WORLDWIDE PDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Jan 7, 2024 – 04:46 pm GMT

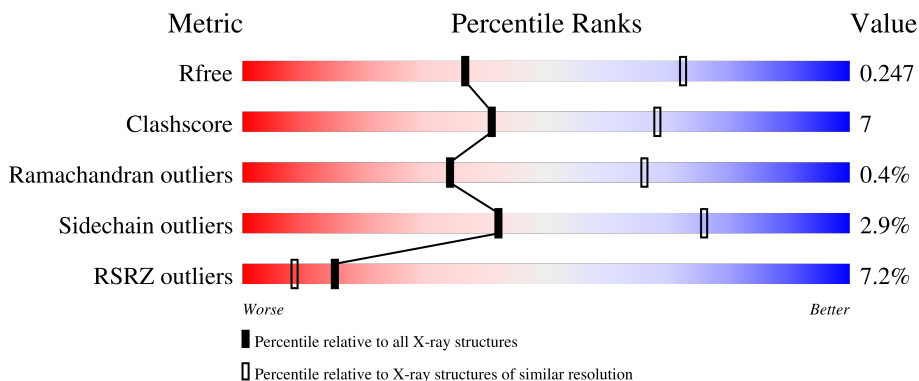|		
PDB ID	:	5ONG
Title	:	X-Ray crystal structure of a nucleosome core particle with its DNA site-specifically crosslinked to the histone octamer
Authors	:	Frouws, T.D.; Barth, P.D.; Richmond, T.J.
Deposited on	:	2017-08-03
Resolution	:	2.80 Å(reported)

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

Metric	Percentile Ranks	Value
Rfree		0.247
Clashscore		7
Ramachandran outliers		0.4%
Sidechain outliers		2.9%
RSRZ outliers		7.2%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
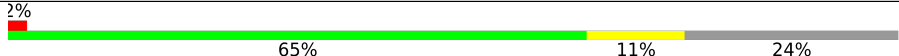
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	I	147	22% / 57% / 42% / •
2	J	147	21% / 59% / 41%
3	A	135	.% / 56% / 11% / • / 29%
3	E	135	.% / 59% / 10% / • / 28%
4	B	103	62% / 14% / 24%

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Mol	Chain	Length	Quality of chain
4	F	103	69% ... 13% ... 18%
5	C	129	2% 73% ... 9% ... 18%
5	G	129	2% 71% ... 11% · 18%
6	D	122	69% ... 7% · 23%
6	H	122	2% 65% ... 11% ... 24%

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	MN	J	102	-	-	-	X

2 Entry composition ⓘ

There are 9 unique types of molecules in this entry. The entry contains 12111 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 DNA (147-MER).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	I	147	Total	C	N	O	P	S	0	0	0
			3014	1440	548	879	146	1			

- Molecule 2 is a DNA chain called DNA (147-MER).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	J	147	Total	C	N	O	P	S	0	0	0
			3013	1440	545	881	146	1			

- Molecule 3 is a protein called Histone H3.2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	96	Total	C	N	O	S	0	0	0
			789	498	151	137	3			
3	E	97	Total	C	N	O	S	0	0	0
			794	501	152	138	3			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	40	CYS	ARG	engineered mutation	UNP P84233
A	102	ALA	GLY	conflict	UNP P84233
A	110	ALA	CYS	engineered mutation	UNP P84233
E	40	CYS	ARG	engineered mutation	UNP P84233
E	102	ALA	GLY	conflict	UNP P84233
E	110	ALA	CYS	engineered mutation	UNP P84233

- Molecule 4 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	78	Total	C	N	O	S	0	0	0
			618	391	120	106	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	84	Total 673	C 424	N 133	O 115	S 1	0	0	0

- Molecule 5 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	C	106	Total 820	C 517	N 160	O 143	0	0	0
5	G	106	Total 818	C 516	N 160	O 142	0	0	0

