



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 01:46 PM EDT

PDB ID : 3AFA / pdb_00003afa
Title : The human nucleosome structure
Authors : Tachiwana, H.; Kagawa, W.; Osakabe, A.; Koichiro, K.; Shiga, T.; Kimura, H.; Kurumizaka, H.
Deposited on : 2010-02-24
Resolution : 2.50 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtrriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

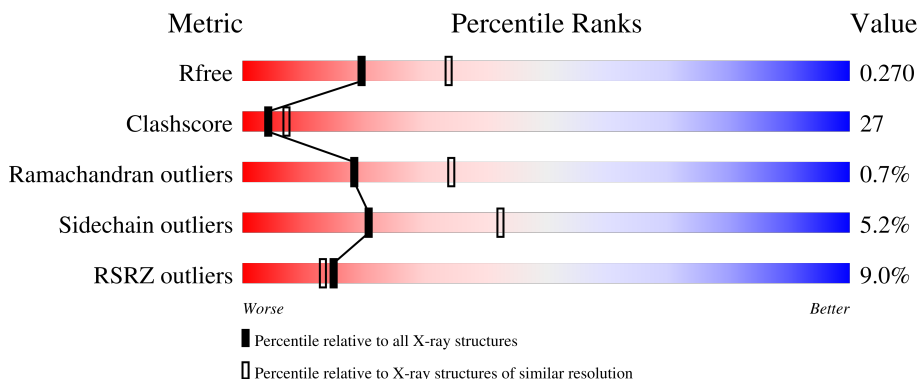
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	
1	E	139	
2	B	106	
2	F	106	
3	C	133	

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Mol	Chain	Length	Quality of chain
3	G	133	<p>2% 58% 17% 22%</p>
4	D	129	<p>5% 46% 22% 7% 26%</p>
4	H	129	<p>3% 57% 12% 29%</p>
5	I	146	<p>23% 11% 88%</p>
5	J	146	<p>25% 8% 91%</p>

2 Entry composition i

There are 8 unique types of molecules in this entry. The entry contains 12198 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
			Total	C	N	O	S			
1	A	97	801	505	155	137	4	0	0	0
1	E	99	816	514	158	140	4	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP P68431
A	-2	SER	-	expression tag	UNP P68431
A	-1	HIS	-	expression tag	UNP P68431
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
			Total	C	N	O	S			
2	B	78	619	391	120	107	1	0	0	0
2	F	84	673	424	133	115	1	0	0	0

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
			Total	C	N	O			
3	C	108	Total	C	N	O	0	0	0
			835	526	165	144			
3	G	104	Total	C	N	O	0	0	0
			805	508	157	140			

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
			Total	C	N	O	S			
4	D	96	Total	C	N	O	S	0	0	0
			755	474	138	141	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 146-MER DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
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 CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 7 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	D	1	Total Mn 1 1	0	0
7	I	3	Total Mn 3 3	0	0
7	J	4	Total Mn 4 4	0	0

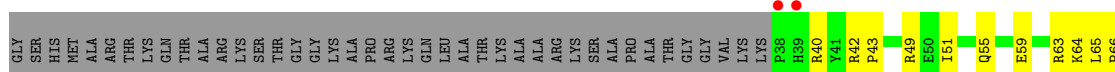
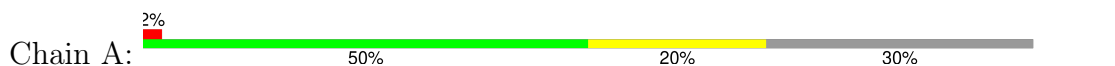
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	19	Total O 19 19	0	0
8	B	15	Total O 15 15	0	0
8	C	19	Total O 19 19	0	0
8	D	17	Total O 17 17	0	0
8	E	33	Total O 33 33	0	0
8	F	26	Total O 26 26	0	0
8	G	15	Total O 15 15	0	0
8	H	13	Total O 13 13	0	0
8	I	15	Total O 15 15	0	0
8	J	11	Total O 11 11	0	0

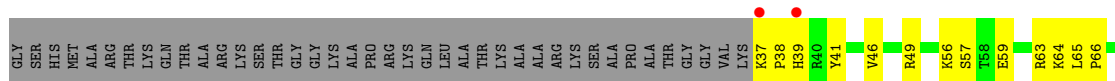
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

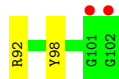
- Molecule 1: Histone H3.1



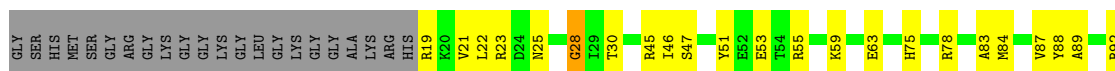
- Molecule 1: Histone H3.1

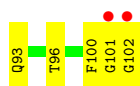


- Molecule 2: Histone H4

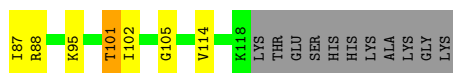


- Molecule 2: Histone H4





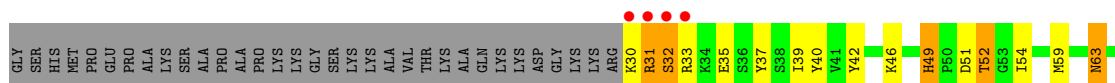
• Molecule 3: Histone H2A type 1-B/E



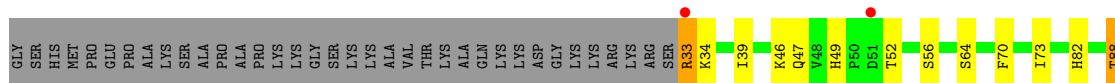
• Molecule 3: Histone H2A type 1-B/E



• Molecule 4: Histone H2B type 1-J

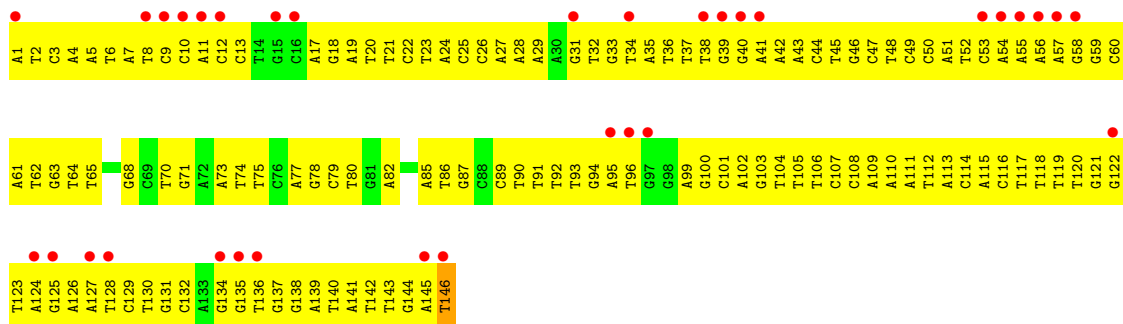


• Molecule 4: Histone H2B type 1-J

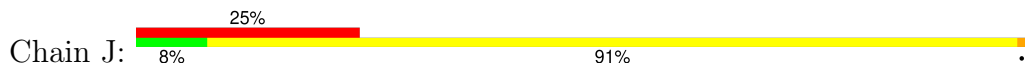


• Molecule 5: 146-MER DNA





● Molecule 5: 146-MER DNA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.84Å 109.51Å 180.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 50.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.50) 99.8 (50.00-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.48 (at 2.51Å)	Xtrriage
Refinement program	CNS 1.2.1	Depositor
R, R_{free}	0.240 , 0.270 0.240 , 0.270	Depositor DCC
R_{free} test set	3693 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	42.4	Xtrriage
Anisotropy	0.352	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 43.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.014 for k,h,-l	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12198	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

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

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	0.95	3/1090 (0.3%)
1	E	0.55	0/828	0.92	1/1109 (0.1%)
2	B	0.48	0/626	1.02	4/837 (0.5%)
2	F	0.59	0/680	1.00	4/908 (0.4%)
3	C	0.53	0/845	0.92	0/1139
3	G	0.49	0/815	0.91	2/1100 (0.2%)
4	D	0.55	0/766	0.96	4/1026 (0.4%)
4	H	0.49	0/730	0.91	1/982 (0.1%)
5	I	0.29	0/3354	0.73	1/5175 (0.0%)
5	J	0.29	0/3354	0.72	1/5175 (0.0%)
All	All	0.42	0/12811	0.83	21/18541 (0.1%)

