



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 10:30 pm GMT

PDB ID : 5CPJ  
Title : Nucleosome containing methylated Sat2R DNA  
Authors : Osakabe, A.; Arimura, Y.; Adachi, F.; Maehara, K.; Ohkawa, Y.; Kurumizaka, H.  
Deposited on : 2015-07-21  
Resolution : 3.15 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

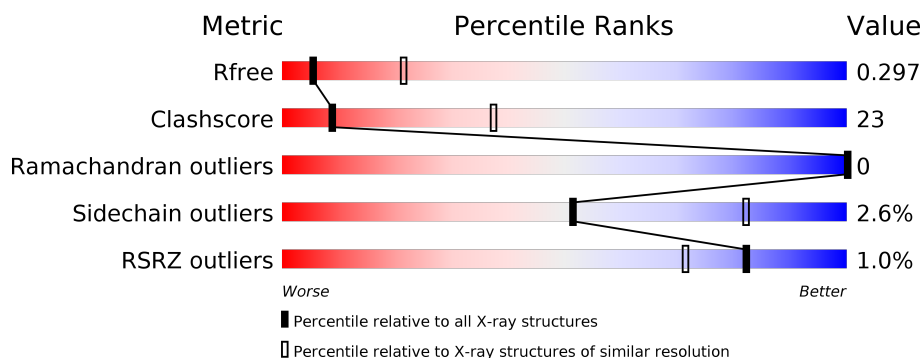
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.15 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 (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	1259 (3.20-3.12)
Clashscore	112137	1397 (3.20-3.12)
Ramachandran outliers	110173	1368 (3.20-3.12)
Sidechain outliers	110143	1367 (3.20-3.12)
RSRZ outliers	101464	1264 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	139	<div> <div>%</div> <div> <div></div> <div>32%</div> <div>33%</div> <div>•</div> <div>32%</div> </div> </div>
1	E	139	<div> <div>%</div> <div> <div></div> <div>35%</div> <div>33%</div> <div>•</div> <div>30%</div> </div> </div>
2	B	106	<div> <div>%</div> <div> <div></div> <div>40%</div> <div>34%</div> <div></div> <div>26%</div> </div> </div>
2	F	106	<div> <div></div> <div> <div>39%</div> <div>40%</div> <div>•</div> <div>21%</div> </div> </div>
3	C	133	<div> <div></div> <div> <div>52%</div> <div>25%</div> <div>••</div> <div>21%</div> </div> </div>
3	G	133	<div> <div></div> <div> <div>44%</div> <div>33%</div> <div>•</div> <div>23%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
4	D	129	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>45%</div><div>26%</div><div>28%</div></div><div><div></div><div></div><div></div></div></div>
4	H	129	<div><div><div></div><div></div><div></div></div><div><div>%</div><div>43%</div><div>25%</div><div>29%</div></div><div><div></div><div></div><div></div></div></div>
5	I	146	<div><div><div></div><div></div><div></div></div><div><div>3%</div><div>27%</div><div>71%</div><div></div></div><div><div></div><div></div><div></div></div></div>
6	J	146	<div><div><div></div><div></div><div></div></div><div><div></div><div>38%</div><div>58%</div><div></div></div><div><div></div><div></div><div></div></div></div>

## 2 Entry composition

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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	94	Total	C	N	O	S	0	0	0
			773	488	147	134	4			
1	E	97	Total	C	N	O	S	0	0	0
			801	505	155	137	4			

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
E	-3	GLY	-	expression tag	UNP P68431
E	-2	SER	-	expression tag	UNP P68431
E	-1	HIS	-	expression tag	UNP P68431

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	78	Total	C	N	O	S	0	0	0
			619	391	120	107	1			
2	F	84	Total	C	N	O	S	0	0	0
			673	424	133	115	1			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP P62805
B	-2	SER	-	expression tag	UNP P62805
B	-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 is a protein called Histone H2A type 1-B/E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	105	Total	C	N	O	0	0	0
			810	511	158	141			
3	G	103	Total	C	N	O	0	0	0
			796	502	155	139			

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
4	D	93	Total	C	N	O	S	0	0	0
			725	456	130	137	2			
4	H	92	Total	C	N	O	S	0	0	0
			719	453	129	135	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 DNA (146-MER).

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

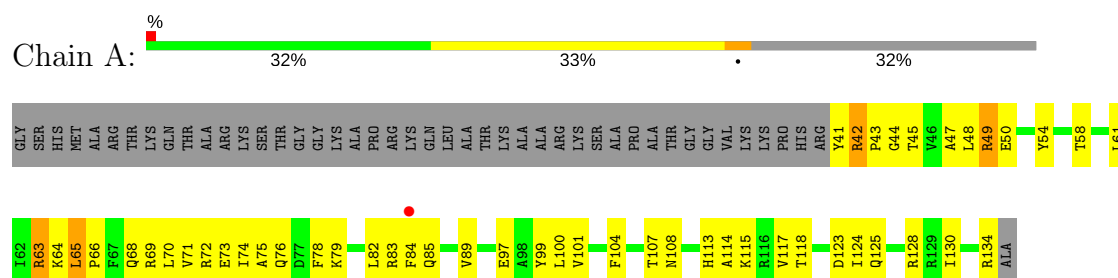
- Molecule 6 is a DNA chain called DNA (146-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	J	146	Total	C	N	O	P	0	0	0
			2973	1432	512	883	146			

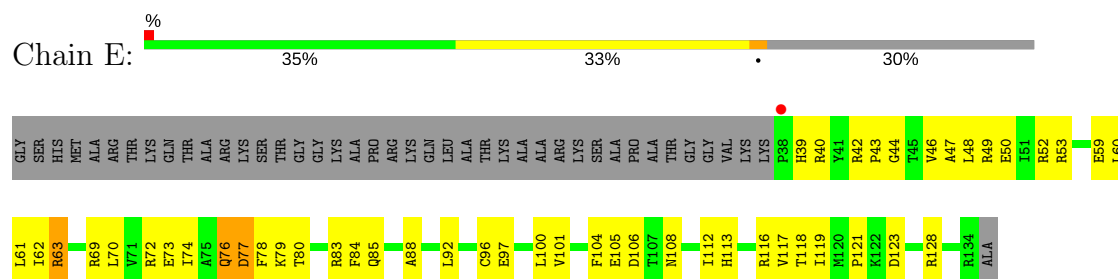
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

