



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:34 PM GMT

PDB ID : 4IR9  
Title : Polymerase-DNA complex  
Authors : Sharma, A.; Nair, D.T.  
Deposited on : 2013-01-14  
Resolution : 2.33 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

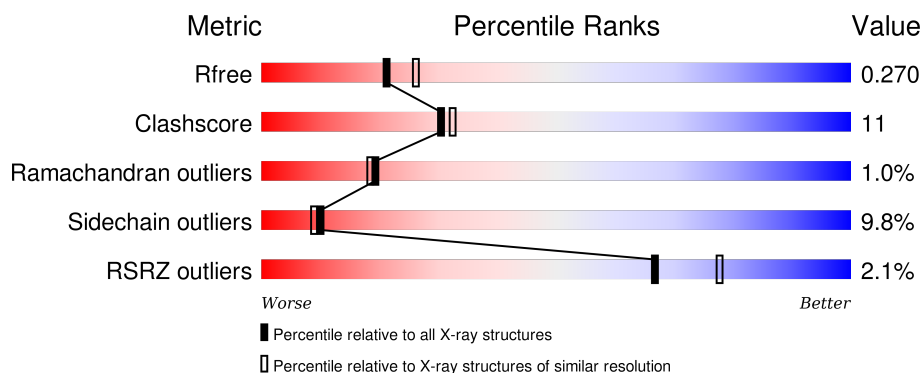
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.33 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	1406 (2.36-2.32)
Clashscore	102246	1509 (2.36-2.32)
Ramachandran outliers	100387	1490 (2.36-2.32)
Sidechain outliers	100360	1491 (2.36-2.32)
RSRZ outliers	91569	1412 (2.36-2.32)

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	B	18	 61% 17% 22%
1	G	18	 44% 39% 17%
2	C	17	 6% 47% 41% 12%
3	H	14	 50% 29% 21%
4	A	352	 4% 71% 21% 5% •

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Mol	Chain	Length	Quality of chain
4	F	352	 A horizontal bar chart showing the quality of chain 4. The bar is divided into three segments: a green segment representing 72%, a yellow segment representing 21%, and a small red segment representing 7%. The text '72%' is centered under the green segment, and '21%' is centered under the yellow segment. To the right of the bar are three dots '...'.

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
6	MG	F	402	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6927 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	18	Total	C	N	O	P	0	0	0
			362	173	64	108	17			
1	B	18	Total	C	N	O	P	0	0	0
			362	173	64	108	17			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	17	Total	C	N	O	P	0	0	0
			344	164	64	100	16			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	14	Total	C	N	O	P	0	0	0
			284	135	54	82	13			

- Molecule 4 is a protein called DNA polymerase IV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	342	Total	C	N	O	S	0	0	0
			2687	1695	494	484	14			
4	A	342	Total	C	N	O	S	0	0	0
			2687	1695	494	484	14			

There are 4 discrepancies between the modelled and reference sequences:

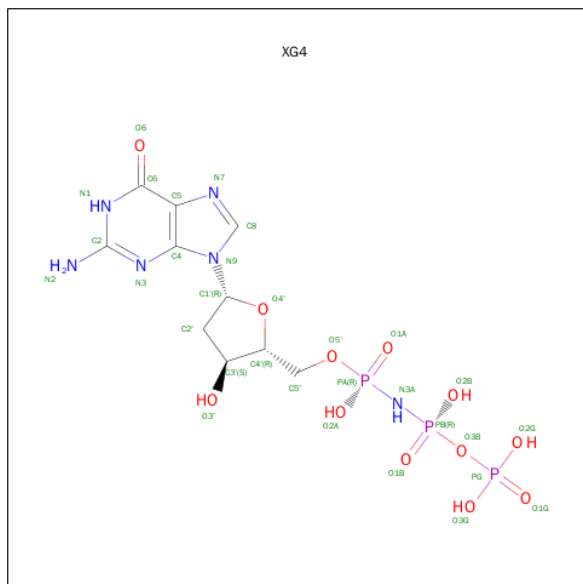
Chain	Residue	Modelled	Actual	Comment	Reference
F	0	GLY	-	EXPRESSION TAG	UNP Q47155

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Chain	Residue	Modelled	Actual	Comment	Reference
F	1	SER	-	EXPRESSION TAG	UNP Q47155
A	0	GLY	-	EXPRESSION TAG	UNP Q47155
A	1	SER	-	EXPRESSION TAG	UNP Q47155

- Molecule 5 is 2'-DEOXY-5'-O-[(R)-HYDROXY{[(R)-HYDROXY(PHOSPHONOOXY)P HOSPHORYL]AMINO}PHOSPHORYL]GUANOSINE (three-letter code: XG4) (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
5	F	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
5	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	Mg	0	0
			2	2		
6	F	2	Total	Mg	0	0
			2	2		

- Molecule 7 is water.

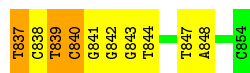
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	7	Total 7	O 7	0	0
7	C	8	Total 8	O 8	0	0
7	G	20	Total 20	O 20	0	0
7	H	15	Total 15	O 15	0	0
7	F	63	Total 63	O 63	0	0
7	A	22	Total 22	O 22	0	0

### 3 Residue-property plots

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.