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	64	LYS	N-CA-C	8.05	119.69	111.07
2	B	30	THR	N-CA-C	6.92	119.89	110.55
2	B	27	GLN	N-CA-C	-6.67	105.01	113.01
2	F	28	GLY	N-CA-C	-6.66	107.35	114.67
2	F	30	THR	N-CA-C	6.20	118.71	110.53
2	B	46	ILE	N-CA-C	6.19	116.78	108.11
1	E	85	GLN	N-CA-C	-6.18	101.13	110.28
3	G	116	LEU	CA-C-N	6.18	126.14	120.21
3	G	116	LEU	C-N-CA	6.18	126.14	120.21
4	D	101	LEU	N-CA-C	6.09	119.18	111.69
5	J	292	DT	C2'-C3'-O3'	-6.06	102.41	111.50
4	D	49	HIS	CA-C-N	6.02	126.45	119.47
4	D	49	HIS	C-N-CA	6.02	126.45	119.47
1	A	85	GLN	N-CA-C	-6.01	101.38	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	46	ILE	N-CA-C	5.91	116.51	107.77
1	A	133	GLU	N-CA-C	-5.91	106.03	113.18
5	I	146	DT	C2'-C3'-O3'	-5.89	102.66	111.50
4	D	52	THR	N-CA-C	5.87	119.39	109.76
4	H	101	LEU	N-CA-C	5.25	119.75	112.45
2	F	101	GLY	N-CA-C	-5.20	108.86	115.31
2	B	35	ARG	N-CA-C	-5.07	105.65	111.07

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	801	0	839	21	0
1	E	816	0	856	37	0
2	B	619	0	659	26	0
2	F	673	0	722	22	0
3	C	835	0	897	42	0
3	G	805	0	861	26	0
4	D	755	0	784	49	0
4	H	719	0	740	18	0
5	I	2990	0	1652	197	0
5	J	2990	0	1652	225	0
6	A	1	0	0	1	0
6	C	1	0	0	0	0
6	E	1	0	0	1	0
6	G	1	0	0	1	0
7	D	1	0	0	0	0
7	I	3	0	0	0	0
7	J	4	0	0	0	0
8	A	19	0	0	0	0
8	B	15	0	0	2	0
8	C	19	0	0	2	0
8	D	17	0	0	1	0
8	E	33	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	F	26	0	0	3	0
8	G	15	0	0	2	0
8	H	13	0	0	1	0
8	I	15	0	0	0	0
8	J	11	0	0	0	0
All	All	12198	0	9662	589	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 27.

