Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2024 – 11:07 AM EST

PDB ID	:	4JJN
Title	:	Crystal structure of heterochromatin protein Sir3 in complex with a silenced yeast nucleosome
Authors	:	Wang, F.; Li, G.; Mohammed, A.; Lu, C.; Currie, M.; Johnson, A.; Moazed, D.
Deposited on	:	2013-03-08
Resolution	:	3.09 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:

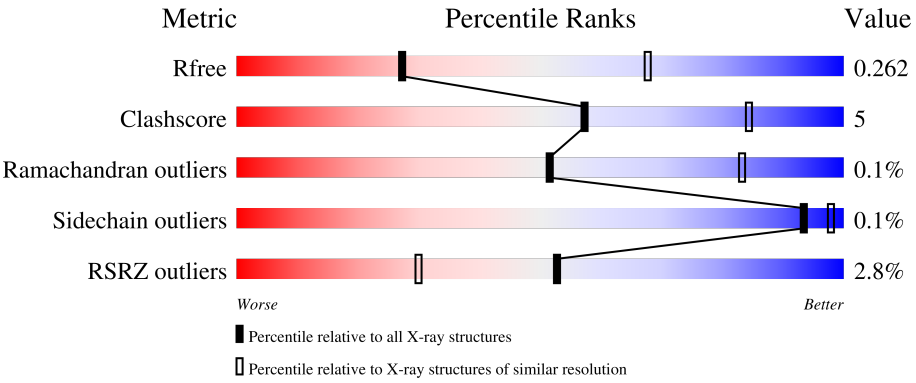
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.09 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	135	6% 61% 11% 27%
1	E	135	4% 61% 10% 29%
2	B	102	7% 76% 11% 13%
2	F	102	9% 75% 15% 11%
3	C	131	% 73% 8% 20%

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Mol	Chain	Length	Quality of chain
3	G	131	2% 73% 8% 19%
4	D	130	3% 66% 7% 27%
4	H	130	2% 59% 12% 29%
5	K	382	43% 10% 46%
5	L	382	48% 7% 45%
6	I	147	% 82% 17%
7	J	147	79% 20%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 15621 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.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	98	Total	C	N	O	0	0	0
			807	511	156	140			
1	E	96	Total	C	N	O	0	0	0
			794	503	154	137			

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	89	Total	C	N	O	0	0	0
			712	448	143	121			
2	F	91	Total	C	N	O	0	0	0
			726	456	146	124			

- Molecule 3 is a protein called Histone H2A.2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	105	Total	C	N	O	0	0	0
			806	505	158	143			
3	G	106	Total	C	N	O	0	0	0
			819	514	161	144			

- Molecule 4 is a protein called Histone H2B.2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	95	Total	C	N	O	S	0	0	0
			742	467	130	144	1			
4	H	92	Total	C	N	O	S	0	0	0
			715	450	123	141	1			

- Molecule 5 is a protein called Regulatory protein SIR3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	K	205	Total	C	N	O	S	0	0	0
			1738	1122	288	326	2			
5	L	211	Total	C	N	O	S	0	0	0
			1776	1146	299	329	2			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	1	SER	-	expression tag	UNP P06701
K	205	ASN	ASP	engineered mutation	UNP P06701
L	1	SER	-	expression tag	UNP P06701
L	205	ASN	ASP	engineered mutation	UNP P06701

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	I	146	Total	C	N	O	P	0	0	0
			2975	1413	540	876	146			

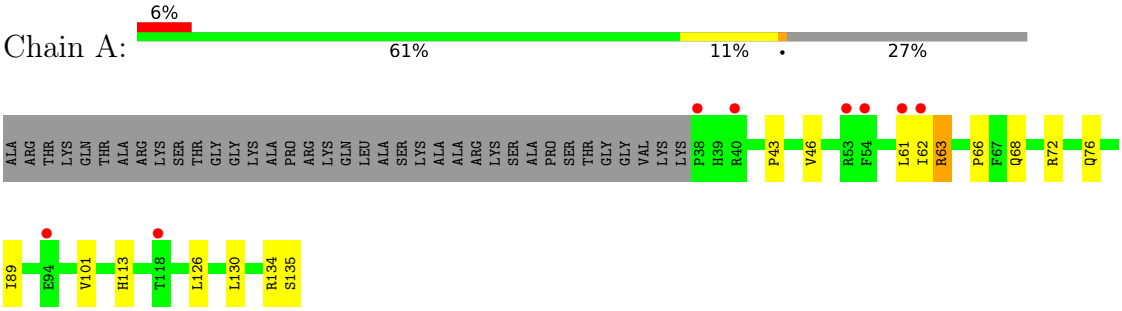
- Molecule 7 is a DNA chain called DNA (146-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	J	146	Total	C	N	O	P	0	0	0
			3011	1425	564	876	146			

