



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:59 AM UTC

PDB ID : 5AY8 / pdb_00005ay8
Title : Crystal structure of human nucleosome containing H3.Y
Authors : Kujirai, T.; Horikoshi, N.; Sato, K.; Maehara, K.; Machida, S.; Osakabe, A.;
Kimura, H.; Ohkawa, Y.; Kurumizaka, H.
Deposited on : 2015-08-10
Resolution : 2.80 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
Xtriage (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

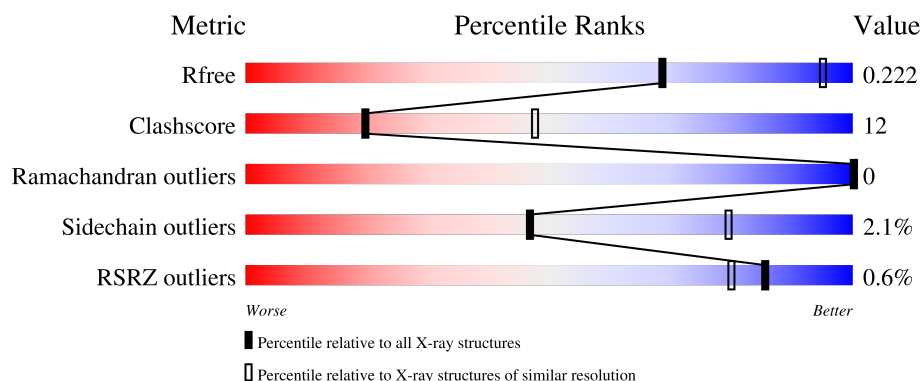
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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.



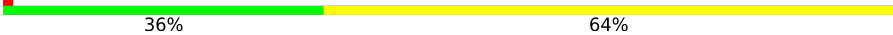
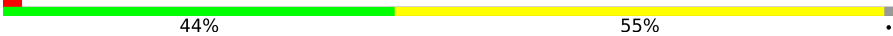
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	% 50% 18% • 30%
1	E	139	54% 13% •• 31%
2	B	106	% 66% 8% 26%
2	F	106	60% 14% 25%
3	C	133	62% 14% • 21%

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Mol	Chain	Length	Quality of chain
3	G	133	 58% 20% 22%
4	D	129	 53% 19% 29%
4	H	129	 57% 13% 29%
5	I	146	 36% 64% .
5	J	146	 44% 55% .

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 11843 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 H3.Y.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	97	Total	C	N	O	S	0	0	0
			794	500	156	135	3			
1	E	96	Total	C	N	O	S	0	0	0
			790	498	155	134	3			

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	78	Total	C	N	O	S	0	0	0
			619	391	120	107	1			
2	F	79	Total	C	N	O	S	0	0	0
			627	395	121	110	1			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP P62805
B	-2	SER	-	expression tag	UNP P62805
B	-1	HIS	-	expression tag	UNP P62805
F	-3	GLY	-	expression tag	UNP P62805
F	-2	SER	-	expression tag	UNP P62805
F	-1	HIS	-	expression tag	UNP P62805

- Molecule 3 is a protein called Histone H2A type 1-B/E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	105	Total	C	N	O	0	0	0
			810	511	158	141			
3	G	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
4	D	92	Total	C	N	O	S	0	0	0
			719	453	129	135	2			
4	H	92	Total	C	N	O	S	0	0	0
			719	453	129	135	2			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-3	GLY	-	expression tag	UNP P06899
D	-2	SER	-	expression tag	UNP P06899
D	-1	HIS	-	expression tag	UNP P06899
H	-3	GLY	-	expression tag	UNP P06899
H	-2	SER	-	expression tag	UNP P06899
H	-1	HIS	-	expression tag	UNP P06899

- Molecule 5 is a DNA chain called DNA (146-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	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
			2972	1421	535	871	145			

- Molecule 6 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mn	0	0
			1	1		
6	G	1	Total	Mn	0	0
			1	1		
6	I	2	Total	Mn	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	J	4	Total 4	Mn 4	0	0

