



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 07:02 am BST

PDB ID : 5GTC  
Title : Crystal structure of complex between DMAP-SH conjugated with a Kaposi's sarcoma herpesvirus LANA peptide (5-15) and nucleosome core particle  
Authors : Arimura, Y.; Kato, D.; Suto, H.; Kurumizaka, H.; Kawashima, S.A.; Yamat-sugu, K.; Kanai, M.  
Deposited on : 2016-08-19  
Resolution : 2.70 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

<https://www.wwpdb.org/validation/2017/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
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

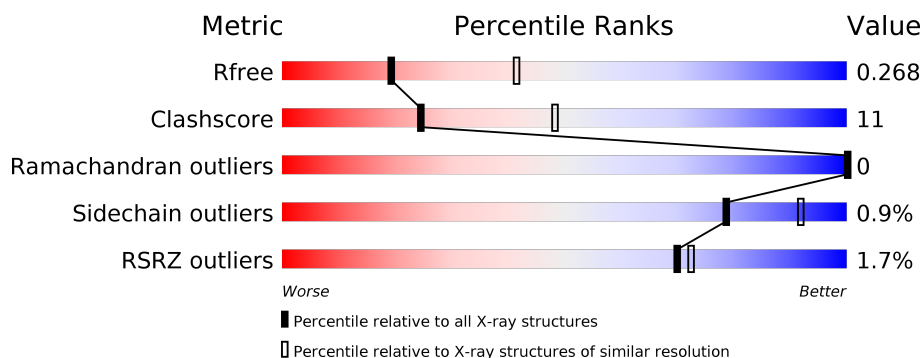
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
$R_{free}$	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	139	<div> <div>%</div> <div> <div></div> <div>56%</div> <div>14%</div> <div>30%</div> </div> </div>
1	E	139	<div> <div>58%</div> <div>12%</div> <div>29%</div> </div>
2	B	106	<div> <div>%</div> <div> <div></div> <div>61%</div> <div>12%</div> <div>26%</div> </div> </div>
2	F	106	<div> <div>69%</div> <div>11%</div> <div>19%</div> </div>
3	C	133	<div> <div>3%</div> <div> <div></div> <div>65%</div> <div>17%</div> <div>19%</div> </div> </div>
3	G	133	<div> <div>%</div> <div> <div></div> <div>61%</div> <div>20%</div> <div>20%</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>55%</div><div>17%</div><div>28%</div></div></div>
4	H	129	<div><div><div></div><div></div><div></div></div><div><div>%</div><div>61%</div><div>9%</div><div>29%</div></div></div>
5	I	146	<div><div><div></div><div></div><div></div></div><div><div>3%</div><div>38%</div><div>57%</div><div>5%</div></div></div>
5	J	146	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>38%</div><div>59%</div><div></div></div></div>
6	K	12	<div><div><div></div><div></div><div></div></div><div><div></div><div>50%</div><div>50%</div><div></div></div></div>

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 12095 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	97	Total	C	N	O	S	0	0	0
			801	505	155	137	4			
1	E	98	Total	C	N	O	S	0	0	0
			807	508	156	139	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	86	Total	C	N	O	S	0	0	0
			694	436	140	117	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	108	Total	C	N	O	0	0	0
			835	526	165	144			
3	G	107	Total	C	N	O	0	0	0
			824	520	161	143			

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
			2990	1431	540	874	145			
5	J	146	Total	C	N	O	P	0	0	0
			2990	1431	540	874	145			

- Molecule 6 is a protein called LANA peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	K	12	Total	C	N	O	S	0	0	1
			81	45	21	14	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	16	NH2	-	amidation	UNP D0UZU1

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	G	1	Total	Cl	0	0
			1	1		
7	A	1	Total	Cl	0	0
			1	1		
7	C	1	Total	Cl	0	0
			1	1		
7	E	1	Total	Cl	0	0
			1	1		

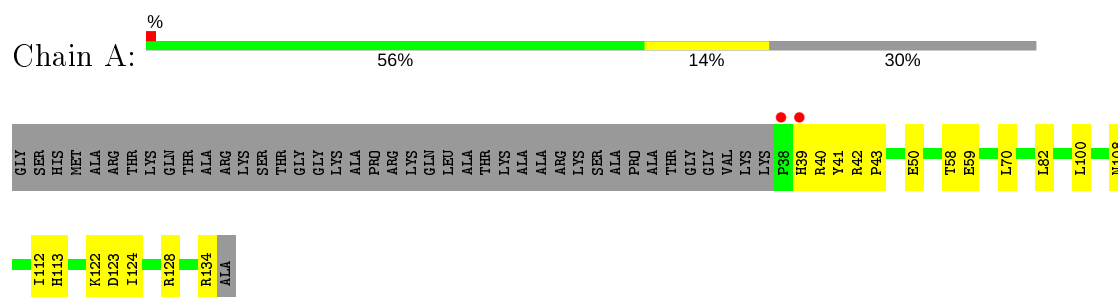
- Molecule 8 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	J	3	Total	Mn	0	0
			3	3		
8	I	2	Total	Mn	0	0
			2	2		
8	E	1	Total	Mn	0	0
			1	1		