All (589) 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:I:51:DA:H2''	5:I:52:DT:H5''	1.25	1.12
5:J:194:DT:H2''	5:J:195:DC:H5'	1.30	1.08
5:I:36:DT:H2''	5:I:37:DT:H5''	1.37	1.07
5:I:128:DT:H2''	5:I:129:DC:H5''	1.32	1.07
5:I:101:DC:H2''	5:I:102:DA:H5'	1.35	1.06
5:J:152:DT:H2''	5:J:153:DA:H5''	1.33	1.05
5:J:164:DG:H2''	5:J:165:DA:H5''	1.40	1.04
5:I:46:DG:H2''	5:I:47:DC:H5''	1.41	1.03
3:C:84:GLN:HE22	3:C:88:ARG:HE	1.05	1.02
5:I:52:DT:H2''	5:I:53:DC:H5'	1.41	1.01
5:I:19:DA:H2''	5:I:20:DT:H5'	1.42	1.01
5:J:241:DA:H2''	5:J:242:DT:H5'	1.40	0.99
5:J:183:DT:H2''	5:J:184:DT:H5'	1.45	0.97
5:I:43:DA:H2''	5:I:44:DC:H5''	1.46	0.97
5:J:152:DT:C2'	5:J:153:DA:H5''	1.96	0.95
1:E:134:ARG:HH11	1:E:134:ARG:HB3	1.33	0.94
5:J:211:DT:H2''	5:J:212:DC:H5'	1.50	0.94
5:J:248:DA:H2''	5:J:249:DG:H5'	1.50	0.94
2:B:75:HIS:CD2	4:D:96:THR:HG21	2.04	0.92
5:I:51:DA:C2'	5:I:52:DT:H5''	2.00	0.92
3:C:42:ARG:HG3	4:D:88:THR:HB	1.50	0.91
5:I:9:DC:H2''	5:I:10:DC:H5'	1.53	0.91
5:I:2:DT:H2''	5:I:3:DC:H5''	1.52	0.90
5:J:157:DA:H2''	5:J:158:DC:H5'	1.51	0.90
5:I:2:DT:C2'	5:I:3:DC:H5''	2.03	0.89
5:I:50:DC:H2''	5:I:51:DA:H5'	1.54	0.88
5:I:40:DG:H2''	5:I:41:DA:H5'	1.55	0.87
5:J:264:DT:H2''	5:J:265:DT:H5'	1.56	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:43:DA:C2'	5:I:44:DC:H5''	2.05	0.86
5:J:266:DT:H2''	5:J:267:DG:C8	2.11	0.86
5:I:130:DT:H2''	5:I:131:DG:H5''	1.58	0.85
5:J:262:DC:H2''	5:J:263:DT:H5'	1.58	0.84
3:C:17:ARG:HH22	3:C:31:HIS:CD2	1.95	0.84
5:I:36:DT:C2'	5:I:37:DT:H5''	2.07	0.84
3:C:101:THR:HG22	8:F:219:HOH:O	1.78	0.82
4:D:122:THR:C	4:D:124:ALA:H	1.86	0.82
5:J:148:DT:H2''	5:J:149:DC:H5'	1.61	0.82
1:E:134:ARG:HB3	1:E:134:ARG:NH1	1.94	0.82
5:I:53:DC:H2''	5:I:54:DA:H5'	1.63	0.81
5:J:238:DT:H2''	5:J:239:DT:H5'	1.61	0.80
5:J:282:DT:H2''	5:J:283:DG:H5'	1.62	0.80
5:J:158:DC:H2''	5:J:159:DC:H5''	1.64	0.80
1:A:63:ARG:HH11	5:I:60:DC:H5''	1.47	0.79
5:J:164:DG:C2'	5:J:165:DA:H5''	2.12	0.79
5:J:192:DG:H2''	5:J:193:DC:H5'	1.62	0.79
5:I:2:DT:C3'	5:I:3:DC:H5''	2.12	0.79
5:I:91:DT:H2''	5:I:92:DT:H5'	1.65	0.78
5:I:5:DA:H2''	5:I:6:DT:H5''	1.64	0.78
4:D:123:SER:C	4:D:125:LYS:H	1.90	0.78
5:I:46:DG:C2'	5:I:47:DC:H5''	2.13	0.78
5:I:128:DT:C2'	5:I:129:DC:H5''	2.13	0.77
5:I:43:DA:H2''	5:I:44:DC:C5'	2.14	0.77
5:J:208:DT:H2''	5:J:209:DG:H5'	1.67	0.77
1:E:37:LYS:HB2	1:E:38:PRO:C	2.10	0.76
5:I:42:DA:H2''	5:I:43:DA:H5'	1.66	0.76
5:I:64:DT:H2''	5:I:65:DT:H5'	1.68	0.76
2:F:59:LYS:O	2:F:63:GLU:HG3	1.85	0.76
5:I:8:DT:H1'	5:I:9:DC:H5''	1.68	0.75
5:I:128:DT:H2''	5:I:129:DC:C5'	2.14	0.75
1:E:64:LYS:HE2	1:E:90:MET:HE1	1.68	0.75
5:J:155:DC:H2''	5:J:156:DC:H5'	1.67	0.75
5:J:149:DC:H1'	5:J:150:DA:H5''	1.69	0.75
5:J:189:DA:H2''	5:J:190:DC:O5'	1.86	0.75
5:J:184:DT:H2''	5:J:185:DG:N7	2.01	0.75
2:B:59:LYS:O	2:B:63:GLU:HG3	1.86	0.74
5:J:158:DC:H2''	5:J:159:DC:C5'	2.18	0.74
5:I:37:DT:H2''	5:I:38:DT:H5'	1.70	0.73
5:J:194:DT:H2''	5:J:195:DC:C5'	2.13	0.73
3:C:84:GLN:HE21	3:C:102:ILE:HD12	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:158:DC:C2'	5:J:159:DC:H5''	2.19	0.72
5:J:168:DC:H1'	5:J:169:DT:H5''	1.72	0.72
1:E:129:ARG:HD3	1:E:135:ALA:HA	1.71	0.72
5:J:219:DA:H2''	5:J:220:DT:H5'	1.71	0.72
5:I:115:DA:H1'	5:I:116:DC:H5''	1.72	0.71
5:J:233:DG:H2''	5:J:234:DC:OP2	1.90	0.71
5:J:279:DA:H2''	5:J:280:DG:H5'	1.70	0.71
5:J:181:DA:H2''	5:J:182:DT:H5''	1.72	0.71
4:D:32:SER:OG	5:I:103:DG:H5''	1.90	0.71
5:J:274:DT:H2''	5:J:275:DC:C5'	2.21	0.71
5:J:275:DC:H2''	5:J:276:DT:H5'	1.72	0.71
5:J:291:DA:C8	5:J:292:DT:H72	2.26	0.71
5:I:5:DA:C2'	5:I:6:DT:H5''	2.21	0.70
5:J:208:DT:H2''	5:J:209:DG:C5'	2.21	0.70
5:J:264:DT:H2''	5:J:265:DT:C5'	2.20	0.70
4:D:46:LYS:HA	4:D:46:LYS:HE2	1.73	0.70
1:E:121:PRO:HB3	2:F:53:GLU:HG3	1.73	0.70
4:D:92:ARG:O	4:D:96:THR:HG22	1.92	0.69
1:E:49:ARG:HG3	1:E:49:ARG:HH11	1.57	0.69
5:J:273:DA:H1'	5:J:274:DT:H5''	1.75	0.69
5:I:50:DC:H2''	5:I:51:DA:C5'	2.21	0.69
5:I:23:DT:H2''	5:I:24:DA:H5'	1.74	0.68
5:J:261:DA:H2''	5:J:262:DC:H5''	1.75	0.68
2:F:19:ARG:HH22	2:F:22:LEU:HD11	1.59	0.68
5:I:20:DT:H1'	5:I:21:DT:H5''	1.76	0.68
3:C:62:ILE:HD11	3:C:83:LEU:HD22	1.76	0.68
5:I:129:DC:H2''	5:I:130:DT:C5	2.29	0.68
5:J:179:DG:H1'	5:J:180:DT:H5''	1.75	0.68
5:I:39:DG:H2''	5:I:40:DG:H5''	1.75	0.68
5:I:106:DT:H1'	5:I:107:DC:H5''	1.75	0.68
5:J:235:DC:H2''	5:J:236:DT:C7	2.24	0.67
5:J:170:DA:H1'	5:J:171:DC:H5''	1.75	0.67
5:J:270:DA:H2''	5:J:271:DG:O5'	1.93	0.67
5:I:47:DC:H2''	5:I:48:DT:C6	2.29	0.67
3:G:31:HIS:CD2	3:G:48:PRO:HG3	2.30	0.67
1:A:63:ARG:NH1	5:I:60:DC:H5''	2.10	0.67
5:J:266:DT:H2''	5:J:267:DG:N7	2.10	0.67
5:I:5:DA:H2''	5:I:6:DT:C5'	2.24	0.67
5:I:115:DA:C2'	5:I:116:DC:H5''	2.25	0.67
5:J:152:DT:C3'	5:J:153:DA:H5''	2.25	0.67
4:D:31:ARG:HA	4:D:31:ARG:CZ	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:44:DC:H2''	5:I:45:DT:O5'	1.95	0.66
1:A:125:GLN:HG2	1:A:134:ARG:HH12	1.60	0.66
3:C:83:LEU:O	3:C:87:ILE:HG12	1.95	0.66
5:I:19:DA:H2''	5:I:20:DT:C5'	2.22	0.66
5:J:290:DG:H2''	5:J:291:DA:OP2	1.96	0.66
3:C:84:GLN:HE22	3:C:88:ARG:NE	1.86	0.66
4:D:37:TYR:H	4:D:63:ASN:HD21	1.44	0.66
5:I:115:DA:H2''	5:I:116:DC:H5''	1.77	0.66
5:I:135:DG:H2''	5:I:136:DT:O5'	1.95	0.66
5:I:137:DG:H2''	5:I:138:DG:OP2	1.96	0.66
5:I:134:DG:H2''	5:I:135:DG:H5'	1.77	0.65
3:C:55:LEU:O	3:C:59:THR:HG23	1.97	0.65
2:B:78:ARG:CD	5:J:248:DA:H5'	2.26	0.65
5:J:261:DA:C2'	5:J:262:DC:H5''	2.27	0.65
5:I:130:DT:C2'	5:I:131:DG:H5''	2.25	0.65
5:I:108:DC:H2''	5:I:109:DA:N7	2.12	0.65
3:G:17:ARG:HH12	3:G:31:HIS:CD2	2.14	0.65
5:J:281:DG:H2''	5:J:282:DT:H5'	1.79	0.64
5:I:3:DC:H2''	5:I:4:DA:C8	2.33	0.64
5:J:254:DC:H2''	5:J:255:DA:N7	2.12	0.64
5:J:152:DT:H2''	5:J:153:DA:C5'	2.19	0.64
5:J:255:DA:H2''	5:J:256:DA:OP2	1.96	0.64
1:E:122:LYS:HB2	6:E:201:CL:CL	2.34	0.64
4:D:31:ARG:CG	5:J:270:DA:H4'	2.27	0.64
4:D:122:THR:C	4:D:124:ALA:N	2.54	0.63
5:I:92:DT:H2''	5:I:93:DT:H5'	1.80	0.63
5:I:108:DC:H2''	5:I:109:DA:C8	2.33	0.63
5:I:117:DT:H1'	5:I:118:DT:H5''	1.79	0.63
3:G:83:LEU:O	3:G:87:ILE:HG12	1.98	0.63
5:I:93:DT:H2''	5:I:94:DG:H5'	1.81	0.63
2:B:29:ILE:N	2:B:29:ILE:HD12	2.14	0.63
5:I:104:DT:H2''	5:I:105:DT:C5'	2.29	0.63
5:J:241:DA:C2'	5:J:242:DT:H5'	2.21	0.63
3:C:38:ASN:HD22	4:H:82:HIS:CE1	2.17	0.62
5:I:34:DT:H2''	5:I:35:DA:H8	1.64	0.62
5:J:197:DA:H1'	5:J:198:DT:H5''	1.80	0.62
8:C:301:HOH:O	4:D:49:HIS:HD2	1.81	0.62
5:I:113:DA:H2''	5:I:114:DC:O5'	2.00	0.62
5:J:163:DA:H2''	5:J:164:DG:OP2	1.98	0.62
5:J:251:DT:H2''	5:J:252:DT:H5'	1.81	0.62
5:J:259:DA:H2''	5:J:260:DC:C5'	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:73:ASN:HB2	8:G:313:HOH:O	1.98	0.62
5:J:149:DC:H2''	5:J:150:DA:H5'	1.81	0.62
5:J:248:DA:H2''	5:J:249:DG:C5'	2.26	0.62
4:H:33:ARG:HD3	4:H:33:ARG:N	2.14	0.62
5:I:77:DA:H1'	5:I:78:DG:H5'	1.82	0.62
5:J:291:DA:N9	5:J:292:DT:H72	2.15	0.62
3:C:64:GLU:O	4:D:49:HIS:HE1	1.83	0.62
5:J:194:DT:C2'	5:J:195:DC:H5'	2.19	0.61
5:J:274:DT:H2''	5:J:275:DC:H5'	1.82	0.61
1:A:121:PRO:HD2	6:A:201:CL:CL	2.37	0.61
5:J:186:DG:H1'	5:J:187:DA:N7	2.15	0.61
5:I:104:DT:H2''	5:I:105:DT:H5''	1.82	0.61
5:I:63:DG:H2''	5:I:64:DT:OP2	1.99	0.61
1:E:41:TYR:OH	5:I:7:DA:H5'	2.01	0.61
4:D:31:ARG:HG2	5:J:270:DA:H4'	1.82	0.61
5:J:288:DT:H1'	5:J:289:DT:H5''	1.82	0.61
5:J:261:DA:H1'	5:J:262:DC:H5''	1.82	0.61
5:I:2:DT:H2''	5:I:3:DC:O4'	2.00	0.61
5:J:284:DG:H2''	5:J:285:DA:C8	2.36	0.61
5:I:101:DC:H2''	5:I:102:DA:C5'	2.21	0.60
1:E:108:ASN:O	1:E:112:ILE:HG12	2.01	0.60
5:J:165:DA:H2''	5:J:166:DT:H5'	1.82	0.60
5:I:34:DT:H2''	5:I:35:DA:C8	2.36	0.60
5:I:58:DG:H2''	5:I:59:DG:C8	2.36	0.59
5:I:139:DA:H2''	5:I:140:DT:H5'	1.84	0.59
1:E:121:PRO:CB	2:F:53:GLU:HG3	2.32	0.59
5:J:242:DT:H1'	5:J:243:DG:H5''	1.84	0.59
5:I:119:DT:H2''	5:I:120:DT:OP2	2.02	0.59
5:I:74:DT:H1'	5:I:75:DT:H5''	1.84	0.59
1:E:65:LEU:HB3	1:E:66:PRO:HD3	1.82	0.59
5:J:181:DA:C2'	5:J:182:DT:H5''	2.32	0.59
3:C:101:THR:HG21	8:F:211:HOH:O	2.03	0.59
5:I:120:DT:H2''	5:I:121:DG:C8	2.38	0.59
1:A:40:ARG:NH2	5:J:229:DA:N3	2.48	0.59
5:J:242:DT:C2'	5:J:243:DG:H5''	2.33	0.59
5:I:93:DT:H1'	5:I:94:DG:H5''	1.85	0.59
5:J:147:DA:C2	5:J:148:DT:C2	2.91	0.59
3:G:42:ARG:HB2	4:H:88:THR:HB	1.84	0.58
3:C:58:LEU:O	3:C:62:ILE:HG23	2.02	0.58
4:D:123:SER:C	4:D:125:LYS:N	2.60	0.58
3:G:101:THR:HG22	8:G:301:HOH:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:3:DC:H2''	5:I:4:DA:N7	2.17	0.58
2:B:32:PRO:HA	2:B:35:ARG:HG3	1.85	0.58
2:F:19:ARG:NH2	2:F:22:LEU:HD11	2.18	0.58
3:G:87:ILE:HD12	3:G:97:LEU:HD12	1.85	0.58
3:C:42:ARG:CG	4:D:88:THR:HB	2.28	0.58
5:J:220:DT:H1'	5:J:221:DT:H5'	1.85	0.58
5:J:271:DG:H4'	5:J:271:DG:OP1	2.03	0.58
1:A:51:ILE:O	1:A:55:GLN:HG3	2.03	0.58
3:G:17:ARG:HH12	3:G:31:HIS:HD2	1.50	0.58
5:J:183:DT:H2''	5:J:184:DT:C5'	2.27	0.58
5:J:154:DT:H2''	5:J:155:DC:O5'	2.03	0.57
5:J:250:DT:H2''	5:J:251:DT:H5'	1.86	0.57
1:A:65:LEU:HB3	1:A:66:PRO:HD3	1.86	0.57
3:C:20:ARG:O	4:D:125:LYS:OXT	2.23	0.57
4:D:80:LEU:HD23	4:D:96:THR:HG23	1.86	0.57
5:J:153:DA:H2''	5:J:154:DT:H5'	1.86	0.57
5:J:285:DA:H1'	5:J:286:DT:H5''	1.86	0.57
5:J:287:DA:H2'	5:J:288:DT:H72	1.85	0.57
5:I:129:DC:H2''	5:I:130:DT:C7	2.34	0.57
5:J:237:DT:H1'	5:J:238:DT:H5''	1.86	0.57
1:A:101:VAL:O	1:A:105:GLU:HG3	2.04	0.57
5:I:118:DT:H2'	5:I:119:DT:H71	1.87	0.57
5:J:211:DT:C2'	5:J:212:DC:H5'	2.27	0.57
4:H:88:THR:HG23	5:J:186:DG:OP1	2.05	0.57
5:I:62:DT:H2''	5:I:63:DG:C8	2.40	0.57
4:D:118:VAL:O	4:D:122:THR:HG23	2.04	0.57
5:I:110:DA:H2''	5:I:111:DA:OP2	2.05	0.57
5:I:114:DC:H4'	5:I:114:DC:OP1	2.05	0.56
5:J:236:DT:H2''	5:J:237:DT:OP2	2.04	0.56
5:J:274:DT:H1'	5:J:275:DC:H5''	1.87	0.56
3:C:62:ILE:CD1	3:C:83:LEU:HD22	2.34	0.56
1:E:85:GLN:HA	5:J:196:DC:OP1	2.05	0.56
5:I:4:DA:H2''	5:I:5:DA:H5'	1.87	0.56
5:I:36:DT:C3'	5:I:37:DT:H5''	2.36	0.56
5:J:242:DT:H2''	5:J:243:DG:C5'	2.35	0.56
1:E:37:LYS:HD3	1:E:39:HIS:HB2	1.87	0.56
5:I:102:DA:H2''	5:I:103:DG:OP2	2.03	0.56
5:J:259:DA:H2''	5:J:260:DC:H5'	1.86	0.56
3:C:76:THR:O	4:D:52:THR:HG23	2.06	0.56
5:I:36:DT:H2''	5:I:37:DT:C5'	2.25	0.56
5:J:274:DT:H2''	5:J:275:DC:H5''	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:238:DT:C2'	5:J:239:DT:H5'	2.32	0.56
5:J:231:DA:H2''	5:J:232:DT:OP2	2.06	0.56
5:I:143:DT:H2''	5:I:144:DG:OP2	2.05	0.56
5:J:157:DA:H2''	5:J:158:DC:C5'	2.30	0.56
5:J:235:DC:H2''	5:J:236:DT:C5	2.41	0.56
5:J:205:DG:H2''	5:J:206:DC:H5''	1.86	0.56
3:C:84:GLN:NE2	3:C:88:ARG:HE	1.88	0.56
5:I:115:DA:C1'	5:I:116:DC:H5''	2.36	0.56
2:B:52:GLU:OE2	2:B:55:ARG:NH1	2.39	0.55
2:B:92:ARG:HH21	4:D:101:LEU:HD22	1.70	0.55
2:F:21:VAL:HG12	2:F:23:ARG:HG3	1.88	0.55
5:J:242:DT:H2''	5:J:243:DG:H5''	1.88	0.55
2:B:46:ILE:O	5:J:227:DG:H3'	2.07	0.55
5:J:153:DA:H1'	5:J:154:DT:H5''	1.87	0.55
5:J:265:DT:H2''	5:J:266:DT:O5'	2.06	0.55
5:J:247:DC:H2''	5:J:248:DA:N7	2.21	0.55
1:A:42:ARG:HH21	5:I:68:DG:P	2.30	0.55
5:I:118:DT:C2'	5:I:119:DT:H71	2.37	0.55
5:I:2:DT:H2''	5:I:3:DC:C5'	2.32	0.55
5:J:281:DG:H2''	5:J:282:DT:C5'	2.37	0.55
5:I:12:DC:H1'	5:I:13:DC:H5''	1.89	0.55
5:I:131:DG:H2''	5:I:132:DC:C5	2.42	0.55
5:J:260:DC:H2''	5:J:261:DA:C8	2.42	0.55
3:C:62:ILE:HD11	3:C:83:LEU:CD2	2.37	0.54
5:I:43:DA:H1'	5:I:44:DC:H5''	1.89	0.54
1:E:46:VAL:HG21	5:I:82:DA:H3'	1.88	0.54
5:J:150:DA:H2''	5:J:151:DA:OP2	2.07	0.54
5:J:205:DG:C2'	5:J:206:DC:H5''	2.37	0.54
3:G:95:LYS:HD3	3:G:95:LYS:C	2.33	0.54
5:I:53:DC:C2'	5:I:54:DA:H5'	2.36	0.54
5:J:287:DA:H2'	5:J:288:DT:C7	2.37	0.54
5:I:124:DA:H2''	5:I:125:DG:OP2	2.07	0.54
5:J:239:DT:H4'	5:J:240:DG:OP1	2.08	0.54
5:I:141:DA:H1'	5:I:142:DT:H5''	1.89	0.54
5:J:149:DC:N4	5:J:150:DA:N6	2.56	0.54
5:I:74:DT:H2''	5:I:75:DT:H5'	1.89	0.54
5:I:51:DA:C3'	5:I:52:DT:H5''	2.37	0.54
5:I:20:DT:H2''	5:I:21:DT:C5'	2.38	0.53
5:I:43:DA:C1'	5:I:44:DC:H5''	2.38	0.53
5:J:284:DG:H2''	5:J:285:DA:H8	1.71	0.53
5:J:155:DC:C2'	5:J:156:DC:H5'	2.36	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:181:DA:H1'	5:J:182:DT:H5''	1.90	0.53
5:J:205:DG:H1'	5:J:206:DC:H5''	1.90	0.53
4:D:30:LYS:N	5:I:104:DT:OP1	2.42	0.53
5:I:104:DT:C2'	5:I:105:DT:H5''	2.38	0.53
5:J:170:DA:H2''	5:J:171:DC:H5''	1.90	0.53
5:I:7:DA:C2	5:J:287:DA:C2	2.97	0.53
5:I:10:DC:H2''	5:I:11:DA:OP2	2.08	0.53
5:I:55:DA:H2''	5:I:56:DA:O5'	2.09	0.53
5:I:7:DA:H1'	5:I:8:DT:H5'	1.90	0.53
5:I:70:DT:H2''	5:I:71:DG:H5'	1.90	0.53
5:I:36:DT:H2''	5:I:37:DT:H6	1.74	0.53
5:I:93:DT:H2''	5:I:94:DG:C5'	2.38	0.53
5:J:229:DA:H2''	5:J:230:DC:H5'	1.90	0.53
3:G:79:ILE:HG12	3:G:82:HIS:CE1	2.44	0.53
5:J:159:DC:H1'	5:J:160:DT:H5'	1.91	0.53
5:J:230:DC:H2''	5:J:231:DA:C8	2.44	0.53
5:J:286:DT:H2''	5:J:287:DA:O5'	2.07	0.53
3:C:71:ARG:NH1	4:D:51:ASP:OD2	2.40	0.52
4:D:120:LYS:HG2	4:D:125:LYS:OXT	2.08	0.52
5:I:106:DT:H2''	5:I:107:DC:H5'	1.90	0.52
5:J:197:DA:H2''	5:J:198:DT:H5'	1.90	0.52
5:J:234:DC:H2''	5:J:235:DC:C5	2.44	0.52
5:I:57:DA:H2''	5:I:58:DG:C8	2.45	0.52
5:I:144:DG:C6	5:I:145:DA:C6	2.97	0.52
