



wwPDB X-ray Structure Validation Summary Report ⓘ

May 16, 2020 – 03:18 pm BST

PDB ID : 1M18
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 : 2.45 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

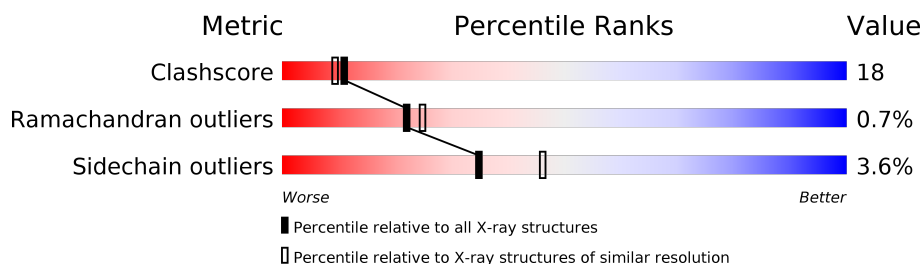
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)

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 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	I	146	51% 47% .
1	J	146	44% 55% .
2	A	135	56% 16% . 27%
2	E	135	59% 12% . 27%
3	B	102	57% 20% . 23%
3	F	102	69% 13% 19%
4	C	129	69% 9% 5% 17%
4	G	129	67% 14% . 18%

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Mol	Chain	Length	Quality of chain
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	1SZ	I	1625	-	-	X	-
7	1SZ	J	1601	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 12676 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	98	Total	C	N	O	S	0	0	0
			808	509	156	140	3			
2	E	99	Total	C	N	O	S	0	0	0
			817	515	158	141	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	83	Total	C	N	O	S	0	0	0
			662	418	129	114	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	106	Total	C	N	O	0	0	0
			818	516	160	142			

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			

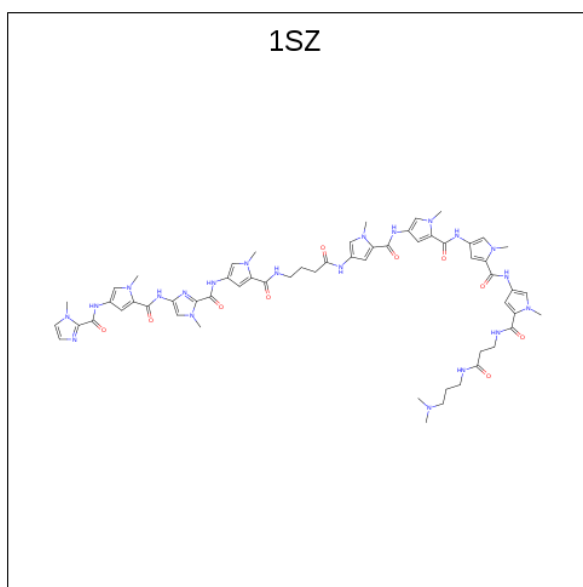
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1229	THR	SER	VARIANT	UNP P02281
H	1429	THR	SER	VARIANT	UNP P02281

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

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

- Molecule 7 is N-[5-[[4-[[5-[[5-[[5-[[3-3-(dimethylamino)propylamino]-3-oxidanylidene-propyl]carbamoyl]-1-methyl-pyrrol-3-yl]carbamoyl]-1-methyl-pyrrol-3-yl]carbamoyl]-1-methyl-pyrrol-3-yl]amino]-4-oxidanylidene-butyl]carbamoyl]-1-methyl-pyrrol-3-yl]-1-methyl-4-[[1-methyl-4-[(1-methylimidazol-2-yl)carbonylamino]pyrrol-2-yl]carbonylamino]imidazole-2-carboxamide (three-letter code: 1SZ) (formula: C₅₈H₇₁N₂₁O₁₀).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	I	1	Total	C	N	O	0	0
			54	36	12	6		
7	J	1	Total	C	N	O	0	0
			89	58	21	10		

- Molecule 8 is water.

