Full wwPDB X-ray Structure Validation Report (i)

Sep 25, 2023 – 07:33 PM EDT

PDB ID	:	6BJY
Title	:	VSV Nucleocapsid with Polyamide Bound
Authors	:	Gumpper, 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

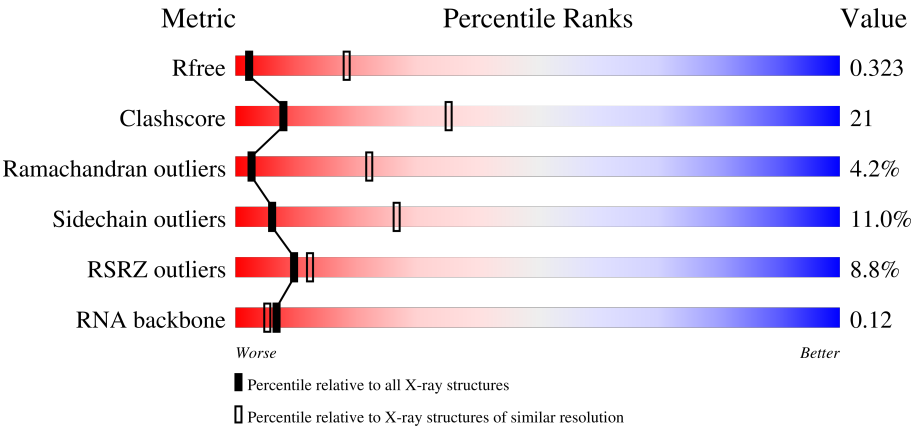
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.46 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.



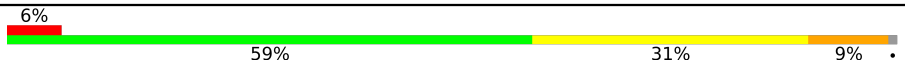
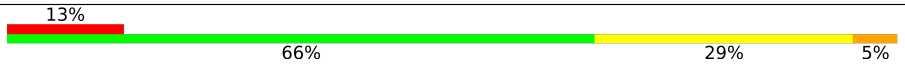
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1291 (3.52-3.40)
Clashscore	141614	1372 (3.52-3.40)
Ramachandran outliers	138981	1337 (3.52-3.40)
Sidechain outliers	138945	1338 (3.52-3.40)
RSRZ outliers	127900	1205 (3.52-3.40)
RNA backbone	3102	1036 (3.96-2.96)

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	R	45	13% 7% 24% 56% 13%
2	A	421	11% 61% 33% 5%
2	B	421	7% 59% 32% 8%
2	C	421	7% 59% 31% 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	D	421	
2	E	421	

2 Entry composition (i)

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.

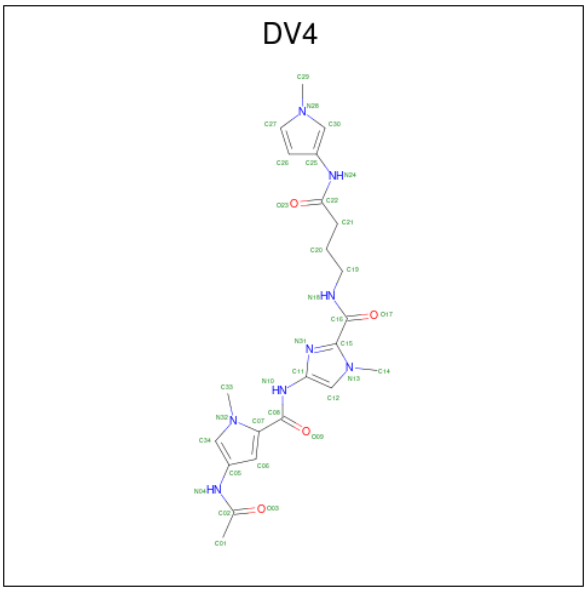
- Molecule 1 is a RNA chain called RNA (45-MER).

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.

