Full wwPDB X-ray Structure Validation Report ⓘ

Nov 13, 2023 – 03:39 PM JST

PDB ID	:	5XM1
Title	:	The mouse nucleosome structure containing H2A, H2B type3-A, H3mm7, and H4
Authors	:	Taguchi, H.; Horikoshi, N.; Kurumizaka, H.
Deposited on	:	2017-05-12
Resolution	:	3.45 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:

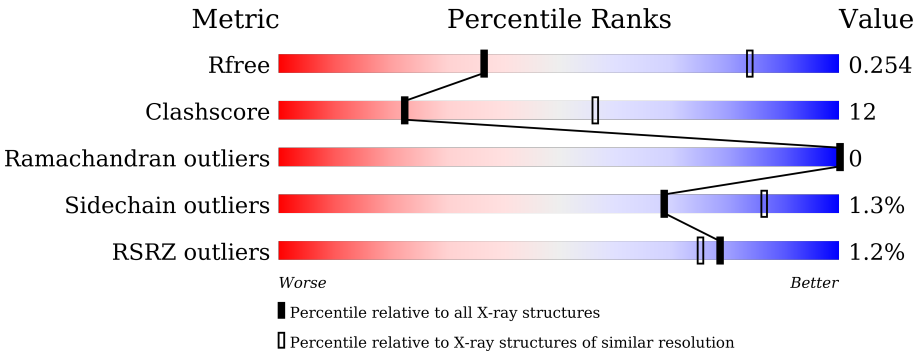
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 3.45 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	1291 (3.52-3.40)
Clashscore	141614	1372 (3.52-3.40)
Ramachandran outliers	138981	1337 (3.52-3.40)
Sidechain outliers	138945	1338 (3.52-3.40)
RSRZ outliers	127900	1205 (3.52-3.40)

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	139	63% 6% 30%
1	E	139	50% 19% 29%
2	B	106	60% 13% 26%
2	F	106	61% 17% 22%
3	C	133	61% 17% 21%
3	G	133	57% 20% 22%

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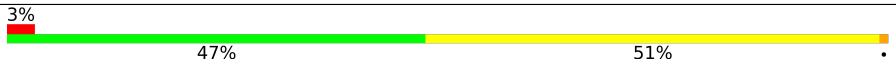
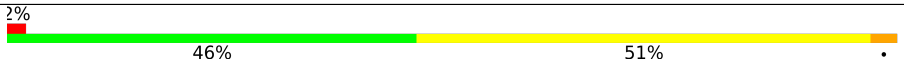
Mol	Chain	Length	Quality of chain
4	D	129	
4	H	129	
5	I	146	
5	J	146	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 11920 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 H3mm7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	97	Total	C	N	O	S	0	0	0
			796	503	155	136	2			
1	E	98	Total	C	N	O	S	0	0	0
			802	506	156	138	2			

- 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	83	Total	C	N	O	S	0	0	0
			662	418	129	114	1			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP P62806
B	-2	SER	-	expression tag	UNP P62806
B	-1	HIS	-	expression tag	UNP P62806
F	-3	GLY	-	expression tag	UNP P62806
F	-2	SER	-	expression tag	UNP P62806
F	-1	HIS	-	expression tag	UNP P62806

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

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 C0HKE1
C	-2	SER	-	expression tag	UNP C0HKE1
C	-1	HIS	-	expression tag	UNP C0HKE1
G	-3	GLY	-	expression tag	UNP C0HKE1
G	-2	SER	-	expression tag	UNP C0HKE1
G	-1	HIS	-	expression tag	UNP C0HKE1

- Molecule 4 is a protein called Histone H2B type 3-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	94	Total	C	N	O	S	0	0	0
			736	461	134	139	2			
4	H	91	Total	C	N	O	S	0	0	0
			710	447	125	136	2			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-3	GLY	-	expression tag	UNP Q9D2U9
D	-2	SER	-	expression tag	UNP Q9D2U9
D	-1	HIS	-	expression tag	UNP Q9D2U9
H	-3	GLY	-	expression tag	UNP Q9D2U9
H	-2	SER	-	expression tag	UNP Q9D2U9
H	-1	HIS	-	expression tag	UNP Q9D2U9

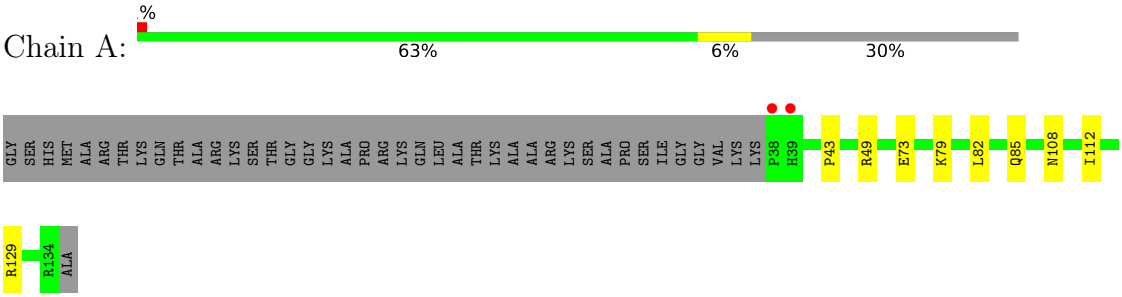
- Molecule 5 is a DNA chain called DNA (146-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	146	Total	C	N	O	P	0	0	0
			2990	1431	540	874	145			
5	J	146	Total	C	N	O	P	0	0	0
			2990	1431	540	874	145			

