



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 05:13 PM UTC

PDB ID : 1M1A / pdb_00001m1a
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 : 2.65 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 types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

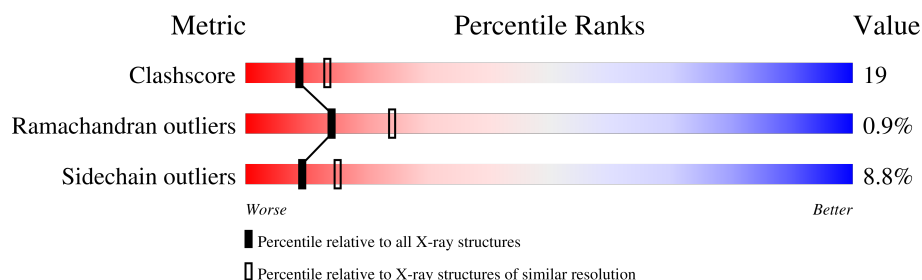
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	
1	J	146	
2	A	135	
2	E	135	
3	B	102	
3	F	102	
4	C	129	
4	G	129	

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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
11	DIB	J	1911	-	-	X	-
7	IMT	J	1901	-	X	-	-
8	PYB	J	1903	-	-	X	-
8	PYB	J	1904	-	-	X	-

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 12378 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 H3.3C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	99	Total	C	N	O	S	0	0	0
			817	515	158	141	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	conflict	UNP P02302
E	686	SER	ARG	conflict	UNP P02302

- Molecule 3 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	80	Total	C	N	O	S	0	0	0
			638	401	125	111	1			
3	F	93	Total	C	N	O	S	0	0	0
			737	463	149	124	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	C	105	Total	C	N	O	0	0	0
			809	510	158	141			

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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	conflict	UNP P06897
G	1099	ARG	GLY	conflict	UNP P06897

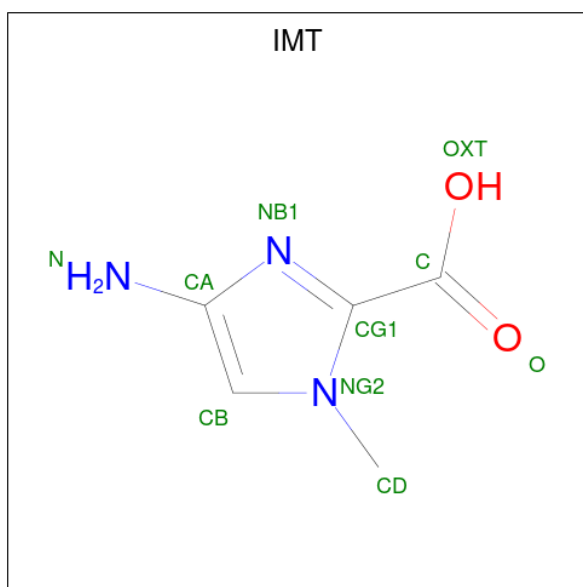
- Molecule 5 is a protein called Histone H2B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	D	93	Total	C	N	O	S	0	0	0
			726	457	130	137	2			
5	H	93	Total	C	N	O	S	0	0	0
			726	457	130	137	2			

- Molecule 6 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

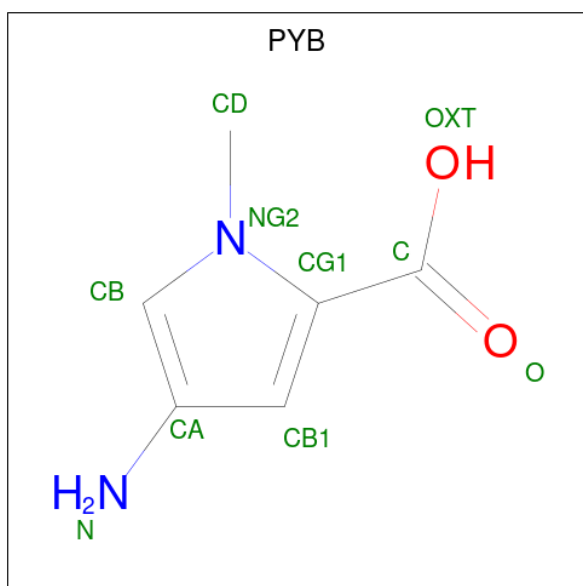
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	I	5	Total	Mn	0	0
			5	5		
6	J	4	Total	Mn	0	0
			4	4		
6	E	1	Total	Mn	0	0
			1	1		

- Molecule 7 is 4-AMINO-(1-METHYLIMIDAZOLE)-2-CARBOXYLIC ACID (CCD ID: IMT) (formula: C₅H₇N₃O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	J	1	Total	C	N	O	0	0
			8	5	2	1		
7	J	1	Total	C	N	O	0	0
			9	5	3	1		

- Molecule 8 is 4-AMINO-(1-METHYLPYRROLE)-2-CARBOXYLIC ACID (CCD ID: PYB) (formula: $C_6H_8N_2O_2$).