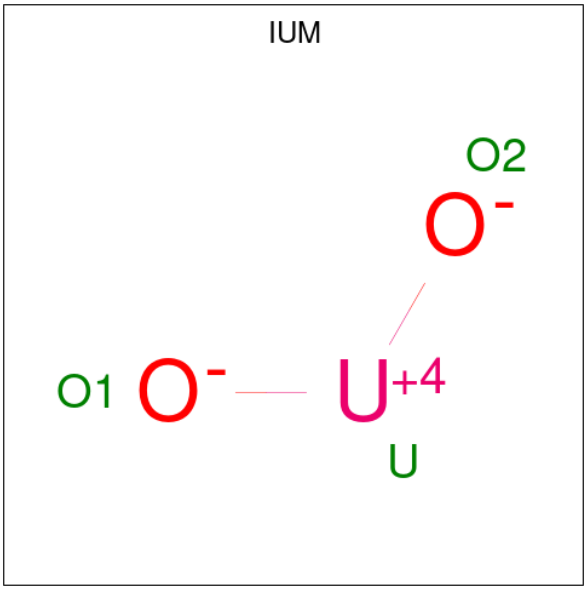
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	421	Total	C	N	O	S	0	0	0
			3327	2118	558	633	18			
2	B	415	Total	C	N	O	S	0	0	0
			3290	2097	552	623	18			
2	C	413	Total	C	N	O	S	0	0	0
			3275	2089	550	618	18			
2	D	416	Total	C	N	O	S	0	0	0
			3298	2103	553	624	18			
2	E	421	Total	C	N	O	S	0	0	0
			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: $C_{22}H_{28}N_8O_4$).



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_2U).



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		

Continued on next page...

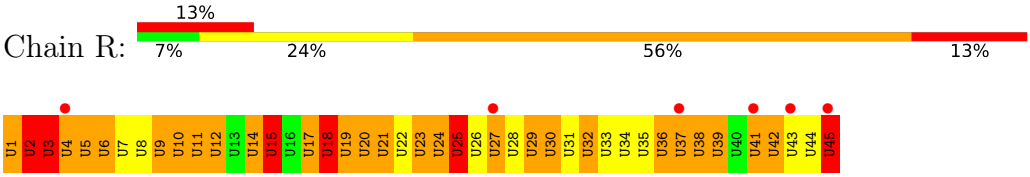
Continued from previous page...

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

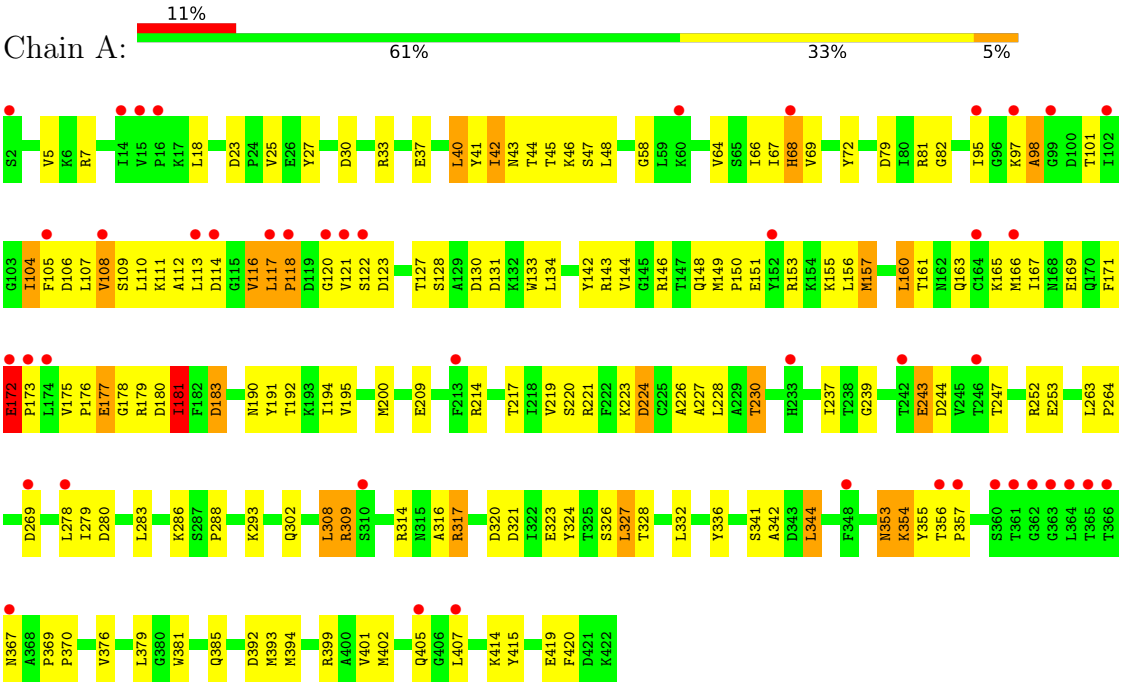
3 Residue-property plots (i)

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.