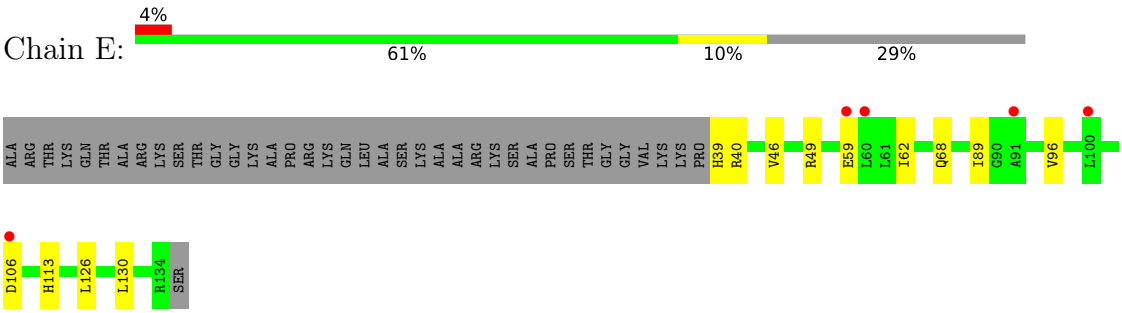
3 Residue-property plots (i)

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

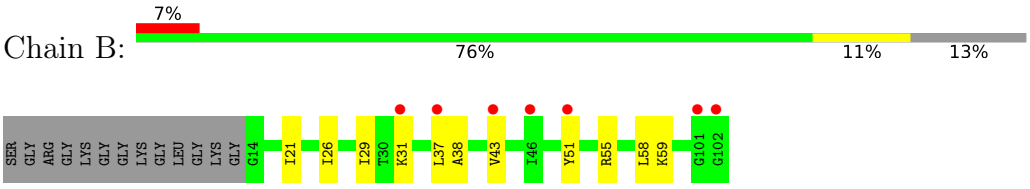
• Molecule 1: Histone H3



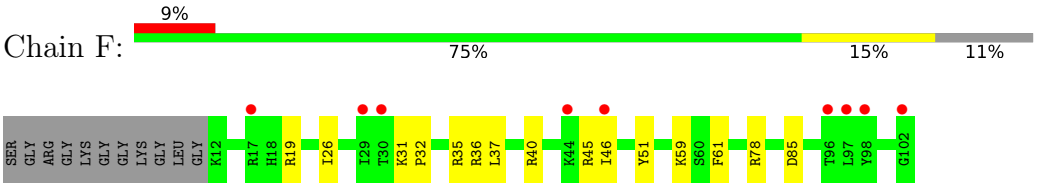
• Molecule 1: Histone H3



• Molecule 2: Histone H4

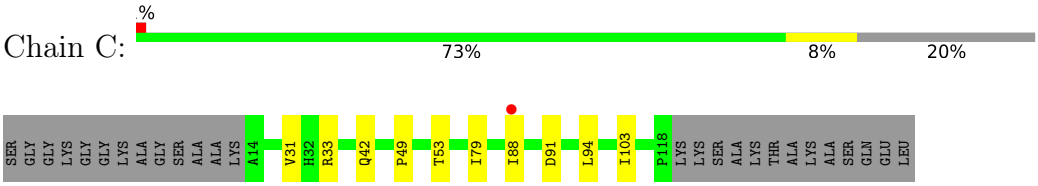


• Molecule 2: Histone H4



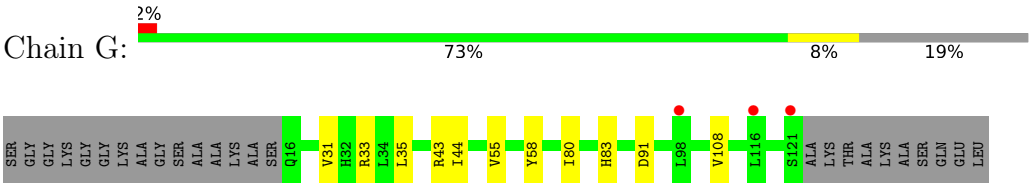
• Molecule 3: Histone H2A.2

Chain C:



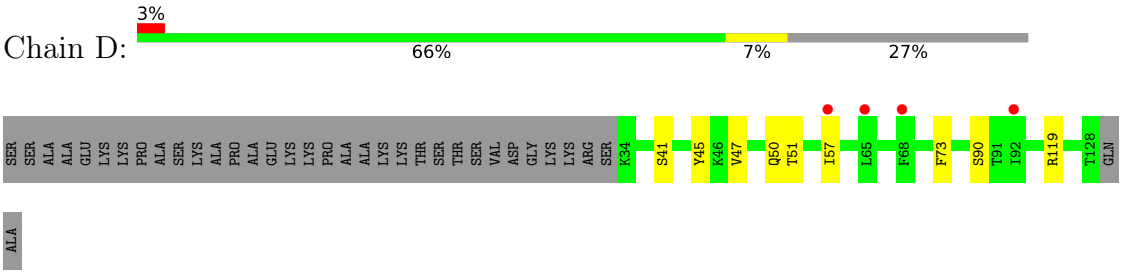
• Molecule 3: Histone H2A.2

Chain G:



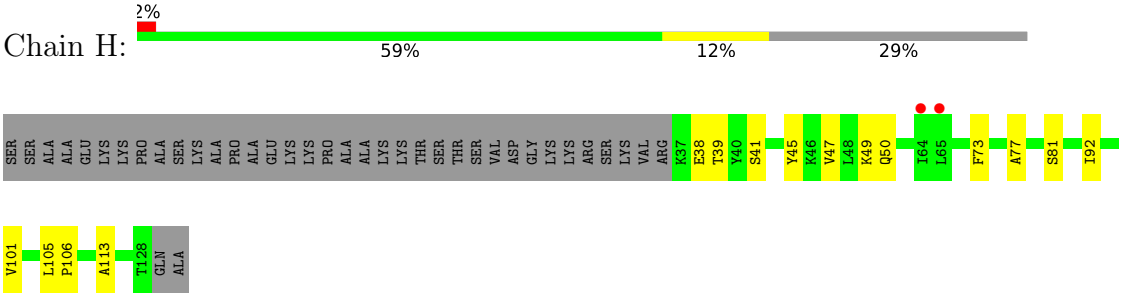
• Molecule 4: Histone H2B.2

Chain D:



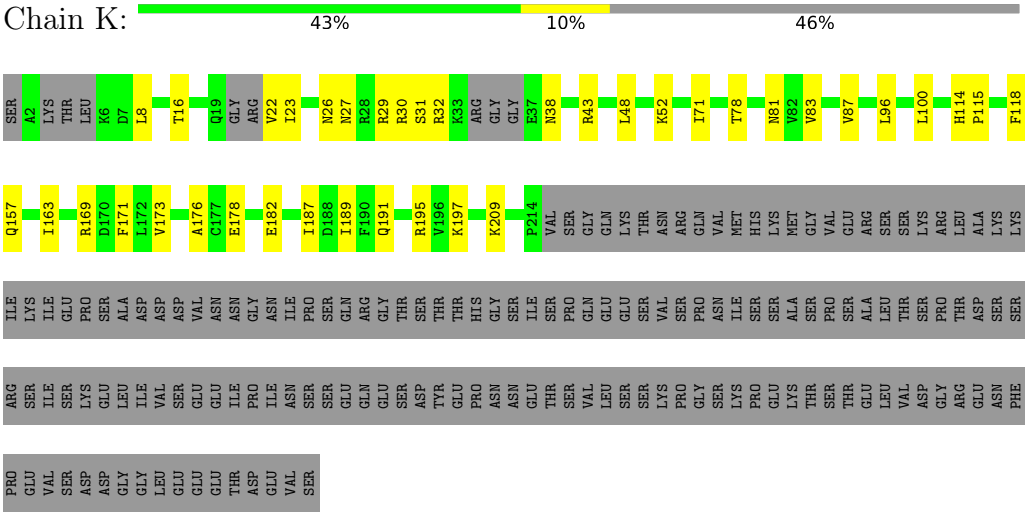
• Molecule 4: Histone H2B.2

Chain H:



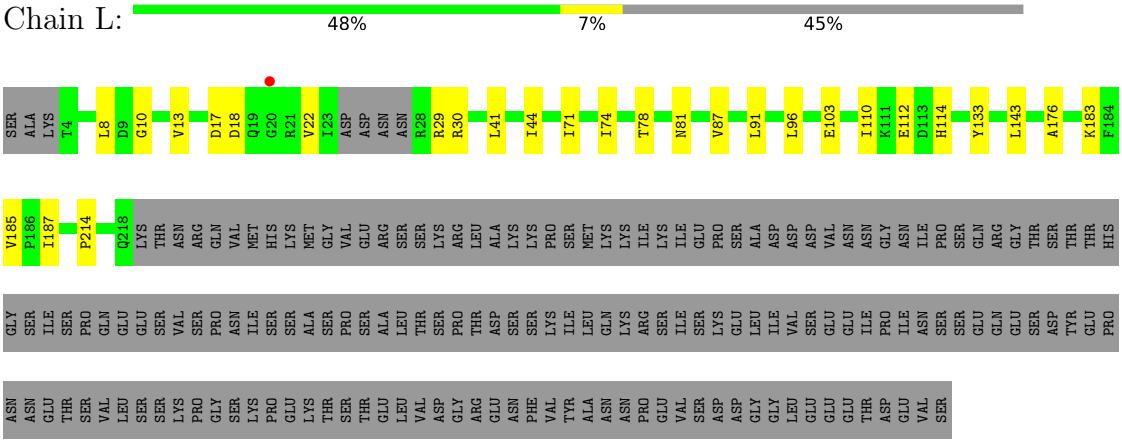
• Molecule 5: Regulatory protein SIR3

Chain K:



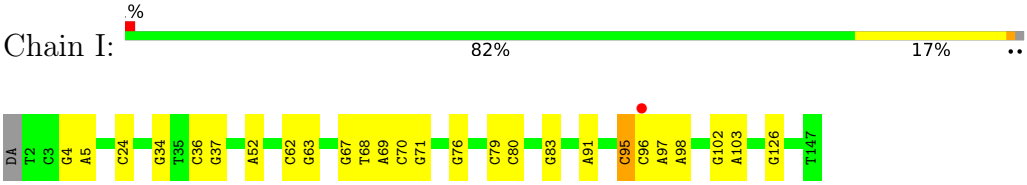
• Molecule 5: Regulatory protein SIR3

Chain L:



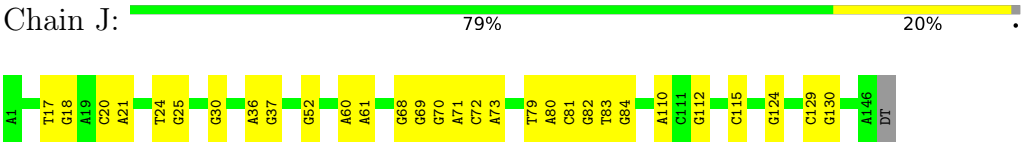
• Molecule 6: DNA (146-MER)

Chain I:



• Molecule 7: DNA (146-MER)

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	103.68Å 103.68Å 556.38Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	85.45 – 3.09 139.09 – 3.09	Depositor EDS
% Data completeness (in resolution range)	97.0 (85.45-3.09) 97.2 (139.09-3.09)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) >$ [1]	1.55 (at 3.07Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.231 , 0.255 0.237 , 0.262	Depositor DCC
R_{free} test set	3037 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	105.3	Xtriage
Anisotropy	0.371	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 160.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.449 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	15621	wwPDB-VP
Average B, all atoms (Å^2)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.21	0/818	0.35	0/1094
1	E	0.21	0/804	0.35	0/1075
2	B	0.20	0/720	0.38	0/961
2	F	0.20	0/734	0.37	0/977
3	C	0.20	0/817	0.37	0/1106
3	G	0.20	0/830	0.35	0/1121
4	D	0.21	0/752	0.37	0/1012
4	H	0.21	0/725	0.38	0/977
5	K	0.22	0/1776	0.38	0/2398
5	L	0.22	0/1816	0.38	0/2452
6	I	0.43	0/3333	0.98	1/5137 (0.0%)
7	J	0.43	0/3381	0.97	0/5221
All	All	0.32	0/16506	0.70	1/23531 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	I	95	DC	O4'-C4'-C3'	-5.63	102.25	104.50

