



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 02:06 PM UTC

PDB ID : 3AN2 / pdb_00003an2
Title : The structure of the centromeric nucleosome containing CENP-A
Authors : Tachiwana, H.; Kagawa, W.; Shiga, T.; Saito, K.; Osakabe, A.; Hayashi-Takanaka, Y.; Park, S.-Y.; Kimura, H.; Kurumizaka, H.
Deposited on : 2010-08-27
Resolution : 3.60 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) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

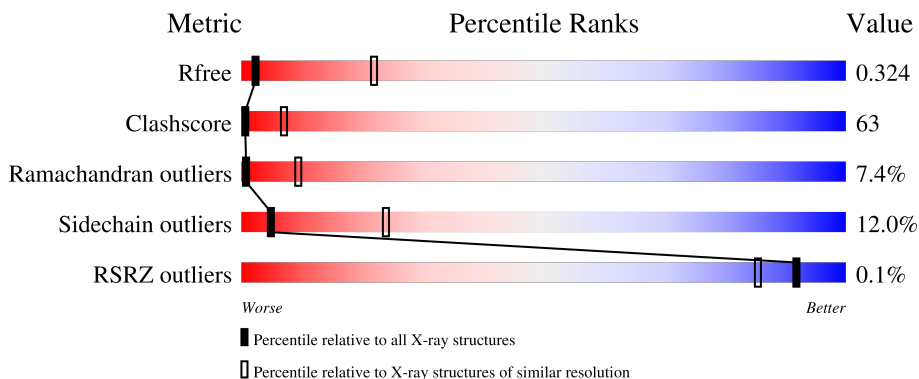
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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.






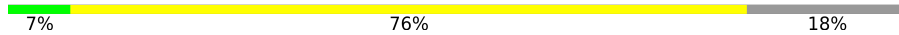
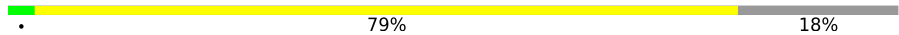
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

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 $\leq 5\%$. 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	A	143	
1	E	143	
2	B	106	
2	F	106	
3	C	133	

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Mol	Chain	Length	Quality of chain
3	G	133	
4	D	129	
4	H	129	
5	I	147	
5	J	147	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10542 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 protein called Histone H3-like centromeric protein A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	89	Total 732	C 477	N 136	O 118	S 1	0	0	0
1	E	83	Total 685	C 449	N 126	O 109	S 1	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P49450
A	-1	SER	-	expression tag	UNP P49450
A	0	HIS	-	expression tag	UNP P49450
E	-2	GLY	-	expression tag	UNP P49450
E	-1	SER	-	expression tag	UNP P49450
E	0	HIS	-	expression tag	UNP P49450

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	78	Total 619	C 391	N 120	O 107	S 1	0	0	0
2	F	79	Total 627	C 395	N 121	O 110	S 1	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP B2R4R0
B	-2	SER	-	expression tag	UNP B2R4R0
B	-1	HIS	-	expression tag	UNP B2R4R0
F	-3	GLY	-	expression tag	UNP B2R4R0
F	-2	SER	-	expression tag	UNP B2R4R0
F	-1	HIS	-	expression tag	UNP B2R4R0

- Molecule 3 is a protein called Histone H2A type 1-B/E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	97	Total	C	N	O	0	0	0
			752	471	148	133			
3	G	100	Total	C	N	O	0	0	0
			773	485	152	136			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	GLY	-	expression tag	UNP P04908
C	-2	SER	-	expression tag	UNP P04908
C	-1	HIS	-	expression tag	UNP P04908
G	-3	GLY	-	expression tag	UNP P04908
G	-2	SER	-	expression tag	UNP P04908
G	-1	HIS	-	expression tag	UNP P04908

- Molecule 4 is a protein called Histone H2B type 1-J.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
4	D	90	Total	C	N	O	Se	0	0	0
			699	441	123	133	2			
4	H	90	Total	C	N	O	Se	0	0	0
			699	441	123	133	2			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-3	GLY	-	expression tag	UNP P06899
D	-2	SER	-	expression tag	UNP P06899
D	-1	HIS	-	expression tag	UNP P06899
H	-3	GLY	-	expression tag	UNP P06899
H	-2	SER	-	expression tag	UNP P06899
H	-1	HIS	-	expression tag	UNP P06899

