



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:08 AM UTC

PDB ID : 9FF4 / pdb\_00009ff4  
Title : The structure of G.kaustophilus T-1 ScoC-17bp dsDNA complex  
Authors : Hadad, N.; Shulami, S.; Pomyalov, S.; Shoham, Y.; Shoham, G.  
Deposited on : 2024-05-22  
Resolution : 2.80 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 : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

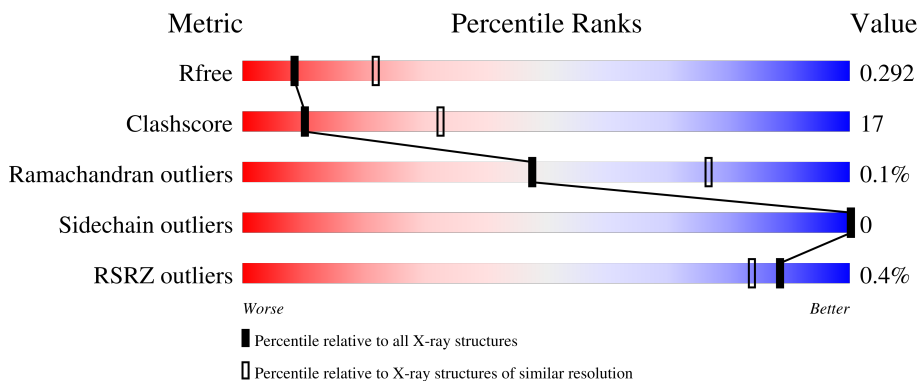
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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.






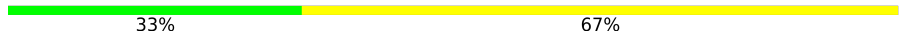
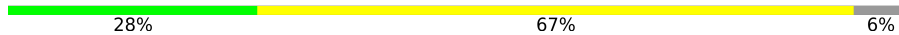
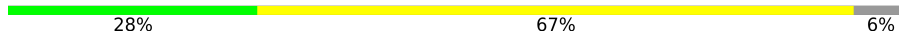
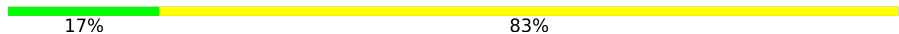
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	207	 62% 24% 14%
1	B	207	 58% 27% 14%
1	C	207	 58% 28% 14%
1	D	207	 54% 32% 14%
2	G	18	 44% 56%

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Mol	Chain	Length	Quality of chain
2	H	18	
2	K	18	
2	M	18	
3	F	18	
3	J	18	
3	L	18	
3	N	18	

## 2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 8911 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 HTH-type transcriptional regulator Hpr.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	178	1484	965	243	268	8	0	0	0
1	C	178	1484	965	243	268	8	0	0	0
1	A	178	1484	965	243	268	8	0	0	0
1	D	178	1484	965	243	268	8	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	202	HIS	-	expression tag	UNP Q5L293
B	203	HIS	-	expression tag	UNP Q5L293
B	204	HIS	-	expression tag	UNP Q5L293
B	205	HIS	-	expression tag	UNP Q5L293
B	206	HIS	-	expression tag	UNP Q5L293
B	207	HIS	-	expression tag	UNP Q5L293
C	202	HIS	-	expression tag	UNP Q5L293
C	203	HIS	-	expression tag	UNP Q5L293
C	204	HIS	-	expression tag	UNP Q5L293
C	205	HIS	-	expression tag	UNP Q5L293
C	206	HIS	-	expression tag	UNP Q5L293
C	207	HIS	-	expression tag	UNP Q5L293
A	202	HIS	-	expression tag	UNP Q5L293
A	203	HIS	-	expression tag	UNP Q5L293
A	204	HIS	-	expression tag	UNP Q5L293
A	205	HIS	-	expression tag	UNP Q5L293
A	206	HIS	-	expression tag	UNP Q5L293
A	207	HIS	-	expression tag	UNP Q5L293
D	202	HIS	-	expression tag	UNP Q5L293
D	203	HIS	-	expression tag	UNP Q5L293
D	204	HIS	-	expression tag	UNP Q5L293

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Chain	Residue	Modelled	Actual	Comment	Reference
D	205	HIS	-	expression tag	UNP Q5L293
D	206	HIS	-	expression tag	UNP Q5L293
D	207	HIS	-	expression tag	UNP Q5L293

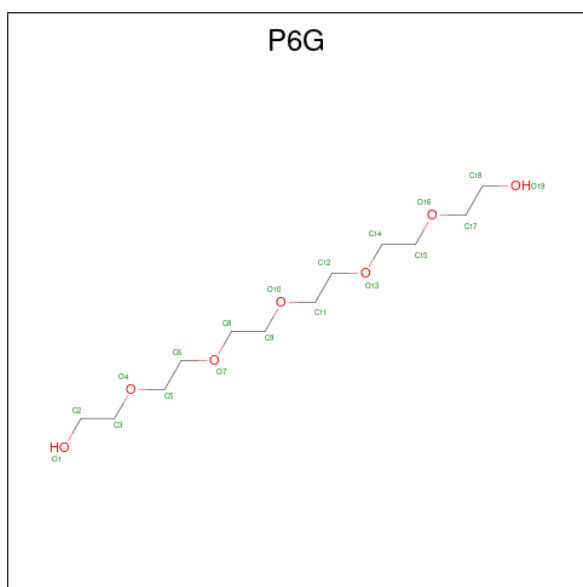
- Molecule 2 is a DNA chain called DNA (5'-D(\*TP\*AP\*AP\*TP\*AP\*AP\*AP\*AP\*TP\*AP\*AP\*AP\*AP\*AP\*AP\*TP\*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	H	18	Total 369	C 179	N 76	O 97	P 17	0	0	0
2	M	17	Total 349	C 169	N 74	O 90	P 16	0	0	0
2	G	18	Total 369	C 179	N 76	O 97	P 17	0	0	0
2	K	17	Total 349	C 169	N 74	O 90	P 16	0	0	0

- Molecule 3 is a DNA chain called DNA (5'-D(\*AP\*GP\*AP\*TP\*TP\*TP\*TP\*TP\*TP\*TP\*TP\*AP\*TP\*TP\*TP\*TP\*AP\*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	L	17	Total 343	C 170	N 49	O 108	P 16	0	0	0
3	F	18	Total 363	C 180	N 51	O 115	P 17	0	0	0
3	J	17	Total 343	C 170	N 49	O 108	P 16	0	0	0
3	N	18	Total 363	C 180	N 51	O 115	P 17	0	0	0