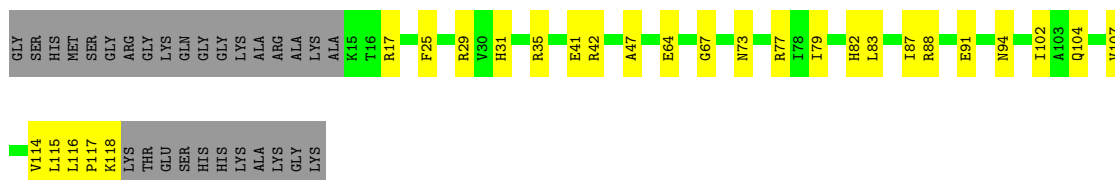
- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	J	2	Total 2	Cl 2	0	0

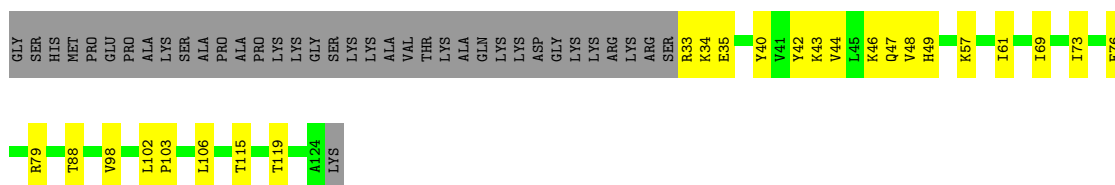
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	1	Total 1	O 1	0	0
8	E	1	Total 1	O 1	0	0
8	G	2	Total 2	O 2	0	0
8	J	4	Total 4	O 4	0	0

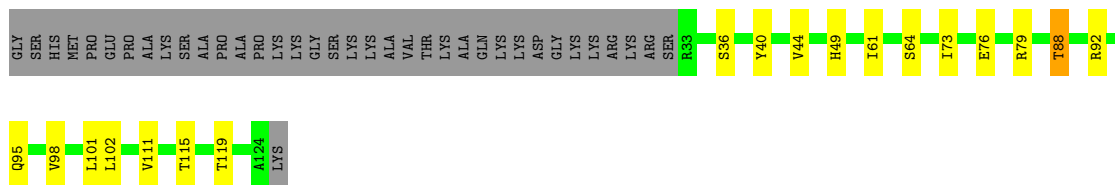
- Molecule 3: Histone H2A type 1-B/E



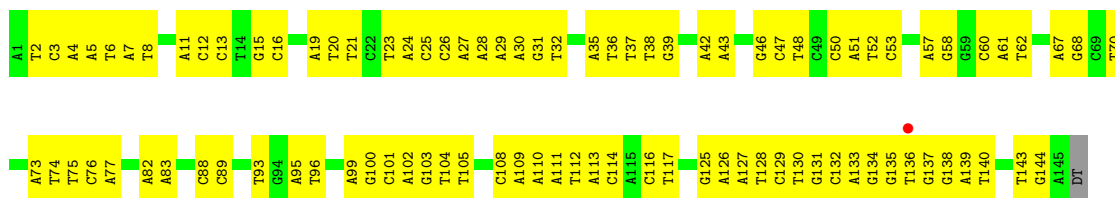
- Molecule 4: Histone H2B type 1-J



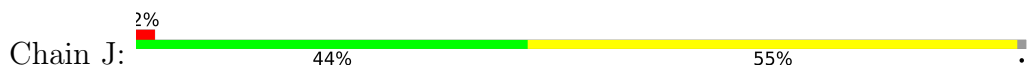
- Molecule 4: Histone H2B type 1-J

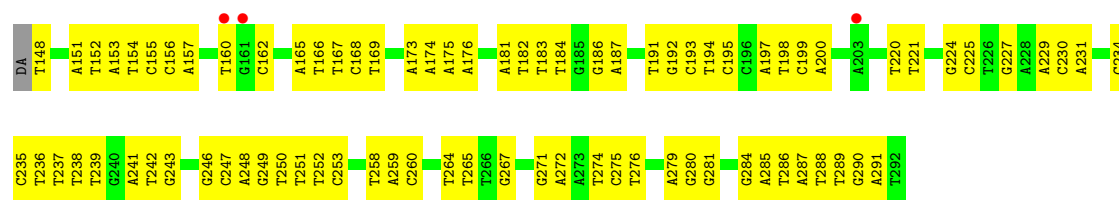


- Molecule 5: DNA (146-MER)



- Molecule 5: DNA (146-MER)





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	101.52Å 101.92Å 175.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.95 – 2.80 48.95 – 2.80	Depositor EDS
% Data completeness (in resolution range)	95.6 (48.95-2.80) 95.4 (48.95-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.201 , 0.249 (Not available) , 0.222	Depositor DCC
R_{free} test set	2196 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	56.3	Xtriage
Anisotropy	0.281	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 47.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.034 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11843	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% 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 ⓘ