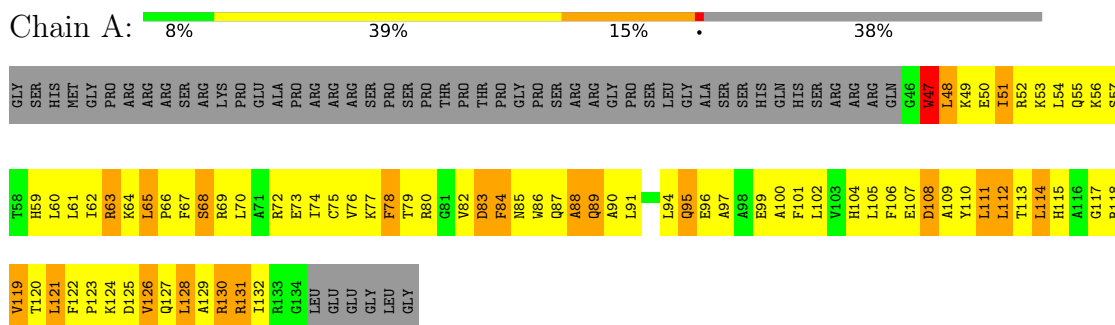
- Molecule 5 is a DNA chain called 147 mer DNA.

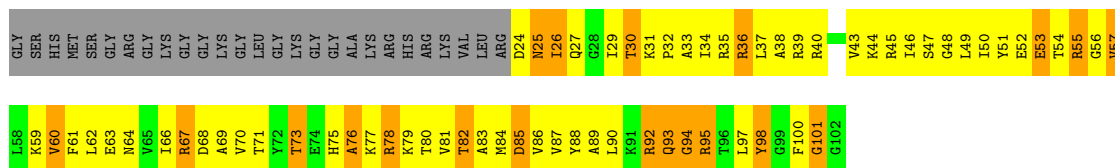
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
5	I	121	Total	C	N	O	P	0	0	0
			2478	1187	448	723	120			
5	J	121	Total	C	N	O	P	0	0	0
			2478	1187	448	723	120			

3 Residue-property plots

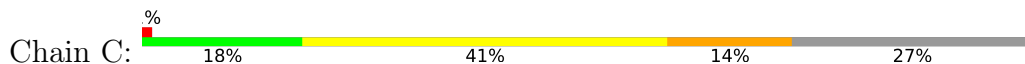
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Histone H3-like centromeric protein A

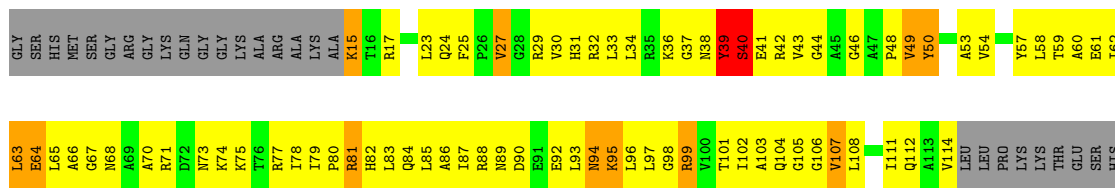
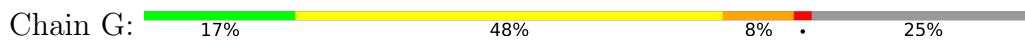




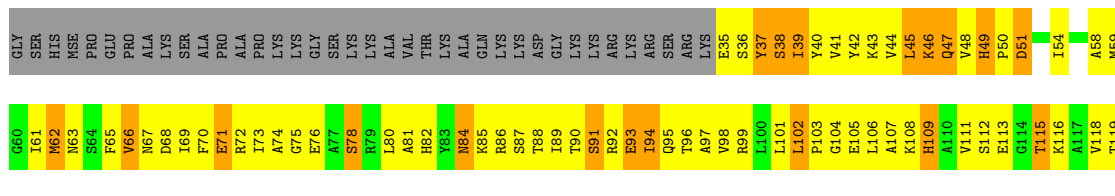
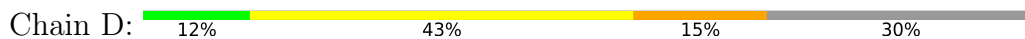
• Molecule 3: Histone H2A type 1-B/E



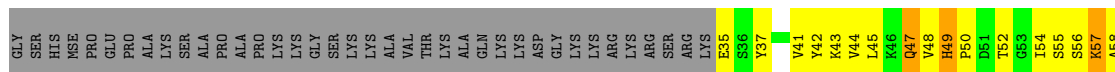
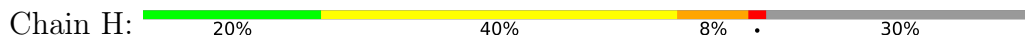
• Molecule 3: Histone H2A type 1-B/E