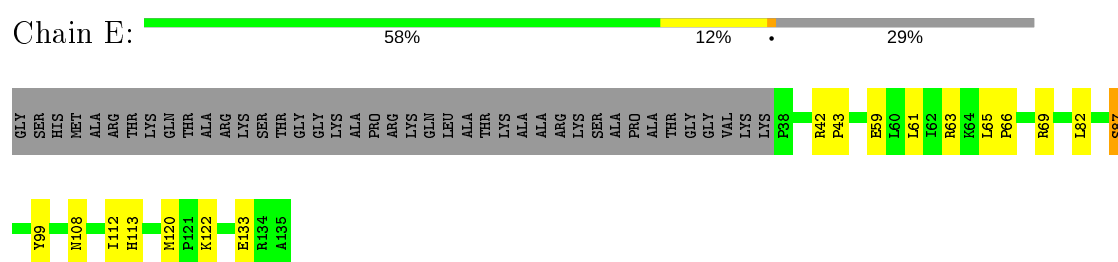
### 3 Residue-property plots [i](#)

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.

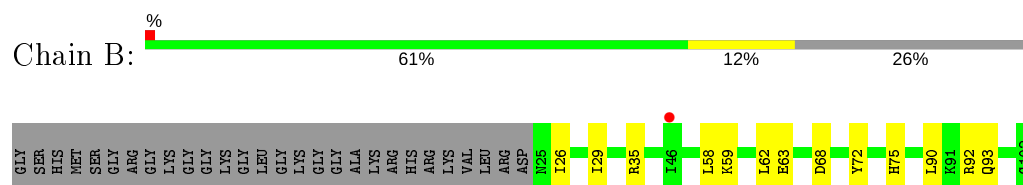
- Molecule 1: Histone H3.1



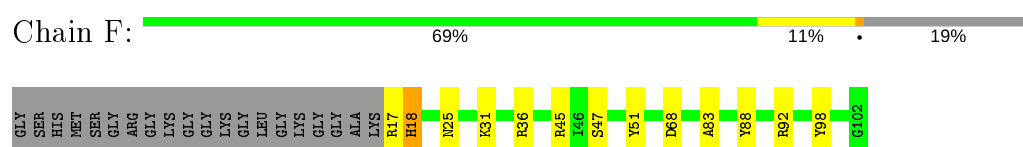
- Molecule 1: Histone H3.1



- Molecule 2: Histone H4

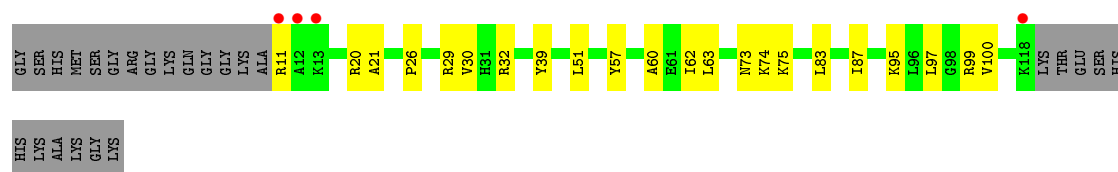


- Molecule 2: Histone H4

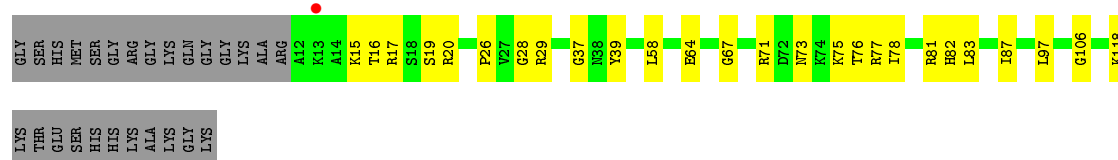


- Molecule 3: Histone H2A type 1-B/E

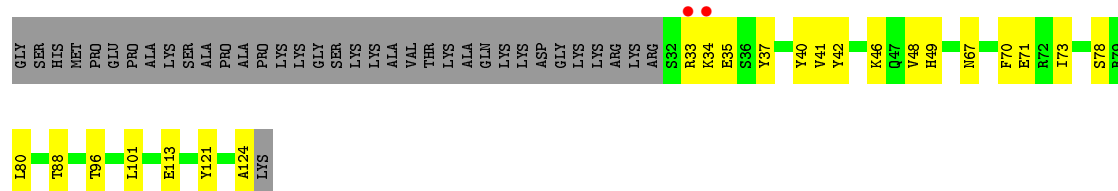




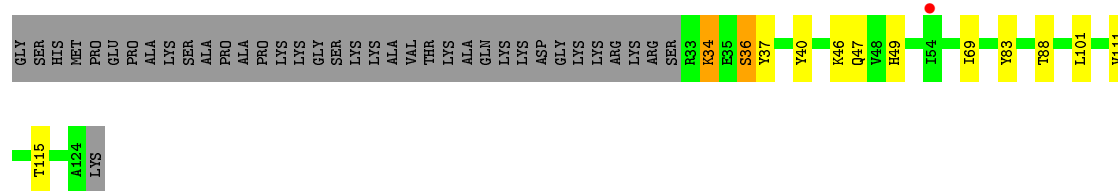
- Molecule 3: Histone H2A type 1-B/E



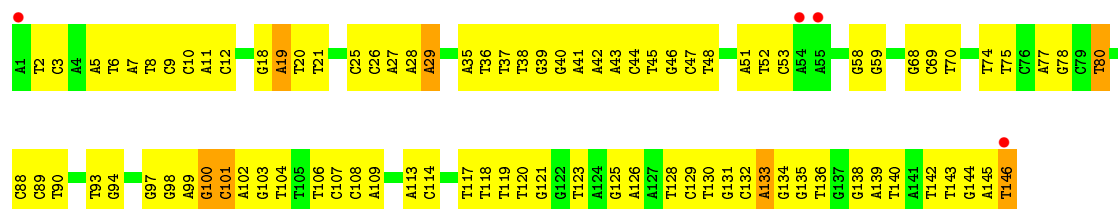
- Molecule 4: Histone H2B type 1-J



- Molecule 4: Histone H2B type 1-J

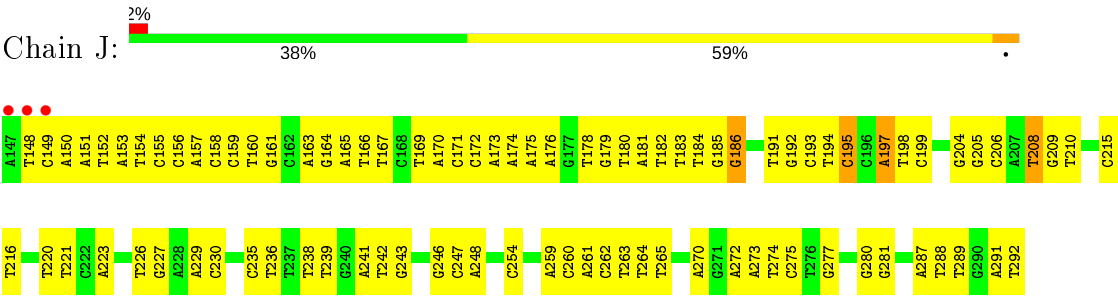


- Molecule 5: DNA (146-MER)



- Molecule 5: DNA (146-MER)





● Molecule 6: LANA peptide



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	107.22Å 109.02Å 176.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.59 – 2.70 48.59 – 2.69	Depositor EDS
% Data completeness (in resolution range)	98.5 (48.59-2.70) 98.0 (48.59-2.69)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.10 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.211 , 0.267 0.213 , 0.268	Depositor DCC
$R_{free}$ test set	2843 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	59.2	Xtriage
Anisotropy	0.500	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 51.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.010 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	12095	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.81% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, MN, NH2

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.49	0/813	0.67	0/1090
1	E	0.67	0/819	0.80	0/1097
2	B	0.55	0/626	0.73	0/837
2	F	0.67	0/702	0.85	0/937
3	C	0.59	0/845	0.77	1/1139 (0.1%)
3	G	0.51	0/834	0.68	0/1125
4	D	0.68	0/736	0.80	0/990
4	H	0.60	0/730	0.69	0/982
5	I	0.86	6/3354 (0.2%)	1.04	5/5175 (0.1%)
5	J	0.90	1/3354 (0.0%)	1.05	4/5175 (0.1%)
6	K	0.49	0/79	0.60	0/101
All	All	0.76	7/12892 (0.1%)	0.93	10/18648 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	100	DG	C3'-O3'	-8.46	1.32	1.44
5	I	29	DA	C3'-O3'	-6.60	1.35	1.44
5	I	19	DA	C3'-O3'	-6.21	1.35	1.44
5	I	28	DA	C3'-O3'	-5.75	1.36	1.44
5	J	223	DA	C3'-O3'	-5.64	1.36	1.44
5	I	80	DT	C1'-N1	5.39	1.56	1.49
5	I	101	DC	P-O5'	-5.33	1.54	1.59

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	197	DA	O5'-P-OP2	-7.59	98.87	105.70
5	J	208	DT	O5'-P-OP2	-6.04	100.27	105.70
3	C	62	ILE	CG1-CB-CG2	-5.83	98.57	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	186	DG	O4'-C1'-N9	5.75	112.03	108.00
5	I	80	DT	O5'-P-OP1	-5.59	100.67	105.70
5	I	133	DA	O4'-C1'-N9	5.58	111.91	108.00
5	I	18	DG	O4'-C1'-N9	5.56	111.89	108.00
5	I	80	DT	OP1-P-OP2	5.50	127.85	119.60
5	I	146	DT	C5-C4-O4	-5.49	121.06	124.90
5	J	195	DC	OP2-P-O3'	5.32	116.91	105.20

There are no chirality outliers.

There are no planarity outliers.