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	807	0	856	22	0
1	E	794	0	843	12	0
2	B	712	0	766	11	0
2	F	726	0	782	11	0
3	C	806	0	844	8	0
3	G	819	0	865	11	0
4	D	742	0	770	8	0
4	H	715	0	735	11	0
5	K	1738	0	1708	25	0
5	L	1776	0	1763	17	0
6	I	2975	0	1639	21	0
7	J	3011	0	1639	28	0
All	All	15621	0	13210	136	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 5.

All (136) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:LEU:HD12	1:E:130:LEU:CD1	1.69	1.22
1:A:130:LEU:CD1	1:E:130:LEU:HD12	1.75	1.16
1:A:130:LEU:HD12	1:E:130:LEU:HD12	0.99	0.98
3:C:79:ILE:HB	4:D:57:ILE:HG22	1.72	0.72
2:B:21:ILE:HD11	5:K:209:LYS:HG2	1.72	0.69
5:K:22:VAL:HG12	5:K:23:ILE:H	1.60	0.66
2:B:26:ILE:HD11	2:B:55:ARG:O	1.96	0.66
1:A:63:ARG:NH2	7:J:60:DA:H4'	2.11	0.65
1:A:63:ARG:HH22	7:J:60:DA:H4'	1.62	0.65
5:K:173:VAL:HG13	5:K:189:ILE:HG12	1.80	0.64
4:H:39:THR:HG22	4:H:41:SER:H	1.65	0.61
5:K:169:ARG:O	5:K:171:PHE:CD1	2.55	0.60
2:B:21:ILE:HD12	5:K:136:ALA:HB3	1.84	0.59
5:L:176:ALA:HB2	5:L:187:ILE:HD13	1.86	0.58
6:I:102:DG:H2"	6:I:103:DA:H5"	1.86	0.57
1:A:62:ILE:HD11	2:B:37:LEU:HD11	1.88	0.56
1:A:63:ARG:HB3	1:A:66:PRO:HD2	1.89	0.55
4:D:119:ARG:NH1	5:K:29:ARG:HE	2.04	0.55
2:F:19:ARG:NE	6:I:52:DA:OP1	2.40	0.55
5:K:8:LEU:HD11	5:K:83:VAL:HG22	1.89	0.55
6:I:34:DG:N2	7:J:115:DC:O2	2.41	0.54
5:K:169:ARG:O	5:K:171:PHE:CE1	2.61	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:26:ILE:HD12	2:B:59:LYS:HD2	1.90	0.53
5:L:185:VAL:HG22	5:L:214:PRO:HB3	1.91	0.53
3:C:33:ARG:NH2	7:J:30:DG:OP1	2.40	0.53
1:E:62:ILE:HD11	2:F:37:LEU:HD11	1.91	0.52
3:G:33:ARG:NH2	4:H:38:GLU:OE1	2.42	0.52
1:A:63:ARG:NH2	7:J:60:DA:O3'	2.44	0.51
3:G:31:VAL:HG13	4:H:73:PHE:HE1	1.76	0.51
3:C:88:ILE:HD12	3:C:103:ILE:HD11	1.92	0.51
2:B:29:ILE:HG13	2:B:58:LEU:HD21	1.93	0.50
5:L:103:GLU:HA	5:L:110:ILE:HG13	1.92	0.50
1:A:126:LEU:HD22	1:E:113:HIS:CG	2.47	0.49
6:I:70:DC:H2"	6:I:71:DG:C8	2.48	0.49
1:A:113:HIS:CG	1:E:126:LEU:HD22	2.47	0.49
6:I:126:DG:O6	7:J:21:DA:N6	2.45	0.49
3:G:91:ASP:OD2	5:L:30:ARG:NH2	2.46	0.48
5:K:115:PRO:HG2	5:K:118:PHE:HB2	1.94	0.48
7:J:81:DC:H2'	7:J:82:DG:C8	2.48	0.48
5:K:176:ALA:HB2	5:K:187:ILE:HD13	1.95	0.48
2:F:26:ILE:HG21	2:F:59:LYS:HD2	1.95	0.48
6:I:37:DG:O6	7:J:110:DA:N6	2.46	0.48
