

wwPDB X-ray Structure Validation Summary Report (i)

Oct 31, 2023 – 11:41 AM JST

PDB ID : 5CPJ

> Title Nucleosome containing methylated Sat2R DNA

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Η.

2015-07-21 Deposited on

3.15 Å(reported) Resolution

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 (i) 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 (1)) were used in the production of this report:

MolProbity 4.02b-467

> 1.8.5 (274361), CSD as541be (2020) Mogul

Xtriage (Phenix) 1.13 EDS 2.36

20191225.v01 (using entries in the PDB archive December 25th 2019) Percentile statistics

> Refmac 5.8.0158

CCP4 7.0.044 (Gargrove) Engh & Huber (2001)

Ideal geometry (proteins) Ideal geometry (DNA, RNA) Parkinson et al. (1996)

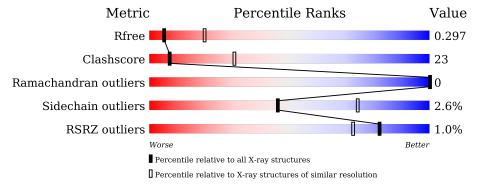
Validation Pipeline (wwPDB-VP) 2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.15 Å.

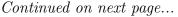
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries},{\rm resolution\ range}(\mathring{\rm A})) \end{array}$
R_{free}	130704	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

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	A	139	32%	33% •	32%
1	Е	139	35%	33% ·	30%
2	В	106	40%	34%	26%
2	F	106	39%	40%	• 21%
3	С	133	52%	25%	•• 21%
3	G	133	44%	33%	• 23%





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Mol	Chain	Length	Quality of chain								
4	D	129	45%	26% •	28%						
4	Н	129	43%	25% •	29%						
5	I	146	25%	71%	5%						
6	J	146	38%	55%	7%						



2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 11916 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 H3.1.

\mathbf{Mol}	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	94	Total 773	C 488		O 134	S 4	0	0	0
1	E	97	Total 801	C 505		O 137	S 4	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP P68431
A	-2	SER	-	expression tag	UNP P68431
A	-1	HIS	-	expression tag	UNP P68431
Е	-3	GLY	-	expression tag	UNP P68431
Е	-2	SER	-	expression tag	UNP P68431
Е	-1	HIS	-	expression tag	UNP P68431

• Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	В	78	Total 619	C 391		O 107		0	0	0
2	F	84	Total 673			O 115	S 1	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	-3	GLY	-	expression tag	UNP P62805
В	-2	SER	-	expression tag	UNP P62805
В	-1	HIS	-	expression tag	UNP P62805
F	-3	GLY	-	expression tag	UNP P62805
F	-2	SER	-	expression tag	UNP P62805
F	-1	HIS	-	expression tag	UNP P62805



• Molecule	3 1	a	protein	called	Histone	H2A	type	I-B/	/E.
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	105	Total	С	N	О	0	0	0
	105	810	511	158	141	0	U	0	
9	C	103	Total	С	N	О	0	0	0
3 G	105	796	502	155	139	0	U	U	

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
С	-3	GLY	-	expression tag	UNP P04908
С	-2	SER	-	expression tag	UNP P04908
С	-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
4	D	93	Total			0	S	0	0	0
			725	456	130	137	2			
1	Н	92	Total	С	N	Ο	S	0	0	0
4	11	92	719	453	129	135	2			U

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
Н	-3	GLY	-	expression tag	UNP P06899
Н	-2	SER	-	expression tag	UNP P06899
Н	-1	HIS	-	expression tag	UNP P06899

• Molecule 5 is a DNA chain called DNA (146-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
5	I	146	Total 3027	C 1448	N 562	O 871	P 146	0	0	0

• Molecule 6 is a DNA chain called DNA (146-MER).