## 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	801	0	839	18	0
1	E	807	0	844	18	0
2	B	619	0	659	16	0
2	F	694	0	742	13	0
3	C	835	0	897	26	0
3	G	824	0	884	23	0
4	D	725	0	745	25	0
4	H	719	0	740	14	0
5	I	2990	0	1652	75	0
5	J	2990	0	1652	73	0
6	K	81	0	84	5	0
7	A	1	0	0	1	0
7	C	1	0	0	0	0
7	E	1	0	0	1	0
7	G	1	0	0	0	0
8	E	1	0	0	0	0
8	I	2	0	0	0	0
8	J	3	0	0	0	0
All	All	12095	0	9738	237	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 11.

All (237) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:154:DT:H2"	5:J:155:DC:H5"	1.45	0.98
5:I:19:DA:H2"	5:I:20:DT:H5'	1.56	0.87
4:H:34:LYS:HD2	5:I:123:DT:OP1	1.78	0.83
5:J:166:DT:H1'	5:J:167:DT:H5'	1.65	0.79
5:I:58:DG:H2"	5:I:59:DG:C8	2.17	0.78
1:E:69:ARG:NH2	5:I:90:DT:OP2	2.19	0.76
5:I:20:DT:H1'	5:I:21:DT:H5'	1.67	0.76
5:J:152:DT:H2"	5:J:153:DA:H5"	1.65	0.76
5:J:170:DA:H2"	5:J:171:DC:H5"	1.67	0.75
5:J:259:DA:H2"	5:J:260:DC:H5"	1.69	0.74
5:J:182:DT:H2"	5:J:183:DT:H5"	1.70	0.73
1:E:87:SER:HB2	2:F:83:ALA:HB2	1.71	0.71
5:I:51:DA:H2"	5:I:52:DT:H5"	1.72	0.70
5:I:40:DG:H2"	5:I:41:DA:C8	2.27	0.69
5:J:179:DG:H1'	5:J:180:DT:H5"	1.76	0.68
5:I:36:DT:H2"	5:I:37:DT:H5"	1.75	0.67
5:I:99:DA:H2"	5:I:100:DG:C8	2.30	0.67
5:I:108:DC:H2"	5:I:109:DA:C8	2.30	0.66
3:C:83:LEU:O	3:C:87:ILE:HG12	1.96	0.66
5:I:11:DA:H1'	5:I:12:DC:H5'	1.77	0.65
5:I:5:DA:H2"	5:I:6:DT:H5"	1.79	0.65
5:J:246:DG:H2"	5:J:247:DC:H5"	1.77	0.65
1:E:108:ASN:O	1:E:112:ILE:HG12	1.96	0.65
5:J:264:DT:H1'	5:J:265:DT:H5'	1.78	0.65
3:C:32:ARG:NH1	5:I:29:DA:OP1	2.30	0.65
5:J:220:DT:H1'	5:J:221:DT:H5'	1.80	0.64
5:J:173:DA:H2"	5:J:174:DA:C8	2.32	0.64
5:J:164:DG:H2"	5:J:165:DA:H5"	1.78	0.63
3:C:20:ARG:HH21	4:D:124:ALA:HA	1.63	0.63
5:I:118:DT:H1'	5:I:119:DT:H5'	1.81	0.63
5:I:106:DT:H1'	5:I:107:DC:H5'	1.79	0.62
1:E:99:TYR:OH	1:E:133:GLU:OE2	2.17	0.62
5:I:125:DG:H2"	5:I:126:DA:H8	1.65	0.62
5:I:74:DT:H1'	5:I:75:DT:H5'	1.82	0.62
2:B:75:HIS:HD2	4:D:96:THR:OG1	1.83	0.62
5:I:8:DT:H1'	5:I:9:DC:H5'	1.82	0.62
2:F:92:ARG:HH21	4:H:101:LEU:HD23	1.66	0.60
3:G:15:LYS:HG3	3:G:20:ARG:HD2	1.83	0.60
5:I:138:DG:N2	5:J:156:DC:O2	2.34	0.60
3:G:77:ARG:HB3	5:I:131:DG:OP1	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:128:DT:H2"	5:I:129:DC:H5"	1.84	0.59
3:G:87:ILE:HD12	3:G:97:LEU:HD12	1.85	0.59
1:E:63:ARG:CZ	5:I:90:DT:H4'	2.32	0.59
5:J:242:DT:H1'	5:J:243:DG:H5'	1.85	0.59
4:D:34:LYS:HG3	5:J:270:DA:OP1	2.03	0.59
3:G:15:LYS:HG2	5:J:178:DT:OP1	2.03	0.59
2:B:92:ARG:HH21	4:D:101:LEU:HD23	1.67	0.59
5:J:229:DA:H1'	5:J:230:DC:H5'	1.85	0.59
5:I:37:DT:H2"	5:I:38:DT:C6	2.38	0.58
5:J:215:DC:H2"	5:J:216:DT:H71	1.86	0.58