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	0.78	0/806	1.04	0/1082
1	E	0.74	0/802	1.05	3/1077 (0.3%)
2	B	0.75	0/626	0.96	2/837 (0.2%)
2	F	0.76	0/634	1.10	3/848 (0.4%)
3	C	0.71	0/820	1.04	2/1107 (0.2%)
3	G	0.77	0/815	1.02	3/1100 (0.3%)
4	D	0.72	0/730	0.99	0/982
4	H	0.71	0/730	0.93	0/982
5	I	0.43	0/3332	0.64	0/5141
5	J	0.45	0/3333	0.67	0/5142
All	All	0.60	0/12628	0.83	13/18298 (0.1%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	31	LYS	CA-C-N	-8.68	110.80	119.56
2	F	31	LYS	C-N-CA	-8.68	110.80	119.56
3	C	73	ASN	N-CA-C	-8.20	102.32	113.30
2	B	31	LYS	CA-C-N	-7.33	112.16	119.56
2	B	31	LYS	C-N-CA	-7.33	112.16	119.56
1	E	117	VAL	N-CA-C	-6.08	107.57	113.53
2	F	46	ILE	N-CA-C	5.82	116.39	107.77
3	G	47	ALA	CA-C-N	-5.72	113.13	119.19
3	G	47	ALA	C-N-CA	-5.72	113.13	119.19
1	E	132	ARG	CA-CB-CG	5.69	125.48	114.10
1	E	102	GLN	N-CA-C	-5.65	106.39	113.28
3	G	73	ASN	N-CA-C	-5.55	105.72	112.88
3	C	114	VAL	CB-CA-C	-5.43	104.12	112.05

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	794	0	837	22	0
1	E	790	0	834	17	0
2	B	619	0	659	7	0
2	F	627	0	663	11	0
3	C	810	0	866	17	0
3	G	805	0	861	20	0
4	D	719	0	740	16	0
4	H	719	0	740	16	0
5	I	2970	0	1640	85	0
5	J	2972	0	1640	80	0
6	A	1	0	0	0	0
6	G	1	0	0	0	0
6	I	2	0	0	0	0
6	J	4	0	0	0	0
7	J	2	0	0	1	0
8	D	1	0	0	0	0
8	E	1	0	0	0	0
8	G	2	0	0	1	0
8	J	4	0	0	0	0
All	All	11843	0	9480	236	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 12.

