



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:48 PM GMT

PDB ID : 1M19  
Title : LIGAND BINDING ALTERS THE STRUCTURE AND DYNAMICS OF NUCLEOSOMAL DNA  
Authors : Suto, R.K.; Edayathumangalam, R.S.; White, C.L.; Melander, C.; Gottesfeld, J.M.; Dervan, P.B.; Luger, K.  
Deposited on : 2002-06-18  
Resolution : 2.30 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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

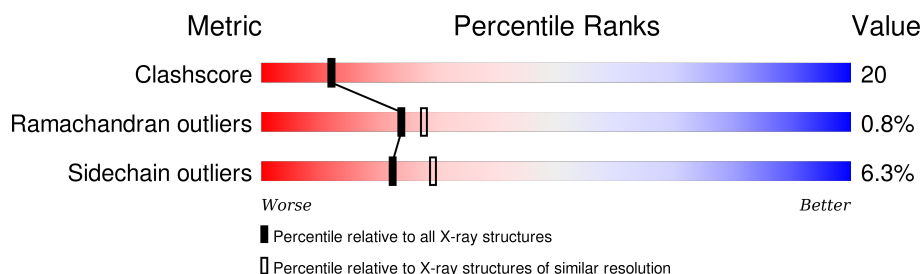
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)

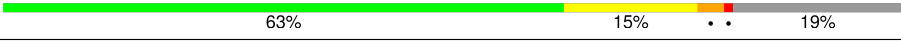


The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	I	146	
1	J	146	
2	A	135	
2	E	135	
3	B	102	
3	F	102	
4	C	129	

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Mol	Chain	Length	Quality of chain
4	G	129	
5	D	125	
5	H	125	

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
7	IMT	I	1961	-	-	X	-
7	PYB	I	1962	-	-	X	-
7	PYB	I	1963	-	-	X	-
7	PYB	I	1964	-	-	X	-
7	PYB	I	1967	-	-	X	-
7	PYB	I	1968	-	-	X	-
7	PYB	I	1969	-	-	X	-
7	PYB	I	2022	-	-	X	-
7	PYB	I	2023	-	-	X	-
7	PYB	I	2024	-	-	X	-
7	PYB	I	2028	-	-	X	-
7	PYB	I	2029	-	-	X	-
7	IMT	J	1901	-	-	X	-
7	PYB	J	1902	-	-	X	-
7	PYB	J	1903	-	-	X	-
7	PYB	J	1904	-	-	X	-
7	ABU	J	1905	-	-	X	-
7	PYB	J	1906	-	-	X	-
7	PYB	J	1907	-	-	X	-
7	PYB	J	1908	-	-	X	-
7	PYB	J	1922	-	-	X	-
7	PYB	J	1923	-	-	X	-
7	PYB	J	1924	-	-	X	-
7	PYB	J	1927	-	-	X	-
7	PYB	J	1928	-	-	X	-
7	PYB	J	1929	-	-	X	-
7	PYB	J	2002	-	-	X	-
7	PYB	J	2003	-	-	X	-
7	PYB	J	2006	-	-	X	-
7	PYB	J	2007	-	-	X	-
7	PYB	J	2008	-	-	X	-
7	PYB	J	2009	-	-	X	-

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 13158 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 Palindromic 146 Base Pair DNA Fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	I	146	Total	C	N	O	P	0	0	0
			2990	1430	541	874	145			
1	J	146	Total	C	N	O	P	0	0	0
			2990	1430	541	874	145			

- Molecule 2 is a protein called Histone H3.2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	100	Total	C	N	O	S	0	0	0
			826	521	160	142	3			
2	E	98	Total	C	N	O	S	0	0	0
			808	509	156	140	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	486	SER	ARG	SEE REMARK 999	UNP P02302
E	686	SER	ARG	SEE REMARK 999	UNP P02302

- Molecule 3 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	79	Total	C	N	O	S	0	0	0
			627	395	121	110	1			
3	F	86	Total	C	N	O	S	0	0	0
			694	436	140	117	1			

- Molecule 4 is a protein called Histone H2A.1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	C	107	Total	C	N	O	0	0	0
			825	520	161	144			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	105	Total	C	N	O	0	0	0
			813	513	159	141			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	899	ARG	GLY	SEE REMARK 999	UNP P06897
G	1099	ARG	GLY	SEE REMARK 999	UNP P06897

- Molecule 5 is a protein called Histone H2B.1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	D	94	Total	C	N	O	S	0	0	0
			736	463	132	139	2			
5	H	94	Total	C	N	O	S	0	0	0
			736	463	132	139	2			

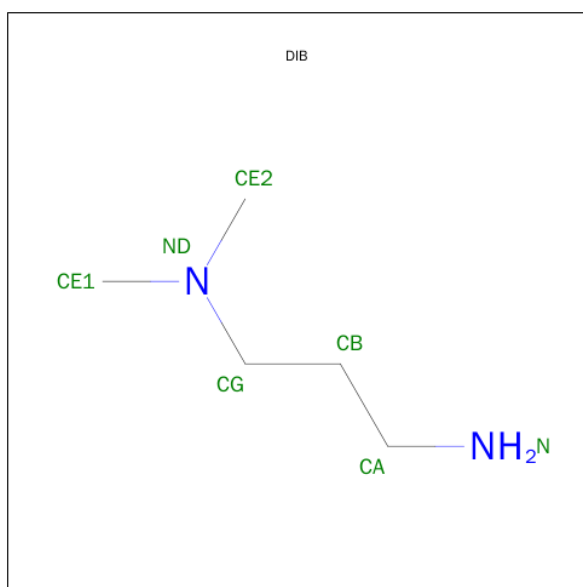
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1229	THR	SER	SEE REMARK 999	UNP P02281
H	1429	THR	SER	SEE REMARK 999	UNP P02281

- Molecule 6 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	J	4	Total	Mn	0	0
			4	4		
6	I	6	Total	Mn	0	0
			6	6		
6	E	1	Total	Mn	0	0
			1	1		

- Molecule 7 is 4-AMINO-(1-METHYLIMIDAZOLE)-2-CARBOXYLIC ACID (three-letter code: DIB, PYB, IMT, BAL, ABU) (formula: C<sub>5</sub>H<sub>14</sub>N<sub>2</sub>, C<sub>6</sub>H<sub>8</sub>N<sub>2</sub>O<sub>2</sub>, C<sub>5</sub>H<sub>7</sub>N<sub>3</sub>O<sub>2</sub>, C<sub>3</sub>H<sub>7</sub>NO<sub>2</sub>, C<sub>4</sub>H<sub>9</sub>NO<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	J	11	Total	C	N	O	0	0
			89	59	20	10		
7	J	11	Total	C	N	O	0	0
			89	59	20	10		
7	I	11	Total	C	N	O	0	0
			89	59	20	10		
7	J	11	Total	C	N	O	0	0
			89	59	20	10		
7	I	11	Total	C	N	O	0	0
			89	59	20	10		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	68	Total	O	0	0
			68	68		
8	B	46	Total	O	0	0
			46	46		
8	C	79	Total	O	0	0
			79	79		
8	D	44	Total	O	0	0
			44	44		
8	E	84	Total	O	0	0
			84	84		
8	F	75	Total	O	0	0
			75	75		
8	G	66	Total	O	0	0
			66	66		

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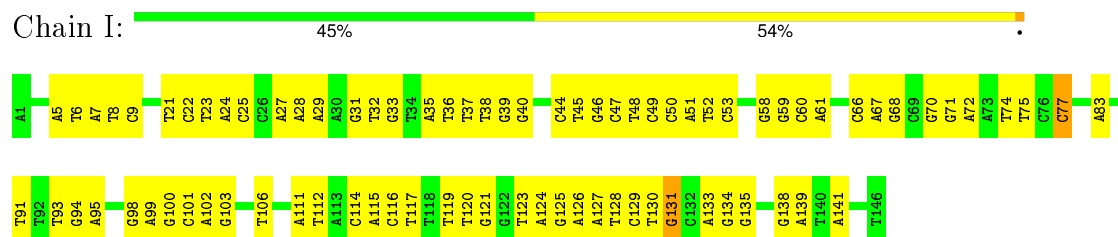
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	H	40	Total 40	O 40	0	0
8	I	88	Total 88	O 88	0	0
8	J	67	Total 67	O 67	0	0

### 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.

Note EDS was not executed.

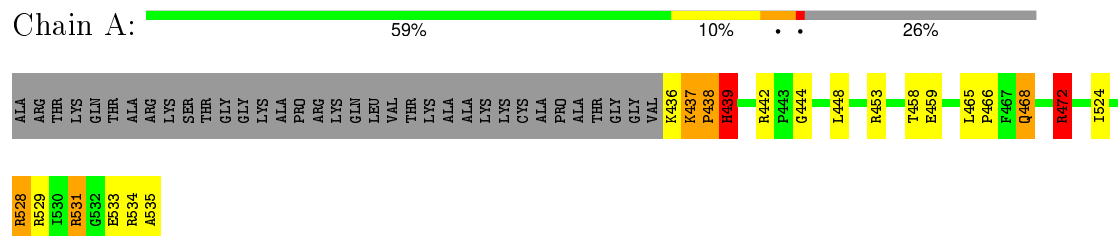
#### • Molecule 1: Palindromic 146 Base Pair DNA Fragment



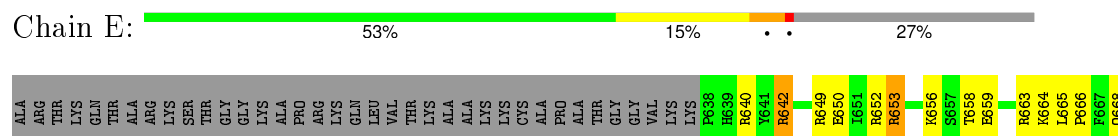
#### • Molecule 1: Palindromic 146 Base Pair DNA Fragment