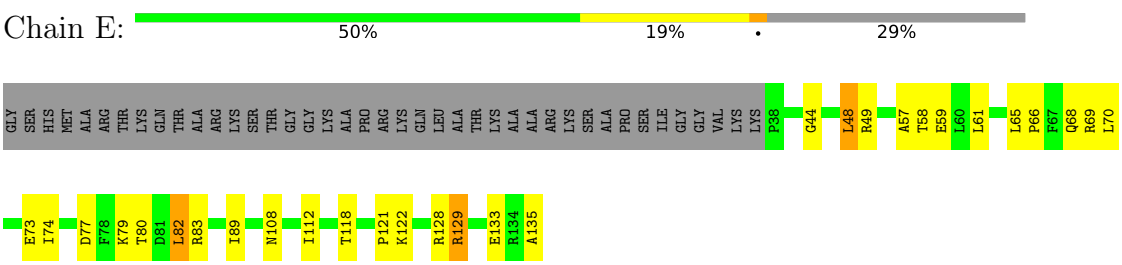
3 Residue-property plots (i)

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.

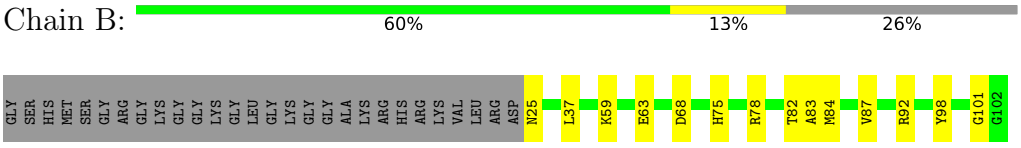
• Molecule 1: Histone H3mm7



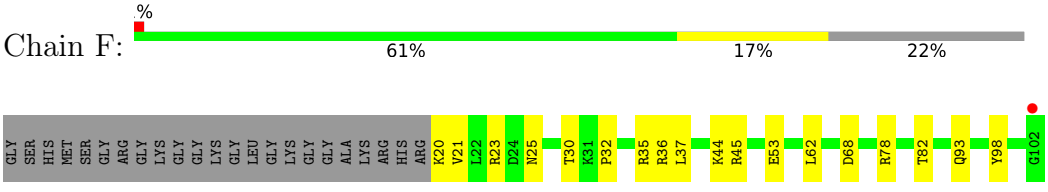
• Molecule 1: Histone H3mm7



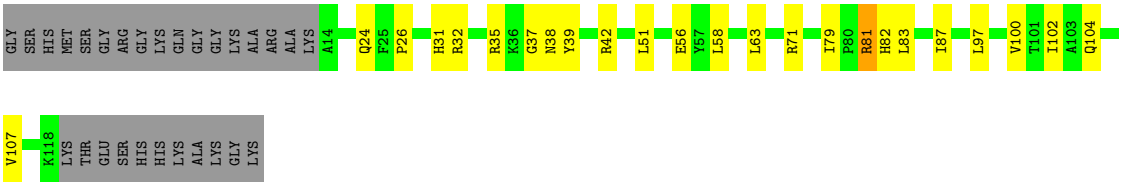
• Molecule 2: Histone H4



• Molecule 2: Histone H4



• Molecule 3: Histone H2A type 1-B

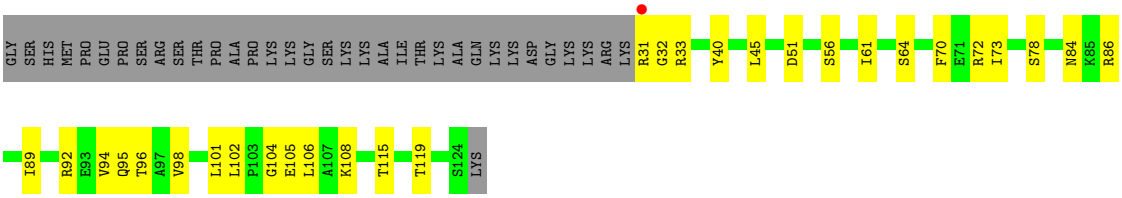


• Molecule 3: Histone H2A type 1-B

Chain G:

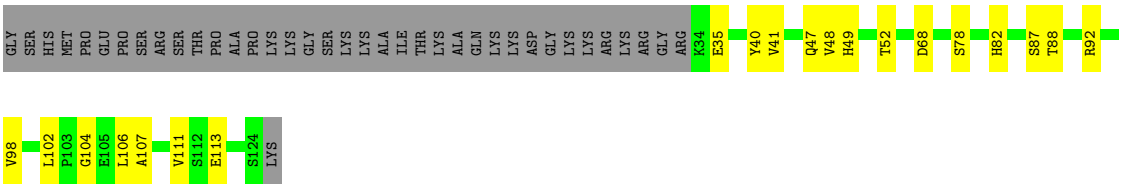
• Molecule 4: Histone H2B type 3-A

Chain D:



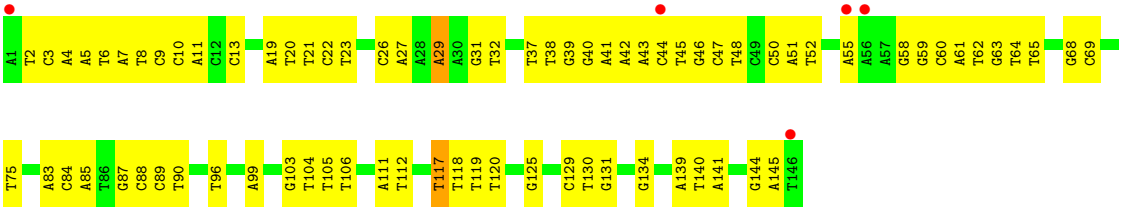
• Molecule 4: Histone H2B type 3-A

Chain H:



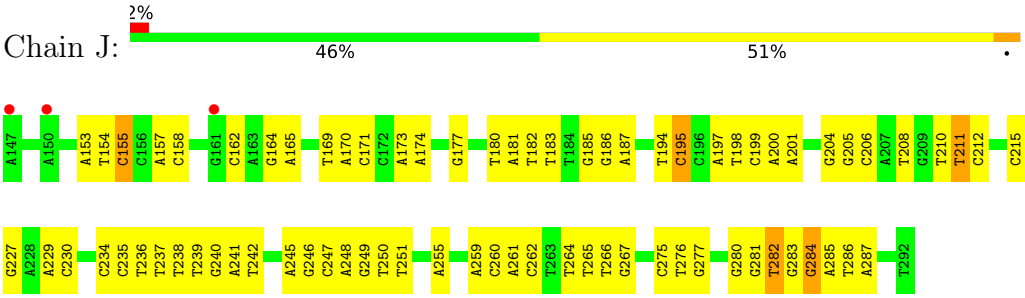
• Molecule 5: DNA (146-MER)

Chain I:



• Molecule 5: DNA (146-MER)

Chain J:


2%
46%
51%
A147 A150 A153 T154 C155 C156 A157 C158 G161 C162 A163 G164 A165 T169 A170 C171 C172 A173 A174 G177 T180 A181 T182 T183 T184 G185 G186 A187 T194 C195 C196 A197 T198 C199 A200 A201 G204 G205 C206 A207 T208 G209 T210 T211 C212 C215 T216 G224 C225 T226
G227 A228 A229 C230 C234 C235 T236 T237 T238 T239 G240 A241 T242 A245 G246 C247 A248 G249 T250 T251 A255 A259 C260 A261 C262 T263 T264 T265 T266 G267 C275 T276 G277 G280 G281 T282 G283 G284 A285 T286 A287 T292

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	105.55Å 109.38Å 176.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.88 – 3.45 34.87 – 3.36	Depositor EDS
% Data completeness (in resolution range)	96.5 (34.88-3.45) 93.5 (34.87-3.36)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.08 (at 3.39Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.200 , 0.254 0.200 , 0.254	Depositor DCC
R_{free} test set	1987 reflections (7.16%)	wwPDB-VP
Wilson B-factor (Å^2)	90.8	Xtriage
Anisotropy	0.688	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 54.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.027 for k,h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11920	wwPDB-VP
Average B, all atoms (Å^2)	112.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% 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 (i)

5.1 Standard geometry (i)

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	0/808	0.63	0/1084
1	E	0.68	1/814 (0.1%)	0.90	2/1091 (0.2%)
2	B	0.49	0/626	0.70	0/837
2	F	0.65	0/669	0.78	0/894
3	C	0.58	0/820	0.72	0/1107
3	G	0.49	0/815	0.74	1/1100 (0.1%)
4	D	0.59	0/747	0.75	0/1004
4	H	0.57	0/721	0.68	0/971
5	I	0.85	1/3354 (0.0%)	1.09	8/5175 (0.2%)
5	J	0.89	2/3354 (0.1%)	1.10	6/5175 (0.1%)
All	All	0.74	4/12728 (0.0%)	0.96	17/18438 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	77	ASP	CB-CG	9.05	1.70	1.51
5	J	195	DC	C3'-O3'	-5.71	1.36	1.44
5	I	89	DC	C3'-O3'	-5.14	1.37	1.44
5	J	284	DG	C3'-O3'	-5.10	1.37	1.44