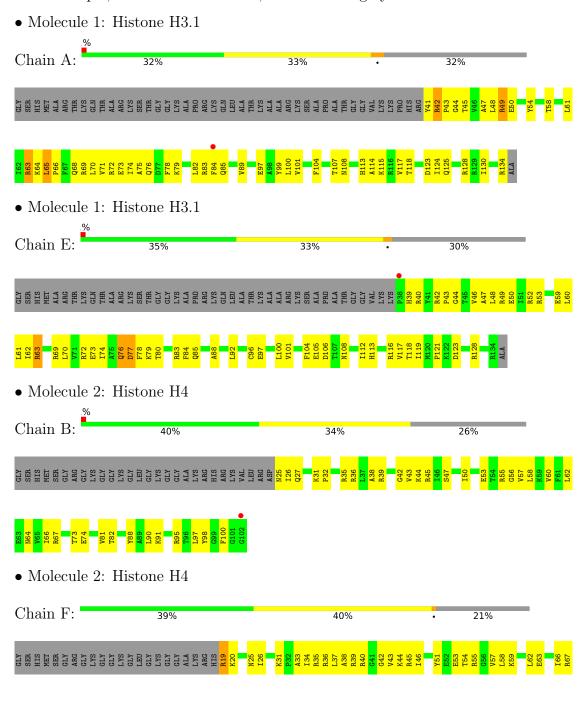


Mol	Chain	Residues		\mathbf{A}_{1}	toms			ZeroOcc	AltConf	Trace
6	J	146	Total	C 1432	N 512	O 883	P 146	0	0	0

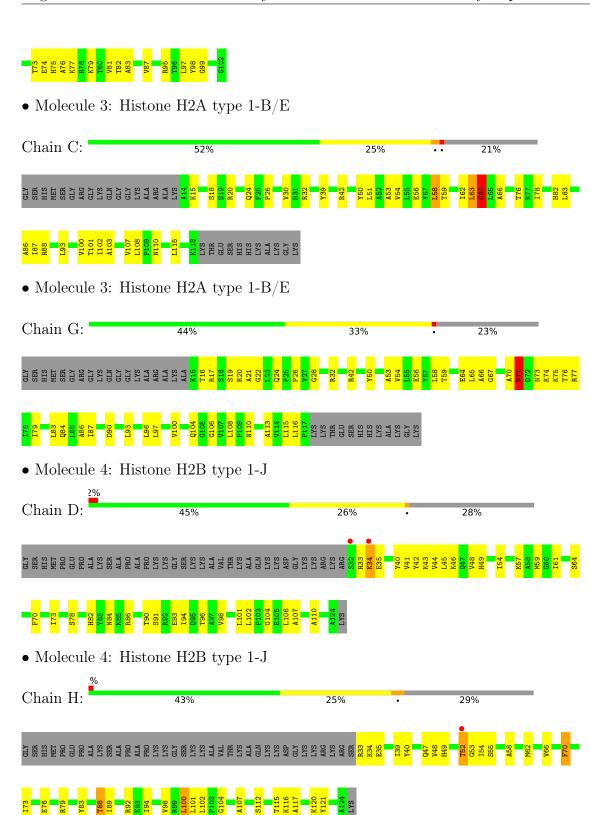


3 Residue-property plots (i)

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.







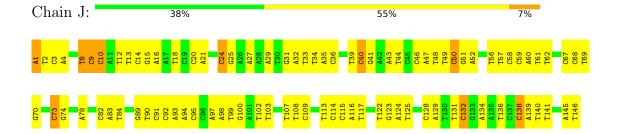


• Molecule 5: DNA (146-MER)





• Molecule 6: DNA (146-MER)





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	103.45Å 108.99Å 173.45Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.90 - 3.15	Depositor
Resolution (A)	46.45 - 3.13	EDS
% Data completeness	99.3 (24.90-3.15)	Depositor
(in resolution range)	98.0 (46.45-3.13)	EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.77 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.235 , 0.295	Depositor
it, it free	0.236 , 0.297	DCC
R_{free} test set	1995 reflections (5.71%)	wwPDB-VP
Wilson B-factor (Å ²)	89.4	Xtriage
Anisotropy	0.576	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.25, 83.1	EDS
L-test for twinning ²	$< L >=0.39, < L^2>=0.22$	Xtriage
Estimated twinning fraction	0.055 for k,h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11916	wwPDB-VP
Average B, all atoms (Å ²)	127.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.96% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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: 5CM