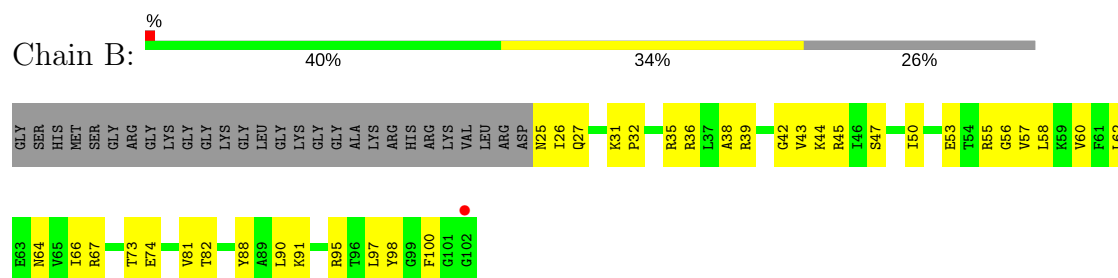
#### • Molecule 1: Histone H3.1



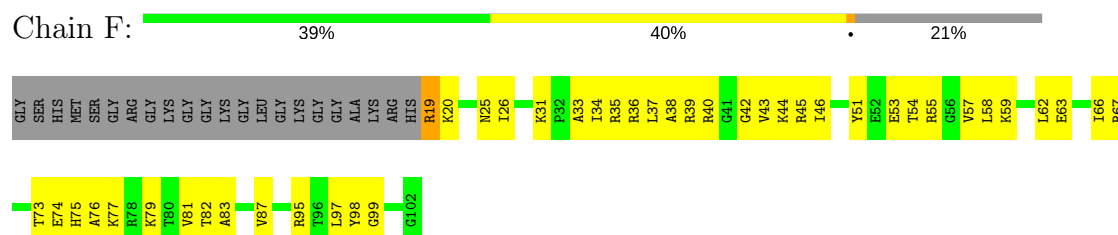
#### • Molecule 1: Histone H3.1



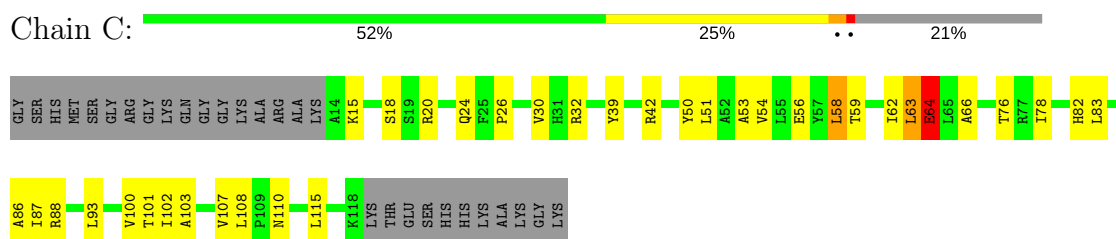
#### • Molecule 2: Histone H4



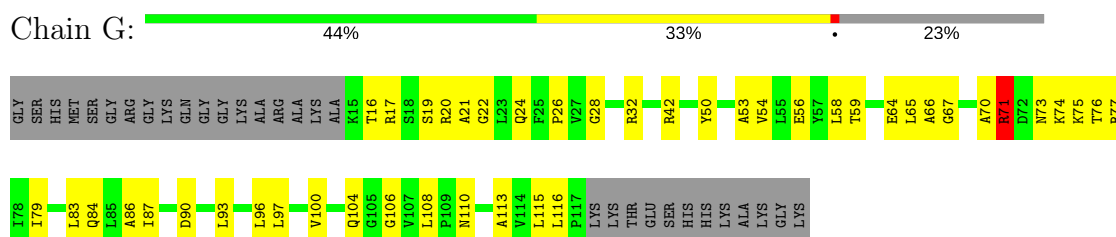
#### • Molecule 2: Histone H4



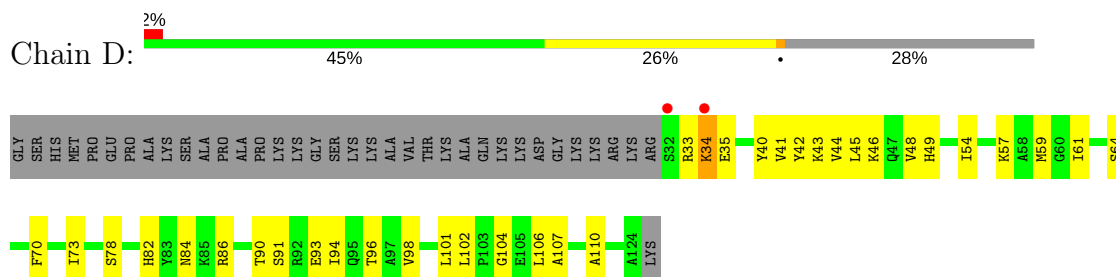
- Molecule 3: Histone H2A type 1-B/E



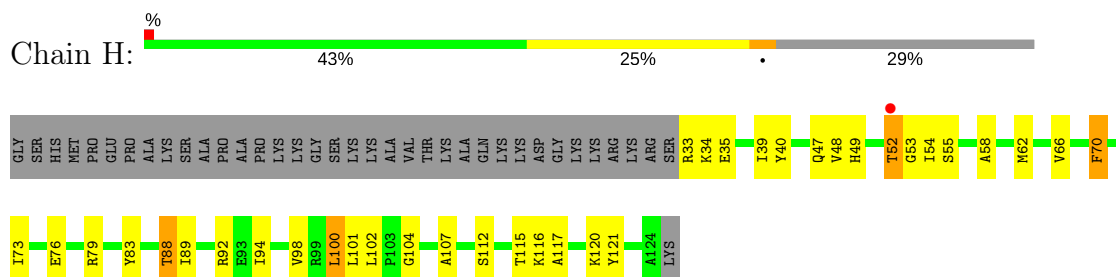
- Molecule 3: Histone H2A type 1-B/E



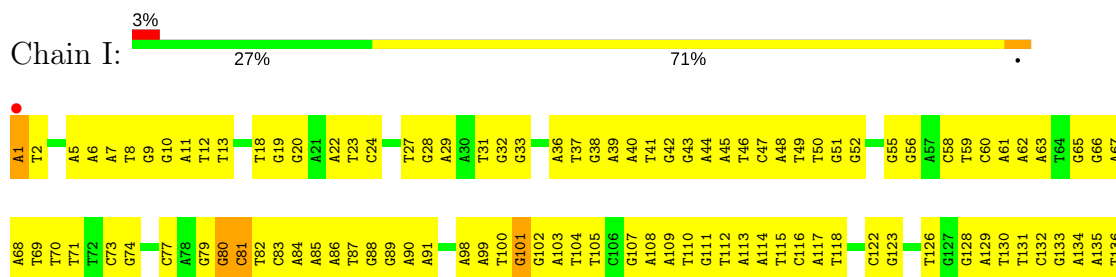
- Molecule 4: Histone H2B type 1-J



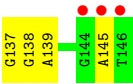
- Molecule 4: Histone H2B type 1-J



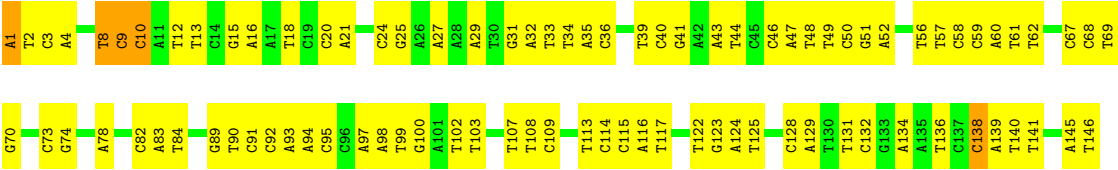
- Molecule 5: DNA (146-MER)







● Molecule 6: DNA (146-MER)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	103.45Å 108.99Å 173.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.90 – 3.15 46.45 – 3.13	Depositor EDS
% Data completeness (in resolution range)	99.3 (24.90-3.15) 98.0 (46.45-3.13)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.17 (at 3.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, $R_{free}$	0.235 , 0.295 0.235 , 0.297	Depositor DCC
$R_{free}$ test set	1965 reflections (5.73%)	DCC
Wilson B-factor (Å <sup>2</sup> )	87.9	Xtriage
Anisotropy	0.554	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 83.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.38$ , $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.056 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 <sup>2</sup> )	127.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.01% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

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	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.57	0/783	0.82	2/1050 (0.2%)
1	E	0.66	0/813	0.92	2/1090 (0.2%)
2	B	0.63	1/626 (0.2%)	0.77	0/837
2	F	0.75	0/680	0.94	2/908 (0.2%)
3	C	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	H	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 mainchain 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

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	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	C	64	GLU	CB-CG	5.84	1.63	1.52
6	J	10	DC	P-O5'	5.57	1.65	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	81	DC	C1'-N1	5.39	1.56	1.49
6	J	78	DA	C3'-O3'	-5.13	1.37	1.44
2	B	88	TYR	CD1-CE1	-5.01	1.31	1.39

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
5	I	80	DG	O5'-P-OP2	-6.44	99.90	105.70
6	J	18	DT	O4'-C1'-N1	6.42	112.49	108.00
4	H	100	LEU	CA-CB-CG	-6.08	101.31	115.30
3	C	63	LEU	CB-CG-CD2	-5.58	101.50	111.00
2	F	95	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	E	63	ARG	CA-CB-CG	-5.39	101.55	113.40
6	J	136	DT	C5-C4-O4	-5.37	121.14	124.90
6	J	138	DC	O4'-C1'-N1	5.36	111.75	108.00
1	E	77	ASP	CB-CG-OD2	5.22	123.00	118.30
2	F	19	ARG	NE-CZ-NH2	-5.13	117.74	120.30
5	I	101	DG	O5'-P-OP2	-5.13	101.08	105.70
3	C	58	LEU	CA-CB-CG	-5.05	103.69	115.30
6	J	136	DT	N3-C4-O4	5.04	122.92	119.90

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 ⓘ

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	E	801	0	839	68	1
2	B	619	0	659	41	0
2	F	673	0	722	74	0
3	C	810	0	866	50	0
3	G	796	0	848	55	0
4	D	725	0	745	37	1
4	H	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.

