



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 20, 2018 – 08:03 PM EST

PDB ID : 6BJY  
Title : VSV Nucleocapsid with Polyamide Bound  
Authors : Gumpfer, R.H.; Luo, M.  
Deposited on : 2017-11-07  
Resolution : 3.46 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030736  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030736

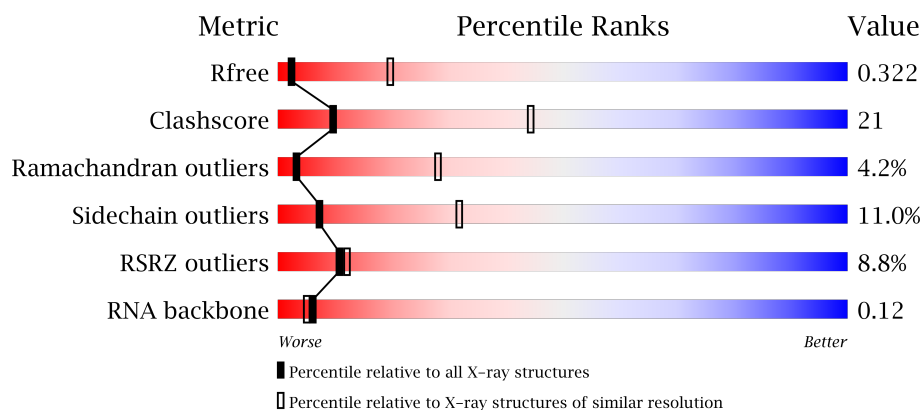
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.46 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))
$R_{free}$	100719	1135 (3.56-3.36)
Clashscore	112137	1040 (3.52-3.40)
Ramachandran outliers	110173	1009 (3.52-3.40)
Sidechain outliers	110143	1010 (3.52-3.40)
RSRZ outliers	101464	1017 (3.54-3.38)
RNA backbone	2435	1020 (4.02-2.86)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	R	45	<div> <div>9%</div> <div>7% 24% 56% 13%</div> </div>
2	A	421	<div> <div>11%</div> <div>61% 33% 5%</div> </div>
2	B	421	<div> <div>7%</div> <div>59% 32% 8% .</div> </div>
2	C	421	<div> <div>7%</div> <div>59% 31% 8% .</div> </div>

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Mol	Chain	Length	Quality of chain
2	D	421	<div><div></div><div>6%</div><div>59%</div><div>31%</div><div>9%</div><div></div></div>
2	E	421	<div><div></div><div>13%</div><div>66%</div><div>29%</div><div>5%</div><div></div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17494 atoms, of which 28 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.

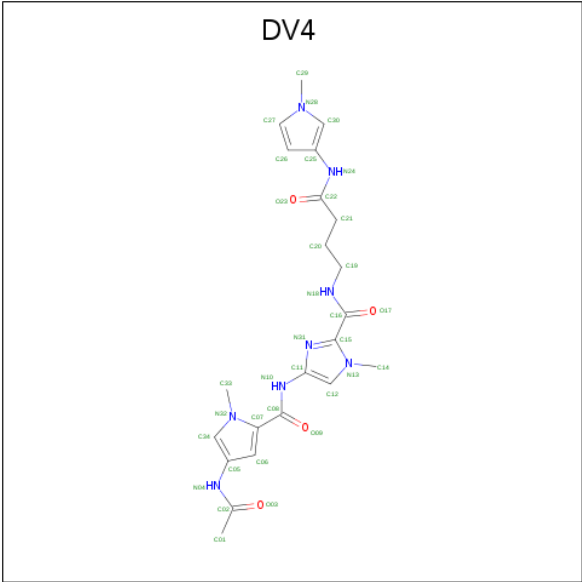
- Molecule 1 is a RNA chain called RNA (45-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	R	45	Total	C	N	O	P	0	0	0
			900	405	90	360	45			

- Molecule 2 is a protein called Nucleoprotein.

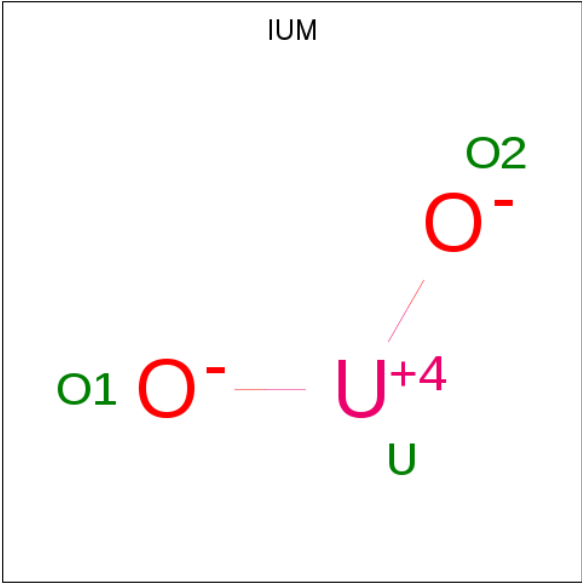
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	421	Total	C	N	O	S	0	0	0
			3327	2118	558	633	18			
2	B	415	Total	C	N	O	S	0	0	0
			3290	2097	552	623	18			
2	C	413	Total	C	N	O	S	0	0	0
			3275	2089	550	618	18			
2	D	416	Total	C	N	O	S	0	0	0
			3298	2103	553	624	18			
2	E	421	Total	C	N	O	S	0	0	0
			3327	2118	558	633	18			

- Molecule 3 is 4-{[4-(acetylamino)-1-methyl-1H-pyrrole-2-carbonyl]amino}-1-methyl-N-{4-[(1-methyl-1H-pyrrol-3-yl)amino]-4-oxobutyl}-1H-imidazole-2-carboxamide (three-letter code: DV4) (formula: C<sub>22</sub>H<sub>28</sub>N<sub>8</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	R	1	Total	C	H	N	O	0	0
			62	22	28	8	4		

- Molecule 4 is URANYL (VI) ION (three-letter code: IUM) (formula: O<sub>2</sub>U).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	U	0	0
			1	1		
4	A	1	Total	U	0	0
			1	1		
4	A	1	Total	U	0	0
			1	1		

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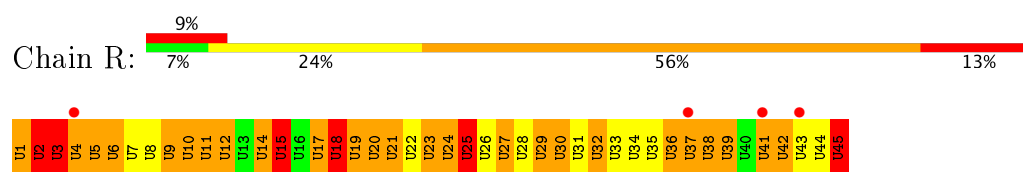
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	U 1	0	0
4	A	1	Total 1	U 1	0	0
4	B	1	Total 1	U 1	0	0
4	B	1	Total 1	U 1	0	0
4	B	1	Total 1	U 1	0	0
4	C	1	Total 1	U 1	0	0
4	C	1	Total 1	U 1	0	0
4	C	1	Total 1	U 1	0	0
4	D	1	Total 1	U 1	0	0
4	D	1	Total 1	U 1	0	0
4	E	1	Total 1	U 1	0	0
4	E	1	Total 1	U 1	0	0

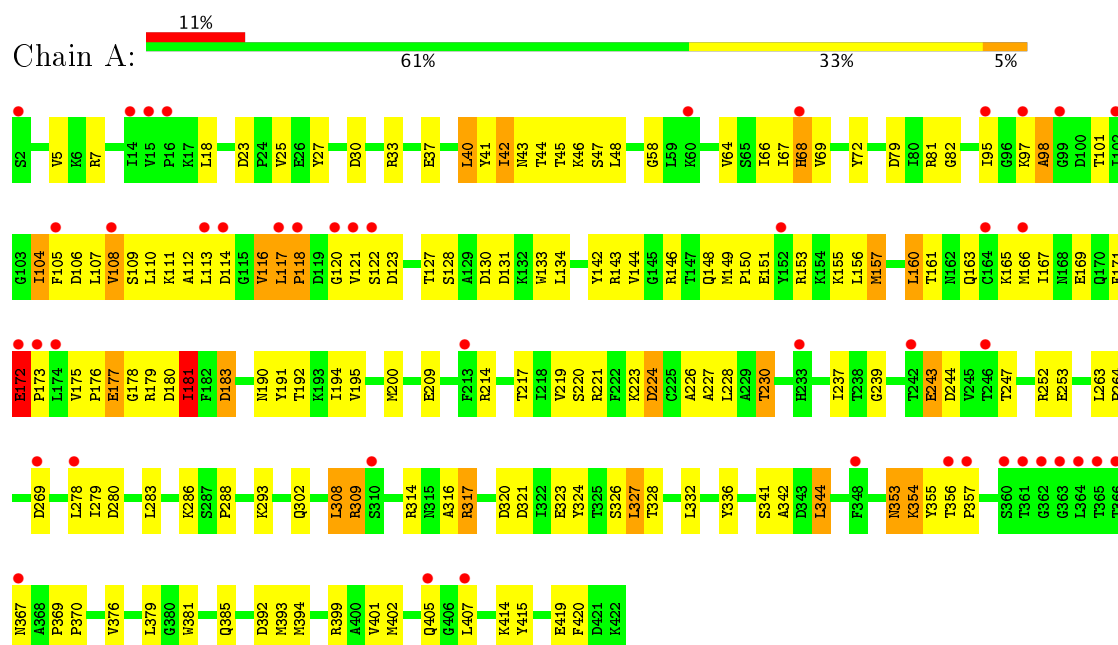
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

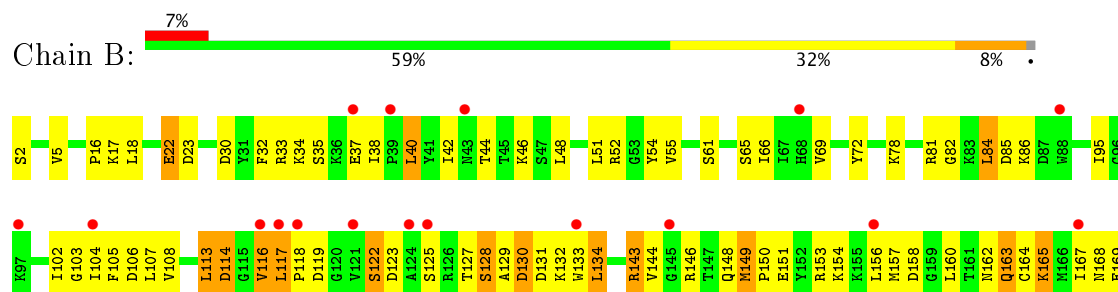
#### • Molecule 1: RNA (45-MER)

