



wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 28, 2016 – 03:33 PM EDT

PDB ID : 5G2E
Title : Structure of the Nap1 H2A H2B complex
Authors : AguilarGurrieri, C.; Larabi, A.; Vinayachandran, V.; Patel, N.A.; Yen, K.;
Reja, R.; Ebong, I.O.; Schoehn, G.; Robinson, C.V.; Pugh, B.F.; Panne, D.
Deposited on : 2016-04-07
Resolution : 6.70 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

<http://wwpdb.org/validation/2016/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	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

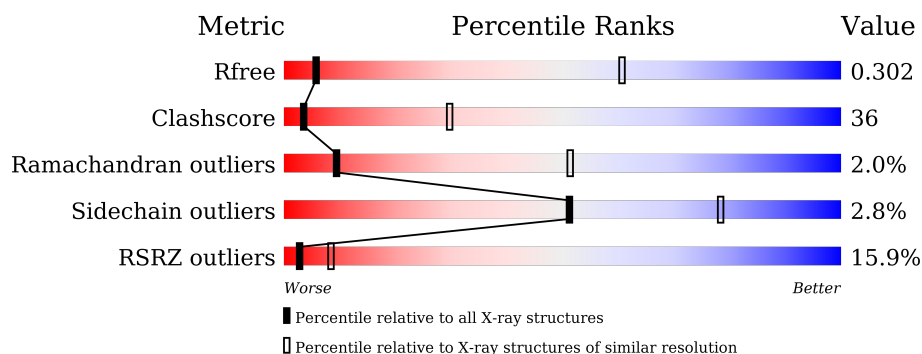
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 6.70 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}	91344	1014 (9.50-3.66)
Clashscore	102246	1062 (9.50-3.70)
Ramachandran outliers	100387	1035 (9.50-3.66)
Sidechain outliers	100360	1005 (9.50-3.66)
RSRZ outliers	91569	1013 (9.50-3.66)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	310	<div> <div>10%</div> <div> <div>35%</div> <div>43%</div> <div>•</div> <div>19%</div> </div> </div>
1	B	310	<div> <div>9%</div> <div> <div>33%</div> <div>45%</div> <div>•</div> <div>21%</div> </div> </div>
1	E	310	<div> <div>13%</div> <div> <div>35%</div> <div>43%</div> <div>•</div> <div>19%</div> </div> </div>
1	F	310	<div> <div>16%</div> <div> <div>34%</div> <div>43%</div> <div>•</div> <div>21%</div> </div> </div>
1	I	310	<div> <div>11%</div> <div> <div>35%</div> <div>43%</div> <div>•</div> <div>19%</div> </div> </div>
1	J	310	<div> <div>18%</div> <div> <div>35%</div> <div>42%</div> <div>•</div> <div>21%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	M	310	
1	N	310	
1	Q	310	
1	R	310	
1	U	310	
1	V	310	
2	C	107	
2	G	107	
2	K	107	
2	O	107	
2	S	107	
2	W	107	
3	D	100	
3	H	100	
3	L	100	
3	P	100	
3	T	100	
3	X	100	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 32814 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 NUCLEOSOME ASSEMBLY PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	252	Total	C	N	O	S	0	0	0
			2067	1328	323	412	4			
1	B	245	Total	C	N	O	S	0	0	0
			2009	1297	315	393	4			
1	E	252	Total	C	N	O	S	0	0	0
			2067	1328	323	412	4			
1	F	245	Total	C	N	O	S	0	0	0
			2009	1297	315	393	4			
1	I	252	Total	C	N	O	S	0	0	0
			2067	1328	323	412	4			
1	J	245	Total	C	N	O	S	0	0	0
			2009	1297	315	393	4			
1	M	252	Total	C	N	O	S	0	0	0
			2067	1328	323	412	4			
1	N	245	Total	C	N	O	S	0	0	0
			2009	1297	315	393	4			
1	Q	252	Total	C	N	O	S	0	0	0
			2067	1328	323	412	4			
1	R	245	Total	C	N	O	S	0	0	0
			2009	1297	315	393	4			
1	U	252	Total	C	N	O	S	0	0	0
			2067	1328	323	412	4			
1	V	245	Total	C	N	O	S	0	0	0
			2009	1297	315	393	4			

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	63	SER	-	EXPRESSION TAG	UNP P25293
A	64	GLN	-	EXPRESSION TAG	UNP P25293
A	65	ASP	-	EXPRESSION TAG	UNP P25293
A	66	PRO	-	EXPRESSION TAG	UNP P25293
A	67	GLU	-	EXPRESSION TAG	UNP P25293