All (480) 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: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
2:B:64:ASN:HD22	2:B:67:ARG:HH21	1.12	0.95
3:G:71:ARG:HD3	3:G:74:LYS:HA	1.50	0.93
1:E:63:ARG:NH2	6:J:60:DA:O3'	2.03	0.91
5:I:139:DA:H61	6:J:8:DT:H3	1.14	0.91
2:F:31:LYS:HG3	2:F:51:TYR:CE1	2.08	0.89
6:J:113:DT:H2''	6:J:114:DC:H5''	1.53	0.89
2:F:19:ARG:NH2	6:J:52:DA:H3'	1.89	0.88
1:E:83:ARG:HE	6:J:51:DG:H5'	1.40	0.85
3:G:32:ARG:NH2	4:H:35:GLU:OE2	2.09	0.84
1:E:121:PRO:HB3	2:F:53:GLU:HG3	1.60	0.83
3:G:24:GLN:NE2	4:H:47:GLN:OE1	2.12	0.82
5:I:101:DG:H8	5:I:101:DG:H5''	1.46	0.81
4:H:33:ARG:HG2	4:H:34:LYS:HD3	1.63	0.80
1:E:100:LEU:HD11	2:F:58:LEU:HD13	1.65	0.79
2:B:39:ARG:O	2:B:42:GLY:N	2.15	0.79
3:G:77:ARG:HG2	4:H:53:GLY:H	1.45	0.79
1:A:118:THR:OG1	2:B:45:ARG:NH1	2.15	0.79
2:B:64:ASN:ND2	2:B:67:ARG:HH21	1.81	0.78
2:B:39:ARG:NH1	2:B:43:VAL:O	2.16	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:115:LEU:HD13	2:F:44:LYS:HD2	1.66	0.76
3:C:39:TYR:O	4:D:78:SER:OG	2.04	0.76
2:F:39:ARG:O	2:F:42:GLY:N	2.16	0.76
5:I:111:DG:H1	6:J:36:DC:H42	1.35	0.74
3:C:76:THR:HG21	6:J:131:DT:H5'	1.69	0.73
2:B:64:ASN:HD22	2:B:67:ARG:NH2	1.86	0.73
3:C:32:ARG:NH2	4:D:35:GLU:OE1	2.21	0.72
2:B:58:LEU:HD21	2:B:62:LEU:HD12	1.72	0.72
5:I:65:DG:H1	6:J:82:DC:H42	1.37	0.72
4:D:34:LYS:NZ	5:I:28:DG:OP1	2.19	0.72
5:I:77:DC:H42	6:J:70:DG:H1	1.38	0.72
1:A:104:PHE:HA	1:A:107:THR:HG22	1.72	0.71
3:G:42:ARG:HB3	4:H:88:THR:HG23	1.72	0.71
1:A:65:LEU:HB2	1:A:68:GLN:CB	2.14	0.71
2:F:45:ARG:CZ	6:J:70:DG:H4'	2.21	0.70
3:G:113:ALA:HA	3:G:116:LEU:HD12	1.74	0.69
4:D:33:ARG:O	4:D:34:LYS:HG2	1.92	0.69
3:C:115:LEU:HD22	2:F:44:LYS:NZ	2.07	0.69
1:E:42:ARG:HG3	1:E:43:PRO:HD2	1.74	0.69
3:G:21:ALA:HB2	4:H:121:TYR:HB2	1.75	0.69
5:I:107:DG:H2''	5:I:108:DA:N7	2.09	0.68
1:A:63:ARG:HD3	6:J:91:DC:H4'	1.76	0.68
1:A:49:ARG:HH21	6:J:8:DT:H4'	1.57	0.68
3:C:115:LEU:HD21	1:E:112:ILE:HD11	1.76	0.68
6:J:138:DC:H2''	6:J:139:DA:N7	2.09	0.68
4:D:33:ARG:HG3	6:J:124:DA:H5'	1.75	0.67
5:I:22:DA:H1'	5:I:23:DT:H5'	1.75	0.67
3:C:100:VAL:HG11	2:F:98:TYR:CE2	2.30	0.67
5:I:145:DA:H61	6:J:1:DA:N6	1.93	0.67
5:I:135:DA:H2''	5:I:136:DT:O4'	1.95	0.66
1:E:117:VAL:HG22	2:F:44:LYS:HZ3	1.60	0.66
1:A:64:LYS:HB2	6:J:92:DC:OP1	1.95	0.66
1:E:46:VAL:HG23	1:E:49:ARG:HD2	1.78	0.66
3:G:67:GLY:HA3	4:H:49:HIS:HD2	1.60	0.66
1:E:85:GLN:NE2	2:F:82:THR:HG22	2.10	0.66
3:G:42:ARG:NH1	5:I:112:DT:H4'	2.11	0.66
5:I:46:DT:H2''	5:I:47:DC:H5''	1.78	0.66
5:I:90:DA:H2''	5:I:91:DA:C8	2.31	0.66
3:C:62:ILE:HD11	3:C:93:LEU:HD22	1.78	0.65
1:A:130:ILE:CD1	1:E:106:ASP:HB3	2.26	0.65
3:C:51:LEU:HB2	4:D:94:ILE:HD12	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:42:ARG:HB3	4:H:88:THR:CG2	2.26	0.65
1:E:69:ARG:O	1:E:72:ARG:N	2.30	0.65
3:G:17:ARG:HH21	3:G:28:GLY:HA2	1.61	0.65
3:G:58:LEU:HD11	4:H:102:LEU:HD21	1.76	0.65
5:I:112:DT:C6	5:I:112:DT:H5'	2.32	0.65
1:A:76:GLN:HA	1:A:79:LYS:O	1.97	0.65
5:I:56:DG:N2	6:J:92:DC:N3	2.45	0.65
1:E:96:CYS:SG	2:F:62:LEU:HD13	2.38	0.64
5:I:73:5CM:H2'	5:I:74:DG:C8	2.32	0.64
1:E:104:PHE:CD2	2:F:38:ALA:HA	2.33	0.64
5:I:101:DG:C8	5:I:101:DG:H5''	2.30	0.64
6:J:27:DA:H5''	6:J:27:DA:H8	1.63	0.64
2:B:47:SER:HB3	2:B:50:ILE:HG12	1.80	0.64
2:F:45:ARG:NH2	6:J:70:DG:O3'	2.31	0.64
1:A:108:ASN:ND2	2:B:43:VAL:HA	2.13	0.63
3:C:24:GLN:N	3:C:56:GLU:OE1	2.27	0.63
1:E:116:ARG:NH1	1:E:118:THR:O	2.32	0.63
1:A:108:ASN:HD22	2:B:43:VAL:HG12	1.63	0.63
1:E:70:LEU:O	1:E:74:ILE:HG12	1.98	0.63
1:E:76:GLN:HA	1:E:79:LYS:O	1.98	0.63
2:B:73:THR:OG1	2:B:81:VAL:HG12	1.99	0.63
4:D:40:TYR:HA	4:D:43:LYS:HG2	1.81	0.63
6:J:31:DG:H2''	6:J:32:DA:H5''	1.80	0.62
1:E:83:ARG:HE	6:J:51:DG:C5'	2.12	0.62
3:G:77:ARG:NH2	6:J:21:DA:OP1	2.32	0.62
4:H:79:ARG:HB3	4:H:83:TYR:CZ	2.35	0.62
1:E:73:GLU:OE1	2:F:25:ASN:ND2	2.21	0.62
3:G:71:ARG:HD3	3:G:74:LYS:CA	2.27	0.62
4:H:98:VAL:HG13	4:H:102:LEU:HD13	1.81	0.62
1:A:64:LYS:HB2	6:J:92:DC:P	2.39	0.62
4:H:76:GLU:OE1	4:H:79:ARG:NH1	2.33	0.62
3:C:83:LEU:O	3:C:87:ILE:HD12	2.00	0.62
3:G:90:ASP:HB3	3:G:93:LEU:HD12	1.81	0.62
2:B:38:ALA:HB1	2:B:43:VAL:HG21	1.83	0.61
1:E:78:PHE:CZ	2:F:67:ARG:HB2	2.36	0.61
1:A:42:ARG:HG2	1:A:43:PRO:HD2	1.82	0.61
4:D:86:ARG:HH21	5:I:39:DA:H5''	1.66	0.61
5:I:86:DA:H61	6:J:61:DT:H3	1.49	0.61
5:I:101:DG:N2	6:J:46:DC:N3	2.49	0.61
5:I:118:DT:H3	6:J:29:DA:H61	1.48	0.61
1:E:46:VAL:HG12	5:I:82:DT:P	2.41	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:104:DT:H2''	5:I:105:DT:H5''	1.82	0.60
3:G:71:ARG:CD	3:G:74:LYS:HA	2.29	0.60
1:E:108:ASN:HD22	2:F:43:VAL:HA	1.64	0.60
5:I:113:DA:H2''	5:I:114:DA:C8	2.36	0.60
6:J:122:DT:H2''	6:J:123:DG:C8	2.37	0.60
3:G:42:ARG:HD2	5:I:111:DG:H4'	1.84	0.60
3:C:100:VAL:HG11	2:F:98:TYR:CD2	2.37	0.60
1:E:63:ARG:HH11	5:I:90:DA:H4'	1.67	0.60
1:E:117:VAL:HG13	2:F:44:LYS:CE	2.23	0.59
4:D:33:ARG:HH22	5:I:27:DT:H4'	1.67	0.59
5:I:83:DC:H2''	5:I:84:DA:H8	1.65	0.59
1:E:63:ARG:HH22	6:J:61:DT:H5'	1.66	0.59
5:I:58:DC:H42	6:J:89:DG:H1	1.50	0.58
3:G:83:LEU:HD12	4:H:58:ALA:HB1	1.85	0.58
