Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:42 PM GMT

PDB ID	:	1LEI
Title	:	The kB DNA sequence from the HLV-LTR functions as an allosteric regulator of HIV transcription
Authors	:	Chen-Park, F.; Huang, D.B.; Ghosh, G.
Deposited on	:	2002-04-09
Resolution	:	2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

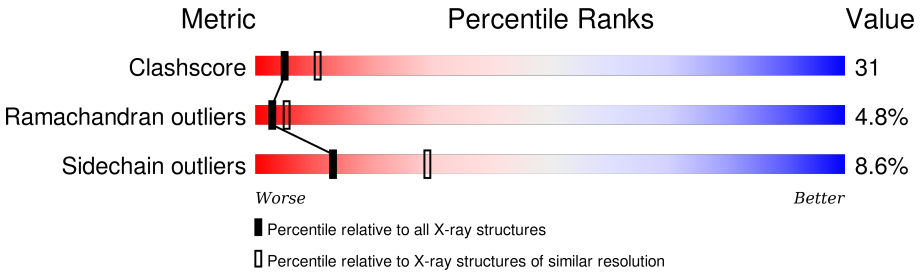
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	C	17	18% 82%
2	D	17	6% 94%
3	A	274	63% 29% 8%
4	B	313	45% 45% 8%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	5IU	D	10	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5344 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 DNA chain called 5'-D(*CP*TP*CP*AP*GP*GP*GP*AP*AP*AP*GP*TP*AP*CP*AP*GP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	17	Total	C	N	O	P	0	0	0
			351	167	73	95	16			

- Molecule 2 is a DNA chain called 5'-D(*TP*CP*TP*GP*5ITP*AP*CP*5ITP*5ITP*5ITP*CP*CP*CP*TP*GP*AP*G)-3'.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	D	17	Total	C	I	N	O	P	0	0	0
			340	161	4	54	105	16			

- Molecule 3 is a protein called NUCLEAR FACTOR NF-KAPPA-B P65 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	273	Total	C	N	O	S	0	0	0
			2176	1356	401	408	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	MET	-	CLONING ARTIFACT	UNP Q04207
A	19	ALA	-	CLONING ARTIFACT	UNP Q04207

- Molecule 4 is a protein called NUCLEAR FACTOR NF-KAPPA-B P50 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	312	Total	C	N	O	S	0	0	0
			2454	1554	428	460	12			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	38	MET	-	INITIATING MET	UNP P25799

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	15	Total O 15 15	0	0
5	B	8	Total O 8 8	0	0

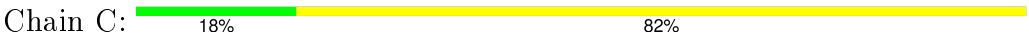
3 Residue-property plots (i)

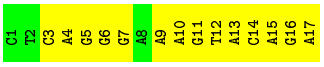
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

• Molecule 1: 5'-D(*CP*TP*CP*AP*GP*GP*GP*AP*AP*AP*GP*TP*AP*CP*AP*GP*A)-3'

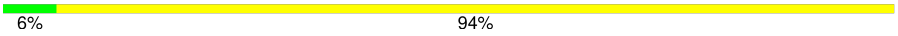
Chain C:





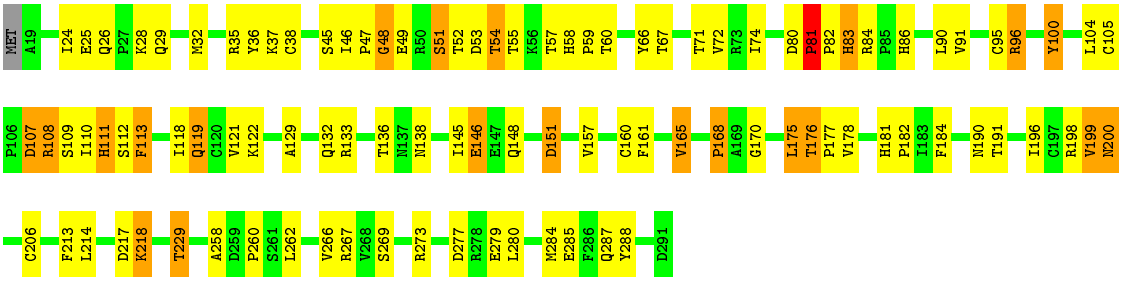
• Molecule 2: 5'-D(*TP*CP*TP*GP*5ITP*AP*CP*5ITP*5ITP*5ITP*CP*CP*CP*TP*GP*AP*G)-3'

Chain D:



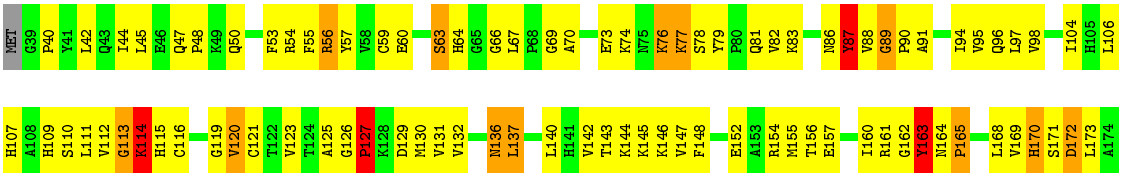
• Molecule 3: NUCLEAR FACTOR NF-KAPPA-B P65 SUBUNIT