- Molecule 4 is HEXAETHYLENE GLYCOL (CCD ID: P6G) (formula: C<sub>12</sub>H<sub>26</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 19 12 7	0	0
4	C	1	Total C O 19 12 7	0	0
4	A	1	Total C O 19 12 7	0	0
4	D	1	Total C O 19 12 7	0	0

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Mg 1 1	0	0
5	A	1	Total Mg 1 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	6	Total O 6 6	0	0
6	C	15	Total O 15 15	0	0
6	A	6	Total O 6 6	0	0

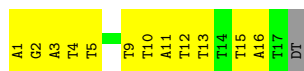
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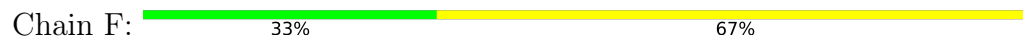
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
6	D	6	Total O 6 6	0	0
6	H	2	Total O 2 2	0	0
6	L	2	Total O 2 2	0	0
6	M	1	Total O 1 1	0	0
6	F	4	Total O 4 4	0	0
6	J	2	Total O 2 2	0	0
6	K	3	Total O 3 3	0	0
6	N	2	Total O 2 2	0	0



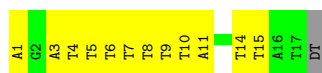




- Molecule 3: DNA (5'-D(\*AP\*GP\*AP\*TP\*TP\*TP\*TP\*TP\*TP\*TP\*AP\*TP\*TP\*TP\*TP\*AP\*T)-3')



- Molecule 3: DNA (5'-D(\*AP\*GP\*AP\*TP\*TP\*TP\*TP\*TP\*TP\*TP\*AP\*TP\*TP\*TP\*TP\*AP\*T)-3')



- Molecule 3: DNA (5'-D(\*AP\*GP\*AP\*TP\*TP\*TP\*TP\*TP\*TP\*TP\*AP\*TP\*TP\*TP\*TP\*AP\*T)-3')



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.63Å 70.55Å 95.47Å 89.77° 81.62° 60.91°	Depositor
Resolution (Å)	48.48 – 2.80 48.48 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.1 (48.48-2.80) 98.1 (48.48-2.80)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.91 (at 2.81Å)	Xtrriage
Refinement program	PHENIX 1.17.1_3660, PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.228 , 0.293 0.231 , 0.292	Depositor DCC
$R_{free}$ test set	1813 reflections (4.63%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	63.6	Xtrriage
Anisotropy	0.819	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 47.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.004 for -h+k,k,-l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8911	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	69.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.32% 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: MG, P6G

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.45	0/1519	0.67	2/2037 (0.1%)
1	B	0.45	0/1519	0.69	1/2037 (0.0%)
1	C	0.49	0/1519	0.72	0/2037
1	D	0.52	0/1519	0.73	0/2037
2	G	0.44	0/417	0.64	0/641
2	H	0.42	0/417	0.62	0/641
2	K	0.41	0/395	0.60	0/607
2	M	0.45	0/395	0.66	0/607
3	F	0.50	0/403	0.75	0/621
3	J	0.42	0/381	0.65	0/587
3	L	0.49	0/381	0.71	0/587
3	N	0.53	0/403	0.84	0/621
All	All	0.47	0/9268	0.70	3/13060 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	28	TRP	CA-CB-CG	-6.20	101.82	113.60
1	A	95	LYS	CA-C-N	6.12	133.23	121.54
1	A	95	LYS	C-N-CA	6.12	133.23	121.54

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1484	0	1482	40	1
1	B	1484	0	1482	57	0
1	C	1484	0	1482	56	1
1	D	1484	0	1482	52	0
2	G	369	0	204	14	0
2	H	369	0	204	19	0
2	K	349	0	192	13	1
2	M	349	0	192	16	0
3	F	363	0	213	9	1
3	J	343	0	201	16	0
3	L	343	0	201	16	0
3	N	363	0	213	19	0
4	A	19	0	26	2	0
4	B	19	0	26	2	0
4	C	19	0	26	2	0
4	D	19	0	26	2	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	6	0	0	0	0
6	B	6	0	0	0	0
6	C	15	0	0	1	0
6	D	6	0	0	0	0
6	F	4	0	0	0	0
6	H	2	0	0	0	0
6	J	2	0	0	1	0
6	K	3	0	0	0	0
6	L	2	0	0	1	0
6	M	1	0	0	0	0
6	N	2	0	0	0	0
All	All	8911	0	7652	273	2

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 17.

