



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 8, 2024 – 06:55 am GMT

PDB ID : 6HB4  
Title : TFAM in Complex with Site-Y  
Authors : Cuppari, A.; Fernandez-Millan, P.; Rubio-Cosials, A.; Tarres-Sole, A.; Lyon-  
nais, S.; Sola, M.  
Deposited on : 2018-08-09  
Resolution : 3.05 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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

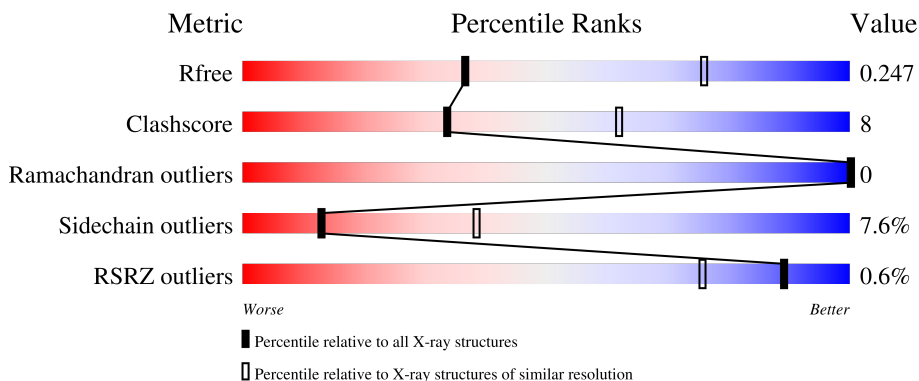
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.05 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.



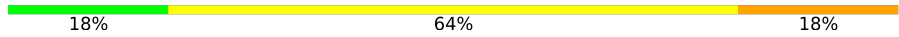
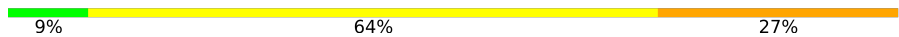



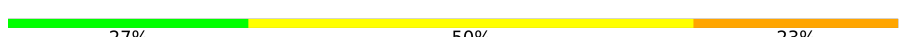
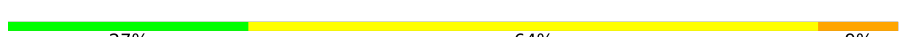
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1754 (3.10-3.02)
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)
RSRZ outliers	127900	1713 (3.10-3.02)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	A	213	<div style="display: flex; align-items: center;"> <div style="width: 10px; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="flex-grow: 1; position: relative;"> <div style="position: absolute; top: -10px; left: 0; right: 0; text-align: center;">%</div> <div style="position: absolute; top: 0; left: 0; right: 0; height: 15px; background: linear-gradient(to right, red 1%, orange 1%, yellow 16%, green 77%, yellow 77%, orange 83%, grey 83%);"></div> <div style="position: absolute; bottom: 0; left: 0; right: 0; text-align: center;">77% 16% 8%</div> </div> </div>
1	D	213	<div style="display: flex; align-items: center;"> <div style="flex-grow: 1; position: relative;"> <div style="position: absolute; top: 0; left: 0; right: 0; height: 15px; background: linear-gradient(to right, green 71%, yellow 71%, orange 80%, grey 80%);"></div> <div style="position: absolute; bottom: 0; left: 0; right: 0; text-align: center;">71% 19% • 9%</div> </div> </div>
1	G	213	<div style="display: flex; align-items: center;"> <div style="flex-grow: 1; position: relative;"> <div style="position: absolute; top: 0; left: 0; right: 0; height: 15px; background: linear-gradient(to right, green 74%, yellow 74%, orange 89%, grey 89%);"></div> <div style="position: absolute; bottom: 0; left: 0; right: 0; text-align: center;">74% 15% • 9%</div> </div> </div>
1	J	213	<div style="display: flex; align-items: center;"> <div style="width: 10px; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="flex-grow: 1; position: relative;"> <div style="position: absolute; top: -10px; left: 0; right: 0; text-align: center;">%</div> <div style="position: absolute; top: 0; left: 0; right: 0; height: 15px; background: linear-gradient(to right, red 1%, orange 1%, yellow 24%, green 64%, yellow 64%, orange 88%, grey 88%);"></div> <div style="position: absolute; bottom: 0; left: 0; right: 0; text-align: center;">64% 24% • 9%</div> </div> </div>
2	B	22	<div style="display: flex; align-items: center;"> <div style="flex-grow: 1; position: relative;"> <div style="position: absolute; top: 0; left: 0; right: 0; height: 15px; background: linear-gradient(to right, green 14%, yellow 68%, orange 82%, grey 82%);"></div> <div style="position: absolute; bottom: 0; left: 0; right: 0; text-align: center;">14% 68% 18%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	E	22	
2	H	22	
2	K	22	
3	C	22	
3	F	22	
3	I	22	
3	L	22	

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
5	1PE	A	303	-	-	X	-
5	1PE	A	304	-	-	X	-
5	1PE	D	301	-	-	X	-

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 10420 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Transcription factor A, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	197	Total 1664	C 1051	N 303	O 304	S 6	0	0	0
1	D	194	Total 1635	C 1034	N 295	O 300	S 6	0	0	0
1	G	193	Total 1626	C 1028	N 293	O 299	S 6	0	0	0
1	J	193	Total 1626	C 1028	N 293	O 299	S 6	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	42	MET	-	initiating methionine	UNP Q00059
A	247	LEU	-	expression tag	UNP Q00059
A	248	GLN	-	expression tag	UNP Q00059
A	249	HIS	-	expression tag	UNP Q00059
A	250	HIS	-	expression tag	UNP Q00059
A	251	HIS	-	expression tag	UNP Q00059
A	252	HIS	-	expression tag	UNP Q00059
A	253	HIS	-	expression tag	UNP Q00059
A	254	HIS	-	expression tag	UNP Q00059
D	42	MET	-	initiating methionine	UNP Q00059
D	247	LEU	-	expression tag	UNP Q00059
D	248	GLN	-	expression tag	UNP Q00059
D	249	HIS	-	expression tag	UNP Q00059
D	250	HIS	-	expression tag	UNP Q00059
D	251	HIS	-	expression tag	UNP Q00059
D	252	HIS	-	expression tag	UNP Q00059
D	253	HIS	-	expression tag	UNP Q00059
D	254	HIS	-	expression tag	UNP Q00059
G	42	MET	-	initiating methionine	UNP Q00059
G	247	LEU	-	expression tag	UNP Q00059
G	248	GLN	-	expression tag	UNP Q00059

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Chain	Residue	Modelled	Actual	Comment	Reference
G	249	HIS	-	expression tag	UNP Q00059
G	250	HIS	-	expression tag	UNP Q00059
G	251	HIS	-	expression tag	UNP Q00059
G	252	HIS	-	expression tag	UNP Q00059
G	253	HIS	-	expression tag	UNP Q00059
G	254	HIS	-	expression tag	UNP Q00059
J	42	MET	-	initiating methionine	UNP Q00059
J	247	LEU	-	expression tag	UNP Q00059
J	248	GLN	-	expression tag	UNP Q00059
J	249	HIS	-	expression tag	UNP Q00059
J	250	HIS	-	expression tag	UNP Q00059
J	251	HIS	-	expression tag	UNP Q00059
J	252	HIS	-	expression tag	UNP Q00059
J	253	HIS	-	expression tag	UNP Q00059
J	254	HIS	-	expression tag	UNP Q00059

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	B	22	Total 450	C 216	N 78	O 134	P 22	0	0	0
2	E	22	Total 491	C 236	N 85	O 146	P 24	0	2	0
2	H	22	Total 511	C 245	N 88	O 153	P 25	0	3	0
2	K	22	Total 533	C 256	N 92	O 159	P 26	0	4	0