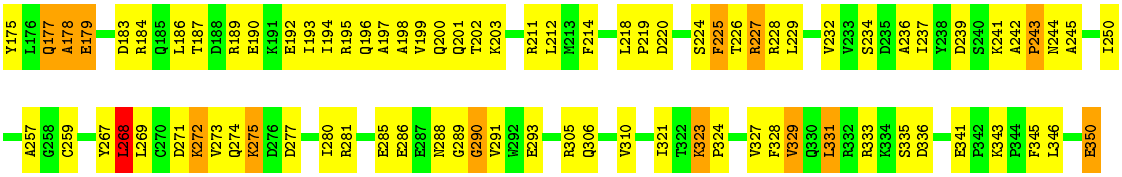
Chain A:



• Molecule 4: NUCLEAR FACTOR NF-KAPPA-B P50 SUBUNIT

Chain B:




Y175 L176 Q177 A178 E179 D183 R184 Q185 L186 T187 D188 R189 E190 K191 E192 I193 I194 R195 Q196 A197 A198 V199 Q200 Q201 T202 K203 R211 L212 M213 F214 L218 P219 D220 S224 F225 T226 R227 R228 L229 V232 Y233 S234 D235 A236 I237 Y238 D239 S240 K241 A242 P243 M244 A245 I250
A257 G258 C259 Y267 L268 L269 C270 D271 K272 V273 Q274 K275 D276 D277 I280 R281 E285 E286 E287 N288 G289 G290 V291 W292 E293 R305 Q306 V310 I321 T322 K323 P324 V327 F328 V329 Q330 L331 R332 R333 K334 S335 D336 E341 P342 K343 P344 F345 L346 E350

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	137.13Å 179.70Å 97.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70	Depositor
% Data completeness (in resolution range)	87.1 (20.00-2.70)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.250 , 0.284	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5344	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5IU

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	C	0.39	0/396	0.77	0/610
2	D	0.53	0/288	0.99	0/437
3	A	0.43	0/2228	0.70	0/3021
4	B	0.37	0/2506	0.61	1/3384 (0.0%)
All	All	0.41	0/5418	0.69	1/7452 (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})
4	B	268	LEU	CA-CB-CG	5.56	128.08	115.30

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	C	351	0	191	19	0
2	D	340	0	184	26	1
3	A	2176	0	2137	100	0
4	B	2454	0	2449	197	0
5	A	15	0	0	0	0
5	B	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5344	0	4961	320	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 31.