#### • Molecule 2: Histone H3.2



#### • Molecule 2: Histone H3.2

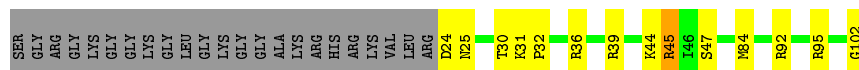






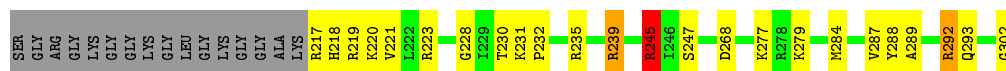
- Molecule 3: Histone H4

Chain B: 64% 13% 23%



- Molecule 3: Histone H4

Chain F: 61% 21% 16%



- Molecule 4: Histone H2A.1

Chain C: 67% 11% 17%



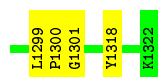
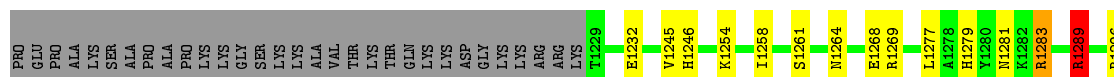
- Molecule 4: Histone H2A.1

Chain G: 63% 15% 19%



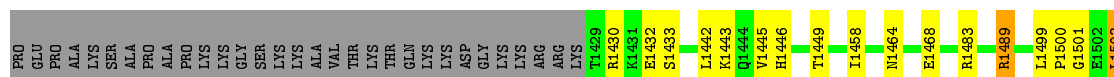
- Molecule 5: Histone H2B.1

Chain D: 60% 14% 25%



- Molecule 5: Histone H2B.1

Chain H: 62% 12% 25%



K1522

## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	107.05Å 109.66Å 183.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	80.00 – 2.30	Depositor
% Data completeness (in resolution range)	97.1 (80.00-2.30)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.214 , 0.253	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13158	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MN, DIB, IMT, BAL, PYB, ABU

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	I	0.50	0/3354	0.77	0/5175
1	J	0.52	0/3354	0.80	1/5175 (0.0%)
2	A	0.70	0/838	0.88	3/1122 (0.3%)
2	E	0.86	0/820	1.01	4/1099 (0.4%)
3	B	0.74	0/634	0.93	1/848 (0.1%)
3	F	0.86	0/702	0.97	1/937 (0.1%)
4	C	0.76	0/835	0.85	1/1127 (0.1%)
4	G	0.65	0/823	0.76	1/1110 (0.1%)
5	D	0.77	0/747	0.84	0/1004
5	H	0.68	0/747	0.79	0/1004
All	All	0.64	0/12854	0.83	12/18601 (0.1%)

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	I	0	4
1	J	0	3
2	A	0	2
2	E	0	2
3	B	0	2
3	F	0	2
4	C	0	1
4	G	0	2
5	D	0	1
All	All	0	19

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	245	ARG	NE-CZ-NH2	-8.32	116.14	120.30
2	E	728	ARG	NE-CZ-NH2	-7.55	116.53	120.30
2	E	672	ARG	NE-CZ-NH2	-7.51	116.55	120.30
3	B	36	ARG	NE-CZ-NH1	-6.62	116.99	120.30
4	G	1081	ARG	NE-CZ-NH2	-6.49	117.06	120.30
2	A	439	HIS	N-CA-C	6.45	128.41	111.00
2	A	531	ARG	NE-CZ-NH2	-6.43	117.08	120.30
2	A	472	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	J	227	DG	C5'-C4'-C3'	-5.66	103.92	114.10
2	E	653	ARG	NE-CZ-NH2	-5.23	117.68	120.30
2	E	652	ARG	CB-CG-CD	5.22	125.17	111.60
4	C	881	ARG	CB-CG-CD	5.15	124.99	111.60

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	472	ARG	Sidechain
2	A	531	ARG	Sidechain
3	B	39	ARG	Sidechain
3	B	45	ARG	Sidechain
4	C	829	ARG	Sidechain
5	D	1289	ARG	Sidechain
2	E	672	ARG	Sidechain
2	E	731	ARG	Sidechain
3	F	239	ARG	Sidechain
3	F	245	ARG	Sidechain
4	G	1081	ARG	Sidechain
4	G	1088	ARG	Sidechain
1	I	131	DG	Sidechain
1	I	135	DG	Sidechain
1	I	67	DA	Sidechain
1	I	77	DC	Sidechain
1	J	147	DA	Sidechain
1	J	214	DG	Sidechain
1	J	226	DT	Sidechain

## 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	I	2990	0	1651	132	0
1	J	2990	0	1651	132	0
2	A	826	0	871	16	0
2	E	808	0	846	23	0
3	B	627	0	663	9	0
3	F	694	0	742	18	0
4	C	825	0	884	23	0
4	G	813	0	872	32	0
5	D	736	0	760	15	0
5	H	736	0	760	15	0
6	E	1	0	0	0	0
6	I	6	0	0	0	0
6	J	4	0	0	0	0
7	I	178	0	137	64	0
7	J	267	0	205	100	0
8	A	68	0	0	1	0
8	B	46	0	0	3	0
8	C	79	0	0	3	0
8	D	44	0	0	4	0
8	E	84	0	0	5	0
8	F	75	0	0	2	0
8	G	66	0	0	1	0
8	H	40	0	0	0	0
8	I	88	0	0	6	0
8	J	67	0	0	5	0
All	All	13158	0	10042	450	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 20.