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Chain	Residue	Modelled	Actual	Comment	Reference
A	68	ASN	-	EXPRESSION TAG	UNP P25293
A	69	LEU	-	EXPRESSION TAG	UNP P25293
A	70	TYR	-	EXPRESSION TAG	UNP P25293
A	71	PHE	-	EXPRESSION TAG	UNP P25293
A	72	GLN	-	EXPRESSION TAG	UNP P25293
A	73	GLY	-	EXPRESSION TAG	UNP P25293
B	63	SER	-	EXPRESSION TAG	UNP P25293
B	64	GLN	-	EXPRESSION TAG	UNP P25293
B	65	ASP	-	EXPRESSION TAG	UNP P25293
B	66	PRO	-	EXPRESSION TAG	UNP P25293
B	67	GLU	-	EXPRESSION TAG	UNP P25293
B	68	ASN	-	EXPRESSION TAG	UNP P25293
B	69	LEU	-	EXPRESSION TAG	UNP P25293
B	70	TYR	-	EXPRESSION TAG	UNP P25293
B	71	PHE	-	EXPRESSION TAG	UNP P25293
B	72	GLN	-	EXPRESSION TAG	UNP P25293
B	73	GLY	-	EXPRESSION TAG	UNP P25293
E	63	SER	-	EXPRESSION TAG	UNP P25293
E	64	GLN	-	EXPRESSION TAG	UNP P25293
E	65	ASP	-	EXPRESSION TAG	UNP P25293
E	66	PRO	-	EXPRESSION TAG	UNP P25293
E	67	GLU	-	EXPRESSION TAG	UNP P25293
E	68	ASN	-	EXPRESSION TAG	UNP P25293
E	69	LEU	-	EXPRESSION TAG	UNP P25293
E	70	TYR	-	EXPRESSION TAG	UNP P25293
E	71	PHE	-	EXPRESSION TAG	UNP P25293
E	72	GLN	-	EXPRESSION TAG	UNP P25293
E	73	GLY	-	EXPRESSION TAG	UNP P25293
F	63	SER	-	EXPRESSION TAG	UNP P25293
F	64	GLN	-	EXPRESSION TAG	UNP P25293
F	65	ASP	-	EXPRESSION TAG	UNP P25293
F	66	PRO	-	EXPRESSION TAG	UNP P25293
F	67	GLU	-	EXPRESSION TAG	UNP P25293
F	68	ASN	-	EXPRESSION TAG	UNP P25293
F	69	LEU	-	EXPRESSION TAG	UNP P25293
F	70	TYR	-	EXPRESSION TAG	UNP P25293
F	71	PHE	-	EXPRESSION TAG	UNP P25293
F	72	GLN	-	EXPRESSION TAG	UNP P25293
F	73	GLY	-	EXPRESSION TAG	UNP P25293
I	63	SER	-	EXPRESSION TAG	UNP P25293
I	64	GLN	-	EXPRESSION TAG	UNP P25293
I	65	ASP	-	EXPRESSION TAG	UNP P25293

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Chain	Residue	Modelled	Actual	Comment	Reference
I	66	PRO	-	EXPRESSION TAG	UNP P25293
I	67	GLU	-	EXPRESSION TAG	UNP P25293
I	68	ASN	-	EXPRESSION TAG	UNP P25293
I	69	LEU	-	EXPRESSION TAG	UNP P25293
I	70	TYR	-	EXPRESSION TAG	UNP P25293
I	71	PHE	-	EXPRESSION TAG	UNP P25293
I	72	GLN	-	EXPRESSION TAG	UNP P25293
I	73	GLY	-	EXPRESSION TAG	UNP P25293
J	63	SER	-	EXPRESSION TAG	UNP P25293
J	64	GLN	-	EXPRESSION TAG	UNP P25293
J	65	ASP	-	EXPRESSION TAG	UNP P25293
J	66	PRO	-	EXPRESSION TAG	UNP P25293
J	67	GLU	-	EXPRESSION TAG	UNP P25293
J	68	ASN	-	EXPRESSION TAG	UNP P25293
J	69	LEU	-	EXPRESSION TAG	UNP P25293
J	70	TYR	-	EXPRESSION TAG	UNP P25293
J	71	PHE	-	EXPRESSION TAG	UNP P25293
J	72	GLN	-	EXPRESSION TAG	UNP P25293
J	73	GLY	-	EXPRESSION TAG	UNP P25293
M	63	SER	-	EXPRESSION TAG	UNP P25293
M	64	GLN	-	EXPRESSION TAG	UNP P25293
M	65	ASP	-	EXPRESSION TAG	UNP P25293
M	66	PRO	-	EXPRESSION TAG	UNP P25293
M	67	GLU	-	EXPRESSION TAG	UNP P25293
M	68	ASN	-	EXPRESSION TAG	UNP P25293
M	69	LEU	-	EXPRESSION TAG	UNP P25293
M	70	TYR	-	EXPRESSION TAG	UNP P25293
M	71	PHE	-	EXPRESSION TAG	UNP P25293
M	72	GLN	-	EXPRESSION TAG	UNP P25293
M	73	GLY	-	EXPRESSION TAG	UNP P25293
N	63	SER	-	EXPRESSION TAG	UNP P25293
N	64	GLN	-	EXPRESSION TAG	UNP P25293
N	65	ASP	-	EXPRESSION TAG	UNP P25293
N	66	PRO	-	EXPRESSION TAG	UNP P25293
N	67	GLU	-	EXPRESSION TAG	UNP P25293
N	68	ASN	-	EXPRESSION TAG	UNP P25293
N	69	LEU	-	EXPRESSION TAG	UNP P25293
N	70	TYR	-	EXPRESSION TAG	UNP P25293
N	71	PHE	-	EXPRESSION TAG	UNP P25293
N	72	GLN	-	EXPRESSION TAG	UNP P25293
N	73	GLY	-	EXPRESSION TAG	UNP P25293
Q	63	SER	-	EXPRESSION TAG	UNP P25293