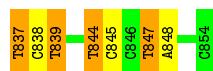
- Molecule 1: DNA (5'-D(P\*TP\*CP\*TP\*CP\*GP\*GP\*GP\*TP\*CP\*CP\*TP\*AP\*GP\*GP\*AP\*CP\*CP\*C)-3')

Chain G: 



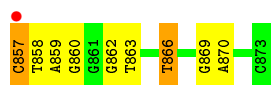
- Molecule 1: DNA (5'-D(P\*TP\*CP\*TP\*CP\*GP\*GP\*GP\*TP\*CP\*CP\*TP\*AP\*GP\*GP\*AP\*CP\*CP\*C)-3')

Chain B: 



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

Chain C: 



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

Chain H: 



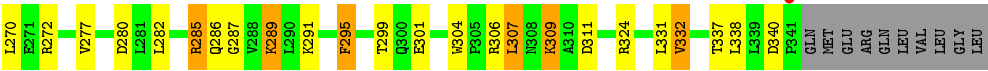
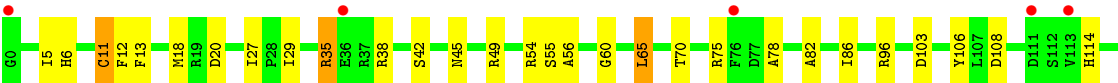
- Molecule 4: DNA polymerase IV

Chain F: 





● Molecule 4: DNA polymerase IV





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.76 Å 57.04 Å 110.70 Å 90.00° 94.76° 90.00°	Depositor
Resolution (Å)	47.66 – 2.33 47.61 – 2.33	Depositor EDS
% Data completeness (in resolution range)	99.3 (47.66-2.33) 99.4 (47.61-2.33)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.19 (at 2.34 Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.211 , 0.272 0.213 , 0.270	Depositor DCC
$R_{free}$ test set	2341 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	48.8	Xtriage
Anisotropy	0.466	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 39.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 46348 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6927	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.59% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: XG4, MG

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	B	1.76	14/404 (3.5%)	2.21	30/621 (4.8%)
1	G	1.65	10/404 (2.5%)	2.28	36/621 (5.8%)
2	C	1.61	10/385 (2.6%)	1.90	22/592 (3.7%)
3	H	1.54	10/318 (3.1%)	1.84	14/489 (2.9%)
4	A	0.67	0/2738	0.88	2/3699 (0.1%)
4	F	0.77	0/2738	1.01	11/3699 (0.3%)
All	All	1.00	44/6987 (0.6%)	1.31	115/9721 (1.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	G	1	0
4	F	0	1
All	All	1	1

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	847	DT	N1-C2	10.78	1.46	1.38
2	C	863	DT	C5-C6	10.78	1.41	1.34
1	B	844	DT	N3-C4	-9.72	1.30	1.38
1	B	847	DT	C4-C5	9.32	1.53	1.45
1	G	844	DT	N1-C6	-9.12	1.31	1.38
1	G	844	DT	N3-C4	-9.03	1.31	1.38
2	C	863	DT	N1-C2	8.97	1.45	1.38
3	H	863	DT	C5-C6	8.47	1.40	1.34
1	B	847	DT	C5-C6	8.20	1.40	1.34
1	B	839	DT	C5-C6	8.18	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	839	DT	C5-C6	8.04	1.40	1.34
2	C	858	DT	C5-C6	7.68	1.39	1.34
1	G	837	DT	N1-C2	7.57	1.44	1.38
3	H	866	DT	N3-C4	-7.52	1.32	1.38
3	H	863	DT	N3-C4	-7.49	1.32	1.38
2	C	866	DT	C5-C6	7.32	1.39	1.34
1	G	837	DT	C5-C6	7.30	1.39	1.34
1	B	837	DT	C5-C6	7.25	1.39	1.34
3	H	866	DT	C5-C6	7.08	1.39	1.34
2	C	863	DT	C4-C5	6.85	1.51	1.45
1	B	844	DT	C5-C6	6.75	1.39	1.34
1	B	847	DT	C2-O2	6.65	1.27	1.22
2	C	863	DT	N3-C4	-6.50	1.33	1.38
1	B	847	DT	N3-C4	-6.47	1.33	1.38
3	H	863	DT	C4-C5	6.40	1.50	1.45
2	C	866	DT	C2-O2	6.19	1.27	1.22
1	B	839	DT	N1-C2	6.15	1.43	1.38
1	B	837	DT	N1-C2	6.05	1.42	1.38
1	B	837	DT	C4-C5	6.04	1.50	1.45
1	G	844	DT	C4-C5	5.95	1.50	1.45
2	C	863	DT	C2-N3	-5.92	1.33	1.37
3	H	863	DT	N1-C2	5.90	1.42	1.38
3	H	863	DT	C2-N3	-5.74	1.33	1.37
2	C	858	DT	N3-C4	-5.64	1.34	1.38
1	G	844	DT	N1-C2	5.63	1.42	1.38
1	G	837	DT	C4-C5	5.58	1.50	1.45
1	B	844	DT	C4-C5	5.56	1.50	1.45
3	H	866	DT	C2-N3	-5.50	1.33	1.37
3	H	866	DT	C3'-O3'	-5.49	1.36	1.44
3	H	866	DT	O3'-P	-5.38	1.54	1.61
1	B	844	DT	N1-C6	-5.31	1.34	1.38
1	G	839	DT	N3-C4	-5.26	1.34	1.38
1	G	847	DT	N1-C6	-5.11	1.34	1.38
2	C	858	DT	N1-C2	5.03	1.42	1.38