All (320) 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)
4:B:285:GLU:HA	4:B:290:GLY:HA3	1.24	1.19
4:B:91:ALA:HB3	4:B:125:ALA:HB3	1.33	1.05
4:B:88:VAL:HG21	4:B:218:LEU:HD22	1.42	1.02
4:B:187:THR:HB	4:B:190:GLU:HG2	1.39	1.02
3:A:51:SER:HB3	3:A:57:THR:H	1.21	1.02
4:B:113:GLY:HA3	4:B:137:LEU:HA	1.39	1.01
3:A:199:VAL:HG23	3:A:214:LEU:HD13	1.46	0.98
3:A:196:ILE:HG23	3:A:214:LEU:HD11	1.46	0.96
4:B:243:PRO:HB2	4:B:274:GLN:HE21	1.40	0.86
4:B:123:VAL:HG21	4:B:132:VAL:HG11	1.58	0.85
4:B:157:GLU:O	4:B:161:ARG:HB2	1.76	0.84
4:B:110:SER:HB2	4:B:119:GLY:HA2	1.57	0.84
3:A:108:ARG:HE	3:A:108:ARG:HA	1.41	0.84
4:B:187:THR:HG22	4:B:189:ARG:H	1.44	0.83
3:A:122:LYS:NZ	3:A:122:LYS:HB2	1.94	0.82
4:B:144:LYS:O	4:B:147:VAL:HG12	1.79	0.81
3:A:229:THR:HG22	3:A:269:SER:HB2	1.62	0.81
1:C:14:DC:H2"	1:C:15:DA:C8	2.15	0.80
4:B:184:ARG:HH12	4:B:186:LEU:HD23	1.46	0.78
4:B:87:TYR:HA	4:B:130:MET:HG3	1.64	0.78
2:D:6:DA:H5"	4:B:306:GLN:NE2	1.99	0.77
1:C:15:DA:H2"	1:C:16:DG:C8	2.19	0.77
4:B:97:LEU:HD21	4:B:111:LEU:HG	1.66	0.77
3:A:262:LEU:HD21	3:A:266:VAL:HG12	1.65	0.77
4:B:125:ALA:O	4:B:130:MET:HE1	1.85	0.77
4:B:86:ASN:O	4:B:88:VAL:HG13	1.84	0.76
4:B:190:GLU:O	4:B:193:ILE:HG12	1.86	0.76
4:B:114:LYS:NZ	4:B:114:LYS:HA	1.99	0.76
2:D:10:5IU:H5'	4:B:59:CYS:SG	2.26	0.76
4:B:90:PRO:HA	4:B:126:GLY:HA2	1.68	0.76
4:B:111:LEU:HD22	4:B:137:LEU:HD12	1.67	0.75
4:B:45:LEU:HB2	4:B:81:GLN:HG3	1.69	0.75
4:B:271:ASP:O	4:B:273:VAL:HG13	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:285:GLU:HA	4:B:290:GLY:CA	2.13	0.75
4:B:152:GLU:OE1	4:B:195:ARG:HG3	1.87	0.75
4:B:114:LYS:HZ3	4:B:114:LYS:HA	1.51	0.75
3:A:262:LEU:HD21	3:A:266:VAL:CG1	2.18	0.74
3:A:81:PRO:HB2	3:A:82:PRO:HD3	1.70	0.74
4:B:187:THR:HB	4:B:190:GLU:CG	2.18	0.73
3:A:199:VAL:HG23	3:A:214:LEU:CD1	2.18	0.73
4:B:243:PRO:HB2	4:B:274:GLN:NE2	2.02	0.73
4:B:104:ILE:HD11	4:B:211:ARG:HH21	1.52	0.73
4:B:57:TYR:HB2	4:B:60:GLU:HG2	1.71	0.72
2:D:6:DA:H2'	2:D:7:DC:C6	2.24	0.72
4:B:94:ILE:HD13	4:B:163:TYR:HB2	1.71	0.72
3:A:108:ARG:NE	3:A:109:SER:H	1.87	0.72
3:A:267:ARG:HH21	3:A:287:GLN:NE2	1.88	0.71
4:B:218:LEU:HB2	4:B:227:ARG:HB3	1.72	0.71
3:A:199:VAL:CG2	3:A:214:LEU:HD13	2.20	0.71
4:B:177:GLN:HE21	4:B:228:ARG:HH11	1.38	0.70
4:B:57:TYR:H	4:B:60:GLU:HG3	1.57	0.70
4:B:173:LEU:HD21	4:B:193:ILE:HD11	1.74	0.69
3:A:200:ASN:HB2	3:A:213:PHE:H	1.56	0.69
4:B:197:ALA:HB1	4:B:201:GLN:HE21	1.57	0.69
2:D:4:DG:H2"	2:D:5:5IU:O5'	1.91	0.68
1:C:3:DC:H1'	1:C:4:DA:C8	2.29	0.68
4:B:109:HIS:ND1	4:B:142:VAL:HG12	2.09	0.67
3:A:184:PHE:HB3	3:A:191:THR:HB	1.76	0.67
4:B:277:ASP:OD1	4:B:333:ARG:HG2	1.94	0.67
1:C:12:DT:H2"	1:C:13:DA:H5'	1.77	0.67
4:B:286:GLU:H	4:B:290:GLY:HA2	1.59	0.66
3:A:95:CYS:SG	3:A:100:TYR:HB2	2.35	0.66
3:A:28:LYS:N	3:A:48:GLY:O	2.29	0.66
3:A:198:ARG:HG2	4:B:267:TYR:OH	1.96	0.65
3:A:46:ILE:HD11	3:A:118:ILE:CD1	2.26	0.65
4:B:178:ALA:HB1	4:B:226:THR:HG22	1.77	0.65
4:B:329:VAL:CG2	4:B:345:PHE:HB2	2.26	0.65
4:B:107:HIS:CD2	4:B:109:HIS:H	2.15	0.65
2:D:14:DT:H2'	2:D:15:DG:C8	2.32	0.65
4:B:42:LEU:HD11	4:B:82:VAL:HG12	1.79	0.64
3:A:80:ASP:HB3	3:A:81:PRO:HD2	1.79	0.63
2:D:2:DC:H2'	2:D:3:DT:O4'	1.99	0.63
3:A:107:ASP:OD2	3:A:107:ASP:N	2.30	0.63
4:B:44:ILE:HD12	4:B:214:PHE:HE2	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:95:VAL:O	4:B:120:VAL:HG23	1.99	0.63
3:A:122:LYS:HZ2	3:A:122:LYS:HB2	1.60	0.63
4:B:147:VAL:HG13	4:B:148:PHE:H	1.63	0.63
4:B:179:GLU:HG2	4:B:179:GLU:O	1.99	0.63