5:J:259:DA:H1'	5:J:260:DC:H5''	1.92	0.52
1:E:121:PRO:HB3	2:F:53:GLU:CG	2.40	0.52
3:G:76:THR:O	4:H:52:THR:HG23	2.09	0.52
2:B:49:LEU:HB3	8:B:211:HOH:O	2.10	0.52
5:J:198:DT:H2''	5:J:199:DC:H5'	1.91	0.52
2:B:58:LEU:HD23	2:B:58:LEU:C	2.36	0.51
3:G:31:HIS:HD2	3:G:48:PRO:HG3	1.75	0.51
5:I:1:DA:C2	5:I:2:DT:C2	2.99	0.51
5:J:159:DC:H2''	5:J:160:DT:O5'	2.11	0.51
5:J:251:DT:H2'	5:J:252:DT:H71	1.91	0.51
5:J:274:DT:C2'	5:J:275:DC:H5''	2.40	0.51
5:J:149:DC:H1'	5:J:150:DA:C5'	2.38	0.51
3:C:42:ARG:O	4:D:88:THR:HA	2.11	0.51
3:G:17:ARG:HG2	4:H:121:TYR:HE1	1.75	0.51
5:I:95:DA:H2''	5:I:96:DT:C5'	2.40	0.51
5:I:122:DG:H1'	5:I:123:DT:H5''	1.92	0.51
5:I:136:DT:H2'	5:I:137:DG:C8	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:101:DC:C2'	5:I:102:DA:H5'	2.25	0.51
5:J:173:DA:H2''	5:J:174:DA:C8	2.46	0.51
4:D:123:SER:CB	4:D:125:LYS:HG3	2.41	0.51
1:E:37:LYS:HB2	1:E:39:HIS:N	2.25	0.51
5:J:250:DT:H2''	5:J:251:DT:C5'	2.40	0.51
5:J:262:DC:H2'	5:J:263:DT:H71	1.92	0.51
5:I:89:DC:H2''	5:I:90:DT:H71	1.92	0.51
5:J:170:DA:C2'	5:J:171:DC:H5''	2.40	0.51
5:J:201:DA:H2''	5:J:202:DA:OP2	2.10	0.51
4:D:69:ILE:O	4:D:73:ILE:HG12	2.10	0.51
5:J:258:DT:H2''	5:J:259:DA:C8	2.45	0.51
5:I:49:DC:H2''	5:I:50:DC:OP2	2.10	0.51
5:I:59:DG:H2''	5:I:60:DC:OP2	2.10	0.51
5:J:205:DG:H2''	5:J:206:DC:C5'	2.41	0.51
5:J:246:DG:H2''	5:J:247:DC:H5'	1.93	0.51
5:J:275:DC:H2''	5:J:276:DT:C5'	2.39	0.51
5:I:37:DT:C2'	5:I:38:DT:H5'	2.39	0.51
5:J:285:DA:H2''	5:J:286:DT:H5'	1.92	0.51
3:C:32:ARG:NH1	5:I:29:DA:OP1	2.42	0.50
2:B:78:ARG:HD3	5:J:248:DA:H5'	1.93	0.50
1:E:57:SER:HB2	1:E:59:GLU:OE2	2.12	0.50
5:I:58:DG:H4'	5:I:58:DG:OP1	2.12	0.50
5:I:8:DT:C1'	5:I:9:DC:H5''	2.40	0.50
5:I:36:DT:H2''	5:I:37:DT:C6	2.46	0.50
5:I:52:DT:C2'	5:I:53:DC:H5'	2.28	0.50
5:J:177:DG:H1'	5:J:178:DT:H5''	1.94	0.50
4:D:84:ASN:O	4:D:86:ARG:HG3	2.11	0.50
3:G:81:ARG:NH2	3:G:107:VAL:O	2.45	0.50
5:J:252:DT:H2''	5:J:253:DC:O5'	2.11	0.50
5:I:146:DT:H5'	5:I:146:DT:C6	2.47	0.50
4:D:54:ILE:HG21	4:D:59:MET:HE2	1.94	0.50
5:J:148:DT:C4	5:J:149:DC:N4	2.79	0.50
5:J:276:DT:H2''	5:J:277:DG:N7	2.26	0.50
5:J:179:DG:C2'	5:J:180:DT:H5''	2.42	0.50
5:J:246:DG:H1'	5:J:247:DC:H5''	1.93	0.50
5:J:249:DG:H1'	5:J:250:DT:H5''	1.93	0.50
2:B:98:TYR:CD1	4:H:64:SER:HB3	2.46	0.49
5:I:46:DG:H2''	5:I:47:DC:C5'	2.28	0.49
5:J:229:DA:H1'	5:J:230:DC:H5''	1.94	0.49
5:J:273:DA:C2'	5:J:274:DT:H5''	2.42	0.49
1:A:113:HIS:CG	1:E:126:LEU:HD22	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:172:DC:H2''	5:J:173:DA:C8	2.48	0.49
5:J:175:DA:H2''	5:J:176:DA:C8	2.46	0.49
3:G:24:GLN:HG3	4:H:47:GLN:OE1	2.12	0.49
5:J:264:DT:H2'	5:J:265:DT:H72	1.94	0.49
5:J:147:DA:N1	5:J:148:DT:C2	2.81	0.49
5:I:139:DA:C8	5:I:140:DT:H72	2.48	0.49
5:J:231:DA:H1'	5:J:232:DT:H5''	1.94	0.49
5:J:170:DA:C1'	5:J:171:DC:H5''	2.43	0.48
5:J:282:DT:H2''	5:J:283:DG:C5'	2.36	0.48
5:J:207:DA:H1'	5:J:208:DT:H5''	1.96	0.48
3:C:38:ASN:ND2	4:H:82:HIS:CE1	2.81	0.48
5:I:61:DA:H1'	5:I:62:DT:H5''	1.95	0.48
5:I:103:DG:H1'	5:I:104:DT:H5''	1.95	0.48
1:E:134:ARG:HH11	1:E:134:ARG:CB	2.16	0.48
5:J:281:DG:H1'	5:J:282:DT:H5''	1.95	0.48
2:B:72:TYR:CE1	4:D:80:LEU:HD13	2.48	0.48
5:I:145:DA:N6	5:J:147:DA:N6	2.61	0.48
1:A:108:ASN:O	1:A:112:ILE:HG12	2.13	0.48
1:E:134:ARG:O	1:E:135:ALA:C	2.55	0.48
5:I:136:DT:H4'	5:I:136:DT:OP1	2.14	0.48
5:J:227:DG:H2''	5:J:228:DA:OP2	2.14	0.48
3:C:17:ARG:NH2	3:C:31:HIS:CD2	2.75	0.48
5:J:261:DA:C1'	5:J:262:DC:H5''	2.43	0.48
2:F:83:ALA:O	2:F:87:VAL:HG23	2.13	0.48
5:I:24:DA:H2''	5:I:25:DC:O5'	2.14	0.48
5:I:52:DT:H2''	5:I:53:DC:C5'	2.27	0.48
5:I:136:DT:C2'	5:I:137:DG:C8	2.97	0.48
5:J:153:DA:H2''	5:J:154:DT:C5'	2.44	0.48
2:F:89:ALA:O	2:F:93:GLN:HG2	2.14	0.47
5:I:131:DG:H2''	5:I:132:DC:C6	2.49	0.47
5:J:291:DA:C2'	5:J:292:DT:H72	2.44	0.47
5:J:193:DC:H2''	5:J:194:DT:H71	1.96	0.47
5:J:273:DA:H2''	5:J:274:DT:H5''	1.96	0.47
3:C:26:PRO:HD3	4:D:40:TYR:CD1	2.49	0.47
5:I:74:DT:H2''	5:I:75:DT:C5'	2.44	0.47
5:J:279:DA:H2''	5:J:280:DG:C5'	2.42	0.47
2:F:92:ARG:NH1	2:F:92:ARG:HB3	2.29	0.47
4:H:88:THR:CG2	5:J:186:DG:OP1	2.62	0.47
5:I:8:DT:C2'	5:I:9:DC:H5''	2.45	0.47
5:I:115:DA:H2''	5:I:116:DC:C5'	2.43	0.47
5:J:190:DC:H2''	5:J:191:DT:O5'	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:29:ILE:N	2:B:29:ILE:CD1	2.78	0.47
1:A:49:ARG:HD2	5:J:155:DC:OP1	2.15	0.47
1:A:125:GLN:CG	1:A:134:ARG:HH12	2.25	0.47
3:C:25:PHE:CZ	3:C:59:THR:HG21	2.50	0.47
2:F:100:PHE:C	2:F:102:GLY:H	2.21	0.47
5:I:114:DC:H2''	5:I:115:DA:C8	2.49	0.47
5:J:246:DG:H1'	5:J:247:DC:C5'	2.44	0.47
5:J:279:DA:H1'	5:J:280:DG:H5''	1.97	0.47
4:D:122:THR:O	4:D:124:ALA:N	2.47	0.47
5:I:130:DT:H2''	5:I:131:DG:C5'	2.39	0.47
5:I:145:DA:C6	5:I:146:DT:O4	2.68	0.47
2:F:84:MET:HE3	2:F:88:TYR:CZ	2.50	0.47
4:H:33:ARG:N	4:H:33:ARG:CD	2.77	0.47
5:J:242:DT:C1'	5:J:243:DG:H5''	2.45	0.47
3:C:26:PRO:HD3	4:D:40:TYR:CG	2.49	0.47
4:H:70:PHE:CD1	4:H:70:PHE:C	2.93	0.47
5:J:283:DG:H2''	5:J:284:DG:OP2	2.15	0.47
1:A:76:GLN:HA	1:A:76:GLN:HE21	1.79	0.46
2:B:92:ARG:HB3	2:B:92:ARG:NH1	2.31	0.46
3:C:51:LEU:HD13	4:D:73:ILE:HG21	1.96	0.46
1:E:49:ARG:HD3	5:I:8:DT:P	2.55	0.46
1:E:131:ARG:HD3	1:E:133:GLU:OE2	2.14	0.46
5:I:22:DC:H1'	5:I:23:DT:H5''	1.96	0.46
3:C:30:VAL:HG13	4:D:70:PHE:HE1	1.81	0.46
1:E:49:ARG:HD3	5:I:7:DA:O3'	2.15	0.46
3:G:77:ARG:HB3	5:I:131:DG:OP1	2.15	0.46
3:G:95:LYS:HD3	3:G:95:LYS:O	2.14	0.46
5:I:20:DT:C1'	5:I:21:DT:H5''	2.45	0.46
2:F:51:TYR:O	2:F:55:ARG:HG3	2.15	0.46
5:I:31:DG:H1'	5:I:32:DT:H5''	1.97	0.46
5:I:33:DG:H2''	5:I:34:DT:O5'	2.14	0.46
3:C:114:VAL:HG23	8:C:317:HOH:O	2.14	0.46
4:D:31:ARG:O	4:D:32:SER:CB	2.63	0.46
1:E:79:LYS:HD3	1:E:80:THR:O	2.16	0.46
5:J:292:DT:H6	5:J:292:DT:H5'	1.79	0.46
3:C:55:LEU:O	3:C:59:THR:CG2	2.62	0.46
2:F:28:GLY:HA3	8:F:215:HOH:O	2.15	0.46
5:I:26:DC:H1'	5:I:27:DA:C5	2.51	0.46
5:J:192:DG:C2'	5:J:193:DC:H5'	2.40	0.46
3:C:29:ARG:HD2	4:D:35:GLU:OE2	2.15	0.46
3:G:64:GLU:O	4:H:49:HIS:HE1	1.99	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:179:DG:H2''	5:J:180:DT:H5''	1.98	0.46
5:J:258:DT:H2''	5:J:259:DA:H8	1.81	0.46
5:I:38:DT:H2''	5:I:39:DG:C8	2.51	0.46
5:I:45:DT:H2''	5:I:46:DG:C8	2.51	0.46
5:J:148:DT:N3	5:J:149:DC:C4	2.84	0.46
5:J:165:DA:C8	5:J:166:DT:H72	2.51	0.45
2:F:45:ARG:CZ	5:I:80:DT:H4'	2.46	0.45
5:J:240:DG:H2''	5:J:241:DA:O5'	2.16	0.45
5:J:273:DA:C1'	5:J:274:DT:H5''	2.44	0.45
1:E:122:LYS:CB	1:E:122:LYS:NZ	2.79	0.45
1:E:63:ARG:HD2	5:I:90:DT:H4'	1.97	0.45
1:E:79:LYS:HD3	1:E:79:LYS:C	2.41	0.45
5:I:99:DA:H1'	5:I:100:DG:H5'	1.98	0.45
5:J:289:DT:H2''	5:J:290:DG:C8	2.50	0.45
5:J:194:DT:C2'	5:J:195:DC:C5'	2.87	0.45
1:A:70:LEU:HD22	2:B:29:ILE:HD11	1.99	0.45
1:E:37:LYS:HD3	1:E:39:HIS:CB	2.47	0.45
5:I:146:DT:H5'	5:I:146:DT:H6	1.81	0.45
1:E:134:ARG:O	1:E:135:ALA:O	2.34	0.45
5:I:73:DA:H1'	5:I:74:DT:H5''	1.97	0.45
5:J:179:DG:C1'	5:J:180:DT:H5''	2.44	0.45
5:J:225:DC:H2''	5:J:226:DT:H71	1.99	0.45
5:J:250:DT:H1'	5:J:251:DT:H5''	1.99	0.45
5:I:145:DA:C4	5:I:146:DT:H73	2.52	0.45
5:I:89:DC:H2''	5:I:90:DT:C7	2.47	0.44
5:I:118:DT:H1'	5:I:119:DT:H5'	2.00	0.44
5:I:136:DT:H2''	5:I:137:DG:H5'	1.99	0.44
5:J:186:DG:H1'	5:J:187:DA:C8	2.51	0.44
5:J:223:DA:H1'	5:J:224:DG:C8	2.53	0.44
3:G:37:GLY:HA3	3:G:39:TYR:CE2	2.52	0.44
5:I:47:DC:H2''	5:I:48:DT:C5	2.52	0.44
5:J:271:DG:H2''	5:J:272:DA:C8	2.52	0.44
5:J:285:DA:H1'	5:J:286:DT:C5'	2.47	0.44
1:A:70:LEU:O	1:A:74:ILE:HG12	2.17	0.44
2:B:78:ARG:HD2	5:J:248:DA:H5'	1.98	0.44
1:E:128:ARG:HD2	1:E:133:GLU:OE1	2.18	0.44
5:I:86:DT:H2''	5:I:87:DG:C8	2.53	0.44
5:J:210:DT:H2''	5:J:211:DT:OP2	2.17	0.44
3:G:15:LYS:HD3	5:J:178:DT:OP1	2.17	0.44
5:I:104:DT:H2''	5:I:105:DT:H5'	2.00	0.44
5:I:106:DT:H1'	5:I:107:DC:C5'	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:120:LYS:O	4:D:125:LYS:HB2	2.18	0.44
1:E:49:ARG:HG3	1:E:49:ARG:NH1	2.30	0.44
5:I:111:DA:H2''	5:I:112:DT:OP2	2.17	0.44
5:I:126:DA:H2''	5:I:127:DA:OP2	2.16	0.44
5:J:269:DT:H2''	5:J:270:DA:OP2	2.17	0.44
5:J:280:DG:H2''	5:J:281:DG:H5'	1.99	0.44
4:D:51:ASP:HB3	8:D:302:HOH:O	2.18	0.44
5:I:20:DT:C2'	5:I:21:DT:H5''	2.47	0.44
5:J:253:DC:C4	5:J:254:DC:N4	2.85	0.44
2:B:92:ARG:NH2	4:D:101:LEU:HD22	2.32	0.44
2:F:75:HIS:HD2	4:H:96:THR:OG1	2.01	0.44
4:H:73:ILE:HD13	4:H:101:LEU:HD12	1.99	0.44
5:I:31:DG:H2''	5:I:32:DT:H5'	2.00	0.44
5:J:176:DA:H2''	5:J:177:DG:OP2	2.18	0.44
5:J:207:DA:H2''	5:J:208:DT:H5'	1.99	0.44
4:D:123:SER:HB3	4:D:125:LYS:HG3	1.99	0.44
5:J:263:DT:H2''	5:J:264:DT:O5'	2.18	0.44
4:H:39:ILE:HG13	8:H:208:HOH:O	2.18	0.44
1:A:43:PRO:HG2	5:I:68:DG:C5'	2.48	0.43
2:B:28:GLY:O	2:B:30:THR:HG23	2.18	0.43
5:J:158:DC:H1'	5:J:159:DC:H5''	2.00	0.43
3:C:42:ARG:HG3	4:D:88:THR:CB	2.35	0.43
1:E:73:GLU:OE1	2:F:25:ASN:ND2	2.46	0.43
3:C:84:GLN:HG3	3:C:105:GLY:HA3	2.00	0.43
1:E:69:ARG:CD	2:F:25:ASN:OD1	2.67	0.43
5:I:46:DG:N2	5:J:248:DA:C2	2.86	0.43
5:J:267:DG:H1'	5:J:268:DG:H5''	2.01	0.43
4:D:88:THR:CG2	5:I:39:DG:OP1	2.66	0.43
3:C:54:VAL:HG21	4:D:98:VAL:HG21	1.99	0.43
5:I:123:DT:H6	5:I:123:DT:H2'	1.72	0.43
5:J:259:DA:H2''	5:J:260:DC:H5''	2.01	0.43
4:H:46:LYS:HA	4:H:46:LYS:HD3	1.83	0.43
5:I:145:DA:C2	5:I:146:DT:C4	3.07	0.43
5:J:169:DT:H2''	5:J:170:DA:H8	1.82	0.43
5:J:206:DC:H2''	5:J:207:DA:C8	2.54	0.43
2:B:31:LYS:HB3	2:B:32:PRO:CD	2.48	0.43
2:F:78:ARG:HD3	5:I:101:DC:H5'	2.00	0.43
5:I:5:DA:H1'	5:I:6:DT:H5''	2.01	0.43
5:I:17:DA:H1'	5:I:18:DG:H5'	2.00	0.43
5:J:161:DG:H1'	5:J:162:DC:H5''	2.01	0.43
3:G:99:ARG:HA	3:G:99:ARG:HD2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:28:DA:H1'	5:I:29:DA:C8	2.54	0.43
5:J:152:DT:H2'	5:J:153:DA:C8	2.53	0.43
5:J:197:DA:H2''	5:J:198:DT:C5'	2.49	0.43
5:J:231:DA:H1'	5:J:232:DT:C5'	2.48	0.43
2:B:92:ARG:HB3	2:B:92:ARG:CZ	2.49	0.43
5:J:152:DT:H2''	5:J:153:DA:O4'	2.18	0.43
5:J:257:DA:H2''	5:J:258:DT:OP2	2.19	0.43
2:F:78:ARG:CD	5:I:101:DC:H5'	2.49	0.42
5:I:91:DT:H1'	5:I:92:DT:H5''	2.01	0.42
3:C:32:ARG:HD3	5:I:29:DA:OP2	2.19	0.42
5:J:215:DC:H2''	5:J:216:DT:H71	2.01	0.42
4:H:116:LYS:HB2	4:H:116:LYS:HE3	1.85	0.42
5:J:259:DA:C2'	5:J:260:DC:H5''	2.48	0.42
2:B:75:HIS:CD2	4:D:96:THR:CG2	2.92	0.42
3:C:17:ARG:HH22	3:C:31:HIS:HD2	1.58	0.42
5:J:200:DA:H2''	5:J:201:DA:H5'	2.01	0.42
1:E:129:ARG:CD	1:E:135:ALA:HA	2.46	0.42
5:I:10:DC:H6	5:I:10:DC:H2'	1.66	0.42
5:I:85:DA:H2''	5:I:86:DT:H5'	2.02	0.42
5:J:225:DC:H2''	5:J:226:DT:C7	2.50	0.42
3:G:99:ARG:HH11	3:G:99:ARG:HG3	1.85	0.42
5:I:20:DT:H2''	5:I:21:DT:H5''	2.02	0.42
3:G:44:GLY:HA3	6:G:201:CL:CL	2.56	0.42
5:I:145:DA:H2''	5:I:146:DT:OP2	2.19	0.42
1:A:63:ARG:HH21	5:J:237:DT:H5''	1.85	0.41
2:B:31:LYS:N	2:B:32:PRO:HD2	2.35	0.41
5:J:192:DG:H1'	5:J:193:DC:H5''	2.02	0.41
5:I:93:DT:H6	5:I:93:DT:H2'	1.77	0.41
5:J:158:DC:C1'	5:J:159:DC:H5''	2.49	0.41
5:I:58:DG:C2'	5:I:59:DG:C8	3.01	0.41
5:I:100:DG:H1'	5:I:101:DC:C5	2.55	0.41
3:C:50:TYR:OH	4:D:95:GLN:HG3	2.20	0.41
4:D:42:TYR:CE2	4:D:46:LYS:HD2	2.55	0.41
3:G:99:ARG:HG3	3:G:99:ARG:NH1	2.35	0.41
5:J:158:DC:H6	5:J:158:DC:H2'	1.73	0.41
1:A:43:PRO:HG2	5:I:68:DG:H5'	2.03	0.41
2:B:31:LYS:HG3	2:B:51:TYR:CE1	2.56	0.41
5:J:208:DT:H2''	5:J:209:DG:H5''	1.98	0.41
3:C:101:THR:HG23	2:F:96:THR:O	2.21	0.41
4:D:31:ARG:O	4:D:32:SER:HB2	2.20	0.41
5:I:63:DG:H1'	5:I:64:DT:H5''	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:20:DT:H2''	5:I:21:DT:H5'	2.02	0.41
5:I:143:DT:H1'	5:I:144:DG:C8	2.56	0.41
5:J:149:DC:H2''	5:J:150:DA:OP2	2.20	0.41
5:I:78:DG:H1'	5:I:79:DC:C5	2.56	0.41
1:A:119:ILE:O	2:B:47:SER:HB3	2.21	0.41
4:D:123:SER:HB2	4:D:125:LYS:HG3	2.03	0.41
2:F:92:ARG:HB3	2:F:92:ARG:CZ	2.50	0.41
3:G:73:ASN:O	3:G:74:LYS:HB2	2.21	0.41
5:I:112:DT:H2''	5:I:113:DA:H5'	2.03	0.41
5:J:235:DC:H2''	5:J:236:DT:H73	2.01	0.41
5:J:256:DA:H2''	5:J:257:DA:OP2	2.20	0.41
1:A:68:GLN:HE21	1:A:89:VAL:HG21	1.85	0.41
5:I:9:DC:C2'	5:I:10:DC:H5'	2.39	0.41
5:I:145:DA:H2''	5:I:146:DT:H71	2.03	0.41
5:J:252:DT:H6	5:J:252:DT:H2'	1.70	0.41
2:B:72:TYR:OH	2:B:92:ARG:HD2	2.21	0.40
3:C:62:ILE:HG13	3:C:63:LEU:N	2.35	0.40
1:E:56:LYS:HB2	1:E:56:LYS:HE3	1.90	0.40
5:J:175:DA:H2''	5:J:176:DA:H8	1.87	0.40
5:J:179:DG:H2''	5:J:180:DT:C5'	2.51	0.40
3:C:25:PHE:HZ	3:C:59:THR:HG21	1.86	0.40
5:I:4:DA:C2	5:J:290:DG:N2	2.89	0.40
5:I:26:DC:O3'	5:I:27:DA:C8	2.74	0.40
8:B:202:HOH:O	3:G:101:THR:HG21	2.20	0.40
3:C:47:ALA:N	3:C:48:PRO:HD2	2.37	0.40
5:J:200:DA:H1'	5:J:201:DA:H5'	2.04	0.40
1:E:97:GLU:O	1:E:101:VAL:HG23	2.22	0.40
5:J:219:DA:H2''	5:J:220:DT:C5'	2.46	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%)	95 (100%)	0	0	100	100
1	E	97/139 (70%)	95 (98%)	1 (1%)	1 (1%)	12	24
2	B	76/106 (72%)	73 (96%)	3 (4%)	0	100	100
2	F	82/106 (77%)	82 (100%)	0	0	100	100
3	C	106/133 (80%)	103 (97%)	3 (3%)	0	100	100
3	G	102/133 (77%)	100 (98%)	2 (2%)	0	100	100
4	D	94/129 (73%)	89 (95%)	2 (2%)	3 (3%)	3	4
4	H	90/129 (70%)	84 (93%)	5 (6%)	1 (1%)	11	22
All	All	742/1014 (73%)	721 (97%)	16 (2%)	5 (1%)	18	34