All (115) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	863	DT	N1-C2-N3	14.90	123.54	114.60
1	G	844	DT	N1-C2-N3	14.88	123.53	114.60
1	B	844	DT	N1-C2-N3	14.78	123.47	114.60
1	B	844	DT	C2-N3-C4	-12.76	119.55	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	863	DT	N1-C2-N3	12.67	122.20	114.60
1	B	847	DT	C2-N3-C4	-12.28	119.83	127.20
1	G	839	DT	N1-C2-N3	11.90	121.74	114.60
1	B	839	DT	N1-C2-N3	11.88	121.73	114.60
1	B	847	DT	N1-C2-N3	11.88	121.73	114.60
1	G	837	DT	N1-C2-N3	11.68	121.61	114.60
1	B	837	DT	C2-N3-C4	-11.56	120.27	127.20
1	B	837	DT	N1-C2-N3	11.50	121.50	114.60
1	G	837	DT	C2-N3-C4	-11.29	120.42	127.20
1	G	844	DT	C6-N1-C2	-11.25	115.67	121.30
3	H	863	DT	N3-C2-O2	-10.76	115.84	122.30
3	H	866	DT	N1-C2-N3	10.68	121.01	114.60
3	H	866	DT	C2-N3-C4	-10.65	120.81	127.20
1	G	844	DT	N1-C2-O2	-10.62	114.61	123.10
1	B	839	DT	C2-N3-C4	-10.61	120.83	127.20
3	H	866	DT	C5-C4-O4	-10.44	117.59	124.90
1	B	839	DT	O4'-C1'-N1	10.29	115.20	108.00
2	C	858	DT	N1-C2-N3	10.05	120.63	114.60
2	C	866	DT	N1-C2-N3	10.00	120.60	114.60
2	C	858	DT	O4'-C4'-C3'	-9.97	100.02	106.00
1	G	839	DT	C2-N3-C4	-9.78	121.33	127.20
3	H	863	DT	C2-N3-C4	-9.76	121.34	127.20
4	F	330	ARG	NE-CZ-NH2	9.70	125.15	120.30
2	C	858	DT	C2-N3-C4	-9.63	121.42	127.20
1	G	847	DT	C2-N3-C4	-9.59	121.44	127.20
1	G	844	DT	N3-C4-O4	9.16	125.39	119.90
2	C	863	DT	N3-C2-O2	-9.15	116.81	122.30
2	C	866	DT	C2-N3-C4	-8.92	121.85	127.20
1	B	847	DT	C5-C6-N1	-8.87	118.38	123.70
3	H	866	DT	N3-C4-C5	8.65	120.39	115.20
1	G	847	DT	C4-C5-C7	8.47	124.08	119.00
1	B	844	DT	N1-C2-O2	-8.43	116.36	123.10
1	G	844	DT	C5-C4-O4	-8.41	119.01	124.90
1	G	844	DT	C2-N3-C4	-8.31	122.21	127.20
2	C	863	DT	C2-N3-C4	-8.28	122.23	127.20
1	G	847	DT	N1-C2-N3	8.23	119.54	114.60
1	G	847	DT	N3-C4-C5	8.11	120.06	115.20
1	G	837	DT	N3-C2-O2	-8.05	117.47	122.30
2	C	858	DT	C5-C4-O4	-8.04	119.27	124.90
1	B	844	DT	C6-C5-C7	-8.00	118.10	122.90
1	G	837	DT	C5'-C4'-C3'	7.98	128.47	114.10
4	F	324	ARG	NE-CZ-NH1	7.85	124.23	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	330	ARG	NE-CZ-NH1	-7.71	116.45	120.30
2	C	863	DT	C5-C6-N1	-7.57	119.16	123.70
1	B	839	DT	C5-C4-O4	-7.31	119.78	124.90
1	B	844	DT	C4-C5-C7	7.31	123.39	119.00
2	C	866	DT	N1-C2-O2	-7.28	117.27	123.10
1	G	839	DT	C5-C4-O4	-7.28	119.80	124.90
1	B	837	DT	N3-C4-C5	7.24	119.54	115.20
3	H	863	DT	C5-C6-N1	-7.23	119.36	123.70
3	H	866	DT	C5-C6-N1	-7.18	119.39	123.70
1	G	840	DC	O5'-P-OP1	-7.18	99.24	105.70
3	H	866	DT	C4'-C3'-C2'	7.13	109.52	103.10