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

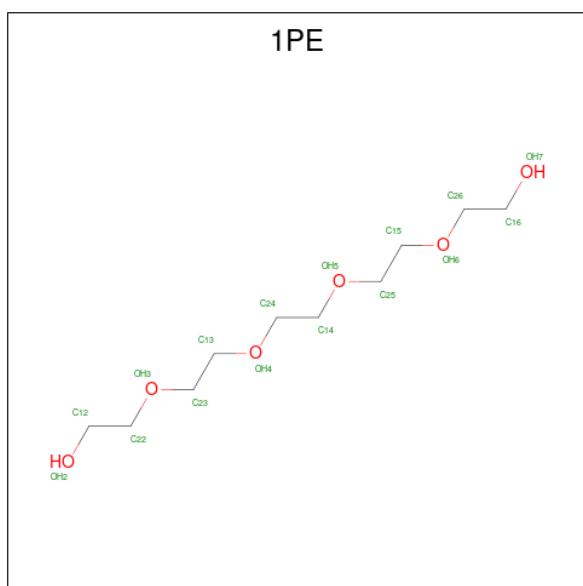
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	C	22	Total 452	C 216	N 84	O 130	P 22	0	0	0
3	F	22	Total 452	C 216	N 84	O 130	P 22	0	0	0
3	I	22	Total 452	C 216	N 84	O 130	P 22	0	0	0
3	L	22	Total 452	C 216	N 84	O 130	P 22	0	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	C O	0	0
			6	3 3		
4	A	1	Total	C O	0	0
			6	3 3		

- Molecule 5 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula:  $C_{10}H_{22}O_6$ ).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	C O	0	0
			16	10 6		

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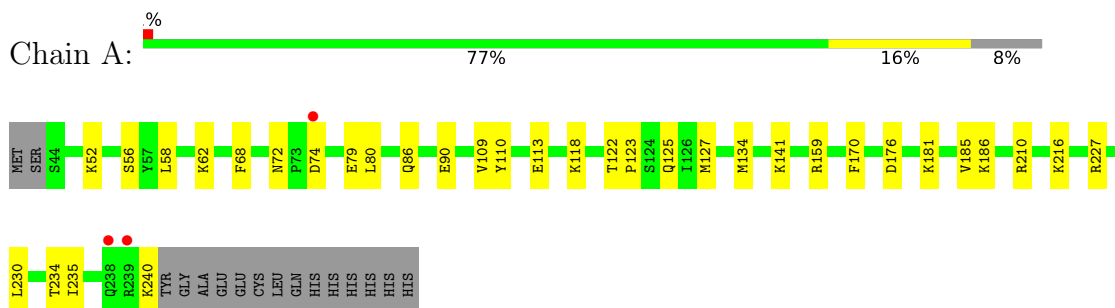
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	16	10	6	0	0
5	D	1	16	10	6	0	0
5	G	1	16	10	6	0	0

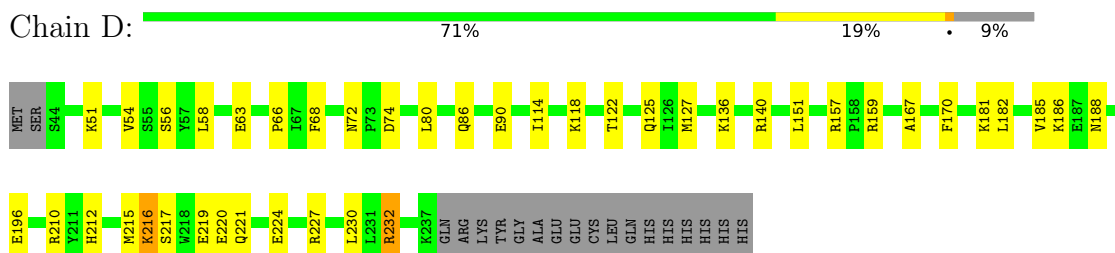
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

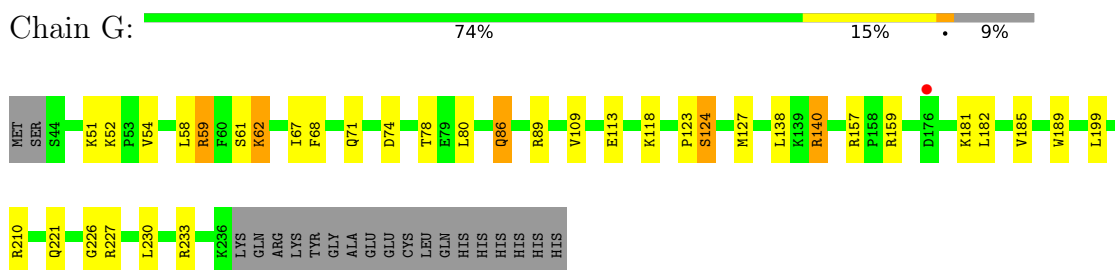
- Molecule 1: Transcription factor A, mitochondrial



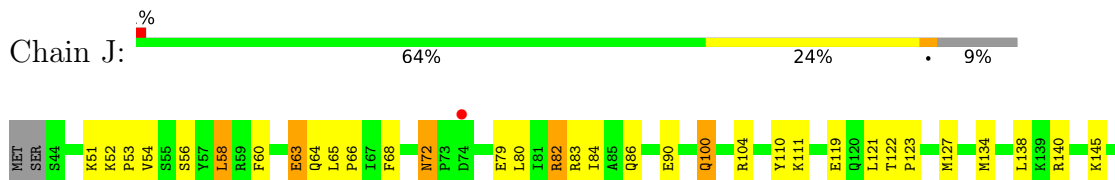
- Molecule 1: Transcription factor A, mitochondrial



- Molecule 1: Transcription factor A, mitochondrial



- Molecule 1: Transcription factor A, mitochondrial







HIS  
HIS  
HIS  
HIS  
HIS

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

Chain B: 14% 68% 18%

C1 T2 G3 T4 G5 G6 A7 G8 A9 A10 A11 T12 T13 C14 A15 A16 T17 T18 G19 T20 T21 A22

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

Chain E: 18% 64% 18%

C1 T2 G3 T4 G5 G6 A7 G8 A9 A10 A11 T12 T13 C14 A15 A16 T17 T18 G19 T20 T21 A22

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

Chain H: 9% 64% 27%

C1 T2 G3 T4 G5 G6 A7 G8 A9 A10 A11 T12 T13 C14 A15 A16 T17 T18 G19 T20 T21 A22

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

Chain K: 14% 55% 32%

C1 T2 G3 T4 G5 G6 A7 G8 A9 A10 A11 T12 T13 C14 A15 A16 T17 T18 G19 T20 T21 A22

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

Chain C: 32% 68%

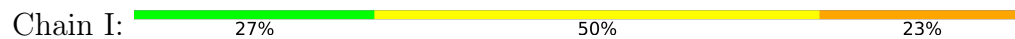
T1 A2 A3 C4 A5 A6 T7 T8 A11 T12 G13 T14 C15 T16 G17 C18 A19 C20 A21 G22

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

Chain F: 36% 50% 14%



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



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



## 4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	157.67Å 140.62Å 108.92Å 90.00° 130.73° 90.00°	Depositor
Resolution (Å)	43.05 – 3.05 43.05 – 3.05	Depositor EDS
% Data completeness (in resolution range)	100.0 (43.05-3.05) 99.9 (43.05-3.05)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.20 (at 3.06Å)	Xtrriage
Refinement program	BUSTER 2.11.2	Depositor
R, $R_{free}$	0.190 , 0.236 0.203 , 0.247	Depositor DCC
$R_{free}$ test set	1739 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	76.4	Xtrriage
Anisotropy	0.292	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 68.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.034 for -h-2*1,-k,l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10420	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	88.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% 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 i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 1PE