2:D:6:DA:H5"	4:B:306:GLN:CD	2.20	0.62
4:B:160:ILE:HG22	4:B:186:LEU:HD21	1.81	0.62
4:B:53:PHE:HE1	4:B:66:GLY:H	1.47	0.62
4:B:56:ARG:O	4:B:140:LEU:HD12	1.99	0.61
4:B:197:ALA:HB1	4:B:201:GLN:NE2	2.15	0.61
4:B:192:GLU:HG2	4:B:196:GLN:HE21	1.64	0.61
4:B:55:PHE:CE2	4:B:239:ASP:HB2	2.36	0.60
4:B:173:LEU:HD21	4:B:193:ILE:CD1	2.31	0.60
4:B:147:VAL:HG13	4:B:148:PHE:N	2.17	0.60
4:B:192:GLU:O	4:B:196:GLN:HG3	2.01	0.60
4:B:161:ARG:HD2	4:B:163:TYR:CE2	2.37	0.60
1:C:11:DG:H3'	3:A:122:LYS:HE3	1.82	0.60
4:B:55:PHE:CD2	4:B:239:ASP:HB2	2.37	0.59
3:A:110:ILE:C	3:A:111:HIS:CD2	2.76	0.59
3:A:111:HIS:CD2	3:A:111:HIS:N	2.71	0.59
3:A:86:HIS:CD2	3:A:157:VAL:HG12	2.38	0.59
4:B:272:LYS:HD2	4:B:306:GLN:OE1	2.02	0.59
3:A:129:ALA:O	3:A:133:ARG:HG2	2.02	0.59
3:A:218:LYS:HE3	3:A:218:LYS:H	1.68	0.58
1:C:12:DT:H1'	1:C:13:DA:H5"	1.84	0.58
4:B:40:PRO:O	4:B:229:LEU:HD22	2.03	0.58
3:A:25:GLU:HB3	3:A:60:THR:HB	1.86	0.58
4:B:212:LEU:HB2	4:B:234:SER:OG	2.04	0.58
3:A:266:VAL:O	3:A:266:VAL:HG13	2.04	0.57
3:A:108:ARG:HE	3:A:108:ARG:CA	2.14	0.57
4:B:177:GLN:HE21	4:B:228:ARG:NH1	2.01	0.57
4:B:154:ARG:HH11	4:B:154:ARG:HG2	1.68	0.57
3:A:32:MET:HE3	3:A:47:PRO:HD3	1.87	0.57
3:A:26:GLN:HG3	3:A:181:HIS:CE1	2.39	0.57
4:B:107:HIS:HD2	4:B:109:HIS:H	1.50	0.57
3:A:196:ILE:CG2	3:A:214:LEU:HD11	2.26	0.57
3:A:190:ASN:OD1	3:A:191:THR:HG23	2.04	0.57
3:A:51:SER:HB3	3:A:57:THR:N	2.06	0.57
4:B:250:ILE:HG23	4:B:268:LEU:HD13	1.85	0.57
3:A:96:ARG:H	3:A:96:ARG:HD2	1.70	0.57
3:A:267:ARG:NH2	3:A:287:GLN:NE2	2.53	0.56
3:A:113:PHE:CD1	3:A:113:PHE:N	2.72	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:323:LYS:HD3	4:B:324:PRO:HD2	1.87	0.56
2:D:6:DA:H2'	2:D:7:DC:H6	1.68	0.56
4:B:169:VAL:O	4:B:170:HIS:HB2	2.04	0.56
3:A:91:VAL:HG13	3:A:119:GLN:HB2	1.87	0.56
4:B:109:HIS:CE1	4:B:142:VAL:H	2.24	0.56
1:C:12:DT:OP2	3:A:38:CYS:SG	2.60	0.56
4:B:112:VAL:O	4:B:113:GLY:O	2.24	0.56
4:B:184:ARG:NH1	4:B:186:LEU:HD23	2.19	0.56
4:B:50:GLN:HG2	4:B:236:ALA:O	2.06	0.56
4:B:48:PRO:HG2	4:B:212:LEU:HD22	1.88	0.56
3:A:132:GLN:O	3:A:136:THR:HG22	2.06	0.56
4:B:54:ARG:HA	4:B:239:ASP:OD1	2.05	0.55
4:B:163:TYR:HD1	4:B:164:ASN:ND2	2.04	0.55
4:B:241:LYS:O	4:B:243:PRO:HD3	2.06	0.55
4:B:163:TYR:CD1	4:B:164:ASN:ND2	2.75	0.55
4:B:155:MET:HE2	4:B:198:ALA:HB2	1.87	0.55
4:B:83:LYS:HD2	4:B:131:VAL:HG22	1.88	0.54
1:C:4:DA:OP2	4:B:63:SER:HB2	2.08	0.54
4:B:143:THR:CG2	4:B:146:LYS:HB2	2.37	0.54
3:A:60:THR:OG1	3:A:112:SER:HB3	2.06	0.54
4:B:323:LYS:CD	4:B:324:PRO:HD2	2.38	0.54
3:A:122:LYS:HB2	3:A:122:LYS:HZ3	1.71	0.54
3:A:46:ILE:HD11	3:A:118:ILE:HD11	1.88	0.54
4:B:42:LEU:HD11	4:B:82:VAL:CG1	2.37	0.54
1:C:6:DG:H2"	1:C:7:DG:C8	2.43	0.54
4:B:171:SER:C	4:B:173:LEU:H	2.11	0.54
4:B:184:ARG:HH11	4:B:184:ARG:HG3	1.72	0.54
4:B:197:ALA:O	4:B:201:GLN:HG3	2.08	0.54
2:D:10:5IU:H5'	4:B:59:CYS:CB	2.38	0.53
4:B:87:TYR:CA	4:B:130:MET:HG3	2.37	0.53
4:B:89:GLY:O	4:B:130:MET:HE3	2.09	0.53
4:B:57:TYR:H	4:B:60:GLU:CG	2.20	0.53
1:C:16:DG:C6	1:C:17:DA:N6	2.77	0.53
3:A:32:MET:HE1	3:A:46:ILE:N	2.24	0.53
4:B:250:ILE:HG23	4:B:268:LEU:CD1	2.40	0.52
3:A:72:VAL:HB	3:A:104:LEU:HD21	1.92	0.52
2:D:9:5IU:H2'	2:D:10:5IU:H6	1.91	0.52
1:C:4:DA:C2	2:D:15:DG:N2	2.78	0.52
2:D:10:5IU:I5	4:B:241:LYS:NZ	3.12	0.52
4:B:162:GLY:O	4:B:164:ASN:N	2.42	0.52
4:B:162:GLY:CA	4:B:178:ALA:HA	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:90:PRO:HA	4:B:126:GLY:CA	2.38	0.51
3:A:66:TYR:CD1	3:A:67:THR:N	2.79	0.51
4:B:196:GLN:O	4:B:200:GLN:HG2	2.10	0.51