All (236) 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:271:DG:H2''	5:J:272:DA:H5''	1.41	1.00
5:I:93:DT:H3	5:J:200:DA:H61	1.28	0.80
5:J:274:DT:H2''	5:J:275:DC:H5''	1.63	0.80
5:J:280:DG:H2''	5:J:281:DG:H5''	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:2:DT:H2''	5:I:3:DC:H5''	1.61	0.80
5:J:152:DT:H2''	5:J:153:DA:H5''	1.63	0.79
5:I:62:DT:O4	5:J:231:DA:N6	2.16	0.77
3:G:17:ARG:HH12	3:G:31:HIS:HD2	1.31	0.76
5:J:279:DA:H2''	5:J:280:DG:H5''	1.66	0.75
5:J:192:DG:H2''	5:J:193:DC:H5''	1.67	0.75
3:G:102:ILE:HG23	4:H:61:ILE:HD13	1.69	0.74
5:I:131:DG:N2	5:J:162:DC:O2	2.20	0.74
1:A:73:GLU:OE2	2:B:25:ASN:ND2	2.20	0.74
5:I:26:DC:N3	5:J:267:DG:N2	2.35	0.74
4:H:88:THR:OG1	5:J:186:DG:OP1	2.08	0.70
5:I:50:DC:H42	5:J:243:DG:H1	1.38	0.70
5:I:128:DT:H5''	5:I:128:DT:H6	1.56	0.70
5:J:182:DT:H2''	5:J:183:DT:H5''	1.75	0.68
1:E:61:LEU:HD12	2:F:37:LEU:HD23	1.76	0.68
5:J:191:DT:H2''	5:J:192:DG:C8	2.28	0.68
5:I:52:DT:H2''	5:I:53:DC:H5'	1.76	0.67
5:J:181:DA:H2''	5:J:182:DT:H5''	1.76	0.67
5:I:133:DA:H2''	5:I:134:DG:H5''	1.77	0.67
5:I:134:DG:H2''	5:I:135:DG:H5'	1.76	0.67
5:I:125:DG:H2''	5:I:126:DA:C8	2.30	0.66
5:J:197:DA:H2''	5:J:198:DT:H5''	1.78	0.65
1:A:115:ARG:HH21	1:E:122:ARG:HH21	1.43	0.65
3:G:91:GLU:OE2	8:G:301:HOH:O	2.13	0.65
5:I:108:DC:H2''	5:I:109:DA:C8	2.31	0.65
1:E:100:LEU:HD11	2:F:58:LEU:HD13	1.79	0.65
4:D:76:GLU:OE2	4:D:79:ARG:NH1	2.29	0.65
5:J:220:DT:H1'	5:J:221:DT:H5'	1.77	0.65
3:C:73:ASN:OD1	3:C:75:LYS:NZ	2.30	0.64
5:I:128:DT:H2''	5:I:129:DC:H5''	1.79	0.64
5:I:143:DT:H2''	5:I:144:DG:C8	2.32	0.63
5:I:36:DT:H2''	5:I:37:DT:H5''	1.81	0.63
3:G:88:ARG:NH1	3:G:94:ASN:OD1	2.26	0.63
5:I:47:DC:H2''	5:I:48:DT:C6	2.34	0.62
1:A:108:ASN:O	1:A:112:ILE:HG12	2.00	0.62
3:G:117:PRO:O	3:G:118:LYS:HB2	1.98	0.62
3:G:79:ILE:HG12	3:G:82:HIS:CE1	2.35	0.61
5:I:46:DG:H2''	5:I:47:DC:H5''	1.82	0.61
5:J:250:DT:H2''	5:J:251:DT:H5''	1.81	0.61
3:C:67:GLY:HA3	4:D:49:HIS:CD2	2.36	0.60
3:C:32:ARG:NH2	4:D:35:GLU:OE2	2.25	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:98:VAL:HG13	4:D:102:LEU:HD22	1.84	0.59
5:J:191:DT:H2''	5:J:192:DG:N7	2.18	0.58
1:E:108:ASN:O	1:E:112:ILE:HG12	2.03	0.58
5:I:129:DC:H2''	5:I:130:DT:C5	2.39	0.58
4:H:95:GLN:OE1	4:H:111:VAL:HG13	2.02	0.58
5:I:73:DA:H2''	5:I:74:DT:H71	1.86	0.57
5:I:74:DT:H1'	5:I:75:DT:H5'	1.85	0.57
5:I:19:DA:H1'	5:I:20:DT:H5'	1.86	0.57
5:J:165:DA:H1'	5:J:166:DT:H5'	1.85	0.57
5:J:284:DG:H2''	5:J:285:DA:H5''	1.86	0.57
5:I:12:DC:H2''	5:I:13:DC:H5'	1.87	0.57
3:C:32:ARG:HD3	5:I:29:DA:OP2	2.05	0.56
5:J:259:DA:H2''	5:J:260:DC:H5''	1.87	0.56
5:I:7:DA:H1'	5:I:8:DT:H5'	1.87	0.56
4:H:73:ILE:HD12	4:H:98:VAL:HG22	1.87	0.56
5:I:68:DG:N2	5:J:225:DC:O2	2.34	0.56
5:J:290:DG:N7	7:J:305:CL:CL	2.76	0.56
