%)	2 (1%)	0	100	100
1	J	141/144 (98%)	139 (99%)	2 (1%)	0	100	100
1	K	141/144 (98%)	140 (99%)	1 (1%)	0	100	100
1	L	140/144 (97%)	139 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	M	141/144 (98%)	139 (99%)	2 (1%)	0	100	100
1	N	140/144 (97%)	138 (99%)	2 (1%)	0	100	100
1	O	140/144 (97%)	139 (99%)	1 (1%)	0	100	100
1	P	141/144 (98%)	139 (99%)	2 (1%)	0	100	100
1	Q	142/144 (99%)	141 (99%)	1 (1%)	0	100	100
1	R	141/144 (98%)	139 (99%)	2 (1%)	0	100	100
1	S	142/144 (99%)	141 (99%)	1 (1%)	0	100	100
1	T	142/144 (99%)	140 (99%)	2 (1%)	0	100	100
1	U	142/144 (99%)	139 (98%)	3 (2%)	0	100	100
1	V	141/144 (98%)	139 (99%)	2 (1%)	0	100	100
1	W	140/144 (97%)	138 (99%)	2 (1%)	0	100	100
1	X	143/144 (99%)	142 (99%)	1 (1%)	0	100	100
1	Y	141/144 (98%)	140 (99%)	1 (1%)	0	100	100
1	Z	141/144 (98%)	139 (99%)	2 (1%)	0	100	100
1	a	142/144 (99%)	140 (99%)	2 (1%)	0	100	100
1	b	141/144 (98%)	139 (99%)	2 (1%)	0	100	100
1	c	142/144 (99%)	140 (99%)	2 (1%)	0	100	100
1	d	141/144 (98%)	139 (99%)	1 (1%)	1 (1%)	22	16
1	e	141/144 (98%)	139 (99%)	2 (1%)	0	100	100
1	f	141/144 (98%)	139 (99%)	2 (1%)	0	100	100
1	g	141/144 (98%)	139 (99%)	2 (1%)	0	100	100
1	h	140/144 (97%)	138 (99%)	2 (1%)	0	100	100
1	i	141/144 (98%)	137 (97%)	4 (3%)	0	100	100
1	j	142/144 (99%)	137 (96%)	5 (4%)	0	100	100
1	k	141/144 (98%)	136 (96%)	5 (4%)	0	100	100
1	l	142/144 (99%)	141 (99%)	1 (1%)	0	100	100
1	m	141/144 (98%)	139 (99%)	2 (1%)	0	100	100
All	All	6780/6912 (98%)	6685 (99%)	93 (1%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	77	SER

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Mol	Chain	Res	Type
1	d	77	SER

### 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	1	125/125 (100%)	122 (98%)	3 (2%)	49	51
1	2	125/125 (100%)	123 (98%)	2 (2%)	62	67
1	3	123/125 (98%)	120 (98%)	3 (2%)	49	51
1	4	127/125 (102%)	125 (98%)	2 (2%)	62	67
1	5	124/125 (99%)	122 (98%)	2 (2%)	62	67
1	6	124/125 (99%)	123 (99%)	1 (1%)	81	86
1	7	123/125 (98%)	121 (98%)	2 (2%)	62	67
1	8	124/125 (99%)	119 (96%)	5 (4%)	31	29
1	9	125/125 (100%)	120 (96%)	5 (4%)	31	29
1	A	126/125 (101%)	124 (98%)	2 (2%)	62	67
1	B	125/125 (100%)	123 (98%)	2 (2%)	62	67
1	C	125/125 (100%)	118 (94%)	7 (6%)	21	17
1	D	124/125 (99%)	120 (97%)	4 (3%)	39	38
1	E	124/125 (99%)	120 (97%)	4 (3%)	39	38
1	F	126/125 (101%)	123 (98%)	3 (2%)	49	51
1	G	125/125 (100%)	121 (97%)	4 (3%)	39	38
1	H	123/125 (98%)	117 (95%)	6 (5%)	25	21
1	I	124/125 (99%)	120 (97%)	4 (3%)	39	38
1	J	124/125 (99%)	119 (96%)	5 (4%)	31	29
1	K	124/125 (99%)	121 (98%)	3 (2%)	49	51
1	L	123/125 (98%)	121 (98%)	2 (2%)	62	67
1	M	124/125 (99%)	122 (98%)	2 (2%)	62	67
1	N	123/125 (98%)	121 (98%)	2 (2%)	62	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	O	123/125 (98%)	117 (95%)	6 (5%)	25	21
1	P	125/125 (100%)	122 (98%)	3 (2%)	49	51
1	Q	125/125 (100%)	122 (98%)	3 (2%)	49	51
1	R	124/125 (99%)	120 (97%)	4 (3%)	39	38
1	S	125/125 (100%)	118 (94%)	7 (6%)	21	17
1	T	125/125 (100%)	121 (97%)	4 (3%)	39	38
1	U	125/125 (100%)	123 (98%)	2 (2%)	62	67
1	V	124/125 (99%)	120 (97%)	4 (3%)	39	38
1	W	123/125 (98%)	120 (98%)	3 (2%)	49	51
1	X	126/125 (101%)	124 (98%)	2 (2%)	62	67
1	Y	124/125 (99%)	119 (96%)	5 (4%)	31	29
1	Z	125/125 (100%)	122 (98%)	3 (2%)	49	51
1	a	125/125 (100%)	121 (97%)	4 (3%)	39	38
1	b	124/125 (99%)	120 (97%)	4 (3%)	39	38
1	c	125/125 (100%)	122 (98%)	3 (2%)	49	51
1	d	124/125 (99%)	121 (98%)	3 (2%)	49	51
1	e	124/125 (99%)	119 (96%)	5 (4%)	31	29
1	f	124/125 (99%)	120 (97%)	4 (3%)	39	38
1	g	125/125 (100%)	120 (96%)	5 (4%)	31	29
1	h	123/125 (98%)	119 (97%)	4 (3%)	38	37
1	i	124/125 (99%)	121 (98%)	3 (2%)	49	51
1	j	125/125 (100%)	119 (95%)	6 (5%)	25	22
1	k	124/125 (99%)	117 (94%)	7 (6%)	21	17
1	l	125/125 (100%)	121 (97%)	4 (3%)	39	38
1	m	124/125 (99%)	121 (98%)	3 (2%)	49	51
All	All	5970/6000 (100%)	5794 (97%)	176 (3%)	42	43