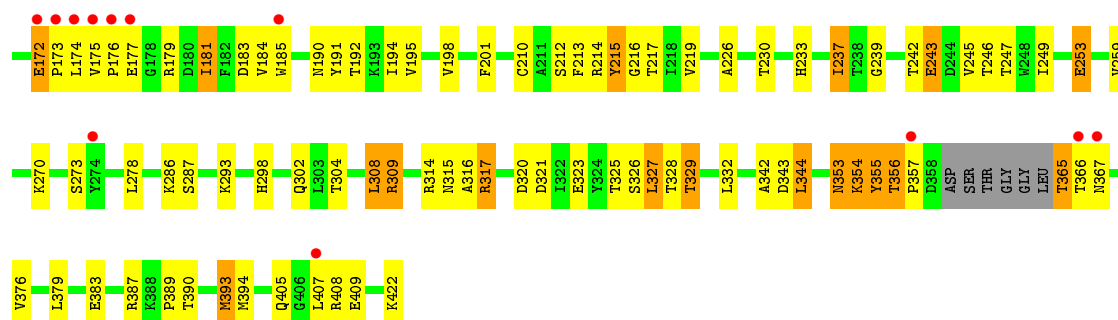


#### • Molecule 2: Nucleoprotein

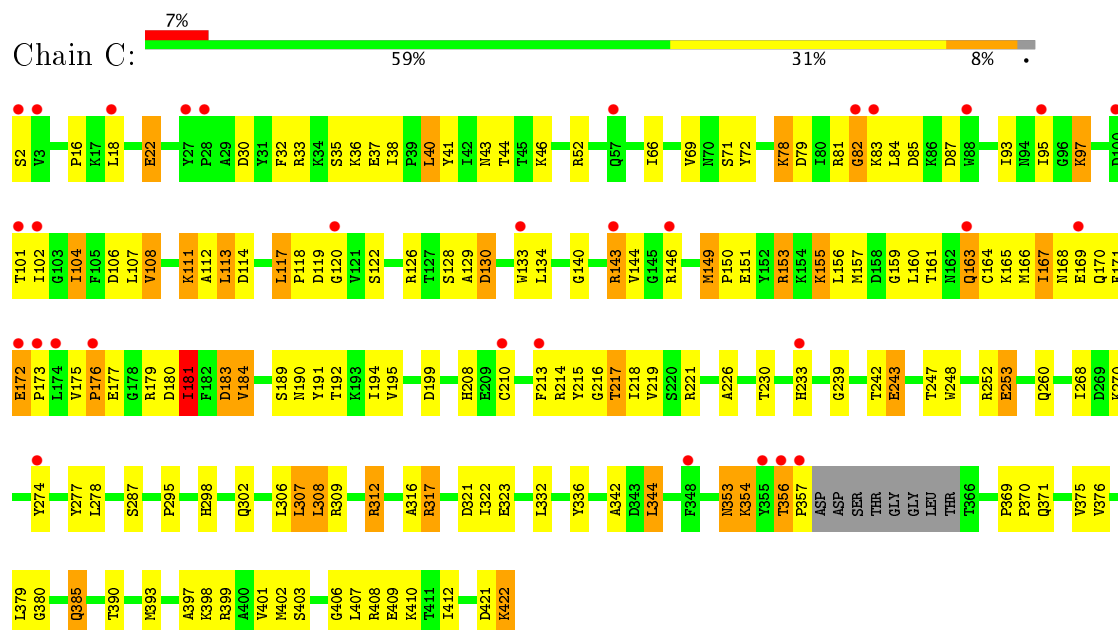


#### • Molecule 2: Nucleoprotein

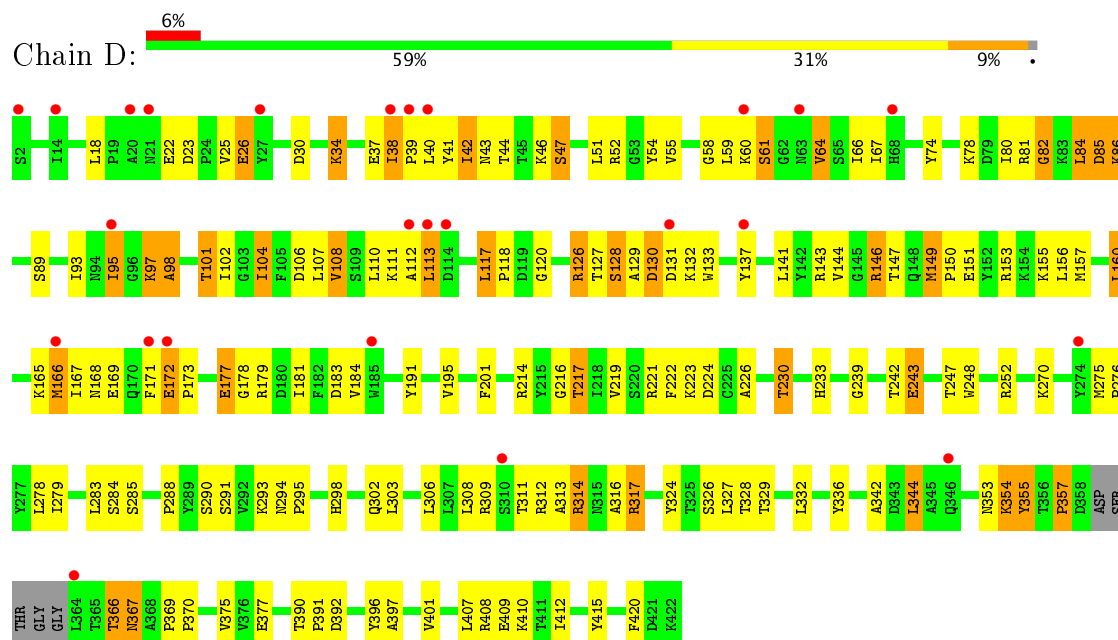




• Molecule 2: Nucleoprotein

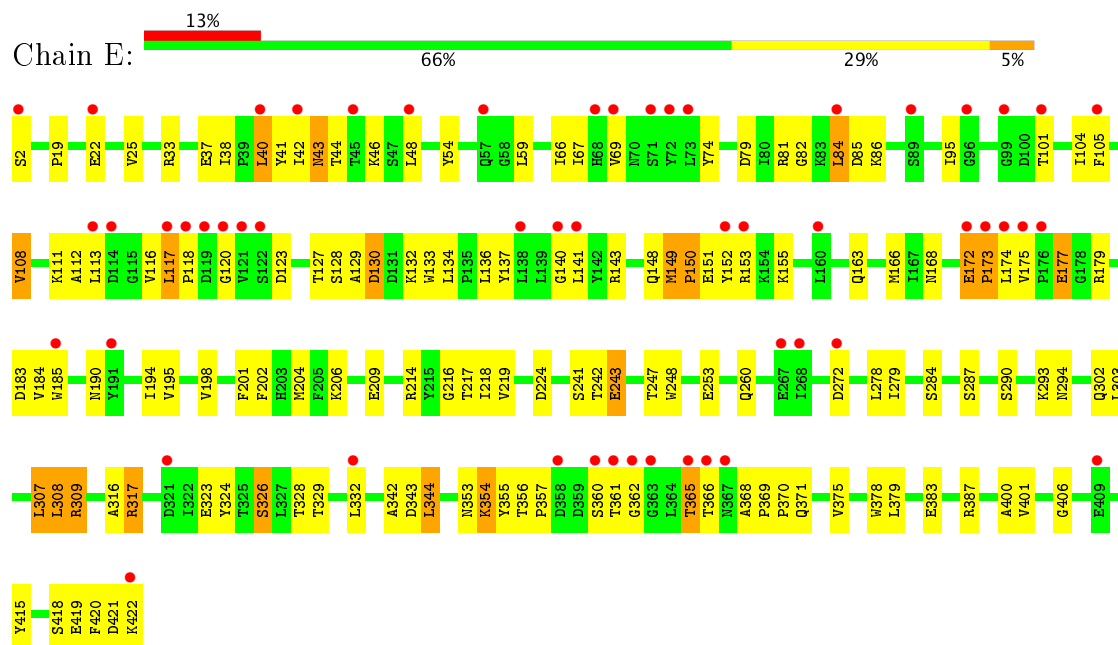


• Molecule 2: Nucleoprotein





● Molecule 2: Nucleoprotein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	75.48Å 165.48Å 234.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.30 – 3.46 46.30 – 3.46	Depositor EDS
% Data completeness (in resolution range)	92.3 (46.30-3.46) 92.3 (46.30-3.46)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.82 (at 3.48Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, $R_{free}$	0.266 , 0.311 0.280 , 0.322	Depositor DCC
$R_{free}$ test set	1998 reflections (5.52%)	DCC
Wilson B-factor (Å <sup>2</sup> )	100.3	Xtriage
Anisotropy	0.630	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 47.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.36$ , $\langle L^2 \rangle = 0.18$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	17494	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	121.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.57% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: DV4, IUM

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	R	0.58	1/989 (0.1%)	1.42	27/1526 (1.8%)
2	A	0.25	0/3403	0.45	0/4607
2	B	0.25	0/3365	0.46	0/4554
2	C	0.25	0/3350	0.48	0/4533
2	D	0.24	0/3373	0.44	0/4565
2	E	0.25	0/3403	0.45	0/4607
All	All	0.28	1/17883 (0.0%)	0.57	27/24392 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	1	U	C4-C5	-5.97	1.38	1.43

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	1	U	O5'-P-OP1	-15.45	91.79	105.70
1	R	1	U	OP1-P-OP2	-10.34	104.09	119.60
1	R	25	U	N3-C2-O2	-9.23	115.74	122.20
1	R	1	U	N1-C2-O2	-9.09	116.44	122.80
1	R	45	U	C6-N1-C2	8.56	126.14	121.00
1	R	1	U	C4-C5-C6	7.83	124.40	119.70
1	R	15	U	N1-C2-O2	7.42	128.00	122.80
1	R	25	U	N1-C2-O2	7.27	127.89	122.80
1	R	15	U	N3-C2-O2	-7.22	117.15	122.20
1	R	45	U	C4-C5-C6	-7.21	115.38	119.70
1	R	1	U	O4'-C1'-N1	7.09	113.87	108.20
1	R	1	U	N3-C4-O4	7.07	124.35	119.40
1	R	45	U	N1-C2-N3	-6.86	110.79	114.90
1	R	18	U	O4'-C1'-N1	6.75	113.60	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	45	U	N3-C4-C5	6.54	118.52	114.60
1	R	15	U	N3-C4-O4	-6.39	114.92	119.40
1	R	1	U	N3-C2-O2	6.29	126.60	122.20
1	R	45	U	C6-N1-C1'	-6.06	112.72	121.20
1	R	2	U	N1-C1'-C2'	6.03	121.84	114.00
1	R	1	U	C5-C4-O4	-5.83	122.40	125.90
1	R	45	U	C3'-C2'-C1'	5.76	106.11	101.50
1	R	2	U	O4'-C1'-N1	5.65	112.72	108.20
1	R	3	U	C5-C6-N1	5.50	125.45	122.70
1	R	15	U	C5-C4-O4	5.45	129.17	125.90
1	R	45	U	N3-C2-O2	5.39	125.98	122.20
1	R	2	U	C5-C6-N1	5.13	125.27	122.70
1	R	45	U	C5-C4-O4	-5.12	122.83	125.90

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	R	900	0	451	158	0
2	A	3327	0	3287	135	0
2	B	3290	0	3253	135	0
2	C	3275	0	3242	147	0
2	D	3298	0	3264	147	0
2	E	3327	0	3287	115	0
3	R	34	28	0	20	0
4	A	5	0	0	0	0
4	B	3	0	0	0	0
4	C	3	0	0	0	0
4	D	2	0	0	0	0
4	E	2	0	0	0	0
All	All	17466	28	16784	736	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 21.