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.64	0/1695	0.74	0/2264
1	D	0.64	0/1666	0.77	1/2227 (0.0%)
1	G	0.58	0/1657	0.72	0/2216
1	J	0.60	0/1657	0.75	0/2216
2	B	1.43	2/503 (0.4%)	2.63	43/774 (5.6%)
2	E	1.42	4/548 (0.7%)	2.36	43/841 (5.1%)
2	H	1.23	1/571 (0.2%)	2.43	47/879 (5.3%)
2	K	1.25	2/595 (0.3%)	2.26	41/914 (4.5%)
3	C	1.29	0/507	1.97	19/780 (2.4%)
3	F	1.31	1/507 (0.2%)	2.03	22/780 (2.8%)
3	I	1.40	3/507 (0.6%)	2.25	37/780 (4.7%)
3	L	1.26	1/507 (0.2%)	2.10	28/780 (3.6%)
All	All	0.96	14/10920 (0.1%)	1.58	281/15451 (1.8%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	22	DG	C3'-O3'	-6.96	1.34	1.44
2	K	3	DG	C3'-O3'	-6.91	1.34	1.44
2	E	3	DG	C3'-O3'	-6.86	1.35	1.44
2	H	17	DT	C3'-O3'	-5.84	1.36	1.44
2	K	10	DC	C1'-N1	5.83	1.56	1.49
2	B	9	DA	N3-C4	5.82	1.38	1.34
3	I	21	DA	C3'-O3'	-5.69	1.36	1.44
2	E	20	DT	N1-C2	5.62	1.42	1.38
3	L	22	DG	C3'-O3'	-5.56	1.36	1.44
2	B	18	DT	C3'-O3'	-5.42	1.36	1.44
2	E	21[A]	DT	N1-C2	5.24	1.42	1.38
2	E	21[B]	DT	N1-C2	5.24	1.42	1.38
3	F	16	DT	C3'-O3'	-5.17	1.37	1.44
3	I	2	DA	C6-N1	5.12	1.39	1.35