All (5) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	85/113 (75%)	83 (98%)	2 (2%)	43	70
1	E	86/113 (76%)	82 (95%)	4 (5%)	23	47
2	B	63/81 (78%)	62 (98%)	1 (2%)	55	79
2	F	69/81 (85%)	68 (99%)	1 (1%)	59	81
3	C	85/102 (83%)	79 (93%)	6 (7%)	13	29
3	G	83/102 (81%)	77 (93%)	6 (7%)	13	28
4	D	82/107 (77%)	74 (90%)	8 (10%)	7	16
4	H	78/107 (73%)	73 (94%)	5 (6%)	16	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	631/806 (78%)	598 (95%)	33 (5%)	21	42

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	GLU
1	A	129	ARG
2	B	58	LEU
3	C	59	THR
3	C	62	ILE
3	C	81	ARG
3	C	84	GLN
3	C	95	LYS
3	C	101	THR
4	D	31	ARG
4	D	33	ARG
4	D	39	ILE
4	D	63	ASN
4	D	71	GLU
4	D	80	LEU
4	D	88	THR
4	D	106	LEU
1	E	79	LYS
1	E	122	LYS
1	E	129	ARG
1	E	134	ARG
2	F	47	SER
3	G	62	ILE
3	G	64	GLU
3	G	81	ARG
3	G	99	ARG
3	G	101	THR
3	G	118	LYS
4	H	33	ARG
4	H	34	LYS
4	H	56	SER
4	H	88	THR
4	H	106	LEU