All (450) 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:J:259:DA:C4'	7:J:1905:ABU:HG1	1.75	1.17
7:J:1911:DIB:HE22	4:C:814:ALA:HB3	1.36	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:249:DG:N2	7:J:1929:PYB:HB1	1.68	1.08
1:J:174:DA:H2''	1:J:175:DA:H5''	1.38	1.05
1:J:259:DA:H4'	7:J:1905:ABU:HG1	1.39	1.03
1:I:93:DT:H2''	1:I:94:DG:H5''	1.43	0.99
1:I:112:DT:H4'	7:I:2025:ABU:HG1	1.47	0.95
1:I:125:DG:H1'	1:I:126:DA:H5'	1.49	0.94
1:J:249:DG:H21	7:J:1929:PYB:HB1	1.30	0.92
3:F:287:VAL:HG11	3:F:302:GLY:HA3	1.51	0.92
1:J:188:DA:N3	7:J:2006:PYB:HB1	1.86	0.90
1:J:287:DA:H5''	8:J:2055:HOH:O	1.75	0.85
8:I:2045:HOH:O	4:G:1075:LYS:HE2	1.78	0.84
1:J:259:DA:H4'	7:J:1905:ABU:CG	2.07	0.83
1:J:174:DA:C2'	1:J:175:DA:H5''	2.08	0.82
4:G:1017:ARG:HH22	4:G:1031:HIS:CD2	1.98	0.81
1:I:112:DT:C4'	7:I:2025:ABU:HG1	2.09	0.81
1:I:37:DT:H2''	1:I:38:DT:C6	2.15	0.81
2:E:664:LYS:HB2	8:E:802:HOH:O	1.80	0.81
1:J:194:DT:H4'	7:J:2011:DIB:HE13	1.63	0.80
7:J:1911:DIB:CE2	4:C:814:ALA:HB3	2.11	0.79
1:I:47:DC:H4'	7:J:1931:DIB:HG2	1.65	0.79
1:I:5:DA:H2''	1:I:6:DT:H5'	1.66	0.78
1:J:192:DG:N3	7:J:2010:BAL:HA2	1.99	0.78
1:I:126:DA:OP2	1:I:126:DA:H3'	1.85	0.77
1:J:149:DC:H2'	1:J:150:DA:C8	2.21	0.76
1:J:260:DC:O2	7:J:1907:PYB:N	2.16	0.76
2:A:528:ARG:HB2	2:A:535:ALA:OXT	1.85	0.76
1:J:147:DA:H2'	1:J:148:DT:H72	1.69	0.75
1:I:115:DA:C2	7:I:2029:PYB:HB1	2.22	0.74
1:I:125:DG:H2''	1:I:126:DA:OP2	1.85	0.74
1:I:68:DG:H1	1:J:225:DC:H42	1.35	0.74
2:A:448:LEU:HD11	3:B:44:LYS:HD2	1.69	0.74
1:J:249:DG:H21	7:J:1929:PYB:CB1	2.01	0.74
1:J:175:DA:H2''	1:J:176:DA:C8	2.23	0.74
2:E:668:GLN:O	2:E:672:ARG:HG2	1.88	0.74
7:I:2031:DIB:HA2	1:J:177:DG:N3	2.02	0.73
5:D:1264:ASN:O	5:D:1268:GLU:HG3	1.89	0.73
1:J:259:DA:O4'	7:J:1905:ABU:HG1	1.89	0.72
8:B:141:HOH:O	4:G:1099:ARG:HD3	1.89	0.72
1:I:111:DA:H4'	4:G:1042:ARG:HH11	1.54	0.72
1:I:133:DA:H2''	1:I:134:DG:H5'	1.72	0.72
1:I:71:DG:H21	7:I:1969:PYB:HB1	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:1017:ARG:HH22	4:G:1031:HIS:HD2	1.37	0.72
4:C:918:LYS:O	4:C:919:LYS:HB2	1.89	0.72
1:J:275:DC:C6	1:J:276:DT:H72	2.25	0.71
1:J:244:DG:H1'	1:J:245:DA:H5'	1.73	0.71
1:J:188:DA:H2''	1:J:189:DA:O5'	1.89	0.70
4:C:855:LEU:O	4:C:859:THR:HG23	1.92	0.70
3:B:95:ARG:HD3	8:B:142:HOH:O	1.92	0.69
1:I:125:DG:H1'	1:I:126:DA:C5'	2.22	0.69
7:I:1971:DIB:HG2	1:J:226:DT:H4'	1.75	0.69
1:J:227:DG:N7	8:J:2021:HOH:O	2.25	0.69
1:I:133:DA:H2''	1:I:134:DG:C5'	2.23	0.69
1:J:172:DC:H1'	1:J:173:DA:C5	2.28	0.69
1:I:31:DG:H2''	1:I:32:DT:H5'	1.74	0.69
1:I:9:DC:H42	1:J:284:DG:H1	1.41	0.69
2:A:534:ARG:O	2:A:534:ARG:HG2	1.93	0.68
1:J:259:DA:C4'	7:J:1905:ABU:CG	2.64	0.67
2:E:663:ARG:NH1	8:E:774:HOH:O	2.27	0.67
1:I:66:DC:H42	1:J:227:DG:H1	1.42	0.67
1:J:174:DA:H2''	1:J:175:DA:C5'	2.19	0.67
1:I:48:DT:H2''	1:I:49:DC:C5	2.30	0.67
3:B:30:THR:HB	3:B:32:PRO:HD2	1.78	0.66
2:E:664:LYS:HE2	8:E:801:HOH:O	1.95	0.66
4:C:832:ARG:NH2	5:D:1232:GLU:OE2	2.27	0.66
1:J:151:DA:H2''	1:J:152:DT:C5'	2.26	0.66
1:I:125:DG:C1'	1:I:126:DA:H5'	2.25	0.65
1:J:149:DC:H6	1:J:149:DC:H5''	1.60	0.65
5:H:1445:VAL:HG12	5:H:1446:HIS:CD2	2.32	0.65
1:J:253:DC:H4'	7:J:1924:PYB:CB	2.26	0.65
1:J:181:DA:H2''	1:J:182:DT:OP2	1.95	0.65
1:I:129:DC:H2'	1:I:130:DT:H71	1.79	0.65
1:I:37:DT:H2''	1:I:38:DT:C5	2.32	0.64
3:F:230:THR:HB	3:F:232:PRO:HD2	1.79	0.64
1:I:68:DG:H1	1:J:225:DC:N4	1.96	0.64
1:J:249:DG:H22	7:J:1929:PYB:HB1	1.62	0.64
1:I:60:DC:H42	1:J:233:DG:H1	1.44	0.64
1:I:93:DT:C2'	1:I:94:DG:H5''	2.22	0.64
1:I:100:DG:OP1	3:F:279:LYS:HE2	1.97	0.64
1:J:182:DT:H2''	1:J:183:DT:C5'	2.28	0.64
1:J:149:DC:H2''	1:J:150:DA:O5'	1.97	0.64
5:D:1281:ASN:O	5:D:1283:ARG:HD3	1.97	0.64
1:I:31:DG:N2	1:I:32:DT:C2	2.67	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:215:DC:OP1	2:E:642:ARG:NH1	2.26	0.63
1:I:119:DT:H2''	1:I:120:DT:C5	2.34	0.63
1:I:116:DC:H4'	7:I:2029:PYB:NG2	2.13	0.63
1:I:5:DA:H2''	1:I:6:DT:C5'	2.29	0.63
2:A:468:GLN:O	2:A:472:ARG:HG2	1.99	0.63
3:F:287:VAL:CG1	3:F:302:GLY:HA3	2.28	0.63
1:J:182:DT:H1'	1:J:183:DT:H5''	1.81	0.63
2:E:725:GLN:HB3	2:E:734:ARG:NH2	2.13	0.62
1:J:149:DC:C2'	1:J:150:DA:C8	2.83	0.62
1:I:22:DC:H2''	1:I:23:DT:O5'	2.00	0.62
7:I:1962:PYB:O	7:I:1963:PYB:HB	2.01	0.61
1:I:115:DA:H2	7:I:2029:PYB:HB1	1.66	0.61
1:J:247:DC:H5	8:J:2019:HOH:O	1.82	0.61
1:J:173:DA:H1'	1:J:174:DA:H5'	1.81	0.60
3:F:277:LYS:HE2	5:H:1489:ARG:NH2	2.16	0.60
1:J:193:DC:H2''	1:J:194:DT:H71	1.83	0.60
1:J:151:DA:H2''	1:J:152:DT:H5''	1.83	0.60
7:J:1927:PYB:O	7:J:1928:PYB:HB	2.01	0.60
1:I:52:DT:H2''	1:I:53:DC:C5	2.37	0.60
7:J:1902:PYB:O	7:J:1903:PYB:HB	2.02	0.59
1:I:71:DG:N2	7:I:1969:PYB:HB1	2.16	0.59
1:I:131:DG:H3'	4:G:1076:THR:HG22	1.84	0.59
5:D:1289:ARG:HD3	8:D:406:HOH:O	2.03	0.59
1:I:21:DT:H6	1:I:21:DT:H5'	1.67	0.59
1:J:184:DT:H2''	1:J:185:DG:N7	2.18	0.59
1:I:99:DA:H2''	1:I:100:DG:C5'	2.33	0.59
1:I:58:DG:H2''	1:I:59:DG:O5'	2.02	0.59
2:A:465:LEU:HB3	2:A:466:PRO:HD3	1.85	0.59
1:I:44:DC:H4'	7:J:1928:PYB:CG1	2.34	0.58
7:I:2022:PYB:O	7:I:2023:PYB:HB	2.03	0.58
5:H:1464:ASN:O	5:H:1468:GLU:HG3	2.03	0.58
1:I:32:DT:O4'	7:J:1901:IMT:NB1	2.37	0.58
1:I:35:DA:H2''	1:I:36:DT:OP2	2.02	0.57
1:J:260:DC:H2''	1:J:261:DA:C8	2.40	0.57
1:I:31:DG:H2''	1:I:32:DT:C5'	2.33	0.57
1:I:35:DA:H1'	1:I:36:DT:H5'	1.86	0.57
1:J:248:DA:N3	7:J:1930:BAL:HA2	2.19	0.57
1:J:170:DA:H2''	1:J:171:DC:OP2	2.05	0.57
1:J:247:DC:C5	8:J:2019:HOH:O	2.52	0.56
1:I:103:DG:N2	7:J:2009:PYB:HB1	2.19	0.56
1:J:183:DT:H2'	1:J:184:DT:H71	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:259:DA:C3'	7:J:1905:ABU:HG1	2.36	0.56
7:J:1905:ABU:OE2	7:J:1906:PYB:HB	2.06	0.56
1:I:99:DA:H2''	1:I:100:DG:H5'	1.88	0.56
7:I:1963:PYB:O	7:I:1964:PYB:HB	2.05	0.56
1:I:114:DC:O2	7:I:2028:PYB:HB1	2.05	0.56
4:C:855:LEU:O	4:C:859:THR:CG2	2.53	0.56
4:G:1063:LEU:HD13	5:H:1442:LEU:HB2	1.87	0.56
4:G:1016:THR:HG23	4:G:1019:SER:OG	2.06	0.56
3:F:289:ALA:O	3:F:293:GLN:HG3	2.06	0.56
7:J:2002:PYB:O	7:J:2003:PYB:HB	2.06	0.55
7:I:1968:PYB:HD1	7:I:1968:PYB:O	2.06	0.55
1:I:38:DT:H4'	4:C:842:ARG:HH21	1.71	0.55
3:F:230:THR:CB	3:F:232:PRO:HD2	2.36	0.55
7:I:1963:PYB:HD1	7:I:1963:PYB:O	2.07	0.55
7:I:1966:PYB:O	7:I:1967:PYB:HB	2.06	0.55
2:A:458:THR:CG2	4:G:1081:ARG:HD3	2.37	0.55
1:J:151:DA:C2'	1:J:152:DT:H5''	2.37	0.55
1:J:284:DG:OP2	1:J:284:DG:H2'	2.07	0.55
7:J:1906:PYB:O	7:J:1906:PYB:HD1	2.07	0.54
1:J:182:DT:C2'	1:J:183:DT:H5''	2.37	0.54
1:I:27:DA:H2''	1:I:28:DA:O5'	2.07	0.54
4:C:914:VAL:HG13	8:C:294:HOH:O	2.06	0.54
7:I:1961:IMT:O	7:I:1962:PYB:HB	2.08	0.54
1:J:197:DA:C5'	2:E:683:ARG:HD2	2.37	0.54
2:E:680:THR:O	2:E:681:ASP:HB2	2.08	0.54
7:J:1928:PYB:O	7:J:1928:PYB:HD1	2.07	0.54
1:I:74:DT:H2'	8:I:2085:HOH:O	2.08	0.54