5 of 176 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	99	LEU
1	T	12	GLU
1	k	3	MET

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Mol	Chain	Res	Type
1	P	12	GLU
1	R	105	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	4	GLN
1	O	4	GLN
1	h	4	GLN
1	L	4	GLN
1	M	129	HIS

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 146 ligands modelled in this entry, 48 are monoatomic - leaving 98 for Mogul analysis.

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	DUR	1	1145	-	14,17,17	1.47	3 (21%)	14,24,24	1.06	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	POP	Z	1146	4	6,8,8	0.71	0	13,13,13	1.53	4 (30%)
2	DUR	6	1145	-	14,17,17	0.98	1 (7%)	14,24,24	1.17	0
3	POP	D	1146	4	6,8,8	1.07	1 (16%)	13,13,13	1.53	4 (30%)
2	DUR	k	1145	-	14,17,17	1.05	2 (14%)	14,24,24	1.40	2 (14%)
2	DUR	Y	1145	-	14,17,17	1.14	1 (7%)	14,24,24	1.43	2 (14%)
2	DUR	G	1145	-	14,17,17	1.08	1 (7%)	14,24,24	0.98	1 (7%)
2	DUR	e	1145	-	14,17,17	1.42	1 (7%)	14,24,24	1.22	2 (14%)
2	DUR	C	1145	-	14,17,17	1.14	2 (14%)	14,24,24	1.35	0
3	POP	F	1146	4	6,8,8	1.01	1 (16%)	13,13,13	1.65	2 (15%)
3	POP	G	1146	4	6,8,8	1.33	1 (16%)	13,13,13	1.85	5 (38%)
3	POP	L	1146	4	6,8,8	0.90	0	13,13,13	1.33	2 (15%)
3	POP	m	1146	4	6,8,8	0.87	0	13,13,13	1.57	2 (15%)
3	POP	f	1146	4	6,8,8	0.66	0	13,13,13	1.63	4 (30%)
3	POP	e	1146	4	6,8,8	1.26	1 (16%)	13,13,13	1.41	3 (23%)
3	POP	N	1146	4	6,8,8	1.17	1 (16%)	13,13,13	1.48	3 (23%)
3	POP	h	1146	4	6,8,8	1.27	1 (16%)	13,13,13	1.50	3 (23%)
3	POP	j	1146	4	6,8,8	0.75	0	13,13,13	1.67	3 (23%)
3	POP	T	1146	4	6,8,8	1.03	0	13,13,13	1.58	4 (30%)
2	DUR	d	1145	-	14,17,17	1.04	1 (7%)	14,24,24	1.09	1 (7%)
3	POP	6	1146	4	6,8,8	0.77	0	13,13,13	1.35	1 (7%)
3	POP	7	1146	4	6,8,8	0.82	0	13,13,13	1.53	3 (23%)
3	POP	2	1146	4	6,8,8	1.06	0	13,13,13	0.95	0
3	POP	3	1146	4	6,8,8	1.19	0	13,13,13	1.36	2 (15%)
3	POP	Y	1146	4	6,8,8	0.93	1 (16%)	13,13,13	1.76	5 (38%)
3	POP	W	1146	4	6,8,8	0.81	0	13,13,13	1.44	2 (15%)
3	POP	M	1146	4	6,8,8	1.12	1 (16%)	13,13,13	1.69	4 (30%)
3	POP	I	1146	4	6,8,8	1.52	2 (33%)	13,13,13	1.51	2 (15%)
2	DUR	L	1145	-	14,17,17	1.43	2 (14%)	14,24,24	1.17	2 (14%)
2	DUR	K	1145	-	14,17,17	1.29	1 (7%)	14,24,24	0.85	0
2	DUR	B	1145	-	14,17,17	0.86	1 (7%)	14,24,24	1.19	0
3	POP	4	1146	4	6,8,8	1.16	1 (16%)	13,13,13	1.67	3 (23%)