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	64	GLN	-	EXPRESSION TAG	UNP P25293
Q	65	ASP	-	EXPRESSION TAG	UNP P25293
Q	66	PRO	-	EXPRESSION TAG	UNP P25293
Q	67	GLU	-	EXPRESSION TAG	UNP P25293
Q	68	ASN	-	EXPRESSION TAG	UNP P25293
Q	69	LEU	-	EXPRESSION TAG	UNP P25293
Q	70	TYR	-	EXPRESSION TAG	UNP P25293
Q	71	PHE	-	EXPRESSION TAG	UNP P25293
Q	72	GLN	-	EXPRESSION TAG	UNP P25293
Q	73	GLY	-	EXPRESSION TAG	UNP P25293
R	63	SER	-	EXPRESSION TAG	UNP P25293
R	64	GLN	-	EXPRESSION TAG	UNP P25293
R	65	ASP	-	EXPRESSION TAG	UNP P25293
R	66	PRO	-	EXPRESSION TAG	UNP P25293
R	67	GLU	-	EXPRESSION TAG	UNP P25293
R	68	ASN	-	EXPRESSION TAG	UNP P25293
R	69	LEU	-	EXPRESSION TAG	UNP P25293
R	70	TYR	-	EXPRESSION TAG	UNP P25293
R	71	PHE	-	EXPRESSION TAG	UNP P25293
R	72	GLN	-	EXPRESSION TAG	UNP P25293
R	73	GLY	-	EXPRESSION TAG	UNP P25293
U	63	SER	-	EXPRESSION TAG	UNP P25293
U	64	GLN	-	EXPRESSION TAG	UNP P25293
U	65	ASP	-	EXPRESSION TAG	UNP P25293
U	66	PRO	-	EXPRESSION TAG	UNP P25293
U	67	GLU	-	EXPRESSION TAG	UNP P25293
U	68	ASN	-	EXPRESSION TAG	UNP P25293
U	69	LEU	-	EXPRESSION TAG	UNP P25293
U	70	TYR	-	EXPRESSION TAG	UNP P25293
U	71	PHE	-	EXPRESSION TAG	UNP P25293
U	72	GLN	-	EXPRESSION TAG	UNP P25293
U	73	GLY	-	EXPRESSION TAG	UNP P25293
V	63	SER	-	EXPRESSION TAG	UNP P25293
V	64	GLN	-	EXPRESSION TAG	UNP P25293
V	65	ASP	-	EXPRESSION TAG	UNP P25293
V	66	PRO	-	EXPRESSION TAG	UNP P25293
V	67	GLU	-	EXPRESSION TAG	UNP P25293
V	68	ASN	-	EXPRESSION TAG	UNP P25293
V	69	LEU	-	EXPRESSION TAG	UNP P25293
V	70	TYR	-	EXPRESSION TAG	UNP P25293
V	71	PHE	-	EXPRESSION TAG	UNP P25293
V	72	GLN	-	EXPRESSION TAG	UNP P25293

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Chain	Residue	Modelled	Actual	Comment	Reference
V	73	GLY	-	EXPRESSION TAG	UNP P25293

- Molecule 2 is a protein called HISTONE H2A TYPE 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	90	Total 699	C 437	N 139	O 123	0	0	0
2	G	90	Total 699	C 437	N 139	O 123	0	0	0
2	K	90	Total 699	C 437	N 139	O 123	0	0	0
2	O	90	Total 699	C 437	N 139	O 123	0	0	0
2	S	90	Total 699	C 437	N 139	O 123	0	0	0
2	W	90	Total 699	C 437	N 139	O 123	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	12	MET	-	EXPRESSION TAG	UNP P06897
C	99	ARG	GLY	CONFLICT	UNP P06897
G	12	MET	-	EXPRESSION TAG	UNP P06897
G	99	ARG	GLY	CONFLICT	UNP P06897
K	12	MET	-	EXPRESSION TAG	UNP P06897
K	99	ARG	GLY	CONFLICT	UNP P06897
O	12	MET	-	EXPRESSION TAG	UNP P06897
O	99	ARG	GLY	CONFLICT	UNP P06897
S	12	MET	-	EXPRESSION TAG	UNP P06897
S	99	ARG	GLY	CONFLICT	UNP P06897
W	12	MET	-	EXPRESSION TAG	UNP P06897
W	99	ARG	GLY	CONFLICT	UNP P06897

- Molecule 3 is a protein called HISTONE H2B 1.1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	89	Total 694	C 439	N 123	O 130	S 2	0	0	0
3	H	89	Total 694	C 439	N 123	O 130	S 2	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	89	Total 694	C 439	N 123	O 130	S 2	0	0	0
3	P	89	Total 694	C 439	N 123	O 130	S 2	0	0	0
3	T	89	Total 694	C 439	N 123	O 130	S 2	0	0	0
3	X	89	Total 694	C 439	N 123	O 130	S 2	0	0	0

