



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 10:46 pm GMT

PDB ID : 3AZL  
Title : Crystal Structure of Human Nucleosome Core Particle Containing H4K77Q mutation  
Authors : Iwasaki, W.; Tachiwana, H.; Kawaguchi, K.; Shibata, T.; Kagawa, W.; Kurumizaka, H.  
Deposited on : 2011-05-25  
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

<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:

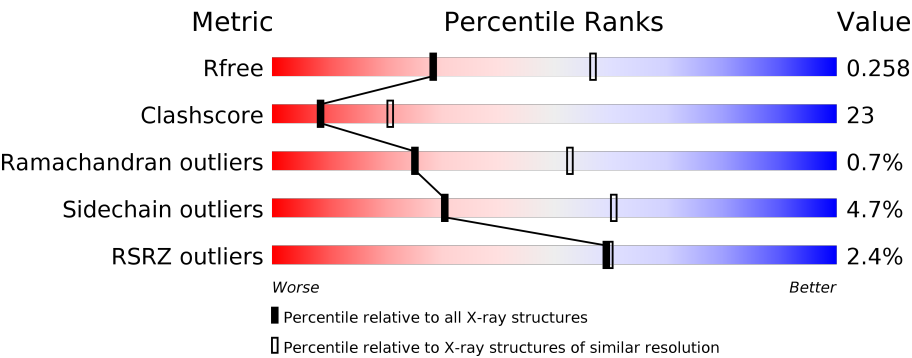
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

# 1 Overall quality at a glance i

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))
$R_{free}$	100719	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (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. 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>55%14%•30%</div></div>
1	E	139	<div>%<div>51%16%••29%</div></div>
2	B	106	<div>%<div>52%20%•26%</div></div>
2	F	106	<div>3%<div>62%18%•19%</div></div>
3	C	133	<div>3%<div>55%22%5%19%</div></div>
3	G	133	<div>2%<div>59%17%•21%</div></div>

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Mol	Chain	Length	Quality of chain
4	D	129	
4	H	129	
5	I	146	
5	J	146	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	MN	E	1001	-	-	-	X
7	MN	I	1004	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 12153 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	99	Total	C	N	O	S	0	0	0
			816	514	158	140	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	390	120	108	1			
2	F	86	Total	C	N	O	S	0	0	0
			694	435	140	118	1			

There are 8 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
B	77	GLN	LYS	ENGINEERED MUTATION	UNP P62805
F	-3	GLY	-	EXPRESSION TAG	UNP P62805
F	-2	SER	-	EXPRESSION TAG	UNP P62805

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-1	HIS	-	EXPRESSION TAG	UNP P62805
F	77	GLN	LYS	ENGINEERED MUTATION	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	105	Total	C	N	O	0	0	0
			810	511	158	141			

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	94	Total	C	N	O	S	0	0	0
			736	462	134	138	2			
4	H	93	Total	C	N	O	S	0	0	0
			725	456	130	137	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 146-MER DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	145	Total	C	N	O	P	0	0	0
			2970	1421	538	867	144			
5	J	145	Total	C	N	O	P	0	0	0
			2969	1421	535	869	144			

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 7 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	J	4	Total	Mn	0	0
			4	4		
7	I	6	Total	Mn	0	0
			6	6		
7	E	1	Total	Mn	0	0
			1	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	21	Total	O	0	0
			21	21		
8	B	15	Total	O	0	0
			15	15		
8	C	19	Total	O	0	0
			19	19		
8	D	10	Total	O	0	0
			10	10		
8	E	36	Total	O	0	0
			36	36		
8	F	23	Total	O	0	0
			23	23		

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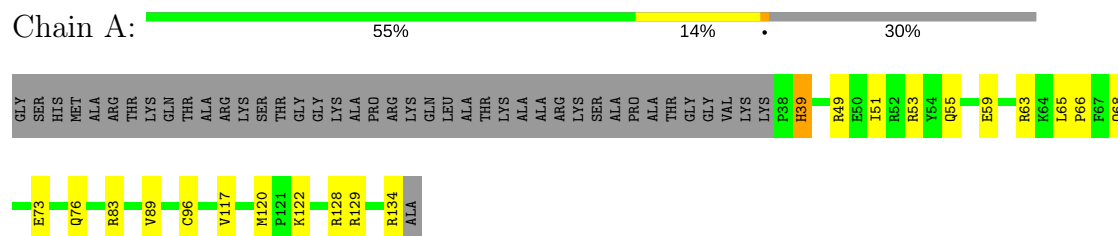
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	G	9	Total 9	O 9	0	0
8	H	9	Total 9	O 9	0	0
8	I	9	Total 9	O 9	0	0
8	J	12	Total 12	O 12	0	0

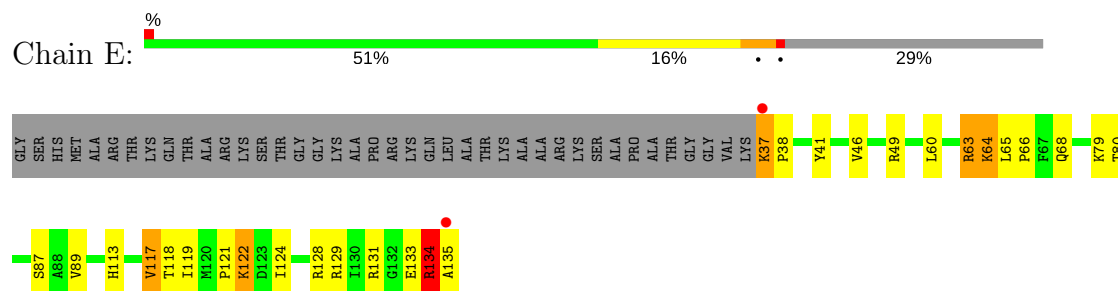
### 3 Residue-property plots [i](#)

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.