1:I:7:DA:C2	1:J:287:DA:C2	2.96	0.54
7:I:1967:PYB:O	7:I:1968:PYB:HB	2.07	0.54
2:E:729:ARG:HD2	2:E:729:ARG:O	2.08	0.54
3:F:268:ASP:OD2	3:F:292:ARG:HD3	2.07	0.54
1:I:126:DA:H1'	1:I:127:DA:O4'	2.07	0.54
7:I:1968:PYB:O	7:I:1969:PYB:HB	2.06	0.54
3:B:31:LYS:HB3	3:B:32:PRO:HD3	1.89	0.53
3:F:231:LYS:O	3:F:235:ARG:HG2	2.08	0.53
7:I:1965:ABU:HG1	1:J:219:DA:O4'	2.09	0.53
7:J:1902:PYB:O	7:J:1903:PYB:CB	2.56	0.53
7:I:2022:PYB:HD1	7:I:2022:PYB:O	2.07	0.53
1:I:115:DA:N3	7:I:2029:PYB:HB1	2.23	0.53
1:J:260:DC:O4'	7:J:1906:PYB:CB1	2.56	0.53
7:J:1922:PYB:HD1	7:J:1922:PYB:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:1928:PYB:O	7:J:1929:PYB:HB	2.07	0.53
7:J:2008:PYB:O	7:J:2009:PYB:HB	2.08	0.53
1:J:147:DA:H2'	1:J:148:DT:C7	2.37	0.53
1:J:187:DA:H1'	7:J:2005:ABU:HG1	1.91	0.52
7:J:1902:PYB:O	7:J:1902:PYB:HD1	2.09	0.52
1:J:180:DT:H2''	1:J:181:DA:C8	2.44	0.52
7:I:1967:PYB:O	7:I:1967:PYB:HD1	2.09	0.52
7:J:1911:DIB:HE22	4:C:814:ALA:CB	2.26	0.52
7:J:1901:IMT:O	7:J:1902:PYB:HB	2.09	0.52
1:J:197:DA:H5''	2:E:683:ARG:CD	2.40	0.52
7:J:2003:PYB:O	7:J:2004:PYB:HB	2.10	0.52
1:I:72:DA:O4'	7:I:1961:IMT:CA	2.58	0.52
7:J:1928:PYB:O	7:J:1929:PYB:CB	2.57	0.52
1:I:117:DT:O4'	7:I:2030:BAL:HA1	2.10	0.52
4:C:918:LYS:HE2	8:C:626:HOH:O	2.10	0.52
7:J:2002:PYB:O	7:J:2002:PYB:HD1	2.10	0.51
1:J:182:DT:H2''	1:J:183:DT:H5'	1.90	0.51
3:F:277:LYS:HE2	5:H:1489:ARG:HH22	1.75	0.51
7:J:1927:PYB:O	7:J:1928:PYB:CB	2.57	0.51
1:J:151:DA:H2''	1:J:152:DT:H5'	1.93	0.51
1:J:255:DA:H2''	1:J:256:DA:OP2	2.09	0.51
7:J:2003:PYB:O	7:J:2003:PYB:HD1	2.10	0.51
4:C:837:GLY:HA3	4:C:839:TYR:CE2	2.46	0.51
1:J:151:DA:OP2	2:A:436:LYS:HE2	2.11	0.51
1:J:263:DT:H2''	1:J:264:DT:H72	1.93	0.51
1:I:83:DA:H5''	2:E:640:ARG:HD3	1.92	0.51
1:J:230:DC:H2''	1:J:231:DA:C8	2.46	0.51
7:J:1908:PYB:HD1	7:J:1908:PYB:O	2.11	0.51
7:I:2022:PYB:O	7:I:2023:PYB:CB	2.54	0.51
1:J:169:DT:C2	1:J:170:DA:C6	2.99	0.51
1:J:268:DG:H5''	1:J:268:DG:H8	1.75	0.51
7:I:2023:PYB:HD1	7:I:2023:PYB:O	2.11	0.50
7:I:2027:PYB:O	7:I:2028:PYB:HB	2.10	0.50
1:J:249:DG:H2''	1:J:250:DT:H71	1.93	0.50
4:G:1064:GLU:OE1	5:H:1445:VAL:HG13	2.11	0.50
7:J:1923:PYB:HD1	7:J:1923:PYB:O	2.11	0.50
4:C:914:VAL:HG11	8:E:817:HOH:O	2.11	0.50
1:J:241:DA:H2''	1:J:242:DT:O5'	2.12	0.50
7:J:1907:PYB:O	7:J:1907:PYB:HD1	2.10	0.50
1:I:138:DG:H2''	1:I:139:DA:OP2	2.11	0.50
1:I:116:DC:H4'	7:I:2029:PYB:CD	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:172:DC:H1'	1:J:173:DA:N7	2.27	0.50
1:I:48:DT:H2''	1:I:49:DC:H5	1.77	0.50
7:I:1963:PYB:O	7:I:1964:PYB:CB	2.59	0.50
1:J:197:DA:H5''	2:E:683:ARG:HD2	1.93	0.50
7:I:1971:DIB:HA2	1:J:224:DG:H21	1.76	0.50
2:E:728:ARG:HD2	2:E:733:GLU:OE1	2.12	0.50
7:J:1927:PYB:HD1	7:J:1927:PYB:O	2.12	0.49
7:J:2007:PYB:O	7:J:2008:PYB:HB	2.12	0.49
3:B:24:ASP:OD1	3:B:25:ASN:N	2.45	0.49
2:E:665:LEU:HB3	2:E:666:PRO:HD3	1.94	0.49
1:J:182:DT:H2''	1:J:183:DT:H5''	1.91	0.49
7:I:1968:PYB:O	7:I:1969:PYB:CB	2.59	0.49
1:I:24:DA:H2''	1:I:25:DC:OP2	2.11	0.49
1:I:130:DT:C4	1:J:162:DC:N4	2.80	0.49
7:I:2021:IMT:O	7:I:2022:PYB:HB	2.13	0.49
2:A:438:PRO:HD2	2:A:439:HIS:H	1.78	0.49
1:I:83:DA:C5'	2:E:640:ARG:HD3	2.43	0.49
7:J:1903:PYB:O	7:J:1904:PYB:HB	2.13	0.49
1:J:187:DA:N3	7:J:2005:ABU:HB1	2.28	0.49
1:J:275:DC:N1	1:J:276:DT:H72	2.28	0.49
1:I:47:DC:O3'	7:J:1931:DIB:HE13	2.13	0.48
7:I:1962:PYB:HD1	7:I:1962:PYB:O	2.13	0.48
4:C:869:ALA:O	4:C:873:ASN:ND2	2.41	0.48
1:J:259:DA:C1'	7:J:1905:ABU:HG1	2.42	0.48
1:I:111:DA:C4'	4:G:1042:ARG:HH11	2.24	0.48
7:J:2002:PYB:O	7:J:2003:PYB:CB	2.60	0.48
4:G:1112:GLN:OE1	8:G:643:HOH:O	2.20	0.48
4:C:867:GLY:HA3	5:D:1246:HIS:CD2	2.48	0.48
7:I:2028:PYB:O	7:I:2028:PYB:HD1	2.13	0.48
4:G:1016:THR:HG23	4:G:1019:SER:CB	2.43	0.48
7:J:1903:PYB:HD1	7:J:1903:PYB:O	2.13	0.48
1:I:114:DC:H42	1:J:179:DG:H1	1.61	0.48
1:I:21:DT:C6	1:I:21:DT:H5'	2.48	0.48
1:I:45:DT:O2	7:J:1929:PYB:C	2.62	0.48
3:B:30:THR:CB	3:B:32:PRO:HD2	2.42	0.48
7:J:2008:PYB:HD1	7:J:2008:PYB:O	2.13	0.48
1:I:8:DT:OP1	2:E:649:ARG:HD2	2.14	0.48
1:I:35:DA:H1'	1:I:36:DT:C5'	2.44	0.48
1:I:38:DT:C4	1:I:39:DG:C6	3.02	0.48
1:I:5:DA:H1'	1:I:6:DT:H5''	1.95	0.48
1:J:269:DT:OP1	4:C:829:ARG:NH2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:47:DC:N4	1:J:245:DA:N6	2.62	0.47
1:I:124:DA:H2''	1:I:125:DG:N7	2.29	0.47
1:I:128:DT:H1'	1:I:129:DC:H5'	1.97	0.47
1:J:194:DT:H4'	7:J:2011:DIB:CE1	2.39	0.47
1:J:207:DA:H5''	8:F:314:HOH:O	2.13	0.47
7:J:2007:PYB:O	7:J:2007:PYB:HD1	2.14	0.47
7:J:2001:IMT:HD2	7:J:2009:PYB:HD2	1.95	0.47
2:A:444:GLY:O	2:A:448:LEU:HD13	2.14	0.47
3:F:231:LYS:N	3:F:232:PRO:CD	2.78	0.47
7:I:1964:PYB:O	7:I:1964:PYB:HD1	2.15	0.47
1:I:33:DG:H21	7:J:1903:PYB:H	1.61	0.47
7:J:1923:PYB:O	7:J:1924:PYB:HB	2.13	0.47
7:J:1926:PYB:O	7:J:1927:PYB:HB	2.15	0.47
1:I:23:DT:O2	1:J:271:DG:N2	2.48	0.47
1:J:260:DC:O4'	7:J:1906:PYB:CA	2.63	0.47
1:J:261:DA:H2''	1:J:262:DC:H5'	1.97	0.47
1:I:131:DG:H3'	4:G:1076:THR:CG2	2.45	0.47
1:J:263:DT:H2''	1:J:264:DT:C7	2.45	0.47
3:F:220:LYS:HG2	3:F:221:VAL:N	2.30	0.47
1:I:77:DC:H42	1:J:216:DG:H1	1.63	0.47
1:J:245:DA:H2''	1:J:246:DG:OP2	2.15	0.47
7:I:2023:PYB:O	7:I:2024:PYB:HB	2.14	0.47
1:J:148:DT:H2''	1:J:149:DC:O5'	2.15	0.47
7:I:2025:ABU:OE2	7:I:2026:PYB:HB	2.15	0.47
3:F:231:LYS:HB3	3:F:232:PRO:HD3	1.97	0.47
1:I:111:DA:H4'	4:G:1042:ARG:NH1	2.27	0.47
4:G:1079:ILE:HG12	4:G:1082:HIS:CE1	2.50	0.47
1:I:116:DC:H4'	7:I:2029:PYB:HD3	1.97	0.46
7:I:2026:PYB:HD1	7:I:2026:PYB:O	2.15	0.46
1:I:112:DT:H5'	4:G:1042:ARG:HD3	1.96	0.46
4:G:1064:GLU:HA	5:H:1445:VAL:HG11	1.95	0.46
1:I:45:DT:H2''	1:I:46:DG:C8	2.50	0.46
1:I:44:DC:H4'	7:J:1928:PYB:NG2	2.29	0.46
7:J:1924:PYB:O	7:J:1924:PYB:HD1	2.16	0.46
3:B:24:ASP:CG	3:B:25:ASN:H	2.19	0.46
1:I:32:DT:O4'	7:J:1901:IMT:CA	2.64	0.46
1:J:259:DA:H2''	1:J:260:DC:C6	2.51	0.46
1:J:259:DA:O4'	7:J:1905:ABU:CG	2.61	0.46
1:J:149:DC:H2'	1:J:150:DA:H8	1.77	0.46
7:I:1966:PYB:O	7:I:1967:PYB:CB	2.60	0.46
7:J:1908:PYB:O	7:J:1909:PYB:HB	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:94:DG:H2''	1:I:95:DA:O5'	2.15	0.46
7:J:2008:PYB:O	7:J:2009:PYB:CB	2.62	0.46
4:G:1076:THR:O	5:H:1449:THR:HG23	2.15	0.46
2:E:729:ARG:HD2	2:E:729:ARG:C	2.35	0.46
4:G:1079:ILE:HB	4:G:1080:PRO:CD	2.46	0.46
7:I:2027:PYB:O	7:I:2028:PYB:CB	2.63	0.46
7:J:1921:IMT:O	7:J:1922:PYB:HB	2.15	0.46
1:I:27:DA:H5''	8:I:2086:HOH:O	2.16	0.46
1:I:127:DA:N3	1:I:128:DT:C2	2.83	0.46
1:I:72:DA:O4'	7:I:1961:IMT:NB1	2.49	0.46
1:J:191:DT:H5'	7:J:2008:PYB:C	2.46	0.46
1:I:125:DG:C6	1:I:126:DA:C5	3.05	0.45
1:I:133:DA:C2'	1:I:134:DG:H5''	2.46	0.45
1:J:257:DA:C8	1:J:258:DT:H72	2.52	0.45
5:D:1300:PRO:HG3	8:D:476:HOH:O	2.16	0.45
7:I:2028:PYB:O	7:I:2029:PYB:HB	2.16	0.45
1:I:127:DA:C4	1:I:128:DT:C4	3.03	0.45