1:A:127:ALA:O	1:A:131:ARG:HG3	2.06	0.55
5:I:132:DC:N4	5:J:160:DT:O4	2.39	0.55
3:G:77:ARG:HB3	5:I:131:DG:OP1	2.06	0.55
5:I:136:DT:H1'	5:I:137:DG:N7	2.22	0.55
5:I:23:DT:H2''	5:I:24:DA:C8	2.42	0.55
1:E:131:ARG:O	1:E:132:ARG:HB2	2.06	0.55
5:J:173:DA:H2''	5:J:174:DA:C8	2.42	0.55
5:J:156:DC:H1'	5:J:157:DA:H5'	1.88	0.54
5:J:194:DT:H2''	5:J:195:DC:H5'	1.89	0.54
5:J:151:DA:H2''	5:J:152:DT:H5''	1.89	0.54
2:B:44:LYS:HD2	3:G:115:LEU:HB3	1.88	0.54
4:H:76:GLU:OE1	4:H:79:ARG:NH1	2.41	0.54
4:H:98:VAL:HG13	4:H:102:LEU:HD22	1.90	0.53
4:H:115:THR:O	4:H:119:THR:HG22	2.09	0.53
5:J:168:DC:H1'	5:J:169:DT:H5''	1.91	0.53
3:C:79:ILE:HG12	3:C:82:HIS:CE1	2.43	0.53
5:I:20:DT:H1'	5:I:21:DT:H5''	1.90	0.53
5:I:113:DA:H2''	5:I:114:DC:H5''	1.88	0.53
1:E:40:ARG:HG3	5:I:83:DA:H5''	1.91	0.53
3:G:67:GLY:HA3	4:H:49:HIS:CD2	2.44	0.53
5:I:112:DT:H1'	5:I:113:DA:H5'	1.91	0.53
5:J:235:DC:H2''	5:J:236:DT:C5	2.43	0.53
5:J:275:DC:H2''	5:J:276:DT:H5'	1.90	0.53
4:D:69:ILE:O	4:D:73:ILE:HG12	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:88:THR:HG22	5:I:39:DG:OP1	2.09	0.52
5:J:175:DA:H2''	5:J:176:DA:C8	2.44	0.52
2:F:30:THR:HB	2:F:32:PRO:HD2	1.92	0.52
5:J:192:DG:C2'	5:J:193:DC:H5''	2.39	0.52
1:A:118:THR:OG1	5:I:70:DT:OP1	2.26	0.52
5:J:241:DA:H1'	5:J:242:DT:H5'	1.92	0.52
5:I:35:DA:H2''	5:I:36:DT:H5''	1.92	0.52
1:A:60:LEU:HD12	1:A:64:LYS:HE3	1.91	0.51
5:I:38:DT:H2''	5:I:39:DG:C8	2.45	0.51
5:I:31:DG:H2''	5:I:32:DT:H5'	1.91	0.51
5:I:60:DC:H2''	5:I:61:DA:C8	2.45	0.51
5:I:6:DT:H2''	5:I:7:DA:C8	2.45	0.51
4:H:40:TYR:O	4:H:44:VAL:HG23	2.10	0.51
5:J:258:DT:H1'	5:J:259:DA:H5'	1.92	0.51
3:G:17:ARG:HH12	3:G:31:HIS:CD2	2.20	0.51
4:D:103:PRO:HG2	4:D:106:LEU:HD12	1.92	0.51
5:J:224:DG:H1'	5:J:225:DC:H5'	1.93	0.51
3:G:41:GLU:HG3	3:G:42:ARG:HG3	1.93	0.51
5:J:183:DT:H2''	5:J:184:DT:H5'	1.93	0.50
5:J:162:DC:H5'	5:J:162:DC:C6	2.46	0.50
5:J:197:DA:C2'	5:J:198:DT:H5''	2.41	0.50
5:I:105:DT:O4	5:J:187:DA:N6	2.45	0.50
5:I:131:DG:H2''	5:I:132:DC:C6	2.47	0.50
5:I:99:DA:H2''	5:I:100:DG:C8	2.46	0.50
3:G:31:HIS:CE1	3:G:35:ARG:HD3	2.46	0.50
5:I:42:DA:H1'	5:I:43:DA:H5'	1.93	0.50
5:J:252:DT:H2''	5:J:253:DC:C6	2.47	0.50
1:A:46:LEU:HB3	5:J:229:DA:P	2.52	0.50
3:C:74:LYS:NZ	5:I:11:DA:OP2	2.40	0.50
5:I:2:DT:H2''	5:I:3:DC:C5'	2.38	0.49
5:J:194:DT:C2'	5:J:195:DC:H5'	2.43	0.49
5:J:152:DT:H2''	5:J:153:DA:C5'	2.39	0.49
2:B:45:ARG:CZ	5:J:227:DG:H4'	2.43	0.48
3:G:42:ARG:HB2	4:H:88:THR:CG2	2.44	0.48
5:I:108:DC:H2''	5:I:109:DA:N7	2.28	0.48
3:C:87:ILE:HD12	3:C:97:LEU:HD12	1.96	0.48
5:J:275:DC:H2'	5:J:276:DT:H71	1.96	0.48
5:J:271:DG:H2''	5:J:272:DA:C5'	2.28	0.47
5:I:26:DC:H42	5:J:267:DG:H1	1.59	0.47
5:I:15:DG:H1'	5:I:16:DC:H5''	1.96	0.47