All (281) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	12	DT	P-O3'-C3'	13.04	135.34	119.70
2	K	8	DG	P-O3'-C3'	12.23	134.38	119.70
2	E	20	DT	P-O3'-C3'	11.82	133.89	119.70
2	B	21	DT	N3-C2-O2	-11.78	115.23	122.30
2	H	8	DG	O4'-C4'-C3'	-11.56	99.06	106.00
2	H	20	DT	P-O3'-C3'	11.53	133.54	119.70
2	K	11	DA	O4'-C1'-N9	11.32	115.92	108.00
2	H	21	DT	P-O3'-C3'	11.14	133.06	119.70
2	B	20	DT	N3-C2-O2	-10.68	115.89	122.30
2	K	10	DC	O4'-C1'-N1	10.45	115.32	108.00
2	E	10	DC	O4'-C1'-N1	10.21	115.15	108.00
2	K	13	DT	O4'-C4'-C3'	-9.90	100.06	106.00
2	H	18	DT	P-O3'-C3'	9.79	131.44	119.70
2	B	10	DC	O4'-C1'-N1	9.70	114.79	108.00
2	B	4	DT	C4-C5-C7	9.69	124.81	119.00
2	B	6	DC	O4'-C1'-N1	9.62	114.73	108.00
2	E	21[A]	DT	N3-C2-O2	-9.55	116.57	122.30
2	E	21[B]	DT	N3-C2-O2	-9.55	116.57	122.30
3	I	16	DT	O4'-C1'-N1	9.36	114.55	108.00
2	B	13	DT	C4-C5-C7	9.34	124.60	119.00
2	B	14	DC	O4'-C1'-N1	9.34	114.54	108.00
2	H	10	DC	O4'-C1'-N1	9.33	114.53	108.00
2	B	4	DT	C6-C5-C7	-9.18	117.39	122.90
3	L	1	DT	N3-C2-O2	-8.92	116.95	122.30
2	K	13	DT	O4'-C1'-N1	8.83	114.18	108.00
2	K	14	DC	O4'-C1'-N1	8.65	114.06	108.00
3	L	1	DT	C6-C5-C7	-8.60	117.74	122.90
3	L	19	DA	O4'-C4'-C3'	-8.44	100.94	106.00
2	E	21[A]	DT	P-O3'-C3'	8.44	129.83	119.70
2	E	21[B]	DT	P-O3'-C3'	8.44	129.83	119.70
3	L	1	DT	N3-C4-O4	-8.39	114.87	119.90
3	I	8	DT	C6-C5-C7	-8.33	117.90	122.90
2	H	2[A]	DT	C6-C5-C7	-8.30	117.92	122.90
2	H	2[B]	DT	C6-C5-C7	-8.30	117.92	122.90
2	B	13	DT	C6-C5-C7	-8.30	117.92	122.90
2	H	13	DT	C4-C5-C7	8.21	123.92	119.00
2	E	14	DC	O4'-C1'-N1	8.21	113.75	108.00
2	B	17	DT	P-O3'-C3'	8.17	129.50	119.70
2	K	21[A]	DT	P-O3'-C3'	8.16	129.49	119.70
2	K	21[B]	DT	P-O3'-C3'	8.16	129.49	119.70
3	I	19	DA	O4'-C4'-C3'	-8.13	101.12	106.00
2	E	4	DT	C6-C5-C7	-8.12	118.03	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	9	DA	P-O3'-C3'	8.10	129.43	119.70
3	I	20	DC	N1-C2-O2	8.10	123.76	118.90
2	E	4	DT	C4-C5-C7	8.08	123.85	119.00
3	I	8	DT	C4-C5-C7	8.06	123.84	119.00
2	K	12	DT	O4'-C1'-N1	8.05	113.64	108.00
2	E	17	DT	P-O3'-C3'	7.97	129.26	119.70
2	E	20	DT	C4-C5-C7	7.93	123.76	119.00
3	F	15	DC	O4'-C1'-N1	7.92	113.55	108.00
2	B	21	DT	P-O3'-C3'	7.90	129.18	119.70
3	I	21	DA	O4'-C1'-N9	-7.89	102.48	108.00
2	H	6	DC	O4'-C1'-N1	7.85	113.50	108.00
3	L	7	DT	O5'-P-OP2	-7.83	98.66	105.70
3	F	13	DG	O4'-C1'-N9	7.82	113.47	108.00
2	H	14	DC	O4'-C1'-N1	7.72	113.41	108.00
2	K	1	DC	P-O3'-C3'	7.63	128.85	119.70
2	B	19	DG	P-O3'-C3'	7.61	128.83	119.70
3	L	18	DC	P-O5'-C5'	7.61	133.07	120.90
3	C	3	DA	N1-C6-N6	7.61	123.16	118.60
2	H	13	DT	C6-C5-C7	-7.60	118.34	122.90
2	E	16	DA	C2-N3-C4	7.59	114.40	110.60
2	B	18	DT	N3-C2-O2	-7.58	117.75	122.30
2	E	20	DT	C6-C5-C7	-7.57	118.36	122.90
2	K	2	DT	O4'-C1'-N1	7.55	113.29	108.00
2	E	6	DC	P-O3'-C3'	7.54	128.74	119.70
2	H	2[A]	DT	C1'-O4'-C4'	-7.53	102.57	110.10
2	H	2[B]	DT	C1'-O4'-C4'	-7.53	102.57	110.10
2	E	20	DT	N3-C2-O2	-7.52	117.79	122.30
3	I	20	DC	O4'-C1'-N1	7.50	113.25	108.00
2	K	16	DA	P-O3'-C3'	7.49	128.68	119.70
2	B	20	DT	P-O3'-C3'	7.48	128.67	119.70
3	I	22	DG	C5-C6-O6	-7.46	124.12	128.60
2	B	21	DT	C6-C5-C7	-7.45	118.43	122.90
3	L	8	DT	C4-C5-C7	7.44	123.46	119.00
2	H	18	DT	O4'-C4'-C3'	7.43	110.46	106.00
3	I	20	DC	N3-C2-O2	-7.40	116.72	121.90
3	C	20	DC	N1-C2-O2	7.39	123.34	118.90
2	B	6	DC	C4'-C3'-C2'	-7.38	96.45	103.10
2	K	21[A]	DT	N3-C2-O2	-7.34	117.90	122.30
2	K	21[B]	DT	N3-C2-O2	-7.34	117.90	122.30
3	F	15	DC	N1-C2-O2	7.32	123.29	118.90
3	F	7	DT	O5'-P-OP2	-7.22	99.20	105.70
3	I	1	DT	C6-C5-C7	-7.22	118.57	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	20	DT	O4'-C1'-C2'	-7.21	100.13	105.90
3	C	7	DT	C5'-C4'-C3'	-7.15	101.22	114.10
2	E	16	DA	P-O3'-C3'	7.06	128.18	119.70
2	B	18	DT	P-O3'-C3'	7.03	128.13	119.70
2	H	2[A]	DT	O4'-C1'-N1	6.99	112.89	108.00
2	H	2[B]	DT	O4'-C1'-N1	6.99	112.89	108.00
2	B	20	DT	C6-C5-C7	-6.99	118.71	122.90
2	H	9	DA	P-O3'-C3'	6.98	128.08	119.70