6:I:62:DC:H2"	6:I:63:DG:H5'	1.96	0.48
1:A:68:GLN:HG3	1:A:89:ILE:HD13	1.97	0.47
5:K:26:ASN:OD1	5:K:27:ASN:N	2.45	0.47
5:L:41:LEU:HG	5:L:74:ILE:HD13	1.97	0.47
6:I:68:DT:H2"	6:I:69:DA:C8	2.50	0.47
1:A:43:PRO:HG2	7:J:69:DG:H5'	1.97	0.47
3:C:91:ASP:HB3	3:C:94:LEU:HB2	1.97	0.47
5:L:10:GLY:O	5:L:44:ILE:N	2.46	0.46
5:L:96:LEU:HD11	5:L:133:TYR:CE1	2.50	0.46
5:K:52:LYS:HD3	5:K:197:LYS:HA	1.98	0.46
5:L:17:ASP:O	5:L:18:ASP:HB2	2.14	0.46
6:I:96:DC:H2'	6:I:97:DA:C8	2.51	0.46
1:E:96:VAL:HG12	2:F:61:PHE:CD2	2.51	0.46
2:F:32:PRO:O	2:F:36:ARG:HG2	2.16	0.46
1:A:63:ARG:NH1	6:I:91:DA:H4'	2.31	0.46
6:I:24:DC:O2	7:J:124:DG:N2	2.48	0.46
5:K:78:THR:OG1	5:K:81:ASN:O	2.29	0.46
5:K:96:LEU:HD11	5:K:133:TYR:CE1	2.50	0.46
5:L:71:ILE:HA	5:L:87:VAL:HG12	1.99	0.45
5:L:71:ILE:HD13	5:L:87:VAL:HG12	1.99	0.45
5:L:183:LYS:HB3	5:L:214:PRO:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:ARG:HA	1:A:135:SER:HA	1.65	0.45
5:K:16:THR:OG1	5:K:38:ASN:HB2	2.16	0.45
5:K:43:ARG:HH21	5:K:48:LEU:HD13	1.82	0.45
4:D:47:VAL:O	4:D:50:GLN:HG2	2.17	0.45
5:L:78:THR:OG1	5:L:81:ASN:O	2.33	0.45
6:I:96:DC:O2	7:J:52:DG:N2	2.38	0.45
4:H:105:LEU:HA	4:H:106:PRO:HD3	1.75	0.44
1:A:43:PRO:HA	6:I:83:DG:H5'	1.99	0.44
5:K:71:ILE:HA	5:K:87:VAL:HG12	1.98	0.44
2:F:35:ARG:HG2	2:F:46:ILE:HD12	1.99	0.44
5:K:114:HIS:HB3	5:K:115:PRO:HD2	2.00	0.44
2:B:26:ILE:HD12	2:B:59:LYS:HB2	1.99	0.44
7:J:20:DC:H2"	7:J:21:DA:C8	2.52	0.44
4:D:51:THR:HG21	5:K:30:ARG:HH12	1.83	0.44
1:A:63:ARG:HD3	1:A:63:ARG:HA	1.41	0.44
1:E:46:VAL:HG22	1:E:49:ARG:HH21	1.83	0.44
1:E:59:GLU:O	2:F:40:ARG:NH2	2.48	0.44
5:L:112:GLU:HB3	5:L:114:HIS:CD2	2.53	0.44
5:K:100:LEU:HD13	5:K:182:GLU:HG2	1.99	0.44
7:J:79:DT:H2"	7:J:80:DA:C8	2.52	0.44
2:B:38:ALA:HB1	2:B:43:VAL:HB	1.99	0.43
3:G:43:ARG:HD3	7:J:112:DG:H4'	1.98	0.43
5:K:191:GLN:O	5:K:195:ARG:HG2	2.18	0.43
7:J:68:DG:H2"	7:J:69:DG:C8	2.54	0.43
4:D:119:ARG:HH12	5:K:29:ARG:HE	1.66	0.43
7:J:72:DC:H2"	7:J:73:DA:C8	2.53	0.43
5:L:8:LEU:HD21	5:L:13:VAL:HG23	1.99	0.43
3:G:44:ILE:HG22	4:H:92:ILE:HB	2.01	0.43
2:B:31:LYS:HG3	2:B:51:TYR:CE1	2.53	0.43
1:E:39:HIS:HA	1:E:40:ARG:HA	1.69	0.43
5:K:157:GLN:HG3	5:K:163:ILE:HG13	1.99	0.43
2:B:21:ILE:HG22	5:K:178:GLU:OE1	2.18	0.43
3:C:31:VAL:HG13	4:D:73:PHE:HE1	1.84	0.43
7:J:24:DT:H2'	7:J:25:DG:C8	2.54	0.42