1:J:271:DG:H2''	1:J:272:DA:OP2	2.16	0.45
5:D:1279:HIS:HB3	8:D:422:HOH:O	2.15	0.45
4:G:1087:VAL:HG12	4:G:1088:ARG:HD3	1.97	0.45
7:J:1907:PYB:O	7:J:1908:PYB:HB	2.16	0.45
3:F:287:VAL:HG11	3:F:302:GLY:CA	2.35	0.45
1:I:47:DC:C3'	7:J:1931:DIB:HE13	2.47	0.45
1:I:127:DA:C2	1:I:128:DT:N3	2.85	0.45
7:J:1923:PYB:O	7:J:1924:PYB:CB	2.64	0.45
4:G:1037:GLY:O	4:G:1038:ASN:HB2	2.15	0.45
1:I:66:DC:N4	1:J:227:DG:H1	2.10	0.45
7:I:1961:IMT:O	7:I:1961:IMT:HD1	2.17	0.45
1:J:268:DG:H5''	1:J:268:DG:C8	2.52	0.45
5:D:1245:VAL:HG23	5:D:1246:HIS:CD2	2.52	0.45
1:I:111:DA:C2'	1:I:112:DT:H71	2.46	0.45
4:G:1016:THR:HG23	4:G:1019:SER:HG	1.81	0.45
1:J:197:DA:H5'	2:E:683:ARG:HD2	1.99	0.45
2:A:437:LYS:HA	2:A:438:PRO:HD3	1.53	0.45
8:B:120:HOH:O	5:D:1296:ARG:HD3	2.16	0.45
5:D:1299:LEU:HA	5:D:1300:PRO:HD3	1.77	0.45
5:H:1443:LYS:HA	5:H:1443:LYS:HD3	1.57	0.45
7:J:2001:IMT:O	7:J:2002:PYB:HB	2.17	0.44
7:J:2003:PYB:O	7:J:2004:PYB:CB	2.63	0.44
1:I:21:DT:C2	1:J:273:DA:C2	3.05	0.44
7:J:1907:PYB:O	7:J:1908:PYB:CB	2.63	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:192:DG:H2''	1:J:193:DC:O5'	2.18	0.44
2:E:663:ARG:CD	8:E:774:HOH:O	2.65	0.44
4:G:1092:GLU:HB3	5:H:1503:LEU:HD22	1.98	0.44
7:I:2021:IMT:CA	1:J:179:DG:O4'	2.66	0.44
7:I:1961:IMT:O	7:I:1962:PYB:CB	2.61	0.44
1:I:36:DT:H2''	1:I:37:DT:H5''	1.98	0.44
1:J:165:DA:C2	1:J:166:DT:N3	2.85	0.44
5:D:1254:LYS:O	5:D:1258:ILE:HG12	2.17	0.44
1:J:147:DA:C2'	1:J:148:DT:H72	2.43	0.44
7:J:1922:PYB:O	7:J:1923:PYB:CB	2.65	0.44
1:I:127:DA:H2''	1:I:128:DT:C6	2.52	0.44
7:J:2004:PYB:O	7:J:2004:PYB:HD1	2.18	0.44
1:J:169:DT:H2''	1:J:170:DA:C8	2.53	0.44
1:I:46:DG:H2''	1:I:47:DC:C5	2.53	0.44
3:B:24:ASP:CG	3:B:25:ASN:N	2.71	0.44
7:J:1905:ABU:OE2	7:J:1906:PYB:CB	2.60	0.44
1:I:46:DG:H1'	1:I:47:DC:C5	2.52	0.44
7:I:1962:PYB:O	7:I:1963:PYB:CB	2.56	0.44
2:A:438:PRO:CD	2:A:439:HIS:H	2.31	0.44
7:J:1904:PYB:HD1	7:J:1904:PYB:O	2.18	0.43
7:I:1969:PYB:O	7:I:1969:PYB:HD1	2.17	0.43
1:I:75:DT:H4'	7:I:1964:PYB:CB	2.48	0.43
7:J:1901:IMT:O	7:J:1902:PYB:CB	2.63	0.43
7:J:2007:PYB:O	7:J:2008:PYB:CB	2.65	0.43
7:J:2009:PYB:O	7:J:2009:PYB:HD1	2.17	0.43
4:G:1032:ARG:HH22	5:H:1432:GLU:CD	2.21	0.43
7:J:2006:PYB:O	7:J:2007:PYB:HB	2.18	0.43
1:J:177:DG:OP1	4:G:1017:ARG:HG3	2.19	0.43
2:A:437:LYS:H	2:A:437:LYS:HD2	1.82	0.43
5:D:1269:ARG:HD3	8:D:275:HOH:O	2.16	0.43
1:J:173:DA:C1'	1:J:174:DA:H5'	2.47	0.43
1:J:182:DT:C1'	1:J:183:DT:H5''	2.47	0.43
1:I:124:DA:H2''	1:I:125:DG:C8	2.54	0.43
1:I:102:DA:H2''	1:I:103:DG:C8	2.54	0.43
7:I:1966:PYB:HD1	7:I:1966:PYB:O	2.19	0.43
1:I:59:DG:H2''	1:I:60:DC:C6	2.53	0.43
1:I:120:DT:H2''	1:I:121:DG:C8	2.54	0.43
1:J:267:DG:H2''	1:J:268:DG:O5'	2.18	0.43
3:F:228:GLY:HA3	8:F:326:HOH:O	2.18	0.43
7:J:1903:PYB:O	7:J:1904:PYB:CB	2.64	0.43
2:A:524:ILE:O	2:A:528:ARG:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:1967:PYB:O	7:I:1968:PYB:CB	2.59	0.43
4:G:1016:THR:HG23	4:G:1019:SER:HB3	2.00	0.43
4:C:817:ARG:HD2	5:D:1318:TYR:OH	2.18	0.43
1:I:38:DT:H4'	4:C:842:ARG:NH2	2.34	0.43
4:G:1017:ARG:NH2	4:G:1031:HIS:HD2	2.12	0.43
2:A:438:PRO:HD2	2:A:439:HIS:N	2.34	0.43
1:I:61:DA:N6	8:I:2076:HOH:O	2.51	0.43
1:I:37:DT:C2'	1:I:38:DT:C5	3.00	0.43
1:I:100:DG:H2''	1:I:101:DC:C6	2.54	0.43
8:J:2027:HOH:O	4:C:875:LYS:HE2	2.18	0.43
7:I:2023:PYB:O	7:I:2024:PYB:CB	2.66	0.43
1:J:183:DT:H2''	1:J:184:DT:C6	2.53	0.43
7:I:2031:DIB:HA2	1:J:177:DG:H21	1.83	0.43
1:I:28:DA:H1'	1:I:29:DA:C8	2.54	0.43
8:A:582:HOH:O	2:E:722:LYS:HE3	2.19	0.43
4:G:1032:ARG:NH2	5:H:1432:GLU:OE2	2.52	0.42
1:J:174:DA:H4'	5:H:1430:ARG:HD3	2.01	0.42
7:I:2028:PYB:O	7:I:2029:PYB:CB	2.67	0.42
1:J:260:DC:H2''	1:J:261:DA:H8	1.85	0.42
4:G:1016:THR:O	4:G:1020:ARG:HG2	2.19	0.42
5:H:1499:LEU:HA	5:H:1500:PRO:HD3	1.81	0.42
7:I:2024:PYB:CD	1:J:183:DT:H4'	2.50	0.42
1:I:101:DC:H2''	1:I:102:DA:C8	2.54	0.42
1:I:21:DT:O2	1:J:273:DA:C2	2.73	0.42
1:I:116:DC:H4'	7:I:2029:PYB:CB	2.49	0.42
5:D:1261:SER:OG	3:F:302:GLY:O	2.29	0.42
7:I:2030:BAL:HB3	1:J:178:DT:O2	2.20	0.42
1:I:99:DA:H2''	1:I:100:DG:H5''	2.01	0.42
1:I:123:DT:H2''	1:I:124:DA:C8	2.55	0.42
4:G:1102:ILE:HG23	5:H:1458:ILE:HD13	2.02	0.42
1:I:99:DA:H1'	1:I:100:DG:H5''	2.02	0.42
7:I:2024:PYB:O	1:J:183:DT:H4'	2.20	0.41
1:I:99:DA:C2'	1:I:100:DG:H5''	2.49	0.41
4:C:881:ARG:HB2	2:E:658:THR:HG21	2.01	0.41
1:I:36:DT:H4'	7:J:1904:PYB:C	2.49	0.41
1:J:259:DA:O4'	7:J:1905:ABU:CB	2.68	0.41
1:I:44:DC:H3'	8:I:2109:HOH:O	2.21	0.41
1:I:45:DT:H5'	7:J:1928:PYB:O	2.19	0.41
1:J:151:DA:H1'	1:J:152:DT:H5''	2.02	0.41
4:G:1079:ILE:HB	4:G:1080:PRO:HD2	2.02	0.41
7:J:1901:IMT:HD1	7:J:1901:IMT:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:1906:PYB:O	7:J:1907:PYB:HB	2.20	0.41
7:I:2021:IMT:O	7:I:2022:PYB:CB	2.66	0.41
1:I:133:DA:H1'	1:I:134:DG:H5''	2.03	0.41
1:I:106:DT:H4'	7:J:2003:PYB:CG1	2.51	0.41
1:I:21:DT:C2	1:J:273:DA:H2	2.38	0.41
2:E:650:GLU:HB3	3:F:239:ARG:HG3	2.02	0.41
7:I:2029:PYB:HD1	7:I:2029:PYB:O	2.20	0.41
7:J:2005:ABU:OE2	7:J:2006:PYB:HB	2.20	0.41
2:A:533:GLU:O	2:A:534:ARG:HB3	2.19	0.41
1:I:40:DG:OP2	5:D:1283:ARG:NH2	2.53	0.41
1:I:91:DT:H5''	2:E:663:ARG:NH2	2.36	0.41
2:A:468:GLN:OE1	2:A:472:ARG:NH2	2.53	0.41
1:J:259:DA:OP1	4:C:842:ARG:HA	2.20	0.41
1:I:36:DT:C2'	1:I:37:DT:H5''	2.50	0.41
1:I:98:DG:H1'	1:I:99:DA:N7	2.36	0.41
7:J:2006:PYB:HD1	7:J:2006:PYB:O	2.20	0.41
1:I:50:DC:H2''	1:I:51:DA:C8	2.55	0.41
3:B:84:MET:HE1	3:B:102:GLY:HA3	2.03	0.41
1:J:262:DC:O4'	7:J:1908:PYB:CB1	2.69	0.41
7:J:1926:PYB:O	7:J:1927:PYB:CB	2.67	0.41
7:I:2031:DIB:HE22	1:J:177:DG:O4'	2.21	0.40
1:J:194:DT:H2''	1:J:195:DC:C6	2.56	0.40
1:I:141:DA:C2	1:J:153:DA:C2	3.09	0.40
1:J:187:DA:C6	1:J:188:DA:N6	2.89	0.40
4:C:829:ARG:HG3	4:C:832:ARG:HH12	1.86	0.40
4:C:879:ILE:HB	4:C:880:PRO:CD	2.52	0.40
7:J:1908:PYB:O	7:J:1909:PYB:CB	2.68	0.40
7:I:2026:PYB:O	7:I:2027:PYB:HB	2.20	0.40
1:J:188:DA:C2'	1:J:189:DA:O5'	2.66	0.40
7:J:2001:IMT:O	7:J:2001:IMT:HD1	2.21	0.40
1:I:70:DG:H21	7:I:1970:BAL:HA2	1.86	0.40
4:C:871:ARG:NH2	8:C:638:HOH:O	2.53	0.40
1:I:106:DT:H4'	7:J:2003:PYB:NG2	2.36	0.40
7:J:1921:IMT:O	7:J:1922:PYB:CB	2.68	0.40
1:I:138:DG:H4'	8:I:2105:HOH:O	2.21	0.40
1:J:262:DC:O4'	7:J:1908:PYB:CA	2.69	0.40
1:J:184:DT:H2''	1:J:185:DG:C8	2.56	0.40
3:F:284:MET:HE3	3:F:288:TYR:CZ	2.56	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	98/135 (73%)	95 (97%)	1 (1%)	2 (2%)	9	7
2	E	96/135 (71%)	96 (100%)	0	0	100	100
3	B	77/102 (76%)	76 (99%)	1 (1%)	0	100	100
3	F	84/102 (82%)	82 (98%)	1 (1%)	1 (1%)	16	16
4	C	105/129 (81%)	103 (98%)	1 (1%)	1 (1%)	19	21
4	G	103/129 (80%)	100 (97%)	3 (3%)	0	100	100
5	D	92/125 (74%)	90 (98%)	1 (1%)	1 (1%)	17	18
5	H	92/125 (74%)	90 (98%)	1 (1%)	1 (1%)	17	18
All	All	747/982 (76%)	732 (98%)	9 (1%)	6 (1%)	24	27