2	C	858	DT	N3-C4-C5	7.12	119.47	115.20
2	C	858	DT	C5-C6-N1	-7.09	119.44	123.70
1	B	847	DT	N3-C4-C5	6.97	119.38	115.20
1	B	844	DT	N3-C4-C5	6.86	119.32	115.20
1	G	837	DT	N3-C4-C5	6.79	119.27	115.20
1	G	841	DG	O5'-P-OP2	-6.63	99.73	105.70
4	F	311	ASP	CB-CG-OD1	-6.61	112.35	118.30
1	G	847	DT	C5-C4-O4	-6.59	120.29	124.90
1	B	837	DT	C5-C6-N1	-6.59	119.75	123.70
1	G	837	DT	O4'-C4'-C3'	6.55	109.93	106.00
2	C	857	DC	C5'-C4'-C3'	6.55	125.89	114.10
1	B	839	DT	N1-C1'-C2'	-6.50	100.25	112.60
1	B	839	DT	N3-C4-C5	6.48	119.09	115.20
1	B	837	DT	C4-C5-C7	6.44	122.86	119.00
1	G	837	DT	C6-C5-C7	-6.39	119.07	122.90
1	B	837	DT	C6-C5-C7	-6.37	119.08	122.90
2	C	858	DT	N3-C2-O2	-6.35	118.49	122.30
1	G	847	DT	C6-C5-C7	-6.27	119.14	122.90
1	B	837	DT	N3-C2-O2	-6.25	118.55	122.30
1	G	839	DT	N3-C4-C5	6.21	118.93	115.20
1	G	837	DT	C5-C6-N1	-6.16	120.00	123.70
4	F	220	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	B	844	DT	C6-N1-C2	-6.04	118.28	121.30
1	G	837	DT	C5'-C4'-O4'	6.01	120.71	109.30
1	G	848	DA	O5'-P-OP2	-5.99	100.31	105.70
3	H	866	DT	N1-C2-O2	-5.98	118.31	123.10
1	B	839	DT	C5-C6-N1	-5.97	120.11	123.70
2	C	866	DT	O4'-C1'-N1	5.95	112.16	108.00
4	F	311	ASP	CB-CG-OD2	5.93	123.64	118.30
1	G	847	DT	OP1-P-OP2	5.82	128.33	119.60
4	F	8	ASP	CB-CG-OD1	5.81	123.53	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	324	ARG	NE-CZ-NH2	-5.80	117.40	120.30
2	C	866	DT	C5-C6-N1	-5.80	120.22	123.70
2	C	858	DT	O4'-C1'-N1	-5.78	103.95	108.00
1	B	844	DT	O4'-C1'-N1	5.75	112.03	108.00
2	C	866	DT	N3-C4-C5	5.73	118.64	115.20
1	B	837	DT	O4'-C1'-N1	5.69	111.98	108.00
1	B	847	DT	N3-C2-O2	-5.67	118.90	122.30
4	F	265	ARG	NE-CZ-NH1	5.66	123.13	120.30
3	H	866	DT	O4'-C4'-C3'	-5.64	102.25	104.50
4	F	338	LEU	CB-CG-CD1	5.58	120.48	111.00
1	G	837	DT	C5-C4-O4	-5.47	121.07	124.90
1	G	837	DT	C4-C5-C7	5.47	122.28	119.00
2	C	870	DA	O5'-P-OP2	-5.47	100.78	105.70
4	A	324	ARG	NE-CZ-NH1	5.45	123.03	120.30
3	H	860	DG	C5'-C4'-C3'	5.44	123.90	114.10
4	F	129	THR	N-CA-CB	5.37	120.50	110.30
1	G	847	DT	O5'-P-OP2	-5.33	100.90	105.70
1	G	839	DT	N1-C2-O2	-5.29	118.86	123.10
3	H	863	DT	C6-N1-C2	-5.29	118.65	121.30
1	G	844	DT	O4'-C1'-N1	5.28	111.70	108.00
1	B	847	DT	O5'-P-OP1	-5.20	101.02	105.70
1	B	839	DT	N1-C2-O2	-5.18	118.95	123.10
1	G	839	DT	C5-C6-N1	-5.18	120.59	123.70
4	F	61	MET	CG-SD-CE	5.14	108.43	100.20
1	G	844	DT	C3'-C2'-C1'	5.08	108.60	102.50
2	C	866	DT	C4-C5-C7	5.07	122.04	119.00
2	C	866	DT	C1'-O4'-C4'	-5.00	105.10	110.10