All (736) 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:R:25:U:H1'	3:R:101:DV4:C21	1.59	1.32
1:R:18:U:O2'	1:R:19:U:H3'	1.23	1.29
1:R:25:U:H1'	3:R:101:DV4:C20	1.72	1.20
2:B:37:GLU:HB2	2:B:108:VAL:HG21	1.18	1.15
2:A:165:LYS:HA	2:E:184:VAL:HG22	1.20	1.11
2:B:172:GLU:HB3	2:B:173:PRO:HD3	1.32	1.07
2:C:117:LEU:HB2	2:C:118:PRO:HD3	1.38	1.05
1:R:26:U:H4'	3:R:101:DV4:C14	1.87	1.04
2:B:117:LEU:HB2	2:B:118:PRO:HD3	1.42	1.02
1:R:11:U:H3'	1:R:12:U:H5''	1.41	1.01
1:R:25:U:C1'	3:R:101:DV4:C21	2.38	1.01
1:R:15:U:O4	2:C:408:ARG:HG3	1.61	1.01
2:A:117:LEU:HB3	2:A:118:PRO:HD3	1.41	1.00
1:R:44:U:C2'	1:R:45:U:H5''	1.91	1.00
1:R:15:U:C4	2:C:408:ARG:HG3	2.00	0.97
1:R:44:U:H2'	1:R:45:U:H5''	1.47	0.95
1:R:2:U:H3'	1:R:3:U:H6	1.27	0.95
2:E:117:LEU:HB2	2:E:118:PRO:HD3	1.49	0.95
1:R:20:U:OP1	2:B:286:LYS:NZ	2.03	0.92
2:D:117:LEU:HB2	2:D:118:PRO:HD3	1.47	0.92
2:E:129:ALA:HB1	2:E:133:TRP:HE1	1.32	0.92
1:R:26:U:C4'	3:R:101:DV4:C14	2.48	0.92
1:R:18:U:H1'	1:R:20:U:OP2	1.70	0.92
1:R:20:U:O2'	1:R:21:U:OP1	1.87	0.91
1:R:27:U:O2'	1:R:29:U:OP2	1.88	0.91
1:R:44:U:C3'	1:R:45:U:H5''	1.96	0.90
1:R:4:U:H2'	2:D:317:ARG:HG3	1.54	0.88
1:R:18:U:HO2'	1:R:19:U:H3'	1.41	0.86
2:B:23:ASP:HB3	2:B:286:LYS:HE3	1.58	0.86
1:R:1:U:OP2	1:R:1:U:H2'	1.74	0.85
2:A:223:LYS:HG2	2:A:224:ASP:OD1	1.76	0.85
1:R:4:U:OP2	2:D:290:SER:HB2	1.77	0.85
2:C:155:LYS:HA	2:C:155:LYS:HE3	1.58	0.84
1:R:17:U:H2'	1:R:18:U:C5'	2.07	0.84
2:B:54:TYR:CE1	2:B:122:SER:HB2	2.13	0.84
2:C:2:SER:HB3	2:D:243:GLU:HG3	1.59	0.84
1:R:2:U:H3'	1:R:3:U:C6	2.14	0.83
1:R:18:U:O2'	1:R:19:U:C3'	2.19	0.82
2:C:38:ILE:HD11	2:C:107:LEU:HB3	1.60	0.82
2:A:175:VAL:HG13	2:A:181:ILE:HD13	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:143:ARG:HE	2:D:155:LYS:HE3	1.45	0.82
1:R:36:U:O2'	1:R:37:U:OP2	1.97	0.82
2:B:174:LEU:HD23	2:B:174:LEU:O	1.81	0.81
1:R:1:U:P	1:R:1:U:H2'	2.21	0.80
3:R:101:DV4:C27	2:A:320:ASP:HB3	2.12	0.80
2:E:43:ASN:ND2	2:E:67:ILE:HG23	1.97	0.79
2:C:199:ASP:HB2	2:C:217:THR:OG1	1.82	0.79
1:R:17:U:O2'	1:R:18:U:OP1	2.00	0.78
2:A:133:TRP:HB3	2:A:167:ILE:HD13	1.64	0.77
2:E:356:THR:HG23	2:E:357:PRO:HD3	1.66	0.77
2:A:165:LYS:HA	2:E:184:VAL:CG2	2.10	0.77
2:D:43:ASN:HB3	2:D:112:ALA:O	1.84	0.77
2:D:43:ASN:ND2	2:D:113:LEU:O	2.17	0.77
2:C:379:LEU:HB3	2:D:354:LYS:HD2	1.68	0.76
2:B:37:GLU:CB	2:B:108:VAL:HG21	2.07	0.76
1:R:3:U:H4'	2:D:224:ASP:CB	2.16	0.75
2:B:104:ILE:HD11	2:B:198:VAL:HG22	1.67	0.75
2:C:133:TRP:HB3	2:C:167:ILE:HG21	1.66	0.75
1:R:20:U:H2'	1:R:21:U:O4'	1.86	0.75
2:A:40:LEU:HD22	2:A:42:ILE:HG12	1.68	0.75
1:R:25:U:H6	3:R:101:DV4:C20	1.99	0.75
1:R:15:U:C5	2:C:408:ARG:HG3	2.22	0.75
2:A:226:ALA:O	2:A:230:THR:HG22	1.86	0.75
1:R:17:U:HO2'	1:R:18:U:P	2.09	0.75
2:C:159:GLY:O	2:C:163:GLN:NE2	2.20	0.75
2:D:143:ARG:HD3	2:D:216:GLY:HA2	1.69	0.75
2:D:324:TYR:O	2:D:328:THR:HG23	1.87	0.74
2:B:103:GLY:N	2:B:106:ASP:OD2	2.16	0.74
2:D:39:PRO:HB3	2:D:110:LEU:HD12	1.69	0.74
1:R:1:U:C5	1:R:2:U:C6	2.74	0.74
1:R:1:U:C5	1:R:2:U:N1	2.55	0.74
2:B:172:GLU:HB3	2:B:173:PRO:CD	2.16	0.74
2:B:84:LEU:HD12	2:B:86:LYS:O	1.88	0.74
2:C:172:GLU:H	2:C:173:PRO:HD2	1.52	0.74
2:B:176:PRO:O	2:B:181:ILE:HD11	1.87	0.73
2:A:223:LYS:NZ	2:A:280:ASP:OD1	2.22	0.73
2:B:104:ILE:HD11	2:B:198:VAL:HA	1.69	0.72
2:D:43:ASN:HB2	2:D:111:LYS:HB3	1.70	0.72
1:R:3:U:H4'	2:D:224:ASP:HB3	1.69	0.72
2:A:324:TYR:O	2:A:328:THR:HG23	1.90	0.72
2:B:146:ARG:O	2:B:146:ARG:HG2	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:89:SER:O	2:D:270:LYS:NZ	2.22	0.72
2:C:191:TYR:O	2:C:195:VAL:HG13	1.90	0.71
1:R:1:U:O2'	1:R:2:U:O4'	2.08	0.71
2:A:379:LEU:HB3	2:B:354:LYS:HD2	1.71	0.71
2:C:171:PHE:O	2:C:172:GLU:HG3	1.89	0.71
2:D:133:TRP:HB3	2:D:167:ILE:HD13	1.73	0.71
2:B:184:VAL:HG13	2:C:165:LYS:HA	1.70	0.71
2:B:355:TYR:CD2	2:B:357:PRO:HD2	2.25	0.71
1:R:1:U:C2'	1:R:1:U:P	2.78	0.71
2:D:195:VAL:HG13	2:D:217:THR:OG1	1.91	0.70
2:B:44:THR:HG21	2:B:116:VAL:HG13	1.71	0.70
2:D:355:TYR:O	2:D:357:PRO:HD3	1.91	0.70
1:R:1:U:C5	1:R:2:U:H1'	2.26	0.70
2:C:140:GLY:HA2	2:C:216:GLY:HA3	1.74	0.70
2:E:224:ASP:OD2	2:E:279:ILE:HG13	1.91	0.69
2:E:324:TYR:O	2:E:328:THR:HG23	1.91	0.69
1:R:39:U:OP2	2:E:287:SER:N	2.26	0.69
2:E:356:THR:CG2	2:E:357:PRO:HD3	2.22	0.69
1:R:25:U:C6	3:R:101:DV4:C20	2.76	0.69
2:B:38:ILE:HD11	2:B:107:LEU:HD13	1.72	0.69
2:C:37:GLU:HB2	2:C:108:VAL:HG21	1.74	0.69
2:C:149:MET:O	2:C:151:GLU:N	2.26	0.68
1:R:15:U:O4	2:C:408:ARG:CG	2.41	0.68
1:R:23:U:H3	3:R:101:DV4:C22	2.05	0.68
2:E:195:VAL:HG13	2:E:217:THR:HG22	1.74	0.68
1:R:17:U:H2'	1:R:18:U:H5''	1.75	0.68
1:R:1:U:H5	1:R:2:U:C6	2.10	0.68
2:D:38:ILE:H	2:D:108:VAL:HG21	1.57	0.68
2:E:174:LEU:HD23	2:E:175:VAL:HG13	1.76	0.68
2:E:130:ASP:O	2:E:132:LYS:HD2	1.93	0.68
2:A:192:THR:O	2:A:195:VAL:HG22	1.94	0.67
2:B:149:MET:O	2:B:151:GLU:N	2.26	0.67
2:B:164:CYS:HA	2:B:168:ASN:H	1.59	0.67
1:R:26:U:O2'	1:R:27:U:H5'	1.93	0.67
1:R:1:U:O2'	1:R:2:U:P	2.53	0.67
2:A:381:TRP:O	2:A:385:GLN:NE2	2.28	0.67
2:B:72:TYR:CE2	2:B:134:LEU:HD12	2.30	0.67
2:B:214:ARG:HA	2:B:217:THR:HG22	1.78	0.66
2:C:353:ASN:N	2:C:353:ASN:OD1	2.29	0.66
1:R:25:U:C1'	3:R:101:DV4:C20	2.64	0.66
2:B:325:THR:O	2:B:329:THR:HG22	1.93	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:325:THR:O	2:B:328:THR:HG22	1.95	0.66
2:A:177:GLU:OE1	2:A:178:GLY:N	2.28	0.66
2:A:41:TYR:O	2:A:42:ILE:HG23	1.96	0.66
2:D:179:ARG:HA	2:D:183:ASP:CG	2.16	0.66
1:R:44:U:H5''	2:E:143:ARG:HH22	1.60	0.65
2:C:117:LEU:HB2	2:C:118:PRO:CD	2.20	0.65
2:A:117:LEU:HB3	2:A:118:PRO:CD	2.19	0.65
2:D:34:LYS:HD2	2:D:34:LYS:N	2.10	0.65
1:R:38:U:H3'	1:R:39:U:H5''	1.77	0.65
1:R:1:U:C6	1:R:2:U:C1'	2.79	0.65
2:E:104:ILE:HD11	2:E:198:VAL:HG22	1.78	0.65
2:D:172:GLU:HB3	2:D:173:PRO:HD3	1.79	0.65
2:B:167:ILE:HG22	2:B:169:GLU:HG2	1.78	0.65
2:B:38:ILE:O	2:B:38:ILE:HG13	1.97	0.65
2:D:156:LEU:O	2:D:160:LEU:HD23	1.97	0.65
2:C:172:GLU:H	2:C:173:PRO:CD	2.10	0.65
2:C:302:GLN:HG2	2:C:316:ALA:CB	2.27	0.65
2:E:37:GLU:HB2	2:E:108:VAL:HG21	1.77	0.65
1:R:23:U:OP2	2:B:317:ARG:NH2	2.31	0.64
1:R:4:U:H2'	2:D:317:ARG:CG	2.26	0.64
2:D:214:ARG:HA	2:D:217:THR:HG22	1.79	0.64
2:B:192:THR:O	2:B:195:VAL:HG22	1.97	0.64
2:E:179:ARG:HA	2:E:183:ASP:CG	2.17	0.64
1:R:18:U:C1'	1:R:20:U:OP2	2.45	0.64
2:A:336:TYR:OH	2:A:392:ASP:OD2	2.11	0.64
2:B:117:LEU:HB2	2:B:118:PRO:CD	2.22	0.64
2:B:184:VAL:HG11	2:C:166:MET:H	1.63	0.64
1:R:44:U:H5''	2:E:143:ARG:NH2	2.12	0.64
1:R:1:U:O2'	1:R:2:U:OP2	2.16	0.63
2:A:317:ARG:CZ	2:A:317:ARG:H	2.12	0.63
1:R:1:U:O2'	1:R:2:U:C5'	2.46	0.63
2:D:171:PHE:CZ	2:D:173:PRO:HG2	2.34	0.62
2:B:52:ARG:NH1	2:B:127:THR:O	2.31	0.62
2:D:117:LEU:HB2	2:D:118:PRO:CD	2.27	0.62
1:R:1:U:C6	1:R:2:U:C6	2.87	0.62
2:B:54:TYR:CD1	2:B:122:SER:HB2	2.34	0.62
2:E:137:TYR:CE1	2:E:141:LEU:HD11	2.35	0.62
1:R:44:U:H2'	1:R:45:U:C5'	2.27	0.62
2:A:191:TYR:O	2:A:195:VAL:HG13	1.99	0.61
2:C:36:LYS:HG3	2:C:93:ILE:HD11	1.82	0.61
1:R:26:U:O4'	3:R:101:DV4:C14	2.47	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:43:ASN:CB	2:D:111:LYS:HB3	2.30	0.61
1:R:23:U:N3	3:R:101:DV4:C21	2.63	0.61
2:A:43:ASN:CG	2:A:111:LYS:HG2	2.21	0.61
2:B:409:GLU:OE2	2:B:409:GLU:N	2.33	0.61
2:A:177:GLU:CD	2:A:178:GLY:H	2.04	0.61
2:C:226:ALA:O	2:C:230:THR:HG23	2.01	0.61
1:R:8:U:H5''	2:D:143:ARG:NH2	2.16	0.61
2:D:149:MET:O	2:D:151:GLU:N	2.34	0.61
2:D:177:GLU:HG2	2:D:178:GLY:H	1.66	0.61
2:A:81:ARG:NH1	2:A:209:GLU:OE2	2.33	0.61
2:C:342:ALA:HB1	2:C:344:LEU:HD23	1.83	0.61
2:D:328:THR:HG21	2:D:415:TYR:OH	2.01	0.61
2:E:59:LEU:HD11	2:E:137:TYR:CE1	2.35	0.61
2:E:172:GLU:H	2:E:173:PRO:HD2	1.65	0.61
2:A:243:GLU:HG3	2:E:2:SER:HB3	1.83	0.60
1:R:1:U:C5	1:R:2:U:C1'	2.84	0.60
2:C:163:GLN:N	2:C:163:GLN:HE21	1.99	0.60
2:C:163:GLN:O	2:C:167:ILE:HG13	2.00	0.60
2:D:366:THR:OG1	2:D:367:ASN:N	2.33	0.60
2:A:354:LYS:HD2	2:E:379:LEU:HB3	1.84	0.60
2:E:370:PRO:HD2	2:E:378:TRP:CH2	2.36	0.60
1:R:2:U:C3'	1:R:3:U:C6	2.84	0.60
1:R:23:U:H2'	1:R:25:U:H5''	1.83	0.60
2:B:2:SER:HB3	2:C:243:GLU:HG3	1.83	0.60
2:E:174:LEU:O	2:E:175:VAL:HG13	2.02	0.60
2:E:302:GLN:HG2	2:E:316:ALA:CB	2.32	0.60
1:R:1:U:P	1:R:1:U:C1'	2.89	0.60
2:E:317:ARG:H	2:E:317:ARG:NE	2.00	0.59
2:B:179:ARG:HA	2:B:183:ASP:CG	2.23	0.59
2:A:79:ASP:OD2	2:A:81:ARG:HD2	2.02	0.59
2:B:317:ARG:CZ	2:B:317:ARG:H	2.15	0.59
2:C:192:THR:O	2:C:195:VAL:HG22	2.03	0.59
2:E:278:LEU:HD13	2:E:284:SER:HB3	1.84	0.59
1:R:30:U:H2'	1:R:31:U:O4'	2.02	0.59
2:A:23:ASP:HB2	2:A:286:LYS:NZ	2.18	0.59
2:A:143:ARG:HD3	2:A:219:VAL:HG11	1.84	0.59
2:C:32:PHE:HA	2:C:35:SER:O	2.03	0.59
2:D:151:GLU:OE1	2:D:155:LYS:NZ	2.29	0.59
1:R:11:U:H3'	1:R:12:U:C5'	2.25	0.59
2:C:164:CYS:HA	2:C:168:ASN:HA	1.85	0.58
1:R:6:U:C4	2:D:408:ARG:HD3	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:354:LYS:HE3	2:E:356:THR:HA	1.84	0.58
2:A:317:ARG:NE	2:A:317:ARG:H	2.01	0.58
2:D:60:LYS:O	2:D:61:SER:HB2	2.04	0.58
2:A:309:ARG:NH1	2:E:419:GLU:OE1	2.35	0.58
1:R:23:U:H3	3:R:101:DV4:C21	2.17	0.58
2:B:118:PRO:O	2:B:119:ASP:HB2	2.03	0.58
2:B:230:THR:HG21	2:B:298:HIS:CE1	2.38	0.58
2:B:390:THR:OG1	2:B:393:MET:HG2	2.03	0.58
2:E:117:LEU:HB2	2:E:118:PRO:CD	2.30	0.58
2:B:144:VAL:HG11	2:B:156:LEU:HG	1.85	0.58
1:R:6:U:C1'	2:D:149:MET:HG3	2.34	0.58
2:A:227:ALA:O	2:A:230:THR:HG23	2.03	0.58
2:B:253:GLU:H	2:B:253:GLU:CD	2.07	0.58
2:C:43:ASN:CG	2:C:112:ALA:HB3	2.24	0.58
2:E:214:ARG:HH21	2:E:218:ILE:HD12	1.69	0.58
2:C:81:ARG:HB2	2:C:208:HIS:HE2	1.69	0.57
1:R:2:U:C2'	1:R:3:U:C6	2.87	0.57
2:B:104:ILE:CD1	2:B:198:VAL:HG22	2.33	0.57
2:D:342:ALA:HB1	2:D:344:LEU:HD23	1.86	0.57
2:A:149:MET:O	2:A:151:GLU:N	2.37	0.57
2:D:302:GLN:HG2	2:D:316:ALA:CB	2.35	0.57
2:A:253:GLU:CD	2:A:253:GLU:H	2.07	0.57
2:A:353:ASN:N	2:A:353:ASN:OD1	2.37	0.57
2:A:43:ASN:ND2	2:A:111:LYS:HG2	2.20	0.57
1:R:1:U:C6	1:R:2:U:H1'	2.38	0.57
2:E:129:ALA:HB1	2:E:133:TRP:NE1	2.11	0.57
2:A:43:ASN:HB2	2:A:112:ALA:H	1.70	0.57
2:C:210:CYS:HB3	2:C:213:PHE:CE2	2.40	0.57
2:A:320:ASP:HA	2:A:324:TYR:OH	2.05	0.56
2:C:317:ARG:NH1	2:C:317:ARG:H	2.03	0.56
2:D:177:GLU:CG	2:D:178:GLY:H	2.19	0.56
2:D:37:GLU:HB2	2:D:108:VAL:HG11	1.87	0.56
2:E:137:TYR:HE1	2:E:141:LEU:HD11	1.69	0.56
2:B:320:ASP:HB3	2:C:312:ARG:NH2	2.20	0.56
2:B:353:ASN:N	2:B:353:ASN:OD1	2.37	0.56
2:D:226:ALA:O	2:D:230:THR:HG23	2.05	0.56
2:A:177:GLU:HG2	2:A:183:ASP:OD2	2.06	0.56
2:E:361:THR:OG1	2:E:362:GLY:N	2.38	0.56
2:C:336:TYR:CG	2:C:393:MET:HG2	2.40	0.56
1:R:4:U:C5'	2:D:291:SER:HB3	2.35	0.56
2:B:323:GLU:O	2:B:327:LEU:HD22	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:309:ARG:HH21	2:E:400:ALA:HB2	1.71	0.56
2:A:328:THR:HG21	2:A:415:TYR:OH	2.05	0.56
1:R:17:U:C2'	1:R:18:U:H5''	2.35	0.56