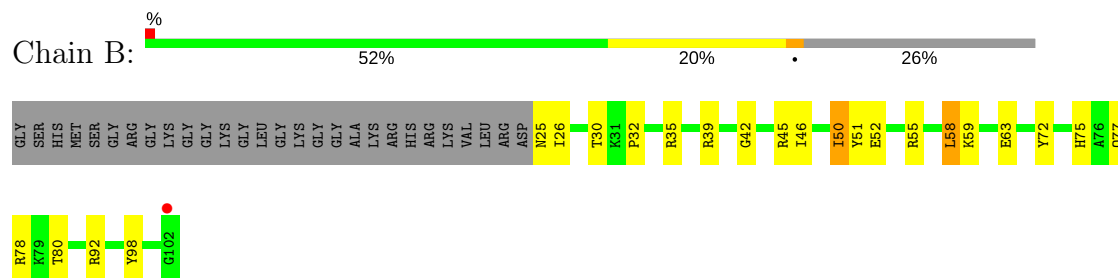
#### • Molecule 1: Histone H3.1



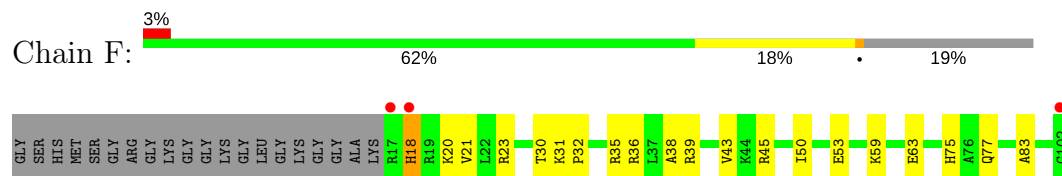
#### • Molecule 1: Histone H3.1



#### • Molecule 2: Histone H4

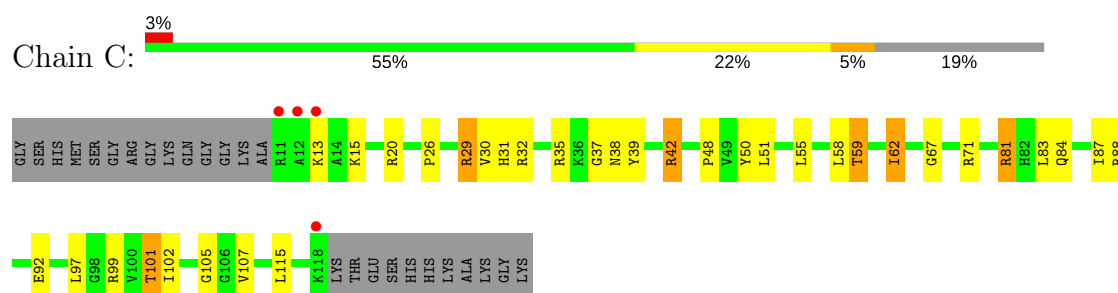


#### • Molecule 2: Histone H4

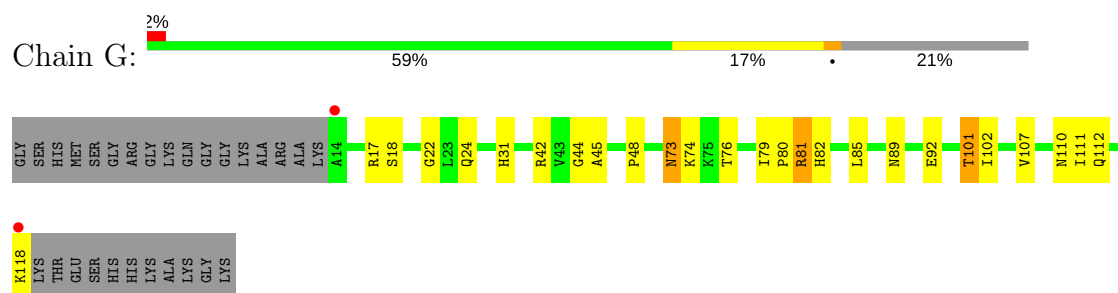


#### • Molecule 3: Histone H2A type 1-B/E

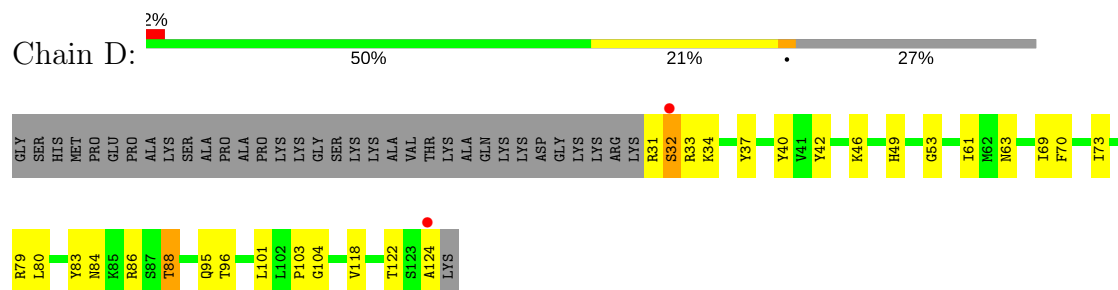




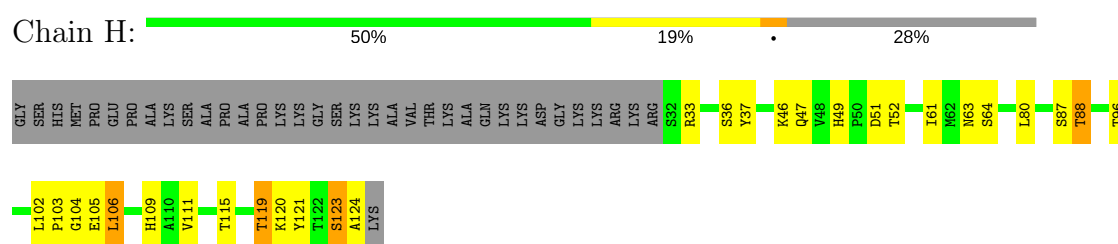
• Molecule 3: Histone H2A type 1-B/E



• Molecule 4: Histone H2B type 1-J



• Molecule 4: Histone H2B type 1-J



• Molecule 5: 146-MER DNA



G131  
C132  
A133  
G134  
G135  
T136  
G137  
G138  
A139  
T140  
A141  
T142  
T143  
G144  
A145  
DT

● Molecule 5: 146-MER DNA



DA  
T148  
C149  
A150  
A151  
T152  
A153  
T154  
C155  
C158  
C159  
T160  
G161  
C162  
A163  
G164  
A165  
T166  
T167  
C168  
T169  
A170  
C171  
C172  
A173  
A174  
A175  
A176  
G177  
T178  
G179  
T180  
A181  
T182  
T183  
T184  
G185  
G186  
A187  
A188  
A189  
C190  
T191  
G192  
C193  
T194  
C195  
C196  
A197  
T198  
C199  
A200  
A201  
A202  
G205  
C206  
A207

T210  
T211  
C212  
G217  
T220  
T221  
C222  
A223  
G224  
C225  
T226  
G227  
A228  
A229  
C230  
A231  
T232  
G233  
C234  
C235  
T236  
T237  
T238  
T239  
G240  
A241  
T242  
G243  
G244  
A245  
G246  
C247  
A248  
G249  
T250  
T251  
T252  
C253  
C254  
A255  
A256  
A257  
T258  
A259  
C260  
A261  
C262  
T263  
T264  
T265  
T266  
G267  
G268  
T269  
A270  
G271  
A272  
A273

T274  
C275  
A279  
G280  
G281  
T282  
G283  
G284  
A285  
T286  
A287  
T288  
T289  
T292

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	106.58Å 109.64Å 182.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.98 – 2.70 42.98 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (42.98-2.70) 99.8 (42.98-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.28 (at 2.69Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.208 , 0.259 0.208 , 0.258	Depositor DCC
$R_{free}$ test set	2996 reflections (5.06%)	DCC
Wilson B-factor (Å <sup>2</sup> )	53.4	Xtriage
Anisotropy	0.407	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 60.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.016 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	12153	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% 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: MN, CL

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	0.46	0/813	0.67	0/1090
1	E	0.55	0/828	0.72	0/1109
2	B	0.48	0/626	0.68	0/838
2	F	0.53	0/702	0.77	0/938
3	C	0.47	0/845	0.66	0/1139
3	G	0.41	0/820	0.62	0/1107
4	D	0.46	0/747	0.66	0/1004
4	H	0.46	0/736	0.62	0/990
5	I	0.42	0/3332	0.81	0/5141
5	J	0.41	0/3330	0.82	0/5138
All	All	0.45	0/12779	0.75	0/18494

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	51	TYR	Sidechain

## 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	26	0
1	E	816	0	856	36	0
2	B	619	0	654	28	0
2	F	694	0	737	24	0
3	C	835	0	897	39	0
3	G	810	0	866	26	0
4	D	736	0	758	32	0
4	H	725	0	745	25	0
5	I	2970	0	1640	163	0
5	J	2969	0	1641	159	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
6	E	1	0	0	1	0
6	G	1	0	0	1	0
7	E	1	0	0	0	0
7	I	6	0	0	0	0
7	J	4	0	0	0	0
8	A	21	0	0	4	0
8	B	15	0	0	1	0
8	C	19	0	0	1	0
8	D	10	0	0	1	0
8	E	36	0	0	1	0
8	F	23	0	0	3	0
8	G	9	0	0	3	0
8	H	9	0	0	1	0
8	I	9	0	0	1	0
8	J	12	0	0	5	0
All	All	12153	0	9633	494	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 23.