2	DUR	O	1145	-	14,17,17	1.33	1 (7%)	14,24,24	1.11	2 (14%)
2	DUR	E	1145	-	14,17,17	0.96	1 (7%)	14,24,24	1.36	2 (14%)
2	DUR	Z	1145	-	14,17,17	1.21	1 (7%)	14,24,24	1.34	1 (7%)
3	POP	l	1146	4	6,8,8	0.79	0	13,13,13	1.13	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	POP	c	1146	4	6,8,8	0.59	0	13,13,13	1.72	3 (23%)
5	PO4	e	1148	-	4,4,4	0.58	0	6,6,6	0.82	0
5	PO4	l	1148	-	4,4,4	1.28	0	6,6,6	1.11	1 (16%)
2	DUR	V	1145	-	14,17,17	1.41	2 (14%)	14,24,24	1.38	1 (7%)
3	POP	a	1146	4	6,8,8	0.85	0	13,13,13	1.36	1 (7%)
2	DUR	3	1145	-	14,17,17	1.02	1 (7%)	14,24,24	0.91	0
2	DUR	D	1145	-	14,17,17	1.05	1 (7%)	14,24,24	1.26	2 (14%)
2	DUR	h	1145	-	14,17,17	1.77	2 (14%)	14,24,24	0.91	0
3	POP	R	1146	4	6,8,8	0.63	0	13,13,13	1.51	3 (23%)
2	DUR	a	1145	-	14,17,17	1.17	1 (7%)	14,24,24	1.28	3 (21%)
2	DUR	c	1145	-	14,17,17	1.44	2 (14%)	14,24,24	1.07	1 (7%)
2	DUR	Q	1145	-	14,17,17	1.05	0	14,24,24	0.84	0
2	DUR	b	1145	-	14,17,17	1.45	1 (7%)	14,24,24	1.17	1 (7%)
2	DUR	f	1145	-	14,17,17	0.84	1 (7%)	14,24,24	1.35	1 (7%)
3	POP	A	1146	4	6,8,8	1.10	0	13,13,13	1.18	1 (7%)
3	POP	8	1146	4	6,8,8	1.15	0	13,13,13	1.25	1 (7%)
3	POP	d	1146	4	6,8,8	0.88	0	13,13,13	1.87	6 (46%)
3	POP	E	1146	4	6,8,8	0.80	0	13,13,13	1.18	1 (7%)
3	POP	i	1146	4	6,8,8	1.02	0	13,13,13	1.39	3 (23%)
3	POP	U	1146	4	6,8,8	0.91	0	13,13,13	1.24	0
2	DUR	N	1145	-	14,17,17	0.89	0	14,24,24	1.26	2 (14%)
2	DUR	P	1145	-	14,17,17	0.69	0	14,24,24	1.22	1 (7%)
3	POP	9	1146	4	6,8,8	0.96	0	13,13,13	1.31	1 (7%)
2	DUR	W	1145	-	14,17,17	1.00	1 (7%)	14,24,24	0.88	0
3	POP	g	1146	4	6,8,8	0.73	0	13,13,13	1.67	3 (23%)
2	DUR	m	1145	-	14,17,17	0.99	1 (7%)	14,24,24	0.63	0
2	DUR	S	1145	-	14,17,17	1.28	1 (7%)	14,24,24	1.21	1 (7%)
2	DUR	J	1145	-	14,17,17	1.55	3 (21%)	14,24,24	1.76	3 (21%)
2	DUR	R	1145	-	14,17,17	1.70	1 (7%)	14,24,24	1.04	0
2	DUR	I	1145	-	14,17,17	1.84	2 (14%)	14,24,24	0.74	0
2	DUR	7	1145	-	14,17,17	1.20	2 (14%)	14,24,24	1.10	2 (14%)
2	DUR	8	1145	-	14,17,17	1.31	1 (7%)	14,24,24	0.87	0
2	DUR	U	1145	-	14,17,17	1.07	0	14,24,24	1.28	1 (7%)
3	POP	k	1146	4	6,8,8	0.79	0	13,13,13	1.60	3 (23%)
2	DUR	g	1145	-	14,17,17	0.91	1 (7%)	14,24,24	1.10	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	POP	1	1146	4	6,8,8	0.90	0	13,13,13	1.48	4 (30%)
3	POP	S	1146	4	6,8,8	1.33	0	13,13,13	0.98	0