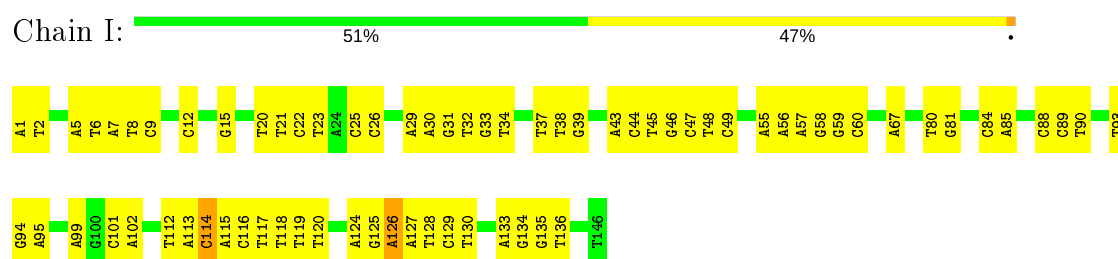
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	I	32	Total	O	0	0
			32	32		
8	J	42	Total	O	0	0
			42	42		
8	A	53	Total	O	0	0
			53	53		
8	B	39	Total	O	0	0
			39	39		
8	C	83	Total	O	0	0
			83	83		
8	D	42	Total	O	0	0
			42	42		
8	E	64	Total	O	0	0
			64	64		
8	F	69	Total	O	0	0
			69	69		
8	G	47	Total	O	0	0
			47	47		
8	H	42	Total	O	0	0
			42	42		

3 Residue-property plots

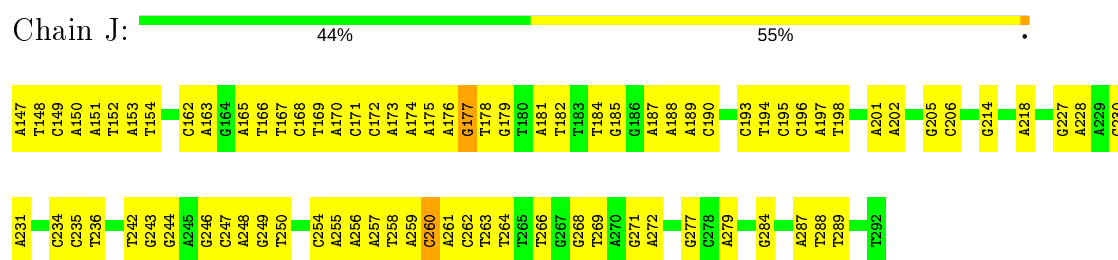
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

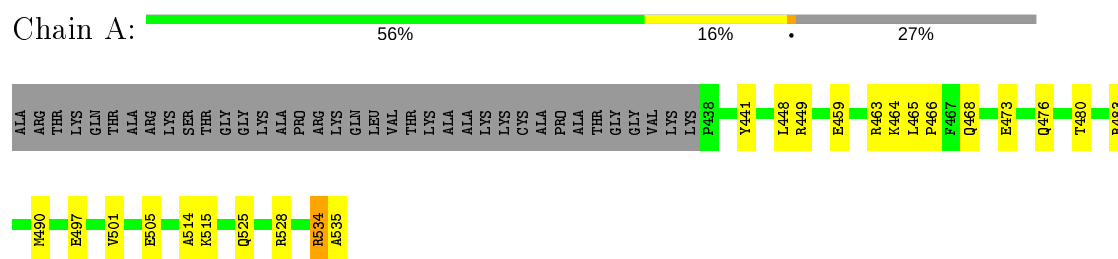
• Molecule 1: Palindromic 146 Base Pair DNA Fragment



