



wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 04:43 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 wwPDB validation summary report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

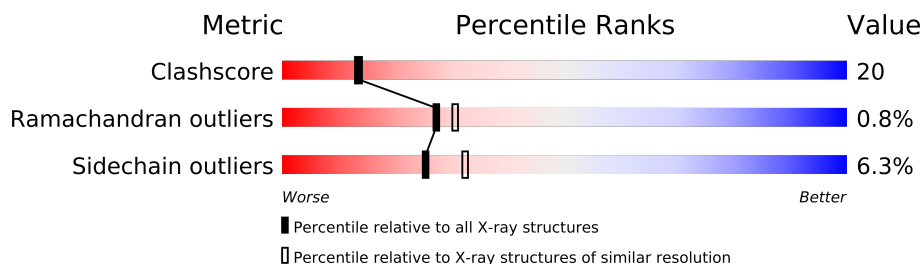
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

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	
4	G	129	
5	D	125	
5	H	125	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 13158 atoms, of which 0 are hydrogen and 0 are deuterium.

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			

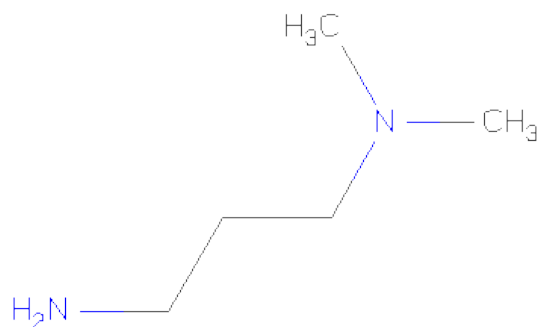
There are 2 discrepancies between the modelled and reference sequences:

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-CARBOXYLICACID (three-letter code: DIB, PYB, IMT, BAL, ABU) (formula: C₅H₁₄N₂, C₆H₈N₂O₂, C₅H₇N₃O₂, C₃H₇NO₂, C₄H₉NO₂).



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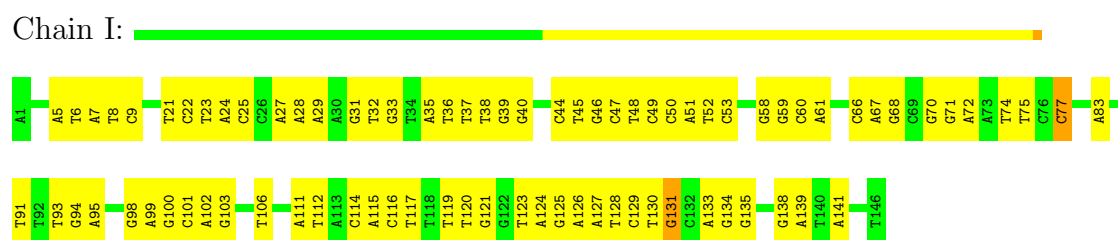
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	H	40	Total 40	O 40	0	0
8	I	88	Total 88	O 88	0	0
8	J	67	Total 67	O 67	0	0

3 Residue-property plots

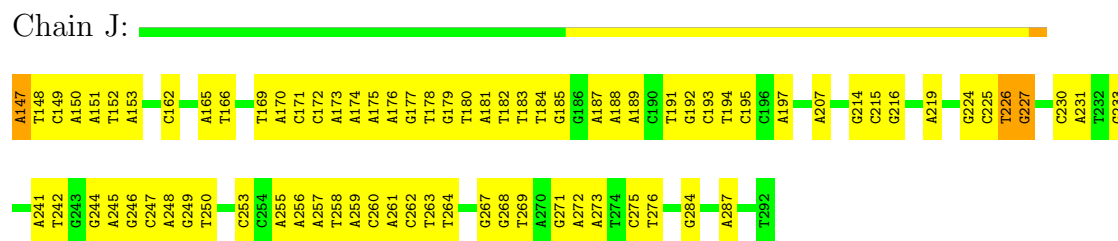
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