5:J:241:DA:H2"	5:J:242:DT:H5'	1.86	0.57
4:H:111:VAL:O	4:H:115:THR:HG23	2.04	0.57
4:H:47:GLN:HB3	6:K:15:GLY:H	1.70	0.57
1:A:43:PRO:HA	5:J:229:DA:H5"	1.87	0.57
5:J:215:DC:H2"	5:J:216:DT:C7	2.35	0.56
5:J:149:DC:H2"	5:J:150:DA:H5"	1.86	0.56
5:J:274:DT:H2"	5:J:275:DC:H5"	1.88	0.56
5:I:125:DG:N2	5:J:169:DT:O2	2.38	0.56
5:J:165:DA:H2"	5:J:166:DT:H5'	1.87	0.56
4:H:88:THR:HG22	5:J:186:DG:OP1	2.07	0.55
5:J:194:DT:H2"	5:J:195:DC:H5'	1.88	0.55
4:H:36:SER:OG	4:H:37:TYR:N	2.39	0.55
5:J:153:DA:H1'	5:J:154:DT:H5'	1.87	0.55
3:G:16:THR:O	3:G:19:SER:OG	2.17	0.55
1:A:70:LEU:HD22	2:B:29:ILE:HD11	1.88	0.55
2:F:68:ASP:OD2	2:F:92:ARG:NH1	2.40	0.54
1:A:108:ASN:O	1:A:112:ILE:HG12	2.07	0.54
5:J:192:DG:H2"	5:J:193:DC:H5'	1.89	0.54
6:K:7:ARG:NH1	6:K:11:GLY:O	2.40	0.54
1:E:61:LEU:HD13	2:F:36:ARG:HB3	1.90	0.54
3:C:26:PRO:HB2	3:C:29:ARG:HB3	1.88	0.54
5:J:235:DC:H2"	5:J:236:DT:C5	2.43	0.54
3:C:74:LYS:HG2	3:C:74:LYS:O	2.08	0.53
3:G:26:PRO:HD3	4:H:40:TYR:CD1	2.43	0.53
3:G:83:LEU:O	3:G:87:ILE:HG12	2.09	0.53
5:I:51:DA:C2'	5:I:52:DT:H5"	2.39	0.53
1:A:42:ARG:NE	5:I:68:DG:OP1	2.35	0.53
5:J:197:DA:H2"	5:J:198:DT:H5'	1.91	0.53
5:J:198:DT:H1'	5:J:199:DC:H5'	1.91	0.53
5:I:7:DA:H1'	5:I:8:DT:H5'	1.89	0.53
3:G:64:GLU:OE2	6:K:12:ARG:NH1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:39:TYR:HB3	4:D:78:SER:HB2	1.91	0.52
5:J:280:DG:H1'	5:J:281:DG:H5'	1.92	0.52
5:J:184:DT:H2''	5:J:185:DG:C8	2.45	0.52
5:J:261:DA:H2''	5:J:262:DC:H5''	1.92	0.52
3:G:71:ARG:NH2	3:G:76:THR:HG22	2.24	0.51
1:E:59:GLU:OE2	1:E:59:GLU:N	2.43	0.51
5:J:247:DC:H2''	5:J:248:DA:N7	2.26	0.51
1:A:41:TYR:HD2	5:J:230:DC:OP1	1.94	0.51
5:J:209:DG:H1'	5:J:210:DT:H5'	1.91	0.51
3:C:39:TYR:OH	4:D:71:GLU:OE1	2.23	0.50
6:K:6:MET:H	6:K:14:THR:HG1	1.55	0.50
1:A:128:ARG:HH12	1:A:134:ARG:HD3	1.75	0.50
3:C:73:ASN:O	3:C:74:LYS:HB3	2.10	0.50
5:I:117:DT:H1'	5:I:118:DT:H5''	1.93	0.50
5:J:148:DT:H2''	5:J:149:DC:H5'	1.93	0.50
5:I:88:DC:N4	5:J:204:DG:O6	2.44	0.50
2:B:59:LYS:O	2:B:63:GLU:HG3	2.12	0.50
5:I:118:DT:H5'	5:I:118:DT:H6	1.77	0.50
5:I:93:DT:H1'	5:I:94:DG:H5'	1.93	0.50
2:B:92:ARG:NH2	4:D:101:LEU:HD23	2.26	0.49
5:J:205:DG:H1'	5:J:206:DC:H5''	1.93	0.49
5:J:288:DT:H1'	5:J:289:DT:H5'	1.94	0.49
3:G:26:PRO:HD3	4:H:40:TYR:CG	2.48	0.49
5:J:172:DC:H2''	5:J:173:DA:C8	2.48	0.49
5:J:175:DA:H2''	5:J:176:DA:C8	2.48	0.49
3:G:17:ARG:NH2	3:G:28:GLY:HA2	2.28	0.48
3:C:11:ARG:NH1	5:J:265:DT:H5''	2.29	0.48
5:I:25:DC:H2''	5:I:26:DC:H6	1.78	0.48
3:C:63:LEU:HD11	4:D:41:VAL:HG13	1.95	0.48
3:G:71:ARG:HD3	3:G:71:ARG:O	2.14	0.48
2:F:88:TYR:CE1	4:H:83:TYR:CZ	3.02	0.48
3:G:29:ARG:NH1	4:H:36:SER:O	2.46	0.47