2	DUR	2	1145	-	14,17,17	0.87	1 (7%)	14,24,24	0.91	0
2	DUR	4	1145	-	14,17,17	0.94	0	14,24,24	1.22	2 (14%)
2	DUR	5	1145	-	14,17,17	1.43	1 (7%)	14,24,24	1.09	1 (7%)
3	POP	5	1146	4	6,8,8	1.03	0	13,13,13	1.19	3 (23%)
3	POP	P	1146	4	6,8,8	1.20	0	13,13,13	1.68	5 (38%)
2	DUR	H	1145	-	14,17,17	1.03	1 (7%)	14,24,24	1.51	3 (21%)
2	DUR	A	1145	-	14,17,17	1.24	1 (7%)	14,24,24	1.51	3 (21%)
3	POP	B	1146	4	6,8,8	1.16	0	13,13,13	1.88	6 (46%)
3	POP	C	1146	4	6,8,8	0.57	0	13,13,13	1.39	3 (23%)
2	DUR	1	1145	-	14,17,17	1.26	2 (14%)	14,24,24	1.41	3 (21%)
3	POP	H	1146	4	6,8,8	1.26	0	13,13,13	1.29	1 (7%)
3	POP	J	1146	4	6,8,8	0.84	0	13,13,13	1.08	1 (7%)
2	DUR	F	1145	-	14,17,17	1.68	3 (21%)	14,24,24	1.17	2 (14%)
2	DUR	9	1145	-	14,17,17	0.91	0	14,24,24	1.18	2 (14%)
2	DUR	j	1145	-	14,17,17	1.20	1 (7%)	14,24,24	1.42	2 (14%)
3	POP	X	1146	4	6,8,8	0.95	0	13,13,13	1.49	2 (15%)
2	DUR	i	1145	-	14,17,17	1.03	1 (7%)	14,24,24	1.13	0
2	DUR	X	1145	-	14,17,17	1.20	2 (14%)	14,24,24	1.19	2 (14%)
3	POP	b	1146	4	6,8,8	1.11	0	13,13,13	1.43	3 (23%)
3	POP	Q	1146	4	6,8,8	1.07	1 (16%)	13,13,13	1.09	1 (7%)
3	POP	K	1146	4	6,8,8	1.41	0	13,13,13	1.12	1 (7%)
2	DUR	T	1145	-	14,17,17	0.90	1 (7%)	14,24,24	1.29	2 (14%)
2	DUR	M	1145	-	14,17,17	1.11	2 (14%)	14,24,24	0.80	0
3	POP	O	1146	4	6,8,8	1.14	0	13,13,13	1.29	2 (15%)
3	POP	V	1146	4	6,8,8	0.89	0	13,13,13	1.71	3 (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	DUR	l	1145	-	-	0/3/18/18	0/2/2/2
3	POP	Z	1146	4	-	2/6/6/6	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DUR	6	1145	-	-	0/3/18/18	0/2/2/2
3	POP	D	1146	4	-	3/6/6/6	-
2	DUR	k	1145	-	-	0/3/18/18	0/2/2/2
2	DUR	Y	1145	-	-	0/3/18/18	0/2/2/2
2	DUR	G	1145	-	-	0/3/18/18	0/2/2/2
2	DUR	e	1145	-	-	0/3/18/18	0/2/2/2
2	DUR	C	1145	-	-	0/3/18/18	0/2/2/2
3	POP	F	1146	4	-	2/6/6/6	-
3	POP	G	1146	4	-	3/6/6/6	-
3	POP	L	1146	4	-	2/6/6/6	-
3	POP	m	1146	4	-	2/6/6/6	-
3	POP	f	1146	4	-	2/6/6/6	-
3	POP	e	1146	4	-	2/6/6/6	-
3	POP	N	1146	4	-	2/6/6/6	-
3	POP	h	1146	4	-	3/6/6/6	-
3	POP	j	1146	4	-	3/6/6/6	-
3	POP	T	1146	4	-	3/6/6/6	-
2	DUR	d	1145	-	-	0/3/18/18	0/2/2/2
3	POP	6	1146	4	-	2/6/6/6	-
3	POP	7	1146	4	-	2/6/6/6	-
3	POP	2	1146	4	-	2/6/6/6	-
3	POP	3	1146	4	-	2/6/6/6	-
3	POP	Y	1146	4	-	3/6/6/6	-
3	POP	W	1146	4	-	3/6/6/6	-
3	POP	M	1146	4	-	2/6/6/6	-
3	POP	I	1146	4	-	3/6/6/6	-