Sometimes 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	113	HIS
2	B	75	HIS
3	C	31	HIS
3	C	38	ASN
3	C	84	GLN
4	D	49	HIS
4	D	63	ASN
2	F	75	HIS
2	F	93	GLN
3	G	31	HIS
3	G	73	ASN
4	H	49	HIS
4	H	63	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 12 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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	97/139 (69%)	-0.06	3 (3%) 51 47	24, 36, 53, 80	0
1	E	99/139 (71%)	-0.26	3 (3%) 52 48	16, 28, 49, 85	0
2	B	78/106 (73%)	-0.16	2 (2%) 57 52	25, 33, 48, 56	0
2	F	84/106 (79%)	-0.26	2 (2%) 59 55	17, 28, 44, 74	0
3	C	108/133 (81%)	-0.09	3 (2%) 55 50	17, 32, 58, 106	0
3	G	104/133 (78%)	-0.07	2 (1%) 66 62	25, 38, 63, 76	0
4	D	96/129 (74%)	0.19	7 (7%) 21 19	23, 34, 76, 104	0
4	H	92/129 (71%)	0.13	4 (4%) 40 35	26, 39, 61, 81	0
5	I	146/146 (100%)	1.38	33 (22%) 2 2	36, 92, 134, 150	0
5	J	146/146 (100%)	1.44	36 (24%) 2 1	43, 92, 137, 161	0
All	All	1050/1306 (80%)	0.34	95 (9%) 15 13	16, 39, 120, 161	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	125	LYS	8.7
2	F	102	GLY	6.4
1	E	135	ALA	5.9
2	B	102	GLY	4.9
4	H	124	ALA	4.6
2	F	101	GLY	4.6
5	J	148	DT	4.6
5	I	146	DT	4.5
5	J	147	DA	4.2
4	D	124	ALA	4.1
5	I	39	DG	4.0
5	J	162	DC	3.8
5	I	96	DT	3.7