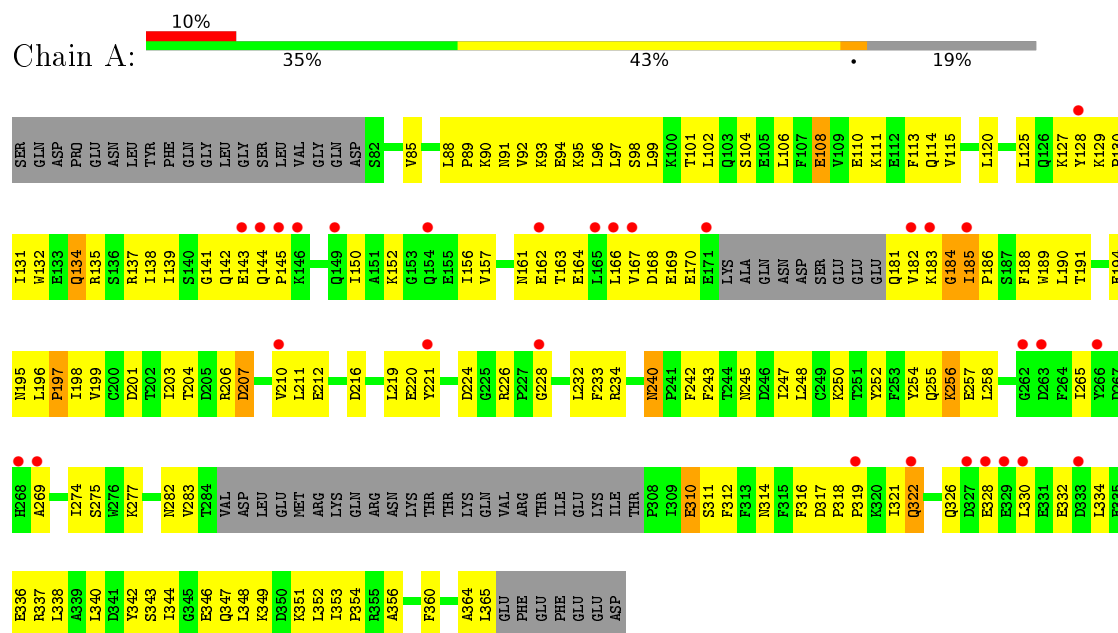
There are 12 discrepancies between the modelled and reference sequences:

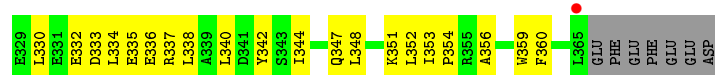
Chain	Residue	Modelled	Actual	Comment	Reference
D	23	MET	-	EXPRESSION TAG	UNP P02281
D	29	THR	SER	CONFLICT	UNP P02281
H	23	MET	-	EXPRESSION TAG	UNP P02281
H	29	THR	SER	CONFLICT	UNP P02281
L	23	MET	-	EXPRESSION TAG	UNP P02281
L	29	THR	SER	CONFLICT	UNP P02281
P	23	MET	-	EXPRESSION TAG	UNP P02281
P	29	THR	SER	CONFLICT	UNP P02281
T	23	MET	-	EXPRESSION TAG	UNP P02281
T	29	THR	SER	CONFLICT	UNP P02281
X	23	MET	-	EXPRESSION TAG	UNP P02281
X	29	THR	SER	CONFLICT	UNP P02281

3 Residue-property plots

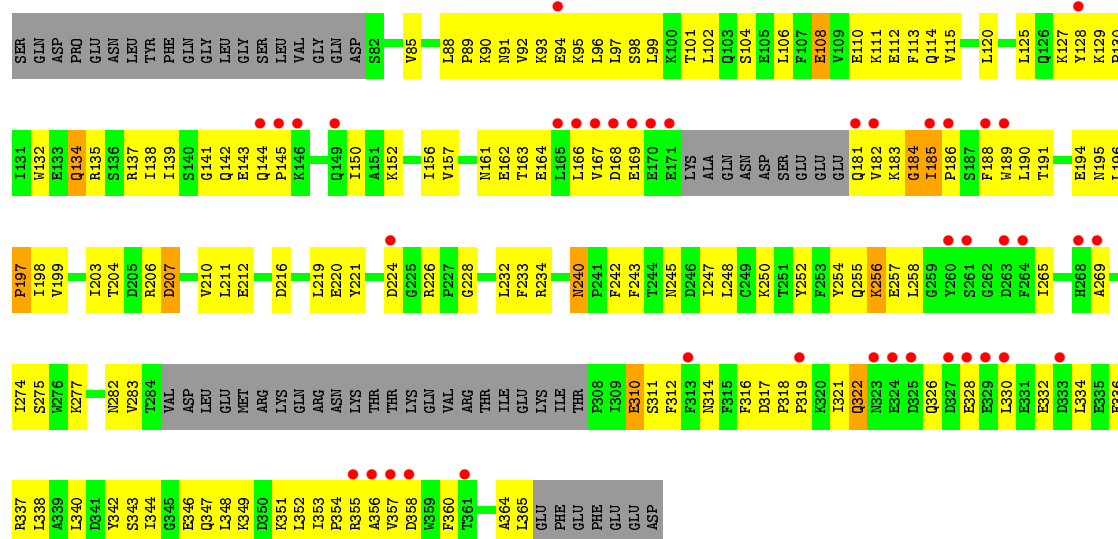
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