2	DUR	L	1145	-	-	0/3/18/18	0/2/2/2
2	DUR	K	1145	-	-	0/3/18/18	0/2/2/2
2	DUR	B	1145	-	-	0/3/18/18	0/2/2/2
3	POP	4	1146	4	-	2/6/6/6	-
2	DUR	O	1145	-	-	0/3/18/18	0/2/2/2
2	DUR	E	1145	-	-	0/3/18/18	0/2/2/2
2	DUR	Z	1145	-	-	0/3/18/18	0/2/2/2
3	POP	l	1146	4	-	2/6/6/6	-
3	POP	c	1146	4	-	3/6/6/6	-
2	DUR	V	1145	-	-	0/3/18/18	0/2/2/2
3	POP	a	1146	4	-	2/6/6/6	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DUR	3	1145	-	-	0/3/18/18	0/2/2/2
2	DUR	D	1145	-	-	0/3/18/18	0/2/2/2
2	DUR	h	1145	-	-	0/3/18/18	0/2/2/2
3	POP	R	1146	4	-	3/6/6/6	-
2	DUR	a	1145	-	-	0/3/18/18	0/2/2/2
2	DUR	c	1145	-	-	0/3/18/18	0/2/2/2
2	DUR	Q	1145	-	-	0/3/18/18	0/2/2/2
2	DUR	b	1145	-	-	0/3/18/18	0/2/2/2
2	DUR	f	1145	-	-	0/3/18/18	0/2/2/2
3	POP	A	1146	4	-	2/6/6/6	-
3	POP	8	1146	4	-	2/6/6/6	-
3	POP	d	1146	4	-	3/6/6/6	-
3	POP	E	1146	4	-	2/6/6/6	-
3	POP	i	1146	4	-	2/6/6/6	-
3	POP	U	1146	4	-	3/6/6/6	-
2	DUR	N	1145	-	-	0/3/18/18	0/2/2/2
2	DUR	P	1145	-	-	0/3/18/18	0/2/2/2
3	POP	9	1146	4	-	2/6/6/6	-
2	DUR	W	1145	-	-	0/3/18/18	0/2/2/2
3	POP	g	1146	4	-	2/6/6/6	-
2	DUR	m	1145	-	-	0/3/18/18	0/2/2/2
2	DUR	S	1145	-	-	0/3/18/18	0/2/2/2
2	DUR	J	1145	-	1/1/3/3	2/3/18/18	0/2/2/2
2	DUR	R	1145	-	-	0/3/18/18	0/2/2/2
2	DUR	I	1145	-	-	0/3/18/18	0/2/2/2
2	DUR	7	1145	-	-	0/3/18/18	0/2/2/2
2	DUR	8	1145	-	-	0/3/18/18	0/2/2/2
2	DUR	U	1145	-	-	0/3/18/18	0/2/2/2
3	POP	k	1146	4	-	2/6/6/6	-
2	DUR	g	1145	-	-	0/3/18/18	0/2/2/2
3	POP	1	1146	4	-	2/6/6/6	-
3	POP	S	1146	4	-	2/6/6/6	-
2	DUR	2	1145	-	-	0/3/18/18	0/2/2/2
2	DUR	4	1145	-	-	0/3/18/18	0/2/2/2
2	DUR	5	1145	-	-	0/3/18/18	0/2/2/2
3	POP	5	1146	4	-	2/6/6/6	-
3	POP	P	1146	4	-	2/6/6/6	-
2	DUR	H	1145	-	-	0/3/18/18	0/2/2/2
2	DUR	A	1145	-	-	0/3/18/18	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	POP	B	1146	4	-	3/6/6/6	-
3	POP	C	1146	4	-	3/6/6/6	-
2	DUR	1	1145	-	-	0/3/18/18	0/2/2/2
3	POP	H	1146	4	-	2/6/6/6	-
3	POP	J	1146	4	-	3/6/6/6	-
2	DUR	F	1145	-	-	0/3/18/18	0/2/2/2
2	DUR	9	1145	-	-	0/3/18/18	0/2/2/2
2	DUR	j	1145	-	-	0/3/18/18	0/2/2/2
3	POP	X	1146	4	-	2/6/6/6	-
2	DUR	i	1145	-	-	0/3/18/18	0/2/2/2
2	DUR	X	1145	-	-	0/3/18/18	0/2/2/2
3	POP	b	1146	4	-	3/6/6/6	-
3	POP	Q	1146	4	-	2/6/6/6	-
3	POP	K	1146	4	-	2/6/6/6	-
2	DUR	T	1145	-	-	2/3/18/18	0/2/2/2
2	DUR	M	1145	-	-	0/3/18/18	0/2/2/2
3	POP	O	1146	4	-	2/6/6/6	-
3	POP	V	1146	4	-	3/6/6/6	-