5:I:139:DA:H2''	5:I:140:DT:H5'	1.96	0.47
5:I:10:DC:H1'	5:I:11:DA:C8	2.50	0.47
2:B:75:HIS:CD2	4:D:96:THR:OG1	2.65	0.47
3:C:21:ALA:HB2	4:D:121:TYR:HB2	1.96	0.47
5:I:45:DT:H2'	5:I:46:DG:C8	2.49	0.47
5:J:272:DA:H2''	5:J:273:DA:H8	1.79	0.47
3:C:30:VAL:HG13	4:D:70:PHE:HE1	1.78	0.47
5:J:272:DA:H2''	5:J:273:DA:C8	2.49	0.47
1:A:39:HIS:CG	1:A:40:ARG:N	2.82	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:26:PRO:HD3	4:D:40:TYR:CG	2.50	0.47
5:I:47:DC:H2"	5:I:48:DT:C5	2.50	0.47
4:D:37:TYR:HE2	4:D:67:ASN:OD1	1.98	0.47
5:J:191:DT:H1'	5:J:192:DG:C8	2.49	0.47
3:C:11:ARG:NH2	5:J:264:DT:O3'	2.40	0.47
3:C:26:PRO:HD3	4:D:40:TYR:CD1	2.50	0.46
5:I:131:DG:H2"	5:I:132:DC:C6	2.49	0.46
1:A:59:GLU:OE1	1:A:59:GLU:N	2.48	0.46
5:I:26:DC:H2"	5:I:27:DA:N7	2.31	0.46
5:I:97:DG:H1'	5:I:98:DG:H5'	1.97	0.46
2:B:26:ILE:HD12	2:B:29:ILE:HD13	1.97	0.46
3:C:26:PRO:HG3	4:D:40:TYR:CE2	2.51	0.46
4:D:33:ARG:HH11	4:D:33:ARG:HG3	1.80	0.46
5:J:158:DC:H2"	5:J:159:DC:H5'	1.98	0.46
5:J:238:DT:H1'	5:J:239:DT:H5'	1.96	0.46
3:C:51:LEU:HD13	4:D:73:ILE:HG21	1.97	0.46
5:J:262:DC:H1'	5:J:263:DT:H5'	1.98	0.46
5:I:120:DT:H2"	5:I:121:DG:C8	2.51	0.46
5:I:2:DT:H2"	5:I:3:DC:H5'	1.98	0.46
3:G:71:ARG:HH22	3:G:76:THR:HG22	1.81	0.45
1:E:69:ARG:HH22	5:I:90:DT:P	2.39	0.45
1:A:122:LYS:HB2	7:A:1001:CL:CL	2.53	0.45
2:B:62:LEU:HD23	2:B:62:LEU:HA	1.58	0.45
2:B:72:TYR:CE1	4:D:80:LEU:HD11	2.51	0.45
5:I:133:DA:H1'	5:I:134:DG:H5"	1.98	0.45
5:I:47:DC:H2"	5:I:48:DT:C6	2.51	0.45
5:I:52:DT:H2"	5:I:53:DC:H5'	1.98	0.45
5:J:157:DA:H1'	5:J:158:DC:H5'	1.98	0.45
1:A:58:THR:HG22	3:G:106:GLY:HA3	1.98	0.45
3:C:73:ASN:O	3:C:75:LYS:HG2	2.16	0.45
1:E:82:LEU:HA	1:E:82:LEU:HD23	1.87	0.45
5:I:125:DG:H2"	5:I:126:DA:C8	2.47	0.45
5:I:113:DA:H2"	5:I:114:DC:O5'	2.17	0.45
5:I:43:DA:H2"	5:I:44:DC:H5"	1.99	0.45
5:I:6:DT:H2"	5:I:7:DA:C8	2.51	0.45
3:G:78:ILE:HA	3:G:82:HIS:HD1	1.82	0.45
5:I:134:DG:H1'	5:I:135:DG:H5'	1.97	0.45
1:E:43:PRO:HG2	5:J:215:DC:H5'	1.99	0.45
3:C:100:VAL:HG11	2:F:98:TYR:CE2	2.52	0.45
4:D:46:LYS:HA	4:D:46:LYS:HD3	1.74	0.44
5:I:132:DC:H2"	5:I:133:DA:C8	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:148:DT:C4	5:J:149:DC:N4	2.85	0.44
1:E:69:ARG:HD2	2:F:25:ASN:OD1	2.18	0.44
3:G:73:ASN:O	3:G:75:LYS:HG3	2.17	0.44
5:I:133:DA:C6	5:I:134:DG:C6	3.05	0.44
5:I:39:DG:H1	5:J:254:DC:H42	1.64	0.44
3:C:57:TYR:HB2	4:D:113:GLU:HG3	2.00	0.44
3:C:32:ARG:NH2	4:D:35:GLU:OE2	2.46	0.44
2:F:31:LYS:HG3	2:F:51:TYR:CE1	2.53	0.44
5:I:7:DA:C2	5:J:287:DA:C2	3.06	0.44
3:G:118:LYS:HE2	3:G:118:LYS:HB2	1.69	0.44
5:J:150:DA:C6	5:J:151:DA:C6	3.06	0.43