4:B:321:ILE:HD12	4:B:323:LYS:O	2.10	0.51
2:D:12:DC:H2'	2:D:13:DC:C6	2.45	0.51
4:B:242:ALA:O	4:B:244:ASN:N	2.43	0.51
4:B:155:MET:HE1	4:B:198:ALA:N	2.26	0.51
3:A:54:THR:HG23	3:A:55:THR:H	1.76	0.51
2:D:15:DG:H2'	2:D:16:DA:C8	2.46	0.51
4:B:250:ILE:HG12	4:B:331:LEU:HD22	1.93	0.51
3:A:132:GLN:O	3:A:136:THR:CG2	2.59	0.51
4:B:44:ILE:HD11	4:B:47:GLN:HA	1.94	0.50
3:A:96:ARG:O	3:A:96:ARG:HD2	2.12	0.50
3:A:24:ILE:HD11	3:A:60:THR:HG22	1.92	0.50
4:B:195:ARG:HH11	4:B:195:ARG:HG2	1.76	0.50
3:A:217:ASP:HA	4:B:305:ARG:HH12	1.77	0.50
4:B:74:LYS:C	4:B:76:LYS:H	2.14	0.50
4:B:143:THR:HG23	4:B:146:LYS:H	1.76	0.50
4:B:156:THR:HG22	4:B:194:ILE:HG21	1.94	0.49
3:A:81:PRO:O	3:A:83:HIS:N	2.44	0.49
2:D:10:5IU:C5'	4:B:59:CYS:SG	2.98	0.49
4:B:333:ARG:HB3	4:B:336:ASP:OD2	2.12	0.49
3:A:29:GLN:HG2	3:A:182:PRO:O	2.12	0.49
4:B:56:ARG:HH11	4:B:56:ARG:HG3	1.77	0.49
4:B:323:LYS:HE3	4:B:324:PRO:HD2	1.94	0.49
4:B:66:GLY:O	4:B:67:LEU:C	2.50	0.49
3:A:121:VAL:HG23	3:A:122:LYS:O	2.13	0.49
2:D:16:DA:N6	2:D:17:DG:C6	2.81	0.49
4:B:113:GLY:O	4:B:114:LYS:O	2.30	0.49
4:B:76:LYS:O	4:B:77:LYS:C	2.52	0.49
3:A:277:ASP:OD1	3:A:279:GLU:HB2	2.13	0.49
4:B:86:ASN:O	4:B:88:VAL:N	2.46	0.48
4:B:87:TYR:HA	4:B:130:MET:CG	2.38	0.48
4:B:137:LEU:O	4:B:137:LEU:HG	2.13	0.48
4:B:184:ARG:NH1	4:B:184:ARG:HG3	2.28	0.48
4:B:54:ARG:HG3	4:B:241:LYS:HB2	1.96	0.48
4:B:48:PRO:CG	4:B:212:LEU:HD22	2.42	0.48
3:A:86:HIS:NE2	3:A:157:VAL:HG12	2.28	0.48
3:A:146:GLU:CD	3:A:146:GLU:H	2.17	0.48
4:B:286:GLU:H	4:B:290:GLY:CA	2.26	0.48
4:B:83:LYS:HB2	4:B:131:VAL:HG22	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:15:DG:H2"	2:D:16:DA:O4'	2.14	0.47
3:A:46:ILE:HD11	3:A:118:ILE:HD12	1.96	0.47
1:C:12:DT:H2'	3:A:38:CYS:HB2	1.95	0.47
3:A:168:PRO:C	3:A:170:GLY:H	2.18	0.47
4:B:152:GLU:O	4:B:156:THR:HG23	2.14	0.47
4:B:114:LYS:CA	4:B:114:LYS:NZ	2.73	0.47
3:A:58:HIS:HB3	3:A:59:PRO:HD2	1.96	0.47
3:A:67:THR:O	3:A:67:THR:HG23	2.13	0.47
4:B:199:VAL:O	4:B:203:LYS:HG3	2.15	0.47
4:B:45:LEU:HD12	4:B:131:VAL:HG13	1.97	0.47
3:A:136:THR:HG23	3:A:138:ASN:HB2	1.95	0.47
4:B:54:ARG:HD2	4:B:241:LYS:HG3	1.96	0.47
4:B:154:ARG:HG2	4:B:154:ARG:NH1	2.29	0.47
4:B:104:ILE:HD11	4:B:211:ARG:NH2	2.25	0.47
4:B:335:SER:OG	4:B:336:ASP:N	2.47	0.47
3:A:104:LEU:HD22	3:A:111:HIS:CE1	2.50	0.46
3:A:176:THR:HA	3:A:177:PRO:HD3	1.78	0.46
4:B:281:ARG:NH1	4:B:293:GLU:OE1	2.46	0.46
4:B:54:ARG:HD2	4:B:241:LYS:CG	2.45	0.46
2:D:9:5IU:H3'	4:B:57:TYR:CE1	2.51	0.46
4:B:115:HIS:CD2	4:B:123:VAL:HG12	2.51	0.46
3:A:32:MET:HE1	3:A:45:SER:C	2.36	0.46
3:A:218:LYS:N	3:A:218:LYS:HE3	2.31	0.46
4:B:87:TYR:HE2	4:B:89:GLY:HA2	1.80	0.46
4:B:160:ILE:HG22	4:B:186:LEU:CD2	2.44	0.46
4:B:114:LYS:HG2	4:B:136:ASN:O	2.15	0.46
4:B:273:VAL:HG22	4:B:306:GLN:O	2.16	0.46
4:B:83:LYS:HD2	4:B:131:VAL:CG2	2.47	0.45
3:A:96:ARG:N	3:A:96:ARG:HD2	2.30	0.45
4:B:143:THR:HG23	4:B:146:LYS:HB2	1.98	0.45
4:B:160:ILE:HG13	4:B:160:ILE:O	2.16	0.45
4:B:96:GLN:HE22	4:B:165:PRO:HD2	1.81	0.45
4:B:67:LEU:HD21	4:B:237:ILE:HD11	1.98	0.45
2:D:6:DA:OP1	4:B:275:LYS:CD	2.65	0.45
2:D:11:DC:H2'	2:D:12:DC:C6	2.52	0.45
3:A:74:ILE:HA	3:A:160:CYS:O	2.17	0.45
2:D:15:DG:H2'	2:D:16:DA:H8	1.80	0.45
4:B:88:VAL:O	4:B:89:GLY:C	2.54	0.45
4:B:98:VAL:HG23	4:B:211:ARG:HB2	1.97	0.45
4:B:87:TYR:CD2	4:B:87:TYR:C	2.90	0.45
2:D:10:5IU:C5'	4:B:59:CYS:HG	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:162:GLY:HA3	4:B:178:ALA:HA	1.98	0.45
4:B:268:LEU:HD23	4:B:280:ILE:HD13	1.98	0.45