The worst 5 of 71 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	R	1145	DUR	C6-N1	-5.55	1.29	1.35
2	h	1145	DUR	C2-N3	-5.15	1.28	1.38
2	F	1145	DUR	C2-N3	-4.66	1.28	1.38
2	I	1145	DUR	C2-N3	-4.56	1.29	1.38
2	J	1145	DUR	C2-N3	-4.51	1.29	1.38

The worst 5 of 182 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	m	1146	POP	O6-P2-O5	4.06	123.17	107.64
3	V	1146	POP	O6-P2-O5	4.04	123.06	107.64
2	J	1145	DUR	O3'-C3'-C4'	3.90	125.03	110.10
3	j	1146	POP	O5-P2-O4	3.36	123.85	110.68
3	7	1146	POP	P2-O-P1	-3.36	121.31	132.83

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	J	1145	DUR	C3'

5 of 117 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	Z	1146	POP	P1-O-P2-O5
3	D	1146	POP	P1-O-P2-O5
3	F	1146	POP	P1-O-P2-O5
3	G	1146	POP	P1-O-P2-O5
3	L	1146	POP	P1-O-P2-O5

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, 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	1	142/144 (98%)	-0.24	0 100 100	14, 24, 44, 53	3 (2%)
1	2	142/144 (98%)	-0.46	0 100 100	13, 23, 39, 50	0
1	3	142/144 (98%)	-0.40	0 100 100	11, 21, 36, 44	1 (0%)
1	4	142/144 (98%)	-0.42	0 100 100	13, 21, 35, 49	0
1	5	142/144 (98%)	-0.23	2 (1%) 75 74	16, 27, 48, 56	2 (1%)
1	6	142/144 (98%)	-0.21	0 100 100	15, 26, 46, 58	3 (2%)
1	7	142/144 (98%)	-0.21	0 100 100	16, 27, 47, 60	0
1	8	142/144 (98%)	-0.44	0 100 100	13, 21, 40, 53	0
1	9	142/144 (98%)	-0.39	0 100 100	11, 22, 38, 53	1 (0%)
1	A	143/144 (99%)	-0.25	1 (0%) 87 87	16, 26, 44, 55	2 (1%)
1	B	142/144 (98%)	-0.33	0 100 100	14, 25, 43, 51	2 (1%)
1	C	142/144 (98%)	-0.17	2 (1%) 75 74	15, 25, 45, 57	2 (1%)
1	D	142/144 (98%)	-0.43	0 100 100	11, 22, 38, 54	2 (1%)
1	E	142/144 (98%)	-0.36	0 100 100	12, 22, 38, 57	1 (0%)
1	F	143/144 (99%)	-0.40	1 (0%) 87 87	11, 21, 40, 48	1 (0%)
1	G	142/144 (98%)	-0.40	0 100 100	11, 20, 37, 50	2 (1%)
1	H	142/144 (98%)	-0.42	1 (0%) 87 87	11, 20, 38, 48	1 (0%)
1	I	142/144 (98%)	-0.47	0 100 100	12, 20, 35, 47	2 (1%)
1	J	142/144 (98%)	-0.39	0 100 100	13, 23, 42, 51	1 (0%)
1	K	142/144 (98%)	-0.30	0 100 100	13, 24, 41, 52	4 (2%)
1	L	142/144 (98%)	-0.41	0 100 100	14, 23, 39, 55	0
1	M	142/144 (98%)	-0.35	1 (0%) 87 87	13, 23, 40, 48	1 (0%)
1	N	142/144 (98%)	-0.37	0 100 100	15, 25, 44, 52	1 (0%)
1	O	142/144 (98%)	-0.32	2 (1%) 75 74	16, 24, 41, 57	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	P	142/144 (98%)	-0.44	0 100 100	11, 20, 38, 48	1 (0%)
1	Q	143/144 (99%)	-0.38	0 100 100	13, 22, 40, 46	0
1	R	142/144 (98%)	-0.40	0 100 100	11, 22, 40, 50	1 (0%)
1	S	142/144 (98%)	-0.38	0 100 100	13, 23, 39, 54	0
1	T	142/144 (98%)	-0.39	0 100 100	13, 24, 45, 56	1 (0%)
1	U	142/144 (98%)	-0.39	0 100 100	13, 23, 42, 50	0
1	V	142/144 (98%)	-0.38	0 100 100	13, 23, 41, 50	1 (0%)
1	W	142/144 (98%)	-0.35	0 100 100	11, 22, 41, 51	0
1	X	142/144 (98%)	-0.43	0 100 100	12, 21, 41, 50	0
1	Y	142/144 (98%)	-0.27	0 100 100	14, 24, 44, 54	1 (0%)
1	Z	142/144 (98%)	-0.30	0 100 100	14, 26, 43, 66	2 (1%)
1	a	143/144 (99%)	-0.43	0 100 100	13, 22, 36, 44	2 (1%)
1	b	143/144 (99%)	-0.36	0 100 100	12, 24, 45, 51	1 (0%)
1	c	142/144 (98%)	-0.31	0 100 100	13, 25, 44, 58	2 (1%)
1	d	142/144 (98%)	-0.31	1 (0%) 87 87	14, 25, 45, 60	0
1	e	142/144 (98%)	-0.36	0 100 100	13, 23, 44, 53	0
1	f	142/144 (98%)	-0.30	0 100 100	13, 24, 42, 49	0
1	g	142/144 (98%)	-0.32	1 (0%) 87 87	14, 23, 42, 57	1 (0%)
1	h	142/144 (98%)	-0.39	0 100 100	11, 21, 40, 48	1 (0%)
1	i	142/144 (98%)	-0.40	2 (1%) 75 74	13, 21, 39, 46	1 (0%)
1	j	143/144 (99%)	-0.37	0 100 100	13, 22, 43, 51	1 (0%)
1	k	142/144 (98%)	-0.32	1 (0%) 87 87	15, 27, 45, 58	1 (0%)
1	l	142/144 (98%)	-0.21	1 (0%) 87 87	16, 28, 50, 63	0
1	m	142/144 (98%)	-0.29	0 100 100	16, 28, 49, 57	0
All	All	6822/6912 (98%)	-0.35	16 (0%) 95 94	11, 24, 43, 66	49 (0%)

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	99	LEU	2.9
1	C	34	VAL	2.8
1	g	101	ASP	2.5
1	i	131	GLY	2.4
1	C	101	ASP	2.4