1:R:34:U:H2'	1:R:35:U:O4'	2.06	0.56
2:D:317:ARG:H	2:D:317:ARG:NE	2.04	0.55
2:A:166:MET:H	2:E:184:VAL:CG1	2.18	0.55
2:B:148:GLN:OE1	2:B:179:ARG:HG3	2.06	0.55
2:C:104:ILE:HD12	2:C:104:ILE:H	1.72	0.55
2:D:129:ALA:HB1	2:D:133:TRP:HE1	1.72	0.55
2:E:253:GLU:CD	2:E:253:GLU:H	2.07	0.55
1:R:2:U:H2'	1:R:3:U:C6	2.42	0.55
1:R:36:U:O2'	1:R:37:U:P	2.65	0.55
2:A:144:VAL:HG11	2:A:156:LEU:HG	1.88	0.55
2:A:146:ARG:HG2	2:A:146:ARG:O	2.06	0.55
1:R:1:U:OP2	1:R:1:U:C2'	2.50	0.55
2:D:38:ILE:H	2:D:108:VAL:CG2	2.20	0.55
2:D:302:GLN:HG3	2:D:313:ALA:HB1	1.89	0.55
2:C:376:VAL:HG13	2:D:354:LYS:HA	1.89	0.55
1:R:1:U:O2'	1:R:2:U:C4'	2.55	0.55
2:C:97:LYS:HD3	2:C:97:LYS:N	2.22	0.54
2:A:180:ASP:N	2:A:183:ASP:OD1	2.34	0.54
1:R:3:U:H4'	2:D:224:ASP:HB2	1.89	0.54
2:D:97:LYS:HD3	2:D:97:LYS:N	2.22	0.54
1:R:12:U:OP2	2:C:287:SER:N	2.40	0.54
2:C:321:ASP:OD1	2:D:233:HIS:ND1	2.39	0.54
1:R:1:U:P	1:R:1:U:O4'	2.66	0.54
2:D:128:SER:OG	2:D:129:ALA:N	2.39	0.54
2:B:270:LYS:HE3	2:B:273:SER:HB2	1.89	0.54
2:D:104:ILE:HD13	2:D:201:PHE:CD2	2.43	0.54
1:R:41:U:O5'	2:E:317:ARG:NH2	2.41	0.54
1:R:26:U:C1'	3:R:101:DV4:C14	2.86	0.54
2:C:149:MET:C	2:C:151:GLU:H	2.10	0.54
1:R:1:U:C5	1:R:2:U:C2	2.96	0.54
2:A:214:ARG:HA	2:A:217:THR:HG22	1.90	0.54
2:D:66:ILE:HD11	2:D:191:TYR:HB2	1.90	0.53
2:B:365:THR:HG23	2:B:366:THR:H	1.72	0.53
2:B:376:VAL:HG13	2:C:354:LYS:HB2	1.90	0.53
2:B:105:PHE:C	2:B:107:LEU:H	2.12	0.53
2:D:146:ARG:HH11	2:D:223:LYS:HE2	1.73	0.53
2:D:248:TRP:CD1	2:D:375:VAL:HG22	2.44	0.53
1:R:29:U:H3'	1:R:30:U:H5''	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:419:GLU:OE2	2:B:309:ARG:HD3	2.09	0.53
2:A:379:LEU:CB	2:B:354:LYS:HD2	2.37	0.53
2:D:224:ASP:OD1	2:D:279:ILE:HG13	2.08	0.53
2:E:79:ASP:HB2	2:E:81:ARG:HG3	1.90	0.53
1:R:29:U:OP1	2:A:286:LYS:NZ	2.29	0.53
2:B:102:ILE:HB	2:B:106:ASP:OD2	2.09	0.53
2:A:323:GLU:CD	2:B:239:GLY:HA3	2.29	0.53
2:B:323:GLU:CD	2:C:239:GLY:HA3	2.30	0.53
2:B:383:GLU:OE1	2:B:387:ARG:HD3	2.09	0.53
2:C:306:LEU:HD22	2:C:412:ILE:HD12	1.91	0.53
2:D:25:VAL:HG11	2:D:288:PRO:HA	1.91	0.53
2:C:146:ARG:HD3	2:C:146:ARG:O	2.09	0.52
2:E:309:ARG:NH2	2:E:400:ALA:HB2	2.24	0.52
2:E:43:ASN:HD22	2:E:67:ILE:HG23	1.71	0.52
2:C:171:PHE:CD1	2:C:173:PRO:HD2	2.44	0.52
2:D:58:GLY:O	2:D:64:VAL:HG22	2.08	0.52
2:E:172:GLU:H	2:E:173:PRO:CD	2.22	0.52
2:E:84:LEU:HD22	2:E:86:LYS:O	2.09	0.52
1:R:8:U:H2'	1:R:9:U:H5''	1.90	0.52
2:D:43:ASN:HB2	2:D:112:ALA:N	2.25	0.52
1:R:21:U:H2'	1:R:22:U:O4'	2.09	0.52
2:B:342:ALA:HB1	2:B:344:LEU:HD23	1.92	0.52
2:C:323:GLU:CD	2:D:239:GLY:HA3	2.30	0.52
2:D:278:LEU:HD13	2:D:284:SER:HB3	1.92	0.52
2:E:149:MET:O	2:E:151:GLU:N	2.42	0.52
1:R:25:U:H1'	3:R:101:DV4:C19	2.37	0.52
2:E:224:ASP:CG	2:E:279:ILE:HG13	2.30	0.52
1:R:9:U:OP2	2:D:143:ARG:NH1	2.37	0.52
1:R:14:U:P	2:C:317:ARG:HH21	2.33	0.52
1:R:17:U:C2'	1:R:18:U:C5'	2.85	0.52
2:C:253:GLU:CD	2:C:253:GLU:H	2.13	0.52
2:A:336:TYR:CD2	2:A:393:MET:HG2	2.45	0.51
2:B:210:CYS:HB3	2:B:213:PHE:CE2	2.45	0.51
2:C:107:LEU:HD23	2:C:274:TYR:HE1	1.74	0.51
2:A:48:LEU:HD22	2:A:48:LEU:H	1.75	0.51
2:D:165:LYS:O	2:D:167:ILE:HG13	2.09	0.51
2:D:143:ARG:HD2	2:D:219:VAL:HG13	1.92	0.51
2:A:227:ALA:HA	2:A:230:THR:CG2	2.40	0.51
2:A:167:ILE:HG22	2:A:169:GLU:HG2	1.92	0.51
2:A:224:ASP:OD1	2:A:224:ASP:N	2.43	0.51
2:B:16:PRO:HB2	2:C:242:THR:HB	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:356:THR:N	2:B:357:PRO:CD	2.74	0.51
2:D:101:THR:OG1	2:D:101:THR:O	2.19	0.51
2:D:38:ILE:N	2:D:108:VAL:HG21	2.25	0.51
2:A:323:GLU:OE1	2:B:239:GLY:HA3	2.11	0.51
2:D:309:ARG:NH1	2:D:396:TYR:OH	2.44	0.51
2:E:204:MET:HE2	2:E:272:ASP:OD2	2.10	0.51
1:R:15:U:O4	2:C:408:ARG:HB2	2.11	0.51
2:D:52:ARG:NH2	2:D:130:ASP:OD2	2.43	0.51
2:D:97:LYS:O	2:D:98:ALA:C	2.49	0.51
2:A:314:ARG:HD3	2:A:407:LEU:HD23	1.92	0.51
1:R:3:U:O2	1:R:3:U:H2'	2.11	0.51
2:A:23:ASP:HB2	2:A:286:LYS:HZ2	1.74	0.50
2:C:214:ARG:O	2:C:216:GLY:N	2.45	0.50
2:C:398:LYS:HD2	2:C:421:ASP:HA	1.93	0.50
2:A:107:LEU:HD21	2:A:200:MET:HE2	1.94	0.50
2:A:133:TRP:HB3	2:A:167:ILE:HG21	1.92	0.50
2:B:329:THR:HG21	2:C:342:ALA:HB2	1.93	0.50
2:A:104:ILE:O	2:A:106:ASP:N	2.44	0.50
2:B:130:ASP:C	2:B:132:LYS:H	2.14	0.50
1:R:30:U:O5'	2:A:224:ASP:OD2	2.30	0.50
1:R:35:U:O2'	1:R:36:U:C6	2.64	0.50
2:A:149:MET:C	2:A:151:GLU:H	2.15	0.50
2:C:104:ILE:H	2:C:104:ILE:CD1	2.21	0.50
2:C:317:ARG:H	2:C:317:ARG:CZ	2.24	0.50
2:C:41:TYR:HB3	2:C:112:ALA:HB2	1.94	0.50
1:R:23:U:C4	3:R:101:DV4:C21	2.95	0.50
1:R:3:U:C5'	1:R:4:U:OP2	2.60	0.50
2:A:133:TRP:CB	2:A:167:ILE:HD13	2.39	0.50
2:D:306:LEU:HD22	2:D:412:ILE:HD12	1.94	0.50
2:A:143:ARG:HD2	2:A:155:LYS:HE2	1.93	0.50
2:B:84:LEU:HD23	2:B:102:ILE:HD11	1.92	0.50
2:D:311:THR:O	2:D:314:ARG:HG2	2.12	0.50
2:C:422:LYS:HB3	2:C:422:LYS:NZ	2.27	0.50
2:B:5:VAL:HG21	2:C:243:GLU:HB3	1.93	0.49
2:C:385:GLN:HG2	2:C:390:THR:CG2	2.42	0.49
2:D:107:LEU:C	2:D:108:VAL:HG22	2.32	0.49
2:C:36:LYS:HG3	2:C:93:ILE:CD1	2.42	0.49
1:R:14:U:O5'	2:C:317:ARG:NH2	2.45	0.49
2:A:25:VAL:HB	2:A:288:PRO:HB3	1.93	0.49
2:B:191:TYR:O	2:B:195:VAL:HG13	2.11	0.49
2:D:143:ARG:HB2	2:D:216:GLY:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:165:LYS:CA	2:E:184:VAL:HG22	2.14	0.49
2:E:33:ARG:HG2	2:E:33:ARG:O	2.12	0.49
2:E:248:TRP:CD1	2:E:375:VAL:HG22	2.47	0.49
2:B:149:MET:C	2:B:151:GLU:H	2.15	0.49
2:C:230:THR:HG21	2:C:298:HIS:CE1	2.48	0.49
2:E:202:PHE:HB2	2:E:214:ARG:HD3	1.94	0.49
2:A:172:GLU:HB2	2:A:173:PRO:CD	2.43	0.49
2:A:58:GLY:HA3	2:A:64:VAL:HB	1.94	0.49
2:A:324:TYR:HD2	2:B:237:ILE:HD11	1.78	0.49
2:B:314:ARG:HH21	2:B:315:ASN:HD21	1.60	0.49
2:D:177:GLU:HG2	2:D:178:GLY:N	2.28	0.49
2:E:243:GLU:O	2:E:247:THR:HG23	2.13	0.49
2:E:342:ALA:HB1	2:E:344:LEU:HD23	1.94	0.49
2:E:379:LEU:O	2:E:383:GLU:HG2	2.13	0.49
1:R:20:U:H2'	1:R:21:U:C4'	2.42	0.49
2:A:321:ASP:OD1	2:B:233:HIS:ND1	2.43	0.49
2:C:83:LYS:HD3	2:C:101:THR:HG22	1.94	0.49
2:C:184:VAL:CG1	2:D:165:LYS:HA	2.43	0.49
2:D:93:ILE:HG22	2:D:95:ILE:HG23	1.94	0.49
1:R:19:U:H2'	1:R:20:U:C6	2.48	0.49
2:A:23:ASP:OD2	2:A:293:LYS:NZ	2.35	0.49
2:D:82:GLY:O	2:D:101:THR:HA	2.12	0.49
2:C:336:TYR:CD2	2:C:393:MET:HG2	2.47	0.49
2:D:126:ARG:HG3	2:D:127:THR:N	2.28	0.49
2:D:74:TYR:O	2:D:78:LYS:HG3	2.12	0.49
1:R:18:U:OP2	1:R:19:U:H5	1.96	0.49
1:R:6:U:O4'	2:D:149:MET:HG3	2.13	0.49
2:A:30:ASP:OD1	2:A:33:ARG:NH1	2.45	0.48
2:A:399:ARG:HB3	2:E:422:LYS:NZ	2.28	0.48
2:B:317:ARG:O	2:B:317:ARG:HG2	2.11	0.48
1:R:38:U:C2'	1:R:39:U:OP1	2.61	0.48
2:A:172:GLU:HB2	2:A:173:PRO:HD3	1.94	0.48
1:R:42:U:C6	2:E:149:MET:HG3	2.49	0.48
2:A:107:LEU:HD12	2:A:107:LEU:N	2.29	0.48
2:A:142:TYR:OH	2:A:223:LYS:NZ	2.38	0.48
2:B:226:ALA:O	2:B:230:THR:HG23	2.13	0.48
2:C:82:GLY:O	2:C:101:THR:HA	2.13	0.48
2:C:140:GLY:O	2:C:144:VAL:HG23	2.13	0.48
2:C:356:THR:N	2:C:357:PRO:HD3	2.29	0.48
2:C:170:GLN:HB3	2:C:171:PHE:H	1.56	0.48
2:D:38:ILE:O	2:D:108:VAL:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:2:U:H2'	1:R:3:U:C1'	2.44	0.48
2:B:366:THR:HG23	2:B:367:ASN:H	1.78	0.48
2:D:41:TYR:HA	2:D:110:LEU:O	2.13	0.48
2:A:172:GLU:CB	2:A:173:PRO:CD	2.91	0.48
2:A:342:ALA:HB1	2:A:344:LEU:HD23	1.96	0.47
2:B:190:ASN:O	2:B:194:ILE:HG13	2.13	0.47
2:B:66:ILE:HD11	2:B:191:TYR:HB2	1.95	0.47
2:C:184:VAL:HG11	2:D:166:MET:H	1.78	0.47
2:D:41:TYR:C	2:D:42:ILE:HG13	2.32	0.47
2:D:60:LYS:HA	2:D:60:LYS:HE2	1.96	0.47
2:A:68:HIS:CE1	2:A:116:VAL:HG12	2.50	0.47
2:D:144:VAL:O	2:D:147:THR:HG22	2.14	0.47
2:D:172:GLU:H	2:D:173:PRO:HD2	1.79	0.47
2:D:230:THR:HG21	2:D:298:HIS:HD1	1.79	0.47
1:R:4:U:H2'	2:D:317:ARG:CD	2.43	0.47
2:C:385:GLN:HG2	2:C:390:THR:HG22	1.96	0.47
2:D:149:MET:N	2:D:149:MET:SD	2.86	0.47
2:E:328:THR:HG21	2:E:415:TYR:OH	2.14	0.47
2:A:109:SER:O	2:A:110:LEU:HD23	2.14	0.47
2:C:164:CYS:SG	2:C:168:ASN:HA	2.55	0.47
2:C:175:VAL:HG23	2:C:176:PRO:HD2	1.95	0.47
2:E:150:PRO:HA	2:E:152:TYR:CE2	2.49	0.47
2:B:123:ASP:C	2:B:125:SER:H	2.18	0.47
2:B:379:LEU:HB3	2:C:354:LYS:HD2	1.96	0.47
2:D:149:MET:C	2:D:151:GLU:H	2.17	0.47
2:A:342:ALA:N	2:E:387:ARG:HH12	2.12	0.47
2:A:143:ARG:HD3	2:A:219:VAL:CG1	2.44	0.47
2:B:104:ILE:HD11	2:B:198:VAL:CG2	2.41	0.47
2:B:48:LEU:H	2:B:48:LEU:HD22	1.79	0.47
2:B:5:VAL:CG2	2:C:243:GLU:HB3	2.45	0.47
2:E:66:ILE:HD13	2:E:185:TRP:CD1	2.49	0.47
2:C:143:ARG:HG3	2:C:144:VAL:N	2.30	0.47
2:E:290:SER:O	2:E:294:ASN:ND2	2.39	0.47
2:E:421:ASP:O	2:E:422:LYS:HB3	2.14	0.47
1:R:6:U:H5'	1:R:7:U:O5'	2.15	0.47
2:A:7:ARG:HH11	2:B:259:VAL:HG21	1.80	0.47
2:B:51:LEU:O	2:B:55:VAL:HG22	2.15	0.47
1:R:30:U:OP1	2:A:279:ILE:HD12	2.14	0.47
2:C:159:GLY:HA2	2:C:163:GLN:HE22	1.80	0.47
2:A:402:MET:SD	2:E:422:LYS:HB2	2.54	0.47
1:R:8:U:C2'	1:R:9:U:H5''	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:122:SER:OG	2:A:123:ASP:N	2.46	0.47
2:C:107:LEU:HD12	2:C:107:LEU:N	2.29	0.47
2:C:117:LEU:CB	2:C:118:PRO:HD3	2.24	0.47
2:E:326:SER:O	2:E:329:THR:HG22	2.14	0.47
1:R:20:U:O2'	1:R:21:U:P	2.72	0.47
2:C:153:ARG:NH2	2:C:176:PRO:HA	2.29	0.47
2:D:37:GLU:HB2	2:D:108:VAL:HG21	1.97	0.47
2:E:54:TYR:HE1	2:E:118:PRO:HB2	1.79	0.47
1:R:11:U:C3'	1:R:12:U:H5''	2.28	0.47
1:R:22:U:H2'	2:B:317:ARG:HE	1.80	0.46
2:E:137:TYR:HA	2:E:163:GLN:NE2	2.29	0.46
1:R:25:U:C6	3:R:101:DV4:C21	2.98	0.46
1:R:1:U:H5	1:R:2:U:N1	2.06	0.46
1:R:45:U:H6	1:R:45:U:H2'	1.29	0.46
2:C:172:GLU:N	2:C:173:PRO:CD	2.78	0.46
2:C:95:ILE:O	2:C:95:ILE:HG22	2.15	0.46
2:D:302:GLN:HG2	2:D:316:ALA:HB3	1.97	0.46
2:D:67:ILE:HD12	2:D:67:ILE:H	1.80	0.46
2:A:354:LYS:HE3	2:A:356:THR:HA	1.96	0.46
2:B:302:GLN:HG2	2:B:316:ALA:CB	2.46	0.46
2:B:37:GLU:HB2	2:B:108:VAL:CG2	2.13	0.46
2:D:43:ASN:HB2	2:D:111:LYS:CB	2.43	0.46
2:E:81:ARG:O	2:E:201:PHE:HZ	1.97	0.46
1:R:1:U:H5	1:R:2:U:C2	2.34	0.46
2:C:38:ILE:O	2:C:38:ILE:HG13	2.15	0.46
2:E:140:GLY:HA2	2:E:216:GLY:HA3	1.97	0.46
2:B:321:ASP:OD1	2:C:233:HIS:ND1	2.45	0.46
2:B:184:VAL:CG1	2:C:166:MET:H	2.26	0.46
2:A:190:ASN:O	2:A:194:ILE:HG13	2.15	0.46
2:B:40:LEU:HD22	2:B:42:ILE:HG13	1.97	0.46
2:C:243:GLU:O	2:C:247:THR:HG23	2.16	0.46
2:C:356:THR:N	2:C:357:PRO:CD	2.78	0.46
1:R:44:U:C3'	1:R:45:U:C5'	2.83	0.46
2:A:177:GLU:OE1	2:A:179:ARG:N	2.43	0.46
2:B:128:SER:O	2:B:130:ASP:N	2.49	0.46
1:R:5:U:H5'	1:R:6:U:OP2	2.16	0.46
2:C:219:VAL:O	2:C:219:VAL:HG12	2.15	0.46
2:D:168:ASN:O	2:D:168:ASN:ND2	2.49	0.46
2:D:85:ASP:N	2:D:85:ASP:OD1	2.40	0.46
1:R:3:U:H5'	1:R:4:U:OP2	2.15	0.46
2:B:66:ILE:HD13	2:B:185:TRP:CD1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:66:ILE:HD12	2:B:69:VAL:CG2	2.46	0.46
2:D:243:GLU:O	2:D:247:THR:HG23	2.15	0.46
1:R:15:U:H3'	1:R:15:U:O2	2.15	0.46
2:A:376:VAL:HG13	2:B:354:LYS:HB2	1.98	0.46
2:D:172:GLU:HB3	2:D:173:PRO:CD	2.43	0.46
2:D:26:GLU:OE2	2:D:285:SER:N	2.38	0.46