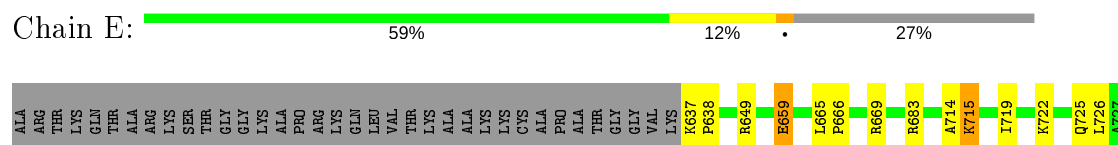
• Molecule 1: Palindromic 146 Base Pair DNA Fragment



• Molecule 2: Histone H3.2



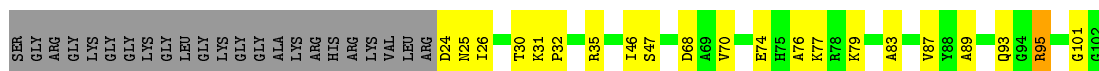
• Molecule 2: Histone H3.2





• Molecule 3: Histone H4

Chain B: 57% 20% 23%



• Molecule 3: Histone H4

Chain F: 69% 13% 19%



• Molecule 4: Histone H2A.1

Chain C: 69% 9% 5% 17%



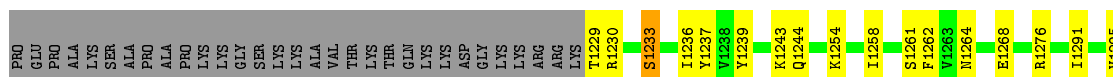
• Molecule 4: Histone H2A.1

Chain G: 67% 14% 18%



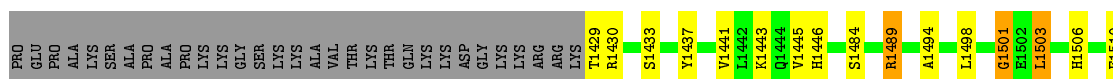
• Molecule 5: Histone H2B.1

Chain D: 61% 14% 25%



• Molecule 5: Histone H2B.1

Chain H: 62% 10% 25%





K1522

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	106.84Å 109.63Å 183.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	60.00 – 2.45	Depositor
% Data completeness (in resolution range)	97.1 (60.00-2.45)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.222 , 0.257	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12676	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

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: 1SZ, MN

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	0.47	1/3354 (0.0%)	0.75	1/5175 (0.0%)
1	J	0.41	2/3354 (0.1%)	0.77	3/5175 (0.1%)
2	A	0.51	0/820	0.66	0/1099
2	E	0.59	0/829	0.73	0/1111
3	B	0.50	0/634	0.70	0/848
3	F	0.59	0/669	0.77	0/894
4	C	0.55	0/835	0.67	0/1127
4	G	0.46	0/828	0.61	0/1117
5	D	0.54	0/747	0.66	0/1004
5	H	0.48	0/747	0.64	0/1004
All	All	0.49	3/12817 (0.0%)	0.73	4/18554 (0.0%)

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	2
1	J	0	1
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	114	DC	O3'-P	-16.23	1.41	1.61
1	J	177	DG	O3'-P	-7.82	1.51	1.61
1	J	260	DC	O3'-P	-5.85	1.54	1.61

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	177	DG	P-O3'-C3'	15.09	137.80	119.70
1	J	260	DC	P-O3'-C3'	10.47	132.27	119.70
1	I	114	DC	P-O3'-C3'	10.19	131.93	119.70
1	J	260	DC	OP1-P-O3'	5.42	117.12	105.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	I	126	DA	Sidechain
1	I	67	DA	Sidechain
1	J	214	DG	Sidechain