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	77	ASP	CB-CG-OD1	10.73	127.96	118.30
5	J	162	DC	O4'-C4'-C3'	-7.98	101.21	106.00
5	I	83	DA	O5'-P-OP2	-7.96	98.54	105.70
1	E	82	LEU	CA-CB-CG	6.77	130.86	115.30
5	I	134	DG	O4'-C1'-N9	6.55	112.59	108.00
5	I	117	DT	N3-C4-O4	5.75	123.35	119.90
5	J	204	DG	O4'-C1'-N9	5.45	111.81	108.00
5	I	117	DT	C5-C4-O4	-5.44	121.09	124.90
5	J	155	DC	O5'-P-OP1	-5.40	100.84	105.70
5	J	282	DT	O4'-C1'-N1	5.36	111.75	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	116	LEU	CA-CB-CG	-5.35	103.00	115.30
5	J	211	DT	N3-C4-O4	5.33	123.10	119.90
5	I	75	DT	C5-C4-O4	-5.24	121.23	124.90
5	I	75	DT	N3-C4-O4	5.24	123.04	119.90
5	I	29	DA	O4'-C1'-N9	5.16	111.61	108.00
5	I	96	DT	N3-C4-O4	5.06	122.94	119.90
5	J	210	DT	OP2-P-O3'	5.01	116.22	105.20

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	796	0	835	6	0
1	E	802	0	840	25	0
2	B	619	0	659	15	0
2	F	662	0	709	15	1
3	C	810	0	866	24	1
3	G	805	0	861	24	0
4	D	736	0	756	24	0
4	H	710	0	727	21	0
5	I	2990	0	1652	79	0
5	J	2990	0	1652	71	0
All	All	11920	0	9557	237	1