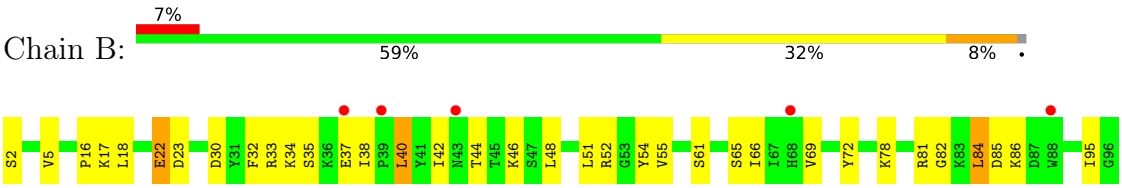
• Molecule 1: RNA (45-MER)

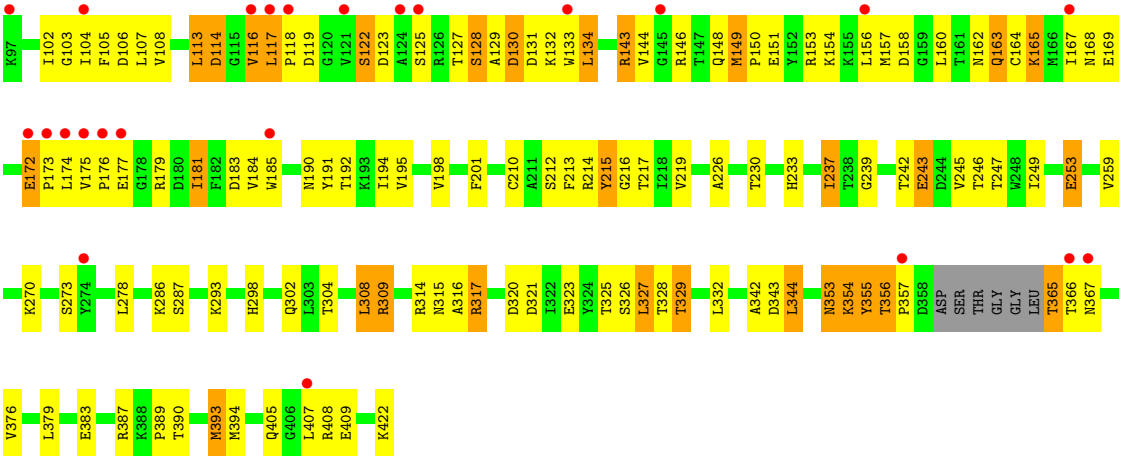


• Molecule 2: Nucleoprotein



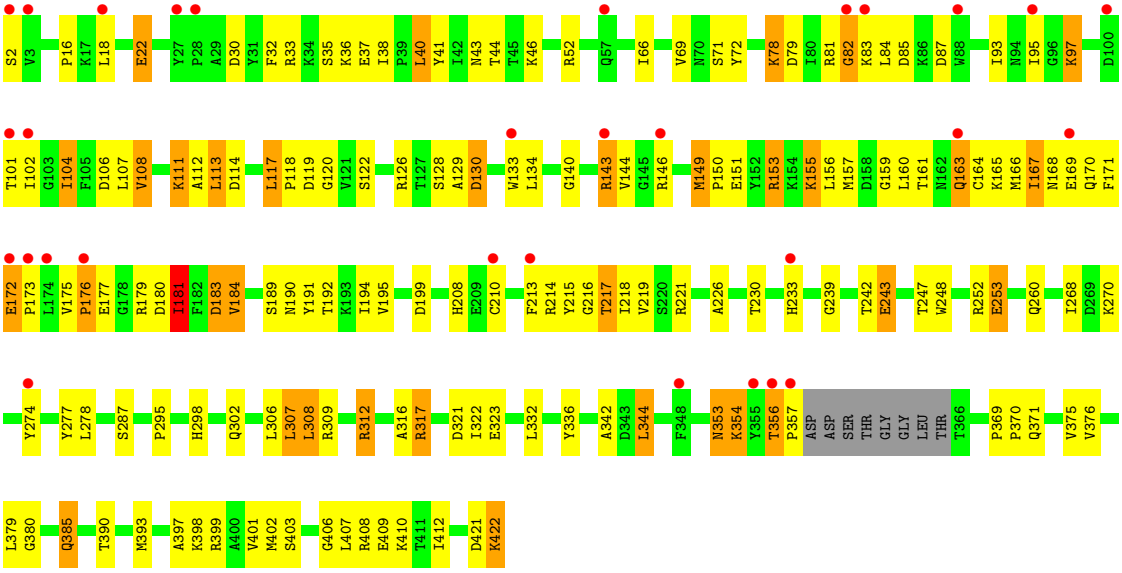
• Molecule 2: Nucleoprotein