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	I	2990	0	1651	132	0
1	J	2990	0	1651	111	0
2	A	808	0	846	27	0
2	E	817	0	858	18	0
3	B	627	0	663	17	0
3	F	662	0	709	17	0
4	C	825	0	884	21	0
4	G	818	0	877	38	0
5	D	736	0	760	17	0
5	H	736	0	760	15	0
6	D	1	0	0	0	0
6	I	4	0	0	0	0
6	J	6	0	0	0	0
7	I	54	0	48	54	0
7	J	89	0	71	40	0
8	A	53	0	0	2	0
8	B	39	0	0	3	0
8	C	83	0	0	3	0
8	D	42	0	0	5	0
8	E	64	0	0	2	0
8	F	69	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	G	47	0	0	1	0
8	H	42	0	0	1	1
8	I	32	0	0	4	1
8	J	42	0	0	4	0
All	All	12676	0	9778	396	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

The worst 5 of 396 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)
7:I:1625:1SZ:C56	4:G:1016:THR:HG22	1.38	1.53
7:I:1625:1SZ:H70	4:G:1016:THR:CB	1.36	1.50
7:I:1625:1SZ:C58	4:G:1016:THR:HB	1.43	1.48
1:I:114:DC:O2	7:I:1625:1SZ:C28	1.76	1.33
1:I:114:DC:H1'	7:I:1625:1SZ:C28	1.65	1.25

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:1654:HOH:O	8:H:512:HOH:O[3_645]	2.08	0.12

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	96/135 (71%)	94 (98%)	2 (2%)	0	100	100
2	E	97/135 (72%)	95 (98%)	1 (1%)	1 (1%)	15	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	B	77/102 (76%)	75 (97%)	2 (3%)	0	100	100
3	F	81/102 (79%)	81 (100%)	0	0	100	100
4	C	105/129 (81%)	102 (97%)	3 (3%)	0	100	100
4	G	104/129 (81%)	101 (97%)	2 (2%)	1 (1%)	15	16
5	D	92/125 (74%)	90 (98%)	0	2 (2%)	6	4
5	H	92/125 (74%)	88 (96%)	3 (3%)	1 (1%)	14	14
All	All	744/982 (76%)	726 (98%)	13 (2%)	5 (1%)	22	25

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	D	1230	ARG
2	E	734	ARG
5	H	1501	GLY
5	D	1301	GLY
4	G	1026	PRO

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	85/111 (77%)	82 (96%)	3 (4%)	36	47
2	E	86/111 (78%)	82 (95%)	4 (5%)	26	34
3	B	64/78 (82%)	63 (98%)	1 (2%)	62	74
3	F	68/78 (87%)	68 (100%)	0	100	100
4	C	85/100 (85%)	75 (88%)	10 (12%)	5	4
4	G	84/100 (84%)	84 (100%)	0	100	100
5	D	80/105 (76%)	79 (99%)	1 (1%)	69	79
5	H	80/105 (76%)	76 (95%)	4 (5%)	24	32
All	All	632/788 (80%)	609 (96%)	23 (4%)	35	46

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	C	884	GLN
4	C	909	PRO
5	H	1503	LEU
4	C	901	THR
4	C	919	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
5	D	1292	GLN
5	H	1506	HIS
5	H	1479	HIS
4	C	884	GLN
4	G	1031	HIS

5.3.3 RNA ⓘ

There are no RNA molecules 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 13 ligands modelled in this entry, 11 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	1SZ	J	1601	-	85,96,96	1.92	19 (22%)	81,137,137	2.19	25 (30%)
7	1SZ	I	1625	-	53,57,96	1.60	9 (16%)	50,79,137	2.62	14 (28%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	1SZ	J	1601	-	-	7/40/80/80	0/8/8/8
7	1SZ	I	1625	-	-	12/29/49/80	0/4/4/8

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	J	1601	1SZ	C3-C5	-8.73	1.46	1.53
7	J	1601	1SZ	C14-C16	-6.72	1.47	1.53
7	I	1625	1SZ	C26-N11	5.41	1.47	1.35
7	I	1625	1SZ	C48-N18	3.45	1.43	1.36
7	J	1601	1SZ	C14-N6	3.40	1.39	1.34