3:C:59:THR:HG21	4:D:41:VAL:HG22	1.85	0.58
5:I:45:DA:H61	6:J:102:DT:H3	1.52	0.58
3:C:102:ILE:HG23	4:D:61:ILE:HG21	1.86	0.58
3:C:15:LYS:HG2	5:I:31:DT:OP1	2.04	0.58
6:J:12:DT:H2''	6:J:13:DT:H5''	1.86	0.57
5:I:107:DG:H2''	5:I:108:DA:C8	2.39	0.57
5:I:112:DT:H6	5:I:112:DT:H5'	1.68	0.57
1:A:68:GLN:HB2	1:A:89:VAL:HG11	1.86	0.57
5:I:90:DA:H61	6:J:57:DT:H3	1.51	0.57
1:A:130:ILE:HD13	1:E:106:ASP:HB3	1.87	0.57
1:A:113:HIS:NE2	1:E:123:ASP:OD1	2.38	0.57
2:F:39:ARG:NH1	2:F:44:LYS:O	2.24	0.57
3:G:17:ARG:NH2	3:G:28:GLY:HA2	2.20	0.57
3:C:42:ARG:HD2	5:I:38:DG:H5''	1.85	0.57
6:J:39:DT:OP2	6:J:39:DT:H2'	2.04	0.57
4:H:101:LEU:HB2	4:H:102:LEU:HD12	1.87	0.57
5:I:44:DA:H61	6:J:103:DT:H3	1.52	0.57
2:F:45:ARG:NH2	6:J:70:DG:H4'	2.19	0.57
1:E:104:PHE:HD2	2:F:38:ALA:HA	1.68	0.57
1:E:46:VAL:HA	1:E:49:ARG:HH11	1.70	0.57
1:E:62:ILE:HD11	2:F:37:LEU:HD11	1.88	0.56
6:J:9:DC:H2''	6:J:10:DC:C6	2.40	0.56
3:G:67:GLY:HA3	4:H:49:HIS:CD2	2.40	0.56
5:I:13:DT:H3	6:J:134:DA:H61	1.53	0.56
5:I:73:5CM:HN41	6:J:74:DG:H1	1.53	0.56
5:I:45:DA:H2''	5:I:46:DT:H5''	1.88	0.56
6:J:40:5CM:H5'	6:J:41:DG:OP1	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:LEU:O	2:B:36:ARG:NH2	2.38	0.55
4:D:33:ARG:HH21	4:D:34:LYS:HE3	1.71	0.55
5:I:70:DT:H1'	5:I:71:DT:H5'	1.86	0.55
6:J:99:DT:H1'	6:J:100:DG:C5	2.40	0.55
2:B:58:LEU:CD2	2:B:62:LEU:HD12	2.37	0.55
2:F:36:ARG:O	2:F:39:ARG:N	2.39	0.55
2:F:44:LYS:CG	2:F:45:ARG:H	2.20	0.55
2:F:44:LYS:HG3	2:F:45:ARG:H	1.71	0.55
5:I:115:DT:H2''	5:I:116:DC:H5''	1.88	0.55
2:F:79:LYS:N	5:I:101:DG:OP1	2.37	0.55
3:C:18:SER:OG	3:C:26:PRO:HA	2.07	0.55
4:D:94:ILE:O	4:D:98:VAL:HG23	2.06	0.55
2:F:26:ILE:O	2:F:55:ARG:HD3	2.06	0.55
2:B:98:TYR:CE2	3:G:100:VAL:HG11	2.42	0.54
1:A:78:PHE:CZ	2:B:67:ARG:HB2	2.42	0.54
3:C:64:GLU:HB2	4:D:49:HIS:CD2	2.42	0.54
5:I:42:DG:H2''	5:I:43:DG:H5'	1.89	0.54
1:A:65:LEU:HA	1:A:68:GLN:H	1.72	0.54
5:I:89:DG:H1'	5:I:90:DA:C8	2.43	0.54
4:D:43:LYS:O	4:D:46:LYS:N	2.39	0.54
5:I:130:DT:H2''	5:I:131:DT:OP2	2.08	0.54
5:I:47:DC:H42	6:J:100:DG:H1	1.54	0.54
5:I:85:DA:H2''	5:I:86:DA:H5''	1.88	0.54
5:I:32:DG:H1	6:J:115:DC:H42	1.56	0.54
1:A:65:LEU:O	1:A:69:ARG:HG3	2.08	0.54
6:J:8:DT:H2''	6:J:9:DC:C5	2.43	0.54
6:J:24:5CM:H2''	6:J:25:DG:C8	2.43	0.54
4:D:57:LYS:O	4:D:61:ILE:HD12	2.08	0.53
1:E:128:ARG:HD3	2:F:57:VAL:HG11	1.91	0.53
5:I:24:DC:H42	6:J:123:DG:H1	1.55	0.53
6:J:40:5CM:H2'	6:J:41:DG:N7	2.23	0.53
1:E:108:ASN:ND2	2:F:43:VAL:HA	2.23	0.53
2:B:45:ARG:NH1	5:I:69:DT:H4'	2.23	0.53
2:B:45:ARG:NH1	5:I:69:DT:O3'	2.42	0.53
4:D:73:ILE:HD13	4:D:101:LEU:HD12	1.91	0.53
1:E:79:LYS:HE3	2:F:74:GLU:OE1	2.09	0.53
3:G:76:THR:HG23	3:G:77:ARG:N	2.24	0.53
5:I:41:DT:H2'	5:I:42:DG:C8	2.44	0.53
3:G:79:ILE:HA	4:H:55:SER:OG	2.08	0.53
1:A:117:VAL:HG13	3:G:115:LEU:HD22	1.91	0.52
3:C:50:TYR:O	3:C:54:VAL:HG23	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:115:LEU:CD1	2:F:44:LYS:HD2	2.39	0.52
3:G:64:GLU:HG3	4:H:49:HIS:CE1	2.43	0.52
5:I:111:DG:H1	6:J:36:DC:N4	2.05	0.52
5:I:117:DA:H2''	5:I:118:DT:H72	1.91	0.52
5:I:65:DG:H1	6:J:82:DC:N4	2.05	0.52
1:A:104:PHE:CD2	2:B:38:ALA:HA	2.44	0.52
3:G:76:THR:OG1	3:G:77:ARG:HG3	2.08	0.52
5:I:133:DG:H21	6:J:15:DG:H22	1.57	0.52
4:D:33:ARG:NH2	5:I:27:DT:H4'	2.24	0.52
6:J:124:DA:C8	6:J:125:DT:H72	2.44	0.52
6:J:27:DA:H5''	6:J:27:DA:C8	2.45	0.52
1:E:61:LEU:HD12	2:F:37:LEU:HD23	1.92	0.52
4:D:90:THR:OG1	4:D:93:GLU:OE2	2.18	0.52
4:H:112:SER:O	4:H:115:THR:HG22	2.09	0.52
1:A:123:ASP:OD1	1:E:113:HIS:NE2	2.43	0.52
3:C:63:LEU:HD22	4:D:45:LEU:HD13	1.91	0.51
1:E:108:ASN:HD22	2:F:43:VAL:HG22	1.75	0.51
3:C:88:ARG:HB2	3:C:108:LEU:HD21	1.93	0.51
5:I:60:DC:H2''	5:I:61:DA:C8	2.46	0.51
5:I:8:DT:H2''	5:I:9:DG:H5''	1.93	0.51
2:B:64:ASN:ND2	2:B:67:ARG:NH2	2.51	0.51
1:A:44:GLY:O	1:A:47:ALA:HB3	2.10	0.51
3:C:108:LEU:O	3:C:110:ASN:N	2.42	0.51
3:G:87:ILE:HD12	3:G:97:LEU:HD12	1.91	0.51
5:I:61:DA:H1'	5:I:62:DA:H5''	1.93	0.51
3:G:77:ARG:HG2	4:H:53:GLY:N	2.21	0.51
3:C:78:ILE:HA	3:C:82:HIS:ND1	2.26	0.51
2:F:62:LEU:O	2:F:66:ILE:HG13	2.10	0.51
4:H:33:ARG:HG2	4:H:34:LYS:CD	2.35	0.51
5:I:90:DA:H2''	5:I:91:DA:H8	1.73	0.51
3:C:58:LEU:HD11	4:D:102:LEU:HD21	1.93	0.51
3:C:101:THR:HB	2:F:97:LEU:HD12	1.93	0.51
3:C:54:VAL:HG13	4:D:110:ALA:HB1	1.92	0.51
1:E:59:GLU:O	2:F:40:ARG:NH2	2.43	0.51
1:A:47:ALA:O	1:A:50:GLU:HG2	2.11	0.50
3:G:64:GLU:HB2	4:H:48:VAL:HG11	1.93	0.50
5:I:137:DG:C6	5:I:138:DG:C6	2.99	0.50
5:I:98:DA:H1'	5:I:99:DA:C5	2.47	0.50
1:E:61:LEU:N	1:E:97:GLU:OE1	2.28	0.50
1:E:97:GLU:HG2	2:F:37:LEU:HD21	1.93	0.50
3:G:77:ARG:HB3	4:H:53:GLY:C	2.32	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:62:MET:O	4:H:66:VAL:HG23	2.11	0.50
2:F:19:ARG:NH2	6:J:52:DA:O5'	2.44	0.50
2:F:19:ARG:HH21	6:J:52:DA:P	2.33	0.50
6:J:61:DT:H2''	6:J:62:DT:H5'	1.93	0.50
4:D:44:VAL:O	4:D:48:VAL:HG22	2.11	0.50
6:J:128:DC:H1'	6:J:129:DA:C8	2.46	0.50
2:F:19:ARG:HH22	6:J:52:DA:C3'	2.08	0.49
1:E:108:ASN:HB2	2:F:43:VAL:HG22	1.93	0.49
3:G:76:THR:O	4:H:52:THR:HG22	2.12	0.49
1:E:117:VAL:O	2:F:44:LYS:HG3	2.11	0.49