5:J:155:DC:H2''	5:J:156:DC:H5'	2.00	0.43
1:A:43:PRO:HG2	5:I:68:DG:H5'	2.00	0.43
1:A:100:LEU:HD11	2:B:58:LEU:HD12	2.01	0.43
3:C:87:ILE:HD12	3:C:97:LEU:HD12	2.00	0.43
2:B:68:ASP:OD2	2:B:92:ARG:NH1	2.52	0.43
5:I:144:DG:C6	5:I:145:DA:C6	3.06	0.43
2:F:45:ARG:CZ	5:I:80:DT:H4'	2.49	0.43
2:F:88:TYR:CE1	4:H:83:TYR:CE1	3.06	0.43
3:G:67:GLY:HA3	4:H:49:HIS:ND1	2.33	0.43
5:J:208:DT:H2''	5:J:209:DG:C8	2.54	0.43
5:I:142:DT:H1'	5:I:143:DT:H5'	1.99	0.43
5:J:152:DT:C2'	5:J:153:DA:H5''	2.43	0.43
5:J:261:DA:C2'	5:J:262:DC:H5''	2.48	0.43
5:J:247:DC:H2''	5:J:248:DA:C8	2.53	0.43
4:D:88:THR:HG22	5:I:39:DG:OP1	2.18	0.43
5:I:135:DG:H2''	5:I:136:DT:O5'	2.18	0.43
5:I:42:DA:H2''	5:I:43:DA:H5'	2.01	0.43
5:J:149:DC:N4	5:J:150:DA:N6	2.66	0.43
5:I:11:DA:C2	5:I:12:DC:C2	3.07	0.42
5:I:130:DT:H2''	5:I:131:DG:C8	2.54	0.42
1:E:42:ARG:NE	5:J:215:DC:OP1	2.52	0.42
5:J:277:DG:H5''	5:J:277:DG:H8	1.83	0.42
5:I:69:DC:H2''	5:I:70:DT:C7	2.49	0.42
5:I:5:DA:C2'	5:I:6:DT:H5''	2.46	0.42
2:B:72:TYR:HE1	4:D:80:LEU:HD11	1.84	0.42
3:G:37:GLY:HA3	3:G:39:TYR:CE2	2.54	0.42
5:I:77:DA:H2''	5:I:78:DG:C8	2.55	0.42
1:E:65:LEU:HB3	1:E:66:PRO:HD3	2.00	0.42
1:A:123:ASP:OD1	1:E:113:HIS:NE2	2.50	0.42
3:C:57:TYR:O	3:C:60:ALA:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:9:DC:H2"	5:I:10:DC:H5'	2.01	0.42
5:J:163:DA:H2"	5:J:164:DG:C8	2.53	0.42
5:J:181:DA:H2"	5:J:182:DT:OP2	2.19	0.42
5:J:226:DT:H2"	5:J:227:DG:C8	2.55	0.42
2:F:17:ARG:HG2	2:F:18:HIS:N	2.34	0.42
5:I:101:DC:H2"	5:I:102:DA:C8	2.54	0.42
5:J:291:DA:C5	5:J:292:DT:H73	2.56	0.41
1:A:113:HIS:CE1	1:E:122:LYS:HG2	2.56	0.41
4:H:46:LYS:HD3	4:H:46:LYS:HA	1.75	0.41
5:I:109:DA:C2	5:J:185:DG:N2	2.89	0.41
3:C:32:ARG:HD3	5:I:29:DA:OP2	2.20	0.41
4:D:42:TYR:CE2	4:D:46:LYS:HE3	2.55	0.41
5:I:35:DA:H2"	5:I:36:DT:OP2	2.20	0.41
5:I:89:DC:H2"	5:I:90:DT:C7	2.50	0.41
1:A:124:ILE:O	1:A:128:ARG:HG3	2.20	0.41
3:C:95:LYS:HA	3:C:95:LYS:HD2	1.81	0.41
3:G:64:GLU:HG3	6:K:12:ARG:NH1	2.36	0.41
2:B:68:ASP:OD2	2:B:93:GLN:NE2	2.53	0.41
1:A:58:THR:CG2	3:G:81:ARG:HD3	2.51	0.41
1:E:120:MET:HG2	2:F:47:SER:HB2	2.03	0.41
5:I:103:DG:H1'	5:I:104:DT:H5"	2.02	0.41
1:A:50:GLU:OE1	2:B:35:ARG:NH1	2.54	0.41
1:E:43:PRO:HG2	5:J:215:DC:C5'	2.50	0.41
2:B:90:LEU:HA	2:B:90:LEU:HD23	1.95	0.40
3:G:58:LEU:HD23	3:G:58:LEU:HA	1.84	0.40
1:E:122:LYS:HB2	7:E:1001:CL:CL	2.58	0.40
3:C:100:VAL:HG11	2:F:98:TYR:CZ	2.56	0.40
4:H:69:ILE:HG23	4:H:69:ILE:HD12	1.86	0.40
5:J:160:DT:H2"	5:J:161:DG:C8	2.56	0.40
1:A:70:LEU:HD22	2:B:29:ILE:CD1	2.51	0.40
4:D:48:VAL:HG23	4:D:49:HIS:CD2	2.57	0.40
5:I:145:DA:C6	5:I:146:DT:O4	2.75	0.40
5:I:88:DC:H2"	5:I:89:DC:C6	2.55	0.40