All (273) 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:48:GLU:HG2	1:A:84:LEU:HD13	1.56	0.87
3:L:15:DT:H2'	3:L:16:DA:C8	2.12	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:1:DA:O5'	6:L:101:HOH:O	1.96	0.83
3:J:1:DA:O5'	6:J:101:HOH:O	1.99	0.81
1:A:48:GLU:HG2	1:A:84:LEU:CD1	2.13	0.77
2:K:13:DA:H2'	2:K:14:DA:C8	2.19	0.76
1:C:9:SER:OG	1:C:12:GLU:HB2	1.86	0.76
1:B:38:TRP:HB2	4:B:301:P6G:H32	1.70	0.73
1:C:73:HIS:HB3	1:C:76:THR:HG23	1.69	0.72
1:A:101:ASN:HB3	1:A:103:TYR:HE1	1.53	0.72
1:B:135:LEU:HG	1:A:138:LEU:HD21	1.72	0.71
1:B:171:ILE:HD12	1:C:18:GLN:HE22	1.55	0.71
3:J:9:DT:H2'	3:J:10:DT:H71	1.73	0.71
1:A:126:ASN:HB2	4:A:301:P6G:H51	1.74	0.69
2:K:6:DA:H2'	2:K:7:DA:C8	2.28	0.69
1:D:69:PHE:HB3	1:D:163:ILE:HD12	1.76	0.68
1:B:100:ARG:NH1	2:M:11:DA:H1'	2.08	0.68
1:D:144:GLU:O	1:D:145:ILE:HD12	1.93	0.68
2:G:4:DT:H2''	2:G:5:DA:C8	2.29	0.68
2:K:13:DA:H2'	2:K:14:DA:H8	1.56	0.67
1:B:146:LEU:HD21	1:D:139:TYR:CD1	2.30	0.67
3:F:16:DA:H2''	3:F:17:DT:H5''	1.76	0.67
3:L:11:DA:H2''	3:L:12:DT:H5''	1.77	0.67
1:D:101:ASN:HA	3:N:12:DT:OP1	1.95	0.66
2:K:2:DA:H2'	2:K:3:DA:C8	2.31	0.66
2:H:11:DA:H4'	2:H:12:DA:OP1	1.96	0.66
1:D:73:HIS:HB3	1:D:76:THR:HG23	1.77	0.65
1:C:176:ILE:HD12	1:C:177:GLU:H	1.61	0.65
1:A:111:GLU:HG2	1:A:115:MET:HE1	1.79	0.65
2:K:12:DA:H2''	2:K:13:DA:O4'	1.97	0.65
2:M:3:DA:H2''	2:M:4:DT:O4'	1.96	0.64
3:L:9:DT:H2'	3:L:10:DT:H71	1.79	0.64
1:C:69:PHE:HB3	1:C:163:ILE:HD12	1.80	0.63
3:L:10:DT:H2''	3:L:11:DA:O5'	1.99	0.63
3:N:12:DT:OP1	3:N:12:DT:H4'	1.97	0.63
1:B:182:LEU:HG	1:C:10:ILE:HG23	1.79	0.63
3:N:16:DA:H2''	3:N:17:DT:O5'	1.99	0.62
2:G:5:DA:H2'	2:G:6:DA:C8	2.34	0.62
3:N:13:DT:H2'	3:N:14:DT:H71	1.80	0.62
3:J:3:DA:H2'	3:J:4:DT:C6	2.34	0.61
2:H:2:DA:H2''	2:H:3:DA:H5''	1.82	0.61
3:J:7:DT:H2'	3:J:8:DT:C6	2.36	0.61
1:B:145:ILE:HG22	1:B:148:MET:HB2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:ASN:O	1:B:51:ILE:HG13	2.01	0.61
1:C:76:THR:HG22	2:H:4:DT:H71	1.82	0.61
2:M:14:DA:H2''	2:M:15:DA:H8	1.66	0.61
1:B:88:GLY:O	1:B:107:THR:HG21	2.01	0.60
1:C:145:ILE:HG22	1:C:148:MET:HB2	1.84	0.60
1:B:100:ARG:HH12	2:M:11:DA:H1'	1.67	0.60
1:D:90:LEU:HD23	1:D:106:LEU:HA	1.83	0.60
1:C:82:LYS:O	1:C:85:GLU:HG3	2.01	0.59
3:F:1:DA:H2''	3:F:2:DG:C8	2.37	0.59
3:N:15:DT:H2'	3:N:16:DA:C8	2.37	0.59
1:A:50:HIS:O	1:A:54:ILE:HG12	2.02	0.59
1:C:14:MET:O	1:C:18:GLN:HG2	2.03	0.58
1:C:38:TRP:HB3	4:C:301:P6G:H21	1.85	0.58
1:A:98:ASP:CG	1:A:100:ARG:HE	2.12	0.58
2:G:5:DA:H8	2:G:5:DA:H5''	1.68	0.57
1:B:50:HIS:O	1:B:54:ILE:HG12	2.03	0.57
1:A:182:LEU:HG	1:D:10:ILE:HG23	1.85	0.57
1:D:31:ILE:HG13	1:D:128:VAL:HG21	1.87	0.57
3:F:5:DT:H1'	3:F:6:DT:H5'	1.85	0.57
3:J:3:DA:H2'	3:J:4:DT:C5	2.39	0.57
1:B:10:ILE:HD12	1:B:10:ILE:H	1.70	0.57
1:B:121:TYR:CE2	1:B:123:PRO:HD3	2.40	0.57
1:B:57:HIS:CE1	1:B:167:ALA:HA	2.39	0.57
1:C:9:SER:OG	1:C:12:GLU:CB	2.52	0.56
1:D:59:LYS:H	1:D:59:LYS:HD2	1.69	0.56
1:D:52:LEU:HD22	1:D:106:LEU:HD21	1.87	0.56
2:G:1:DT:H6	2:G:1:DT:H5''	1.70	0.56
1:C:138:LEU:HD13	1:C:138:LEU:C	2.30	0.56
1:D:112:GLU:O	1:D:116:LYS:HG2	2.04	0.56
2:H:5:DA:H5''	2:H:5:DA:H8	1.70	0.56
3:F:11:DA:H2''	3:F:12:DT:H5''	1.87	0.56
1:C:82:LYS:NZ	6:C:401:HOH:O	2.10	0.56
1:A:62:SER:HB2	2:K:13:DA:OP1	2.06	0.56
1:A:149:MET:SD	1:D:23:LEU:HD11	2.45	0.56
1:D:67:ALA:HB1	1:D:72:MET:O	2.06	0.56
2:H:3:DA:H61	3:F:17:DT:H3	1.52	0.56
3:J:1:DA:HO5'	3:N:18:DT:HO3'	1.51	0.56
3:J:1:DA:O5'	3:N:18:DT:O3'	2.20	0.56
3:J:1:DA:C8	3:N:18:DT:H2''	2.41	0.55
2:K:15:DA:H2'	2:K:16:DA:C8	2.41	0.55
3:L:3:DA:H2	2:M:17:DT:H3	1.55	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:47:ASN:O	1:D:51:ILE:HG13	2.06	0.55
1:B:28:TRP:HA	1:B:31:ILE:HB	1.89	0.55
1:A:67:ALA:HB1	1:A:72:MET:O	2.07	0.55
3:L:15:DT:H2'	3:L:16:DA:H8	1.70	0.55
1:B:94:LYS:HD3	1:B:101:ASN:O	2.08	0.54
2:G:3:DA:H2''	2:G:4:DT:H5'	1.88	0.54