5:J:182:DT:H2''	5:J:183:DT:C6	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:274:DT:C2'	5:J:275:DC:H5''	2.41	0.47
1:A:43:PRO:HG2	5:I:68:DG:H5'	1.97	0.47
5:I:101:DC:H2'	5:I:102:DA:C8	2.50	0.47
3:C:43:VAL:N	5:J:259:DA:OP1	2.32	0.47
5:J:238:DT:H1'	5:J:239:DT:H5'	1.96	0.47
5:J:289:DT:H2''	5:J:290:DG:C8	2.49	0.47
3:C:32:ARG:HH22	4:D:35:GLU:CD	2.19	0.47
5:I:127:DA:H2''	5:I:128:DT:OP2	2.14	0.47
3:G:29:ARG:NH1	4:H:36:SER:O	2.47	0.47
1:A:60:LEU:HD13	1:A:93:GLN:NE2	2.31	0.46
1:A:100:LEU:HD11	2:B:58:LEU:HD13	1.97	0.46
3:C:24:GLN:N	3:C:56:GLU:OE1	2.40	0.46
3:C:26:PRO:HG3	4:D:40:TYR:CE2	2.51	0.46
5:I:67:DA:N6	5:J:225:DC:N3	2.64	0.46
5:J:246:DG:H2''	5:J:247:DC:H5''	1.98	0.46
1:A:68:GLN:HG3	1:A:89:ILE:CD1	2.44	0.46
2:F:35:ARG:O	2:F:39:ARG:HG2	2.16	0.46
5:J:271:DG:C2'	5:J:272:DA:H5''	2.28	0.46
1:A:61:LEU:H	1:A:97:GLU:CD	2.24	0.46
2:F:70:VAL:O	2:F:74:GLU:HG3	2.15	0.46
5:I:116:DC:H1'	5:I:117:DT:H5'	1.97	0.46
5:J:247:DC:H2''	5:J:248:DA:C8	2.50	0.46
5:J:166:DT:H1'	5:J:167:DT:H5''	1.98	0.46
3:C:42:ARG:HG3	4:D:88:THR:HB	1.98	0.45
5:I:104:DT:H2''	5:I:105:DT:H5''	1.98	0.45
3:G:83:LEU:O	3:G:87:ILE:HG12	2.16	0.45
1:E:97:GLU:O	1:E:101:VAL:HG23	2.16	0.45
5:J:252:DT:H72	5:J:253:DC:N4	2.30	0.45
1:E:39:HIS:CE1	5:J:291:DA:H5'	2.51	0.45
5:I:5:DA:H2''	5:I:6:DT:H5''	1.97	0.45
5:I:6:DT:H2''	5:I:7:DA:H8	1.80	0.45
5:I:101:DC:H5''	5:I:101:DC:H6	1.82	0.45
5:J:148:DT:O4'	5:J:148:DT:P	2.74	0.45
5:J:153:DA:H1'	5:J:154:DT:H5'	1.99	0.45
5:I:57:DA:H2''	5:I:58:DG:C8	2.51	0.44
5:I:76:DC:H2''	5:I:77:DA:N7	2.33	0.44
5:J:285:DA:H2''	5:J:286:DT:H5'	1.99	0.44
4:D:115:THR:O	4:D:119:THR:HG23	2.17	0.44
1:E:62:LEU:HD22	2:F:29:ILE:HG23	2.00	0.44
5:I:88:DC:H2''	5:I:89:DC:C6	2.52	0.44
5:I:128:DT:H5''	5:I:128:DT:C6	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:100:VAL:HG11	2:F:98:TYR:CE2	2.51	0.44
1:E:50:GLU:HB2	2:F:39:ARG:HD2	2.00	0.44
5:J:250:DT:H6	5:J:250:DT:H2'	1.67	0.44
1:A:94:GLU:OE2	3:G:104:GLN:NE2	2.37	0.43
3:C:30:VAL:HG21	3:C:52:ALA:HB2	1.99	0.43
5:I:3:DC:H2''	5:I:4:DA:C8	2.53	0.43
5:J:151:DA:C2'	5:J:152:DT:H5''	2.48	0.43
5:J:264:DT:H1'	5:J:265:DT:H5'	2.00	0.43
5:I:38:DT:H2''	5:I:39:DG:N7	2.33	0.43
1:A:69:ARG:HH22	5:J:237:DT:P	2.41	0.43
2:B:98:TYR:CD1	4:H:64:SER:HB3	2.53	0.43
3:G:88:ARG:HA	3:G:88:ARG:HD3	1.87	0.43
5:I:52:DT:C2'	5:I:53:DC:H5'	2.47	0.43
5:I:95:DA:H2''	5:I:96:DT:OP2	2.17	0.43
5:I:136:DT:H1'	5:I:137:DG:C8	2.54	0.43
5:I:27:DA:H2''	5:I:28:DA:C8	2.52	0.43
1:A:61:LEU:HD12	2:B:37:LEU:HD23	2.01	0.43
3:C:115:LEU:CD2	1:E:117:VAL:HG22	2.48	0.43
4:D:34:LYS:O	4:D:34:LYS:HG3	2.17	0.43
5:I:25:DC:H2''	5:I:26:DC:C6	2.53	0.43
5:I:29:DA:H2''	5:I:30:DA:C8	2.54	0.43
5:I:134:DG:C2'	5:I:135:DG:H5'	2.45	0.43
3:C:81:ARG:HD3	1:E:58:THR:CG2	2.49	0.42