2:D:30:ASP:O	2:D:34:LYS:HE3	2.17	0.46
2:E:224:ASP:OD1	2:E:279:ILE:HG13	2.16	0.46
1:R:17:U:H2'	1:R:18:U:H5'	1.93	0.46
2:A:356:THR:N	2:A:357:PRO:CD	2.79	0.45
2:B:17:LYS:HG3	2:C:268:ILE:HD11	1.98	0.45
1:R:21:U:OP2	2:B:287:SER:N	2.47	0.45
2:A:172:GLU:CB	2:A:173:PRO:HD3	2.46	0.45
2:A:401:VAL:HG21	2:A:420:PHE:HB2	1.99	0.45
2:A:67:ILE:HD12	2:A:67:ILE:H	1.81	0.45
2:E:116:VAL:HG12	2:E:117:LEU:N	2.31	0.45
2:E:278:LEU:CD1	2:E:284:SER:HB3	2.46	0.45
1:R:20:U:C3'	1:R:21:U:H5''	2.45	0.45
1:R:44:U:H3'	1:R:45:U:H5''	1.90	0.45
2:C:180:ASP:N	2:C:183:ASP:OD1	2.49	0.45
2:D:166:MET:CE	2:D:166:MET:HA	2.46	0.45
2:D:355:TYR:C	2:D:357:PRO:HD3	2.35	0.45
2:E:190:ASN:O	2:E:194:ILE:HG13	2.16	0.45
2:E:43:ASN:CG	2:E:67:ILE:HG23	2.36	0.45
2:A:43:ASN:HB2	2:A:111:LYS:HA	1.97	0.45
2:B:33:ARG:HB2	2:B:33:ARG:HE	1.52	0.45
2:C:190:ASN:O	2:C:194:ILE:HG13	2.16	0.45
2:D:224:ASP:OD2	2:D:279:ILE:HG13	2.16	0.45
2:D:40:LEU:HG	2:D:42:ILE:HD11	1.97	0.45
2:D:130:ASP:C	2:D:132:LYS:H	2.19	0.45
2:E:43:ASN:N	2:E:43:ASN:OD1	2.32	0.45
1:R:1:U:O2'	1:R:2:U:O5'	2.34	0.45
2:A:18:LEU:HD22	2:B:242:THR:HG21	1.98	0.45
2:A:323:GLU:O	2:A:327:LEU:HD22	2.16	0.45
2:D:59:LEU:HB3	2:D:172:GLU:HG2	1.99	0.45
2:E:172:GLU:N	2:E:173:PRO:HD2	2.31	0.45
2:A:157:MET:O	2:A:161:THR:HG23	2.17	0.45
2:E:41:TYR:HB3	2:E:112:ALA:HB2	1.98	0.45
2:E:241:SER:OG	2:E:243:GLU:HG2	2.17	0.45
2:E:66:ILE:HD12	2:E:69:VAL:CG2	2.47	0.45
1:R:27:U:C4	3:R:101:DV4:O17	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:181:ILE:H	2:B:181:ILE:HG13	1.67	0.45
1:R:1:U:C6	1:R:2:U:O4'	2.70	0.45
2:C:295:PRO:HB2	2:C:322:ILE:HG21	1.99	0.45
2:B:163:GLN:O	2:B:167:ILE:HB	2.16	0.44
2:D:169:GLU:OE2	2:D:169:GLU:HA	2.17	0.44
2:E:136:LEU:HD22	2:E:163:GLN:CG	2.47	0.44
2:E:317:ARG:H	2:E:317:ARG:CZ	2.30	0.44
2:A:356:THR:CG2	2:A:357:PRO:HD3	2.48	0.44
2:B:81:ARG:O	2:B:201:PHE:HZ	1.99	0.44
2:B:214:ARG:O	2:B:216:GLY:N	2.49	0.44
2:C:43:ASN:OD1	2:C:112:ALA:HB3	2.17	0.44
2:C:143:ARG:HB2	2:C:219:VAL:HG21	1.98	0.44
2:D:54:TYR:CE1	2:D:118:PRO:HG2	2.52	0.44
2:A:341:SER:HA	2:E:387:ARG:HH22	1.81	0.44
2:A:399:ARG:HB3	2:E:422:LYS:HZ1	1.82	0.44
2:A:5:VAL:HG21	2:B:243:GLU:HB3	2.00	0.44
2:E:303:LEU:O	2:E:307:LEU:HD22	2.17	0.44
1:R:26:U:H1'	3:R:101:DV4:C14	2.48	0.44
2:E:40:LEU:HD22	2:E:42:ILE:HG12	1.99	0.44
1:R:15:U:O4	2:C:408:ARG:CB	2.66	0.44
2:B:157:MET:O	2:B:160:LEU:HG	2.17	0.44
2:C:165:LYS:O	2:C:167:ILE:HG12	2.18	0.44
2:E:419:GLU:O	2:E:422:LYS:HE3	2.16	0.44
2:C:93:ILE:HG22	2:C:95:ILE:HG13	1.99	0.44
2:D:52:ARG:NH1	2:D:127:THR:O	2.50	0.44
1:R:35:U:HO2'	1:R:36:U:H6	1.60	0.44
2:A:214:ARG:O	2:A:217:THR:HG22	2.18	0.44
2:D:137:TYR:CE2	2:D:141:LEU:HD11	2.52	0.44
2:D:52:ARG:NE	2:D:130:ASP:OD1	2.50	0.44
2:D:54:TYR:CZ	2:D:118:PRO:HG2	2.53	0.44
2:E:365:THR:OG1	2:E:366:THR:N	2.50	0.44
2:A:414:LYS:HA	2:A:414:LYS:HE3	2.00	0.44
2:A:97:LYS:O	2:A:98:ALA:C	2.55	0.44
2:B:165:LYS:HE3	2:B:165:LYS:HA	2.00	0.44
2:C:30:ASP:HA	2:C:33:ARG:HB3	2.00	0.44
2:B:149:MET:SD	2:B:149:MET:N	2.91	0.44
2:C:199:ASP:OD2	2:C:277:TYR:OH	2.34	0.44
2:C:380:GLY:HA2	2:D:354:LYS:NZ	2.32	0.44
2:C:410:LYS:HA	2:C:410:LYS:HD2	1.84	0.44
1:R:1:U:HO2'	1:R:1:U:H6	1.66	0.44
2:C:233:HIS:CE1	2:C:312:ARG:HE	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:278:LEU:HD23	2:B:278:LEU:H	1.83	0.43
2:B:389:PRO:HA	2:B:393:MET:SD	2.57	0.43
2:C:369:PRO:HA	2:C:370:PRO:HD3	1.93	0.43
2:D:38:ILE:HG13	2:D:108:VAL:HG23	2.00	0.43
1:R:4:U:H5''	2:D:291:SER:HB3	2.00	0.43
2:A:217:THR:O	2:A:220:SER:OG	2.32	0.43
2:A:278:LEU:HA	2:A:283:LEU:HD12	1.99	0.43
2:D:137:TYR:OH	2:D:173:PRO:HD3	2.18	0.43
2:B:133:TRP:HB3	2:B:167:ILE:HD13	2.00	0.43
2:B:184:VAL:HG21	2:C:164:CYS:O	2.19	0.43
2:C:278:LEU:HD23	2:C:278:LEU:H	1.83	0.43
2:C:16:PRO:HB2	2:D:242:THR:OG1	2.19	0.43
2:D:51:LEU:O	2:D:55:VAL:HG22	2.18	0.43
2:E:137:TYR:HA	2:E:163:GLN:HE22	1.83	0.43
2:E:370:PRO:HG2	2:E:378:TRP:CD2	2.53	0.43
2:A:44:THR:O	2:A:46:LYS:HD2	2.17	0.43
2:B:113:LEU:HB3	2:B:114:ASP:H	1.62	0.43
1:R:17:U:C5'	2:C:143:ARG:HH12	2.32	0.43
1:R:14:U:C5'	2:C:317:ARG:HH22	2.31	0.43
2:E:353:ASN:OD1	2:E:353:ASN:N	2.45	0.43
1:R:1:U:C6	1:R:1:U:P	3.12	0.43
2:A:27:TYR:CZ	2:A:263:LEU:HD22	2.54	0.43
2:B:22:GLU:O	2:B:23:ASP:C	2.57	0.43
2:C:129:ALA:HB1	2:C:133:TRP:NE1	2.33	0.43
2:B:422:LYS:NZ	2:C:399:ARG:O	2.46	0.43
2:D:34:LYS:HD2	2:D:34:LYS:H	1.84	0.43
2:A:356:THR:HG23	2:A:357:PRO:HD3	2.00	0.43
2:C:308:LEU:O	2:C:309:ARG:HB2	2.18	0.43
2:D:157:MET:HA	2:D:160:LEU:CD2	2.49	0.43
2:D:230:THR:HG21	2:D:298:HIS:ND1	2.33	0.43
2:D:401:VAL:HG21	2:D:420:PHE:HB2	2.00	0.43
2:D:81:ARG:O	2:D:201:PHE:HZ	2.02	0.43
2:E:143:ARG:HE	2:E:155:LYS:HE3	1.84	0.43
2:E:44:THR:HA	2:E:111:LYS:HE2	2.01	0.43
2:A:37:GLU:HB2	2:A:108:VAL:HG21	2.01	0.43
2:B:65:SER:HB2	2:B:117:LEU:HD11	2.00	0.43
2:C:302:GLN:HG2	2:C:316:ALA:HB2	2.00	0.43
2:C:40:LEU:C	2:C:40:LEU:HD22	2.39	0.43
1:R:43:U:H2'	1:R:44:U:C6	2.54	0.43
1:R:9:U:C3'	1:R:10:U:H5''	2.49	0.43
2:B:245:VAL:O	2:B:249:ILE:HD12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:326:SER:O	2:B:329:THR:HG23	2.19	0.43
2:C:72:TYR:OH	2:C:130:ASP:HA	2.18	0.43
1:R:20:U:H2'	1:R:21:U:C5'	2.49	0.43
2:A:243:GLU:O	2:A:247:THR:HG23	2.19	0.42
2:B:134:LEU:HA	2:B:134:LEU:HD22	1.78	0.42
2:B:212:SER:HA	2:B:215:TYR:CZ	2.54	0.42
2:D:18:LEU:H	2:D:18:LEU:HD23	1.84	0.42
2:D:222:PHE:N	2:D:276:PRO:O	2.51	0.42
2:E:104:ILE:HG23	2:E:105:PHE:CD2	2.54	0.42
2:A:42:ILE:O	2:A:42:ILE:HD12	2.19	0.42
2:B:212:SER:HA	2:B:215:TYR:CE2	2.54	0.42
1:R:5:U:C4'	2:D:317:ARG:NH2	2.81	0.42
2:E:172:GLU:N	2:E:173:PRO:CD	2.81	0.42
2:A:66:ILE:O	2:A:69:VAL:HG22	2.19	0.42
2:B:243:GLU:O	2:B:247:THR:HG23	2.18	0.42
2:C:113:LEU:HB3	2:C:114:ASP:H	1.57	0.42
2:B:179:ARG:O	2:C:161:THR:HG22	2.19	0.42
2:B:129:ALA:O	2:B:133:TRP:CD1	2.72	0.42
1:R:17:U:H3'	2:C:143:ARG:HH22	1.83	0.42
1:R:20:U:H2'	1:R:21:U:H5''	2.01	0.42
2:B:293:LYS:HA	2:B:293:LYS:HD3	1.83	0.42
2:C:78:LYS:NZ	2:C:78:LYS:HA	2.34	0.42
2:C:78:LYS:HZ2	2:C:78:LYS:HA	1.85	0.42
2:D:157:MET:HA	2:D:160:LEU:HD21	2.01	0.42
2:D:294:ASN:N	2:D:295:PRO:HD3	2.34	0.42
2:B:354:LYS:HE3	2:B:356:THR:HA	2.01	0.42
2:D:275:MET:HB3	2:D:276:PRO:HD3	2.01	0.42
2:D:336:TYR:OH	2:D:392:ASP:OD2	2.20	0.42
1:R:6:U:H3'	2:D:408:ARG:HH12	1.85	0.42
2:E:369:PRO:HA	2:E:370:PRO:HD3	1.89	0.42
2:C:175:VAL:CG2	2:C:176:PRO:HD2	2.50	0.42
2:E:149:MET:C	2:E:151:GLU:H	2.22	0.42
2:C:175:VAL:HG12	2:C:181:ILE:HG23	2.00	0.42
2:E:279:ILE:HD13	2:E:284:SER:O	2.20	0.42
1:R:25:U:O2'	3:R:101:DV4:C19	2.68	0.42
2:A:160:LEU:HD13	2:A:171:PHE:CE2	2.55	0.42
2:A:269:ASP:HA	2:E:19:PRO:HA	2.02	0.42
2:C:278:LEU:HD23	2:C:278:LEU:N	2.35	0.42
2:D:303:LEU:CD2	2:D:328:THR:HA	2.50	0.42
2:D:66:ILE:HG23	2:D:67:ILE:HD12	2.02	0.42
2:E:40:LEU:HD22	2:E:42:ILE:CG1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:17:U:O2'	1:R:18:U:H5''	2.20	0.42
1:R:24:U:C4	2:B:408:ARG:HD3	2.54	0.42
2:A:166:MET:H	2:E:184:VAL:HG13	1.85	0.41
2:A:41:TYR:O	2:A:190:ASN:ND2	2.53	0.41
2:A:239:GLY:HA3	2:E:323:GLU:CD	2.40	0.41
1:R:38:U:C3'	1:R:39:U:H5''	2.46	0.41
2:A:308:LEU:O	2:A:309:ARG:HB2	2.19	0.41
2:C:104:ILE:HD12	2:C:104:ILE:N	2.35	0.41
2:C:248:TRP:CD1	2:C:375:VAL:HG22	2.55	0.41
2:D:84:LEU:HD12	2:D:86:LYS:O	2.20	0.41
2:E:137:TYR:HD2	2:E:163:GLN:OE1	2.03	0.41
2:D:314:ARG:H	2:D:314:ARG:HG2	1.67	0.41
2:E:293:LYS:HD2	2:E:293:LYS:HA	1.91	0.41
1:R:15:U:C4	2:C:408:ARG:CG	2.89	0.41
1:R:27:U:H4'	1:R:29:U:C5	2.55	0.41
2:B:84:LEU:HD22	2:B:84:LEU:HA	1.95	0.41
2:C:33:ARG:HG3	2:C:33:ARG:O	2.19	0.41
2:E:152:TYR:CD1	2:E:153:ARG:N	2.89	0.41
2:E:356:THR:N	2:E:357:PRO:CD	2.84	0.41
2:E:42:ILE:HD13	2:E:74:TYR:HB2	2.03	0.41
2:A:328:THR:HG21	2:A:415:TYR:CE2	2.55	0.41
2:C:111:LYS:HB3	2:C:111:LYS:HE3	1.79	0.41
2:C:44:THR:HG22	2:C:71:SER:OG	2.19	0.41
2:D:224:ASP:CG	2:D:279:ILE:HG13	2.41	0.41
2:E:44:THR:CB	2:E:46:LYS:HZ2	2.34	0.41
1:R:19:U:OP2	2:C:218:ILE:HD12	2.21	0.41
2:A:18:LEU:HD23	2:A:18:LEU:H	1.85	0.41
2:A:293:LYS:HD3	2:A:293:LYS:HA	1.87	0.41
2:A:369:PRO:HA	2:A:370:PRO:HD3	1.95	0.41
2:E:177:GLU:HG2	2:E:179:ARG:H	1.84	0.41
2:A:166:MET:N	2:E:184:VAL:HG13	2.36	0.41
2:E:25:VAL:HG11	2:E:260:GLN:OE1	2.20	0.41
2:E:366:THR:C	2:E:368:ALA:H	2.23	0.41
1:R:1:U:H6	1:R:2:U:C6	2.38	0.41
2:A:308:LEU:HA	2:A:308:LEU:HD12	1.81	0.41
2:A:302:GLN:HG2	2:A:316:ALA:CB	2.51	0.41
2:C:149:MET:C	2:C:151:GLU:N	2.73	0.41
2:D:369:PRO:HA	2:D:370:PRO:HD3	1.97	0.41
2:D:46:LYS:O	2:D:47:SER:O	2.39	0.41
2:E:308:LEU:HD12	2:E:308:LEU:HA	1.86	0.41
2:E:66:ILE:O	2:E:69:VAL:HG22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:278:LEU:HD23	2:A:278:LEU:H	1.85	0.41
2:B:48:LEU:N	2:B:48:LEU:HD22	2.35	0.41
2:B:184:VAL:CG1	2:C:165:LYS:HA	2.44	0.41
2:D:410:LYS:HA	2:D:410:LYS:HD2	1.89	0.41
1:R:15:U:C5'	1:R:15:U:O2	2.68	0.41
2:A:148:GLN:NE2	2:A:179:ARG:HB2	2.36	0.41
2:A:149:MET:C	2:A:151:GLU:N	2.74	0.41
2:A:336:TYR:CG	2:A:393:MET:HG2	2.55	0.41
1:R:26:U:H3'	2:B:143:ARG:NH2	2.35	0.41
2:B:246:THR:HA	2:B:249:ILE:HD13	2.03	0.41
2:C:52:ARG:NH2	2:C:130:ASP:OD2	2.54	0.41
2:C:179:ARG:HA	2:C:183:ASP:CG	2.42	0.41
2:C:308:LEU:HA	2:C:308:LEU:HD12	1.85	0.41
1:R:31:U:H5'	1:R:32:U:OP1	2.20	0.41
2:C:307:LEU:HA	2:C:307:LEU:HD13	1.91	0.41
2:C:402:MET:O	2:C:403:SER:OG	2.30	0.41
2:A:72:TYR:OH	2:A:130:ASP:HB2	2.21	0.40
2:C:270:LYS:HB3	2:C:270:LYS:NZ	2.36	0.40
2:A:43:ASN:HB3	2:A:44:THR:H	1.64	0.40
2:B:304:THR:O	2:B:308:LEU:HD22	2.21	0.40
2:B:366:THR:HG23	2:B:367:ASN:N	2.36	0.40
1:R:14:U:P	2:C:317:ARG:NH2	2.93	0.40
2:E:317:ARG:H	2:E:317:ARG:CD	2.34	0.40
2:E:401:VAL:HG21	2:E:420:PHE:HB2	2.02	0.40
2:A:244:ASP:O	2:A:247:THR:OG1	2.29	0.40
2:B:32:PHE:HA	2:B:35:SER:O	2.21	0.40
2:C:169:GLU:HA	2:C:169:GLU:OE1	2.22	0.40
2:D:278:LEU:HA	2:D:283:LEU:HD12	2.04	0.40
2:D:293:LYS:C	2:D:295:PRO:HD3	2.42	0.40
1:R:31:U:O3'	2:A:317:ARG:NH2	2.54	0.40
1:R:5:U:O4'	2:D:317:ARG:NH2	2.48	0.40
2:B:143:ARG:HB2	2:B:216:GLY:O	2.20	0.40
2:C:397:ALA:O	2:C:401:VAL:HG22	2.21	0.40
2:C:66:ILE:HD12	2:C:69:VAL:CG2	2.51	0.40
2:D:104:ILE:HG12	2:D:104:ILE:H	1.38	0.40
2:D:390:THR:HB	2:D:391:PRO:HD2	2.03	0.40
2:E:127:THR:O	2:E:129:ALA:N	2.47	0.40
2:A:127:THR:OG1	2:A:128:SER:N	2.54	0.40
2:B:72:TYR:OH	2:B:134:LEU:HB3	2.21	0.40
2:D:397:ALA:O	2:D:401:VAL:HG22	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	
2	A	419/421 (100%)	357 (85%)	41 (10%)	21 (5%)	2	23
2	B	411/421 (98%)	355 (86%)	41 (10%)	15 (4%)	4	32
2	C	409/421 (97%)	354 (87%)	39 (10%)	16 (4%)	3	30
2	D	412/421 (98%)	360 (87%)	34 (8%)	18 (4%)	3	27
2	E	419/421 (100%)	356 (85%)	46 (11%)	17 (4%)	3	29
All	All	2070/2105 (98%)	1782 (86%)	201 (10%)	87 (4%)	3	28