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:125:DG:N2	5:J:169:DT:O2	2.03	0.91
5:I:55:DA:H61	5:J:238:DT:H3	1.18	0.87
1:E:121:PRO:HB3	2:F:53:GLU:HG3	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:30:THR:HB	2:F:32:PRO:HD2	1.63	0.80
5:I:11:DA:N6	5:J:282:DT:O4	2.16	0.79
5:I:20:DT:H2"	5:I:21:DT:H5"	1.66	0.77
3:C:32:ARG:NH1	5:I:29:DA:OP1	2.18	0.75
5:J:275:DC:H2"	5:J:276:DT:H5'	1.71	0.72
1:E:69:ARG:NH2	5:I:90:DT:OP2	2.23	0.71
5:I:19:DA:C2'	5:I:20:DT:H5"	2.21	0.71
3:C:83:LEU:O	3:C:87:ILE:HG12	1.91	0.71
5:I:42:DA:H2"	5:I:43:DA:H5'	1.73	0.70
2:B:68:ASP:OD2	2:B:92:ARG:NH1	2.24	0.70
3:G:93:LEU:HD23	4:H:106:LEU:HD11	1.75	0.67
1:E:83:ARG:HH22	5:I:99:DA:H4'	1.60	0.67
4:H:88:THR:HG22	5:J:186:DG:OP1	1.95	0.67
3:C:81:ARG:NH2	3:C:107:VAL:O	2.28	0.67
5:I:19:DA:H2"	5:I:20:DT:H5"	1.75	0.66
4:H:104:GLY:HA2	4:H:107:ALA:H	1.61	0.66
3:G:16:THR:HA	5:J:177:DG:H5"	1.77	0.66
5:I:46:DG:H2"	5:I:47:DC:H6	1.61	0.65
5:I:50:DC:H5'	5:I:50:DC:C6	2.33	0.64
3:G:32:ARG:NH2	4:H:35:GLU:OE2	2.26	0.63
3:G:83:LEU:O	3:G:87:ILE:HG12	1.98	0.63
5:I:10:DC:H2'	5:I:11:DA:C8	2.35	0.62
1:E:129:ARG:HD3	1:E:135:ALA:HA	1.82	0.62
5:I:22:DC:H1'	5:I:23:DT:H5"	1.81	0.62
5:I:9:DC:H5"	5:I:9:DC:H6	1.65	0.61
5:J:164:DG:H2"	5:J:165:DA:H5"	1.82	0.61
2:F:68:ASP:OD2	2:F:93:GLN:NE2	2.33	0.61
5:I:84:DC:H2'	5:I:85:DA:C8	2.36	0.61
3:C:58:LEU:HD11	4:D:102:LEU:HD11	1.82	0.61
3:C:102:ILE:HG23	4:D:61:ILE:HD13	1.82	0.61
2:B:59:LYS:O	2:B:63:GLU:HB2	2.01	0.60
1:E:108:ASN:O	1:E:112:ILE:HG12	2.02	0.60
5:J:264:DT:H1'	5:J:265:DT:H5'	1.83	0.60
5:I:51:DA:H2"	5:I:52:DT:H5"	1.83	0.59
1:E:70:LEU:O	1:E:74:ILE:HG13	2.03	0.59
5:J:266:DT:H2"	5:J:267:DG:C5	2.38	0.59
1:A:79:LYS:HB3	1:A:82:LEU:HD11	1.85	0.58
5:J:215:DC:H2"	5:J:216:DT:H71	1.86	0.58
5:I:8:DT:H2"	5:I:9:DC:H5"	1.86	0.58
1:E:79:LYS:HD2	1:E:80:THR:H	1.68	0.58
5:J:186:DG:H1'	5:J:187:DA:N7	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:50:DC:H5'	5:I:50:DC:H6	1.68	0.57
4:H:87:SER:HB3	5:J:185:DG:H3'	1.86	0.57
5:I:58:DG:H2'	5:I:59:DG:C8	2.39	0.57
1:E:44:GLY:O	1:E:48:LEU:HD12	2.04	0.57
1:E:48:LEU:HD11	2:F:44:LYS:HD2	1.86	0.57
5:J:241:DA:H2"	5:J:242:DT:H5'	1.85	0.57
5:I:61:DA:H1'	5:I:62:DT:H5'	1.87	0.57
5:J:182:DT:H1'	5:J:183:DT:H5'	1.87	0.57
5:J:277:DG:H8	5:J:277:DG:H5"	1.70	0.56
5:J:237:DT:H1'	5:J:238:DT:H5'	1.87	0.56
5:I:144:DG:H2"	5:I:145:DA:H5'	1.88	0.56
5:I:26:DC:H2"	5:I:27:DA:N7	2.20	0.56
5:I:40:DG:H2"	5:I:41:DA:H5'	1.87	0.56
3:C:24:GLN:N	3:C:56:GLU:OE1	2.33	0.56
5:I:31:DG:H2"	5:I:32:DT:H5'	1.87	0.56
5:J:181:DA:H1'	5:J:182:DT:H5"	1.88	0.56
5:I:5:DA:H2"	5:I:6:DT:H5"	1.89	0.55
5:I:13:DC:H42	5:J:280:DG:H22	1.55	0.55
5:J:285:DA:H1'	5:J:286:DT:H5'	1.88	0.55
3:C:87:ILE:CG2	3:C:97:LEU:HD12	2.36	0.55
5:J:250:DT:H2"	5:J:251:DT:H5"	1.88	0.55
5:I:20:DT:H2"	5:I:21:DT:C5'	2.36	0.55
4:D:104:GLY:O	4:D:106:LEU:N	2.39	0.55
5:I:46:DG:H2"	5:I:47:DC:C6	2.40	0.55
5:J:226:DT:H2"	5:J:227:DG:C8	2.42	0.55
5:J:281:DG:H2"	5:J:282:DT:H5'	1.87	0.55
4:H:92:ARG:HG2	4:H:92:ARG:HH11	1.72	0.55
5:I:105:DT:H2"	5:I:106:DT:H5'	1.88	0.54
5:J:194:DT:H1'	5:J:195:DC:H5'	1.89	0.54
5:J:170:DA:H2"	5:J:171:DC:H5"	1.90	0.54
4:D:73:ILE:HD12	4:D:98:VAL:HG22	1.91	0.53
4:H:98:VAL:HG13	4:H:102:LEU:HD22	1.91	0.53
5:I:7:DA:C2	5:J:287:DA:C2	2.97	0.53
3:G:24:GLN:HG3	4:H:47:GLN:NE2	2.24	0.53
1:E:61:LEU:HD12	2:F:37:LEU:HD23	1.92	0.52
1:E:61:LEU:HD13	2:F:36:ARG:HB3	1.92	0.52
1:E:121:PRO:CB	2:F:53:GLU:HG3	2.36	0.52
3:C:42:ARG:HD2	5:I:38:DT:H5"	1.90	0.52
5:J:225:DC:H2"	5:J:226:DT:H71	1.91	0.52
5:J:287:DA:H5"	5:J:287:DA:H8	1.75	0.52
2:B:98:TYR:OH	4:H:68:ASP:OD2	2.21	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:83:ARG:HD2	5:J:197:DA:H5'	1.92	0.51
3:G:26:PRO:HB2	3:G:29:ARG:HB3	1.91	0.51
5:I:43:DA:H2"	5:I:44:DC:H5"	1.93	0.51
5:J:186:DG:H1'	5:J:187:DA:C8	2.46	0.51
1:E:83:ARG:NH2	5:I:99:DA:H4'	2.25	0.50
1:A:108:ASN:O	1:A:112:ILE:HG12	2.10	0.50
5:I:19:DA:H2'	5:I:20:DT:C6	2.47	0.50
5:J:239:DT:H2"	5:J:240:DG:H5'	1.93	0.50
3:C:79:ILE:HG12	3:C:82:HIS:CE1	2.47	0.50
3:G:39:TYR:O	4:H:78:SER:OG	2.26	0.50
2:B:75:HIS:ND1	4:D:96:THR:HG21	2.27	0.50
3:C:26:PRO:HD3	4:D:40:TYR:CD1	2.47	0.50
2:F:35:ARG:HB3	2:F:35:ARG:NH1	2.26	0.50
3:G:26:PRO:HD3	4:H:40:TYR:CD1	2.46	0.50
4:D:72:ARG:HB3	4:D:101:LEU:HD11	1.92	0.50
5:I:2:DT:H2'	5:I:3:DC:C6	2.47	0.50
5:J:245:DA:H2"	5:J:246:DG:N7	2.27	0.49
5:J:281:DG:H2"	5:J:282:DT:C5'	2.43	0.49
3:C:38:ASN:HD22	4:H:82:HIS:HE1	1.60	0.49
5:I:6:DT:H2"	5:I:7:DA:C8	2.47	0.49
5:I:45:DT:H2'	5:I:46:DG:C8	2.47	0.49
5:J:170:DA:H2	5:J:171:DC:C2	2.30	0.49
5:I:37:DT:O4	5:J:255:DA:N6	2.46	0.49
1:A:85:GLN:HG3	2:B:82:THR:HA	1.94	0.49
5:I:3:DC:H2"	5:I:4:DA:C8	2.48	0.49
3:G:57:TYR:HB2	4:H:113:GLU:HG3	1.95	0.49
5:J:277:DG:H5"	5:J:277:DG:C8	2.47	0.49
3:C:71:ARG:NH1	4:D:51:ASP:OD2	2.41	0.48
3:G:73:ASN:OD1	3:G:75:LYS:HE2	2.12	0.48
4:D:78:SER:HA	4:D:89:ILE:HD11	1.95	0.48
5:J:287:DA:H5"	5:J:287:DA:C8	2.47	0.48
1:E:73:GLU:OE1	2:F:25:ASN:HB2	2.13	0.48
1:E:118:THR:HA	2:F:45:ARG:HB3	1.95	0.48
3:C:87:ILE:HG21	3:C:97:LEU:HD12	1.95	0.48