1:A:130:LEU:HD22	1:E:106:ASP:HB3	2.01	0.42
1:A:72:ARG:O	1:A:76:GLN:HG2	2.19	0.42
2:F:78:ARG:NH2	2:F:85:ASP:OD2	2.51	0.42
2:F:31:LYS:HG3	2:F:51:TYR:CE1	2.55	0.42
7:J:83:DT:H2"	7:J:84:DG:C8	2.54	0.42
5:K:31:SER:HA	5:K:32:ARG:HA	1.55	0.42
7:J:129:DC:H2"	7:J:130:DG:C8	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:VAL:HG21	6:I:83:DG:H3'	2.01	0.42
4:D:41:SER:O	4:D:45:TYR:HD2	2.03	0.42
3:G:55:VAL:HG13	4:H:113:ALA:HB1	2.02	0.41
4:H:45:TYR:CE2	4:H:49:LYS:HE3	2.55	0.41
5:L:41:LEU:HD13	5:L:143:LEU:HD11	2.02	0.41
5:L:91:LEU:HB2	5:L:133:TYR:HB2	2.02	0.41
3:G:80:ILE:HG12	3:G:83:HIS:CE1	2.54	0.41
6:I:4:DG:H2"	6:I:5:DA:C8	2.55	0.41
1:E:68:GLN:HG3	1:E:89:ILE:HD13	2.01	0.41
3:G:33:ARG:HH22	4:H:38:GLU:CD	2.22	0.41
7:J:17:DT:H2"	7:J:18:DG:C8	2.55	0.41
3:C:33:ARG:HH21	7:J:30:DG:P	2.43	0.41
2:F:45:ARG:NE	7:J:81:DC:H4'	2.35	0.41
6:I:97:DA:H2'	6:I:98:DA:C8	2.56	0.41
3:G:35:LEU:HD12	3:G:35:LEU:HA	1.92	0.41
6:I:67:DG:N2	7:J:81:DC:O2	2.51	0.41
3:C:49:PRO:O	3:C:53:THR:OG1	2.25	0.41
2:F:35:ARG:NH2	7:J:82:DG:OP2	2.53	0.41
1:A:61:LEU:HD12	2:B:37:LEU:HD23	2.01	0.41
4:H:47:VAL:O	4:H:50:GLN:HG2	2.20	0.41
7:J:70:DG:H2"	7:J:71:DA:C8	2.56	0.41
1:A:101:VAL:HG11	3:G:108:VAL:HG21	2.02	0.41
3:C:42:GLN:HB3	4:D:90:SER:HB2	2.03	0.41
6:I:36:DC:H2'	6:I:37:DG:C8	2.54	0.41
4:H:101:VAL:HG13	4:H:105:LEU:HD12	2.03	0.41
6:I:76:DG:O6	7:J:71:DA:N6	2.53	0.41
6:I:95:DC:H2'	6:I:96:DC:C6	2.56	0.41
4:H:77:ALA:O	4:H:81:SER:OG	2.31	0.40
1:A:63:ARG:HH21	7:J:61:DA:P	2.45	0.40
6:I:79:DC:H2"	6:I:80:DC:C5	2.56	0.40
3:G:58:TYR:CE1	5:L:29:ARG:HD2	2.56	0.40
7:J:36:DA:H2"	7:J:37:DG:C8	2.55	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	96/135 (71%)	93 (97%)	3 (3%)	0	100	100
1	E	94/135 (70%)	89 (95%)	5 (5%)	0	100	100
2	B	87/102 (85%)	84 (97%)	3 (3%)	0	100	100
2	F	89/102 (87%)	85 (96%)	4 (4%)	0	100	100
3	C	103/131 (79%)	101 (98%)	2 (2%)	0	100	100
3	G	104/131 (79%)	103 (99%)	1 (1%)	0	100	100
4	D	93/130 (72%)	92 (99%)	1 (1%)	0	100	100
4	H	90/130 (69%)	88 (98%)	2 (2%)	0	100	100
5	K	198/382 (52%)	185 (93%)	13 (7%)	0	100	100
5	L	207/382 (54%)	191 (92%)	15 (7%)	1 (0%)	29	64
All	All	1161/1760 (66%)	1111 (96%)	49 (4%)	1 (0%)	51	83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	L	22	VAL