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	Bo	nd lengths	Bond angles		
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z >5	
1	A	0.57	0/783	0.82	$2/1050 \ (0.2\%)$	
1	Е	0.66	0/813	0.92	2/1090~(0.2%)	
2	В	0.63	1/626~(0.2%)	0.77	0/837	
2	F	0.75	0/680	0.94	2/908~(0.2%)	
3	С	0.65	1/820~(0.1%)	0.90	2/1107~(0.2%)	
3	G	0.54	0/806	0.84	1/1089 (0.1%)	
4	D	0.65	0/736	0.85	1/990 (0.1%)	
4	Н	0.55	0/730	0.81	1/982 (0.1%)	
5	I	0.79	$2/3264 \ (0.1\%)$	1.02	2/5028~(0.0%)	
6	J	0.83	$4/3188 \; (0.1\%)$	1.08	5/4898~(0.1%)	
All	All	0.73	8/12446 (0.1%)	0.97	18/17979 (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 maintain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
3	G	0	1
4	D	0	1
All	All	0	3

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

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	Observed(A)	Ideal(Å)
6	J	1	DA	OP3-P	-10.48	1.48	1.61
5	I	1	DA	OP3-P	-9.96	1.49	1.61
6	J	8	DT	C3'-O3'	-6.26	1.35	1.44
3	С	64	GLU	CB-CG	5.84	1.63	1.52
6	J	10	DC	P-O5'	5.57	1.65	1.59



The worst !	5	of	18	bond	angle	outliers	are	listed	below:
TITO WOLDO	_	\sim $_{\perp}$		OILG	WII SIC	Cathere	COL C	IID CCC	CIC III.

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
6	J	9	DC	O5'-P-OP2	-12.32	94.61	105.70
4	D	106	LEU	CA-CB-CG	7.83	133.31	115.30
1	A	63	ARG	NE-CZ-NH2	-7.44	116.58	120.30
3	G	71	ARG	CG-CD-NE	7.21	126.95	111.80
1	A	49	ARG	NE-CZ-NH1	6.83	123.71	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	65	LEU	Peptide
4	D	34	LYS	Peptide
3	G	71	ARG	Peptide

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	773	0	811	60	0
1	Е	801	0	839	68	1
2	В	619	0	659	41	0
2	F	673	0	722	74	0
3	С	810	0	866	50	0
3	G	796	0	848	55	0
4	D	725	0	745	37	1
4	Н	719	0	740	45	0
5	I	3027	0	1663	131	0
6	J	2973	0	1669	113	0
All	All	11916	0	9562	480	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 23.

The worst 5 of 480 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
1:A:65:LEU:HB2	1:A:68:GLN:HB3	1.27	1.13
2:F:19:ARG:HH22	6:J:52:DA:H3'	1.22	1.02
1:E:117:VAL:HG13	2:F:44:LYS:HE2	1.43	1.00
1:E:63:ARG:HD2	5:I:90:DA:H4'	1.47	0.97
4:H:88:THR:OG1	6:J:40:5CM:OP1	1.85	0.95

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

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
4:D:48:VAL:O	1:E:77:ASP:OD2[3_555]	2.07	0.13

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	Perce	ntiles
1	A	92/139 (66%)	88 (96%)	4 (4%)	0	100	100
1	E	95/139 (68%)	90 (95%)	5 (5%)	0	100	100
2	В	76/106 (72%)	74 (97%)	2 (3%)	0	100	100
2	F	82/106 (77%)	79 (96%)	3 (4%)	0	100	100
3	\mathbf{C}	103/133 (77%)	100 (97%)	3 (3%)	0	100	100
3	G	101/133 (76%)	97 (96%)	4 (4%)	0	100	100
4	D	91/129 (70%)	89 (98%)	2 (2%)	0	100	100
4	Н	90/129 (70%)	88 (98%)	2 (2%)	0	100	100
All	All	730/1014 (72%)	705 (97%)	25 (3%)	0	100	100

There are no Ramachandran outliers to report.