3:A:84:ARG:NH2	3:A:151:ASP:O	2.47	0.45
4:B:291:VAL:HG22	4:B:291:VAL:O	2.16	0.45
4:B:91:ALA:HB3	4:B:125:ALA:CB	2.24	0.45
3:A:258:ALA:O	3:A:260:PRO:HD3	2.16	0.45
4:B:106:LEU:HG	4:B:168:LEU:HB3	1.98	0.45
4:B:232:VAL:O	4:B:232:VAL:HG23	2.17	0.45
4:B:224:SER:O	4:B:226:THR:N	2.50	0.45
4:B:69:GLY:HA3	4:B:79:TYR:N	2.32	0.45
4:B:259:CYS:SG	4:B:350:GLU:HA	2.57	0.45
4:B:126:GLY:N	4:B:127:PRO:CD	2.79	0.45
3:A:198:ARG:O	3:A:214:LEU:HD12	2.17	0.45
1:C:12:DT:H1'	1:C:13:DA:C5'	2.47	0.45
4:B:220:ASP:OD2	4:B:224:SER:N	2.45	0.44
1:C:3:DC:H1'	1:C:4:DA:N7	2.32	0.44
4:B:87:TYR:HD2	4:B:87:TYR:C	2.20	0.44
4:B:190:GLU:O	4:B:194:ILE:HG12	2.17	0.44
4:B:114:LYS:HB3	4:B:115:HIS:H	1.54	0.44
3:A:200:ASN:HA	3:A:200:ASN:HD22	1.48	0.44
3:A:37:LYS:HG2	3:A:119:GLN:HE22	1.83	0.44
3:A:161:PHE:HB2	3:A:178:VAL:HG22	2.00	0.44
4:B:219:PRO:HG3	4:B:225:PHE:HE2	1.82	0.44
3:A:110:ILE:C	3:A:111:HIS:HD2	2.21	0.44
3:A:104:LEU:HB3	3:A:111:HIS:HE1	1.83	0.44
2:D:4:DG:O6	3:A:35:ARG:NH2	2.51	0.44
4:B:129:ASP:O	4:B:130:MET:HE2	2.17	0.43
3:A:100:TYR:CD2	3:A:100:TYR:C	2.92	0.43
3:A:37:LYS:HG2	3:A:119:GLN:NE2	2.33	0.43
4:B:250:ILE:HG12	4:B:331:LEU:CD2	2.48	0.43
3:A:24:ILE:HD11	3:A:60:THR:CG2	2.49	0.43
2:D:10:5IU:I5	4:B:60:GLU:CD	3.26	0.43
3:A:206:CYS:HA	3:A:288:TYR:HD2	1.83	0.43
4:B:56:ARG:NH1	4:B:56:ARG:HG3	2.33	0.43
4:B:327:VAL:HG23	4:B:328:PHE:N	2.33	0.43
4:B:179:GLU:O	4:B:179:GLU:CG	2.66	0.43
2:D:7:DC:OP1	4:B:274:GLN:NE2	2.52	0.43
3:A:206:CYS:HA	3:A:288:TYR:CD2	2.54	0.43
4:B:114:LYS:C	4:B:116:CYS:H	2.23	0.42
4:B:268:LEU:HD12	4:B:269:LEU:N	2.33	0.42
4:B:323:LYS:CE	4:B:324:PRO:HD2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:80:ASP:CB	3:A:81:PRO:HD2	2.49	0.42
3:A:190:ASN:OD1	3:A:191:THR:N	2.52	0.42
3:A:262:LEU:HD21	3:A:266:VAL:HG11	1.98	0.42
4:B:165:PRO:HB3	4:B:228:ARG:NH2	2.34	0.42
1:C:11:DG:OP2	3:A:36:TYR:OH	2.31	0.42
4:B:286:GLU:OE2	4:B:286:GLU:HA	2.20	0.42
3:A:108:ARG:NE	3:A:108:ARG:CA	2.82	0.42
3:A:108:ARG:CZ	3:A:109:SER:H	2.32	0.42
3:A:66:TYR:CE2	3:A:165:VAL:HB	2.55	0.42
4:B:275:LYS:HE3	4:B:275:LYS:HB2	1.87	0.42
4:B:45:LEU:CB	4:B:81:GLN:HE21	2.32	0.41
4:B:47:GLN:O	4:B:70:ALA:HB2	2.20	0.41
4:B:114:LYS:O	4:B:116:CYS:N	2.48	0.41
3:A:52:THR:OG1	3:A:54:THR:HG23	2.20	0.41
4:B:195:ARG:HG2	4:B:195:ARG:NH1	2.35	0.41
1:C:5:DG:H4'	1:C:6:DG:OP1	2.21	0.41
1:C:6:DG:N2	2:D:13:DC:O2	2.53	0.41
1:C:9:DA:H2"	1:C:10:DA:C8	2.55	0.41
1:C:4:DA:H2'	4:B:64:HIS:O	2.20	0.41
3:A:90:LEU:O	3:A:95:CYS:SG	2.79	0.41
4:B:329:VAL:HG23	4:B:343:LYS:O	2.21	0.41
4:B:114:LYS:CE	4:B:114:LYS:HA	2.51	0.41
4:B:55:PHE:N	4:B:239:ASP:OD1	2.42	0.41
4:B:47:GLN:HA	4:B:48:PRO:HD3	1.87	0.41
3:A:145:ILE:HD13	3:A:148:GLN:NE2	2.35	0.41
3:A:175:LEU:HA	3:A:175:LEU:HD12	1.72	0.41
4:B:97:LEU:HD12	4:B:109:HIS:C	2.41	0.41
4:B:57:TYR:O	4:B:60:GLU:HB2	2.21	0.40
3:A:262:LEU:HA	3:A:262:LEU:HD12	1.88	0.40
3:A:273:ARG:HG3	3:A:280:LEU:HD23	2.03	0.40
4:B:145:LYS:HB2	4:B:145:LYS:HE3	1.80	0.40
4:B:175:TYR:HD1	4:B:175:TYR:H	1.67	0.40
4:B:171:SER:O	4:B:173:LEU:N	2.53	0.40
4:B:109:HIS:CE1	4:B:142:VAL:HG12	2.56	0.40
4:B:155:MET:CE	4:B:198:ALA:HB2	2.49	0.40
4:B:88:VAL:CG2	4:B:218:LEU:HD22	2.31	0.40
4:B:160:ILE:HG22	4:B:186:LEU:CG	2.51	0.40
3:A:267:ARG:HD3	3:A:285:GLU:CD	2.41	0.40
3:A:168:PRO:C	3:A:170:GLY:N	2.74	0.40
4:B:257:ALA:HA	4:B:346:LEU:O	2.22	0.40
4:B:147:VAL:HG13	4:B:202:THR:HG23	2.03	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)
2:D:1:DT:O4	2:D:1:DT:O4[6_555]	1.77	0.43