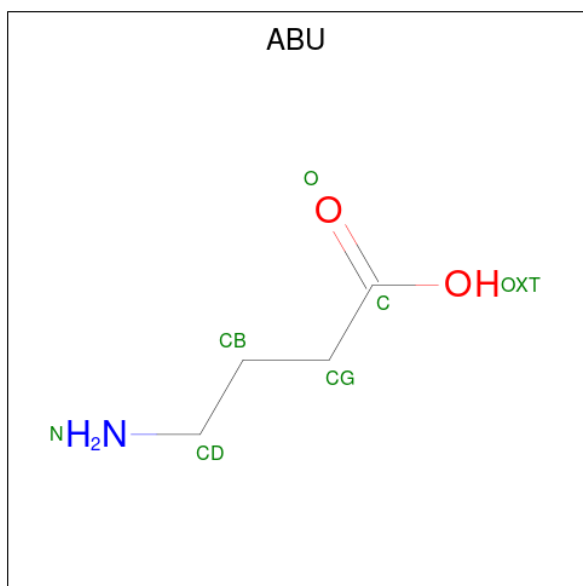
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	J	1	Total	C	N	O	0	0
			9	6	2	1		

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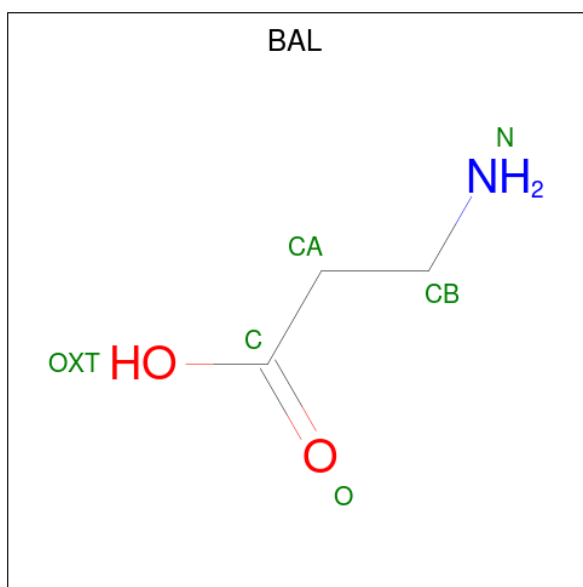
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	J	1	Total	C	N	O	0	0
			9	6	2	1		
8	J	1	Total	C	N	O	0	0
			9	6	2	1		
8	J	1	Total	C	N	O	0	0
			9	6	2	1		
8	J	1	Total	C	N	O	0	0
			9	6	2	1		
8	J	1	Total	C	N	O	0	0
			9	6	2	1		

- Molecule 9 is GAMMA-AMINO-BUTANOIC ACID (CCD ID: ABU) (formula: $C_4H_9NO_2$).



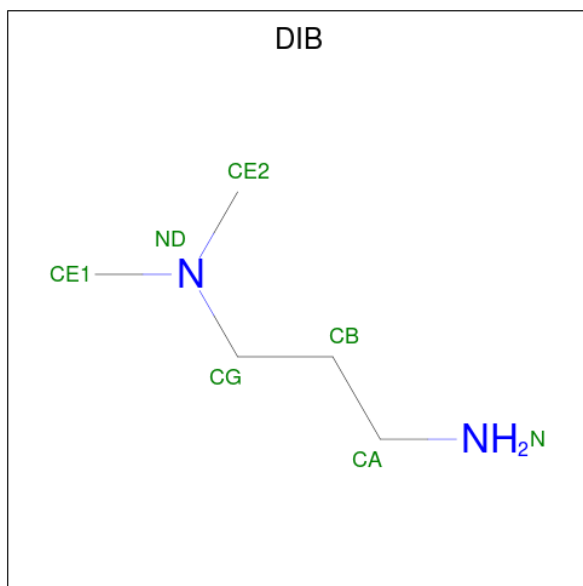
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	J	1	Total	C	N	O	0	0
			6	4	1	1		

- Molecule 10 is BETA-ALANINE (CCD ID: BAL) (formula: $C_3H_7NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	J	1	Total	C	N	O	0	0
			5	3	1	1		

- Molecule 11 is 3-AMINO-(DIMETHYLPROPYLAMINE) (CCD ID: DIB) (formula: $C_5H_{14}N_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	J	1	Total	C	N	0	0
			7	5	2		

- Molecule 12 is water.