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	Percei	ntiles
1	A	82/113 (73%)	81 (99%)	1 (1%)	71	87
1	E	85/113 (75%)	83 (98%)	2 (2%)	49	76
2	В	63/81 (78%)	60 (95%)	3 (5%)	25	59
2	F	69/81 (85%)	69 (100%)	0	100	100
3	C	83/102 (81%)	82 (99%)	1 (1%)	71	87
3	G	82/102 (80%)	80 (98%)	2 (2%)	49	76
4	D	79/107 (74%)	76 (96%)	3 (4%)	33	65
4	Н	78/107 (73%)	74 (95%)	4 (5%)	24	56
All	All	621/806 (77%)	605 (97%)	16 (3%)	46	74

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	Н	88	THR
4	Н	70	PHE
1	Е	52	ARG
4	Н	52	THR
4	D	96	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	Ε	85	GLN
1	Ε	108	ASN
3	G	73	ASN
2	В	64	ASN
1	A	108	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.



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

12 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	Trino	Chain	Dag	Link	Во	ond leng	ths	В	ond ang	gles
MIOI	Type	Chain	Res	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	5CM	I	73	6,5	17,21,22	0.99	2 (11%)	24,30,33	1.48	4 (16%)
6	5CM	J	132	6	17,21,22	1.12	1 (5%)	24,30,33	1.34	3 (12%)
5	5CM	I	122	6,5	17,21,22	1.11	1 (5%)	24,30,33	1.46	4 (16%)
6	5CM	J	73	6,5	17,21,22	0.96	1 (5%)	24,30,33	1.47	3 (12%)
6	5CM	J	50	6,5	17,21,22	1.09	1 (5%)	24,30,33	1.46	4 (16%)
6	5CM	J	40	6,5	17,21,22	1.05	1 (5%)	24,30,33	1.49	4 (16%)
5	5CM	I	96	6,5	17,21,22	1.10	1 (5%)	24,30,33	1.58	4 (16%)
5	5CM	I	132	6,5	17,21,22	1.10	1 (5%)	24,30,33	1.59	3 (12%)
6	5CM	J	14	6	17,21,22	1.04	2 (11%)	24,30,33	1.23	3 (12%)
6	5CM	J	24	6,5	17,21,22	1.08	1 (5%)	24,30,33	1.58	4 (16%)
5	5CM	I	106	5	17,21,22	1.11	2 (11%)	24,30,33	1.40	3 (12%)
5	5CM	I	14	6,5	17,21,22	1.01	2 (11%)	24,30,33	1.71	4 (16%)

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
5	5CM	I	73	6,5	-	2/7/21/22	0/2/2/2
6	5CM	J	132	6	-	2/7/21/22	0/2/2/2
5	5CM	I	122	6,5	-	2/7/21/22	0/2/2/2
6	5CM	J	73	6,5	-	0/7/21/22	0/2/2/2
6	5CM	J	50	6,5	-	0/7/21/22	0/2/2/2
6	5CM	J	40	6,5	-	3/7/21/22	0/2/2/2
5	5CM	I	96	6,5	-	3/7/21/22	0/2/2/2
5	5CM	I	132	6,5	-	1/7/21/22	0/2/2/2
6	5CM	J	14	6	-	0/7/21/22	0/2/2/2

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	.,	10	1

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	5CM	J	24	6,5	-	5/7/21/22	0/2/2/2
5	5CM	I	106	5	-	2/7/21/22	0/2/2/2
5	5CM	I	14	6,5	-	2/7/21/22	0/2/2/2