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	95/139 (68%)	95 (100%)	0	0	100	100
1	E	96/139 (69%)	95 (99%)	1 (1%)	0	100	100
2	B	76/106 (72%)	75 (99%)	1 (1%)	0	100	100
2	F	84/106 (79%)	83 (99%)	1 (1%)	0	100	100
3	C	106/133 (80%)	105 (99%)	1 (1%)	0	100	100
3	G	105/133 (79%)	104 (99%)	1 (1%)	0	100	100
4	D	91/129 (70%)	89 (98%)	2 (2%)	0	100	100
4	H	90/129 (70%)	87 (97%)	3 (3%)	0	100	100
6	K	10/12 (83%)	9 (90%)	1 (10%)	0	100	100
All	All	753/1026 (73%)	742 (98%)	11 (2%)	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	85/113 (75%)	84 (99%)	1 (1%)	71	88
1	E	85/113 (75%)	84 (99%)	1 (1%)	71	88
2	B	63/81 (78%)	63 (100%)	0	100	100
2	F	71/81 (88%)	70 (99%)	1 (1%)	67	86
3	C	85/102 (83%)	84 (99%)	1 (1%)	71	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	G	84/102 (82%)	84 (100%)	0	100	100
4	D	79/107 (74%)	79 (100%)	0	100	100
4	H	78/107 (73%)	76 (97%)	2 (3%)	46	75
6	K	8/8 (100%)	8 (100%)	0	100	100
All	All	638/814 (78%)	632 (99%)	6 (1%)	78	92