2:F:77:LYS:HZ2	4:H:92:ARG:NH2	2.10	0.49
1:E:70:LEU:HD11	1:E:74:ILE:HD11	1.94	0.49
3:G:108:LEU:O	3:G:110:ASN:N	2.43	0.49
6:J:67:DC:H2''	6:J:68:DC:C5	2.48	0.49
1:E:43:PRO:HG2	6:J:69:DT:H5'	1.95	0.49
5:I:1:DA:H5''	5:I:1:DA:H8	1.77	0.49
5:I:79:DG:H2''	5:I:80:DG:C8	2.48	0.49
2:B:56:GLY:O	2:B:60:VAL:HG23	2.12	0.49
1:E:117:VAL:CG2	2:F:44:LYS:HZ3	2.25	0.49
4:H:104:GLY:O	4:H:107:ALA:HB3	2.12	0.49
1:E:69:ARG:NH2	5:I:90:DA:OP2	2.37	0.49
5:I:126:DT:O4	6:J:20:DC:N4	2.45	0.49
1:A:70:LEU:O	1:A:74:ILE:HG12	2.13	0.48
6:J:58:DC:H4'	6:J:59:DC:H5'	1.94	0.48
1:A:69:ARG:NH2	6:J:91:DC:OP1	2.46	0.48
4:D:70:PHE:C	4:D:70:PHE:CD2	2.86	0.48
1:E:42:ARG:HG3	1:E:43:PRO:CD	2.40	0.48
1:E:50:GLU:O	1:E:53:ARG:HB3	2.13	0.48
3:G:77:ARG:HH22	6:J:21:DA:P	2.35	0.48
2:B:45:ARG:CZ	5:I:69:DT:H4'	2.42	0.48
3:C:59:THR:CG2	4:D:41:VAL:HG22	2.43	0.48
3:G:84:GLN:NE2	3:G:106:GLY:O	2.46	0.48
5:I:122:5CM:H2'	5:I:123:DG:C8	2.48	0.48
6:J:108:DT:H2''	6:J:109:DC:C5	2.48	0.48
1:E:83:ARG:NE	6:J:51:DG:H5'	2.18	0.48
1:A:45:THR:HA	1:A:48:LEU:HD12	1.95	0.48
1:A:65:LEU:HD22	1:A:68:GLN:NE2	2.28	0.48
1:A:99:TYR:HA	2:B:95:ARG:NH1	2.28	0.48
6:J:50:5CM:H2''	6:J:51:DG:C8	2.49	0.48
3:G:24:GLN:N	3:G:56:GLU:OE1	2.35	0.48
1:E:60:LEU:HD23	1:E:60:LEU:HA	1.66	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:61:LEU:HD13	2:F:36:ARG:HB3	1.95	0.48
1:A:58:THR:O	3:G:104:GLN:NE2	2.47	0.48
5:I:101:DG:H2'	5:I:102:DG:C8	2.49	0.48
5:I:45:DA:H2''	5:I:46:DT:O4'	2.14	0.48
1:A:71:VAL:HG13	2:B:66:ILE:HD11	1.95	0.48
3:C:115:LEU:HD22	2:F:44:LYS:CE	2.43	0.48
5:I:132:5CM:HN41	6:J:15:DG:H1	1.62	0.48
5:I:11:DA:H2''	5:I:12:DT:O5'	2.13	0.47
5:I:19:DG:H2''	5:I:20:DG:C8	2.49	0.47
5:I:48:DA:H2''	5:I:49:DT:OP2	2.14	0.47
3:G:26:PRO:HD3	4:H:40:TYR:CD1	2.49	0.47
5:I:51:DG:H2''	5:I:52:DG:C8	2.49	0.47
1:A:64:LYS:HB3	1:A:66:PRO:HD2	1.96	0.47
3:G:66:ALA:HA	3:G:86:ALA:HB2	1.95	0.47
5:I:62:DA:H1'	5:I:63:DA:H5'	1.97	0.47
5:I:87:DT:H2''	5:I:88:DG:C8	2.49	0.47
3:C:26:PRO:HD3	4:D:40:TYR:CE1	2.50	0.47
6:J:59:DC:H2''	6:J:60:DA:H5''	1.96	0.47
3:G:19:SER:O	3:G:22:GLY:N	2.46	0.47
5:I:98:DA:H1'	5:I:99:DA:N7	2.30	0.47
1:E:60:LEU:HD22	1:E:97:GLU:OE2	2.15	0.47
2:F:19:ARG:HG3	2:F:20:LYS:N	2.30	0.47
5:I:74:DG:H22	6:J:73:5CM:C2	2.28	0.47
6:J:33:DT:H2''	6:J:34:DT:C6	2.50	0.47
6:J:94:DA:H2''	6:J:95:DC:O4'	2.15	0.47
1:A:65:LEU:HD13	1:A:68:GLN:NE2	2.30	0.46
1:E:85:GLN:HE22	2:F:82:THR:HG22	1.78	0.46
5:I:1:DA:H2'	5:I:2:DT:H72	1.96	0.46
1:A:43:PRO:HG2	5:I:68:DA:H5'	1.97	0.46
1:E:117:VAL:HA	2:F:44:LYS:NZ	2.29	0.46
3:G:32:ARG:HH22	4:H:35:GLU:CD	2.16	0.46
6:J:145:DA:H2''	6:J:146:DT:H5''	1.97	0.46
4:H:73:ILE:HD13	4:H:101:LEU:HD12	1.97	0.46
3:G:73:ASN:OD1	3:G:73:ASN:O	2.34	0.46
5:I:7:DA:H61	6:J:139:DA:N6	2.14	0.46
5:I:23:DT:H3	6:J:124:DA:H61	1.63	0.46
3:G:58:LEU:HD23	3:G:58:LEU:HA	1.67	0.46
4:H:70:PHE:C	4:H:70:PHE:CD2	2.89	0.46
1:A:114:ALA:O	1:A:115:LYS:HB2	2.16	0.46
1:A:49:ARG:NH2	6:J:8:DT:H4'	2.29	0.46
3:C:59:THR:HG22	3:C:63:LEU:HD12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:90:LEU:HB3	2:B:95:ARG:O	2.15	0.46
4:H:34:LYS:HD3	4:H:34:LYS:N	2.31	0.46
2:F:34:ILE:HD13	2:F:54:THR:HB	1.98	0.45
3:C:64:GLU:HA	4:D:49:HIS:HD2	1.80	0.45
4:D:104:GLY:O	4:D:107:ALA:HB3	2.15	0.45
3:C:15:LYS:HG3	3:C:20:ARG:HD3	1.98	0.45
1:A:85:GLN:NE2	2:B:82:THR:HG22	2.31	0.45
1:E:117:VAL:CB	2:F:44:LYS:HZ3	2.30	0.45
5:I:10:DG:H1'	5:I:11:DA:C8	2.51	0.45
6:J:43:DA:H2''	6:J:44:DT:O4'	2.17	0.45
6:J:89:DG:H2''	6:J:90:DT:C5	2.51	0.45
2:F:75:HIS:O	4:H:92:ARG:NH1	2.49	0.45
1:A:108:ASN:HD22	2:B:43:VAL:HA	1.80	0.45
1:A:73:GLU:OE1	2:B:25:ASN:ND2	2.41	0.45
5:I:8:DT:C4	5:I:9:DG:C6	3.05	0.45
6:J:60:DA:C8	6:J:60:DA:H5''	2.52	0.45
1:A:61:LEU:HD13	2:B:36:ARG:HB3	1.99	0.45
1:E:44:GLY:O	1:E:47:ALA:HB3	2.17	0.45
1:E:63:ARG:HG2	5:I:91:DA:OP1	2.17	0.45
5:I:98:DA:H2	6:J:49:DT:H3	1.64	0.45
2:F:62:LEU:HA	2:F:62:LEU:HD12	1.81	0.45
5:I:110:DT:H2''	5:I:111:DG:C8	2.52	0.45
5:I:8:DT:H2''	5:I:9:DG:C8	2.52	0.45
2:F:38:ALA:HB3	2:F:46:ILE:HD11	1.99	0.45
4:H:112:SER:HA	4:H:115:THR:HG22	1.98	0.45
5:I:103:DA:H1'	5:I:104:DT:H5'	2.00	0.45
5:I:33:DG:OP2	5:I:33:DG:H8	2.00	0.45
5:I:36:DA:H1'	5:I:37:DT:H5''	1.99	0.45
5:I:109:DA:H2''	5:I:110:DT:H71	1.99	0.44
3:C:66:ALA:HA	3:C:86:ALA:HB2	1.98	0.44
4:D:84:ASN:N	4:D:84:ASN:HD22	2.15	0.44
5:I:139:DA:OP2	5:I:139:DA:H8	2.00	0.44
6:J:20:DC:H2''	6:J:21:DA:N7	2.32	0.44
1:A:50:GLU:OE2	2:B:35:ARG:NH2	2.51	0.44
5:I:66:DG:H2''	5:I:67:DA:C8	2.52	0.44
5:I:99:DA:H2''	5:I:100:DT:C6	2.52	0.44
1:A:104:PHE:HD1	1:A:104:PHE:HA	1.66	0.44
3:C:62:ILE:CD1	3:C:93:LEU:HD13	2.46	0.44
1:A:72:ARG:HG2	1:A:84:PHE:CE2	2.53	0.44
4:D:42:TYR:O	4:D:45:LEU:HB3	2.18	0.44
1:E:39:HIS:HD2	1:E:40:ARG:N	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:GLN:HG2	1:A:134:ARG:HH22	1.83	0.44
4:D:64:SER:HB3	2:F:98:TYR:CD1	2.53	0.44
6:J:73:5CM:H2'	6:J:74:DG:C8	2.52	0.44
6:J:35:DA:H1'	6:J:36:DC:H5''	1.99	0.44
6:J:97:DA:H2''	6:J:98:DA:OP2	2.16	0.44
4:H:100:LEU:HA	4:H:100:LEU:HD23	1.56	0.44
5:I:41:DT:C4	5:I:42:DG:C6	3.06	0.44
5:I:58:DC:N4	6:J:89:DG:H1	2.15	0.44