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	G	837	DT	C4'

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	F	292	PHE	Peptide

## 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	B	362	0	204	8	0
1	G	362	0	204	12	0
2	C	344	0	192	4	1
3	H	284	0	158	7	0
4	A	2687	0	2739	66	1
4	F	2687	0	2739	56	0
5	A	31	0	13	1	0
5	F	31	0	13	0	0
6	A	2	0	0	0	0
6	F	2	0	0	0	0
7	A	22	0	0	3	0
7	B	7	0	0	0	0
7	C	8	0	0	1	0
7	F	63	0	0	8	0
7	G	20	0	0	4	0
7	H	15	0	0	5	0
All	All	6927	0	6262	144	1

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 11.

All (144) 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)
4:A:18:MET:CE	4:A:45:ASN:HD22	1.67	1.08
4:F:129:THR:N	7:F:550:HOH:O	1.89	1.06
4:F:18:MET:CE	4:F:45:ASN:HD22	1.71	1.02
1:G:837:DT:O3'	7:G:902:HOH:O	1.84	0.94
4:A:129:THR:N	7:A:521:HOH:O	1.96	0.93
4:F:18:MET:HE3	4:F:45:ASN:HD22	1.34	0.93
4:A:18:MET:HE3	4:A:45:ASN:HD22	1.36	0.88
1:G:838:DC:P	7:G:902:HOH:O	2.32	0.85
3:H:863:DT:O4'	7:H:912:HOH:O	1.94	0.84
4:F:57:MET:HE3	4:F:62:ALA:HA	1.60	0.83
2:C:869:DG:N7	7:C:907:HOH:O	2.10	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:57:MET:CE	4:F:62:ALA:HA	2.09	0.82
4:F:129:THR:O	4:F:132:ASN:O	1.97	0.82
2:C:857:DC:H2'	2:C:857:DC:O2	1.78	0.82
4:A:128:GLN:O	4:A:129:THR:OG1	1.96	0.81
4:F:157:LYS:NZ	7:F:549:HOH:O	1.99	0.79
4:F:10:ASP:OD2	4:F:137:THR:HG23	1.86	0.76
4:F:291:LYS:O	7:F:523:HOH:O	2.05	0.74
4:F:125:GLU:O	4:F:129:THR:CG2	2.36	0.74
4:F:57:MET:HE3	4:F:62:ALA:CA	2.17	0.74
3:H:862:DG:N3	7:H:912:HOH:O	2.21	0.73
4:F:125:GLU:O	4:F:129:THR:HG23	1.88	0.72
3:H:869:DG:N7	7:H:914:HOH:O	2.22	0.72
3:H:866:DT:O4	7:H:907:HOH:O	2.08	0.71
1:B:838:DC:OP1	4:A:35:ARG:NE	2.25	0.69
4:F:210:MET:HE2	4:F:211:LEU:HD13	1.74	0.69
3:H:870:DA:N7	7:H:902:HOH:O	2.25	0.68
4:A:233:ASP:OD1	4:A:233:ASP:N	2.27	0.68
1:B:844:DT:H2''	1:B:845:DC:H5'	1.76	0.66
4:F:331:LEU:O	7:F:523:HOH:O	2.14	0.66
1:G:843:DG:OP1	4:F:240:ARG:NH1	2.30	0.65
1:G:838:DC:OP1	7:G:902:HOH:O	2.15	0.64
4:A:18:MET:CE	4:A:45:ASN:ND2	2.51	0.64
4:F:128:GLN:O	4:F:129:THR:HG23	1.99	0.62
4:F:210:MET:CE	4:F:211:LEU:HD13	2.31	0.61
4:F:294:ASP:OD1	4:F:327:ARG:HD2	2.00	0.61
1:B:847:DT:H2''	1:B:848:DA:OP2	2.01	0.61
4:A:238:ARG:HH12	4:A:240:ARG:CA	2.15	0.60
4:A:129:THR:O	4:A:132:ASN:O	2.19	0.60
4:A:96:ARG:C	4:A:234:VAL:HG21	2.22	0.59
1:G:840:DC:H5'	4:F:40:VAL:HG13	1.85	0.59
4:F:331:LEU:N	7:F:523:HOH:O	2.05	0.58
4:A:287:GLY:HA3	4:A:301:GLU:HB3	1.84	0.58
4:F:18:MET:HE3	4:F:45:ASN:ND2	2.12	0.58
4:A:128:GLN:HA	7:A:521:HOH:O	2.03	0.57
4:A:130:ILE:O	4:A:134:LEU:HB2	2.03	0.57
4:F:300:GLN:NE2	4:F:319:THR:OG1	2.37	0.57
4:A:267:TYR:CG	4:A:309:LYS:HG3	2.40	0.57
4:A:331:LEU:C	4:A:331:LEU:HD23	2.26	0.56
1:B:837:DT:H2''	1:B:838:DC:O5'	2.04	0.56
2:C:866:DT:OP2	4:A:285:ARG:NH1	2.35	0.56
4:A:146:LYS:HG3	4:A:230:ASP:OD2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:18:MET:HE3	4:A:45:ASN:ND2	2.15	0.55
1:B:837:DT:H2"	1:B:838:DC:C5'	2.36	0.55
4:A:231:GLU:O	4:A:232:ARG:HB3	2.07	0.55
4:F:125:GLU:O	4:F:128:GLN:O	2.24	0.55
4:A:75:ARG:NH1	4:A:78:ALA:HB2	2.22	0.55
4:A:267:TYR:OH	4:A:307:LEU:HD13	2.08	0.54
4:F:308:ASN:HB2	7:F:538:HOH:O	2.07	0.54
4:F:203:VAL:O	4:F:206:CYS:HB2	2.07	0.54
4:F:302:HIS:HE1	4:F:315:THR:HG21	1.72	0.53
4:A:29:ILE:HD13	4:A:70:THR:HB	1.92	0.52
4:F:57:MET:HE3	4:F:62:ALA:N	2.24	0.52
1:B:837:DT:H2"	1:B:838:DC:H5'	1.90	0.52
4:A:125:GLU:O	4:A:128:GLN:O	2.28	0.52
1:G:839:DT:C4	4:F:295:PHE:CE2	2.97	0.51