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\text{\AA})$	Ideal(A)
5	I	122	5CM	C6-C5	3.70	1.40	1.34
5	I	96	5CM	C6-C5	3.43	1.40	1.34
6	J	132	5CM	C6-C5	3.37	1.40	1.34
6	J	24	5CM	C6-C5	3.34	1.40	1.34
5	I	132	5CM	C6-C5	3.34	1.40	1.34

The worst 5 of 43 bond angle outliers are listed below:

Mo	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^{o})$	$\mathbf{Ideal}(^o)$
5	I	14	5CM	O4'-C1'-N1	4.78	116.40	107.86
5	I	96	5CM	O4'-C1'-N1	4.77	116.38	107.86
5	I	132	5CM	O4'-C1'-N1	4.59	116.06	107.86
6	J	24	5CM	O4'-C1'-N1	4.50	115.91	107.86
5	I	73	5CM	O4'-C1'-N1	4.10	115.19	107.86

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	I	14	5CM	C3'-C4'-C5'-O5'
5	I	14	5CM	O4'-C4'-C5'-O5'
5	I	96	5CM	C3'-C4'-C5'-O5'
6	J	24	5CM	O4'-C4'-C5'-O5'
6	J	40	5CM	O4'-C4'-C5'-O5'

There are no ring outliers.

8 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	I	73	5CM	2	0
6	J	132	5CM	1	0
5	I	122	5CM	2	0
6	J	73	5CM	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	J	50	5CM	1	0
6	J	40	5CM	3	0
5	I	132	5CM	1	0
6	J	24	5CM	1	0

5.5 Carbohydrates (i)

There are no monosaccharides 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 (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, 95^{th} 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>	$\# \mathrm{RSRZ}{>}2$	$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q < 0.9
1	A	94/139~(67%)	0.11	1 (1%) 80 70	69, 104, 143, 163	0
1	E	97/139~(69%)	-0.07	1 (1%) 82 73	47, 75, 124, 152	0
2	В	78/106~(73%)	0.04	1 (1%) 77 66	70, 96, 117, 123	0
2	F	84/106 (79%)	-0.02	0 100 100	48, 71, 93, 123	0
3	С	105/133~(78%)	-0.18	0 100 100	50, 75, 102, 139	0
3	G	103/133~(77%)	-0.03	0 100 100	68, 92, 138, 151	0
4	D	93/129~(72%)	-0.01	2 (2%) 62 47	55, 74, 101, 151	0
4	Н	92/129 (71%)	0.02	1 (1%) 80 70	57, 91, 122, 142	0
5	I	140/146~(95%)	-0.39	4 (2%) 51 35	116, 170, 194, 203	0
6	J	140/146 (95%)	-0.40	0 100 100	111, 171, 195, 206	0
All	All	1026/1306 (78%)	-0.12	10 (0%) 82 73	47, 94, 186, 206	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Е	38	PRO	6.5
4	D	32	SER	4.7
5	I	145	DA	4.0
5	I	144	DG	3.5
5	I	146	DT	3.1

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

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, 95^{th} 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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
5	5CM	I	96	20/21	0.70	0.32	173,191,200,201	0
6	5CM	J	14	20/21	0.77	0.24	192,202,208,210	0
6	5CM	J	24	20/21	0.78	0.18	181,194,201,201	0
5	5CM	I	106	20/21	0.80	0.22	177,180,196,198	0
6	5CM	J	132	20/21	0.83	0.18	126,172,177,177	0
5	5CM	I	73	20/21	0.84	0.19	146,158,160,162	0
5	5CM	I	14	20/21	0.84	0.14	183,195,220,223	0
6	5CM	J	40	20/21	0.87	0.17	128,165,170,171	0
6	5CM	J	73	20/21	0.88	0.09	136,142,150,158	0
5	5CM	I	132	20/21	0.88	0.16	172,188,191,192	0
5	5CM	I	122	20/21	0.90	0.14	126,158,166,166	0
6	5CM	J	50	20/21	0.92	0.11	110,134,156,157	0

6.3 Carbohydrates (i)

There are no monosaccharides 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.