1:E:92:LEU:HA	1:E:92:LEU:HD23	1.79	0.43
2:F:45:ARG:HG3	5:I:81:DC:C5'	2.48	0.43
4:H:102:LEU:N	4:H:102:LEU:HD12	2.33	0.43
5:I:1:DA:H2'	5:I:2:DT:C7	2.48	0.43
5:I:37:DT:H2''	5:I:38:DG:H8	1.83	0.43
5:I:128:DG:H2''	5:I:129:DA:H8	1.83	0.43
5:I:9:DG:H8	5:I:9:DG:H5''	1.83	0.43
1:A:41:TYR:N	6:J:84:DT:OP1	2.51	0.43
3:G:96:LEU:HG	3:G:97:LEU:HD23	2.00	0.43
1:A:78:PHE:CE1	2:B:67:ARG:HB2	2.53	0.43
1:A:75:ALA:O	1:A:78:PHE:HB2	2.19	0.43
3:C:115:LEU:O	1:E:48:LEU:HD21	2.18	0.43
3:G:67:GLY:O	3:G:70:ALA:HB3	2.18	0.43
5:I:60:DC:H2''	5:I:61:DA:H8	1.82	0.43
3:C:107:VAL:HG12	3:C:108:LEU:N	2.34	0.43
3:C:115:LEU:HD22	2:F:44:LYS:HZ1	1.83	0.43
5:I:108:DA:H2''	5:I:109:DA:C8	2.54	0.43
6:J:131:DT:H2''	6:J:132:5CM:O4'	2.17	0.43
3:C:50:TYR:O	3:C:53:ALA:HB3	2.17	0.43
5:I:77:DC:N4	6:J:70:DG:H1	2.11	0.43
1:A:124:ILE:O	1:A:128:ARG:HG3	2.18	0.43
2:F:35:ARG:HG2	2:F:46:ILE:HD12	2.00	0.43
3:G:66:ALA:O	3:G:70:ALA:HB2	2.18	0.43
4:H:39:ILE:HD12	5:I:122:5CM:OP2	2.19	0.43
5:I:22:DA:H2''	5:I:23:DT:OP2	2.18	0.43
6:J:20:DC:H2''	6:J:21:DA:C8	2.54	0.43
1:A:134:ARG:HB2	1:A:134:ARG:HE	1.58	0.43
2:F:83:ALA:O	2:F:87:VAL:HG23	2.18	0.43
4:D:54:ILE:HD13	4:D:59:MET:HE1	2.01	0.43
1:A:123:ASP:OD1	1:E:113:HIS:CE1	2.72	0.43
1:E:84:PHE:CE2	2:F:81:VAL:HG21	2.54	0.43
5:I:134:DA:H2''	5:I:135:DA:H8	1.84	0.43
6:J:59:DC:C4	6:J:60:DA:C6	3.07	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:LEU:HD23	1:A:100:LEU:HA	1.89	0.42
3:C:54:VAL:HG21	4:D:98:VAL:HG21	2.00	0.42
3:C:59:THR:HG22	3:C:63:LEU:CD1	2.48	0.42
5:I:37:DT:H2''	5:I:38:DG:C8	2.53	0.42
2:B:26:ILE:HG23	2:B:27:GLN:HG3	2.00	0.42
1:A:83:ARG:HE	5:I:49:DT:H4'	1.83	0.42
2:F:33:ALA:HA	2:F:36:ARG:CZ	2.49	0.42
2:F:44:LYS:CG	2:F:45:ARG:N	2.81	0.42
3:G:50:TYR:O	3:G:54:VAL:HG23	2.19	0.42
5:I:39:DA:H2''	5:I:40:DA:C8	2.53	0.42
3:G:19:SER:C	3:G:22:GLY:H	2.22	0.42
6:J:122:DT:H2''	6:J:123:DG:H8	1.82	0.42
6:J:60:DA:H2''	6:J:61:DT:C6	2.54	0.42
3:G:50:TYR:O	3:G:53:ALA:HB3	2.19	0.42
2:B:32:PRO:HA	2:B:35:ARG:HG2	2.01	0.42
3:C:30:VAL:HG13	4:D:70:PHE:CE1	2.55	0.42
1:E:79:LYS:HG3	1:E:80:THR:N	2.33	0.42
5:I:9:DG:C8	5:I:9:DG:H5''	2.53	0.42
6:J:15:DG:H1'	6:J:16:DA:H5''	2.01	0.42
6:J:89:DG:H2''	6:J:90:DT:C6	2.54	0.42
6:J:99:DT:H4'	6:J:100:DG:H5'	2.01	0.42
2:B:44:LYS:HB2	3:G:115:LEU:HD13	2.01	0.42
2:B:53:GLU:O	2:B:57:VAL:HG23	2.19	0.42
3:C:62:ILE:HG23	3:C:62:ILE:HD12	1.79	0.42
5:I:51:DG:H2''	5:I:52:DG:H5''	2.01	0.42
6:J:116:DA:H2'	6:J:117:DT:C6	2.55	0.42
6:J:2:DT:H2'	6:J:2:DT:H6	1.72	0.42
1:E:104:PHE:HD2	2:F:37:LEU:O	2.03	0.42
3:G:77:ARG:NH2	4:H:54:ILE:O	2.52	0.42
3:G:42:ARG:CB	4:H:88:THR:HG23	2.47	0.42
3:G:16:THR:O	3:G:20:ARG:HG3	2.20	0.42
3:C:103:ALA:HB3	4:D:61:ILE:HD11	2.01	0.41
5:I:100:DT:H3	6:J:47:DA:H61	1.68	0.41
5:I:90:DA:N6	6:J:57:DT:H3	2.16	0.41
1:A:65:LEU:CA	1:A:68:GLN:H	2.33	0.41
2:B:26:ILE:HG13	2:B:55:ARG:HB3	2.02	0.41
2:B:97:LEU:HD21	2:B:100:PHE:CD2	2.54	0.41
4:D:33:ARG:HG3	6:J:123:DG:O3'	2.21	0.41
1:E:85:GLN:O	1:E:88:ALA:N	2.45	0.41
2:F:44:LYS:H	2:F:44:LYS:HG2	1.26	0.41
2:F:59:LYS:NZ	2:F:63:GLU:OE2	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:89:ILE:HG21	4:H:89:ILE:HD13	1.80	0.41
1:A:97:GLU:O	1:A:101:VAL:HG23	2.21	0.41
5:I:5:DA:H2''	5:I:6:DA:C8	2.56	0.41
3:C:115:LEU:CD2	1:E:112:ILE:HD11	2.48	0.41
5:I:45:DA:N6	6:J:102:DT:H3	2.18	0.41
1:E:119:ILE:CD1	2:F:43:VAL:HG11	2.51	0.41
2:F:45:ARG:HG3	5:I:81:DC:H5''	2.02	0.41
3:G:26:PRO:HD3	4:H:40:TYR:CG	2.56	0.41
3:G:71:ARG:HD3	3:G:75:LYS:N	2.36	0.41
5:I:27:DT:H2''	5:I:28:DG:O5'	2.20	0.41
6:J:56:DT:H2''	6:J:57:DT:H71	2.01	0.41
6:J:83:DA:C5	6:J:84:DT:C4	3.08	0.41
2:B:58:LEU:C	2:B:58:LEU:HD23	2.41	0.41
3:C:58:LEU:HD23	3:C:58:LEU:HA	1.83	0.41
3:C:103:ALA:HB2	2:F:99:GLY:HA3	2.02	0.41
3:G:77:ARG:HH21	4:H:54:ILE:H	1.67	0.41
3:C:64:GLU:HA	4:D:49:HIS:CD2	2.55	0.41
5:I:50:DT:H1'	5:I:51:DG:H5'	2.02	0.41
6:J:60:DA:N3	6:J:61:DT:N3	2.68	0.41
1:A:50:GLU:OE1	2:B:39:ARG:NE	2.54	0.41
3:C:62:ILE:HA	3:C:62:ILE:HD13	1.86	0.41
5:I:28:DG:H1'	5:I:29:DA:C8	2.56	0.41
6:J:107:DT:H2'	6:J:108:DT:H71	2.02	0.41
5:I:55:DG:O6	6:J:92:DC:N4	2.54	0.41
6:J:92:DC:H1'	6:J:93:DA:H5'	2.02	0.41
1:A:54:TYR:CZ	2:B:36:ARG:HD2	2.56	0.41
5:I:118:DT:H3	6:J:29:DA:N6	2.17	0.41
1:A:63:ARG:HH22	5:I:60:DC:H4'	1.85	0.40
4:H:101:LEU:HD23	4:H:101:LEU:HA	1.70	0.40
5:I:59:DT:C4	5:I:60:DC:N4	2.89	0.40
2:B:39:ARG:HD3	2:B:39:ARG:HA	1.74	0.40
1:E:101:VAL:O	1:E:105:GLU:HG3	2.20	0.40
2:F:77:LYS:HD3	2:F:77:LYS:HA	1.90	0.40
6:J:3:DC:H2''	6:J:4:DA:O4'	2.21	0.40
1:A:125:GLN:HG2	1:A:134:ARG:HH12	1.86	0.40
2:F:62:LEU:HG	2:F:66:ILE:CD1	2.52	0.40
5:I:13:DT:H3	6:J:134:DA:N6	2.18	0.40
5:I:18:DT:H2''	5:I:19:DG:C8	2.56	0.40
5:I:7:DA:N6	6:J:139:DA:H61	2.20	0.40
6:J:140:DT:H2''	6:J:141:DT:O4'	2.22	0.40
6:J:47:DA:H1'	6:J:48:DT:C6	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:88:ARG:HB3	3:C:108:LEU:HD11	2.02	0.40
2:F:73:THR:O	2:F:76:ALA:HB3	2.22	0.40
4:H:94:ILE:O	4:H:98:VAL:HG23	2.21	0.40
1:A:82:LEU:HA	1:A:82:LEU:HD23	1.87	0.40
4:H:116:LYS:O	4:H:117:ALA:C	2.59	0.40