3:G:32:ARG:HG2	3:G:36:LYS:HD3	1.96	0.48
2:B:78:ARG:HD3	5:J:248:DA:H5"	1.94	0.48
3:C:100:VAL:HG11	2:F:98:TYR:CE2	2.49	0.48
5:I:5:DA:C2'	5:I:6:DT:H5"	2.44	0.48
1:A:49:ARG:HD2	5:J:155:DC:P	2.53	0.47
5:I:5:DA:H1'	5:I:6:DT:H5"	1.96	0.47
5:I:37:DT:H2"	5:I:38:DT:H72	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:235:DC:H2"	5:J:236:DT:C5	2.49	0.47
5:I:62:DT:H2"	5:I:63:DG:C8	2.49	0.47
5:J:261:DA:H1'	5:J:262:DC:H5"	1.96	0.47
5:I:111:DA:H2"	5:I:112:DT:O5'	2.13	0.47
3:C:31:HIS:CE1	3:C:35:ARG:HH11	2.33	0.47
1:E:65:LEU:HB3	1:E:66:PRO:HD3	1.96	0.47
5:I:55:DA:N6	5:J:238:DT:H3	2.00	0.47
3:C:38:ASN:ND2	3:G:40:SER:HA	2.30	0.47
4:H:92:ARG:HG2	4:H:92:ARG:NH1	2.29	0.47
5:I:46:DG:H2"	5:I:47:DC:H5"	1.96	0.47
5:I:139:DA:H2"	5:I:140:DT:H5'	1.97	0.47
4:H:49:HIS:HB3	4:H:52:THR:OG1	2.15	0.47
5:I:47:DC:N4	5:J:245:DA:N1	2.62	0.47
5:I:47:DC:N4	5:J:245:DA:C6	2.83	0.46
5:I:111:DA:H2'	5:I:112:DT:H72	1.96	0.46
5:J:157:DA:H2"	5:J:158:DC:C6	2.50	0.46
2:B:98:TYR:CE2	3:G:100:VAL:HG11	2.49	0.46
5:I:69:DC:H42	5:J:224:DG:H1	1.62	0.46
5:J:200:DA:H1'	5:J:201:DA:H5'	1.98	0.46
5:J:259:DA:H1'	5:J:260:DC:H5'	1.97	0.46
1:E:68:GLN:HG3	1:E:89:ILE:HD13	1.98	0.46
3:G:85:LEU:HD23	3:G:108:LEU:CD2	2.46	0.46
5:I:10:DC:H2'	5:I:11:DA:H8	1.81	0.46
5:J:205:DG:H2"	5:J:206:DC:H5"	1.98	0.45
3:C:63:LEU:HD13	4:D:45:LEU:HB2	1.97	0.45
3:C:51:LEU:HD13	4:D:73:ILE:HG21	1.98	0.45
3:G:27:VAL:HG11	3:G:49:VAL:HG22	1.99	0.45
5:I:84:DC:H2"	5:I:85:DA:H5'	1.99	0.45
5:J:153:DA:H2"	5:J:154:DT:H5'	1.97	0.45
4:D:101:LEU:O	4:D:101:LEU:HD23	2.16	0.45
4:D:84:ASN:O	4:D:86:ARG:HG3	2.17	0.45
2:B:83:ALA:O	2:B:87:VAL:HG23	2.16	0.45
5:J:275:DC:H2'	5:J:276:DT:H72	1.98	0.45
2:B:78:ARG:CD	5:J:248:DA:H5"	2.47	0.45
3:C:102:ILE:CG2	4:D:61:ILE:HD13	2.46	0.45
3:G:67:GLY:HA3	4:H:49:HIS:CD2	2.52	0.45
5:I:20:DT:C2'	5:I:21:DT:H5"	2.40	0.45
5:J:229:DA:H2"	5:J:230:DC:H5'	1.98	0.45
2:B:78:ARG:HD3	5:J:248:DA:H3'	1.99	0.44
5:J:197:DA:H1'	5:J:198:DT:H5'	1.99	0.44
5:J:248:DA:H2"	5:J:249:DG:C5'	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:37:GLY:HA3	3:C:39:TYR:CE1	2.52	0.44
5:J:248:DA:H2"	5:J:249:DG:H5"	1.99	0.44
2:F:20:LYS:HD2	2:F:21:VAL:H	1.83	0.44
3:G:31:HIS:ND1	3:G:48:PRO:HG3	2.32	0.44
4:D:70:PHE:CD1	4:D:70:PHE:C	2.90	0.44
3:C:87:ILE:HG23	3:C:97:LEU:HD12	2.00	0.44
3:G:42:ARG:HD2	5:J:185:DG:H4'	2.00	0.44
5:J:283:DG:H1'	5:J:284:DG:C8	2.53	0.44
3:C:81:ARG:HD2	1:E:58:THR:CG2	2.48	0.44
4:D:105:GLU:OE1	4:D:108:LYS:HD2	2.18	0.44
5:I:87:DG:H4'	5:I:88:DC:H5'	2.00	0.44
1:E:128:ARG:HD2	1:E:133:GLU:OE1	2.18	0.43
5:I:117:DT:H2'	5:I:118:DT:H71	1.99	0.43
2:F:78:ARG:NH1	2:F:82:THR:HG23	2.33	0.43
5:I:42:DA:H61	5:J:251:DT:H3	1.65	0.43
3:G:75:LYS:HB3	5:I:131:DG:OP1	2.17	0.43
5:I:60:DC:H2"	5:I:61:DA:C8	2.54	0.43
5:I:60:DC:H2"	5:I:61:DA:H5'	2.01	0.43
5:I:42:DA:H2"	5:I:43:DA:H8	1.83	0.43
5:I:119:DT:H1'	5:I:120:DT:H5'	2.00	0.43
4:D:56:SER:OG	5:I:19:DA:OP2	2.34	0.43
1:E:69:ARG:HH22	5:I:90:DT:P	2.41	0.43
4:D:94:VAL:O	4:D:98:VAL:HG23	2.19	0.42
4:D:115:THR:O	4:D:119:THR:HG23	2.19	0.42
3:C:104:GLN:NE2	3:C:104:GLN:HA	2.34	0.42
5:I:103:DG:H2"	5:I:104:DT:H5"	2.01	0.42
5:J:236:DT:H2"	5:J:237:DT:H71	2.01	0.42
5:J:208:DT:H6	5:J:208:DT:H2'	1.62	0.42
2:B:37:LEU:HD23	2:B:37:LEU:HA	1.78	0.42
4:H:106:LEU:HD23	4:H:106:LEU:HA	1.90	0.42
3:G:77:ARG:NH1	5:I:131:DG:H5"	2.34	0.42
5:I:144:DG:H2"	5:I:145:DA:C5'	2.49	0.42
5:J:194:DT:H2"	5:J:195:DC:C6	2.55	0.42
5:J:225:DC:H2"	5:J:226:DT:C7	2.49	0.42
4:H:48:VAL:HG23	4:H:49:HIS:ND1	2.35	0.42
3:C:63:LEU:HA	3:C:63:LEU:HD23	1.77	0.41
4:D:64:SER:HB3	2:F:98:TYR:CD1	2.55	0.41
3:G:37:GLY:HA3	3:G:39:TYR:CE2	2.55	0.41
3:G:116:LEU:HD23	3:G:116:LEU:HA	1.71	0.41
4:H:107:ALA:O	4:H:111:VAL:HG23	2.20	0.41
5:I:9:DC:H6	5:I:9:DC:C5'	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:198:DT:H1'	5:J:199:DC:H5'	2.01	0.41
2:B:84:MET:SD	2:B:101:GLY:HA3	2.60	0.41
5:J:180:DT:H6	5:J:180:DT:H2'	1.75	0.41
5:J:211:DT:H2"	5:J:212:DC:H5'	2.03	0.41
5:J:234:DC:H2"	5:J:235:DC:C5	2.54	0.41
3:G:26:PRO:HD3	4:H:40:TYR:CE1	2.55	0.41
5:J:246:DG:H1'	5:J:247:DC:H5'	2.02	0.41
1:A:43:PRO:HG2	5:I:68:DG:H5'	2.03	0.41
2:F:62:LEU:HA	2:F:62:LEU:HD23	1.77	0.41
5:I:40:DG:H2"	5:I:41:DA:C8	2.55	0.41
5:J:173:DA:H2"	5:J:174:DA:C8	2.56	0.41
5:I:38:DT:H2"	5:I:39:DG:O4'	2.20	0.41
5:I:47:DC:H2"	5:I:48:DT:O4'	2.20	0.41
4:D:106:LEU:HD23	4:D:106:LEU:HA	1.90	0.41
5:I:31:DG:C2'	5:I:32:DT:H5'	2.51	0.41
2:B:92:ARG:HB3	2:B:92:ARG:CZ	2.51	0.41
1:E:49:ARG:HG3	1:E:49:ARG:HH11	1.86	0.41
1:E:57:ALA:HB1	1:E:59:GLU:HG2	2.01	0.41
5:I:64:DT:H2"	5:I:65:DT:H5'	2.03	0.41
5:I:141:DA:C2	5:J:153:DA:C2	3.09	0.41
1:A:73:GLU:OE2	2:B:25:ASN:HB2	2.21	0.41
1:E:83:ARG:NH2	5:I:99:DA:O3'	2.54	0.41
3:G:59:THR:HG21	4:H:41:VAL:HG22	2.02	0.41
5:J:264:DT:H2"	5:J:265:DT:H5'	2.03	0.41
4:D:92:ARG:O	4:D:95:GLN:HB3	2.21	0.40
4:D:31:ARG:HA	4:D:32:GLY:HA2	1.54	0.40
2:B:75:HIS:O	4:D:92:ARG:NH2	2.42	0.40
1:E:83:ARG:HH22	5:I:99:DA:C4'	2.30	0.40
5:I:129:DC:H2"	5:I:130:DT:C5	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:56:GLU:OE2	2:F:23:ARG:NH2[3_544]	2.15	0.05