2	H	19	DG	O4'-C1'-N9	-6.96	103.13	108.00
2	H	2[A]	DT	C4-C5-C7	6.96	123.17	119.00
2	H	2[B]	DT	C4-C5-C7	6.96	123.17	119.00
2	K	20[A]	DT	P-O3'-C3'	6.92	128.00	119.70
2	K	20[B]	DT	P-O3'-C3'	6.92	128.00	119.70
3	F	7	DT	N3-C2-O2	-6.91	118.15	122.30
2	B	16	DA	P-O3'-C3'	6.90	127.97	119.70
2	H	2[A]	DT	C4'-C3'-C2'	-6.89	96.90	103.10
2	H	2[B]	DT	C4'-C3'-C2'	-6.89	96.90	103.10
3	L	1	DT	C4-C5-C7	6.89	123.13	119.00
2	E	20	DT	P-O5'-C5'	6.88	131.91	120.90
2	K	12	DT	C1'-O4'-C4'	-6.85	103.25	110.10
3	C	11	DA	P-O3'-C3'	6.81	127.87	119.70
3	I	2	DA	N1-C6-N6	6.80	122.68	118.60
3	F	20	DC	O4'-C1'-N1	6.80	112.76	108.00
3	L	20	DC	O4'-C1'-N1	6.80	112.76	108.00
3	I	2	DA	N9-C4-C5	-6.79	103.09	105.80
3	F	8	DT	C6-C5-C7	-6.78	118.83	122.90
3	C	15	DC	O4'-C1'-N1	6.76	112.73	108.00
3	C	20	DC	N3-C2-O2	-6.74	117.18	121.90
2	H	4	DT	C4-C5-C7	6.71	123.03	119.00
3	I	3	DA	N1-C6-N6	6.70	122.62	118.60
3	I	15	DC	O4'-C1'-N1	6.67	112.67	108.00
2	K	4	DT	C4-C5-C7	6.66	123.00	119.00
3	F	3	DA	O4'-C1'-N9	-6.63	103.36	108.00
2	B	12	DT	N3-C2-O2	-6.56	118.36	122.30
3	C	19	DA	O4'-C4'-C3'	-6.56	101.88	104.50
3	F	3	DA	N1-C6-N6	6.54	122.53	118.60
3	C	5	DA	P-O3'-C3'	6.54	127.55	119.70
3	L	8	DT	C6-C5-C7	-6.51	119.00	122.90
2	H	2[A]	DT	O4'-C4'-C3'	-6.50	101.90	104.50
2	H	2[B]	DT	O4'-C4'-C3'	-6.50	101.90	104.50
2	K	6	DC	O4'-C1'-N1	6.46	112.52	108.00
2	H	1[A]	DC	O4'-C1'-N1	6.45	112.52	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1[B]	DC	O4'-C1'-N1	6.45	112.52	108.00
2	E	13	DT	C4-C5-C7	6.43	122.86	119.00
3	L	1	DT	C5-C4-O4	6.42	129.39	124.90
3	C	8	DT	C6-C5-C7	-6.41	119.05	122.90
2	B	17	DT	N3-C2-O2	-6.40	118.46	122.30
3	I	1	DT	C4-C5-C7	6.35	122.81	119.00
2	H	1[A]	DC	P-O3'-C3'	6.34	127.31	119.70
2	H	1[B]	DC	P-O3'-C3'	6.34	127.31	119.70
2	B	6	DC	C5'-C4'-C3'	-6.34	102.69	114.10
2	K	10	DC	C6-N1-C2	-6.32	117.77	120.30
3	L	7	DT	O5'-P-OP1	6.31	118.27	110.70
2	K	17	DT	P-O3'-C3'	6.30	127.26	119.70
2	K	11	DA	P-O3'-C3'	6.29	127.25	119.70
3	C	1	DT	C5-C6-N1	-6.29	119.93	123.70
2	B	18	DT	N3-C4-O4	-6.28	116.13	119.90
2	H	6	DC	P-O3'-C3'	6.26	127.22	119.70
2	K	18	DT	P-O3'-C3'	6.22	127.17	119.70
2	E	18	DT	O4'-C4'-C3'	6.21	109.72	106.00
3	I	11	DA	N1-C6-N6	6.19	122.31	118.60
2	E	17	DT	N3-C2-O2	-6.17	118.60	122.30
2	H	16	DA	O4'-C1'-N9	6.17	112.32	108.00
3	F	7	DT	C4'-C3'-C2'	-6.17	97.55	103.10
2	H	16	DA	P-O3'-C3'	6.17	127.10	119.70
2	B	18	DT	O4'-C4'-C3'	6.16	109.69	106.00
2	B	20	DT	N3-C4-O4	-6.13	116.22	119.90
3	L	15	DC	O4'-C1'-N1	6.12	112.28	108.00
2	E	21[A]	DT	N1-C2-O2	6.09	127.97	123.10
2	E	21[B]	DT	N1-C2-O2	6.09	127.97	123.10
2	E	4	DT	N3-C4-O4	-6.08	116.25	119.90
3	C	4	DC	C5-C6-N1	-6.01	117.99	121.00
2	B	11	DA	P-O3'-C3'	6.00	126.90	119.70
3	C	8	DT	C4-C5-C7	5.98	122.59	119.00
3	C	13	DG	O4'-C1'-N9	5.98	112.19	108.00
3	C	1	DT	C4-C5-C6	5.97	121.58	118.00
2	E	21[A]	DT	N3-C4-O4	-5.95	116.33	119.90
2	E	21[B]	DT	N3-C4-O4	-5.95	116.33	119.90
3	I	22	DG	C6-N1-C2	-5.94	121.53	125.10
3	I	22	DG	O4'-C1'-N9	-5.94	103.84	108.00
2	H	13	DT	N3-C4-O4	-5.92	116.35	119.90
3	L	21	DA	O4'-C1'-N9	-5.92	103.86	108.00
2	B	21	DT	N3-C4-O4	-5.92	116.35	119.90
3	I	13	DG	O4'-C1'-N9	5.92	112.14	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	13	DG	O4'-C1'-N9	5.91	112.14	108.00
2	E	19	DG	P-O3'-C3'	5.91	126.79	119.70
2	K	2	DT	C1'-O4'-C4'	-5.85	104.25	110.10
3	F	7	DT	O5'-P-OP1	5.84	117.72	110.70
3	I	5	DA	P-O3'-C3'	5.84	126.71	119.70
2	E	6	DC	O4'-C1'-N1	5.82	112.08	108.00
2	K	6	DC	P-O3'-C3'	5.82	126.69	119.70
2	B	22	DA	N1-C6-N6	5.81	122.08	118.60
3	I	6	DA	P-O3'-C3'	5.80	126.66	119.70
3	L	3	DA	C4-C5-N7	5.80	113.60	110.70
3	C	6	DA	O5'-P-OP2	-5.78	100.50	105.70
3	I	19	DA	C5-C6-N1	5.76	120.58	117.70
2	B	22	DA	OP1-P-OP2	5.74	128.21	119.60
3	F	19	DA	O4'-C4'-C3'	-5.73	102.21	104.50
3	F	13	DG	P-O5'-C5'	5.69	130.01	120.90
2	E	4	DT	N3-C2-O2	-5.68	118.89	122.30
3	I	21	DA	O3'-P-O5'	-5.67	93.22	104.00
2	E	2	DT	N3-C2-O2	-5.66	118.90	122.30
2	K	2	DT	C4'-C3'-C2'	-5.65	98.01	103.10