- Molecule 6 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	94	Total 735	C 463	N 132	O 138	S 2	0	0	0
6	H	93	Total 726	C 457	N 130	O 137	S 2	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	29	THR	SER	conflict	UNP P02281
H	29	THR	SER	conflict	UNP P02281

- Molecule 7 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	I	10	Total 10	Mn 10	0	0
7	J	9	Total 9	Mn 9	0	0
7	E	1	Total 1	Mn 1	0	0

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total 1	Cl 1	0	0
8	D	1	Total 1	Cl 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	E	1	Total 1	Cl 1	0	0
8	G	1	Total 1	Cl 1	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	I	16	Total 16	O 16	0	0
9	J	17	Total 17	O 17	0	0
9	A	3	Total 3	O 3	0	0
9	B	4	Total 4	O 4	0	0
9	C	12	Total 12	O 12	0	0
9	D	5	Total 5	O 5	0	0
9	E	10	Total 10	O 10	0	0
9	F	11	Total 11	O 11	0	0
9	G	4	Total 4	O 4	0	0
9	H	5	Total 5	O 5	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 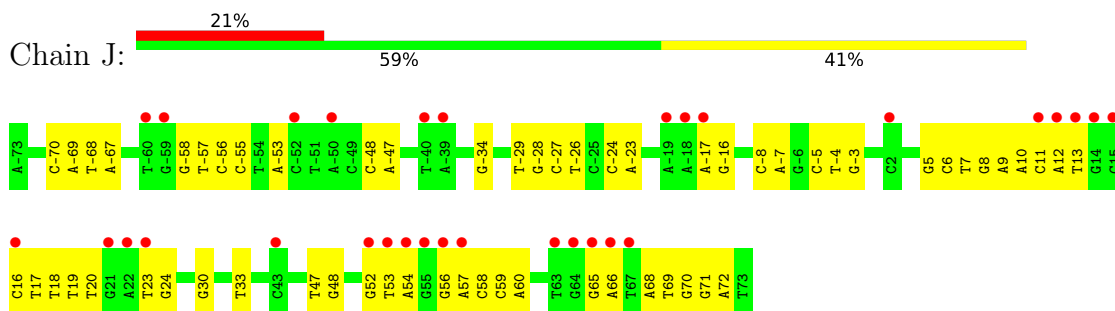view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron 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.
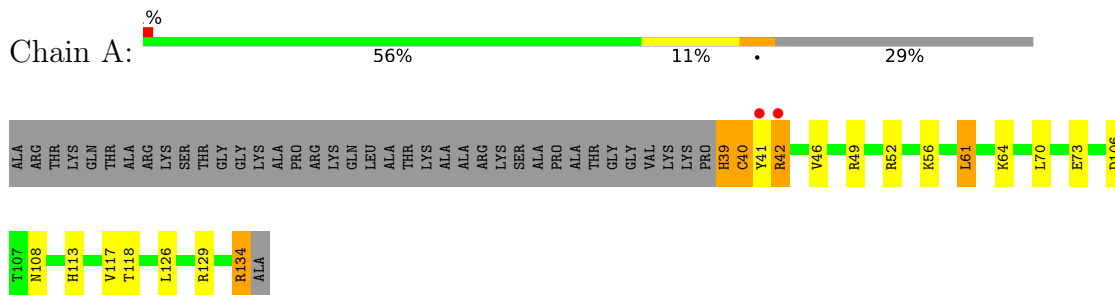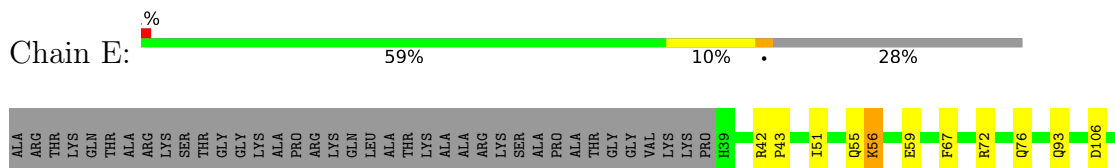
- Molecule 1: DNA (147-MER)