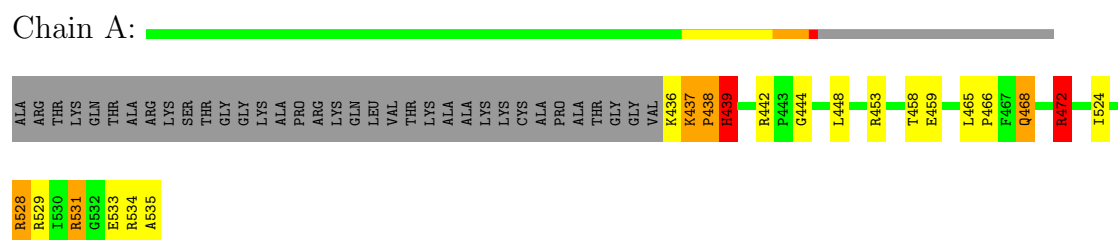
• Molecule 1: Palindromic 146 Base Pair DNA Fragment



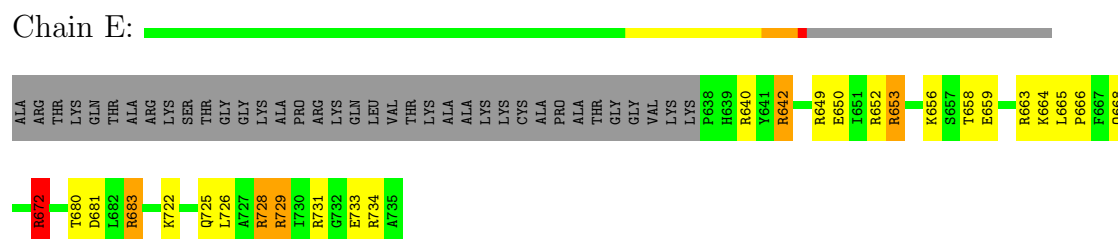
• Molecule 1: Palindromic 146 Base Pair DNA Fragment



• Molecule 2: Histone H3.2



• Molecule 2: Histone H3.2



• Molecule 3: Histone H4

SER	GLY	ARG	GLY	LYS	GLY	GLY	LYS	GLY	LEU	GLY	LYS	GLY	ALA	LYS	ARG	HIS	ARG	LYS	VAL	LEU	ARG	D24	N25	T30	K31	P32	R36	R39	K44	R45	I46	S47	M84	R92	R95	G102
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- Chain F: 

[illegible]

- Chain C:

[illegible]

- Chain G:

SER	GLY	ARG	GLY	LYS	GLN	GLY	GLY	LYS	THR	ARG	ALA	LYS	ALA	R1015	T1016	R1017	S1018	S1019	R1020		H1031	R1032		G1037	N1038		R1042		L1063	E1064		R1071		K1075	T1076		I1079	P1080	R1081	H1082		V1087	R1088		E1092		R1099		I1102		Q1112		K1119	THR	GLU	SER	ALA	LYS
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ALA
LYS
SER
LYS

- Chain D: 

L1299	P1300	G1301		Y1318	K1322	PRO GLU ALA LYS SER ALA PRO PRO PRO LYS LYS GLY SER LYS LYS ALA VAL THR LYS THR GLN LYS ASP GLY LYS ARG ARG LYS	T1229	E1232	V1245 H1246	K1264	I1268	S1261	N1264	E1268 R1269	L1277	A1278	H1279	Y1280	M1281	K1282	R1283	F1289	T1292
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- Chain H:

K1522	PRO	GLU	ALA	LYS	SER	ALA	PRO	ALA	PRO	LYS	LYS	GLY	SER	LYS	ALA	VAL	THR	LYS	THR	GLN	LYS	ASP	GLY	LYS	LYS	ARG	ARG	LYS	T1429	K1430	R1431	E1432	S1433	L1442	K1443	G1444	V1445	H1446	T1449	I1458	N1464	E1468	R1483	R1489	L1499	P1500	G1501	E1502
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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, α , β , γ	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 ²)	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.

The worst 5 of 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

There are no chirality outliers.

5 of 19 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
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

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 20.