• Molecule 1: NUCLEOSOME ASSEMBLY PROTEIN

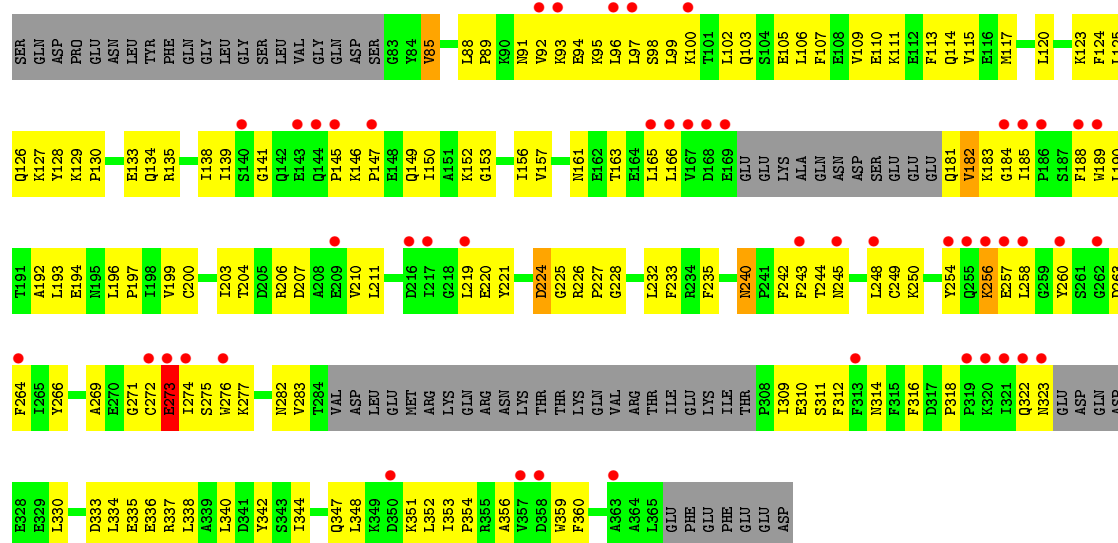




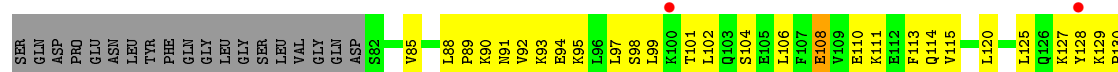
• Molecule 1: NUCLEOSOME ASSEMBLY PROTEIN