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%)	92 (97%)	3 (3%)	0	100	100
1	E	96/139 (69%)	90 (94%)	6 (6%)	0	100	100
2	B	76/106 (72%)	74 (97%)	2 (3%)	0	100	100
2	F	81/106 (76%)	79 (98%)	2 (2%)	0	100	100
3	C	103/133 (77%)	99 (96%)	4 (4%)	0	100	100
3	G	102/133 (77%)	97 (95%)	5 (5%)	0	100	100
4	D	92/129 (71%)	88 (96%)	4 (4%)	0	100	100
4	H	89/129 (69%)	87 (98%)	2 (2%)	0	100	100
All	All	734/1014 (72%)	706 (96%)	28 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	82/111 (74%)	81 (99%)	1 (1%)	71	87
1	E	82/111 (74%)	78 (95%)	4 (5%)	25	57
2	B	63/81 (78%)	63 (100%)	0	100	100
2	F	68/81 (84%)	68 (100%)	0	100	100
3	C	83/102 (81%)	82 (99%)	1 (1%)	71	87
3	G	83/102 (81%)	82 (99%)	1 (1%)	71	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	D	81/110 (74%)	80 (99%)	1 (1%)	71 87
4	H	79/110 (72%)	79 (100%)	0	100 100
All	All	621/808 (77%)	613 (99%)	8 (1%)	69 86