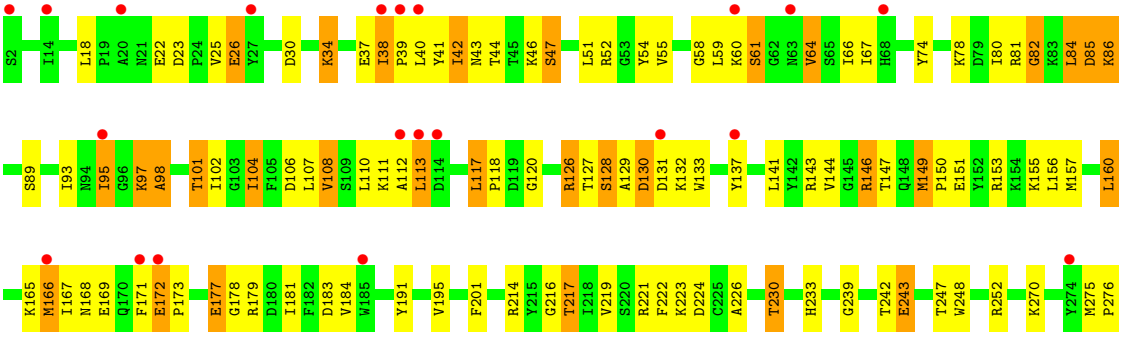
• Molecule 2: Nucleoprotein

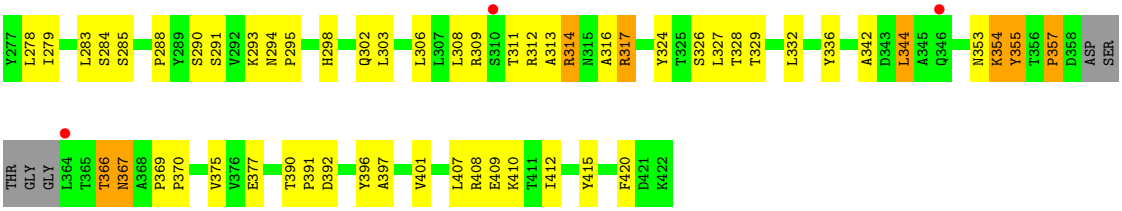
Chain C:



• Molecule 2: Nucleoprotein

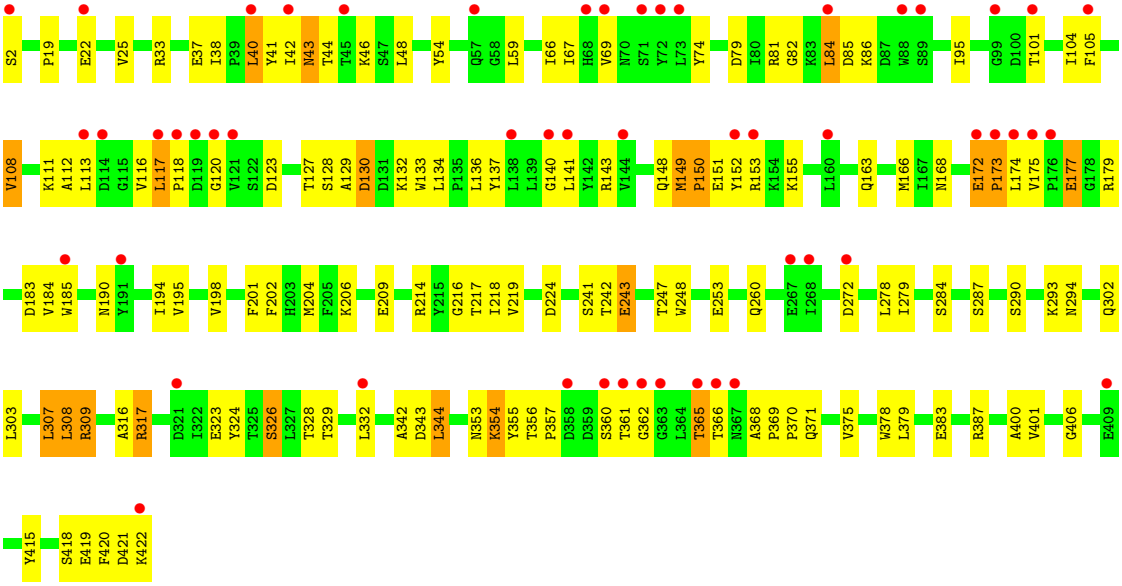
Chain D:





• Molecule 2: Nucleoprotein

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	2.82 (at 3.48Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.266 , 0.311 0.281 , 0.323	Depositor DCC
R_{free} test set	1999 reflections (5.52%)	wwPDB-VP
Wilson B-factor (Å^2)	100.3	Xtriage
Anisotropy	0.630	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 47.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.36$, $< L^2 > = 0.18$	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^2)	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.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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(^{o})	Ideal(^{o})
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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 (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	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
1:R:44:U:C2'	1:R:45:U:H5"	1.91	1.00
2:A:117:LEU:HB3	2:A:118:PRO:HD3	1.41	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:18:U:H1'	1:R:20:U:OP2	1.70	0.92
1:R:26:U:C4'	3:R:101:DV4:C14	2.48	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

Continued on next page...

Continued from previous page...

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:O	2:B:174:LEU:HD23	1.81	0.81
1:R:1:U:H2'	1:R:1:U:P	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:15:U:C5	2:C:408:ARG:HG3	2.22	0.75
1:R:25:U:H6	3:R:101:DV4:C20	1.99	0.75
1:R:17:U:HO2'	1:R:18:U:P	2.09	0.75
2:A:226:ALA:O	2:A:230:THR:HG22	1.86	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
1:R:1:U:C5	1:R:2:U:C6	2.74	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:89:SER:O	2:D:270:LYS:NZ	2.22	0.72
1:R:1:U:O2'	1:R:2:U:O4'	2.08	0.71
2:C:191:TYR:O	2:C:195:VAL:HG13	1.90	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:P	1:R:1:U:C2'	2.78	0.71
2:D:195:VAL:HG13	2:D:217:THR:OG1	1.91	0.70
1:R:1:U:C5	1:R:2:U:H1'	2.26	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
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
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:C:149:MET:O	2:C:151:GLU:N	2.26	0.68
1:R:17:U:H2'	1:R:18:U:H5"	1.75	0.68
2:E:195:VAL:HG13	2:E:217:THR:HG22	1.74	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
1:R:26:U:O2'	1:R:27:U:H5'	1.93	0.67
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: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
1:R:25:U:C1'	3:R:101:DV4:C20	2.64	0.66
2:B:214:ARG:HA	2:B:217:THR:HG22	1.78	0.66
2:C:353:ASN:OD1	2:C:353:ASN:N	2.29	0.66
2:B:325:THR:O	2:B:329:THR:HG22	1.93	0.66

Continued on next page...

Continued from previous page...

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
1:R:38:U:H3'	1:R:39:U:H5"	1.77	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: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:38:ILE:HG13	2:B:38:ILE:O	1.97	0.65
2:B:167:ILE:HG22	2:B:169:GLU:HG2	1.78	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
1:R:18:U:C1'	1:R:20:U:OP2	2.45	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:44:U:H5"	2:E:143:ARG:NH2	2.12	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:1:U:O2'	1:R:2:U:OP2	2.16	0.63
1:R:1:U:O2'	1:R:2:U:C5'	2.46	0.63
2:A:317:ARG:CZ	2:A:317:ARG:H	2.12	0.63
2:D:171:PHE:CZ	2:D:173:PRO:HG2	2.34	0.62
1:R:1:U:C6	1:R:2:U:C6	2.87	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:23:U:N3	3:R:101:DV4:C21	2.63	0.61
2:D:43:ASN:CB	2:D:111:LYS:HB3	2.30	0.61
2:A:43:ASN:CG	2:A:111:LYS:HG2	2.21	0.61
2:B:409:GLU:N	2:B:409:GLU:OE2	2.33	0.61
2:A:177:GLU:CD	2:A:178:GLY:H	2.04	0.61
1:R:8:U:H5"	2:D:143:ARG:NH2	2.16	0.61
2:C:226:ALA:O	2:C:230:THR:HG23	2.01	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:HE21	2:C:163:GLN:N	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
1:R:2:U:C3'	1:R:3:U:C6	2.84	0.60
2:E:370:PRO:HD2	2:E:378:TRP:CH2	2.36	0.60
1:R:23:U:H2'	1:R:25:U:H5"	1.83	0.60
1:R:1:U:P	1:R:1:U:C1'	2.89	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
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
1:R:30:U:H2'	1:R:31:U:O4'	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
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
1:R:11:U:H3'	1:R:12:U:C5'	2.25	0.59
2:D:151:GLU:OE1	2:D:155:LYS:NZ	2.29	0.59
1:R:6:U:C4	2:D:408:ARG:HD3	2.38	0.58
2:C:164:CYS:HA	2:C:168:ASN:HA	1.85	0.58

Continued on next page...