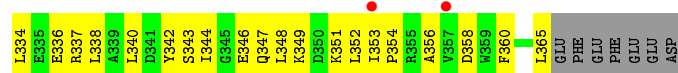


• Molecule 1: NUCLEOSOME ASSEMBLY PROTEIN

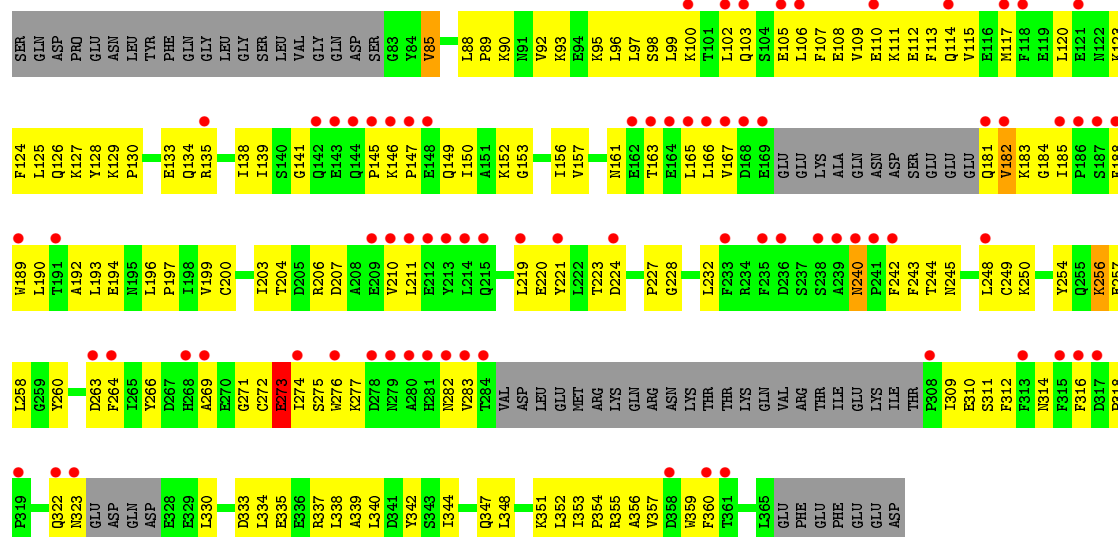


• Molecule 1: NUCLEOSOME ASSEMBLY PROTEIN

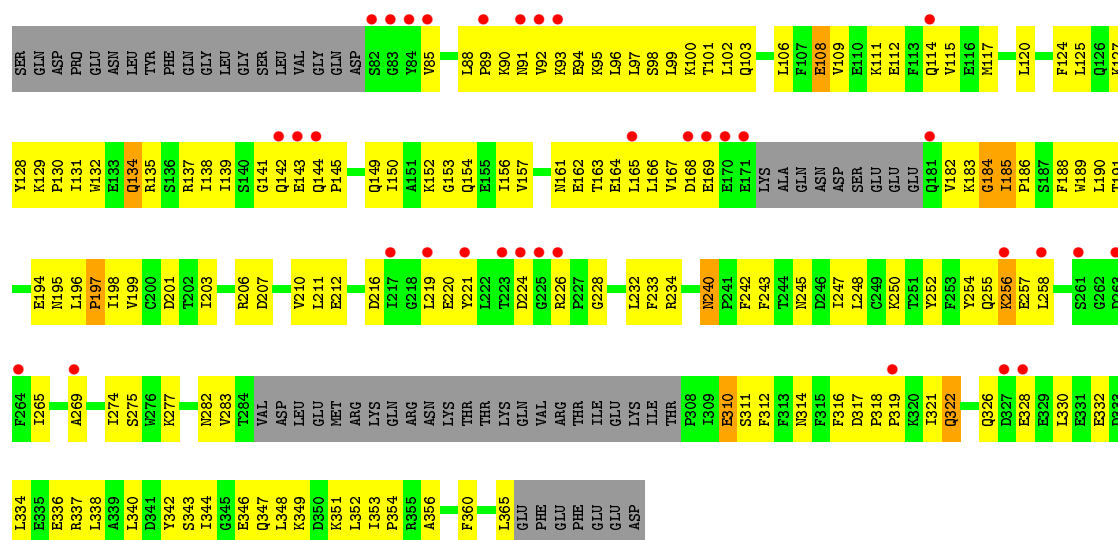




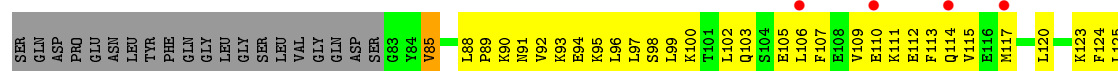
• Molecule 1: NUCLEOSOME ASSEMBLY PROTEIN

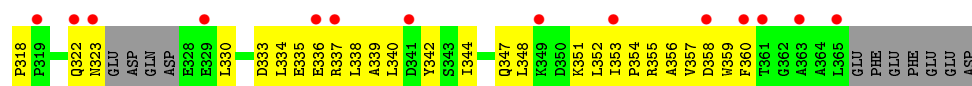


• Molecule 1: NUCLEOSOME ASSEMBLY PROTEIN

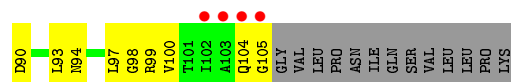
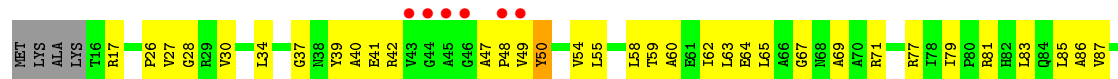


• Molecule 1: NUCLEOSOME ASSEMBLY PROTEIN

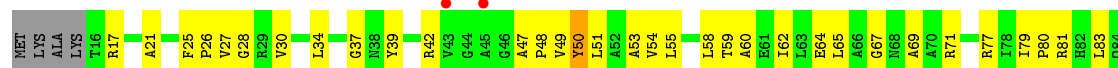




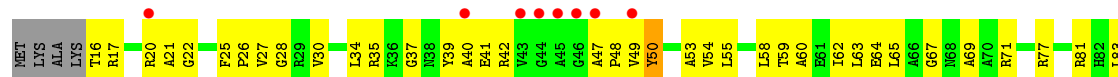
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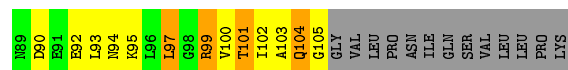
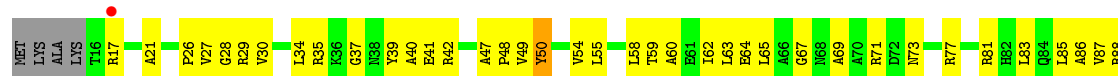
• Molecule 2: HISTONE H2A TYPE 1



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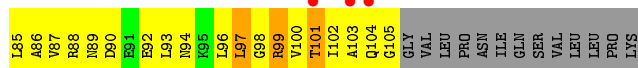
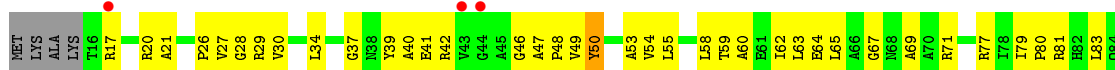


• Molecule 2: HISTONE H2A TYPE 1





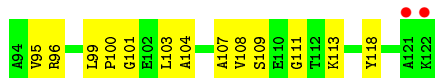
• Molecule 2: HISTONE H2A TYPE 1



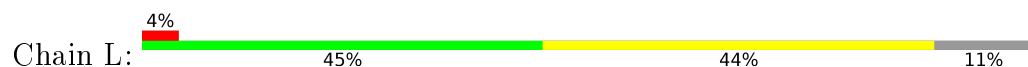
• Molecule 3: HISTONE H2B 1.1



• Molecule 3: HISTONE H2B 1.1

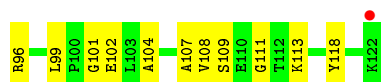


• Molecule 3: HISTONE H2B 1.1

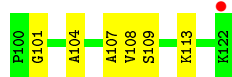


• Molecule 3: HISTONE H2B 1.1

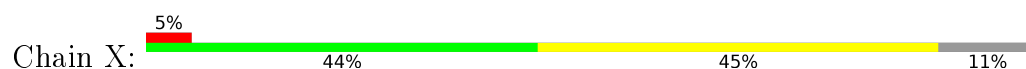




• Molecule 3: HISTONE H2B 1.1



• Molecule 3: HISTONE H2B 1.1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	111.47Å 211.13Å 126.57Å 90.00° 99.72° 90.00°	Depositor
Resolution (Å)	50.00 – 6.70 56.52 – 6.72	Depositor EDS
% Data completeness (in resolution range)	97.0 (50.00-6.70) 98.1 (56.52-6.72)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 6.69Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.263 , 0.310 0.267 , 0.302	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	276.9	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 344.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.77	EDS
Total number of atoms	32814	wwPDB-VP
Average B, all atoms (Å ²)	363.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.41% 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