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Mol	Chain	Res	Type	RSRZ
5	J	161	DG	3.7
5	I	56	DA	3.7
1	A	38	PRO	3.6
5	I	40	DG	3.6
5	J	149	DC	3.6
3	C	12	ALA	3.5
5	I	55	DA	3.5
3	G	15	LYS	3.3
4	D	30	LYS	3.3
1	A	39	HIS	3.2
5	I	57	DA	3.1
5	J	167	DT	3.1
5	J	240	DG	3.0
5	J	242	DT	3.0
5	I	1	DA	3.0
5	J	163	DA	3.0
5	I	136	DT	2.9
1	E	37	LYS	2.9
5	I	124	DA	2.9
5	I	58	DG	2.9
5	J	180	DT	2.9
5	J	150	DA	2.9
2	B	101	GLY	2.7
5	J	241	DA	2.7
5	J	182	DT	2.7
5	J	243	DG	2.7
5	J	284	DG	2.7
5	J	235	DC	2.7
5	J	181	DA	2.7
5	I	9	DC	2.7
5	J	168	DC	2.6
3	G	118	LYS	2.6
5	J	285	DA	2.6
5	I	38	DT	2.6
5	J	234	DC	2.6
3	C	11	ARG	2.5
5	I	122	DG	2.5
5	J	173	DA	2.5
4	D	31	ARG	2.5
5	J	157	DA	2.5
5	I	54	DA	2.5
4	D	32	SER	2.5