3:L:4:DT:H2''	3:L:5:DT:H5''	1.88	0.54
2:H:7:DA:H2'	2:H:8:DA:C8	2.42	0.54
1:B:182:LEU:HD21	1:C:11:LYS:HG3	1.88	0.54
1:C:98:ASP:OD2	1:C:100:ARG:NH2	2.39	0.53
1:B:148:MET:HE2	1:C:23:LEU:HD13	1.89	0.53
2:H:1:DT:H2''	2:H:2:DA:C8	2.44	0.53
1:C:138:LEU:HD13	1:C:138:LEU:O	2.09	0.53
2:H:5:DA:H5''	2:H:5:DA:C8	2.44	0.53
2:H:2:DA:H61	3:F:18:DT:C7	2.21	0.53
2:H:4:DT:H2''	2:H:5:DA:C8	2.44	0.53
2:M:4:DT:H2'	2:M:5:DA:C8	2.43	0.53
3:J:3:DA:N6	2:K:16:DA:H61	2.07	0.53
2:M:2:DA:H2''	2:M:3:DA:O4'	2.09	0.53
1:D:76:THR:HG21	2:G:4:DT:OP2	2.09	0.52
2:H:4:DT:H2''	2:H:5:DA:N7	2.24	0.52
1:C:37:ARG:HH21	4:C:301:P6G:H31	1.75	0.52
1:C:95:LYS:HE2	1:C:103:TYR:CZ	2.45	0.52
1:A:62:SER:OG	1:A:65:GLU:HB2	2.10	0.52
1:A:148:MET:SD	1:D:148:MET:HE2	2.50	0.52
2:K:2:DA:H4'	2:K:3:DA:OP1	2.09	0.52
1:B:101:ASN:OD1	2:M:12:DA:H5''	2.09	0.51
1:D:34:ASP:OD2	1:D:126:ASN:HA	2.10	0.51
2:G:11:DA:H4'	2:G:12:DA:OP1	2.09	0.51
3:N:4:DT:H2'	3:N:5:DT:C6	2.45	0.51
1:C:136:ARG:HD2	1:C:142:PHE:CE2	2.44	0.51
1:A:182:LEU:HD21	1:D:11:LYS:HG2	1.92	0.51
1:A:100:ARG:HG3	2:K:12:DA:H4'	1.94	0.50
1:B:12:GLU:OE1	1:C:136:ARG:NH2	2.45	0.50
3:F:7:DT:H1'	3:F:8:DT:H5'	1.93	0.50
1:D:106:LEU:HD22	1:D:110:GLY:HA3	1.92	0.50
1:A:135:LEU:HD22	1:A:139:TYR:CE2	2.47	0.50
3:L:3:DA:C2'	3:L:4:DT:H5'	2.42	0.50
1:C:178:GLN:HG2	1:C:183:VAL:HG11	1.94	0.50
1:D:50:HIS:O	1:D:54:ILE:HG12	2.12	0.50
2:H:2:DA:C2'	2:H:3:DA:H5''	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:122:ASP:HB3	1:C:125:LYS:HD3	1.93	0.49
1:D:52:LEU:HD21	1:D:84:LEU:HD23	1.93	0.49
1:B:149:MET:HG2	1:C:23:LEU:HD11	1.94	0.49
1:B:171:ILE:HD12	1:C:18:GLN:NE2	2.23	0.49
1:C:134:PRO:HB2	1:D:138:LEU:HD21	1.93	0.49
1:B:51:ILE:HG23	1:B:66:ILE:HD12	1.95	0.49
1:D:107:THR:O	1:D:110:GLY:N	2.46	0.49
1:B:136:ARG:HA	1:B:141:LYS:O	2.13	0.48
1:C:98:ASP:OD1	2:H:12:DA:H5'	2.13	0.48
3:L:1:DA:O5'	3:F:18:DT:O3'	2.29	0.48
1:A:128:VAL:HA	1:D:155:ILE:HD11	1.95	0.48
1:A:101:ASN:HB3	1:A:103:TYR:CE1	2.41	0.48
3:N:2:DG:H2''	3:N:3:DA:C8	2.48	0.48
1:B:138:LEU:HD21	1:A:138:LEU:HD22	1.94	0.48
1:D:89:LEU:CD2	1:D:110:GLY:HA2	2.43	0.48
3:N:11:DA:H2''	3:N:12:DT:O4'	2.13	0.48
1:D:119:GLU:HG2	1:D:183:VAL:HG12	1.96	0.48
1:B:111:GLU:O	1:B:115:MET:HG2	2.14	0.47
1:C:47:ASN:ND2	2:H:3:DA:O5'	2.46	0.47
1:C:152:VAL:HG12	1:C:161:MET:CE	2.45	0.47
1:D:175:PHE:HB3	1:D:182:LEU:HD22	1.96	0.47
2:M:12:DA:H2''	2:M:13:DA:H8	1.80	0.47
3:J:5:DT:H2'	3:J:6:DT:C6	2.50	0.47
3:N:12:DT:H5''	3:N:12:DT:H6	1.78	0.47
1:B:182:LEU:HD23	1:B:182:LEU:HA	1.80	0.47
1:C:170:ASN:O	1:C:174:ASP:HB2	2.14	0.47
1:A:37:ARG:NH2	4:A:301:P6G:O1	2.45	0.47
3:L:3:DA:H2''	3:L:4:DT:H5'	1.97	0.47
1:B:75:SER:HB2	3:L:4:DT:H71	1.97	0.47
1:C:52:LEU:HD21	1:C:84:LEU:HD22	1.97	0.47
1:A:106:LEU:HD21	1:A:114:LEU:HD22	1.96	0.47
2:H:7:DA:H2'	2:H:8:DA:H8	1.79	0.47
1:C:100:ARG:NH1	3:F:10:DT:H1'	2.30	0.46
2:G:11:DA:H2''	2:G:12:DA:O5'	2.16	0.46
1:B:176:ILE:HG22	1:B:177:GLU:N	2.30	0.46
3:N:11:DA:H2''	3:N:12:DT:C5'	2.45	0.46
1:B:50:HIS:CE1	1:B:70:GLY:HA2	2.51	0.46
1:D:125:LYS:HB2	4:D:301:P6G:O19	2.16	0.46
1:D:146:LEU:CD2	1:D:150:CYS:SG	3.03	0.46
1:A:89:LEU:HD22	1:A:110:GLY:HA2	1.96	0.46
1:D:45:ASN:OD1	1:D:48:GLU:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:SER:HA	1:A:74:VAL:HG23	1.97	0.46
1:D:76:THR:HG22	2:G:4:DT:H71	1.97	0.46
1:C:97:ASP:OD1	1:C:97:ASP:N	2.49	0.46
3:N:6:DT:C6	3:N:7:DT:H72	2.51	0.46
1:A:49:HIS:CE1	1:A:53:TRP:CD1	3.04	0.46
2:H:1:DT:H2''	2:H:2:DA:N7	2.31	0.46
3:J:7:DT:H2'	3:J:8:DT:H6	1.79	0.46
1:B:175:PHE:HB3	1:B:182:LEU:HD22	1.97	0.46
1:A:25:LYS:NZ	1:D:50:HIS:ND1	2.61	0.46
1:B:89:LEU:C	1:B:107:THR:HG22	2.41	0.45
2:M:15:DA:H2''	2:M:16:DA:O5'	2.16	0.45
1:C:28:TRP:O	1:C:32:GLU:N	2.47	0.45
1:A:31:ILE:HG12	1:A:128:VAL:HG21	1.99	0.45
1:C:51:ILE:HG13	1:C:72:MET:HE1	1.98	0.45
1:D:7:HIS:CG	1:D:8:TYR:H	2.35	0.45
1:D:9:SER:HB2	1:D:12:GLU:H	1.81	0.45