Continued from previous page...

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:H	2:A:317:ARG:NE	2.01	0.58
1:R:23:U:H3	3:R:101:DV4:C21	2.17	0.58
2:A:309:ARG:NH1	2:E:419:GLU:OE1	2.35	0.58
2:D:60:LYS:O	2:D:61:SER:HB2	2.04	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
1:R:6:U:C1'	2:D:149:MET:HG3	2.34	0.58
2:B:144:VAL:HG11	2:B:156:LEU:HG	1.85	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
1:R:2:U:C2'	1:R:3:U:C6	2.87	0.57
2:C:81:ARG:HB2	2:C:208:HIS:HE2	1.69	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:43:ASN:ND2	2:A:111:LYS:HG2	2.20	0.57
2:A:253:GLU:CD	2:A:253:GLU:H	2.07	0.57
2:A:353:ASN:OD1	2:A:353:ASN:N	2.37	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:H	2:C:317:ARG:NH1	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
1:R:4:U:C5'	2:D:291:SER:HB3	2.35	0.56
2:C:336:TYR:CG	2:C:393:MET:HG2	2.40	0.56
2:B:323:GLU:O	2:B:327:LEU:HD22	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:309:ARG:HH21	2:E:400:ALA:HB2	1.71	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:A:328:THR:HG21	2:A:415:TYR:OH	2.05	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
1:R:2:U:H2'	1:R:3:U:C6	2.42	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:36:U:O2'	1:R:37:U:P	2.65	0.55
1:R:1:U:OP2	1:R:1:U:C2'	2.50	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:O2'	1:R:2:U:C4'	2.55	0.55
2:C:376:VAL:HG13	2:D:354:LYS:HA	1.89	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:97:LYS:HD3	2:C:97:LYS:N	2.22	0.54
1:R:3:U:H4'	2:D:224:ASP:HB2	1.89	0.54
2:A:180:ASP:N	2:A:183:ASP:OD1	2.34	0.54
2:D:97:LYS:N	2:D:97:LYS:HD3	2.22	0.54
1:R:1:U:P	1:R:1:U:O4'	2.66	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
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
1:R:26:U:C1'	3:R:101:DV4:C14	2.86	0.54
1:R:41:U:O5'	2:E:317:ARG:NH2	2.41	0.54
2:D:104:ILE:HD13	2:D:201:PHE:CD2	2.43	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
1:R:29:U:H3'	1:R:30:U:H5"	1.91	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

Continued on next page...

Continued from previous page...

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:O	2:C:146:ARG:HD3	2.09	0.52
2:E:43:ASN:HD22	2:E:67:ILE:HG23	1.71	0.52
2:E:309:ARG:NH2	2:E:400:ALA:HB2	2.24	0.52
1:R:8:U:H2'	1:R:9:U:H5"	1.90	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:84:LEU:HD22	2:E:86:LYS:O	2.09	0.52
2:E:172:GLU:H	2:E:173:PRO:CD	2.22	0.52
1:R:21:U:H2'	1:R:22:U:O4'	2.09	0.52
2:D:43:ASN:HB2	2:D:112:ALA:N	2.25	0.52
1:R:25:U:H1'	3:R:101:DV4:C19	2.37	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:9:U:OP2	2:D:143:ARG:NH1	2.37	0.52
2:E:224:ASP:CG	2:E:279:ILE:HG13	2.30	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:H	2:A:48:LEU:HD22	1.75	0.51
2:D:143:ARG:HD2	2:D:219:VAL:HG13	1.92	0.51
2:D:165:LYS:O	2:D:167:ILE:HG13	2.09	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

Continued on next page...

Continued from previous page...