3	C	21	DA	O4'-C1'-N9	-5.64	104.05	108.00
2	B	19	DG	N3-C2-N2	-5.63	115.96	119.90
3	L	3	DA	C5-N7-C8	-5.60	101.10	103.90
3	I	3	DA	C5-C6-N6	-5.58	119.24	123.70
3	I	7	DT	C4'-C3'-C2'	-5.58	98.08	103.10
3	F	7	DT	C5'-C4'-C3'	5.56	124.10	114.10
2	H	18	DT	OP1-P-OP2	5.54	127.91	119.60
3	F	3	DA	C5-C6-N6	-5.53	119.27	123.70
2	K	18	DT	N3-C2-O2	-5.53	118.98	122.30
2	E	10	DC	C1'-O4'-C4'	-5.53	104.57	110.10
3	I	15	DC	O4'-C1'-C2'	-5.52	101.48	105.90
3	L	18	DC	C4'-C3'-C2'	5.51	108.06	103.10
2	B	21	DT	N1-C2-O2	5.49	127.50	123.10
2	H	15	DA	O4'-C1'-N9	5.48	111.83	108.00
3	I	7	DT	C6-C5-C7	-5.47	119.61	122.90
3	I	1	DT	N3-C4-O4	-5.47	116.62	119.90
2	K	20[A]	DT	N3-C2-O2	-5.46	119.02	122.30
2	K	20[B]	DT	N3-C2-O2	-5.46	119.02	122.30
3	I	3	DA	C4-C5-N7	5.45	113.43	110.70
2	H	4	DT	C6-C5-C7	-5.44	119.63	122.90
2	E	16	DA	O4'-C1'-N9	-5.44	104.19	108.00
2	K	4	DT	C6-C5-C7	-5.43	119.64	122.90
2	B	19	DG	N1-C6-O6	5.43	123.16	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	5	DA	N9-C4-C5	-5.42	103.63	105.80
3	I	7	DT	C5'-C4'-C3'	5.42	123.86	114.10
2	E	13	DT	C6-C5-C7	-5.41	119.66	122.90
3	L	13	DG	P-O3'-C3'	5.41	126.19	119.70
3	L	7	DT	C4'-C3'-C2'	-5.40	98.24	103.10
2	K	10	DC	N1-C2-O2	5.39	122.13	118.90
3	F	4	DC	P-O3'-C3'	5.39	126.16	119.70
3	F	8	DT	C4-C5-C7	5.38	122.23	119.00
3	L	5	DA	OP1-P-OP2	5.38	127.67	119.60
3	I	2	DA	N1-C2-N3	-5.38	126.61	129.30
3	F	12	DT	C6-C5-C7	-5.37	119.68	122.90
3	I	2	DA	C4-C5-N7	5.37	113.39	110.70
2	E	13	DT	O4'-C4'-C3'	-5.37	102.35	104.50
2	K	22[A]	DA	N1-C6-N6	5.34	121.80	118.60
2	K	22[B]	DA	N1-C6-N6	5.34	121.80	118.60
2	E	12	DT	N3-C2-O2	-5.34	119.10	122.30
2	B	10	DC	C1'-O4'-C4'	-5.31	104.79	110.10
2	K	19[A]	DG	C5-C6-O6	-5.31	125.41	128.60
2	K	19[B]	DG	C5-C6-O6	-5.31	125.41	128.60
3	F	12	DT	C4-C5-C7	5.29	122.17	119.00
2	E	21[A]	DT	P-O5'-C5'	5.28	129.35	120.90
2	E	21[B]	DT	P-O5'-C5'	5.28	129.35	120.90
2	H	2[A]	DT	O5'-P-OP2	-5.28	100.95	105.70
2	H	2[B]	DT	O5'-P-OP2	-5.28	100.95	105.70
2	B	11	DA	N1-C6-N6	5.28	121.77	118.60
3	F	20	DC	N1-C2-O2	5.27	122.06	118.90
2	B	22	DA	O5'-P-OP2	-5.27	100.96	105.70
2	H	2[A]	DT	P-O3'-C3'	5.24	125.99	119.70
2	H	2[B]	DT	P-O3'-C3'	5.24	125.99	119.70
2	H	16	DA	C4'-C3'-C2'	5.24	107.81	103.10
2	H	19	DG	P-O3'-C3'	5.22	125.97	119.70
3	L	3	DA	P-O3'-C3'	5.22	125.97	119.70
3	C	3	DA	C5-C6-N6	-5.21	119.53	123.70
2	E	8	DG	O4'-C1'-N9	5.21	111.65	108.00
2	E	20	DT	N1-C2-O2	5.20	127.26	123.10
2	H	21	DT	N3-C4-O4	-5.19	116.78	119.90
3	I	7	DT	C1'-O4'-C4'	-5.19	104.91	110.10
2	K	22[A]	DA	O4'-C1'-C2'	5.19	110.05	105.90
2	K	22[B]	DA	O4'-C1'-C2'	5.19	110.05	105.90
2	B	3	DG	N7-C8-N9	5.18	115.69	113.10
2	K	8	DG	O4'-C1'-N9	5.17	111.62	108.00
2	K	14	DC	O4'-C4'-C3'	-5.17	102.43	104.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	12	DT	O4'-C1'-N1	5.17	111.61	108.00
2	K	10	DC	N1-C1'-C2'	5.15	122.38	112.60
2	K	4	DT	P-O3'-C3'	5.14	125.87	119.70
3	L	12	DT	C6-C5-C7	-5.14	119.81	122.90
3	C	13	DG	P-O5'-C5'	5.14	129.12	120.90
2	H	17	DT	P-O3'-C3'	5.14	125.86	119.70
3	I	13	DG	P-O5'-C5'	5.12	129.09	120.90
2	B	18	DT	C5-C6-N1	-5.11	120.64	123.70
2	B	6	DC	O4'-C1'-C2'	-5.10	101.82	105.90
2	B	14	DC	N3-C4-C5	5.10	123.94	121.90
2	E	18	DT	N3-C2-O2	-5.10	119.24	122.30
3	I	1	DT	N3-C2-O2	-5.10	119.24	122.30
3	F	3	DA	C5-N7-C8	-5.08	101.36	103.90
2	B	1	DC	P-O3'-C3'	5.08	125.80	119.70
2	H	11	DA	P-O3'-C3'	5.08	125.80	119.70
3	L	3	DA	OP1-P-OP2	5.08	127.21	119.60
3	I	2	DA	C5-C6-N6	-5.07	119.64	123.70
3	C	20	DC	O4'-C1'-N1	5.06	111.54	108.00
3	F	21	DA	O4'-C1'-N9	-5.05	104.46	108.00
2	B	8	DG	C3'-C2'-C1'	-5.05	96.44	102.50
2	E	2	DT	O4'-C1'-N1	5.05	111.53	108.00
1	D	114	ILE	N-CA-CB	5.04	122.40	110.80
3	L	5	DA	N1-C6-N6	5.04	121.62	118.60
2	E	18	DT	C1'-O4'-C4'	-5.04	105.06	110.10
2	B	9	DA	P-O3'-C3'	5.04	125.74	119.70
2	H	21	DT	P-O5'-C5'	5.03	128.94	120.90
2	E	1	DC	OP2-P-O3'	5.02	116.25	105.20
3	I	5	DA	N9-C4-C5	-5.02	103.79	105.80
3	L	1	DT	C1'-O4'-C4'	-5.01	105.09	110.10