All (494) 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:285:DA:H2''	5:J:286:DT:H5'	1.23	1.16
5:J:192:DG:H2''	5:J:193:DC:H5''	1.24	1.12
5:I:104:DT:H2''	5:I:105:DT:H5''	1.43	1.00
5:I:23:DT:H2''	5:I:24:DA:H5''	1.40	0.99
5:J:239:DT:H2''	5:J:240:DG:H5''	1.46	0.97
5:I:131:DG:H2''	5:I:132:DC:C5	2.00	0.96
5:J:149:DC:H2''	5:J:150:DA:H5'	1.49	0.94
5:J:192:DG:C2'	5:J:193:DC:H5''	1.98	0.94
5:I:51:DA:H2''	5:I:52:DT:H5'	1.48	0.93
5:I:52:DT:H2''	5:I:53:DC:H5''	1.50	0.91
5:I:55:DA:H2''	5:I:56:DA:H5''	1.53	0.90
5:I:42:DA:H2''	5:I:43:DA:H5'	1.55	0.87
5:I:93:DT:H2''	5:I:94:DG:H5'	1.57	0.87
5:J:281:DG:H2''	5:J:282:DT:H5'	1.55	0.87
5:I:55:DA:C2'	5:I:56:DA:H5''	2.05	0.87
5:I:142:DT:H2''	5:I:143:DT:H5'	1.54	0.86
5:J:266:DT:H2''	5:J:267:DG:N7	1.90	0.85
3:C:62:ILE:HD11	3:C:83:LEU:HD22	1.58	0.85
4:H:37:TYR:H	4:H:63:ASN:HD21	1.24	0.85
5:J:248:DA:H2''	5:J:249:DG:H5'	1.58	0.85
5:I:52:DT:C2'	5:I:53:DC:H5''	2.07	0.84
5:J:164:DG:H2''	5:J:165:DA:H5''	1.59	0.84
5:I:43:DA:H2''	5:I:44:DC:H5''	1.61	0.83
5:I:31:DG:H2''	5:I:32:DT:H5'	1.60	0.83
5:J:172:DC:H2''	5:J:173:DA:H5''	1.62	0.82
5:I:99:DA:H2''	5:I:100:DG:H5'	1.61	0.81
5:J:192:DG:H2''	5:J:193:DC:C5'	2.09	0.81
5:J:286:DT:C2'	5:J:287:DA:H5''	2.11	0.81
4:D:46:LYS:HA	4:D:46:LYS:HE2	1.63	0.80
5:I:36:DT:H1'	5:I:37:DT:H5'	1.64	0.80
1:E:63:ARG:NH1	1:E:63:ARG:H	1.79	0.79
5:I:50:DC:H2''	5:I:51:DA:H5''	1.62	0.79
5:I:55:DA:C3'	5:I:56:DA:H5''	2.13	0.79
5:J:150:DA:H2''	5:J:151:DA:OP2	1.82	0.79
5:J:181:DA:H1'	5:J:182:DT:H5''	1.65	0.79
5:J:189:DA:H2''	5:J:190:DC:O5'	1.81	0.79
3:C:84:GLN:HE22	3:C:88:ARG:HE	1.27	0.78
3:G:102:ILE:HG23	4:H:61:ILE:HD13	1.65	0.78
5:J:235:DC:H2''	5:J:236:DT:C7	2.13	0.78
5:J:270:DA:H2''	5:J:271:DG:O5'	1.84	0.78
5:I:23:DT:C2'	5:I:24:DA:H5''	2.14	0.78
4:H:88:THR:HG23	5:J:186:DG:OP1	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:17:ARG:HH12	3:G:31:HIS:HD2	1.31	0.78
5:J:266:DT:H2''	5:J:267:DG:C8	2.20	0.77
5:I:17:DA:H2''	5:I:18:DG:H5''	1.67	0.77
5:I:43:DA:C2'	5:I:44:DC:H5''	2.15	0.76
5:J:286:DT:H2''	5:J:287:DA:H5''	1.65	0.76
5:J:239:DT:C2'	5:J:240:DG:H5''	2.15	0.76
5:I:50:DC:H2''	5:I:51:DA:C5'	2.14	0.76
4:D:118:VAL:O	4:D:122:THR:HG23	1.86	0.75
5:I:104:DT:H2''	5:I:105:DT:C5'	2.15	0.75
1:E:133:GLU:O	1:E:134:ARG:HB2	1.87	0.74
5:I:104:DT:C2'	5:I:105:DT:H5''	2.17	0.74
5:J:286:DT:H1'	5:J:287:DA:H5''	1.68	0.74
5:I:115:DA:H2''	5:I:116:DC:H5''	1.70	0.74
5:J:241:DA:H1'	5:J:242:DT:H5'	1.69	0.74
5:J:262:DC:H4'	5:J:263:DT:OP1	1.87	0.73
3:G:42:ARG:HB2	4:H:88:THR:HB	1.69	0.73
5:I:8:DT:H2''	5:I:9:DC:OP2	1.89	0.73
5:J:182:DT:H2''	5:J:183:DT:H5'	1.70	0.73
1:E:63:ARG:HB2	1:E:63:ARG:HH11	1.54	0.73
2:B:59:LYS:O	2:B:63:GLU:HG3	1.88	0.72
5:I:16:DC:H2''	5:I:17:DA:OP2	1.89	0.72
5:J:285:DA:C2'	5:J:286:DT:H5'	2.12	0.72
5:J:244:DG:H1'	5:J:245:DA:H5'	1.70	0.72
1:E:68:GLN:HG3	1:E:89:VAL:HG11	1.72	0.72
5:J:284:DG:H2''	5:J:285:DA:H8	1.54	0.72
5:I:34:DT:H2''	5:I:35:DA:H8	1.54	0.71
5:J:165:DA:H2''	5:J:166:DT:H5'	1.71	0.71
5:I:35:DA:H2''	5:I:36:DT:OP2	1.90	0.70
1:E:37:LYS:N	1:E:38:PRO:HA	2.07	0.70
5:I:3:DC:H2''	5:I:4:DA:C8	2.26	0.70
3:G:31:HIS:CD2	3:G:48:PRO:HG2	2.27	0.70
5:J:211:DT:H2''	5:J:212:DC:H5'	1.74	0.70
5:J:182:DT:H1'	5:J:183:DT:H5''	1.73	0.69
5:J:284:DG:H2''	5:J:285:DA:C8	2.26	0.69
3:C:62:ILE:HD11	3:C:83:LEU:CD2	2.23	0.69
5:I:134:DG:H2''	5:I:135:DG:H5'	1.75	0.69
5:J:253:DC:H3'	8:J:2008:HOH:O	1.93	0.69
3:C:55:LEU:O	3:C:59:THR:HG23	1.93	0.68
5:J:271:DG:H2''	5:J:272:DA:H5'	1.76	0.68
1:A:120:MET:HA	2:B:50:ILE:HD11	1.76	0.68
2:F:59:LYS:O	2:F:63:GLU:HG3	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:79:LYS:HD3	1:E:80:THR:N	2.09	0.68
4:H:119:THR:HG22	4:H:120:LYS:N	2.08	0.67
5:I:106:DT:H1'	5:I:107:DC:H5''	1.76	0.67
1:A:63:ARG:HH12	2:B:30:THR:CG2	2.08	0.67
5:I:50:DC:C2'	5:I:51:DA:H5''	2.24	0.67
5:I:52:DT:H2''	5:I:53:DC:C5'	2.23	0.66
4:H:37:TYR:H	4:H:63:ASN:ND2	1.90	0.66
5:I:110:DA:H2''	5:I:111:DA:OP2	1.95	0.66
5:J:286:DT:C1'	5:J:287:DA:H5''	2.25	0.66
5:I:55:DA:OP1	5:I:55:DA:H4'	1.96	0.66
2:B:92:ARG:HB3	2:B:92:ARG:NH1	2.10	0.66
1:E:49:ARG:HG3	1:E:49:ARG:HH11	1.61	0.66
5:J:179:DG:H2''	5:J:180:DT:OP2	1.95	0.66
5:I:54:DA:H4'	5:I:54:DA:OP1	1.95	0.66
5:J:187:DA:H2''	5:J:188:DA:O5'	1.96	0.66
5:J:205:DG:H2''	5:J:206:DC:H5'	1.77	0.66
5:I:31:DG:H2''	5:I:32:DT:C5'	2.25	0.65
5:I:26:DC:H2''	5:I:27:DA:C8	2.30	0.65
1:A:120:MET:HA	2:B:50:ILE:CD1	2.26	0.65
5:I:26:DC:H2''	5:I:27:DA:C5	2.32	0.65
1:A:120:MET:CA	2:B:50:ILE:HD11	2.27	0.65
5:I:115:DA:C2'	5:I:116:DC:H5''	2.27	0.65
3:C:102:ILE:HG23	4:D:61:ILE:HD13	1.78	0.65
5:J:241:DA:H2''	5:J:242:DT:OP2	1.94	0.65
5:I:43:DA:H2''	5:I:44:DC:C5'	2.26	0.65
5:I:26:DC:H2''	5:I:27:DA:N7	2.11	0.65
5:J:161:DG:H2''	5:J:162:DC:OP2	1.95	0.65
5:I:10:DC:H2''	5:I:11:DA:C8	2.32	0.64
5:J:205:DG:H1'	5:J:206:DC:H5''	1.79	0.64
1:E:63:ARG:CB	1:E:63:ARG:HH11	2.11	0.64
3:G:76:THR:O	4:H:52:THR:HG23	1.98	0.63
5:J:250:DT:H2''	5:J:251:DT:OP2	1.97	0.63
4:D:88:THR:HG23	5:I:39:DG:OP1	1.98	0.63
3:G:17:ARG:HH12	3:G:31:HIS:CD2	2.14	0.63
5:J:153:DA:H1'	5:J:154:DT:H5''	1.79	0.63
2:B:92:ARG:HH21	4:D:101:LEU:HD12	1.64	0.63
3:G:110:ASN:HA	8:G:2006:HOH:O	1.98	0.63
3:C:30:VAL:HG13	4:D:70:PHE:HE1	1.64	0.63
2:F:31:LYS:HB3	2:F:32:PRO:HD3	1.81	0.62
5:J:233:DG:H2''	5:J:234:DC:OP2	1.96	0.62
1:E:121:PRO:HB3	2:F:53:GLU:HG3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:34:DT:H2''	5:I:35:DA:C8	2.35	0.62