3:N:10:DT:H2''	3:N:11:DA:O5'	2.16	0.45
3:N:14:DT:H2''	3:N:15:DT:O5'	2.16	0.45
1:B:89:LEU:O	1:B:107:THR:HG22	2.17	0.45
1:D:57:HIS:CE1	1:D:167:ALA:HA	2.52	0.45
3:J:3:DA:H2''	3:J:4:DT:H5'	1.99	0.45
1:B:121:TYR:CD2	1:B:123:PRO:HD3	2.52	0.45
1:C:178:GLN:HG2	1:C:183:VAL:CG1	2.47	0.44
2:G:3:DA:H2''	2:G:4:DT:C5'	2.47	0.44
1:D:37:ARG:HH11	4:D:301:P6G:H171	1.81	0.44
2:K:2:DA:H2''	2:K:3:DA:O5'	2.18	0.44
1:B:146:LEU:HD23	1:B:146:LEU:C	2.43	0.44
2:M:14:DA:H2''	2:M:15:DA:C8	2.48	0.44
1:C:152:VAL:HG12	1:C:161:MET:HE1	2.00	0.44
1:B:82:LYS:O	1:B:86:GLU:HG3	2.18	0.44
1:A:118:MET:HE1	1:D:14:MET:HE1	1.99	0.44
1:B:78:PHE:CZ	2:M:14:DA:H5''	2.52	0.44
3:J:8:DT:H2'	3:J:9:DT:H6	1.83	0.44
1:D:176:ILE:HD12	1:D:177:GLU:H	1.83	0.44
1:B:31:ILE:HD12	1:C:24:SER:OG	2.18	0.43
1:B:94:LYS:HE2	1:B:94:LYS:HB2	1.85	0.43
1:B:175:PHE:O	1:C:11:LYS:HE2	2.18	0.43
2:G:6:DA:H2'	2:G:7:DA:C8	2.53	0.43
1:C:118:MET:HE3	1:C:118:MET:HB3	1.66	0.43
1:B:58:PHE:CZ	1:B:166:ARG:HD3	2.54	0.43
1:C:33:LYS:HG3	1:C:34:ASP:N	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:LEU:C	1:C:138:LEU:CD1	2.91	0.43
1:A:48:GLU:CG	1:A:84:LEU:CD1	2.90	0.43
1:A:88:GLY:O	1:A:107:THR:HG21	2.18	0.43
1:B:182:LEU:HD11	1:C:11:LYS:HA	2.01	0.43
1:A:23:LEU:HD11	1:D:149:MET:SD	2.59	0.43
1:A:115:MET:HG3	1:A:175:PHE:HE2	1.82	0.43
2:K:7:DA:C2	2:K:8:DA:C4	3.06	0.43
3:L:12:DT:H1'	3:L:13:DT:H5'	2.01	0.43
1:B:24:SER:HB3	1:C:27:LEU:HD23	2.00	0.43
1:C:115:MET:HB3	1:C:115:MET:HE3	1.57	0.43
2:M:12:DA:H2''	2:M:13:DA:C8	2.54	0.42
2:H:9:DT:H2''	2:H:10:DA:C8	2.54	0.42
1:B:90:LEU:HD23	1:B:90:LEU:HA	1.79	0.42
1:C:160:PHE:CD1	1:C:161:MET:HE2	2.54	0.42
1:A:136:ARG:HD2	1:A:142:PHE:CE2	2.54	0.42
3:L:3:DA:C8	3:L:3:DA:H5''	2.54	0.42
1:B:94:LYS:NZ	2:M:14:DA:OP1	2.53	0.42
1:A:118:MET:HB3	1:A:118:MET:HE3	1.74	0.42
3:L:1:DA:C6	3:L:2:DG:C6	3.08	0.42
1:C:135:LEU:HD13	1:D:138:LEU:HD13	2.00	0.42
2:M:2:DA:H2''	2:M:3:DA:H5''	2.01	0.42
1:B:80:PHE:O	1:B:84:LEU:HG	2.19	0.42
2:G:12:DA:H2''	2:G:13:DA:O5'	2.19	0.42
1:B:171:ILE:CD1	1:C:18:GLN:HE22	2.29	0.42
1:C:148:MET:HE3	1:C:148:MET:HA	2.02	0.42
1:A:52:LEU:HB3	1:A:114:LEU:HD11	2.02	0.42
1:D:49:HIS:CE1	1:D:53:TRP:CD1	3.08	0.42
1:A:19:ARG:NH2	1:D:143:PRO:O	2.39	0.41
1:A:47:ASN:O	1:A:51:ILE:HG13	2.20	0.41
1:A:144:GLU:C	1:A:145:ILE:HG12	2.45	0.41
2:H:17:DT:H2'	2:H:18:DC:C6	2.56	0.41
2:K:4:DT:H2''	2:K:5:DA:C8	2.55	0.41
1:C:35:TRP:O	1:C:38:TRP:HD1	2.03	0.41
1:C:149:MET:HB3	1:C:149:MET:HE3	1.79	0.41
1:D:111:GLU:HG2	1:D:115:MET:SD	2.60	0.41
1:C:76:THR:HG22	2:H:4:DT:H6	1.85	0.41
1:C:160:PHE:HD1	1:C:161:MET:HE2	1.84	0.41
1:A:24:SER:OG	1:D:31:ILE:HD13	2.20	0.41
1:D:90:LEU:HD23	1:D:90:LEU:HA	1.94	0.41
1:D:122:ASP:OD2	1:D:125:LYS:HD2	2.20	0.41
3:N:14:DT:H4'	3:N:15:DT:OP1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:THR:OG1	3:L:3:DA:OP2	2.28	0.41
1:B:155:ILE:HD11	1:C:128:VAL:HA	2.03	0.41
1:D:52:LEU:HB2	1:D:114:LEU:HD21	2.03	0.41
1:D:121:TYR:CE2	1:D:123:PRO:HG3	2.56	0.41
1:D:136:ARG:HD2	1:D:142:PHE:CE2	2.55	0.41
3:J:8:DT:H2'	3:J:9:DT:H71	2.03	0.41
3:J:10:DT:H2''	3:J:11:DA:O4'	2.19	0.41
1:B:32:GLU:HG3	1:B:46:ILE:HD12	2.03	0.41
1:B:134:PRO:O	1:B:138:LEU:HD23	2.21	0.41
2:G:7:DA:C2	2:G:8:DA:C4	3.09	0.41
1:C:109:LYS:O	1:C:113:VAL:HG13	2.21	0.41
1:B:28:TRP:O	1:B:32:GLU:N	2.44	0.40
1:B:67:ALA:HB1	1:B:72:MET:O	2.21	0.40
1:D:47:ASN:HD22	2:G:3:DA:H5''	1.85	0.40
1:D:48:GLU:HA	1:D:51:ILE:HD12	2.03	0.40
2:M:13:DA:H2'	2:M:14:DA:C8	2.56	0.40
1:B:91:SER:O	1:B:104:ILE:HA	2.20	0.40
1:B:115:MET:HE1	1:B:175:PHE:CZ	2.56	0.40
1:A:27:LEU:HD12	1:A:27:LEU:HA	1.89	0.40
3:J:14:DT:H2'	3:J:15:DT:H71	2.02	0.40
3:N:13:DT:H2''	3:N:14:DT:O5'	2.21	0.40
1:B:38:TRP:HZ3	4:B:301:P6G:H121	1.87	0.40
1:D:35:TRP:CE2	1:D:46:ILE:HG23	2.56	0.40
1:B:112:GLU:O	1:B:116:LYS:HG2	2.21	0.40
3:N:11:DA:H2''	3:N:12:DT:C4'	2.51	0.40