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1664	0	1721	22	0
1	D	1635	0	1687	30	0
1	G	1626	0	1674	31	0
1	J	1626	0	1674	36	0
2	B	450	0	250	3	0
2	E	491	0	273	5	0
2	H	511	0	285	14	0
2	K	533	0	296	17	0
3	C	452	0	248	1	0
3	F	452	0	248	6	0
3	I	452	0	248	9	0
3	L	452	0	248	8	0
4	A	12	0	16	0	0
5	A	32	0	44	22	0
5	D	16	0	22	11	0
5	G	16	0	22	4	0
All	All	10420	0	8956	155	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (155) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:MET:CE	1:A:134:MET:SD	2.01	1.48
5:A:304:1PE:C16	5:A:304:1PE:H251	1.54	1.28
5:A:303:1PE:C16	5:A:303:1PE:H251	1.70	1.20
5:A:304:1PE:C25	5:A:304:1PE:H161	1.68	1.20
1:D:118:LYS:HE2	5:D:301:1PE:H242	1.24	1.17
1:J:157:ARG:HG2	3:L:7:DT:H5'	1.30	1.11
5:A:303:1PE:H142	5:A:303:1PE:H231	1.31	1.11
5:A:303:1PE:H251	5:A:303:1PE:H161	1.32	1.10
5:A:303:1PE:H142	5:A:303:1PE:C23	1.93	0.97
1:G:157:ARG:HG2	3:I:7:DT:H5'	1.44	0.95
1:J:140:ARG:NH2	3:L:16:DT:H3'	1.84	0.93
1:G:118:LYS:HD2	5:G:301:1PE:H261	1.46	0.93
1:G:140:ARG:NH2	2:K:22[B]:DA:H2''	1.85	0.92
5:A:304:1PE:H251	5:A:304:1PE:H161	0.93	0.91
5:A:303:1PE:H251	5:A:303:1PE:H162	1.54	0.90
1:D:157:ARG:HG2	3:F:7:DT:H5'	1.54	0.89
1:D:224:GLU:OE1	1:G:123:PRO:HD2	1.71	0.89
1:G:140:ARG:NH2	2:K:22[B]:DA:C2'	2.37	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:301:1PE:H242	5:D:301:1PE:H151	1.57	0.86
1:D:118:LYS:HZ1	5:D:301:1PE:H261	1.42	0.85
1:D:118:LYS:HE2	5:D:301:1PE:C24	2.07	0.82
1:D:118:LYS:NZ	5:D:301:1PE:H261	1.93	0.82
1:G:140:ARG:HH21	2:K:22[B]:DA:C2'	1.93	0.80
5:A:303:1PE:H161	5:A:303:1PE:C25	2.11	0.79
1:G:118:LYS:HE2	5:G:301:1PE:H131	1.63	0.78
5:A:304:1PE:H251	5:A:304:1PE:H162	1.64	0.77
2:H:22:DA:H2''	2:K:1:DC:P	2.25	0.76
5:A:303:1PE:C23	5:A:303:1PE:C14	2.68	0.71
2:H:3[B]:DG:O6	3:I:19:DA:N6	2.24	0.70
1:J:157:ARG:CG	3:L:7:DT:H5'	2.18	0.69
1:G:52:LYS:HB2	2:H:2[A]:DT:H5'	1.75	0.69
2:H:2[B]:DT:O4	3:I:20:DC:N4	2.26	0.68
1:G:68:PHE:HB3	1:G:80:LEU:HD22	1.77	0.66
1:D:118:LYS:HE2	5:D:301:1PE:H151	1.76	0.66
1:G:140:ARG:HH22	2:K:22[B]:DA:H2''	1.59	0.66
1:G:54:VAL:HG12	2:H:2[A]:DT:H2''	1.78	0.65
1:D:220:GLU:OE2	1:G:124:SER:HB2	1.98	0.64
1:A:235:ILE:HD12	1:A:240:LYS:HA	1.79	0.64
1:J:51:LYS:HB3	2:K:2:DT:H5''	1.81	0.63
2:H:16:DA:H2''	2:H:17:DT:O5'	1.99	0.61
5:D:301:1PE:H151	5:D:301:1PE:C24	2.30	0.60
2:H:2[B]:DT:H2'	2:H:3[B]:DG:C8	2.37	0.60
1:A:118:LYS:HD2	5:A:304:1PE:H142	1.83	0.60
3:F:16:DT:H2''	3:F:17:DG:C8	2.36	0.60
1:D:136:LYS:NZ	1:D:140:ARG:HH22	2.00	0.59
1:G:140:ARG:HH21	2:K:22[B]:DA:C3'	2.15	0.59
1:A:68:PHE:HB3	1:A:80:LEU:HD22	1.85	0.59
1:G:118:LYS:CE	5:G:301:1PE:H131	2.31	0.59
1:D:216:LYS:HD3	1:J:121:LEU:O	2.02	0.58
1:A:141:LYS:HE2	5:A:303:1PE:H221	1.83	0.58
3:C:16:DT:H2''	3:C:17:DG:C8	2.40	0.57
1:D:220:GLU:O	1:D:224:GLU:HG3	2.04	0.57
1:J:68:PHE:HB3	1:J:80:LEU:HD22	1.86	0.57
1:D:68:PHE:HB3	1:D:80:LEU:HD22	1.87	0.57
2:K:21[A]:DT:H2''	2:K:22[A]:DA:C8	2.40	0.56
3:L:16:DT:H2''	3:L:17:DG:C8	2.40	0.56
1:J:192:LEU:HD22	1:J:196:GLU:HG2	1.86	0.56
1:D:118:LYS:CE	5:D:301:1PE:H242	2.16	0.55
1:G:138:LEU:HD21	1:J:138:LEU:HD21	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:3[B]:DG:C8	2:H:4:DT:H73	2.41	0.55
5:A:303:1PE:C16	5:A:303:1PE:C25	2.57	0.55
1:G:189:TRP:NE1	2:H:17:DT:OP1	2.35	0.55
5:A:303:1PE:H252	3:F:4:DC:H5''	1.89	0.54
1:J:140:ARG:HH22	3:L:16:DT:H3'	1.65	0.54
1:D:157:ARG:HD3	3:F:6:DA:H1'	1.89	0.54
2:H:3[B]:DG:N7	2:H:4:DT:H73	2.22	0.54
5:A:304:1PE:C16	5:A:304:1PE:C25	2.41	0.54
1:J:63:GLU:O	1:J:66:PRO:HD2	2.07	0.54
1:G:78:THR:HG23	3:I:19:DA:C4'	2.38	0.53
1:A:118:LYS:HE3	5:A:304:1PE:H262	1.89	0.53
1:G:157:ARG:CG	3:I:7:DT:H5''	2.30	0.53
1:G:181:LYS:O	1:G:185:VAL:HG23	2.09	0.53
1:A:170:PHE:O	1:A:181:LYS:NZ	2.42	0.52
1:A:234:THR:HA	1:A:240:LYS:HB3	1.91	0.52
5:A:303:1PE:OH6	2:E:22[A]:DA:H5''	2.10	0.52
1:G:78:THR:HG23	3:I:19:DA:H4'	1.92	0.52
1:J:63:GLU:OE1	1:J:64:GLN:HG2	2.08	0.52
1:J:58:LEU:HD21	2:K:3:DG:C4	2.45	0.52
1:G:59:ARG:O	1:G:62:LYS:HG2	2.10	0.51
1:D:63:GLU:O	1:D:66:PRO:HD2	2.10	0.51
1:D:122:THR:OG1	1:D:125:GLN:HG3	2.10	0.51
3:I:16:DT:H2'	3:I:17:DG:C8	2.45	0.51
2:K:22[A]:DA:C2	3:L:2:DA:C2	2.99	0.51
1:G:226:GLY:O	1:J:227:ARG:HD3	2.11	0.51
1:G:109:VAL:O	1:G:113:GLU:HG3	2.11	0.50
1:J:227:ARG:HB3	1:J:230:LEU:HD12	1.93	0.50
1:G:67:ILE:O	1:G:71:GLN:HG2	2.11	0.50
1:J:82:ARG:HD3	3:L:19:DA:O3'	2.12	0.50
2:H:22:DA:C2	3:I:2:DA:C2	3.00	0.49
1:J:182:LEU:HD22	2:K:14:DC:C2	2.47	0.49
1:D:215:MET:O	1:D:219:GLU:HG3	2.13	0.49
2:H:3[B]:DG:C8	2:H:4:DT:C7	2.96	0.49
1:J:60:PHE:CZ	1:J:64:GLN:HG3	2.48	0.49
1:J:140:ARG:HH21	3:L:16:DT:H3'	1.74	0.49
1:G:58:LEU:HA	1:G:61:SER:HB3	1.95	0.48
1:A:235:ILE:H	1:A:240:LYS:HD2	1.79	0.48
1:J:165:TYR:OH	1:J:188:ASN:HB3	2.14	0.48
1:J:223:ILE:HD11	1:J:231:LEU:HD21	1.96	0.48
1:G:227:ARG:HD2	1:J:227:ARG:CD	2.43	0.48
1:D:227:ARG:HB3	1:D:230:LEU:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:86:GLN:HG3	1:J:90:GLU:OE1	2.14	0.47
1:G:123:PRO:O	1:G:127:MET:HG3	2.14	0.47
3:I:16:DT:O4'	3:I:16:DT:OP2	2.33	0.47
2:E:2:DT:H2'	2:E:3:DG:C8	2.50	0.47
1:J:54:VAL:HG12	2:K:2:DT:H2''	1.96	0.46
1:J:65:LEU:HA	1:J:84:ILE:HD11	1.97	0.46
1:D:212:HIS:NE2	1:J:119:GLU:HG2	2.30	0.46
1:D:54:VAL:HG11	2:E:3:DG:H5'	1.98	0.46
1:J:162:TYR:O	1:J:166:VAL:HG23	2.15	0.46
1:G:227:ARG:HB3	1:G:230:LEU:HD12	1.98	0.45
2:E:21[A]:DT:H2''	2:E:22[A]:DA:C8	2.51	0.45
1:D:167:ALA:HA	3:F:9:DG:H5'	1.98	0.45
1:D:170:PHE:O	1:D:181:LYS:NZ	2.49	0.45
1:A:86:GLN:HG3	1:A:90:GLU:OE1	2.16	0.45
1:G:86:GLN:HA	1:G:89:ARG:NH1	2.32	0.45
1:J:181:LYS:O	1:J:185:VAL:HG23	2.17	0.45
1:A:234:THR:HA	1:A:240:LYS:HD2	1.99	0.45
5:A:304:1PE:H141	5:A:304:1PE:H152	1.77	0.45
2:B:2:DT:H2'	2:B:3:DG:C8	2.52	0.45
1:G:182:LEU:HD21	2:H:15:DA:C4	2.52	0.45
1:A:227:ARG:HB3	1:A:230:LEU:HD12	2.00	0.44
1:J:79:GLU:HA	1:J:82:ARG:HE	1.83	0.44
1:J:53:PRO:HD3	1:J:110:TYR:HB2	1.99	0.44
1:J:100:GLN:OE1	1:J:104:ARG:NH2	2.51	0.44
1:A:109:VAL:O	1:A:113:GLU:HG3	2.17	0.44
2:B:18:DT:H2''	2:B:19:DG:C8	2.53	0.44
1:D:86:GLN:HG3	1:D:90:GLU:OE1	2.17	0.44
5:D:301:1PE:H232	5:D:301:1PE:H241	1.54	0.44
1:A:122:THR:OG1	1:A:125:GLN:HG3	2.18	0.44
1:A:181:LYS:O	1:A:185:VAL:HG23	2.18	0.44
5:A:303:1PE:H162	3:F:4:DC:H4'	2.00	0.43
1:D:217:SER:HA	1:J:123:PRO:HG3	2.00	0.43
1:A:123:PRO:O	1:A:127:MET:HG3	2.19	0.43
1:D:181:LYS:O	1:D:185:VAL:HG23	2.18	0.43
5:G:301:1PE:H142	5:G:301:1PE:H151	1.77	0.43
1:A:62:LYS:HG3	2:B:4:DT:H5'	2.01	0.42
1:A:134:MET:CE	1:A:134:MET:CG	2.94	0.42
1:D:216:LYS:HE2	1:J:119:GLU:O	2.19	0.42
2:H:21:DT:H2''	2:H:22:DA:C8	2.54	0.42
1:A:127:MET:HE2	1:D:127:MET:HB2	2.01	0.42
2:K:9:DA:H2''	2:K:10:DC:O4'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:LYS:HG2	1:A:110:TYR:CZ	2.55	0.42
2:K:9:DA:H2''	2:K:10:DC:C6	2.55	0.42
1:A:141:LYS:NZ	5:A:303:1PE:OH6	2.53	0.41
1:G:140:ARG:NH2	2:K:22[B]:DA:H2'	2.32	0.41
1:A:141:LYS:HE2	5:A:303:1PE:C22	2.49	0.41
1:J:122:THR:O	1:J:123:PRO:C	2.59	0.41
1:D:232:ARG:H	1:D:232:ARG:HG2	1.51	0.41
2:K:9:DA:H8	2:K:9:DA:OP2	2.04	0.41
1:D:118:LYS:HZ3	5:D:301:1PE:H261	1.79	0.41
1:J:72:ASN:OD1	1:J:83:ARG:NH2	2.53	0.41
1:D:182:LEU:HD22	2:E:14:DC:C2	2.55	0.41
5:D:301:1PE:H222	5:D:301:1PE:H131	1.69	0.41
1:J:52:LYS:CG	2:K:2:DT:H5'	2.51	0.41
1:J:233:ARG:HD3	1:J:233:ARG:HA	1.99	0.41