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	Interatomic distance (Å)	Clash overlap (Å)
4:D:48:VAL:O	1:E:77:ASP:OD2[3_555]	2.07	0.13

## 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	92/139 (66%)	88 (96%)	4 (4%)	0	100	100
1	E	95/139 (68%)	90 (95%)	5 (5%)	0	100	100
2	B	76/106 (72%)	74 (97%)	2 (3%)	0	100	100
2	F	82/106 (77%)	79 (96%)	3 (4%)	0	100	100
3	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	H	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 ⓘ

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	82/113 (73%)	81 (99%)	1 (1%)	75	91
1	E	85/113 (75%)	83 (98%)	2 (2%)	54	83
2	B	63/81 (78%)	60 (95%)	3 (5%)	30	68
2	F	69/81 (85%)	69 (100%)	0	100	100
3	C	83/102 (81%)	82 (99%)	1 (1%)	75	91
3	G	82/102 (80%)	80 (98%)	2 (2%)	54	83
4	D	79/107 (74%)	76 (96%)	3 (4%)	38	74
4	H	78/107 (73%)	74 (95%)	4 (5%)	28	65
All	All	621/806 (77%)	605 (97%)	16 (3%)	51	82

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	ARG
2	B	31	LYS
2	B	74	GLU
2	B	91	LYS
3	C	64	GLU
4	D	82	HIS
4	D	91	SER
4	D	96	THR
1	E	52	ARG
1	E	76	GLN
3	G	59	THR
3	G	65	LEU
4	H	52	THR
4	H	70	PHE
4	H	88	THR
4	H	120	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	ASN
2	B	64	ASN
4	D	49	HIS
1	E	85	GLN
1	E	108	ASN
3	G	73	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	5CM	I	106	5	14,21,22	1.57	1 (7%)	18,30,33	1.45	4 (22%)
5	5CM	I	122	5,6	14,21,22	1.53	1 (7%)	18,30,33	1.51	4 (22%)
5	5CM	I	132	5,6	14,21,22	1.50	1 (7%)	18,30,33	1.74	2 (11%)
5	5CM	I	14	5,6	14,21,22	1.49	1 (7%)	18,30,33	1.83	4 (22%)
5	5CM	I	73	5,6	14,21,22	1.48	1 (7%)	18,30,33	1.53	3 (16%)
5	5CM	I	96	5,6	14,21,22	1.67	2 (14%)	18,30,33	1.56	1 (5%)
6	5CM	J	132	6	14,21,22	1.51	1 (7%)	18,30,33	1.42	2 (11%)
6	5CM	J	14	6	14,21,22	1.55	1 (7%)	18,30,33	1.13	3 (16%)
6	5CM	J	24	5,6	14,21,22	1.57	1 (7%)	18,30,33	1.64	4 (22%)
6	5CM	J	40	5,6	14,21,22	1.52	1 (7%)	18,30,33	1.57	4 (22%)
6	5CM	J	50	5,6	14,21,22	1.46	1 (7%)	18,30,33	1.55	2 (11%)
6	5CM	J	73	5,6	14,21,22	1.31	1 (7%)	18,30,33	1.67	5 (27%)