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	438	PRO
2	A	439	HIS
5	H	1501	GLY
4	C	919	LYS
5	D	1301	GLY
3	F	218	HIS

### 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	
2	A	87/111 (78%)	79 (91%)	8 (9%)	11	13
2	E	85/111 (77%)	78 (92%)	7 (8%)	14	17
3	B	64/78 (82%)	61 (95%)	3 (5%)	32	43
3	F	71/78 (91%)	65 (92%)	6 (8%)	13	16
4	C	85/100 (85%)	80 (94%)	5 (6%)	24	32
4	G	84/100 (84%)	80 (95%)	4 (5%)	31	42
5	D	80/105 (76%)	77 (96%)	3 (4%)	40	54
5	H	80/105 (76%)	76 (95%)	4 (5%)	30	41
All	All	636/788 (81%)	596 (94%)	40 (6%)	22	29

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	437	LYS
2	A	442	ARG
2	A	453	ARG
2	A	459	GLU
2	A	468	GLN
2	A	472	ARG
2	A	528	ARG
2	A	529	ARG
3	B	45	ARG
3	B	47	SER
3	B	92	ARG
4	C	829	ARG
4	C	832	ARG
4	C	859	THR
4	C	881	ARG
4	C	918	LYS
5	D	1277	LEU
5	D	1283	ARG
5	D	1289	ARG
2	E	642	ARG
2	E	653	ARG
2	E	656	LYS
2	E	659	GLU
2	E	683	ARG
2	E	726	LEU
2	E	729	ARG
3	F	217	ARG