Chain I:
22%
57%   42%

- Molecule 2: DNA (147-MER)

Chain J:
21%
59%   41%

- Molecule 3: Histone H3.2

Chain A:
%
56%   11%   29%

- Molecule 3: Histone H3.2

Chain E:
%
59%   10%   28%

H113 L126 R129 I130 R131 R134 A135

• Molecule 4: Histone H4

Chain B:

62% 14% 24%

MET SER GLY ARG GLY LYS GLY GLY LYS GLY LEU GLY LYS GLY GLY ALA LYS ARG HIS ARG LYS VAL LEU ARG ASP N25 I29 T30 K31 P32 R35 R36 V43 K44 R45 K59 L62 E63 I66 K91 T96 G102

• Molecule 4: Histone H4

Chain F:

69% 13% 18%

MET SER GLY ARG GLY LYS GLY GLY LYS GLY LEU GLY LYS GLY GLY ALA LYS ARG HIS R19 R23 T30 K31 P32 R35 R40 I46 L62 V65 K77 Q93 T96 G102

• Molecule 5: Histone H2A

Chain C:

2%

73% 9% 18%

SER GLY ARG GLY LYS GLN GLY GLY LYS THR ARG ALA LYS ALA K15 R29 V30 H31 Y39 P48 L55 L58 T59 L63 E64 L93 T101 I102 K118 K119 T120 GLU SER SER LYS SER ALA LYS SER LYS

• Molecule 5: Histone H2A

Chain G:

2%

71% 11% • 18%

SER GLY ARG GLY LYS GLN GLY GLY LYS THR ARG ALA LYS A14 K15 H31 R32 R35 K36 G37 N38 Y39 L51 L63 G67 R77 I78 I79 H82 L97 V100 P109 L115 K119 THR GLU SER SER LYS SER ALA LYS SER LYS

• Molecule 6: Histone H2B 1.1

Chain D:

69% 7% • 23%

ALA LYS SER ALA PRO ALA PRO LYS LYS GLY SER LYS LYS ALA VAL THR LYS THR GLN LYS LYS ASP GLY LYS LYS ARG ARG K28 S33 V41 H46 I58 M59 N60 V66 S75 R83 G101 A121 LYS

• Molecule 6: Histone H2B 1.1

Chain H:

2%

65% 11% 24%

ALA LYS SER ALA PRO ALA PRO LYS LYS GLY SER LYS LYS ALA VAL THR LYS THR GLN LYS LYS ASP GLY LYS LYS ARG ARG LYS T29 R30 K31 E32 L42 V45 H46 G50 E73 R83 T87 S88 R89 E90 I91 Q92 T93 A94 G101 V108 A121 LYS

4   Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	106.24Å 183.13Å 109.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.50 – 2.80 29.50 – 2.80	Depositor EDS
% Data completeness (in resolution range)	89.4 (29.50-2.80) 89.5 (29.50-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.17 (at 2.80Å)	Xtriage
Refinement program	PHENIX (dev_2447: ???)	Depositor
R, R_{free}	0.206 , 0.247 0.206 , 0.247	Depositor DCC
R_{free} test set	4814 reflections (10.07%)	wwPDB-VP
Wilson B-factor (Å^2)	62.2	Xtriage
Anisotropy	0.567	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 68.0	EDS
L-test for twinning[2]	$< |L| > = 0.45, < L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.042 for l,-k,h	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	12111	wwPDB-VP
Average B, all atoms (Å^2)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, G47, 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	0.51	0/3352	0.95	0/5169
2	J	0.50	0/3350	0.97	0/5166
3	A	0.26	0/800	0.40	0/1074
3	E	0.25	0/805	0.38	0/1081
4	B	0.24	0/625	0.42	0/837
4	F	0.24	0/680	0.43	0/908
5	C	0.23	0/830	0.41	0/1120
5	G	0.25	0/828	0.41	0/1117
6	D	0.24	0/746	0.40	0/1004
6	H	0.24	0/737	0.39	0/993
All	All	0.40	0/12753	0.77	0/18469