The worst 5 of 450 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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
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

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%)	11	8
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%)	19	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	C	105/129 (81%)	103 (98%)	1 (1%)	1 (1%)	22	23
4	G	103/129 (80%)	100 (97%)	3 (3%)	0	100	100
5	D	92/125 (74%)	90 (98%)	1 (1%)	1 (1%)	21	21
5	H	92/125 (74%)	90 (98%)	1 (1%)	1 (1%)	21	21
All	All	747/982 (76%)	732 (98%)	9 (1%)	6 (1%)	27	30

5 of 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

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%)	13	15
2	E	85/111 (77%)	78 (92%)	7 (8%)	17	19
3	B	64/78 (82%)	61 (95%)	3 (5%)	36	47
3	F	71/78 (91%)	65 (92%)	6 (8%)	15	18
4	C	85/100 (85%)	80 (94%)	5 (6%)	28	35
4	G	84/100 (84%)	80 (95%)	4 (5%)	35	46
5	D	80/105 (76%)	77 (96%)	3 (4%)	44	59
5	H	80/105 (76%)	76 (95%)	4 (5%)	34	45
All	All	636/788 (81%)	596 (94%)	40 (6%)	25	32

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	D	1289	ARG

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Mol	Chain	Res	Type
2	E	659	GLU
5	H	1433	SER
2	E	653	ARG
2	E	683	ARG