All (87) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	105	PHE
2	A	113	LEU
2	B	113	LEU
2	B	128	SER
2	C	113	LEU
2	C	172	GLU
2	D	47	SER
2	D	98	ALA
2	D	357	PRO
2	D	366	THR
2	E	113	LEU
2	E	177	GLU
2	A	45	THR
2	A	98	ALA
2	A	108	VAL
2	A	120	GLY
2	A	172	GLU
2	A	176	PRO
2	A	344	LEU
2	A	367	ASN
2	B	172	GLU

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Mol	Chain	Res	Type
2	B	344	LEU
2	C	108	VAL
2	C	120	GLY
2	C	128	SER
2	C	406	GLY
2	D	61	SER
2	D	120	GLY
2	D	177	GLU
2	E	108	VAL
2	E	120	GLY
2	E	365	THR
2	E	406	GLY
2	A	42	ILE
2	A	117	LEU
2	B	114	ASP
2	B	150	PRO
2	C	117	LEU
2	C	150	PRO
2	C	215	TYR
2	C	344	LEU
2	D	113	LEU
2	D	150	PRO
2	D	344	LEU
2	E	360	SER
2	E	371	GLN
2	A	47	SER
2	A	104	ILE
2	A	150	PRO
2	B	61	SER
2	B	117	LEU
2	B	130	ASP
2	B	131	ASP
2	B	177	GLU
2	C	22	GLU
2	C	130	ASP
2	D	130	ASP
2	D	172	GLU
2	E	128	SER
2	E	150	PRO
2	E	168	ASN
2	E	173	PRO
2	E	344	LEU