5:I:67:DA:H2''	5:I:68:DG:C8	2.54	0.42
5:J:198:DT:H2''	5:J:199:DC:H5'	2.01	0.42
5:J:280:DG:C2'	5:J:281:DG:H5'	2.41	0.42
3:G:42:ARG:HB2	4:H:88:THR:HG23	2.01	0.42
1:A:46:LEU:HD12	1:A:46:LEU:HA	1.80	0.42
1:E:131:ARG:NH1	1:E:133:GLU:OE2	2.53	0.42
5:I:139:DA:H1'	5:I:140:DT:H5'	2.02	0.42
5:J:229:DA:H1'	5:J:230:DC:H5'	2.01	0.42
5:I:51:DA:H2''	5:I:52:DT:H5''	2.01	0.42
5:J:193:DC:H2''	5:J:194:DT:C5	2.55	0.42
1:A:60:LEU:HD22	1:A:93:GLN:HG2	2.01	0.42
1:A:120:MET:O	1:A:123:ASP:HB2	2.20	0.42
5:J:220:DT:H6	5:J:220:DT:H2'	1.71	0.42
5:I:110:DA:H2''	5:I:111:DA:C8	2.54	0.42
1:A:126:LEU:HD22	1:E:113:HIS:CG	2.54	0.42
1:E:43:PRO:HA	5:I:82:DA:H5'	2.02	0.42
1:E:124:MET:HE3	2:F:57:VAL:HG21	2.00	0.42
5:I:102:DA:H2''	5:I:103:DG:C8	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:99:DA:C6	5:I:100:DG:C2	3.08	0.41
2:F:92:ARG:NH1	4:H:101:LEU:HD23	2.34	0.41
3:G:25:PHE:HE1	4:H:44:VAL:HG21	1.85	0.41
5:I:138:DG:C2	5:I:139:DA:C4	3.08	0.41
4:D:57:LYS:O	4:D:61:ILE:HG12	2.20	0.41
5:J:234:DC:H2''	5:J:235:DC:C6	2.55	0.41
3:C:31:HIS:CD2	3:C:48:PRO:HG3	2.56	0.41
5:I:5:DA:C2'	5:I:6:DT:H5''	2.50	0.41
5:J:248:DA:H2''	5:J:249:DG:C8	2.55	0.41
4:D:44:VAL:O	4:D:48:VAL:HG22	2.20	0.41
2:F:75:HIS:O	4:H:92:ARG:NH2	2.54	0.41
1:A:65:LEU:HB3	1:A:66:PRO:HD3	2.03	0.41
4:D:42:TYR:CE2	4:D:46:LYS:HE3	2.56	0.41
4:D:43:LYS:O	4:D:47:GLN:HG3	2.19	0.41
5:I:111:DA:C4	5:I:112:DT:H72	2.56	0.41
5:I:116:DC:H6	5:I:116:DC:H2'	1.76	0.41
5:J:162:DC:H6	5:J:162:DC:H2'	1.65	0.41
5:I:46:DG:H2''	5:I:47:DC:C6	2.56	0.41
1:A:78:ILE:HD13	2:B:67:ARG:HA	2.02	0.40
3:G:116:LEU:HD23	3:G:116:LEU:HA	1.79	0.40
1:E:40:ARG:O	5:J:290:DG:H5''	2.22	0.40
5:I:6:DT:H5'	5:I:6:DT:H6	1.86	0.40
5:I:36:DT:H2''	5:I:37:DT:C6	2.57	0.40
5:J:154:DT:H2''	5:J:155:DC:C6	2.56	0.40
5:J:287:DA:H1'	5:J:288:DT:H5'	2.03	0.40
5:J:275:DC:C2'	5:J:276:DT:H5'	2.52	0.40
1:A:124:MET:HE2	1:A:124:MET:HB3	1.62	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	94/139 (68%)	92 (98%)	2 (2%)	0	100	100
2	B	76/106 (72%)	74 (97%)	2 (3%)	0	100	100
2	F	77/106 (73%)	76 (99%)	1 (1%)	0	100	100
3	C	103/133 (77%)	101 (98%)	2 (2%)	0	100	100
3	G	102/133 (77%)	99 (97%)	3 (3%)	0	100	100
4	D	90/129 (70%)	88 (98%)	2 (2%)	0	100	100
4	H	90/129 (70%)	88 (98%)	2 (2%)	0	100	100
All	All	727/1014 (72%)	711 (98%)	16 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	83/112 (74%)	80 (96%)	3 (4%)	31	66
1	E	83/112 (74%)	80 (96%)	3 (4%)	31	66
2	B	63/81 (78%)	63 (100%)	0	100	100
2	F	64/81 (79%)	64 (100%)	0	100	100
3	C	83/102 (81%)	81 (98%)	2 (2%)	43	77
3	G	83/102 (81%)	80 (96%)	3 (4%)	31	66
4	D	78/107 (73%)	77 (99%)	1 (1%)	61	86
4	H	78/107 (73%)	77 (99%)	1 (1%)	61	86
All	All	615/804 (76%)	602 (98%)	13 (2%)	47	79