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	195/213 (92%)	189 (97%)	6 (3%)	0	100	100
1	D	192/213 (90%)	189 (98%)	3 (2%)	0	100	100
1	G	191/213 (90%)	189 (99%)	2 (1%)	0	100	100
1	J	191/213 (90%)	185 (97%)	6 (3%)	0	100	100
All	All	769/852 (90%)	752 (98%)	17 (2%)	0	100	100

There are no Ramachandran outliers to report.



### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	183/197 (93%)	173 (94%)	10 (6%)	21	50
1	D	180/197 (91%)	166 (92%)	14 (8%)	12	37
1	G	179/197 (91%)	167 (93%)	12 (7%)	16	43
1	J	179/197 (91%)	160 (89%)	19 (11%)	6	23
All	All	721/788 (92%)	666 (92%)	55 (8%)	13	38

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	SER
1	A	58	LEU
1	A	72	ASN
1	A	74	ASP
1	A	79	GLU
1	A	159	ARG
1	A	176	ASP
1	A	186	LYS
1	A	210	ARG
1	A	216	LYS
1	D	51	LYS
1	D	56	SER
1	D	58	LEU
1	D	72	ASN
1	D	74	ASP
1	D	151	LEU
1	D	159	ARG
1	D	186	LYS
1	D	188	ASN
1	D	196	GLU
1	D	210	ARG
1	D	216	LYS
1	D	221	GLN
1	D	232	ARG

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Mol	Chain	Res	Type
1	G	51	LYS
1	G	59	ARG
1	G	62	LYS
1	G	74	ASP
1	G	86	GLN
1	G	124	SER
1	G	140	ARG
1	G	159	ARG
1	G	199	LEU
1	G	210	ARG
1	G	221	GLN
1	G	233	ARG
1	J	56	SER
1	J	58	LEU
1	J	63	GLU
1	J	72	ASN
1	J	82	ARG
1	J	100	GLN
1	J	111	LYS
1	J	127	MET
1	J	134	MET
1	J	145	LYS
1	J	159	ARG
1	J	171	GLN
1	J	176	ASP
1	J	179	GLN
1	J	186	LYS
1	J	194	ASP
1	J	210	ARG
1	J	216	LYS
1	J	221	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	188	ASN
1	A	202	GLN
1	D	202	GLN
1	G	71	GLN
1	G	72	ASN
1	G	188	ASN
1	J	203	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](#)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	1PE	A	303	-	15,15,15	0.85	0	14,14,14	1.44	3 (21%)
4	GOL	A	301	-	5,5,5	0.21	0	5,5,5	0.53	0
5	1PE	G	301	-	15,15,15	0.68	0	14,14,14	0.81	0
4	GOL	A	302	-	5,5,5	0.08	0	5,5,5	0.18	0
5	1PE	A	304	-	15,15,15	0.87	0	14,14,14	0.86	0
5	1PE	D	301	-	15,15,15	0.79	0	14,14,14	1.64	4 (28%)

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	1PE	A	303	-	-	10/13/13/13	-
4	GOL	A	301	-	-	4/4/4/4	-
5	1PE	G	301	-	-	7/13/13/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	302	-	-	0/4/4/4	-
5	1PE	A	304	-	-	6/13/13/13	-
5	1PE	D	301	-	-	8/13/13/13	-

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	301	1PE	C25-OH5-C14	3.21	127.18	113.29
5	D	301	1PE	OH5-C14-C24	3.17	124.68	110.39
5	D	301	1PE	C26-OH6-C15	-2.62	101.92	113.29
5	A	303	1PE	OH4-C24-C14	2.54	121.85	110.39
5	D	301	1PE	OH5-C25-C15	2.44	121.38	110.39
5	A	303	1PE	OH6-C15-C25	2.04	119.60	110.39
5	A	303	1PE	C24-OH4-C13	2.04	122.12	113.29

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	304	1PE	C15-C25-OH5-C14
5	A	304	1PE	C25-C15-OH6-C26
5	A	304	1PE	C16-C26-OH6-C15
5	D	301	1PE	C13-C23-OH3-C22
5	G	301	1PE	C14-C24-OH4-C13
5	G	301	1PE	C15-C25-OH5-C14
5	A	303	1PE	C16-C26-OH6-C15
5	D	301	1PE	C15-C25-OH5-C14
5	A	303	1PE	C23-C13-OH4-C24
5	A	303	1PE	C14-C24-OH4-C13
5	A	303	1PE	C15-C25-OH5-C14
5	A	303	1PE	C25-C15-OH6-C26
5	D	301	1PE	C23-C13-OH4-C24
5	D	301	1PE	C24-C14-OH5-C25
5	A	303	1PE	OH2-C12-C22-OH3
5	A	303	1PE	OH6-C15-C25-OH5
5	G	301	1PE	OH5-C14-C24-OH4
5	D	301	1PE	OH6-C15-C25-OH5
5	G	301	1PE	OH6-C15-C25-OH5
5	A	303	1PE	OH5-C14-C24-OH4
5	D	301	1PE	OH4-C13-C23-OH3

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Mol	Chain	Res	Type	Atoms
5	D	301	1PE	OH2-C12-C22-OH3
5	A	304	1PE	OH6-C15-C25-OH5
5	G	301	1PE	OH2-C12-C22-OH3
4	A	301	GOL	O1-C1-C2-C3
4	A	301	GOL	C1-C2-C3-O3
5	A	304	1PE	OH7-C16-C26-OH6
5	D	301	1PE	OH7-C16-C26-OH6
5	A	304	1PE	OH4-C13-C23-OH3
5	G	301	1PE	OH4-C13-C23-OH3
5	A	303	1PE	OH7-C16-C26-OH6
4	A	301	GOL	O1-C1-C2-O2
4	A	301	GOL	O2-C2-C3-O3
5	A	303	1PE	OH4-C13-C23-OH3
5	G	301	1PE	OH7-C16-C26-OH6

There are no ring outliers.

4 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	303	1PE	14	0
5	G	301	1PE	4	0
5	A	304	1PE	8	0
5	D	301	1PE	11	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	197/213 (92%)	-0.30	3 (1%) 73 51	38, 69, 118, 145	0
1	D	194/213 (91%)	-0.38	0 100 100	36, 72, 132, 200	0
1	G	193/213 (90%)	-0.20	1 (0%) 91 79	33, 92, 136, 150	0
1	J	193/213 (90%)	-0.14	2 (1%) 82 63	37, 87, 205, 288	0
2	B	22/22 (100%)	-0.52	0 100 100	49, 76, 93, 102	0
2	E	22/22 (100%)	-0.41	0 100 100	55, 73, 94, 98	0
2	H	22/22 (100%)	0.02	0 100 100	67, 94, 126, 140	0
2	K	22/22 (100%)	-0.12	0 100 100	71, 109, 159, 161	0
3	C	22/22 (100%)	-0.44	0 100 100	50, 71, 99, 114	0
3	F	22/22 (100%)	-0.42	0 100 100	51, 73, 110, 119	0
3	I	22/22 (100%)	-0.30	0 100 100	64, 87, 120, 128	0
3	L	22/22 (100%)	-0.13	0 100 100	67, 109, 159, 163	0
All	All	953/1028 (92%)	-0.26	6 (0%) 89 76	33, 81, 144, 288	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	74	ASP	3.8
1	A	238	GLN	3.5
1	A	239	ARG	3.0
1	J	174	LYS	2.5
1	A	74	ASP	2.3
1	G	176	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 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(Å <sup>2</sup> )	Q<0.9
5	1PE	A	304	16/16	0.81	0.23	69,97,106,107	0
5	1PE	D	301	16/16	0.81	0.26	73,93,103,105	0
5	1PE	G	301	16/16	0.82	0.32	74,106,125,125	0
5	1PE	A	303	16/16	0.83	0.33	76,101,113,114	0
4	GOL	A	301	6/6	0.83	0.29	73,87,91,91	0
4	GOL	A	302	6/6	0.94	0.13	72,83,86,86	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.