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	3014	0	1663	47	0
2	J	3013	0	1664	47	0
3	A	789	0	824	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	794	0	829	12	0
4	B	618	0	659	12	0
4	F	673	0	722	6	0
5	C	820	0	879	10	0
5	G	818	0	877	12	0
6	D	735	0	760	9	0
6	H	726	0	747	10	0
7	E	1	0	0	0	0
7	I	10	0	0	0	0
7	J	9	0	0	0	0
8	A	1	0	0	0	0
8	D	1	0	0	0	0
8	E	1	0	0	0	0
8	G	1	0	0	0	0
9	A	3	0	0	0	0
9	B	4	0	0	0	0
9	C	12	0	0	0	0
9	D	5	0	0	0	0
9	E	10	0	0	1	0
9	F	11	0	0	1	0
9	G	4	0	0	1	0
9	H	5	0	0	0	0
9	I	16	0	0	0	0
9	J	17	0	0	1	0
All	All	12111	0	9624	152	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 7.

The worst 5 of 152 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:I:56:DG:N2	2:J:-56:DC:O2	2.06	0.88
4:F:40:ARG:O	9:F:201:HOH:O	1.95	0.84
1:I:-27:DC:H2"	1:I:-26:DT:H71	1.66	0.77
1:I:39:DT:OP2	5:G:35:ARG:NH2	2.20	0.74
3:E:51:ILE:O	3:E:55:GLN:HB2	1.91	0.71

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	
3	A	94/135 (70%)	92 (98%)	1 (1%)	1 (1%)	14	41
3	E	95/135 (70%)	94 (99%)	1 (1%)	0	100	100
4	B	76/103 (74%)	75 (99%)	1 (1%)	0	100	100
4	F	82/103 (80%)	77 (94%)	5 (6%)	0	100	100
5	C	104/129 (81%)	102 (98%)	2 (2%)	0	100	100
5	G	104/129 (81%)	102 (98%)	2 (2%)	0	100	100
6	D	92/122 (75%)	91 (99%)	0	1 (1%)	14	41
6	H	91/122 (75%)	89 (98%)	1 (1%)	1 (1%)	14	41
All	All	738/978 (76%)	722 (98%)	13 (2%)	3 (0%)	34	66

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	D	101	GLY
3	A	40	CYS
6	H	101	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	83/109 (76%)	78 (94%)	5 (6%)	19	48
3	E	83/109 (76%)	79 (95%)	4 (5%)	25	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	B	63/79 (80%)	63 (100%)	0	100	100
4	F	69/79 (87%)	65 (94%)	4 (6%)	20	50
5	C	85/101 (84%)	84 (99%)	1 (1%)	71	92
5	G	84/101 (83%)	82 (98%)	2 (2%)	49	81
6	D	80/102 (78%)	78 (98%)	2 (2%)	47	80
6	H	79/102 (78%)	79 (100%)	0	100	100
All	All	626/782 (80%)	608 (97%)	18 (3%)	42	76

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	F	93	GLN
5	G	77	ARG
5	G	51	LEU
3	E	56	LYS
4	F	23	ARG

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

Mol	Chain	Res	Type
3	A	108	ASN
6	D	44	GLN
6	D	46	HIS
6	H	92	GLN

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	#$|Z| > 2$
2	G47	J	70	7,1,3,2	19,27,28	1.33	3 (15%)	17,38,41	0.78	1 (5%)
1	G47	I	70	1,3,2	19,27,28	1.25	2 (10%)	17,38,41	0.73	1 (5%)

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
2	G47	J	70	7,1,3,2	-	3/7/25/26	0/3/3/3
1	G47	I	70	1,3,2	-	2/7/25/26	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	70	G47	C6A-N2	-3.43	1.38	1.46
1	I	70	G47	C6A-N2	-3.39	1.38	1.46
1	I	70	G47	C8-N7	-2.37	1.31	1.35
2	J	70	G47	C8-N7	-2.33	1.31	1.35
2	J	70	G47	C7A-SG	2.33	1.89	1.80