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	ILE
1	A	117	VAL

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Mol	Chain	Res	Type
1	A	124	MET
3	C	42	ARG
3	C	114	VAL
4	D	33	ARG
1	E	117	VAL
1	E	124	MET
1	E	130	LEU
3	G	64	GLU
3	G	107	VAL
3	G	114	VAL
4	H	88	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
3	G	73	ASN
4	H	82	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.49	1 (1%) 79 72	31, 40, 75, 87	0
1	E	96/139 (69%)	-0.56	0 100 100	31, 44, 68, 95	0
2	B	78/106 (73%)	-0.55	1 (1%) 75 66	32, 42, 57, 64	0
2	F	79/106 (74%)	-0.57	0 100 100	32, 42, 63, 84	0
3	C	105/133 (78%)	-0.46	0 100 100	32, 46, 67, 88	0
3	G	104/133 (78%)	-0.43	0 100 100	32, 44, 69, 93	0
4	D	92/129 (71%)	-0.46	0 100 100	34, 48, 64, 96	0
4	H	92/129 (71%)	-0.57	0 100 100	33, 44, 72, 90	0
5	I	145/146 (99%)	0.22	1 (0%) 84 77	53, 89, 124, 138	0
5	J	145/146 (99%)	0.11	3 (2%) 63 54	51, 90, 128, 145	0
All	All	1033/1306 (79%)	-0.32	6 (0%) 85 80	31, 50, 116, 145	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	38	PRO	2.9
2	B	102	GLY	2.8
5	J	161	DG	2.8
5	J	160	DT	2.6
5	J	203	DA	2.4
5	I	136	DT	2.2

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
6	MN	I	202	1/1	0.77	0.13	117,117,117,117	0
7	CL	J	305	1/1	0.87	0.12	72,72,72,72	0
6	MN	J	302	1/1	0.89	0.08	95,95,95,95	0
6	MN	A	201	1/1	0.92	0.20	77,77,77,77	0
6	MN	J	304	1/1	0.93	0.08	93,93,93,93	0
7	CL	J	306	1/1	0.94	0.13	75,75,75,75	0
6	MN	I	201	1/1	0.97	0.14	89,89,89,89	0
6	MN	G	201	1/1	0.97	0.05	78,78,78,78	0
6	MN	J	303	1/1	0.98	0.07	71,71,71,71	0
6	MN	J	301	1/1	0.98	0.13	78,78,78,78	0

6.5 Other polymers [i](#)

There are no such residues in this entry.