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	129	ARG
3	C	81	ARG
4	D	33	ARG
1	E	48	LEU
1	E	82	LEU
1	E	122	LYS
1	E	129	ARG
3	G	90	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	31	HIS
3	C	73	ASN
4	H	47	GLN
4	H	82	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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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	97/139 (69%)	0.02	2 (2%) 63 61	64, 83, 118, 151	0
1	E	98/139 (70%)	-0.04	0 100 100	50, 67, 96, 122	0
2	B	78/106 (73%)	-0.11	0 100 100	64, 79, 99, 102	0
2	F	83/106 (78%)	-0.14	1 (1%) 79 75	50, 64, 78, 120	0
3	C	105/133 (78%)	-0.21	0 100 100	54, 71, 96, 126	0
3	G	104/133 (78%)	-0.11	0 100 100	66, 82, 111, 122	0
4	D	94/129 (72%)	-0.19	1 (1%) 80 77	54, 74, 100, 143	0
4	H	91/129 (70%)	-0.07	0 100 100	61, 81, 104, 114	0
5	I	146/146 (100%)	-0.06	5 (3%) 45 43	87, 149, 185, 203	0
5	J	146/146 (100%)	-0.09	3 (2%) 63 61	93, 149, 185, 193	0
All	All	1042/1306 (79%)	-0.10	12 (1%) 79 75	50, 82, 168, 203	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	I	146	DT	12.9
5	I	55	DA	5.3
5	I	44	DC	3.4
2	F	102	GLY	3.3
5	J	147	DA	3.0
5	I	56	DA	2.8
1	A	38	PRO	2.7
5	J	150	DA	2.4
5	I	1	DA	2.2
5	J	161	DG	2.1
1	A	39	HIS	2.1
4	D	31	ARG	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 (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.