5.1 Standard geometry

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	0.26	0/2112	0.45	0/2853
1	B	0.26	0/2053	0.46	0/2772
1	E	0.26	0/2112	0.45	0/2853
1	F	0.26	0/2053	0.46	0/2772
1	I	0.26	0/2112	0.45	0/2853
1	J	0.26	0/2053	0.46	0/2772
1	M	0.26	0/2112	0.45	0/2853
1	N	0.26	0/2053	0.46	0/2772
1	Q	0.26	0/2112	0.45	0/2853
1	R	0.26	0/2053	0.46	0/2772
1	U	0.26	0/2112	0.45	0/2853
1	V	0.26	0/2053	0.46	0/2772
2	C	0.22	0/707	0.41	0/953
2	G	0.38	0/707	0.57	0/953
2	K	0.22	0/707	0.62	2/953 (0.2%)
2	O	0.30	0/707	1.09	3/953 (0.3%)
2	S	62.54	2/707 (0.3%)	1.51	3/953 (0.3%)
2	W	0.21	0/707	0.40	0/953
3	D	0.24	0/705	0.42	0/949
3	H	0.24	0/705	0.42	0/949
3	L	0.24	0/705	0.42	0/949
3	P	0.24	0/705	0.42	0/949
3	T	0.24	0/705	0.42	0/949
3	X	0.24	0/705	0.42	0/949
All	All	9.09	2/33462 (0.0%)	0.52	8/45162 (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
2	K	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	S	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	105	GLY	C-O	1662.54	27.83	1.23
2	S	94	ASN	C-N	-28.57	0.68	1.34

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	105	GLY	CA-C-O	-43.57	42.17	120.60
2	O	95	LYS	O-C-N	-22.19	87.19	122.70
2	O	95	LYS	CA-C-N	15.51	151.33	117.20
2	O	95	LYS	C-N-CA	14.63	158.27	121.70
2	K	94	ASN	O-C-N	-13.31	101.40	122.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	K	94	ASN	Mainchain
2	S	94	ASN	Mainchain

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	2067	0	1986	156	0
1	B	2009	0	1946	150	0
1	E	2067	0	1986	176	0
1	F	2009	0	1946	169	0
1	I	2067	0	1986	172	0
1	J	2009	0	1946	141	0
1	M	2067	0	1986	192	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	N	2009	0	1946	172	0
1	Q	2067	0	1986	197	0
1	R	2009	0	1946	164	0
1	U	2067	0	1986	183	0
1	V	2009	0	1946	155	0
2	C	699	0	735	59	0
2	G	699	0	732	81	0
2	K	699	0	733	115	0
2	O	699	0	735	108	0
2	S	699	0	734	65	0
2	W	699	0	733	98	0
3	D	694	0	716	41	0
3	H	694	0	716	53	0
3	L	694	0	715	63	0
3	P	694	0	714	47	0
3	T	694	0	714	52	0
3	X	694	0	713	55	0
All	All	32814	0	32282	2358	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 36.

The worst 5 of 2358 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)
2:S:94:ASN:C	2:S:95:LYS:CA	1.79	1.48
2:S:94:ASN:CA	2:S:95:LYS:N	1.74	1.48
2:W:99:ARG:NH2	2:W:102:ILE:CG1	1.71	1.48
2:W:99:ARG:NH2	2:W:102:ILE:HG12	1.20	1.48
2:K:103:ALA:CA	2:O:81:ARG:NH1	1.88	1.36

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	
1	A	246/310 (79%)	208 (85%)	31 (13%)	7 (3%)	6	44
1	B	237/310 (76%)	202 (85%)	31 (13%)	4 (2%)	11	55
1	E	246/310 (79%)	209 (85%)	30 (12%)	7 (3%)	6	44
1	F	237/310 (76%)	202 (85%)	31 (13%)	4 (2%)	11	55
1	I	246/310 (79%)	209 (85%)	30 (12%)	7 (3%)	6	44
1	J	237/310 (76%)	202 (85%)	31 (13%)	4 (2%)	11	55
1	M	246/310 (79%)	209 (85%)	30 (12%)	7 (3%)	6	44
1	N	237/310 (76%)	201 (85%)	32 (14%)	4 (2%)	11	55
1	Q	246/310 (79%)	208 (85%)	31 (13%)	7 (3%)	6	44
1	R	237/310 (76%)	202 (85%)	31 (13%)	4 (2%)	11	55
1	U	246/310 (79%)	208 (85%)	31 (13%)	7 (3%)	6	44
1	V	237/310 (76%)	201 (85%)	32 (14%)	4 (2%)	11	55
2	C	88/107 (82%)	87 (99%)	1 (1%)	0	100	100
2	G	88/107 (82%)	84 (96%)	3 (3%)	1 (1%)	17	63
2	K	88/107 (82%)	84 (96%)	2 (2%)	2 (2%)	8	48
2	O	88/107 (82%)	87 (99%)	1 (1%)	0	100	100
2	S	88/107 (82%)	85 (97%)	2 (2%)	1 (1%)	17	63
2	W	88/107 (82%)	86 (98%)	1 (1%)	1 (1%)	17	63
3	D	87/100 (87%)	84 (97%)	2 (2%)	1 (1%)	17	63
3	H	87/100 (87%)	84 (97%)	2 (2%)	1 (1%)	17	63
3	L	87/100 (87%)	84 (97%)	2 (2%)	1 (1%)	17	63
3	P	87/100 (87%)	84 (97%)	2 (2%)	1 (1%)	17	63
3	T	87/100 (87%)	84 (97%)	2 (2%)	1 (1%)	17	63
3	X	87/100 (87%)	84 (97%)	2 (2%)	1 (1%)	17	63
All	All	3948/4962 (80%)	3478 (88%)	393 (10%)	77 (2%)	9	51