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
3	A	271/274 (99%)	239 (88%)	26 (10%)	6 (2%)	8 22
4	B	310/313 (99%)	249 (80%)	39 (13%)	22 (7%)	1 2
All	All	581/587 (99%)	488 (84%)	65 (11%)	28 (5%)	3 5

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	B	87	TYR
4	B	114	LYS
4	B	127	PRO
4	B	225	PHE
3	A	48	GLY
3	A	81	PRO
3	A	83	HIS
4	B	63	SER
4	B	113	GLY
4	B	136	ASN
4	B	163	TYR
4	B	170	HIS
4	B	172	ASP
4	B	243	PRO
4	B	275	LYS
4	B	290	GLY
3	A	49	GLU

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Mol	Chain	Res	Type
4	B	73	GLU
4	B	77	LYS
4	B	137	LEU
4	B	165	PRO
4	B	177	GLN
4	B	289	GLY
3	A	151	ASP
4	B	178	ALA
4	B	245	ALA
4	B	89	GLY
3	A	165	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
3	A	242/243 (100%)	220 (91%)	22 (9%)	12 26
4	B	268/269 (100%)	246 (92%)	22 (8%)	14 32
All	All	510/512 (100%)	466 (91%)	44 (9%)	13 29

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	51	SER
3	A	53	ASP
3	A	54	THR
3	A	71	THR
3	A	81	PRO
3	A	96	ARG
3	A	100	TYR
3	A	105	CYS
3	A	107	ASP
3	A	108	ARG
3	A	111	HIS
3	A	113	PHE