## 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 monosaccharides 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, 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	B-factors( $\text{\AA}^2$ )	Q<0.9
5	PO4	l	1148	5/5	0.90	0.37	40,46,51,61	0
5	PO4	e	1148	5/5	0.94	0.14	49,54,55,61	0
2	DUR	Y	1145	16/16	0.95	0.12	14,17,20,20	0
2	DUR	l	1145	16/16	0.95	0.08	14,18,19,20	0
4	MG	M	1147	1/1	0.95	0.05	19,19,19,19	0
4	MG	d	1147	1/1	0.96	0.06	22,22,22,22	0
2	DUR	C	1145	16/16	0.96	0.11	16,18,22,22	0
2	DUR	J	1145	16/16	0.96	0.10	13,14,16,16	0
2	DUR	i	1145	16/16	0.96	0.09	15,16,19,19	0
2	DUR	k	1145	16/16	0.97	0.10	17,18,20,20	0
4	MG	Z	1147	1/1	0.97	0.05	21,21,21,21	0
2	DUR	V	1145	16/16	0.97	0.09	12,14,16,17	0
2	DUR	3	1145	16/16	0.97	0.12	12,13,15,16	0
2	DUR	D	1145	16/16	0.97	0.09	13,14,17,20	0
2	DUR	h	1145	16/16	0.97	0.09	11,13,14,14	0
2	DUR	c	1145	16/16	0.97	0.09	16,17,19,21	0
2	DUR	Q	1145	16/16	0.97	0.09	14,15,17,20	0
4	MG	B	1147	1/1	0.97	0.04	18,18,18,18	0
4	MG	H	1147	1/1	0.97	0.09	16,16,16,16	0
2	DUR	W	1145	16/16	0.97	0.11	14,15,17,17	0
2	DUR	S	1145	16/16	0.97	0.09	12,15,17,17	0
4	MG	4	1147	1/1	0.97	0.06	15,15,15,15	0
2	DUR	R	1145	16/16	0.97	0.08	12,13,15,15	0
2	DUR	I	1145	16/16	0.97	0.09	10,13,14,15	0
2	DUR	8	1145	16/16	0.97	0.09	12,13,14,15	0
2	DUR	g	1145	16/16	0.97	0.09	14,16,18,19	0
2	DUR	2	1145	16/16	0.97	0.08	12,14,17,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	DUR	4	1145	16/16	0.97	0.08	11,12,13,14	0
2	DUR	K	1145	16/16	0.97	0.11	14,16,18,18	0
2	DUR	B	1145	16/16	0.97	0.09	18,19,20,20	0
2	DUR	F	1145	16/16	0.97	0.07	12,14,15,16	0
2	DUR	j	1145	16/16	0.97	0.10	14,16,17,20	0
2	DUR	Z	1145	16/16	0.97	0.10	17,19,22,22	0
2	DUR	e	1145	16/16	0.97	0.09	14,15,16,16	0
2	DUR	T	1145	16/16	0.97	0.08	14,18,20,20	0
2	DUR	N	1145	16/16	0.98	0.12	15,17,20,20	0
4	MG	E	1147	1/1	0.98	0.06	17,17,17,17	0
2	DUR	P	1145	16/16	0.98	0.09	13,14,16,17	0
4	MG	D	1147	1/1	0.98	0.09	15,15,15,15	0
2	DUR	m	1145	16/16	0.98	0.08	15,20,23,23	0
4	MG	k	1147	1/1	0.98	0.09	21,21,21,21	0
2	DUR	d	1145	16/16	0.98	0.10	14,15,17,18	0
4	MG	F	1147	1/1	0.98	0.06	14,14,14,14	0
4	MG	b	1147	1/1	0.98	0.09	16,16,16,16	0
4	MG	7	1147	1/1	0.98	0.10	20,20,20,20	0
2	DUR	7	1145	16/16	0.98	0.08	15,18,21,24	0
2	DUR	L	1145	16/16	0.98	0.10	14,15,18,19	0
2	DUR	U	1145	16/16	0.98	0.09	15,16,17,18	0
4	MG	C	1147	1/1	0.98	0.06	13,13,13,13	0
2	DUR	l	1145	16/16	0.98	0.10	17,20,23,23	0
2	DUR	G	1145	16/16	0.98	0.10	11,13,14,14	0
2	DUR	a	1145	16/16	0.98	0.07	15,16,17,17	0
2	DUR	5	1145	16/16	0.98	0.07	17,20,22,22	0
2	DUR	H	1145	16/16	0.98	0.07	12,14,15,15	0
2	DUR	A	1145	16/16	0.98	0.10	16,18,20,20	0
2	DUR	O	1145	16/16	0.98	0.10	16,18,21,21	0
4	MG	6	1147	1/1	0.98	0.09	19,19,19,19	0
2	DUR	E	1145	16/16	0.98	0.10	13,14,15,15	0
2	DUR	9	1145	16/16	0.98	0.10	13,14,16,17	0
2	DUR	b	1145	16/16	0.98	0.11	13,15,17,19	0
2	DUR	f	1145	16/16	0.98	0.09	15,16,19,22	0
2	DUR	6	1145	16/16	0.98	0.10	19,21,23,23	0
2	DUR	X	1145	16/16	0.98	0.07	12,14,15,20	0
4	MG	U	1147	1/1	0.98	0.10	15,15,15,15	0
2	DUR	M	1145	16/16	0.98	0.11	14,17,18,19	0
3	POP	T	1146	9/9	0.99	0.07	13,16,18,19	0
4	MG	J	1147	1/1	0.99	0.12	17,17,17,17	0
3	POP	6	1146	9/9	0.99	0.07	18,21,22,24	0
3	POP	R	1146	9/9	0.99	0.07	13,14,15,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	POP	7	1146	9/9	0.99	0.09	18,20,22,23	0