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	I	1625	1SZ	C27-N11-C26	-14.23	102.60	127.50
7	J	1601	1SZ	C14-C16-N8	10.43	125.02	113.69
7	J	1601	1SZ	C3-C5-N3	6.17	120.39	113.69
7	I	1625	1SZ	C35-C33-C34	3.95	107.98	106.05
7	J	1601	1SZ	C27-N11-C26	-3.77	120.90	127.50

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

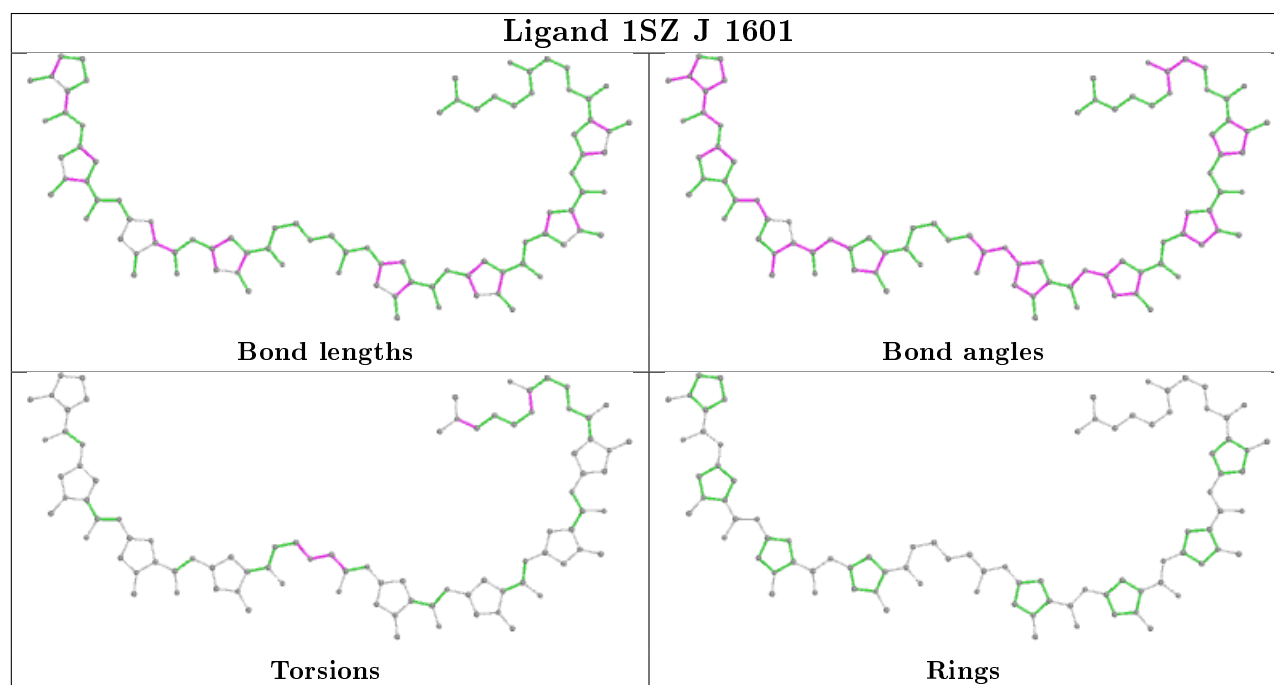
Mol	Chain	Res	Type	Atoms
7	I	1625	1SZ	C23-C24-C25-C26
7	J	1601	1SZ	C23-C24-C25-C26
7	J	1601	1SZ	C52-C53-N20-C54
7	J	1601	1SZ	O10-C53-N20-C54
7	I	1625	1SZ	O5-C26-N11-C27