All (2) 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)
1:C:116:LYS:NZ	3:F:1:DA:O3'[1_455]	2.17	0.03
1:A:119:GLU:OE1	2:K:2:DA:O5'[1_655]	2.18	0.02

## 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	176/207 (85%)	169 (96%)	7 (4%)	0	100	100
1	B	176/207 (85%)	168 (96%)	8 (4%)	0	100	100
1	C	176/207 (85%)	171 (97%)	5 (3%)	0	100	100
1	D	176/207 (85%)	171 (97%)	4 (2%)	1 (1%)	21	51
All	All	704/828 (85%)	679 (96%)	24 (3%)	1 (0%)	48	77

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	145	ILE

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	160/186 (86%)	160 (100%)	0	100	100
1	B	160/186 (86%)	160 (100%)	0	100	100
1	C	160/186 (86%)	160 (100%)	0	100	100
1	D	160/186 (86%)	160 (100%)	0	100	100
All	All	640/744 (86%)	640 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

Mol	Chain	Res	Type
1	B	57	HIS
1	B	170	ASN
1	C	18	GLN
1	C	154	ASN
1	A	7	HIS

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Mol	Chain	Res	Type
1	A	126	ASN
1	D	126	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	$\# Z  > 2$
4	P6G	A	301	-	18,18,18	0.22	0	17,17,17	0.22	0
4	P6G	C	301	-	18,18,18	0.21	0	17,17,17	0.21	0
4	P6G	D	301	-	18,18,18	0.24	0	17,17,17	0.21	0
4	P6G	B	301	-	18,18,18	0.25	0	17,17,17	0.14	0

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
4	P6G	A	301	-	-	4/16/16/16	-
4	P6G	C	301	-	-	6/16/16/16	-
4	P6G	D	301	-	-	5/16/16/16	-
4	P6G	B	301	-	-	4/16/16/16	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	301	P6G	O13-C14-C15-O16
4	B	301	P6G	O10-C11-C12-O13
4	A	301	P6G	O10-C11-C12-O13
4	C	301	P6G	O16-C17-C18-O19
4	D	301	P6G	C12-C11-O10-C9
4	D	301	P6G	O13-C14-C15-O16
4	C	301	P6G	O4-C5-C6-O7
4	D	301	P6G	C9-C8-O7-C6
4	B	301	P6G	C5-C6-O7-C8
4	A	301	P6G	C14-C15-O16-C17
4	B	301	P6G	O4-C5-C6-O7
4	C	301	P6G	C8-C9-O10-C11
4	C	301	P6G	C12-C11-O10-C9
4	B	301	P6G	C6-C5-O4-C3
4	D	301	P6G	C5-C6-O7-C8
4	C	301	P6G	C15-C14-O13-C12
4	D	301	P6G	O10-C11-C12-O13
4	A	301	P6G	O13-C14-C15-O16
4	A	301	P6G	C9-C8-O7-C6