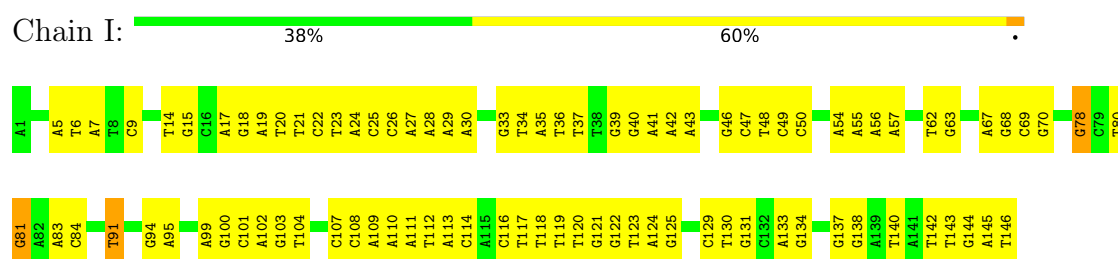
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	I	11	Total 11	O 11	0	0
12	J	28	Total 28	O 28	0	0
12	A	24	Total 24	O 24	0	0
12	B	17	Total 17	O 17	0	0
12	C	30	Total 30	O 30	0	0
12	D	8	Total 8	O 8	0	0
12	E	35	Total 35	O 35	0	0
12	F	40	Total 40	O 40	0	0
12	G	16	Total 16	O 16	0	0
12	H	11	Total 11	O 11	0	0

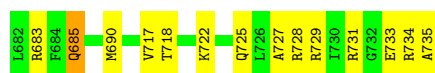
3 Residue-property plots

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

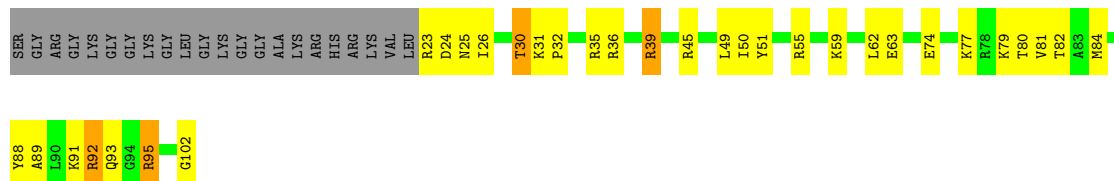
• Molecule 1: Palindromic 146 Base Pair DNA Fragment