5:J:249:DG:H1'	5:J:250:DT:H5''	1.82	0.62
5:J:167:DT:H1'	5:J:168:DC:H5''	1.81	0.62
1:E:41:TYR:OH	5:I:7:DA:H5'	2.00	0.62
5:I:118:DT:H2''	5:I:119:DT:OP2	1.99	0.61
5:I:108:DC:H2''	5:I:109:DA:C8	2.35	0.61
5:I:137:DG:H2''	5:I:138:DG:OP2	2.00	0.61
5:I:99:DA:C2'	5:I:100:DG:H5'	2.29	0.61
3:C:67:GLY:HA3	4:D:49:HIS:CD2	2.36	0.61
3:C:92:GLU:HG2	4:D:103:PRO:HG2	1.82	0.61
5:J:255:DA:H2''	5:J:256:DA:OP2	2.00	0.60
3:C:87:ILE:HD12	3:C:102:ILE:HD11	1.82	0.60
5:I:129:DC:H2''	5:I:130:DT:C7	2.31	0.60
5:I:17:DA:C2'	5:I:18:DG:H5''	2.29	0.60
5:J:159:DC:H1'	5:J:160:DT:H5'	1.83	0.60
5:J:235:DC:H2''	5:J:236:DT:H71	1.81	0.60
1:A:49:ARG:HD2	5:J:155:DC:OP1	2.02	0.60
5:J:252:DT:H2''	5:J:253:DC:O5'	2.02	0.60
5:J:259:DA:H2''	5:J:260:DC:H5'	1.84	0.60
4:H:88:THR:CG2	5:J:186:DG:OP1	2.49	0.60
5:I:113:DA:H1'	5:I:114:DC:H5''	1.83	0.60
5:I:23:DT:H2''	5:I:24:DA:C5'	2.25	0.59
5:I:93:DT:H2''	5:I:94:DG:C5'	2.30	0.59
3:C:51:LEU:HD13	4:D:73:ILE:HG21	1.84	0.59
4:D:122:THR:C	4:D:124:ALA:H	2.04	0.59
5:I:144:DG:H1'	5:I:145:DA:H5''	1.84	0.59
5:J:239:DT:H2''	5:J:240:DG:C5'	2.28	0.59
4:D:42:TYR:CE2	4:D:46:LYS:HD2	2.37	0.59
5:J:195:DC:H1'	5:J:196:DC:C5	2.37	0.59
5:J:242:DT:H2''	5:J:243:DG:H5'	1.84	0.59
3:C:101:THR:HG21	8:F:2011:HOH:O	2.03	0.59
3:C:50:TYR:OH	4:D:95:GLN:HG3	2.02	0.59
5:I:139:DA:H2''	5:I:140:DT:H5'	1.84	0.59
5:I:62:DT:H2''	5:I:63:DG:H5'	1.84	0.58
5:I:46:DG:H2''	5:I:47:DC:C6	2.37	0.58
2:F:35:ARG:HG2	2:F:35:ARG:HH11	1.68	0.58
5:I:22:DC:H1'	5:I:23:DT:H5''	1.85	0.58
5:J:246:DG:H1'	5:J:247:DC:H5'	1.86	0.58
5:J:261:DA:H2''	5:J:262:DC:OP2	2.04	0.58
2:B:46:ILE:O	5:J:227:DG:H3'	2.04	0.58
3:C:31:HIS:ND1	3:C:48:PRO:HG3	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:63:DG:H2''	5:I:64:DT:OP2	2.04	0.57
5:J:164:DG:C2'	5:J:165:DA:H5''	2.32	0.57
5:J:182:DT:H2''	5:J:183:DT:C5'	2.34	0.57
5:J:236:DT:H2''	5:J:237:DT:OP2	2.04	0.57
5:J:286:DT:H2''	5:J:287:DA:C5'	2.35	0.57
5:J:264:DT:H2''	5:J:265:DT:OP2	2.04	0.57
5:I:114:DC:H2''	5:I:115:DA:C8	2.40	0.57
1:A:63:ARG:HH12	2:B:30:THR:HG23	1.69	0.57
5:I:9:DC:H1'	5:I:10:DC:H5''	1.87	0.57
5:J:234:DC:H2''	5:J:235:DC:C5	2.41	0.56
4:H:111:VAL:O	4:H:115:THR:HG23	2.06	0.56
5:J:248:DA:H2''	5:J:249:DG:C5'	2.33	0.56
4:D:37:TYR:H	4:D:63:ASN:HD21	1.52	0.56
5:I:122:DG:H1'	5:I:123:DT:H5''	1.86	0.56
5:I:135:DG:H2''	5:I:136:DT:H5'	1.88	0.56
2:F:45:ARG:CZ	5:I:80:DT:H4'	2.35	0.56
4:D:80:LEU:HD21	4:D:96:THR:CG2	2.36	0.56
5:J:243:DG:H2''	5:J:244:DG:OP2	2.05	0.56
5:I:24:DA:H2''	5:I:25:DC:C6	2.41	0.56
3:C:15:LYS:HB2	3:C:20:ARG:HH12	1.70	0.56
3:C:35:ARG:HD3	8:J:2011:HOH:O	2.05	0.56
5:J:230:DC:H2''	5:J:231:DA:C8	2.41	0.56
1:A:65:LEU:HB3	1:A:66:PRO:HD3	1.87	0.55
5:I:129:DC:H2''	5:I:130:DT:H73	1.87	0.55
5:I:142:DT:C2'	5:I:143:DT:H5'	2.33	0.55
5:I:63:DG:H1'	5:I:64:DT:H5'	1.88	0.55
2:F:77:GLN:HG2	8:F:2022:HOH:O	2.06	0.55
5:I:51:DA:C2'	5:I:52:DT:H5'	2.28	0.55
5:I:77:DA:C2	5:J:217:DG:N2	2.75	0.55
1:E:60:LEU:HD12	1:E:64:LYS:HE3	1.88	0.55
1:A:39:HIS:ND1	1:A:39:HIS:C	2.60	0.55
1:A:96:CYS:SG	2:B:58:LEU:HD21	2.47	0.55
5:I:43:DA:H1'	5:I:44:DC:H5''	1.88	0.55
5:J:241:DA:H1'	5:J:242:DT:C5'	2.36	0.55
4:D:31:ARG:HG3	4:D:31:ARG:O	2.06	0.54
2:F:35:ARG:O	2:F:39:ARG:HG2	2.08	0.54
5:I:31:DG:H1'	5:I:32:DT:H5''	1.89	0.54
5:I:73:DA:H2''	5:I:74:DT:H5'	1.87	0.54
5:J:154:DT:H6	5:J:154:DT:H5'	1.72	0.54
2:B:32:PRO:HA	2:B:35:ARG:HG3	1.88	0.54
4:H:51:ASP:HB3	8:H:209:HOH:O	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:92:DT:H1'	5:I:93:DT:H5''	1.89	0.54
4:D:88:THR:CG2	5:I:39:DG:OP1	2.55	0.54
5:J:201:DA:H2''	5:J:202:DA:OP2	2.08	0.54
3:G:73:ASN:HB2	8:G:2007:HOH:O	2.08	0.54
5:J:229:DA:H2''	5:J:230:DC:H5'	1.89	0.54
1:E:63:ARG:HH11	1:E:63:ARG:H	1.54	0.54
4:D:79:ARG:HG2	4:D:83:TYR:CZ	2.42	0.54
1:E:63:ARG:NH2	2:F:30:THR:H	2.06	0.54
5:I:58:DG:H2'	5:I:59:DG:C8	2.43	0.54
5:I:88:DC:H2''	5:I:89:DC:C6	2.42	0.54
5:I:96:DT:H2''	5:I:97:DG:OP2	2.09	0.54
3:G:92:GLU:HB3	4:H:106:LEU:HD22	1.90	0.53
5:I:37:DT:H2''	5:I:38:DT:OP2	2.07	0.53
5:I:49:DC:H2''	5:I:50:DC:OP2	2.07	0.53
5:J:181:DA:H1'	5:J:182:DT:C5'	2.35	0.53
1:A:49:ARG:HD2	5:J:155:DC:P	2.49	0.53
5:I:50:DC:H2''	5:I:51:DA:H5'	1.88	0.53
5:J:179:DG:H1'	5:J:180:DT:H5''	1.90	0.53
1:E:65:LEU:HB3	1:E:66:PRO:HD3	1.90	0.53
5:I:128:DT:H2''	5:I:129:DC:C6	2.44	0.53
5:J:154:DT:H2''	5:J:155:DC:O5'	2.08	0.53
1:A:51:ILE:HD12	2:B:42:GLY:HA2	1.91	0.53
1:E:122:LYS:HB3	6:E:1002:CL:CL	2.46	0.53
2:F:23:ARG:HD3	8:F:2020:HOH:O	2.09	0.52
3:G:45:ALA:O	3:G:48:PRO:HD2	2.09	0.52
5:I:138:DG:H2''	5:I:139:DA:OP2	2.08	0.52
5:I:63:DG:H1'	5:I:64:DT:C5'	2.39	0.52
3:C:87:ILE:HD12	3:C:102:ILE:CD1	2.40	0.52
5:J:177:DG:H1'	5:J:178:DT:H5''	1.90	0.52
5:J:259:DA:H2''	5:J:260:DC:C5'	2.39	0.52
5:J:182:DT:H6	5:J:182:DT:H5'	1.74	0.52
5:J:197:DA:H2''	5:J:198:DT:H5'	1.90	0.52
5:I:141:DA:H1'	5:I:142:DT:H5''	1.92	0.52
5:I:58:DG:C2'	5:I:59:DG:C8	2.93	0.52
5:J:183:DT:H2'	5:J:184:DT:H71	1.92	0.52
1:A:63:ARG:HH12	2:B:30:THR:HG21	1.75	0.52
3:C:26:PRO:HD3	4:D:40:TYR:CD1	2.44	0.52
1:E:129:ARG:HD3	1:E:135:ALA:HA	1.91	0.52
3:G:81:ARG:HD3	3:G:81:ARG:O	2.10	0.51
5:I:28:DA:H1'	5:I:29:DA:C8	2.45	0.51
3:C:42:ARG:NH1	5:I:38:DT:H4'	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:87:ILE:HD13	3:C:97:LEU:CD1	2.40	0.51
2:B:26:ILE:CG1	2:B:55:ARG:HB3	2.41	0.51
3:C:31:HIS:CD2	3:C:35:ARG:HH11	2.28	0.51
1:A:73:GLU:OE2	2:B:25:ASN:HB2	2.11	0.51