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Mol	Chain	Res	Type	RSRZ
5	J	254	DC	2.4
5	J	249	DG	2.4
5	I	53	DC	2.4
5	J	263	DT	2.4
1	A	134	ARG	2.4
5	I	97	DG	2.4
5	I	128	DT	2.4
5	J	183	DT	2.3
5	I	16	DC	2.3
5	J	283	DG	2.3
5	J	246	DG	2.3
5	I	41	DA	2.3
5	I	127	DA	2.3
4	H	33	ARG	2.3
5	I	8	DT	2.2
5	I	15	DG	2.2
5	J	172	DC	2.2
5	I	125	DG	2.2
4	H	51	ASP	2.2
5	I	95	DA	2.2
5	I	145	DA	2.2
3	C	73	ASN	2.2
4	D	123	SER	2.2
5	I	135	DG	2.2
5	J	233	DG	2.2
5	J	201	DA	2.2
5	J	286	DT	2.1
5	I	134	DG	2.1
5	I	10	DC	2.1
5	J	244	DG	2.1
5	J	253	DC	2.1
1	E	39	HIS	2.1
5	I	34	DT	2.1
5	I	11	DA	2.0
5	J	245	DA	2.0
4	D	33	ARG	2.0
5	I	12	DC	2.0
4	H	121	TYR	2.0
5	I	31	DG	2.0
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 oligosaccharides 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, 95th 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(Å ²)	Q<0.9
7	MN	I	202	1/1	0.81	0.12	101,101,101,101	0
7	MN	I	201	1/1	0.84	0.17	111,111,111,111	0
7	MN	J	302	1/1	0.85	0.13	86,86,86,86	0
7	MN	J	301	1/1	0.90	0.11	97,97,97,97	0
7	MN	I	203	1/1	0.91	0.21	79,79,79,79	0
6	CL	E	201	1/1	0.97	0.07	40,40,40,40	0
6	CL	A	201	1/1	0.97	0.06	46,46,46,46	0
7	MN	J	303	1/1	0.97	0.10	68,68,68,68	0
7	MN	J	304	1/1	0.97	0.12	64,64,64,64	0
6	CL	G	201	1/1	0.98	0.07	38,38,38,38	0
6	CL	C	201	1/1	0.98	0.04	40,40,40,40	0
7	MN	D	201	1/1	0.99	0.10	32,32,32,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.