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Mol	Chain	Res	Type
2	A	264	PRO
2	B	122	SER
2	C	176	PRO
2	D	128	SER
2	D	131	ASP
2	A	121	VAL
2	A	131	ASP
2	B	343	ASP
2	D	117	LEU
2	E	117	LEU
2	E	172	GLU
2	E	343	ASP
2	A	82	GLY
2	A	181	ILE
2	C	181	ILE
2	D	82	GLY
2	E	82	GLY
2	B	82	GLY
2	C	82	GLY
2	B	356	THR
2	A	118	PRO
2	D	80	ILE
2	D	181	ILE
2	C	356	THR

### 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	
2	A	362/362 (100%)	329 (91%)	33 (9%)	11	41
2	B	358/362 (99%)	317 (88%)	41 (12%)	6	29
2	C	356/362 (98%)	306 (86%)	50 (14%)	4	21
2	D	359/362 (99%)	314 (88%)	45 (12%)	5	26
2	E	362/362 (100%)	333 (92%)	29 (8%)	14	48
All	All	1797/1810 (99%)	1599 (89%)	198 (11%)	7	32

All (198) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	40	LEU
2	A	68	HIS
2	A	95	ILE
2	A	101	THR
2	A	114	ASP
2	A	116	VAL
2	A	134	LEU
2	A	153	ARG
2	A	157	MET
2	A	160	LEU
2	A	163	GLN
2	A	172	GLU
2	A	177	GLU
2	A	181	ILE
2	A	183	ASP
2	A	221	ARG
2	A	224	ASP
2	A	228	LEU
2	A	230	THR
2	A	237	ILE
2	A	243	GLU
2	A	252	ARG
2	A	308	LEU
2	A	309	ARG
2	A	317	ARG
2	A	326	SER
2	A	327	LEU
2	A	332	LEU
2	A	353	ASN
2	A	354	LYS
2	A	355	TYR
2	A	394	MET
2	A	405	GLN
2	B	18	LEU
2	B	22	GLU
2	B	30	ASP
2	B	34	LYS
2	B	40	LEU
2	B	46	LYS
2	B	78	LYS
2	B	84	LEU
2	B	85	ASP

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Mol	Chain	Res	Type
2	B	95	ILE
2	B	116	VAL
2	B	134	LEU
2	B	143	ARG
2	B	149	MET
2	B	153	ARG
2	B	154	LYS
2	B	158	ASP
2	B	162	ASN
2	B	163	GLN
2	B	165	LYS
2	B	175	VAL
2	B	181	ILE
2	B	215	TYR
2	B	219	VAL
2	B	237	ILE
2	B	243	GLU
2	B	253	GLU
2	B	308	LEU
2	B	309	ARG
2	B	317	ARG
2	B	327	LEU
2	B	329	THR
2	B	332	LEU
2	B	353	ASN
2	B	354	LYS
2	B	355	TYR
2	B	365	THR
2	B	393	MET
2	B	394	MET
2	B	405	GLN
2	B	407	LEU
2	C	18	LEU
2	C	22	GLU
2	C	40	LEU
2	C	46	LYS
2	C	78	LYS
2	C	79	ASP
2	C	84	LEU
2	C	85	ASP
2	C	87	ASP
2	C	97	LYS

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Mol	Chain	Res	Type
2	C	102	ILE
2	C	104	ILE
2	C	106	ASP
2	C	111	LYS
2	C	119	ASP
2	C	122	SER
2	C	126	ARG
2	C	134	LEU
2	C	143	ARG
2	C	149	MET
2	C	153	ARG
2	C	155	LYS
2	C	156	LEU
2	C	157	MET
2	C	160	LEU
2	C	163	GLN
2	C	167	ILE
2	C	177	GLU
2	C	181	ILE
2	C	183	ASP
2	C	184	VAL
2	C	189	SER
2	C	217	THR
2	C	221	ARG
2	C	243	GLU
2	C	252	ARG
2	C	253	GLU
2	C	260	GLN
2	C	307	LEU
2	C	308	LEU
2	C	312	ARG
2	C	317	ARG
2	C	332	LEU
2	C	353	ASN
2	C	354	LYS
2	C	371	GLN
2	C	385	GLN
2	C	407	LEU
2	C	409	GLU
2	C	422	LYS
2	D	22	GLU
2	D	23	ASP

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Mol	Chain	Res	Type
2	D	26	GLU
2	D	34	LYS
2	D	38	ILE
2	D	42	ILE
2	D	44	THR
2	D	64	VAL
2	D	84	LEU
2	D	85	ASP
2	D	86	LYS
2	D	95	ILE
2	D	97	LYS
2	D	101	THR
2	D	102	ILE
2	D	104	ILE
2	D	106	ASP
2	D	108	VAL
2	D	126	ARG
2	D	146	ARG
2	D	149	MET
2	D	153	ARG
2	D	160	LEU
2	D	166	MET
2	D	184	VAL
2	D	217	THR
2	D	221	ARG
2	D	230	THR
2	D	243	GLU
2	D	252	ARG
2	D	308	LEU
2	D	312	ARG
2	D	314	ARG
2	D	317	ARG
2	D	326	SER
2	D	327	LEU
2	D	329	THR
2	D	332	LEU
2	D	353	ASN
2	D	354	LYS
2	D	355	TYR
2	D	367	ASN
2	D	377	GLU
2	D	407	LEU