5:I:103:DG:H1'	5:I:104:DT:H5''	1.92	0.51
5:J:172:DC:C2'	5:J:173:DA:H5''	2.38	0.51
1:A:63:ARG:HH21	5:J:237:DT:H5''	1.76	0.51
1:A:83:ARG:O	2:B:80:THR:HA	2.11	0.51
2:F:30:THR:OG1	2:F:32:PRO:HD2	2.10	0.51
5:I:5:DA:H1'	5:I:6:DT:H5''	1.92	0.51
5:J:153:DA:H1'	5:J:154:DT:C5'	2.40	0.51
5:J:242:DT:H1'	5:J:243:DG:C5'	2.41	0.51
5:I:1:DA:H1'	5:I:2:DT:C6	2.46	0.51
2:F:20:LYS:HG2	2:F:21:VAL:N	2.26	0.51
1:E:63:ARG:NH2	2:F:30:THR:HG23	2.26	0.51
1:A:76:GLN:HA	1:A:76:GLN:NE2	2.26	0.50
2:F:30:THR:CB	2:F:32:PRO:HD2	2.41	0.50
5:J:287:DA:H1'	5:J:288:DT:H5'	1.94	0.50
4:H:80:LEU:HD11	4:H:96:THR:HG22	1.93	0.50
5:J:279:DA:H1'	5:J:280:DG:H5'	1.93	0.50
5:I:119:DT:H2''	5:I:120:DT:OP2	2.10	0.50
5:I:86:DT:H2''	5:I:87:DG:C8	2.47	0.50
5:J:170:DA:H1'	5:J:171:DC:H5''	1.92	0.50
5:J:241:DA:C1'	5:J:242:DT:H5'	2.40	0.50
5:J:245:DA:H2''	5:J:246:DG:OP2	2.12	0.50
4:D:33:ARG:HD2	5:J:269:DT:H4'	1.93	0.50
3:C:87:ILE:HD13	3:C:97:LEU:HD12	1.92	0.50
4:D:84:ASN:O	4:D:86:ARG:HG3	2.12	0.50
5:I:73:DA:H1'	5:I:74:DT:H5''	1.93	0.50
5:J:179:DG:H1'	5:J:180:DT:C5'	2.42	0.50
5:J:260:DC:H2''	5:J:261:DA:C8	2.47	0.50
4:D:53:GLY:HA3	8:I:2007:HOH:O	2.12	0.49
5:J:266:DT:H2''	5:J:267:DG:C5	2.47	0.49
4:H:119:THR:CG2	4:H:120:LYS:N	2.76	0.49
5:I:43:DA:C1'	5:I:44:DC:H5''	2.41	0.49
3:G:81:ARG:NH2	3:G:107:VAL:O	2.45	0.49
5:I:115:DA:H2''	5:I:116:DC:C5'	2.41	0.49
5:I:9:DC:H2''	5:I:10:DC:H5'	1.94	0.49
5:I:100:DG:H1'	5:I:101:DC:C6	2.48	0.49
5:I:41:DA:H2''	5:I:42:DA:C8	2.47	0.49
5:I:48:DT:H1'	5:I:49:DC:C6	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:153:DA:H2''	5:J:154:DT:OP2	2.13	0.49
5:J:227:DG:H2''	5:J:228:DA:OP2	2.12	0.49
2:B:92:ARG:HB3	2:B:92:ARG:CZ	2.42	0.49
5:I:143:DT:H2''	5:I:144:DG:C8	2.48	0.49
5:I:29:DA:H2''	5:I:30:DA:H8	1.76	0.49
1:A:96:CYS:SG	2:B:58:LEU:CD2	3.01	0.49
3:C:26:PRO:HD3	4:D:40:TYR:CG	2.48	0.49
5:J:190:DC:H5'	8:J:2012:HOH:O	2.12	0.49
5:I:99:DA:H1'	5:I:100:DG:C5'	2.42	0.49
1:E:133:GLU:O	1:E:134:ARG:CB	2.55	0.48
1:E:37:LYS:N	1:E:38:PRO:CA	2.75	0.48
5:I:5:DA:C2'	5:I:6:DT:H5''	2.43	0.48
3:C:15:LYS:HB2	3:C:20:ARG:NH1	2.27	0.48
3:C:29:ARG:HD2	3:C:32:ARG:HH22	1.78	0.48
5:J:181:DA:H2''	5:J:182:DT:OP2	2.13	0.48
2:B:58:LEU:O	2:B:58:LEU:HD22	2.13	0.48
4:D:31:ARG:HH11	4:D:31:ARG:HG2	1.78	0.48
1:E:49:ARG:HG3	1:E:49:ARG:NH1	2.28	0.48
3:C:58:LEU:O	3:C:62:ILE:HG23	2.14	0.48
4:D:69:ILE:HG22	4:D:73:ILE:HD12	1.96	0.48
1:E:37:LYS:HB2	1:E:38:PRO:O	2.13	0.48
5:I:35:DA:H1'	5:I:36:DT:H5'	1.94	0.48
5:J:182:DT:H1'	5:J:183:DT:C5'	2.42	0.48
1:E:37:LYS:N	1:E:37:LYS:HD3	2.27	0.48
5:J:200:DA:H1'	5:J:201:DA:H5'	1.96	0.48
5:J:242:DT:H1'	5:J:243:DG:H5''	1.96	0.48
5:I:26:DC:H4'	5:I:26:DC:OP1	2.13	0.48
1:A:68:GLN:HE21	1:A:89:VAL:HG21	1.79	0.47
5:I:57:DA:H2''	5:I:58:DG:C8	2.49	0.47
3:C:62:ILE:HD12	3:C:62:ILE:O	2.14	0.47
3:G:79:ILE:HG12	3:G:82:HIS:CE1	2.49	0.47
5:I:52:DT:C1'	5:I:53:DC:H5''	2.44	0.47
5:I:5:DA:H2''	5:I:6:DT:C5'	2.45	0.47
5:J:226:DT:H2''	5:J:227:DG:C8	2.50	0.47
5:I:14:DT:H4'	5:I:15:DG:H5'	1.96	0.47
5:J:158:DC:H1'	5:J:159:DC:H5''	1.97	0.47
3:C:42:ARG:HB2	4:D:88:THR:HB	1.96	0.47
5:J:258:DT:H2''	5:J:259:DA:C8	2.50	0.47
1:E:49:ARG:HD3	5:I:8:DT:OP1	2.15	0.46
3:G:24:GLN:HG3	4:H:47:GLN:OE1	2.15	0.46
5:I:27:DA:C6	5:I:28:DA:C6	3.03	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:166:DT:H2'	5:J:167:DT:H71	1.97	0.46
5:J:220:DT:H1'	5:J:221:DT:H5''	1.96	0.46
5:J:265:DT:H2''	5:J:266:DT:O5'	2.15	0.46
5:I:115:DA:H1'	5:I:116:DC:H5''	1.97	0.46
3:C:115:LEU:CD2	1:E:117:VAL:HG22	2.45	0.46
5:J:281:DG:C2'	5:J:282:DT:H5'	2.37	0.46
5:I:133:DA:H1'	5:I:134:DG:H5''	1.98	0.46
5:I:90:DT:H2''	5:I:91:DT:H5'	1.98	0.46
1:A:53:ARG:HG2	8:A:2019:HOH:O	2.15	0.46
3:G:92:GLU:OE1	4:H:105:GLU:HB2	2.14	0.46
1:A:128:ARG:NH1	8:A:2021:HOH:O	2.50	0.46
2:B:52:GLU:OE2	2:B:55:ARG:NH1	2.49	0.46
5:I:46:DG:H2''	5:I:47:DC:C5	2.50	0.46
5:I:52:DT:H1'	5:I:53:DC:H5''	1.97	0.46
2:F:45:ARG:NH2	5:I:80:DT:H4'	2.31	0.46
5:J:182:DT:C1'	5:J:183:DT:H5''	2.43	0.46
1:A:51:ILE:O	1:A:55:GLN:HG3	2.16	0.45
5:J:281:DG:H2''	5:J:282:DT:C5'	2.38	0.45
5:J:280:DG:H1'	5:J:281:DG:H5''	1.99	0.45
3:C:15:LYS:CB	3:C:20:ARG:NH1	2.79	0.45
4:D:122:THR:C	4:D:124:ALA:N	2.69	0.45
1:A:122:LYS:HG2	1:E:113:HIS:HE1	1.81	0.45
1:E:46:VAL:HG21	5:I:82:DA:H3'	1.97	0.45
5:I:101:DC:H2''	5:I:102:DA:O4'	2.16	0.45
8:A:2020:HOH:O	3:G:111:ILE:HD12	2.16	0.45
5:I:20:DT:H2''	5:I:21:DT:OP2	2.16	0.45
5:I:40:DG:H2''	5:I:41:DA:H5'	1.97	0.45
5:J:176:DA:H2''	5:J:177:DG:OP2	2.17	0.45
4:D:31:ARG:CG	4:D:31:ARG:O	2.64	0.45
2:F:20:LYS:HG2	2:F:21:VAL:H	1.81	0.45
5:J:224:DG:C2'	5:J:225:DC:H5''	2.47	0.45
2:F:18:HIS:N	2:F:18:HIS:ND1	2.64	0.45
2:F:30:THR:HB	2:F:32:PRO:HD2	1.99	0.45
5:I:125:DG:H2''	5:I:126:DA:O5'	2.17	0.45
5:I:15:DG:H2''	5:I:16:DC:OP2	2.16	0.45
3:G:18:SER:O	3:G:22:GLY:N	2.50	0.45
3:G:44:GLY:HA3	6:G:1001:CL:CL	2.54	0.45
5:I:116:DC:H2'	5:I:117:DT:H71	1.99	0.44
5:I:131:DG:H2''	5:I:132:DC:C4	2.48	0.44
1:E:134:ARG:HE	1:E:134:ARG:HB3	1.47	0.44
5:I:123:DT:H6	5:I:123:DT:H2'	1.67	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:210:DT:H2''	5:J:211:DT:C6	2.52	0.44
3:G:79:ILE:HB	3:G:80:PRO:CD	2.47	0.44
5:I:58:DG:H2''	5:I:59:DG:C8	2.52	0.44
3:G:85:LEU:O	3:G:89:ASN:HB2	2.18	0.44
5:I:8:DT:H1'	5:I:9:DC:H5'	1.99	0.44
5:J:221:DT:H1'	5:J:222:DC:H5'	2.00	0.44
5:J:271:DG:OP1	5:J:271:DG:H4'	2.18	0.44
1:E:122:LYS:HE2	8:E:2030:HOH:O	2.17	0.44