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Mol	Chain	Res	Type
3	A	119	GLN
3	A	146	GLU
3	A	168	PRO
3	A	175	LEU
3	A	176	THR
3	A	199	VAL
3	A	200	ASN
3	A	218	LYS
3	A	229	THR
3	A	284	MET
4	B	56	ARG
4	B	76	LYS
4	B	78	SER
4	B	87	TYR
4	B	114	LYS
4	B	120	VAL
4	B	121	CYS
4	B	127	PRO
4	B	163	TYR
4	B	172	ASP
4	B	179	GLU
4	B	183	ASP
4	B	227	ARG
4	B	268	LEU
4	B	272	LYS
4	B	288	ASN
4	B	310	VAL
4	B	323	LYS
4	B	329	VAL
4	B	331	LEU
4	B	341	GLU
4	B	350	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	29	GLN
3	A	111	HIS
3	A	114	GLN
3	A	137	ASN
3	A	148	GLN
3	A	181	HIS

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Mol	Chain	Res	Type
3	A	200	ASN
3	A	220	GLN
3	A	287	GLN
4	B	81	GLN
4	B	96	GLN
4	B	107	HIS
4	B	115	HIS
4	B	141	HIS
4	B	177	GLN
4	B	196	GLN
4	B	274	GLN
4	B	279	GLN
4	B	288	ASN
4	B	320	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)

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	5IU	D	10	1,2	12,21,22	6.28	3 (25%)	14,30,33	3.76	1 (7%)
2	5IU	D	5	1,2	12,21,22	6.18	3 (25%)	14,30,33	3.82	2 (14%)
2	5IU	D	8	1,2	12,21,22	5.87	3 (25%)	14,30,33	3.94	2 (14%)
2	5IU	D	9	1,2	12,21,22	5.94	3 (25%)	14,30,33	3.96	2 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means

no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	5IU	D	10	1,2	-	0/3/21/22	0/2/2/2
2	5IU	D	5	1,2	-	0/3/21/22	0/2/2/2
2	5IU	D	8	1,2	-	0/3/21/22	0/2/2/2
2	5IU	D	9	1,2	-	0/3/21/22	0/2/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	10	5IU	C5-I5	-21.33	1.63	2.10
2	D	5	5IU	C5-I5	-21.01	1.64	2.10
2	D	9	5IU	C5-I5	-20.13	1.65	2.10
2	D	8	5IU	C5-I5	-19.84	1.66	2.10
2	D	9	5IU	C4-N3	2.47	1.37	1.33
2	D	10	5IU	C6-N1	2.48	1.38	1.35
2	D	5	5IU	C4-N3	2.62	1.38	1.33
2	D	8	5IU	C4-N3	2.67	1.38	1.33
2	D	5	5IU	C6-N1	2.82	1.39	1.35
2	D	10	5IU	C4-N3	3.00	1.38	1.33
2	D	8	5IU	C6-N1	3.25	1.39	1.35
2	D	9	5IU	C6-N1	3.27	1.39	1.35

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	5	5IU	O4'-C1'-N1	2.02	111.21	107.72
2	D	8	5IU	C2'-C1'-N1	2.24	119.60	114.16
2	D	9	5IU	C2'-C1'-N1	2.33	119.83	114.16
2	D	10	5IU	C4-N3-C2	13.85	127.22	115.25
2	D	5	5IU	C4-N3-C2	14.03	127.37	115.25
2	D	9	5IU	C4-N3-C2	14.33	127.63	115.25
2	D	8	5IU	C4-N3-C2	14.35	127.66	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	10	5IU	7	0
2	D	5	5IU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	9	5IU	2	0

5.5 Carbohydrates (i)

There are no carbohydrates 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

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.