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Mol	Chain	Res	Type
3	F	219	ARG
3	F	223	ARG
3	F	245	ARG
3	F	247	SER
3	F	292	ARG
4	G	1016	THR
4	G	1020	ARG
4	G	1042	ARG
4	G	1071	ARG
5	H	1433	SER
5	H	1483	ARG
5	H	1489	ARG
5	H	1503	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
4	C	838	ASN
5	D	1264	ASN
5	D	1292	GLN
4	G	1031	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 66 ligands modelled in this entry, 11 are monoatomic - leaving 55 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
7	IMT	I	1961	7	6,8,10	1.27	1 (16%)	5,10,14	2.41	3 (60%)
7	PYB	I	1962	7	8,9,10	1.54	2 (25%)	4,12,14	4.01	2 (50%)
7	PYB	I	1963	7	8,9,10	1.45	2 (25%)	4,12,14	3.92	2 (50%)
7	PYB	I	1964	7	8,9,10	1.76	3 (37%)	4,12,14	3.51	2 (50%)
7	ABU	I	1965	7	5,5,6	1.53	1 (20%)	4,4,6	0.40	0
7	PYB	I	1966	7	8,9,10	1.75	2 (25%)	4,12,14	3.77	2 (50%)
7	PYB	I	1967	7	8,9,10	1.46	2 (25%)	4,12,14	3.80	2 (50%)
7	PYB	I	1968	7	8,9,10	1.61	2 (25%)	4,12,14	3.90	2 (50%)
7	PYB	I	1969	7	8,9,10	1.75	3 (37%)	4,12,14	3.48	2 (50%)
7	BAL	I	1970	7	3,4,5	0.72	0	0,3,5	0.00	-
7	DIB	I	1971	7	6,6,6	0.71	0	6,6,6	0.45	0
7	IMT	I	2021	7	6,8,10	1.17	1 (16%)	5,10,14	2.45	3 (60%)
7	PYB	I	2022	7	8,9,10	1.42	2 (25%)	4,12,14	3.93	2 (50%)
7	PYB	I	2023	7	8,9,10	1.41	2 (25%)	4,12,14	3.70	2 (50%)
7	PYB	I	2024	7	8,9,10	1.49	1 (12%)	4,12,14	3.48	2 (50%)
7	ABU	I	2025	7	5,5,6	1.53	1 (20%)	4,4,6	0.47	0
7	PYB	I	2026	7	8,9,10	1.46	1 (12%)	4,12,14	3.75	2 (50%)
7	PYB	I	2027	7	8,9,10	1.56	2 (25%)	4,12,14	3.86	2 (50%)
7	PYB	I	2028	7	8,9,10	1.52	2 (25%)	4,12,14	3.71	2 (50%)
7	PYB	I	2029	7	8,9,10	1.62	1 (12%)	4,12,14	3.51	2 (50%)
7	BAL	I	2030	7	3,4,5	0.91	0	0,3,5	0.00	-
7	DIB	I	2031	7	6,6,6	0.69	0	6,6,6	0.44	0
7	IMT	J	1901	7	6,8,10	1.24	1 (16%)	5,10,14	2.45	2 (40%)
7	PYB	J	1902	7	8,9,10	1.61	2 (25%)	4,12,14	3.86	2 (50%)
7	PYB	J	1903	7	8,9,10	1.63	2 (25%)	4,12,14	3.88	2 (50%)
7	PYB	J	1904	7	8,9,10	1.80	3 (37%)	4,12,14	3.46	2 (50%)
7	ABU	J	1905	7	5,5,6	1.57	1 (20%)	4,4,6	0.45	0
7	PYB	J	1906	7	8,9,10	1.55	2 (25%)	4,12,14	3.96	2 (50%)
7	PYB	J	1907	7	8,9,10	1.71	2 (25%)	4,12,14	3.80	2 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	PYB	J	1908	7	8,9,10	1.54	2 (25%)	4,12,14	3.74	2 (50%)
7	PYB	J	1909	7	8,9,10	1.74	2 (25%)	4,12,14	3.57	2 (50%)
7	BAL	J	1910	7	3,4,5	0.73	0	0,3,5	0.00	-
7	DIB	J	1911	7	6,6,6	0.63	0	6,6,6	0.35	0
7	IMT	J	1921	7	6,8,10	1.48	1 (16%)	5,10,14	2.49	3 (60%)
7	PYB	J	1922	7	8,9,10	1.47	2 (25%)	4,12,14	3.89	2 (50%)
7	PYB	J	1923	7	8,9,10	1.45	2 (25%)	4,12,14	3.82	2 (50%)
7	PYB	J	1924	7	8,9,10	1.49	1 (12%)	4,12,14	3.65	2 (50%)
7	ABU	J	1925	7	5,5,6	1.54	1 (20%)	4,4,6	0.48	0
7	PYB	J	1926	7	8,9,10	1.66	2 (25%)	4,12,14	3.65	2 (50%)
7	PYB	J	1927	7	8,9,10	1.46	2 (25%)	4,12,14	3.87	2 (50%)
7	PYB	J	1928	7	8,9,10	1.20	0	4,12,14	4.02	2 (50%)
7	PYB	J	1929	7	8,9,10	1.47	1 (12%)	4,12,14	3.61	2 (50%)
7	BAL	J	1930	7	3,4,5	0.71	0	0,3,5	0.00	-
7	DIB	J	1931	7	6,6,6	0.72	0	6,6,6	0.40	0
7	IMT	J	2001	7	6,8,10	1.26	1 (16%)	5,10,14	2.51	3 (60%)
7	PYB	J	2002	7	8,9,10	1.38	1 (12%)	4,12,14	3.87	2 (50%)
7	PYB	J	2003	7	8,9,10	1.48	2 (25%)	4,12,14	3.79	2 (50%)
7	PYB	J	2004	7	8,9,10	1.60	1 (12%)	4,12,14	3.46	2 (50%)
7	ABU	J	2005	7	5,5,6	1.55	1 (20%)	4,4,6	0.44	0
7	PYB	J	2006	7	8,9,10	1.55	1 (12%)	4,12,14	3.67	2 (50%)
7	PYB	J	2007	7	8,9,10	1.60	2 (25%)	4,12,14	3.68	2 (50%)
7	PYB	J	2008	7	8,9,10	1.51	2 (25%)	4,12,14	3.81	2 (50%)
7	PYB	J	2009	7	8,9,10	1.60	2 (25%)	4,12,14	3.74	2 (50%)
7	BAL	J	2010	7	3,4,5	1.01	0	0,3,5	0.00	-
7	DIB	J	2011	7	6,6,6	0.68	0	6,6,6	0.58	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
7	IMT	I	1961	7	-	0/0/2/4	0/1/1/1
7	PYB	I	1962	7	-	0/0/2/4	0/1/1/1
7	PYB	I	1963	7	-	0/0/2/4	0/1/1/1
7	PYB	I	1964	7	-	0/0/2/4	0/1/1/1
7	ABU	I	1965	7	-	0/3/3/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PYB	I	1966	7	-	0/0/2/4	0/1/1/1
7	PYB	I	1967	7	-	0/0/2/4	0/1/1/1
7	PYB	I	1968	7	-	0/0/2/4	0/1/1/1
7	PYB	I	1969	7	-	0/0/2/4	0/1/1/1
7	BAL	I	1970	7	-	0/1/2/3	0/0/0/0
7	DIB	I	1971	7	-	0/4/4/4	0/0/0/0
7	IMT	I	2021	7	-	0/0/2/4	0/1/1/1
7	PYB	I	2022	7	-	0/0/2/4	0/1/1/1
7	PYB	I	2023	7	-	0/0/2/4	0/1/1/1
7	PYB	I	2024	7	-	0/0/2/4	0/1/1/1
7	ABU	I	2025	7	-	0/3/3/4	0/0/0/0
7	PYB	I	2026	7	-	0/0/2/4	0/1/1/1
7	PYB	I	2027	7	-	0/0/2/4	0/1/1/1
7	PYB	I	2028	7	-	0/0/2/4	0/1/1/1
7	PYB	I	2029	7	-	0/0/2/4	0/1/1/1
7	BAL	I	2030	7	-	0/1/2/3	0/0/0/0
7	DIB	I	2031	7	-	0/4/4/4	0/0/0/0
7	IMT	J	1901	7	-	0/0/2/4	0/1/1/1
7	PYB	J	1902	7	-	0/0/2/4	0/1/1/1
7	PYB	J	1903	7	-	0/0/2/4	0/1/1/1
7	PYB	J	1904	7	-	0/0/2/4	0/1/1/1
7	ABU	J	1905	7	-	0/3/3/4	0/0/0/0
7	PYB	J	1906	7	-	0/0/2/4	0/1/1/1
7	PYB	J	1907	7	-	0/0/2/4	0/1/1/1
7	PYB	J	1908	7	-	0/0/2/4	0/1/1/1
7	PYB	J	1909	7	-	0/0/2/4	0/1/1/1
7	BAL	J	1910	7	-	0/1/2/3	0/0/0/0
7	DIB	J	1911	7	-	0/4/4/4	0/0/0/0
7	IMT	J	1921	7	-	0/0/2/4	0/1/1/1
7	PYB	J	1922	7	-	0/0/2/4	0/1/1/1
7	PYB	J	1923	7	-	0/0/2/4	0/1/1/1
7	PYB	J	1924	7	-	0/0/2/4	0/1/1/1
7	ABU	J	1925	7	-	0/3/3/4	0/0/0/0
7	PYB	J	1926	7	-	0/0/2/4	0/1/1/1
7	PYB	J	1927	7	-	0/0/2/4	0/1/1/1
7	PYB	J	1928	7	-	0/0/2/4	0/1/1/1
7	PYB	J	1929	7	-	0/0/2/4	0/1/1/1
7	BAL	J	1930	7	-	0/1/2/3	0/0/0/0
7	DIB	J	1931	7	-	0/4/4/4	0/0/0/0
7	IMT	J	2001	7	-	0/0/2/4	0/1/1/1
7	PYB	J	2002	7	-	0/0/2/4	0/1/1/1
7	PYB	J	2003	7	-	0/0/2/4	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PYB	J	2004	7	-	0/0/2/4	0/1/1/1
7	ABU	J	2005	7	-	0/3/3/4	0/0/0/0
7	PYB	J	2006	7	-	0/0/2/4	0/1/1/1
7	PYB	J	2007	7	-	0/0/2/4	0/1/1/1
7	PYB	J	2008	7	-	0/0/2/4	0/1/1/1
7	PYB	J	2009	7	-	0/0/2/4	0/1/1/1
7	BAL	J	2010	7	-	0/1/2/3	0/0/0/0
7	DIB	J	2011	7	-	0/4/4/4	0/0/0/0

All (73) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	J	1905	ABU	OE2-CD	-3.51	1.23	1.42
7	I	2025	ABU	OE2-CD	-3.40	1.23	1.42
7	J	1925	ABU	OE2-CD	-3.40	1.23	1.42
7	J	2005	ABU	OE2-CD	-3.39	1.23	1.42
7	I	1965	ABU	OE2-CD	-3.28	1.24	1.42
7	J	1927	PYB	CG1-C	-2.11	1.42	1.46
7	I	1969	PYB	CB-CA	2.11	1.41	1.37
7	I	2027	PYB	CB1-CA	2.13	1.41	1.39
7	I	2023	PYB	CB-NG2	2.14	1.41	1.38
7	J	1923	PYB	CB1-CA	2.17	1.41	1.39
7	I	1964	PYB	CB-CA	2.18	1.41	1.37
7	J	1926	PYB	CB-CA	2.19	1.41	1.37
7	I	1969	PYB	CB1-CA	2.20	1.41	1.39
7	I	1963	PYB	CB-NG2	2.21	1.41	1.38
7	J	1909	PYB	CB1-CA	2.23	1.41	1.39
7	J	1904	PYB	CB-CA	2.24	1.41	1.37
7	J	2008	PYB	CB1-CA	2.30	1.41	1.39
7	J	2007	PYB	CB1-CA	2.31	1.41	1.39
7	J	2003	PYB	CB1-CA	2.32	1.41	1.39
7	I	2028	PYB	CB1-CA	2.33	1.41	1.39
7	J	1904	PYB	CB1-CA	2.33	1.41	1.39
7	I	1964	PYB	CB1-CA	2.35	1.41	1.39
7	J	1906	PYB	CB-NG2	2.36	1.41	1.38
7	J	1922	PYB	CB1-CA	2.39	1.41	1.39
7	I	2023	PYB	CB1-CA	2.40	1.41	1.39
7	I	2022	PYB	CB1-CA	2.40	1.41	1.39
7	J	2009	PYB	CB1-CA	2.49	1.41	1.39
7	I	2021	IMT	CB-NG2	2.50	1.42	1.37
7	I	1967	PYB	CB1-CA	2.53	1.41	1.39
7	J	1901	IMT	CB-NG2	2.56	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	J	1908	PYB	CB1-CA	2.56	1.41	1.39
7	I	1961	IMT	CB-NG2	2.56	1.42	1.37
7	I	1962	PYB	CB-NG2	2.57	1.41	1.38
7	I	1962	PYB	CB1-CA	2.58	1.41	1.39
7	J	1922	PYB	CB-NG2	2.60	1.41	1.38
7	I	1966	PYB	CB1-CA	2.61	1.41	1.39
7	J	2001	IMT	CB-NG2	2.62	1.42	1.37
7	J	1903	PYB	CB-NG2	2.62	1.41	1.38
7	J	1923	PYB	CB-NG2	2.63	1.41	1.38
7	J	2003	PYB	CB-NG2	2.63	1.41	1.38
7	I	1967	PYB	CB-NG2	2.65	1.41	1.38
7	I	2022	PYB	CB-NG2	2.67	1.42	1.38
7	J	1902	PYB	CB-NG2	2.70	1.42	1.38
7	J	1927	PYB	CB-NG2	2.71	1.42	1.38
7	I	1963	PYB	CB1-CA	2.72	1.41	1.39
7	I	1968	PYB	CB-NG2	2.73	1.42	1.38
7	J	1908	PYB	CB-NG2	2.76	1.42	1.38
7	J	1902	PYB	CB1-CA	2.82	1.41	1.39
7	J	1929	PYB	CB-NG2	2.82	1.42	1.38
7	J	2002	PYB	CB-NG2	2.82	1.42	1.38
7	J	1907	PYB	CB1-CA	2.85	1.41	1.39
7	J	1906	PYB	CB1-CA	2.89	1.42	1.39
7	J	1903	PYB	CB1-CA	2.89	1.42	1.39
7	I	1968	PYB	CB1-CA	2.94	1.42	1.39
7	J	2008	PYB	CB-NG2	2.96	1.42	1.38
7	J	2009	PYB	CB-NG2	2.96	1.42	1.38
7	I	2026	PYB	CB-NG2	2.96	1.42	1.38
7	I	2028	PYB	CB-NG2	2.97	1.42	1.38
7	J	1924	PYB	CB-NG2	3.00	1.42	1.38
7	J	1921	IMT	CB-NG2	3.00	1.43	1.37
7	J	1907	PYB	CB-NG2	3.02	1.42	1.38
7	I	2027	PYB	CB-NG2	3.16	1.42	1.38
7	I	2024	PYB	CB-NG2	3.21	1.42	1.38
7	I	1966	PYB	CB-NG2	3.28	1.42	1.38
7	J	2007	PYB	CB-NG2	3.29	1.42	1.38
7	J	2004	PYB	CB-NG2	3.31	1.42	1.38
7	I	1969	PYB	CB-NG2	3.32	1.42	1.38
7	J	2006	PYB	CB-NG2	3.36	1.42	1.38
7	J	1926	PYB	CB-NG2	3.37	1.43	1.38
7	I	1964	PYB	CB-NG2	3.41	1.43	1.38
7	J	1909	PYB	CB-NG2	3.55	1.43	1.38
7	J	1904	PYB	CB-NG2	3.56	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	2029	PYB	CB-NG2	3.61	1.43	1.38