- Molecule 3: Histone H4

Chain B: 47% 27% 0% 22%



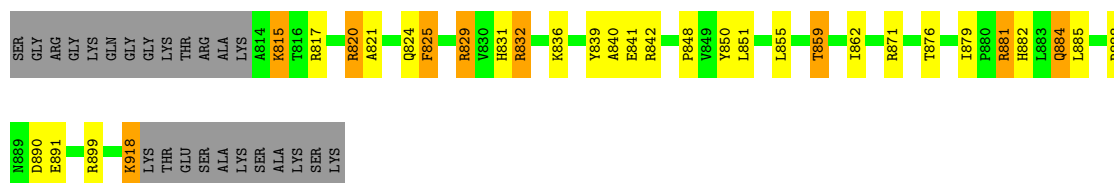
- Molecule 3: Histone H4

Chain F: 68% 16% 5% 9%



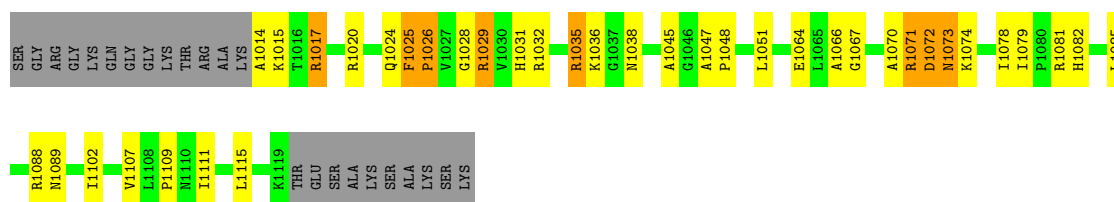
- Molecule 4: Histone H2A type 1

Chain C: 57% 18% 7% 19%



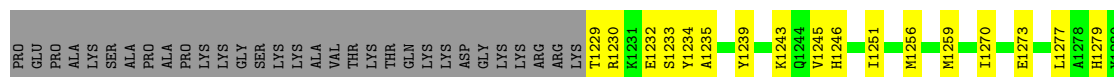
- Molecule 4: Histone H2A type 1

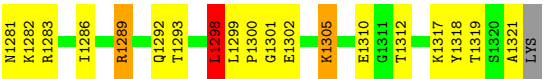
Chain G: 53% 23% 6% 18%



- Molecule 5: Histone H2B

Chain D: 46% 26% 0% 26%





● Molecule 5: Histone H2B



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	106.72Å 109.20Å 177.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	60.00 – 2.65	Depositor
% Data completeness (in resolution range)	96.9 (60.00-2.65)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.223 , 0.267	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12378	wwPDB-VP
Average B, all atoms (Å ²)	88.0	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: BAL, PYB, DIB, ABU, IMT, 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	0.30	0/3354	0.68	1/5175 (0.0%)
1	J	0.31	0/3354	0.66	0/5175
2	A	0.67	0/829	1.01	1/1111 (0.1%)
2	E	0.81	0/820	1.13	2/1099 (0.2%)
3	B	0.67	0/645	1.08	1/862 (0.1%)
3	F	0.77	1/745 (0.1%)	1.21	4/992 (0.4%)
4	C	0.74	0/819	1.17	6/1106 (0.5%)
4	G	0.60	0/828	1.11	5/1117 (0.4%)
5	D	0.74	0/737	1.10	1/993 (0.1%)
5	H	0.68	0/737	1.09	5/993 (0.5%)
All	All	0.54	1/12868 (0.0%)	0.89	26/18623 (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	3
1	J	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	260	VAL	CA-CB	-5.26	1.47	1.54

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	1298	LEU	N-CA-C	8.97	122.34	111.40
4	G	1025	PHE	CA-C-N	7.86	129.66	119.84
4	G	1025	PHE	C-N-CA	7.86	129.66	119.84
3	F	230	THR	N-CA-C	7.54	120.73	110.55
1	I	81	DG	C5'-C4'-C3'	-6.91	104.53	114.90

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	I	7	DA	Sidechain
1	I	78	DG	Sidechain
1	I	91	DT	Sidechain
1	J	213	DA	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	107	0
1	J	2990	0	1651	115	0
2	A	817	0	858	42	0
2	E	808	0	846	31	0
3	B	638	0	676	28	0
3	F	737	0	793	24	0
4	C	809	0	864	31	0
4	G	818	0	877	37	0
5	D	726	0	747	32	0
5	H	726	0	747	25	0
6	E	1	0	0	0	0
6	I	5	0	0	0	0
6	J	4	0	0	0	0
7	J	17	0	9	1	0
8	J	54	0	36	15	0
9	J	6	0	0	1	0
10	J	5	0	4	0	0
11	J	7	0	13	6	0
12	A	24	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	B	17	0	0	1	0
12	C	30	0	0	1	0
12	D	8	0	0	0	0
12	E	35	0	0	4	0
12	F	40	0	0	5	0
12	G	16	0	0	0	0
12	H	11	0	0	0	0
12	I	11	0	0	2	0
12	J	28	0	0	2	0
All	All	12378	0	9772	405	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 19.

The worst 5 of 405 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)
3:F:295:ARG:HD2	12:F:156:HOH:O	1.36	1.19
4:C:918:LYS:H	4:C:918:LYS:HD2	1.17	1.08
1:J:247:DC:H2''	1:J:248:DA:H5''	1.37	1.03
5:H:1445:VAL:HG12	5:H:1446:HIS:HD2	1.29	0.96
3:F:287:VAL:HG11	3:F:302:GLY:HA3	1.48	0.96

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	97/135 (72%)	95 (98%)	2 (2%)	0	100	100
2	E	96/135 (71%)	92 (96%)	3 (3%)	1 (1%)	12	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	B	78/102 (76%)	73 (94%)	5 (6%)	0	100	100
3	F	91/102 (89%)	86 (94%)	3 (3%)	2 (2%)	5	9
4	C	103/129 (80%)	98 (95%)	5 (5%)	0	100	100
4	G	104/129 (81%)	99 (95%)	3 (3%)	2 (2%)	6	10
5	D	91/125 (73%)	89 (98%)	1 (1%)	1 (1%)	11	19
5	H	91/125 (73%)	85 (93%)	5 (6%)	1 (1%)	11	19
All	All	751/982 (76%)	717 (96%)	27 (4%)	7 (1%)	14	24

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	D	1301	GLY
5	H	1501	GLY
4	G	1072	ASP
2	E	681	ASP
3	F	217	ARG