8:B:2004:HOH:O	3:G:101:THR:HG21	2.17	0.44
5:I:6:DT:H2''	5:I:7:DA:C8	2.53	0.44
5:I:95:DA:H2''	5:I:96:DT:OP2	2.17	0.44
2:F:38:ALA:HB1	2:F:43:VAL:HB	2.00	0.44
5:J:282:DT:H2''	5:J:283:DG:C8	2.52	0.44
5:I:106:DT:H2''	5:I:107:DC:H5'	2.00	0.44
5:J:210:DT:H2'	5:J:211:DT:H71	1.99	0.44
5:J:225:DC:H2''	5:J:226:DT:C6	2.52	0.44
5:J:235:DC:H2''	5:J:236:DT:C5	2.52	0.44
5:J:273:DA:H2''	5:J:274:DT:OP2	2.18	0.43
3:C:84:GLN:HG3	3:C:105:GLY:HA3	2.00	0.43
5:J:282:DT:H6	5:J:282:DT:H2'	1.70	0.43
1:A:76:GLN:HA	1:A:76:GLN:HE21	1.81	0.43
1:E:124:ILE:O	1:E:128:ARG:HG3	2.19	0.43
5:J:263:DT:H1'	5:J:264:DT:H5'	1.99	0.43
3:G:73:ASN:O	3:G:74:LYS:HB2	2.18	0.43
5:I:99:DA:H1'	5:I:100:DG:H5'	2.00	0.43
5:I:36:DT:C2'	5:I:37:DT:H71	2.47	0.43
5:I:54:DA:C4'	5:I:54:DA:OP1	2.64	0.43
5:J:151:DA:H2''	5:J:152:DT:OP2	2.17	0.43
1:A:122:LYS:HG2	1:E:113:HIS:CE1	2.54	0.43
5:I:136:DT:H2'	5:I:136:DT:H6	1.69	0.43
5:J:205:DG:H1'	5:J:206:DC:C5'	2.48	0.43
1:A:117:VAL:HG12	1:A:117:VAL:O	2.19	0.43
2:F:21:VAL:HG12	2:F:23:ARG:HG3	2.01	0.43
4:D:34:LYS:HG2	5:J:270:DA:OP1	2.18	0.43
3:C:37:GLY:HA3	3:C:39:TYR:CE2	2.54	0.43
1:E:87:SER:HB3	2:F:83:ALA:HB2	1.99	0.43
4:H:123:SER:O	4:H:124:ALA:C	2.57	0.43
1:E:119:ILE:HG13	2:F:50:ILE:HG13	2.01	0.43
5:I:5:DA:H2''	5:I:6:DT:H5''	1.99	0.43
5:J:224:DG:H2''	5:J:225:DC:H5''	2.01	0.43
2:B:35:ARG:O	2:B:39:ARG:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:49:HIS:HB3	4:H:52:THR:OG1	2.19	0.43
5:J:197:DA:H1'	5:J:198:DT:C5'	2.49	0.43
5:J:287:DA:H2'	5:J:288:DT:H72	2.00	0.43
5:I:111:DA:C8	5:I:112:DT:H72	2.54	0.42
5:J:188:DA:H2''	5:J:189:DA:O5'	2.19	0.42
2:B:78:ARG:CD	5:J:248:DA:H5'	2.49	0.42
5:I:47:DC:N4	5:J:245:DA:N6	2.67	0.42
3:C:84:GLN:HE22	3:C:88:ARG:NE	2.04	0.42
1:E:134:ARG:O	1:E:134:ARG:NE	2.52	0.42
1:E:118:THR:HA	2:F:45:ARG:HB3	2.01	0.42
5:I:17:DA:H1'	5:I:18:DG:H5''	2.01	0.42
4:H:102:LEU:HA	4:H:103:PRO:HD3	1.90	0.42
2:B:98:TYR:CD1	4:H:64:SER:HB3	2.53	0.42
5:I:18:DG:H2''	5:I:19:DA:C8	2.54	0.42
5:J:165:DA:H2'	5:J:166:DT:H72	2.00	0.42
4:D:80:LEU:HD21	4:D:96:THR:HG21	2.00	0.42
5:I:58:DG:H8	5:I:58:DG:H5''	1.83	0.42
4:H:33:ARG:HH11	4:H:33:ARG:HB3	1.84	0.42
5:I:102:DA:H2''	5:I:103:DG:C8	2.55	0.42
5:J:189:DA:C2'	5:J:190:DC:O5'	2.61	0.42
5:J:197:DA:H1'	5:J:198:DT:H5''	2.01	0.42
3:C:38:ASN:HA	8:C:2013:HOH:O	2.20	0.42
4:D:42:TYR:O	4:D:46:LYS:HG2	2.20	0.42
2:F:36:ARG:O	2:F:39:ARG:HB2	2.20	0.42
5:J:173:DA:H2''	5:J:174:DA:C8	2.55	0.42
3:G:81:ARG:HD3	3:G:81:ARG:C	2.40	0.42
5:I:29:DA:H2''	5:I:30:DA:C8	2.54	0.42
5:I:34:DT:C2'	5:I:35:DA:C8	3.01	0.42
5:I:91:DT:H1'	5:I:92:DT:H5'	2.02	0.42
5:J:182:DT:C2'	5:J:183:DT:C5'	2.97	0.42
5:J:249:DG:H2''	5:J:250:DT:H5'	2.02	0.42
5:J:274:DT:H2''	5:J:275:DC:OP2	2.20	0.42
3:C:35:ARG:CD	8:J:2011:HOH:O	2.65	0.41
3:G:17:ARG:HG2	4:H:121:TYR:HE1	1.85	0.41
4:H:46:LYS:HA	4:H:46:LYS:HD3	1.82	0.41
5:J:288:DT:H1'	5:J:289:DT:H5'	2.00	0.41
4:D:86:ARG:NH1	8:D:210:HOH:O	2.50	0.41
5:I:117:DT:H2''	5:I:118:DT:OP2	2.19	0.41
5:I:40:DG:H1'	5:I:41:DA:H5''	2.02	0.41
5:J:268:DG:H2''	5:J:269:DT:C6	2.56	0.41
2:B:75:HIS:C	2:B:77:GLN:H	2.22	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:109:DA:H2''	5:I:110:DA:OP2	2.20	0.41
5:I:7:DA:C2	5:J:287:DA:C2	3.07	0.41
5:J:166:DT:C2'	5:J:167:DT:H71	2.51	0.41
2:B:58:LEU:C	2:B:58:LEU:HD22	2.40	0.41
2:F:75:HIS:HD2	4:H:96:THR:OG1	2.04	0.41
5:I:26:DC:C2'	5:I:27:DA:N7	2.81	0.41
1:E:63:ARG:HE	5:J:207:DA:H5''	1.84	0.41
3:C:31:HIS:CD2	3:C:35:ARG:NH1	2.89	0.41
3:G:44:GLY:O	3:G:48:PRO:HD3	2.21	0.41
5:J:183:DT:H5'	5:J:183:DT:H6	1.86	0.41
3:C:81:ARG:NH2	3:C:107:VAL:O	2.39	0.41
3:C:13:LYS:HD3	3:C:15:LYS:NZ	2.36	0.41
2:B:26:ILE:HG13	2:B:55:ARG:HD3	2.03	0.41
5:J:210:DT:C2'	5:J:211:DT:H71	2.51	0.41
3:C:26:PRO:HB2	3:C:29:ARG:HB3	2.03	0.41
1:E:131:ARG:HD3	1:E:133:GLU:OE2	2.20	0.41
5:J:159:DC:H2''	5:J:160:DT:O5'	2.20	0.41
4:D:32:SER:HB2	5:I:103:DG:OP1	2.21	0.41
5:I:120:DT:H2''	5:I:121:DG:C8	2.56	0.41
3:G:112:GLN:HG2	8:G:2002:HOH:O	2.21	0.41
5:I:7:DA:H2''	5:I:8:DT:OP2	2.21	0.41
4:H:87:SER:OG	5:J:185:DG:H3'	2.20	0.41
5:J:242:DT:H1'	5:J:243:DG:H5'	2.03	0.41
3:C:84:GLN:HE21	3:C:102:ILE:HD12	1.86	0.41
5:J:184:DT:O3'	5:J:185:DG:C8	2.74	0.41
1:A:134:ARG:HD2	8:A:2021:HOH:O	2.20	0.40
5:J:190:DC:C5'	8:J:2012:HOH:O	2.69	0.40
2:B:45:ARG:CZ	5:J:227:DG:H4'	2.50	0.40
5:I:99:DA:H1'	5:I:100:DG:H5''	2.02	0.40
5:I:31:DG:C2'	5:I:32:DT:C5'	2.97	0.40
5:I:84:DC:H2''	5:I:85:DA:C8	2.56	0.40
5:J:231:DA:H2''	5:J:232:DT:OP2	2.22	0.40
4:H:37:TYR:N	4:H:63:ASN:HD21	2.03	0.40
5:I:113:DA:C2	5:J:181:DA:C2	3.10	0.40
5:J:195:DC:H1'	5:J:196:DC:C6	2.57	0.40
5:I:14:DT:H1'	5:I:15:DG:C5	2.57	0.40
5:I:59:DG:H2''	5:I:60:DC:OP2	2.20	0.40
5:J:280:DG:H1'	5:J:281:DG:C5'	2.51	0.40
2:B:72:TYR:OH	2:B:92:ARG:HD2	2.21	0.40
5:I:82:DA:C6	5:I:83:DA:C6	3.09	0.40
5:J:154:DT:C6	5:J:154:DT:H5'	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:225:DC:H2''	5:J:226:DT:C5	2.57	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	95/139 (68%)	93 (98%)	2 (2%)	0	100	100
1	E	97/139 (70%)	94 (97%)	2 (2%)	1 (1%)	18	43
2	B	76/106 (72%)	74 (97%)	2 (3%)	0	100	100
2	F	84/106 (79%)	82 (98%)	2 (2%)	0	100	100
3	C	106/133 (80%)	101 (95%)	5 (5%)	0	100	100
3	G	103/133 (77%)	97 (94%)	6 (6%)	0	100	100
4	D	92/129 (71%)	88 (96%)	2 (2%)	2 (2%)	8	20
4	H	91/129 (70%)	89 (98%)	0	2 (2%)	8	20
All	All	744/1014 (73%)	718 (96%)	21 (3%)	5 (1%)	25	53