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	86/112 (77%)	85 (99%)	1 (1%)	71	88
1	E	84/112 (75%)	84 (100%)	0	100	100
2	B	74/80 (92%)	74 (100%)	0	100	100
2	F	75/80 (94%)	75 (100%)	0	100	100
3	C	83/98 (85%)	83 (100%)	0	100	100
3	G	85/98 (87%)	85 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	83/109 (76%)	83 (100%)	0	100	100
4	H	80/109 (73%)	80 (100%)	0	100	100
5	K	195/355 (55%)	195 (100%)	0	100	100
5	L	198/355 (56%)	198 (100%)	0	100	100
All	All	1043/1508 (69%)	1042 (100%)	1 (0%)	93	98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
4	H	112	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	98/135 (72%)	0.68	8 (8%) 11 4	27, 51, 97, 123	0
1	E	96/135 (71%)	0.65	5 (5%) 27 12	29, 49, 94, 115	0
2	B	89/102 (87%)	0.83	7 (7%) 12 5	23, 41, 73, 87	0
2	F	91/102 (89%)	0.73	9 (9%) 7 2	20, 41, 75, 87	0
3	C	105/131 (80%)	0.22	1 (0%) 82 67	22, 40, 73, 105	0
3	G	106/131 (80%)	0.34	3 (2%) 53 30	21, 40, 78, 144	0
4	D	95/130 (73%)	0.23	4 (4%) 36 18	19, 38, 76, 91	0
4	H	92/130 (70%)	0.19	2 (2%) 62 41	18, 37, 69, 75	0
5	K	205/382 (53%)	-0.16	0 100 100	28, 60, 111, 124	0
5	L	211/382 (55%)	-0.12	1 (0%) 91 81	27, 57, 127, 147	0
6	I	146/147 (99%)	-0.50	1 (0%) 87 75	70, 119, 163, 171	0
7	J	146/147 (99%)	-0.51	0 100 100	70, 118, 161, 168	0
All	All	1480/2054 (72%)	0.11	41 (2%) 53 30	18, 54, 134, 171	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	102	GLY	9.1
2	F	17	ARG	4.5
1	E	60	LEU	4.5
3	G	121	SER	4.0
5	L	20	GLY	3.7
2	B	46	ILE	3.7
1	E	59	GLU	3.7
1	A	40	ARG	3.7
2	F	29	ILE	3.4
1	A	38	PRO	3.3
1	A	61	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
2	F	98	TYR	2.9
2	F	30	THR	2.9
2	B	51	TYR	2.9
1	A	62	ILE	2.8
2	F	46	ILE	2.7
2	B	31	LYS	2.7
2	F	44	LYS	2.7
2	B	101	GLY	2.7
4	D	68	PHE	2.6
4	D	92	ILE	2.6
3	G	98	LEU	2.6
3	C	88	ILE	2.5
2	F	97	LEU	2.5
1	A	54	PHE	2.4
4	H	64	ILE	2.4
3	G	116	LEU	2.4
2	F	102	GLY	2.4
4	H	65	LEU	2.4
1	A	53	ARG	2.3
2	B	43	VAL	2.3
2	B	37	LEU	2.2
4	D	57	ILE	2.2
6	I	96	DC	2.2
1	A	94	GLU	2.1
1	E	91	ALA	2.1
2	F	96	THR	2.1
4	D	65	LEU	2.1
1	E	100	LEU	2.1
1	E	106	ASP	2.1
1	A	118	THR	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 monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.