5 of 77 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	185	ILE
1	A	322	GLN
1	B	273	GLU

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Mol	Chain	Res	Type
1	E	185	ILE
1	E	322	GLN

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	
1	A	228/282 (81%)	220 (96%)	8 (4%)	43	74
1	B	221/282 (78%)	216 (98%)	5 (2%)	58	82
1	E	228/282 (81%)	220 (96%)	8 (4%)	43	74
1	F	221/282 (78%)	216 (98%)	5 (2%)	58	82
1	I	228/282 (81%)	220 (96%)	8 (4%)	43	74
1	J	221/282 (78%)	216 (98%)	5 (2%)	58	82
1	M	228/282 (81%)	220 (96%)	8 (4%)	43	74
1	N	221/282 (78%)	216 (98%)	5 (2%)	58	82
1	Q	228/282 (81%)	220 (96%)	8 (4%)	43	74
1	R	221/282 (78%)	216 (98%)	5 (2%)	58	82
1	U	228/282 (81%)	220 (96%)	8 (4%)	43	74
1	V	221/282 (78%)	216 (98%)	5 (2%)	58	82
2	C	70/85 (82%)	69 (99%)	1 (1%)	74	89
2	G	70/85 (82%)	62 (89%)	8 (11%)	7	32
2	K	70/85 (82%)	66 (94%)	4 (6%)	25	62
2	O	70/85 (82%)	65 (93%)	5 (7%)	18	55
2	S	70/85 (82%)	68 (97%)	2 (3%)	50	78
2	W	70/85 (82%)	67 (96%)	3 (4%)	35	70
3	D	75/86 (87%)	75 (100%)	0	100	100
3	H	75/86 (87%)	75 (100%)	0	100	100
3	L	75/86 (87%)	75 (100%)	0	100	100
3	P	75/86 (87%)	75 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	T	75/86 (87%)	75 (100%)	0	100	100
3	X	75/86 (87%)	75 (100%)	0	100	100
All	All	3564/4410 (81%)	3463 (97%)	101 (3%)	51	78

5 of 101 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	240	ASN
1	M	212	GLU
1	V	161	ASN
1	J	273	GLU
2	K	104	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 112 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	195	ASN
1	M	314	ASN
1	V	161	ASN
1	J	245	ASN
3	L	92	GLN

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 carbohydrates 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 [i](#)

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(Å ²)	Q<0.9
1	A	252/310 (81%)	0.87	30 (11%) 6 11	232, 361, 461, 501	0
1	B	245/310 (79%)	0.93	29 (11%) 6 12	281, 404, 471, 558	0
1	E	252/310 (81%)	0.99	41 (16%) 2 8	233, 361, 461, 502	0
1	F	245/310 (79%)	1.16	49 (20%) 1 7	281, 404, 470, 559	0
1	I	252/310 (81%)	1.01	34 (13%) 4 10	234, 362, 461, 502	0
1	J	245/310 (79%)	1.22	56 (22%) 1 6	281, 404, 471, 559	0
1	M	252/310 (81%)	0.88	43 (17%) 2 8	237, 362, 462, 502	0
1	N	245/310 (79%)	1.42	77 (31%) 1 5	280, 405, 470, 559	0
1	Q	252/310 (81%)	0.81	34 (13%) 4 10	235, 361, 461, 502	0
1	R	245/310 (79%)	1.44	72 (29%) 1 5	278, 406, 471, 559	0
1	U	252/310 (81%)	0.88	36 (14%) 4 9	235, 362, 462, 502	0
1	V	245/310 (79%)	1.55	85 (34%) 0 4	280, 405, 471, 559	0
2	C	90/107 (84%)	0.85	10 (11%) 7 12	159, 291, 414, 456	0
2	G	90/107 (84%)	0.48	2 (2%) 65 61	162, 288, 414, 457	0
2	K	90/107 (84%)	0.65	10 (11%) 7 12	164, 278, 362, 388	0
2	O	90/107 (84%)	0.37	1 (1%) 82 78	164, 278, 363, 388	0
2	S	90/107 (84%)	0.44	1 (1%) 82 78	164, 278, 363, 388	0
2	W	90/107 (84%)	0.65	6 (6%) 21 23	166, 290, 427, 456	0
3	D	89/100 (89%)	0.55	3 (3%) 49 46	196, 300, 396, 464	0
3	H	89/100 (89%)	0.64	6 (6%) 21 23	200, 302, 393, 464	0
3	L	89/100 (89%)	0.47	4 (4%) 37 36	199, 302, 393, 464	0
3	P	89/100 (89%)	0.60	6 (6%) 21 23	196, 302, 393, 462	0
3	T	89/100 (89%)	0.40	4 (4%) 37 36	197, 302, 392, 464	0
3	X	89/100 (89%)	0.56	5 (5%) 28 28	200, 302, 394, 462	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	4056/4962 (81%)	0.95	644 (15%) 3 8	159, 363, 464, 559	0

The worst 5 of 644 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	145	PRO	9.1
1	I	328	GLU	8.5
1	J	274	ILE	8.2
1	V	186	PRO	8.0
1	M	181	GLN	7.6

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 carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.