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	70	G47	O6-C6-C5	2.16	128.59	124.37
1	I	70	G47	O6-C6-C5	2.11	128.49	124.37

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	I	70	G47	N1-C2-N2-C6A
1	I	70	G47	N3-C2-N2-C6A
2	J	70	G47	N1-C2-N2-C6A
2	J	70	G47	N3-C2-N2-C6A
2	J	70	G47	C7A-C6A-N2-C2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	I	70	G47	2	0

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 24 ligands modelled in this entry, 24 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	I	146/147 (99%)	1.29	33 (22%)	0	0	70, 129, 180, 193	0
2	J	146/147 (99%)	1.32	31 (21%)	0	0	70, 126, 173, 218	0
3	A	96/135 (71%)	0.60	2 (2%)	63	54	39, 61, 98, 132	0
3	E	97/135 (71%)	0.51	1 (1%)	82	77	27, 45, 93, 138	0
4	B	78/103 (75%)	0.39	0	100	100	38, 57, 80, 86	0
4	F	84/103 (81%)	0.33	0	100	100	28, 45, 65, 106	0
5	C	106/129 (82%)	0.36	3 (2%)	53	43	26, 47, 79, 162	0
5	G	106/129 (82%)	0.50	3 (2%)	53	43	39, 67, 102, 144	0
6	D	94/122 (77%)	0.23	0	100	100	31, 51, 85, 115	0
6	H	93/122 (76%)	0.29	2 (2%)	62	52	35, 64, 97, 126	0
All	All	1046/1272 (82%)	0.66	75 (7%)	15	8	26, 64, 157, 218	0

The worst 5 of 75 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	G	119	LYS	8.6
5	C	120	THR	7.7
5	G	14	ALA	5.9
2	J	55	DG	5.8
2	J	54	DA	5.2

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
2	G47	J	70	25/26	0.88	0.21	104,115,131,150	0
1	G47	I	70	25/26	0.89	0.21	101,118,149,165	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
7	MN	I	108	1/1	0.58	0.15	133,133,133,133	1
7	MN	I	101	1/1	0.63	0.07	148,148,148,148	0
7	MN	I	103	1/1	0.68	0.28	174,174,174,174	0
7	MN	J	102	1/1	0.77	0.53	128,128,128,128	0
7	MN	J	103	1/1	0.78	0.08	133,133,133,133	0
7	MN	J	104	1/1	0.78	0.10	148,148,148,148	0
7	MN	J	101	1/1	0.79	0.20	131,131,131,131	0
7	MN	I	104	1/1	0.80	0.12	154,154,154,154	0
7	MN	I	109	1/1	0.82	0.19	103,103,103,103	1
7	MN	I	102	1/1	0.83	0.18	136,136,136,136	0
7	MN	I	107	1/1	0.83	0.09	125,125,125,125	0
8	CL	A	201	1/1	0.83	0.21	50,50,50,50	1
7	MN	I	106	1/1	0.84	0.17	117,117,117,117	0
7	MN	I	105	1/1	0.86	0.23	103,103,103,103	0
7	MN	J	107	1/1	0.87	0.29	100,100,100,100	0
7	MN	J	106	1/1	0.89	0.09	104,104,104,104	0
8	CL	D	201	1/1	0.91	0.20	68,68,68,68	0
7	MN	J	108	1/1	0.92	0.23	101,101,101,101	0
8	CL	G	201	1/1	0.92	0.27	63,63,63,63	0
7	MN	I	110	1/1	0.95	0.11	110,110,110,110	0
8	CL	E	202	1/1	0.96	0.10	53,53,53,53	1
7	MN	J	109	1/1	0.96	0.24	93,93,93,93	0
7	MN	J	105	1/1	0.98	0.17	93,93,93,93	0
7	MN	E	201	1/1	0.99	0.27	42,42,42,42	0

6.5 Other polymers ⓘ

There are no such residues in this entry.