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	86/111 (78%)	81 (94%)	5 (6%)	18	31
2	E	85/111 (77%)	79 (93%)	6 (7%)	13	23
3	B	65/78 (83%)	55 (85%)	10 (15%)	2	3
3	F	74/78 (95%)	67 (90%)	7 (10%)	8	13
4	C	83/100 (83%)	74 (89%)	9 (11%)	6	9
4	G	84/100 (84%)	77 (92%)	7 (8%)	10	18
5	D	79/105 (75%)	74 (94%)	5 (6%)	16	29
5	H	79/105 (75%)	72 (91%)	7 (9%)	9	15
All	All	635/788 (81%)	579 (91%)	56 (9%)	9	15

5 of 56 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	D	1312	THR
5	H	1516	THR
3	F	210	LEU
5	H	1513	LYS
5	H	1429	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
4	G	1068	ASN
4	G	1073	ASN
5	H	1479	HIS
5	H	1446	HIS
5	D	1281	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 21 ligands modelled in this entry, 10 are monoatomic - leaving 11 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
8	PYB	J	1907	8	8,9,10	2.02	3 (37%)	6,12,14	2.92	4 (66%)
7	IMT	J	1902	8,7	7,9,10	1.87	2 (28%)	5,12,14	2.62	3 (60%)
9	ABU	J	1905	8	5,5,6	1.67	1 (20%)	4,4,6	0.43	0
11	DIB	J	1911	10	6,6,6	0.83	0	6,6,6	0.53	0
10	BAL	J	1910	11,8	3,4,5	0.42	0	3,3,5	1.33	0
8	PYB	J	1904	8,9	8,9,10	1.80	3 (37%)	6,12,14	2.77	4 (66%)
8	PYB	J	1909	8,10	8,9,10	1.82	3 (37%)	6,12,14	2.89	3 (50%)
8	PYB	J	1903	8,7	8,9,10	1.84	3 (37%)	6,12,14	2.72	3 (50%)
8	PYB	J	1908	8	8,9,10	1.76	3 (37%)	6,12,14	2.89	2 (33%)
8	PYB	J	1906	8,9	8,9,10	1.56	2 (25%)	6,12,14	2.70	2 (33%)
7	IMT	J	1901	7	7,8,10	1.84	4 (57%)	9,10,14	2.17	5 (55%)

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
8	PYB	J	1907	8	-	0/2/2/4	0/1/1/1
7	IMT	J	1902	8,7	-	2/2/2/4	0/1/1/1
9	ABU	J	1905	8	-	3/3/3/4	-
11	DIB	J	1911	10	-	2/4/4/4	-
10	BAL	J	1910	11,8	-	0/1/2/3	-
8	PYB	J	1904	8,9	-	0/2/2/4	0/1/1/1
8	PYB	J	1909	8,10	-	0/2/2/4	0/1/1/1
8	PYB	J	1903	8,7	-	0/2/2/4	0/1/1/1
8	PYB	J	1908	8	-	0/2/2/4	0/1/1/1
8	PYB	J	1906	8,9	-	0/2/2/4	0/1/1/1
7	IMT	J	1901	7	-	0/2/2/4	0/1/1/1

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	J	1905	ABU	OXT-C	-3.73	1.23	1.42
8	J	1904	PYB	CB-CA	3.20	1.40	1.35
8	J	1907	PYB	CB-CA	3.18	1.40	1.35
8	J	1908	PYB	CB-CA	3.15	1.40	1.35
8	J	1903	PYB	CB-CA	3.14	1.40	1.35

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	J	1909	PYB	CD-NG2-CG1	5.02	131.46	126.62
8	J	1904	PYB	CD-NG2-CG1	4.85	131.30	126.62
8	J	1907	PYB	CD-NG2-CG1	4.82	131.27	126.62
8	J	1908	PYB	CD-NG2-CG1	4.55	131.00	126.62
8	J	1906	PYB	CD-NG2-CG1	4.55	131.00	126.62

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	J	1902	IMT	O-C-CG1-NB1
9	J	1905	ABU	OXT-C-CG-CB
7	J	1902	IMT	O-C-CG1-NG2
11	J	1911	DIB	N-CA-CB-CG
11	J	1911	DIB	CB-CG-ND-CE2

There are no ring outliers.

9 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	J	1907	PYB	2	0
7	J	1902	IMT	1	0
9	J	1905	ABU	1	0
11	J	1911	DIB	6	0
8	J	1904	PYB	6	0
8	J	1909	PYB	3	0
8	J	1903	PYB	4	0
8	J	1908	PYB	3	0
8	J	1906	PYB	1	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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.