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	134	ARG
4	D	32	SER
4	D	104	GLY
4	H	104	GLY
4	H	123	SER

### 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%)	82 (96%)	3 (4%)	41	72
1	E	86/113 (76%)	80 (93%)	6 (7%)	18	40
2	B	63/81 (78%)	61 (97%)	2 (3%)	44	75
2	F	71/81 (88%)	70 (99%)	1 (1%)	71	90
3	C	85/102 (83%)	77 (91%)	8 (9%)	10	23
3	G	83/102 (81%)	79 (95%)	4 (5%)	30	59
4	D	80/107 (75%)	79 (99%)	1 (1%)	73	91
4	H	79/107 (74%)	74 (94%)	5 (6%)	21	46
All	All	632/806 (78%)	602 (95%)	30 (5%)	30	60

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	HIS
1	A	59	GLU
1	A	129	ARG
2	B	50	ILE
2	B	58	LEU
3	C	29	ARG
3	C	42	ARG
3	C	59	THR
3	C	62	ILE
3	C	71	ARG
3	C	81	ARG
3	C	99	ARG
3	C	101	THR
4	D	88	THR
1	E	37	LYS
1	E	63	ARG
1	E	64	LYS
1	E	117	VAL
1	E	122	LYS

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Mol	Chain	Res	Type
1	E	134	ARG
2	F	18	HIS
3	G	73	ASN
3	G	81	ARG
3	G	101	THR
3	G	118	LYS
4	H	36	SER
4	H	88	THR
4	H	106	LEU
4	H	109	HIS
4	H	119	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	76	GLN
1	A	108	ASN
2	B	64	ASN
2	B	75	HIS
3	C	24	GLN
3	C	84	GLN
4	D	63	ASN
1	E	68	GLN
1	E	76	GLN
2	F	75	HIS
3	G	31	HIS
3	G	73	ASN
4	H	63	ASN
4	H	95	GLN