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	I	1962	PYB	O-C-CG1	-5.49	115.09	124.44
7	I	2022	PYB	O-C-CG1	-5.36	115.31	124.44
7	J	1902	PYB	O-C-CG1	-5.33	115.36	124.44
7	I	1963	PYB	O-C-CG1	-5.31	115.40	124.44
7	I	1968	PYB	O-C-CG1	-5.25	115.50	124.44
7	J	1906	PYB	O-C-CG1	-5.17	115.64	124.44
7	J	1928	PYB	O-C-CG1	-5.06	115.82	124.44
7	J	2008	PYB	O-C-CG1	-5.05	115.84	124.44
7	J	1922	PYB	O-C-CG1	-5.00	115.93	124.44
7	J	1903	PYB	O-C-CG1	-4.95	116.02	124.44
7	J	2002	PYB	O-C-CG1	-4.90	116.10	124.44
7	J	1907	PYB	O-C-CG1	-4.87	116.14	124.44
7	I	1967	PYB	O-C-CG1	-4.80	116.26	124.44
7	I	2027	PYB	O-C-CG1	-4.79	116.29	124.44
7	J	1923	PYB	O-C-CG1	-4.74	116.38	124.44
7	J	2003	PYB	O-C-CG1	-4.72	116.41	124.44
7	J	1908	PYB	O-C-CG1	-4.64	116.54	124.44
7	I	1966	PYB	O-C-CG1	-4.64	116.54	124.44
7	J	1927	PYB	O-C-CG1	-4.62	116.57	124.44
7	I	2023	PYB	O-C-CG1	-4.56	116.68	124.44
7	I	2028	PYB	O-C-CG1	-4.52	116.75	124.44
7	J	2007	PYB	O-C-CG1	-4.50	116.78	124.44
7	J	1929	PYB	O-C-CG1	-4.47	116.83	124.44
7	I	2026	PYB	O-C-CG1	-4.35	117.03	124.44
7	J	2009	PYB	O-C-CG1	-4.33	117.06	124.44
7	J	2006	PYB	O-C-CG1	-4.28	117.15	124.44
7	J	1924	PYB	O-C-CG1	-4.19	117.30	124.44
7	I	1964	PYB	O-C-CG1	-4.17	117.35	124.44
7	I	1969	PYB	O-C-CG1	-3.96	117.70	124.44
7	I	2029	PYB	O-C-CG1	-3.83	117.92	124.44
7	J	1904	PYB	O-C-CG1	-3.83	117.93	124.44
7	J	1909	PYB	O-C-CG1	-3.81	117.95	124.44
7	J	1926	PYB	O-C-CG1	-3.81	117.95	124.44
7	J	2004	PYB	O-C-CG1	-3.73	118.09	124.44
7	I	2024	PYB	O-C-CG1	-3.57	118.36	124.44
7	J	2001	IMT	CB-NG2-CG1	-2.37	105.36	108.41
7	I	1961	IMT	CB-NG2-CG1	-2.17	105.61	108.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	J	1921	IMT	CB-NG2-CG1	-2.17	105.61	108.41
7	I	2021	IMT	CB-NG2-CG1	-2.09	105.72	108.41
7	J	1921	IMT	CD-NG2-CG1	3.15	131.37	126.54
7	I	2021	IMT	CD-NG2-CG1	3.16	131.38	126.54
7	I	1961	IMT	CD-NG2-CG1	3.18	131.41	126.54
7	J	1901	IMT	CD-NG2-CG1	3.18	131.42	126.54
7	J	2001	IMT	CD-NG2-CG1	3.26	131.54	126.54
7	I	1961	IMT	CA-NB1-CG1	3.55	109.03	104.34
7	J	2001	IMT	CA-NB1-CG1	3.68	109.20	104.34
7	I	2021	IMT	CA-NB1-CG1	3.73	109.26	104.34
7	J	1901	IMT	CA-NB1-CG1	3.73	109.28	104.34
7	J	1921	IMT	CA-NB1-CG1	3.84	109.42	104.34
7	J	1902	PYB	CD-NG2-CG1	5.37	130.76	124.54
7	J	2008	PYB	CD-NG2-CG1	5.45	130.85	124.54
7	I	2022	PYB	CD-NG2-CG1	5.45	130.85	124.54
7	I	1968	PYB	CD-NG2-CG1	5.48	130.89	124.54
7	J	1929	PYB	CD-NG2-CG1	5.49	130.90	124.54
7	I	1964	PYB	CD-NG2-CG1	5.49	130.90	124.54
7	I	1963	PYB	CD-NG2-CG1	5.54	130.96	124.54
7	J	2007	PYB	CD-NG2-CG1	5.56	130.98	124.54
7	J	1907	PYB	CD-NG2-CG1	5.58	131.00	124.54
7	I	1969	PYB	CD-NG2-CG1	5.58	131.01	124.54
7	J	1904	PYB	CD-NG2-CG1	5.60	131.02	124.54
7	I	1967	PYB	CD-NG2-CG1	5.60	131.03	124.54
7	J	1908	PYB	CD-NG2-CG1	5.61	131.04	124.54
7	J	2004	PYB	CD-NG2-CG1	5.61	131.04	124.54
7	I	1962	PYB	CD-NG2-CG1	5.62	131.05	124.54
7	I	2023	PYB	CD-NG2-CG1	5.62	131.05	124.54
7	I	2028	PYB	CD-NG2-CG1	5.64	131.07	124.54
7	J	2006	PYB	CD-NG2-CG1	5.67	131.11	124.54
7	J	1922	PYB	CD-NG2-CG1	5.67	131.11	124.54
7	J	1906	PYB	CD-NG2-CG1	5.68	131.11	124.54
7	I	1966	PYB	CD-NG2-CG1	5.68	131.12	124.54
7	I	2029	PYB	CD-NG2-CG1	5.68	131.12	124.54
7	J	2003	PYB	CD-NG2-CG1	5.69	131.12	124.54
7	J	2002	PYB	CD-NG2-CG1	5.69	131.13	124.54
7	I	2024	PYB	CD-NG2-CG1	5.73	131.18	124.54
7	J	1903	PYB	CD-NG2-CG1	5.74	131.19	124.54
7	J	1923	PYB	CD-NG2-CG1	5.74	131.19	124.54
7	J	1924	PYB	CD-NG2-CG1	5.74	131.19	124.54
7	I	2027	PYB	CD-NG2-CG1	5.77	131.22	124.54
7	J	1909	PYB	CD-NG2-CG1	5.81	131.26	124.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	I	2026	PYB	CD-NG2-CG1	5.82	131.28	124.54
7	J	2009	PYB	CD-NG2-CG1	5.86	131.32	124.54
7	J	1927	PYB	CD-NG2-CG1	5.86	131.32	124.54
7	J	1928	PYB	CD-NG2-CG1	5.87	131.34	124.54
7	J	1926	PYB	CD-NG2-CG1	5.95	131.43	124.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

53 monomers are involved in 164 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	I	1961	IMT	5	0
7	I	1962	PYB	5	0
7	I	1963	PYB	5	0
7	I	1964	PYB	4	0
7	I	1965	ABU	1	0
7	I	1966	PYB	3	0
7	I	1967	PYB	5	0
7	I	1968	PYB	5	0
7	I	1969	PYB	5	0
7	I	1970	BAL	1	0
7	I	1971	DIB	2	0
7	I	2021	IMT	3	0
7	I	2022	PYB	5	0
7	I	2023	PYB	5	0
7	I	2024	PYB	4	0
7	I	2025	ABU	3	0
7	I	2026	PYB	3	0
7	I	2027	PYB	3	0
7	I	2028	PYB	6	0
7	I	2029	PYB	10	0
7	I	2030	BAL	2	0
7	I	2031	DIB	3	0
7	J	1901	IMT	5	0
7	J	1902	PYB	5	0
7	J	1903	PYB	6	0
7	J	1904	PYB	4	0
7	J	1905	ABU	11	0
7	J	1906	PYB	6	0
7	J	1907	PYB	5	0

*Continued on next page...*

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	J	1908	PYB	7	0
7	J	1909	PYB	2	0
7	J	1911	DIB	3	0
7	J	1921	IMT	2	0
7	J	1922	PYB	4	0
7	J	1923	PYB	4	0
7	J	1924	PYB	4	0
7	J	1926	PYB	2	0
7	J	1927	PYB	5	0
7	J	1928	PYB	8	0
7	J	1929	PYB	7	0
7	J	1930	BAL	1	0
7	J	1931	DIB	3	0
7	J	2001	IMT	3	0
7	J	2002	PYB	4	0
7	J	2003	PYB	7	0
7	J	2004	PYB	3	0
7	J	2005	ABU	3	0
7	J	2006	PYB	4	0
7	J	2007	PYB	4	0
7	J	2008	PYB	6	0
7	J	2009	PYB	5	0
7	J	2010	BAL	1	0
7	J	2011	DIB	2	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 ⓘ

EDS was not executed - this section will therefore be empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.