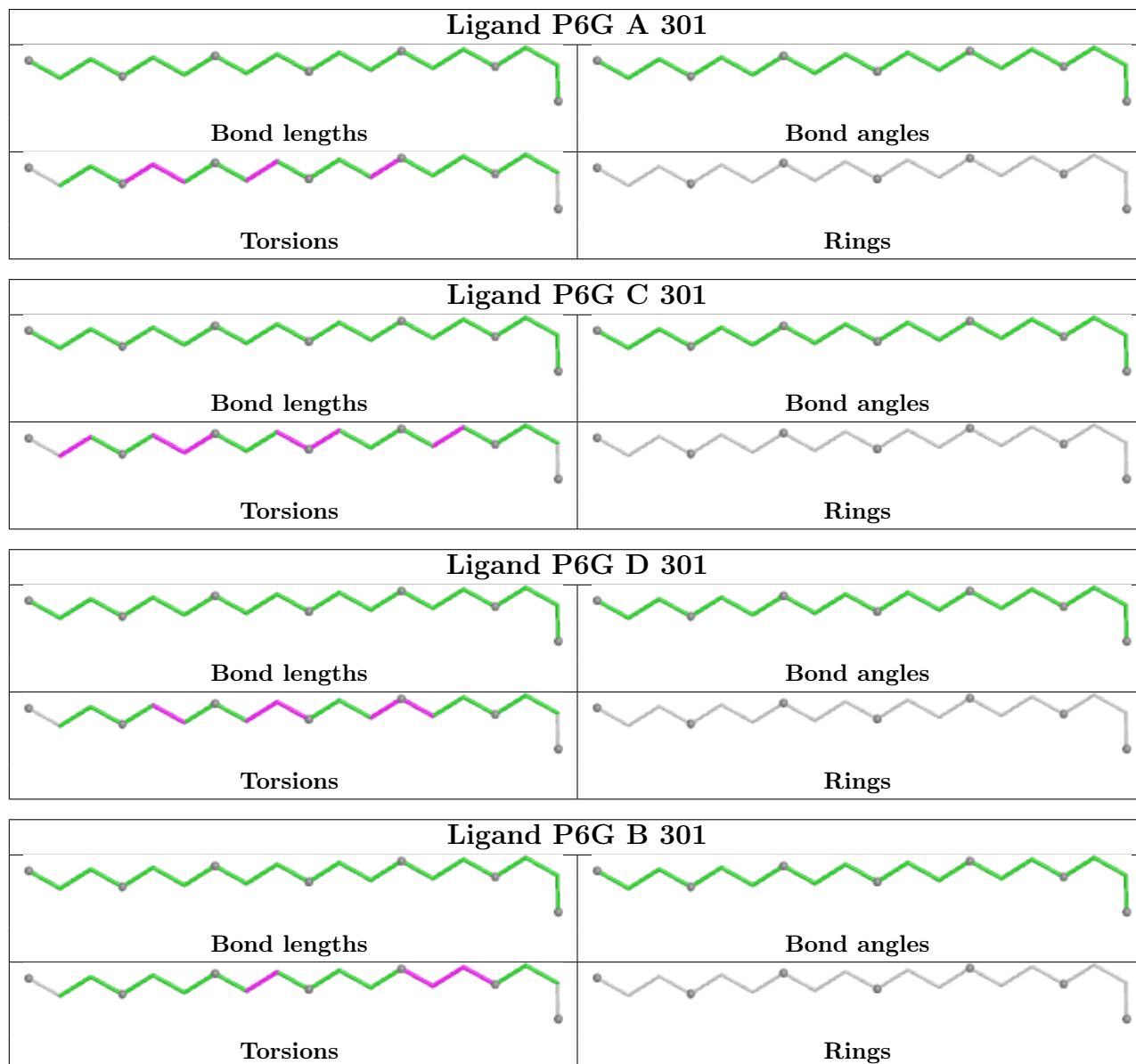
There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	301	P6G	2	0
4	C	301	P6G	2	0
4	D	301	P6G	2	0
4	B	301	P6G	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 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	178/207 (85%)	0.06	1 (0%) 85 80	41, 64, 88, 98	0
1	B	178/207 (85%)	0.03	1 (0%) 85 80	40, 63, 86, 100	0
1	C	178/207 (85%)	-0.11	1 (0%) 85 80	41, 57, 76, 88	0
1	D	178/207 (85%)	-0.17	0 100 100	40, 56, 80, 91	0
2	G	18/18 (100%)	-0.18	0 100 100	63, 77, 101, 110	0
2	H	18/18 (100%)	-0.21	0 100 100	64, 78, 102, 104	0
2	K	17/18 (94%)	0.49	0 100 100	81, 96, 122, 124	0
2	M	17/18 (94%)	0.00	0 100 100	72, 81, 113, 117	0
3	F	18/18 (100%)	-0.15	0 100 100	57, 79, 112, 112	0
3	J	17/18 (94%)	0.45	0 100 100	76, 94, 120, 120	0
3	L	17/18 (94%)	0.07	0 100 100	69, 84, 108, 109	0
3	N	18/18 (100%)	-0.03	0 100 100	65, 79, 112, 116	0
All	All	852/972 (87%)	-0.03	3 (0%) 88 84	40, 62, 96, 124	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	148	MET	3.0
1	A	180	GLY	2.1
1	B	104	ILE	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](#)

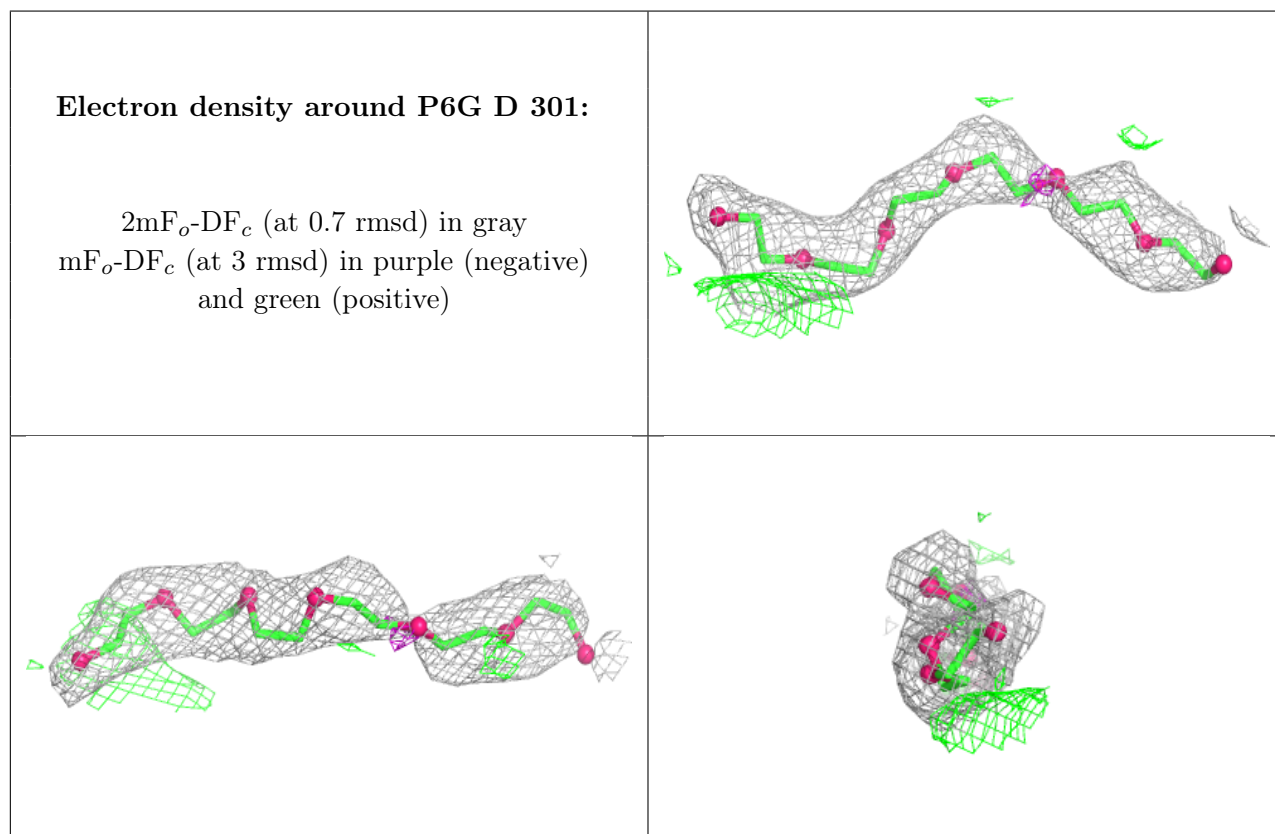
There are no oligosaccharides in this entry.