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	LEU
3	C	99	ARG
1	E	87	SER
2	F	18	HIS
4	H	34	LYS
4	H	36	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	HIS
2	B	75	HIS
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 ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 10 ligands modelled in this entry, 10 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	97/139 (69%)	0.09	2 (2%) 63 65	51, 69, 99, 126	0
1	E	98/139 (70%)	-0.08	0 100 100	35, 49, 73, 99	0
2	B	78/106 (73%)	0.09	1 (1%) 77 78	51, 64, 79, 94	0
2	F	86/106 (81%)	0.04	0 100 100	36, 46, 66, 102	0
3	C	108/133 (81%)	0.07	4 (3%) 41 41	35, 53, 82, 124	0
3	G	107/133 (80%)	-0.01	1 (0%) 84 85	49, 64, 98, 105	0
4	D	93/129 (72%)	0.14	2 (2%) 62 63	39, 55, 76, 102	0
4	H	92/129 (71%)	0.18	1 (1%) 80 82	46, 62, 84, 105	0
5	I	146/146 (100%)	-0.23	4 (2%) 54 55	67, 116, 149, 160	0
5	J	146/146 (100%)	-0.28	3 (2%) 63 65	67, 119, 147, 158	0
6	K	11/12 (91%)	-0.50	0 100 100	62, 73, 84, 93	0
All	All	1062/1318 (80%)	-0.03	18 (1%) 70 72	35, 66, 135, 160	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	I	146	DT	16.1
3	C	11	ARG	3.8
3	C	12	ALA	3.2
1	A	39	HIS	3.1
1	A	38	PRO	3.1
4	D	33	ARG	3.0
3	C	13	LYS	3.0
5	J	147	DA	2.9
3	C	118	LYS	2.9
2	B	46	ILE	2.8
4	H	54	ILE	2.7
5	I	55	DA	2.5

*Continued on next page...*

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Mol	Chain	Res	Type	RSRZ
4	D	34	LYS	2.5
5	I	1	DA	2.5
5	J	148	DT	2.4
5	J	149	DC	2.3
3	G	13	LYS	2.1
5	I	54	DA	2.1

## 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](#)

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<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	B-factors( $\text{\AA}^2$ )	Q<0.9
8	MN	J	2001	1/1	0.78	0.32	132,132,132,132	0
8	MN	I	2002	1/1	0.78	0.17	127,127,127,127	0
7	CL	E	1001	1/1	0.91	0.22	77,77,77,77	0
7	CL	G	1001	1/1	0.91	0.09	68,68,68,68	0
8	MN	I	2001	1/1	0.92	0.07	140,140,140,140	0
7	CL	A	1001	1/1	0.96	0.51	83,83,83,83	0
8	MN	J	2002	1/1	0.96	0.05	108,108,108,108	0
7	CL	C	1001	1/1	0.97	0.11	66,66,66,66	0
8	MN	J	2003	1/1	0.97	0.24	95,95,95,95	0
8	MN	E	1002	1/1	0.98	0.31	54,54,54,54	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.