1:G:837:DT:H2"	1:G:838:DC:C5'	2.40	0.51
4:A:291:LYS:HB3	4:A:331:LEU:HB3	1.91	0.51
4:F:82:ALA:O	4:F:86:ILE:HG23	2.11	0.51
4:A:6:HIS:CE1	4:A:150:LYS:HD2	2.46	0.51
4:F:57:MET:CE	4:F:62:ALA:CA	2.80	0.50
4:F:31:ILE:N	4:F:31:ILE:HD12	2.26	0.50
4:A:280:ASP:O	4:A:282:LEU:HD12	2.11	0.50
4:F:88:GLU:O	4:F:91:SER:OG	2.20	0.50
4:F:35:ARG:NH1	7:F:562:HOH:O	2.44	0.50
4:A:146:LYS:NZ	4:A:232:ARG:HH11	2.10	0.50
4:F:55:SER:O	4:F:56:ALA:HB3	2.12	0.50
4:A:96:ARG:CA	4:A:234:VAL:HG21	2.41	0.49
2:C:859:DA:H2"	2:C:860:DG:C8	2.48	0.49
4:A:304:TRP:CD1	4:A:306:ARG:O	2.64	0.49
4:A:225:ARG:NH2	4:A:232:ARG:NH2	2.60	0.49
4:A:231:GLU:O	4:A:232:ARG:CB	2.60	0.49
4:A:232:ARG:C	4:A:233:ASP:OD1	2.51	0.49
4:A:106:TYR:CE2	4:A:146:LYS:HB2	2.47	0.49
4:A:129:THR:HA	4:A:132:ASN:HB2	1.94	0.48
3:H:860:DG:H2"	3:H:861:DG:OP2	2.12	0.48
4:A:11:CYS:O	4:A:12:PHE:C	2.52	0.48
4:A:238:ARG:NH1	4:A:240:ARG:N	2.61	0.48
4:A:269:GLU:OE1	4:A:272:ARG:HD2	2.13	0.48
4:A:238:ARG:HH12	4:A:240:ARG:N	2.12	0.47
4:F:176:LEU:HD12	4:F:200:CYS:SG	2.54	0.47
4:F:128:GLN:O	4:F:129:THR:CG2	2.62	0.47
4:A:45:ASN:O	4:A:49:ARG:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:132:ASN:O	4:F:133:GLU:HB2	2.15	0.47
4:A:238:ARG:HH12	4:A:240:ARG:HA	1.80	0.47
4:A:134:LEU:O	4:A:135:GLN:HB2	2.15	0.47
4:F:127:ARG:HD2	4:F:138:ALA:O	2.14	0.47
4:A:20:ASP:OD2	4:A:75:ARG:NH2	2.47	0.46
4:F:27:ILE:HG13	4:F:28:PRO:HD2	1.96	0.46
4:F:141:GLY:HA3	4:F:152:ALA:HB3	1.98	0.46
4:F:306:ARG:O	4:F:307:LEU:C	2.52	0.46
4:F:212:LEU:HD21	4:F:220:ARG:HB2	1.97	0.46
4:A:235:ASN:O	4:A:237:GLU:N	2.47	0.45
1:G:840:DC:H2'	1:G:840:DC:O5'	2.18	0.44
4:A:289:LYS:HB2	4:A:299:THR:HG22	1.98	0.44
1:G:839:DT:OP2	4:F:330:ARG:NH1	2.37	0.44
1:G:838:DC:C5'	7:G:902:HOH:O	2.65	0.44
4:A:239:LEU:HD13	4:A:277:VAL:HG13	2.00	0.44
4:A:13:PHE:CD2	5:A:401:XG4:H2'A	2.52	0.44
4:F:131:PHE:HA	4:F:136:LEU:O	2.17	0.44
4:A:304:TRP:HD1	4:A:306:ARG:O	2.00	0.43
4:A:82:ALA:O	4:A:86:ILE:HG23	2.18	0.43
4:A:238:ARG:HD2	4:A:238:ARG:HA	1.66	0.43
4:F:143:ALA:HB1	4:F:144:PRO:CD	2.48	0.43
4:F:106:TYR:O	4:F:107:LEU:HD23	2.19	0.43
4:A:285:ARG:HG3	4:A:337:THR:OG1	2.19	0.42
4:F:12:PHE:CD2	4:F:103:ASP:HB3	2.55	0.42
4:F:139:SER:HA	4:F:160:GLY:O	2.19	0.42
3:H:866:DT:OP2	4:F:285:ARG:NH1	2.44	0.42
1:G:837:DT:H2''	1:G:838:DC:H5'	2.02	0.42
4:F:173:LEU:O	4:F:200:CYS:HB2	2.19	0.42
4:A:27:ILE:O	4:A:29:ILE:HG12	2.19	0.42
4:F:249:MET:SD	4:F:249:MET:N	2.93	0.42
4:F:57:MET:HE2	4:F:62:ALA:HB2	2.02	0.42
4:A:55:SER:O	4:A:56:ALA:HB3	2.20	0.42
4:F:179:ALA:O	7:F:534:HOH:O	2.21	0.42
4:A:5:ILE:HD12	4:A:123:ALA:HB2	2.02	0.42
1:B:837:DT:O3'	4:A:35:ARG:NH2	2.51	0.41
4:A:286:GLN:NE2	4:A:311:ASP:OD2	2.47	0.41
1:B:839:DT:H2'	4:A:295:PHE:CZ	2.55	0.41
4:A:144:PRO:HD3	4:A:164:ILE:O	2.21	0.41
4:A:96:ARG:HB3	4:A:234:VAL:HG21	2.03	0.41
4:A:108:ASP:C	4:A:108:ASP:OD2	2.59	0.41
4:A:245:VAL:HG23	4:A:270:LEU:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:35:ARG:NE	4:A:60:GLY:HA3	2.36	0.41
4:F:132:ASN:O	4:F:133:GLU:CB	2.68	0.41
4:A:331:LEU:HD23	4:A:332:VAL:N	2.36	0.41
4:A:29:ILE:CD1	4:A:70:THR:HB	2.51	0.41
4:F:169:VAL:HB	4:F:170:PRO:HD3	2.01	0.41
4:A:131:PHE:HB3	7:A:521:HOH:O	2.21	0.41
1:G:842:DG:H2'	1:G:843:DG:O4'	2.21	0.40
4:A:11:CYS:SG	4:A:49:ARG:NH2	2.94	0.40
4:F:207:ASP:OD2	4:F:209:VAL:HB	2.22	0.40
4:A:65:LEU:HD12	4:A:65:LEU:HA	1.87	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:862:DG:OP1	4:A:118:SER:OG[2_445]	2.19	0.01