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Mol	Chain	Res	Type
2	D	409	GLU
2	E	22	GLU
2	E	38	ILE
2	E	40	LEU
2	E	43	ASN
2	E	48	LEU
2	E	84	LEU
2	E	85	ASP
2	E	95	ILE
2	E	101	THR
2	E	123	ASP
2	E	130	ASP
2	E	134	LEU
2	E	148	GLN
2	E	149	MET
2	E	166	MET
2	E	206	LYS
2	E	209	GLU
2	E	219	VAL
2	E	242	THR
2	E	243	GLU
2	E	307	LEU
2	E	308	LEU
2	E	309	ARG
2	E	317	ARG
2	E	326	SER
2	E	332	LEU
2	E	354	LYS
2	E	355	TYR
2	E	418	SER

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

Mol	Chain	Res	Type
2	C	163	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	R	44/45 (97%)	31 (70%)	5 (11%)

All (31) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	R	2	U
1	R	3	U
1	R	4	U
1	R	5	U
1	R	6	U
1	R	9	U
1	R	10	U
1	R	11	U
1	R	12	U
1	R	14	U
1	R	15	U
1	R	17	U
1	R	18	U
1	R	19	U
1	R	21	U
1	R	23	U
1	R	24	U
1	R	25	U
1	R	27	U
1	R	28	U
1	R	29	U
1	R	30	U
1	R	32	U
1	R	33	U
1	R	36	U
1	R	37	U
1	R	38	U
1	R	39	U
1	R	41	U
1	R	42	U
1	R	45	U

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	R	5	U
1	R	17	U
1	R	20	U
1	R	36	U
1	R	38	U

## 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 15 are modelled with single atom - leaving 1 for Mogul analysis.

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
3	DV4	R	101	-	31,36,36	2.34	13 (41%)	31,50,50	3.66	15 (48%)

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
3	DV4	R	101	-	-	3/14/27/27	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	101	DV4	C30-N28	-4.00	1.32	1.38
3	R	101	DV4	O17-C16	-2.80	1.17	1.23
3	R	101	DV4	O23-C22	-2.72	1.17	1.23
3	R	101	DV4	O09-C08	-2.66	1.17	1.23
3	R	101	DV4	O03-C02	-2.40	1.17	1.23
3	R	101	DV4	C15-N31	-2.17	1.31	1.34
3	R	101	DV4	C05-N04	2.18	1.45	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	101	DV4	C25-N24	2.19	1.45	1.41
3	R	101	DV4	C11-N10	2.42	1.45	1.40
3	R	101	DV4	C08-N10	4.20	1.46	1.35
3	R	101	DV4	C22-N24	4.25	1.45	1.35
3	R	101	DV4	C02-N04	5.40	1.45	1.35
3	R	101	DV4	C16-N18	5.50	1.46	1.33

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	R	101	DV4	O09-C08-N10	-5.81	110.43	123.69
3	R	101	DV4	C05-N04-C02	-4.04	121.23	128.03
3	R	101	DV4	O17-C16-N18	-3.60	115.15	122.59
3	R	101	DV4	O17-C16-C15	-3.52	115.46	120.37
3	R	101	DV4	C25-N24-C22	-2.78	122.52	127.49
3	R	101	DV4	O23-C22-C21	-2.71	116.93	122.01
3	R	101	DV4	C20-C21-C22	-2.61	106.00	113.32
3	R	101	DV4	O03-C02-N04	-2.17	120.24	123.06
3	R	101	DV4	O03-C02-C01	-2.16	118.13	122.06
3	R	101	DV4	C14-N13-C15	2.18	129.47	126.39
3	R	101	DV4	C11-N10-C08	3.35	137.09	128.02
3	R	101	DV4	C21-C22-N24	3.35	120.53	114.53
3	R	101	DV4	C07-C08-N10	3.47	137.23	117.79
3	R	101	DV4	C01-C02-N04	4.50	121.63	115.02
3	R	101	DV4	C15-C16-N18	15.31	129.39	115.80

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	R	101	DV4	O09-C08-N10-C11
3	R	101	DV4	C07-C08-N10-C11
3	R	101	DV4	C15-C16-N18-C19

There are no ring outliers.

1 monomer is involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	R	101	DV4	20	0

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	R	45/45 (100%)	0.77	4 (8%) 10 12	104, 149, 197, 237	0
2	A	421/421 (100%)	0.56	45 (10%) 7 8	56, 112, 185, 250	0
2	B	415/421 (98%)	0.41	29 (6%) 17 17	54, 107, 170, 314	0
2	C	413/421 (98%)	0.43	31 (7%) 15 15	53, 110, 178, 258	0
2	D	416/421 (98%)	0.43	25 (6%) 23 21	58, 116, 180, 225	0
2	E	421/421 (100%)	0.72	54 (12%) 4 6	63, 125, 197, 246	0
All	All	2131/2150 (99%)	0.51	188 (8%) 11 12	53, 115, 185, 314	0

All (188) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	361	THR	15.2
2	E	2	SER	11.7
2	C	2	SER	10.6
2	E	366	THR	10.2
2	E	176	PRO	7.5
2	A	360	SER	7.1
2	C	357	PRO	7.0
2	C	101	THR	6.8
2	B	172	GLU	6.6
2	E	118	PRO	6.1
2	B	117	LEU	6.0
2	E	367	ASN	5.4
2	C	274	TYR	5.3
2	A	364	LEU	5.3
2	B	177	GLU	5.2
2	C	173	PRO	5.2
2	E	365	THR	5.1
2	D	113	LEU	5.1
2	C	213	PHE	5.1

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Mol	Chain	Res	Type	RSRZ
2	E	153	ARG	5.0
2	A	120	GLY	4.9
2	E	173	PRO	4.9
2	A	363	GLY	4.7
2	D	39	PRO	4.6
2	E	72	TYR	4.6
2	E	113	LEU	4.4
2	A	121	VAL	4.4
2	B	176	PRO	4.4
2	E	22	GLU	4.3
2	C	174	LEU	4.3
2	E	101	THR	4.3
2	E	360	SER	4.2
2	E	141	LEU	4.2
2	D	112	ALA	4.2
2	C	163	GLN	4.2
2	C	356	THR	4.2
2	E	175	VAL	4.1
2	D	166	MET	4.0
2	C	100	ASP	4.0
2	D	131	ASP	3.9
2	A	2	SER	3.9
2	D	114	ASP	3.9
2	D	2	SER	3.9
2	E	363	GLY	3.9
2	A	166	MET	3.8
2	E	105	PHE	3.8
2	A	114	ASP	3.7
2	A	108	VAL	3.7
2	A	407	LEU	3.7
2	E	119	ASP	3.7
2	A	102	ILE	3.7
2	B	274	TYR	3.7
2	C	95	ILE	3.6
2	C	27	TYR	3.6
2	E	361	THR	3.6
2	E	68	HIS	3.6
2	E	362	GLY	3.5
2	B	367	ASN	3.5
2	A	172	GLU	3.4
2	A	113	LEU	3.4
2	C	169	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
2	C	172	GLU	3.4
2	E	69	VAL	3.4
2	A	365	THR	3.4
2	D	68	HIS	3.3
2	C	83	LYS	3.3
2	D	63	ASN	3.3
2	D	40	LEU	3.3
2	C	88	TRP	3.3
2	D	274	TYR	3.2
2	B	43	ASN	3.2
2	A	310	SER	3.2
2	A	269	ASP	3.1
2	B	173	PRO	3.1
2	A	366	THR	3.1
2	C	133	TRP	3.1
2	D	38	ILE	3.1
2	B	133	TRP	3.0
2	E	99	GLY	3.0
2	D	171	PHE	3.0
2	D	95	ILE	3.0
2	B	174	LEU	3.0
2	C	28	PRO	3.0
2	A	105	PHE	3.0
2	B	68	HIS	3.0
2	D	27	TYR	3.0
2	B	121	VAL	2.9
2	E	120	GLY	2.9
2	A	362	GLY	2.9
2	E	422	LYS	2.9
2	B	124	ALA	2.8
2	E	332	LEU	2.8
2	A	367	ASN	2.8
2	E	185	TRP	2.8
2	E	40	LEU	2.8
2	E	272	ASP	2.8
2	D	172	GLU	2.8
2	B	175	VAL	2.8
2	E	117	LEU	2.8
2	B	37	GLU	2.7
2	B	97	LYS	2.7
2	A	152	TYR	2.7
2	A	97	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
2	A	348	PHE	2.7
2	A	233	HIS	2.7
2	D	60	LYS	2.6
2	E	174	LEU	2.6
2	A	118	PRO	2.6
2	B	88	TRP	2.6
2	D	364	LEU	2.6
2	A	122	SER	2.5
2	A	14	ILE	2.5
2	C	146	ARG	2.5
2	D	14	ILE	2.5
2	E	172	GLU	2.5
2	E	89	SER	2.5
2	B	145	GLY	2.5
2	E	84	LEU	2.5
2	E	121	VAL	2.4
1	R	41	U	2.4
2	E	45	THR	2.4
2	A	213	PHE	2.4
2	A	99	GLY	2.4
2	A	164	CYS	2.4
2	C	18	LEU	2.4
2	B	185	TRP	2.4
2	E	267	GLU	2.4
2	A	68	HIS	2.4
2	A	15	VAL	2.4
2	E	152	TYR	2.4
2	E	42	ILE	2.4
2	D	137	TYR	2.4
2	B	125	SER	2.3
2	D	310	SER	2.3
2	E	160	LEU	2.3
2	A	246	THR	2.3
1	R	43	U	2.3
2	E	57	GLN	2.3
2	D	20	ALA	2.3
2	C	57	GLN	2.3
2	E	138	LEU	2.3
2	E	358	ASP	2.3
2	A	95	ILE	2.3
2	A	173	PRO	2.3
2	A	60	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
2	A	278	LEU	2.3
2	A	242	THR	2.3
2	B	156	LEU	2.3
2	C	3	VAL	2.3
2	C	82	GLY	2.3
2	B	39	PRO	2.3
2	C	143	ARG	2.3
2	A	405	GLN	2.3
2	A	356	THR	2.2
2	A	117	LEU	2.2
2	C	102	ILE	2.2
2	B	104	ILE	2.2
2	C	348	PHE	2.2
2	D	185	TRP	2.2
2	A	357	PRO	2.2
2	E	140	GLY	2.2
2	A	16	PRO	2.2
2	D	346	GLN	2.2
2	E	409	GLU	2.2
2	C	210	CYS	2.2
1	R	37	U	2.2
2	B	357	PRO	2.2
2	E	73	LEU	2.1
2	B	116	VAL	2.1
2	B	167	ILE	2.1
2	C	176	PRO	2.1
2	B	366	THR	2.1
2	C	355	TYR	2.1
1	R	4	U	2.1
2	E	114	ASP	2.1
2	E	71	SER	2.1
2	A	174	LEU	2.1
2	B	118	PRO	2.1
2	E	96	GLY	2.1
2	B	407	LEU	2.1
2	E	191	TYR	2.0
2	D	21	ASN	2.0
2	E	268	ILE	2.0
2	C	120	GLY	2.0
2	C	233	HIS	2.0
2	E	122	SER	2.0
2	E	321	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
2	E	48	LEU	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	DV4	R	101	34/34	0.69	0.32	1.17	78,121,148,163	0
4	IUM	B	501	1/3	0.96	0.21	-0.77	164,164,164,164	0
4	IUM	E	501	1/3	0.94	0.17	-	144,144,144,144	0
4	IUM	E	502	1/3	0.89	0.14	-	203,203,203,203	0
4	IUM	C	502	1/3	0.82	0.23	-	144,144,144,144	0
4	IUM	B	502	1/3	0.84	0.14	-	130,130,130,130	0
4	IUM	A	502	1/3	0.81	0.22	-	104,104,104,104	0
4	IUM	C	501	1/3	0.97	0.16	-	146,146,146,146	0
4	IUM	A	505	1/3	0.91	0.19	-	125,125,125,125	0
4	IUM	D	502	1/3	0.73	0.25	-	131,131,131,131	0
4	IUM	B	503	1/3	0.94	0.14	-	194,194,194,194	0
4	IUM	A	501	1/3	0.97	0.18	-	128,128,128,128	0
4	IUM	A	504	1/3	0.97	0.14	-	175,175,175,175	0
4	IUM	C	503	1/3	0.98	0.16	-	144,144,144,144	0
4	IUM	A	503	1/3	0.86	0.16	-	169,169,169,169	0
4	IUM	D	501	1/3	0.91	0.21	-	150,150,150,150	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.