### 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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 15 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 [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	97/139 (69%)	-0.07	0 100 100	32, 45, 73, 103	0
1	E	99/139 (71%)	0.02	2 (2%) 65 66	27, 38, 68, 106	0
2	B	78/106 (73%)	-0.08	1 (1%) 77 78	31, 44, 65, 89	0
2	F	86/106 (81%)	0.07	3 (3%) 44 44	24, 38, 65, 112	0
3	C	108/133 (81%)	0.05	4 (3%) 42 41	25, 43, 77, 137	0
3	G	105/133 (78%)	-0.10	2 (1%) 67 68	31, 48, 78, 99	0
4	D	94/129 (72%)	0.08	2 (2%) 64 65	29, 45, 76, 110	0
4	H	93/129 (72%)	0.01	0 100 100	31, 47, 85, 106	0
5	I	145/146 (99%)	0.25	7 (4%) 31 29	48, 98, 143, 163	0
5	J	145/146 (99%)	0.25	4 (2%) 53 54	51, 102, 149, 156	0
All	All	1050/1306 (80%)	0.07	25 (2%) 59 60	24, 50, 130, 163	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	11	ARG	9.0
2	F	102	GLY	7.2
3	C	12	ALA	6.8
1	E	37	LYS	4.5
3	C	13	LYS	4.2
5	I	55	DA	3.7
1	E	135	ALA	3.6
5	J	263	DT	2.8
5	I	106	DT	2.8
5	J	162	DC	2.7
5	I	56	DA	2.6
5	J	148	DT	2.6
2	B	102	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
3	G	14	ALA	2.5
5	I	44	DC	2.4
3	G	118	LYS	2.4
2	F	18	HIS	2.4
4	D	32	SER	2.4
5	I	42	DA	2.3
3	C	118	LYS	2.3
2	F	17	ARG	2.3
4	D	124	ALA	2.2
5	I	33	DG	2.2
5	I	104	DT	2.1
5	J	262	DC	2.0

## 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. 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
7	MN	E	1001	1/1	0.99	0.26	4.42	39,39,39,39	0
7	MN	I	1004	1/1	0.88	0.20	2.58	96,96,96,96	0
6	CL	G	1001	1/1	0.96	0.19	1.06	54,54,54,54	0
6	CL	C	1001	1/1	0.97	0.10	-3.03	51,51,51,51	0
7	MN	I	1005	1/1	0.74	0.07	-	112,112,112,112	0
6	CL	A	1001	1/1	0.96	0.10	-	63,63,63,63	0
6	CL	E	1002	1/1	0.98	0.15	-	60,60,60,60	0
7	MN	I	1006	1/1	0.63	0.22	-	128,128,128,128	0
7	MN	J	1001	1/1	0.94	0.12	-	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
7	MN	I	1001	1/1	0.43	0.22	-	131,131,131,131	0
7	MN	I	1002	1/1	0.79	0.15	-	133,133,133,133	0
7	MN	J	1004	1/1	0.89	0.19	-	77,77,77,77	0
7	MN	J	1003	1/1	0.97	0.09	-	78,78,78,78	0
7	MN	I	1003	1/1	0.92	0.27	-	90,90,90,90	0
7	MN	J	1002	1/1	0.90	0.15	-	92,92,92,92	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.