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	A	340/352 (97%)	313 (92%)	22 (6%)	5 (2%)	13	10
4	F	340/352 (97%)	317 (93%)	21 (6%)	2 (1%)	30	32
All	All	680/704 (97%)	630 (93%)	43 (6%)	7 (1%)	19	18

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	F	293	ASP
4	A	232	ARG
4	A	236	SER

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Mol	Chain	Res	Type
4	F	133	GLU
4	A	217	LYS
4	A	11	CYS
4	A	234	VAL

### 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	
4	A	286/297 (96%)	254 (89%)	32 (11%)	7	7
4	F	286/297 (96%)	262 (92%)	24 (8%)	14	14
All	All	572/594 (96%)	516 (90%)	56 (10%)	10	9

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	F	37	ARG
4	F	42	SER
4	F	112	SER
4	F	121	LEU
4	F	129	THR
4	F	134	LEU
4	F	136	LEU
4	F	157	LYS
4	F	176	LEU
4	F	197	LEU
4	F	211	LEU
4	F	239	LEU
4	F	243	VAL
4	F	247	ARG
4	F	266	LEU
4	F	276	LYS
4	F	291	LYS
4	F	293	ASP
4	F	306	ARG

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Mol	Chain	Res	Type
4	F	307	LEU
4	F	318	LYS
4	F	330	ARG
4	F	331	LEU
4	F	338	LEU
4	A	35	ARG
4	A	38	ARG
4	A	42	SER
4	A	54	ARG
4	A	65	LEU
4	A	103	ASP
4	A	114	HIS
4	A	133	GLU
4	A	135	GLN
4	A	136	LEU
4	A	146	LYS
4	A	186	LYS
4	A	206	CYS
4	A	207	ASP
4	A	210	MET
4	A	222	LEU
4	A	227	GLN
4	A	233	ASP
4	A	236	SER
4	A	237	GLU
4	A	238	ARG
4	A	239	LEU
4	A	240	ARG
4	A	266	LEU
4	A	285	ARG
4	A	289	LYS
4	A	295	PHE
4	A	307	LEU
4	A	309	LYS
4	A	332	VAL
4	A	338	LEU
4	A	340	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
4	F	45	ASN

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Mol	Chain	Res	Type
4	F	116	HIS
4	F	128	GLN
4	F	132	ASN
4	F	300	GLN
4	A	45	ASN
4	A	84	ASN
4	A	132	ASN
4	A	235	ASN
4	A	300	GLN
4	A	308	ASN
4	A	335	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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
5	XG4	A	401	6	28,33,33	2.24	6 (21%)	35,52,52	2.33	13 (37%)
5	XG4	F	401	6	28,33,33	1.80	7 (25%)	35,52,52	2.36	15 (42%)