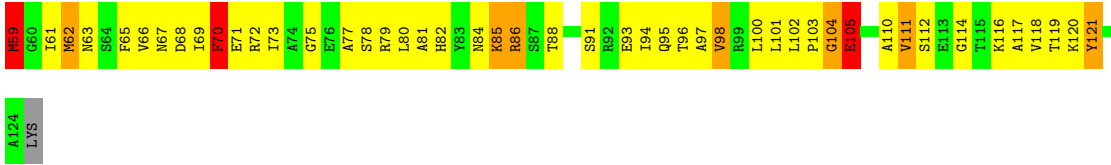


• Molecule 4: Histone H2B type 1-J

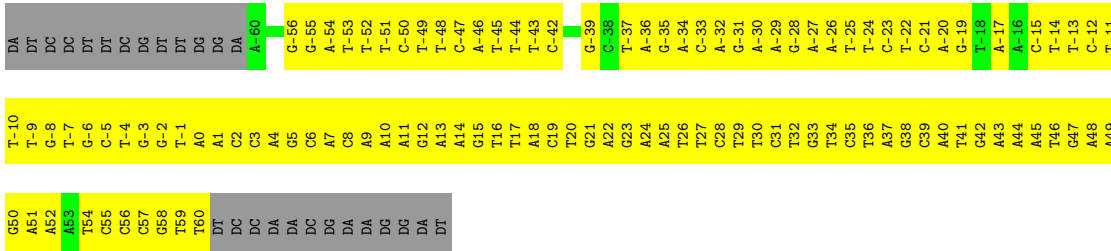
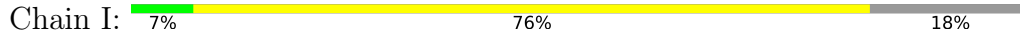


• Molecule 4: Histone H2B type 1-J

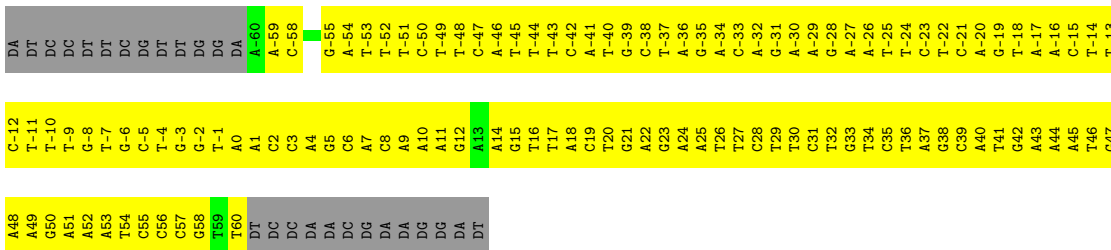
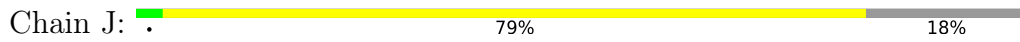




• Molecule 5: 147 mer DNA



• Molecule 5: 147 mer DNA



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	65.84Å 83.29Å 176.83Å 90.00° 100.70° 90.00°	Depositor
Resolution (Å)	50.00 – 3.60 50.00 – 3.60	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.60) 95.1 (50.00-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.96 (at 3.57Å)	Xtrriage
Refinement program	CNS 1.21	Depositor
R, R_{free}	0.271 , 0.325 0.271 , 0.324	Depositor DCC
R_{free} test set	1089 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	85.5	Xtrriage
Anisotropy	0.441	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 104.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.20$	Xtrriage
Estimated twinning fraction	0.339 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	10542	wwPDB-VP
Average B, all atoms (Å ²)	106.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.91% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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](#)

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	A	0.49	0/747	1.10	10/1006 (1.0%)
1	E	0.45	0/697	1.12	8/936 (0.9%)
2	B	0.54	0/626	1.11	5/837 (0.6%)
2	F	0.66	0/634	1.38	11/848 (1.3%)
3	C	0.59	0/761	1.12	7/1027 (0.7%)
3	G	0.67	0/782	1.21	8/1055 (0.8%)
4	D	0.66	0/708	1.41	13/951 (1.4%)
4	H	0.61	0/708	1.23	12/951 (1.3%)
5	I	0.28	0/2780	0.67	0/4289
5	J	0.29	0/2780	0.67	0/4289
All	All	0.47	0/11223	0.96	74/16189 (0.5%)

There are no bond length outliers.