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:38:ILE:N	2:D:108:VAL:HG21	2.25	0.51
2:D:101:THR:O	2:D:101:THR:OG1	2.19	0.51
1:R:15:U:O4	2:C:408:ARG:HB2	2.11	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
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
1:R:3:U:H2'	1:R:3:U:O2	2.11	0.51
2:A:314:ARG:HD3	2:A:407:LEU:HD23	1.92	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
1:R:3:U:C5'	1:R:4:U:OP2	2.60	0.50
1:R:23:U:C4	3:R:101:DV4:C21	2.95	0.50
2:A:149:MET:C	2:A:151:GLU:H	2.15	0.50
2:C:41:TYR:HB3	2:C:112:ALA:HB2	1.94	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: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:NZ	2:C:422:LYS:HB3	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:A:165:LYS:CA	2:E:184:VAL:HG22	2.14	0.49
2:B:191:TYR:O	2:B:195:VAL:HG13	2.11	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:143:ARG:HB2	2:D:216:GLY:O	2.12	0.49
2:E:33:ARG:O	2:E:33:ARG:HG2	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
1:R:20:U:H2'	1:R:21:U:C4'	2.42	0.49
2:A:58:GLY:HA3	2:A:64:VAL:HB	1.94	0.49
2:A:172:GLU:HB2	2:A:173:PRO:CD	2.43	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:19:U:H2'	1:R:20:U:C6	2.48	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
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
1:R:6:U:O4'	2:D:149:MET:HG3	2.13	0.49
1:R:18:U:OP2	1:R:19:U:H5	1.96	0.49
2:C:336:TYR:CD2	2:C:393:MET:HG2	2.47	0.49
2:D:74:TYR:O	2:D:78:LYS:HG3	2.12	0.49
2:D:126:ARG:HG3	2:D:127:THR:N	2.28	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
1:R:38:U:C2'	1:R:39:U:OP1	2.61	0.48
2:B:317:ARG:O	2:B:317:ARG:HG2	2.11	0.48
1:R:42:U:C6	2:E:149:MET:HG3	2.49	0.48
2:A:172:GLU:HB2	2:A:173:PRO:HD3	1.94	0.48
2:A:107:LEU:N	2:A:107:LEU:HD12	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
1:R:2:U:H2'	1:R:3:U:C1'	2.44	0.48
2:C:170:GLN:HB3	2:C:171:PHE:H	1.56	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:38:ILE:O	2:D:108:VAL:HG23	2.13	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:66:ILE:HD11	2:B:191:TYR:HB2	1.95	0.47
2:B:190:ASN:O	2:B:194:ILE:HG13	2.13	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:HE2	2:D:60:LYS:HA	1.96	0.47
1:R:4:U:H2'	2:D:317:ARG:CD	2.43	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
2:C:385:GLN:HG2	2:C:390:THR:HG22	1.96	0.47
2:D:149:MET:SD	2:D:149:MET:N	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:A:342:ALA:N	2:E:387:ARG:HH12	2.12	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:143:ARG:HD3	2:A:219:VAL:CG1	2.44	0.47
2:B:5:VAL:CG2	2:C:243:GLU:HB3	2.45	0.47
2:B:48:LEU:H	2:B:48:LEU:HD22	1.79	0.47
2:B:104:ILE:HD11	2:B:198:VAL:CG2	2.41	0.47
2:E:66:ILE:HD13	2:E:185:TRP:CD1	2.49	0.47
1:R:6:U:H5'	1:R:7:U:O5'	2.15	0.47
1:R:30:U:OP1	2:A:279:ILE:HD12	2.14	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
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:8:U:C2'	1:R:9:U:H5"	2.44	0.47
2:A:402:MET:SD	2:E:422:LYS:HB2	2.54	0.47
2:C:159:GLY:HA2	2:C:163:GLN:HE22	1.80	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:20:U:O2'	1:R:21:U:P	2.72	0.47
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:11:U:C3'	1:R:12:U:H5"	2.28	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:1:U:H5	1:R:2:U:N1	2.06	0.46
1:R:22:U:H2'	2:B:317:ARG:HE	1.80	0.46
1:R:25:U:C6	3:R:101:DV4:C21	2.98	0.46
1:R:45:U:H6	1:R:45:U:H2'	1.29	0.46
2:E:137:TYR:HA	2:E:163:GLN:NE2	2.29	0.46
2:C:95:ILE:HG22	2:C:95:ILE:O	2.15	0.46
2:C:172:GLU:N	2:C:173:PRO:CD	2.78	0.46
2:D:67:ILE:HD12	2:D:67:ILE:H	1.80	0.46
2:D:302:GLN:HG2	2:D:316:ALA:HB3	1.97	0.46
1:R:1:U:H5	1:R:2:U:C2	2.34	0.46
2:A:354:LYS:HE3	2:A:356:THR:HA	1.96	0.46
2:B:37:GLU:HB2	2:B:108:VAL:CG2	2.13	0.46