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
5	XG4	A	401	6	-	0/13/34/34	0/3/3/3
5	XG4	F	401	6	-	0/13/34/34	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	401	XG4	C4-N3	-3.24	1.30	1.35
5	A	401	XG4	PA-O2A	-2.65	1.49	1.56
5	F	401	XG4	PA-O2A	-2.36	1.50	1.56
5	F	401	XG4	PB-O1B	2.00	1.48	1.46
5	F	401	XG4	C8-N7	2.08	1.38	1.34
5	A	401	XG4	C6-C5	2.49	1.46	1.41
5	F	401	XG4	C6-C5	2.66	1.46	1.41
5	A	401	XG4	C5-C4	2.95	1.47	1.40
5	F	401	XG4	C5-C4	3.39	1.48	1.40
5	A	401	XG4	PB-O3B	4.30	1.64	1.59
5	F	401	XG4	PA-O1A	4.46	1.51	1.46
5	A	401	XG4	PA-O1A	6.38	1.53	1.46
5	A	401	XG4	PB-O1B	6.51	1.53	1.46

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	401	XG4	O1B-PB-N3A	-5.07	104.13	111.90
5	A	401	XG4	O3B-PB-N3A	-4.71	93.48	106.44
5	A	401	XG4	C5-C6-N1	-4.64	117.24	123.59
5	F	401	XG4	O3B-PB-N3A	-4.53	93.98	106.44
5	F	401	XG4	C4-C5-N7	-4.46	105.37	109.48
5	F	401	XG4	C5-C6-N1	-4.01	118.11	123.59
5	A	401	XG4	C6-C5-C4	-3.80	116.36	120.90
5	A	401	XG4	PG-O3B-PB	-3.26	121.75	132.67
5	A	401	XG4	N3-C2-N1	-3.15	122.65	127.44
5	F	401	XG4	C2'-C1'-N9	-3.08	106.67	114.16
5	F	401	XG4	O1A-PA-N3A	-2.64	107.85	111.90
5	F	401	XG4	C6-C5-C4	-2.55	117.85	120.90
5	A	401	XG4	C2'-C1'-N9	-2.51	108.06	114.16
5	A	401	XG4	C1'-N9-C4	-2.33	123.21	127.16
5	F	401	XG4	N3-C2-N1	-2.12	124.22	127.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	401	XG4	O1A-PA-N3A	-2.01	108.82	111.90
5	F	401	XG4	O4'-C1'-N9	2.22	111.56	107.72
5	A	401	XG4	O2B-PB-O3B	2.45	116.19	105.09
5	F	401	XG4	N2-C2-N1	2.64	121.57	117.20
5	F	401	XG4	C6-N1-C2	2.69	119.68	115.94
5	F	401	XG4	O2B-PB-O3B	3.14	119.36	105.09
5	F	401	XG4	O2B-PB-O1B	3.49	117.28	110.00
5	F	401	XG4	O2G-PG-O1G	3.61	122.21	110.58
5	F	401	XG4	O2A-PA-O1A	3.63	117.58	110.00
5	A	401	XG4	O2B-PB-O1B	3.73	117.79	110.00
5	A	401	XG4	O2A-PA-O1A	3.74	117.80	110.00
5	A	401	XG4	O1B-PB-N3A	3.79	117.71	111.90
5	A	401	XG4	C6-N1-C2	5.59	123.70	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	401	XG4	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	B	18/18 (100%)	-0.39	0 100 100	42, 60, 100, 104	0
1	G	18/18 (100%)	-0.29	0 100 100	36, 52, 100, 105	0
2	C	17/17 (100%)	-0.38	1 (5%) 26 37	46, 57, 71, 152	0
3	H	14/14 (100%)	-0.30	0 100 100	35, 52, 88, 110	0
4	A	342/352 (97%)	0.18	14 (4%) 41 53	36, 58, 93, 128	0
4	F	342/352 (97%)	0.05	1 (0%) 94 97	30, 49, 71, 102	0
All	All	751/771 (97%)	0.07	16 (2%) 67 78	30, 54, 86, 152	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	A	239	LEU	10.0
4	A	0	GLY	9.0
4	A	236	SER	5.6
4	A	234	VAL	5.0
2	C	857	DC	4.7
4	A	341	PRO	4.4
4	A	237	GLU	3.9
4	A	129	THR	3.3
4	A	238	ARG	3.1
4	A	76	PHE	2.9
4	A	36	GLU	2.8
4	F	341	PRO	2.5
4	A	113	VAL	2.4
4	A	214	ARG	2.4
4	A	119	ALA	2.2
4	A	111	ASP	2.1

## 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
6	MG	F	402	1/1	0.99	0.21	2.15	20,20,20,20	0
5	XG4	A	401	31/31	0.96	0.12	0.05	43,51,57,57	0
5	XG4	F	401	31/31	0.99	0.14	-0.12	30,32,36,39	0
6	MG	A	402	1/1	0.97	0.10	-0.98	30,30,30,30	0
6	MG	F	403	1/1	0.97	0.07	-	57,57,57,57	0
6	MG	A	403	1/1	0.80	0.31	-	104,104,104,104	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.