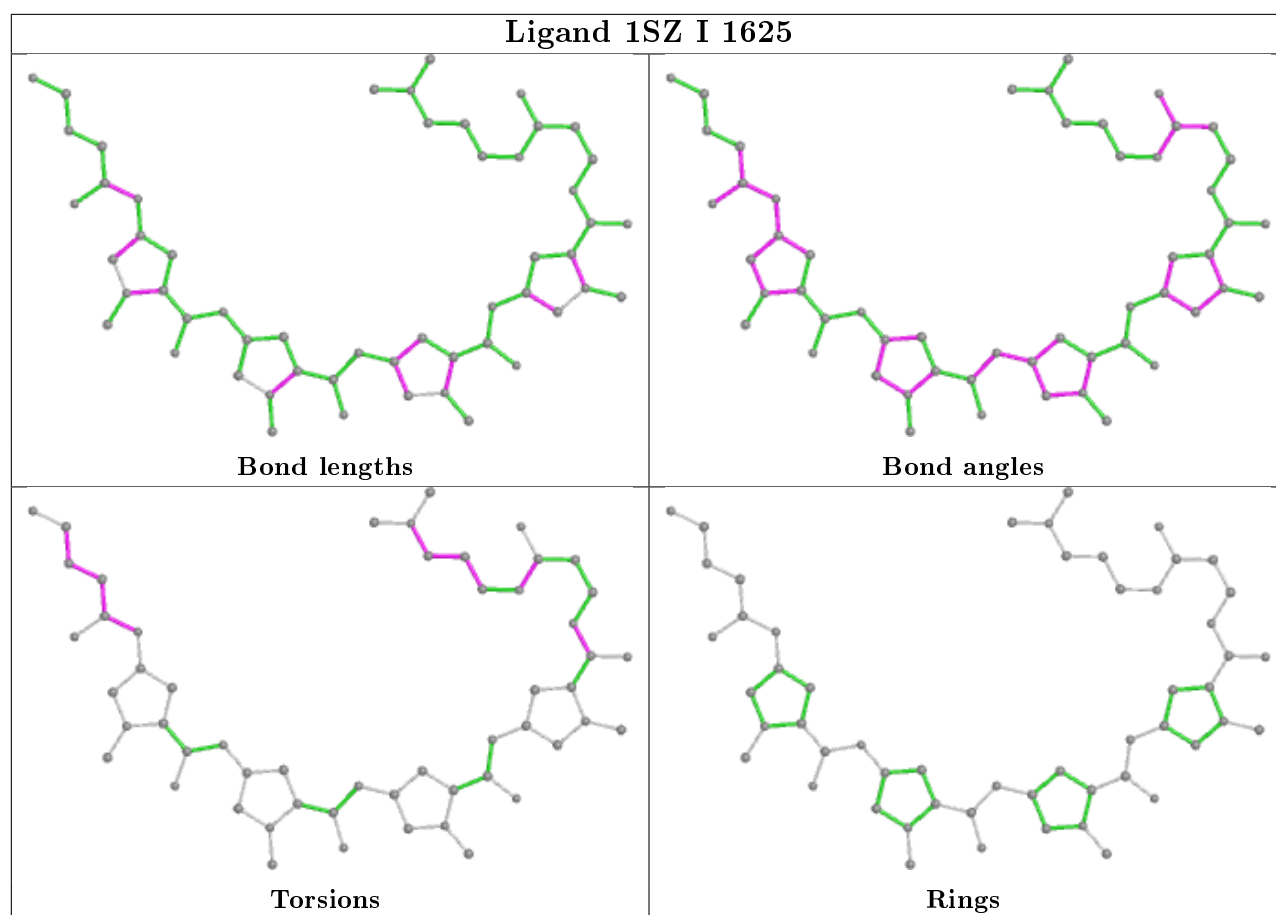
There are no ring outliers.

2 monomers are involved in 94 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	J	1601	1SZ	40	0
7	I	1625	1SZ	54	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](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.