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 ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	2.79	2 (33%)	4,10,14	2.96	4 (100%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	PYB	I	1962	7	9,9,10	1.86	3 (33%)	8,12,14	2.13	2 (25%)
7	PYB	I	1963	7	9,9,10	1.77	3 (33%)	8,12,14	2.07	1 (12%)
7	PYB	I	1964	7	9,9,10	2.06	4 (44%)	8,12,14	2.12	2 (25%)
7	ABU	I	1965	7	3,5,6	0.47	0	2,4,6	0.65	0
7	PYB	I	1966	7	9,9,10	2.24	5 (55%)	8,12,14	2.13	2 (25%)
7	PYB	I	1967	7	9,9,10	1.80	3 (33%)	8,12,14	2.09	1 (12%)
7	PYB	I	1968	7	9,9,10	1.98	4 (44%)	8,12,14	2.03	1 (12%)
7	PYB	I	1969	7	9,9,10	2.12	5 (55%)	8,12,14	2.15	2 (25%)
7	BAL	I	1970	7	4,4,5	8.99	1 (25%)	1,3,5	0.53	0
7	DIB	I	1971	7	6,6,6	0.69	0	6,6,6	0.44	0
7	IMT	I	2021	7	6,8,10	2.71	2 (33%)	4,10,14	3.02	4 (100%)
7	PYB	I	2022	7	9,9,10	1.77	2 (22%)	8,12,14	2.03	1 (12%)
7	PYB	I	2023	7	9,9,10	1.70	3 (33%)	8,12,14	2.15	2 (25%)
7	PYB	I	2024	7	9,9,10	1.70	2 (22%)	8,12,14	2.25	2 (25%)
7	ABU	I	2025	7	3,5,6	0.18	0	2,4,6	0.34	0
7	PYB	I	2026	7	9,9,10	1.79	2 (22%)	8,12,14	2.24	2 (25%)
7	PYB	I	2027	7	9,9,10	1.90	3 (33%)	8,12,14	2.22	2 (25%)
7	PYB	I	2028	7	9,9,10	1.84	2 (22%)	8,12,14	2.11	2 (25%)
7	PYB	I	2029	7	9,9,10	1.87	1 (11%)	8,12,14	2.17	2 (25%)
7	BAL	I	2030	7	4,4,5	9.09	2 (50%)	1,3,5	0.01	0
7	DIB	I	2031	7	6,6,6	0.67	0	6,6,6	0.46	0
7	IMT	J	1901	7	6,8,10	2.89	3 (50%)	4,10,14	3.10	4 (100%)
7	PYB	J	1902	7	9,9,10	1.92	3 (33%)	8,12,14	1.99	1 (12%)
7	PYB	J	1903	7	9,9,10	2.02	4 (44%)	8,12,14	2.14	1 (12%)
7	PYB	J	1904	7	9,9,10	2.08	4 (44%)	8,12,14	2.16	2 (25%)
7	ABU	J	1905	7	3,5,6	0.14	0	2,4,6	0.32	0
7	PYB	J	1906	7	9,9,10	2.04	4 (44%)	8,12,14	2.10	1 (12%)
7	PYB	J	1907	7	9,9,10	2.15	4 (44%)	8,12,14	2.08	2 (25%)
7	PYB	J	1908	7	9,9,10	1.93	4 (44%)	8,12,14	2.09	1 (12%)
7	PYB	J	1909	7	9,9,10	2.24	6 (66%)	8,12,14	2.21	2 (25%)
7	BAL	J	1910	7	4,4,5	8.95	1 (25%)	1,3,5	0.19	0
7	DIB	J	1911	7	6,6,6	0.61	0	6,6,6	0.35	0
7	IMT	J	1921	7	6,8,10	3.04	3 (50%)	4,10,14	3.03	4 (100%)
7	PYB	J	1922	7	9,9,10	1.71	2 (22%)	8,12,14	2.18	2 (25%)
7	PYB	J	1923	7	9,9,10	1.73	2 (22%)	8,12,14	2.20	2 (25%)
7	PYB	J	1924	7	9,9,10	1.77	2 (22%)	8,12,14	2.22	2 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	ABU	J	1925	7	3,5,6	0.33	0	2,4,6	0.57	0
7	PYB	J	1926	7	9,9,10	1.77	2 (22%)	8,12,14	2.45	3 (37%)
7	PYB	J	1927	7	9,9,10	1.56	1 (11%)	8,12,14	2.44	3 (37%)
7	PYB	J	1928	7	9,9,10	1.46	1 (11%)	8,12,14	2.29	2 (25%)
7	PYB	J	1929	7	9,9,10	1.73	2 (22%)	8,12,14	2.10	2 (25%)
7	BAL	J	1930	7	4,4,5	9.00	1 (25%)	1,3,5	0.38	0
7	DIB	J	1931	7	6,6,6	0.70	0	6,6,6	0.40	0
7	IMT	J	2001	7	6,8,10	2.61	2 (33%)	4,10,14	2.97	4 (100%)
7	PYB	J	2002	7	9,9,10	1.67	2 (22%)	8,12,14	2.17	2 (25%)
7	PYB	J	2003	7	9,9,10	1.81	3 (33%)	8,12,14	2.15	2 (25%)
7	PYB	J	2004	7	9,9,10	1.84	2 (22%)	8,12,14	2.16	2 (25%)
7	ABU	J	2005	7	3,5,6	0.33	0	2,4,6	0.28	0
7	PYB	J	2006	7	9,9,10	1.93	3 (33%)	8,12,14	2.15	2 (25%)
7	PYB	J	2007	7	9,9,10	1.91	2 (22%)	8,12,14	2.11	2 (25%)
7	PYB	J	2008	7	9,9,10	1.85	2 (22%)	8,12,14	2.03	1 (12%)
7	PYB	J	2009	7	9,9,10	1.98	3 (33%)	8,12,14	2.22	2 (25%)
7	BAL	J	2010	7	4,4,5	9.13	2 (50%)	1,3,5	0.00	0
7	DIB	J	2011	7	6,6,6	0.66	0	6,6,6	0.53	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	-	0/2/3/4	0/0/0/0
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PYB	I	2024	7	-	0/0/2/4	0/1/1/1
7	ABU	I	2025	7	-	0/2/3/4	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	-	0/2/3/4	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	-	0/2/3/4	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
7	PYB	J	2004	7	-	0/0/2/4	0/1/1/1
7	ABU	J	2005	7	-	0/2/3/4	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

The worst 5 of 119 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	J	2010	BAL	O-C	18.09	1.23	1.11
7	I	2030	BAL	O-C	18.06	1.23	1.11
7	J	1930	BAL	O-C	17.91	1.23	1.11
7	I	1970	BAL	O-C	17.88	1.23	1.11
7	J	1910	BAL	O-C	17.80	1.23	1.11

The worst 5 of 83 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	J	1926	PYB	CD-NG2-CG1	5.63	131.43	125.59
7	J	1928	PYB	CD-NG2-CG1	5.55	131.34	125.59
7	J	2009	PYB	CD-NG2-CG1	5.53	131.32	125.59
7	J	1927	PYB	CD-NG2-CG1	5.54	131.32	125.59
7	I	2026	PYB	CD-NG2-CG1	5.49	131.28	125.59

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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.