### 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.

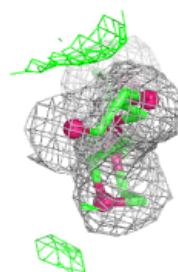
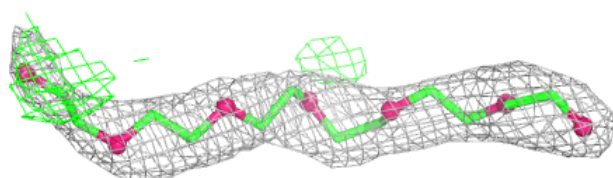
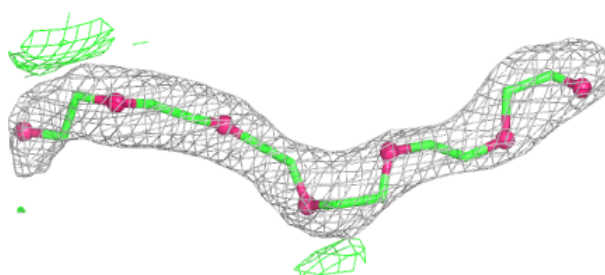
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	MG	A	302	1/1	0.66	0.24	66,66,66,66	0
4	P6G	D	301	19/19	0.85	0.14	48,54,69,72	0
5	MG	B	302	1/1	0.86	0.20	63,63,63,63	0
4	P6G	B	301	19/19	0.89	0.13	56,62,66,67	0
4	P6G	C	301	19/19	0.89	0.12	46,55,61,62	0
4	P6G	A	301	19/19	0.89	0.14	48,62,68,70	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

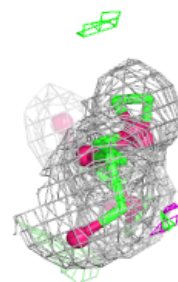
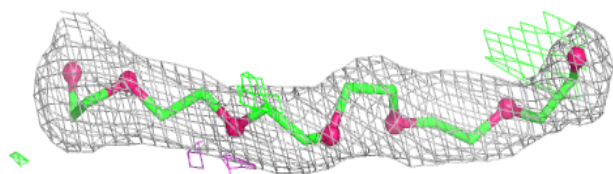
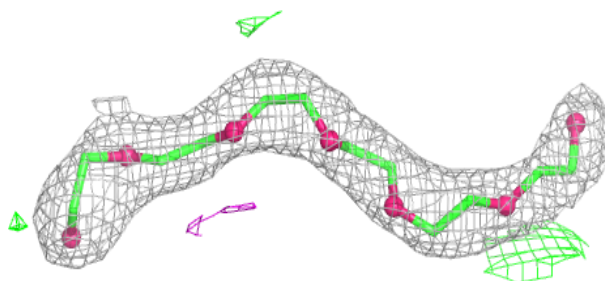


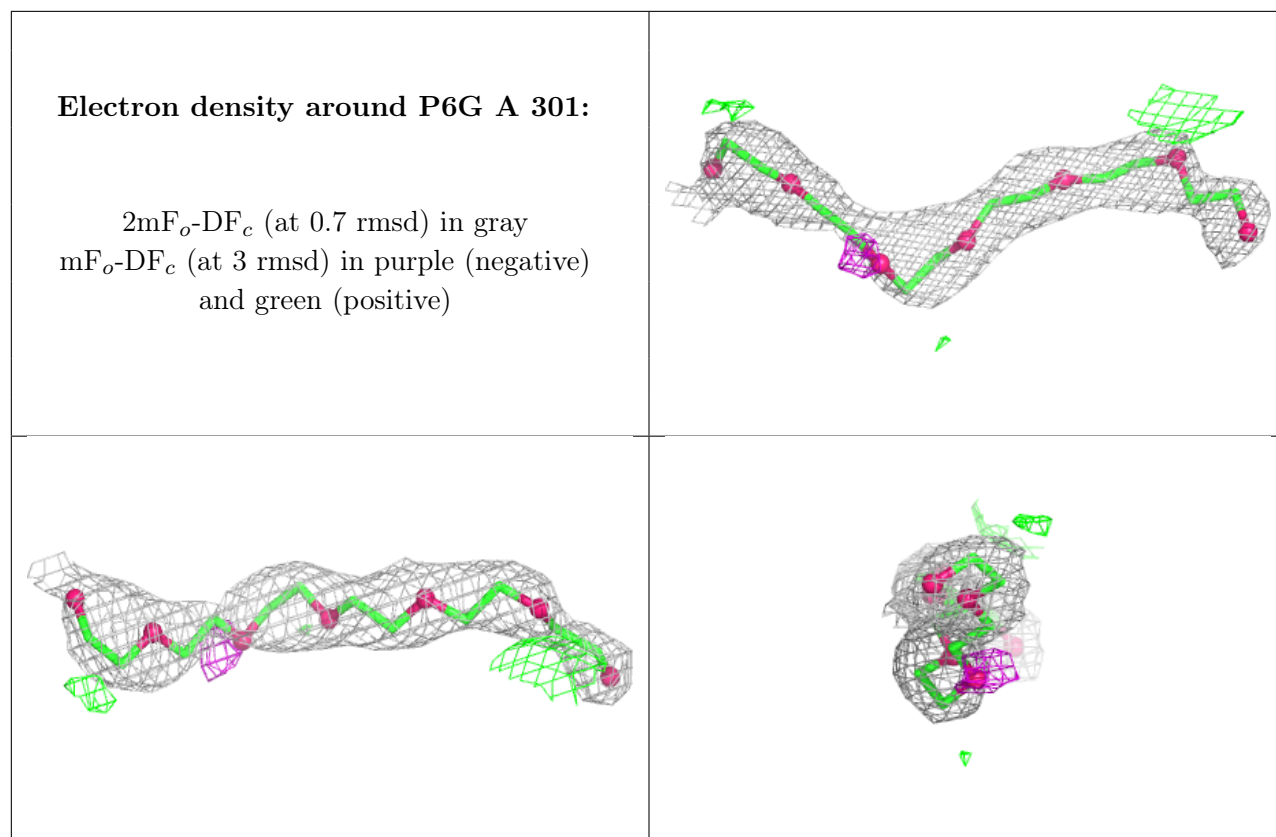
**Electron density around P6G B 301:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around P6G C 301:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.