The worst 5 of 74 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	76	ALA	N-CA-C	-12.46	84.25	110.80
4	D	78	SER	N-CA-C	-10.62	99.71	111.07
2	F	85	ASP	N-CA-C	-10.48	98.80	111.69
4	D	47	GLN	N-CA-C	-10.06	99.30	112.68
2	F	76	ALA	CA-C-N	-9.04	108.08	122.73

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	A	732	0	770	139	0
1	E	685	0	731	140	0
2	B	619	0	659	135	0
2	F	627	0	663	125	0
3	C	752	0	792	118	0
3	G	773	0	819	100	0
4	D	699	0	714	103	0
4	H	699	0	714	78	0
5	I	2478	0	1370	224	0
5	J	2478	0	1370	273	0
All	All	10542	0	8602	1197	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 63.

The worst 5 of 1197 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)
5:I:-9:DT:H2''	5:I:-8:DG:H5'	1.30	1.14
5:J:-52:DT:H2''	5:J:-51:DT:H5''	1.13	1.11
5:J:52:DA:H2''	5:J:53:DA:H5''	1.24	1.10
5:I:-30:DA:H2''	5:I:-29:DA:H5''	1.32	1.09
5:J:21:DG:H2''	5:J:22:DA:H5'	1.36	1.08

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
1	A	87/143 (61%)	63 (72%)	15 (17%)	9 (10%)	0 5
1	E	79/143 (55%)	59 (75%)	16 (20%)	4 (5%)	1 15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	76/106 (72%)	44 (58%)	18 (24%)	14 (18%)	0	1
2	F	77/106 (73%)	61 (79%)	13 (17%)	3 (4%)	2	20
3	C	95/133 (71%)	72 (76%)	19 (20%)	4 (4%)	2	19
3	G	98/133 (74%)	72 (74%)	21 (21%)	5 (5%)	1	15
4	D	88/129 (68%)	65 (74%)	16 (18%)	7 (8%)	1	8
4	H	88/129 (68%)	63 (72%)	20 (23%)	5 (6%)	1	13
All	All	688/1022 (67%)	499 (72%)	138 (20%)	51 (7%)	1	9

5 of 51 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	47	SER
2	B	49	LEU
2	B	99	GLY
4	D	49	HIS
1	E	118	ARG

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	
1	A	75/120 (62%)	66 (88%)	9 (12%)	5	24
1	E	71/120 (59%)	65 (92%)	6 (8%)	10	35
2	B	63/81 (78%)	55 (87%)	8 (13%)	4	22
2	F	64/81 (79%)	56 (88%)	8 (12%)	4	22
3	C	77/102 (76%)	67 (87%)	10 (13%)	4	21
3	G	79/102 (78%)	70 (89%)	9 (11%)	5	26
4	D	76/104 (73%)	67 (88%)	9 (12%)	5	24
4	H	76/104 (73%)	65 (86%)	11 (14%)	3	18
All	All	581/814 (71%)	511 (88%)	70 (12%)	5	24

5 of 70 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	G	101	THR
4	H	49	HIS
4	H	85	LYS
3	C	88	ARG
3	C	84	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	25	ASN
3	G	68	ASN
3	G	31	HIS
3	G	73	ASN
3	C	31	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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(Å ²)	Q<0.9
1	A	89/143 (62%)	-0.81	0 100 100	58, 82, 103, 124	0
1	E	83/143 (58%)	-0.71	0 100 100	58, 80, 96, 102	0
2	B	78/106 (73%)	-0.87	0 100 100	51, 73, 94, 98	0
2	F	79/106 (74%)	-0.89	0 100 100	50, 68, 96, 102	0
3	C	97/133 (72%)	-0.76	1 (1%) 79 54	43, 66, 84, 93	0
3	G	100/133 (75%)	-0.80	0 100 100	36, 65, 93, 112	0
4	D	88/129 (68%)	-0.80	0 100 100	44, 67, 87, 92	0
4	H	88/129 (68%)	-0.84	0 100 100	35, 63, 80, 88	0
5	I	121/147 (82%)	-0.26	0 100 100	95, 147, 179, 195	0
5	J	121/147 (82%)	-0.28	0 100 100	80, 149, 183, 192	0
All	All	944/1316 (71%)	-0.67	1 (0%) 92 85	35, 77, 165, 195	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	74	LYS	2.2

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.