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	106	5	-	0/3/21/22	0/2/2/2
5	5CM	I	122	5,6	-	0/3/21/22	0/2/2/2
5	5CM	I	132	5,6	-	0/3/21/22	0/2/2/2
5	5CM	I	14	5,6	-	0/3/21/22	0/2/2/2
5	5CM	I	73	5,6	-	0/3/21/22	0/2/2/2
5	5CM	I	96	5,6	-	0/3/21/22	0/2/2/2
6	5CM	J	132	6	-	0/3/21/22	0/2/2/2
6	5CM	J	14	6	-	0/3/21/22	0/2/2/2
6	5CM	J	24	5,6	-	0/3/21/22	0/2/2/2
6	5CM	J	40	5,6	-	0/3/21/22	0/2/2/2
6	5CM	J	50	5,6	-	0/3/21/22	0/2/2/2
6	5CM	J	73	5,6	-	0/3/21/22	0/2/2/2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	96	5CM	O5'-C5'	-2.15	1.41	1.44
6	J	73	5CM	C5-C4	4.31	1.47	1.41
5	I	73	5CM	C5-C4	4.83	1.48	1.41
6	J	50	5CM	C5-C4	5.03	1.48	1.41
5	I	14	5CM	C5-C4	5.03	1.48	1.41
5	I	132	5CM	C5-C4	5.08	1.48	1.41
5	I	106	5CM	C5-C4	5.11	1.48	1.41
6	J	40	5CM	C5-C4	5.20	1.49	1.41
6	J	14	5CM	C5-C4	5.26	1.49	1.41
6	J	132	5CM	C5-C4	5.27	1.49	1.41
6	J	24	5CM	C5-C4	5.30	1.49	1.41
5	I	122	5CM	C5-C4	5.33	1.49	1.41
5	I	96	5CM	C5-C4	5.57	1.49	1.41

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	14	5CM	C2'-C1'-N1	-2.99	107.18	114.23
5	I	14	5CM	C5-C6-N1	-2.79	119.13	122.15
6	J	73	5CM	C5A-C5-C4	-2.48	119.10	121.65
5	I	122	5CM	C5A-C5-C4	-2.47	119.11	121.65
6	J	40	5CM	O4'-C4'-C3'	-2.42	99.87	105.68
5	I	122	5CM	C5-C6-N1	-2.26	119.70	122.15
6	J	73	5CM	C5-C6-N1	-2.23	119.74	122.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	J	40	5CM	C5-C6-N1	-2.20	119.77	122.15
6	J	24	5CM	C5-C6-N1	-2.19	119.78	122.15
6	J	14	5CM	C5-C6-N1	-2.17	119.80	122.15
5	I	73	5CM	C5-C6-N1	-2.17	119.80	122.15
5	I	106	5CM	C2'-C1'-N1	-2.09	109.30	114.23
5	I	106	5CM	C5-C6-N1	-2.06	119.92	122.15
6	J	73	5CM	C2'-C1'-N1	-2.05	109.40	114.23
6	J	24	5CM	O3'-C3'-C2'	2.02	118.18	110.83
6	J	14	5CM	N4-C4-N3	2.05	120.03	117.00
5	I	14	5CM	N4-C4-N3	2.17	120.20	117.00
5	I	73	5CM	N4-C4-N3	2.20	120.26	117.00
6	J	14	5CM	O4'-C1'-N1	2.29	111.64	107.78
6	J	40	5CM	N4-C4-N3	2.34	120.46	117.00
6	J	24	5CM	N4-C4-N3	2.40	120.54	117.00
5	I	106	5CM	N4-C4-N3	2.55	120.76	117.00
5	I	122	5CM	N4-C4-N3	2.63	120.89	117.00
6	J	73	5CM	N4-C4-N3	2.67	120.95	117.00
5	I	132	5CM	N4-C4-N3	2.86	121.23	117.00
5	I	122	5CM	O4'-C1'-N1	2.93	112.72	107.78
6	J	132	5CM	N4-C4-N3	3.00	121.44	117.00
6	J	132	5CM	O4'-C1'-N1	3.09	112.99	107.78
6	J	50	5CM	N4-C4-N3	3.14	121.64	117.00
5	I	106	5CM	O4'-C1'-N1	3.33	113.40	107.78
6	J	40	5CM	O4'-C1'-N1	3.73	114.06	107.78
6	J	50	5CM	O4'-C1'-N1	3.98	114.49	107.78
6	J	73	5CM	O4'-C1'-N1	4.25	114.94	107.78
5	I	73	5CM	O4'-C1'-N1	4.40	115.19	107.78
6	J	24	5CM	O4'-C1'-N1	4.82	115.91	107.78
5	I	132	5CM	O4'-C1'-N1	4.91	116.06	107.78
5	I	96	5CM	O4'-C1'-N1	5.10	116.38	107.78
5	I	14	5CM	O4'-C1'-N1	5.12	116.40	107.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 13 short contacts:

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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	J	132	5CM	1	0
6	J	24	5CM	1	0
6	J	40	5CM	3	0
6	J	50	5CM	1	0
6	J	73	5CM	2	0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	94/139 (67%)	0.11	1 (1%) 80 68	69, 104, 143, 163	0
1	E	97/139 (69%)	-0.07	1 (1%) 82 71	47, 75, 124, 152	0
2	B	78/106 (73%)	0.05	1 (1%) 77 64	70, 96, 117, 123	0
2	F	84/106 (79%)	-0.02	0 100 100	48, 71, 93, 123	0
3	C	105/133 (78%)	-0.18	0 100 100	50, 75, 102, 139	0
3	G	103/133 (77%)	-0.02	0 100 100	68, 92, 138, 151	0
4	D	93/129 (72%)	-0.01	2 (2%) 62 46	55, 74, 101, 151	0
4	H	92/129 (71%)	0.02	1 (1%) 80 68	57, 91, 122, 142	0
5	I	140/146 (95%)	-0.39	4 (2%) 52 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 71	47, 94, 186, 206	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	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	3.2
5	I	1	DA	3.0
1	A	84	PHE	2.5
4	H	52	THR	2.4
4	D	34	LYS	2.3
2	B	102	GLY	2.1

## 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
6	5CM	J	24	20/21	0.78	0.18	-	181,194,201,201	0
5	5CM	I	14	20/21	0.84	0.14	-	183,195,220,223	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
6	5CM	J	40	20/21	0.87	0.17	-	128,165,170,171	0
5	5CM	I	106	20/21	0.80	0.22	-	177,180,196,198	0
6	5CM	J	50	20/21	0.92	0.11	-	110,134,156,157	0
5	5CM	I	96	20/21	0.70	0.32	-	173,191,200,201	0
5	5CM	I	132	20/21	0.88	0.16	-	172,188,191,192	0
6	5CM	J	14	20/21	0.77	0.24	-	192,202,208,210	0
5	5CM	I	122	20/21	0.90	0.14	-	126,158,166,166	0
6	5CM	J	73	20/21	0.88	0.09	-	136,142,150,158	0

## 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.