4	MG	X	1147	1/1	0.99	0.08	16,16,16,16	0
3	POP	2	1146	9/9	0.99	0.08	13,14,16,17	0
3	POP	3	1146	9/9	0.99	0.07	14,16,17,18	0
4	MG	I	1147	1/1	0.99	0.04	11,11,11,11	0
3	POP	Y	1146	9/9	0.99	0.06	15,17,18,19	0
4	MG	O	1147	1/1	0.99	0.05	20,20,20,20	0
4	MG	K	1147	1/1	0.99	0.07	15,15,15,15	0
4	MG	f	1147	1/1	0.99	0.05	17,17,17,17	0
3	POP	W	1146	9/9	0.99	0.08	10,13,15,16	0
3	POP	8	1146	9/9	0.99	0.06	14,16,17,17	0
3	POP	d	1146	9/9	0.99	0.07	19,20,22,23	0
4	MG	3	1147	1/1	0.99	0.09	17,17,17,17	0
3	POP	E	1146	9/9	0.99	0.06	15,16,17,18	0
3	POP	Z	1146	9/9	0.99	0.10	16,18,19,20	0
4	MG	T	1147	1/1	0.99	0.07	17,17,17,17	0
3	POP	U	1146	9/9	0.99	0.08	16,17,19,19	0
4	MG	G	1147	1/1	0.99	0.04	14,14,14,14	0
3	POP	M	1146	9/9	0.99	0.06	13,19,20,20	0
4	MG	W	1147	1/1	0.99	0.07	12,12,12,12	0
4	MG	l	1147	1/1	0.99	0.04	18,18,18,18	0
3	POP	9	1146	9/9	0.99	0.07	14,14,16,16	0
3	POP	I	1146	9/9	0.99	0.08	11,13,15,17	0
3	POP	g	1146	9/9	0.99	0.08	13,15,16,19	0
4	MG	a	1147	1/1	0.99	0.05	15,15,15,15	0
3	POP	F	1146	9/9	0.99	0.07	11,13,13,13	0
4	MG	8	1147	1/1	0.99	0.07	17,17,17,17	0
3	POP	G	1146	9/9	0.99	0.06	12,14,15,16	0
4	MG	c	1147	1/1	0.99	0.07	15,15,15,15	0
3	POP	D	1146	9/9	0.99	0.07	11,15,17,17	0
4	MG	5	1147	1/1	0.99	0.08	18,18,18,18	0
4	MG	j	1147	1/1	0.99	0.07	13,13,13,13	0
3	POP	4	1146	9/9	0.99	0.08	14,14,16,17	0
3	POP	k	1146	9/9	0.99	0.07	19,23,24,25	0
4	MG	N	1147	1/1	0.99	0.05	14,14,14,14	0
4	MG	m	1147	1/1	0.99	0.10	17,17,17,17	0
3	POP	1	1146	9/9	0.99	0.06	18,19,21,24	0
4	MG	A	1147	1/1	0.99	0.09	21,21,21,21	0
3	POP	S	1146	9/9	0.99	0.06	13,15,18,21	0
3	POP	L	1146	9/9	0.99	0.09	16,17,19,21	0
3	POP	m	1146	9/9	0.99	0.08	18,20,21,22	0
4	MG	V	1147	1/1	0.99	0.07	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	POP	5	1146	9/9	0.99	0.07	17,19,20,20	0
3	POP	P	1146	9/9	0.99	0.07	14,15,17,17	0
4	MG	2	1147	1/1	0.99	0.05	11,11,11,11	0
3	POP	l	1146	9/9	0.99	0.06	15,19,22,23	0
3	POP	c	1146	9/9	0.99	0.06	14,16,18,18	0
3	POP	B	1146	9/9	0.99	0.06	16,18,20,23	0
3	POP	a	1146	9/9	0.99	0.09	13,15,16,17	0
3	POP	C	1146	9/9	0.99	0.07	17,18,22,22	0
4	MG	g	1147	1/1	0.99	0.11	16,16,16,16	0
3	POP	J	1146	9/9	0.99	0.08	15,18,19,20	0
3	POP	e	1146	9/9	0.99	0.07	16,18,20,20	0
3	POP	N	1146	9/9	0.99	0.08	16,18,19,20	0
4	MG	e	1147	1/1	0.99	0.04	18,18,18,18	0
4	MG	h	1147	1/1	0.99	0.04	15,15,15,15	0
3	POP	X	1146	9/9	0.99	0.07	15,16,18,19	0
3	POP	h	1146	9/9	0.99	0.07	17,18,19,19	0
3	POP	j	1146	9/9	0.99	0.08	13,14,16,17	0
3	POP	b	1146	9/9	0.99	0.06	15,17,20,21	0
3	POP	Q	1146	9/9	0.99	0.08	11,12,14,14	0
4	MG	S	1147	1/1	0.99	0.08	14,14,14,14	0
4	MG	i	1147	1/1	0.99	0.05	14,14,14,14	0
3	POP	K	1146	9/9	0.99	0.07	13,15,18,21	0
4	MG	9	1147	1/1	0.99	0.09	17,17,17,17	0
3	POP	A	1146	9/9	0.99	0.07	18,19,21,25	0
4	MG	P	1147	1/1	0.99	0.11	13,13,13,13	0
4	MG	R	1147	1/1	0.99	0.10	12,12,12,12	0
4	MG	l	1147	1/1	0.99	0.05	18,18,18,18	0
3	POP	O	1146	9/9	0.99	0.07	16,17,22,23	0
3	POP	V	1146	9/9	0.99	0.09	14,16,17,20	0
4	MG	Y	1147	1/1	1.00	0.03	16,16,16,16	0
3	POP	i	1146	9/9	1.00	0.09	13,16,19,21	0
4	MG	L	1147	1/1	1.00	0.05	17,17,17,17	0
3	POP	H	1146	9/9	1.00	0.07	14,15,16,17	0
3	POP	f	1146	9/9	1.00	0.07	13,15,17,17	0
4	MG	Q	1147	1/1	1.00	0.06	10,10,10,10	0

## 6.5 Other polymers

There are no such residues in this entry.