2:B:302:GLN:HG2	2:B:316:ALA:CB	2.46	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
2:C:38:ILE:HG13	2:C:38:ILE:O	2.15	0.46
2:E:140:GLY:HA2	2:E:216:GLY:HA3	1.97	0.46
2:B:184:VAL:CG1	2:C:166:MET:H	2.26	0.46
2:B:321:ASP:OD1	2:C:233:HIS:ND1	2.45	0.46
1:R:44:U:C3'	1:R:45:U:C5'	2.83	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:5:U:H5'	1:R:6:U:OP2	2.16	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:3:U:H5'	1:R:4:U:OP2	2.15	0.46
2:C:219:VAL:HG12	2:C:219:VAL:O	2.15	0.46
2:D:85:ASP:OD1	2:D:85:ASP:N	2.40	0.46
2:D:168:ASN:O	2:D:168:ASN:ND2	2.49	0.46
1:R:15:U:H3'	1:R:15:U:O2	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:66:ILE:HD13	2:B:185:TRP:CD1	2.51	0.46
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:17:U:H2'	1:R:18:U:H5'	1.93	0.46
2:A:376:VAL:HG13	2:B:354:LYS:HB2	1.98	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:D:172:GLU:HB3	2:D:173:PRO:CD	2.43	0.46
2:E:224:ASP:OD1	2:E:279:ILE:HG13	2.16	0.46
1:R:21:U:OP2	2:B:287:SER:N	2.47	0.45
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: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:A:67:ILE:HD12	2:A:67:ILE:H	1.81	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: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
2:C:180:ASP:N	2:C:183:ASP:OD1	2.49	0.45
2:D:166:MET:HA	2:D:166:MET:CE	2.46	0.45
2:D:355:TYR:C	2:D:357:PRO:HD3	2.35	0.45
2:E:43:ASN:CG	2:E:67:ILE:HG23	2.36	0.45
2:E:190:ASN:O	2:E:194:ILE:HG13	2.16	0.45
2:A:43:ASN:HB2	2:A:111:LYS:HA	1.97	0.45
2:B:33:ARG:HE	2:B:33:ARG:HB2	1.52	0.45
2:C:190:ASN:O	2:C:194:ILE:HG13	2.16	0.45
2:D:40:LEU:HG	2:D:42:ILE:HD11	1.97	0.45
2:D:224:ASP:OD2	2:D:279:ILE:HG13	2.16	0.45
1:R:1:U:O2'	1:R:2:U:O5'	2.34	0.45
2:D:130:ASP:C	2:D:132:LYS:H	2.19	0.45
2:E:43:ASN:OD1	2:E:43:ASN:N	2.32	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
1:R:27:U:C4	3:R:101:DV4:O17	2.70	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:66:ILE:HD12	2:E:69:VAL:CG2	2.47	0.45
2:E:241:SER:OG	2:E:243:GLU:HG2	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:1:U:C6	1:R:2:U:O4'	2.70	0.45
2:B:181:ILE:H	2:B:181:ILE:HG13	1.67	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:HA	2:D:169:GLU:OE2	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
1:R:26:U:H1'	3:R:101:DV4:C14	2.48	0.44
2:A:5:VAL:HG21	2:B:243:GLU:HB3	2.00	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:E:303:LEU:O	2:E:307:LEU:HD22	2.17	0.44
1:R:15:U:O4	2:C:408:ARG:CB	2.66	0.44
2:E:40:LEU:HD22	2:E:42:ILE:HG12	1.99	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
1:R:35:U:HO2'	1:R:36:U:H6	1.60	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
2:A:214:ARG:O	2:A:217:THR:HG22	2.18	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:D:137:TYR:CE2	2:D:141:LEU:HD11	2.52	0.44
2:E:365:THR:OG1	2:E:366:THR:N	2.50	0.44
2:A:97:LYS:O	2:A:98:ALA:C	2.55	0.44
2:A:414:LYS:HE3	2:A:414:LYS:HA	2.00	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
1:R:1:U:HO2'	1:R:1:U:H6	1.66	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:HD2	2:C:410:LYS:HA	1.84	0.44
2:C:233:HIS:CE1	2:C:312:ARG:HE	2.36	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:4:U:H5”	2:D:291:SER:HB3	2.00	0.43
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
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:16:PRO:HB2	2:D:242:THR:OG1	2.19	0.43
2:C:278:LEU:H	2:C:278:LEU:HD23	1.83	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
1:R:1:U:P	1:R:1:U:C6	3.12	0.43
1:R:14:U:C5’	2:C:317:ARG:HH22	2.31	0.43
1:R:17:U:C5’	2:C:143:ARG:HH12	2.32	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
2:E:353:ASN:OD1	2:E:353:ASN:N	2.45	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:B:422:LYS:NZ	2:C:399:ARG:O	2.46	0.43
2:C:129:ALA:HB1	2:C:133:TRP:NE1	2.33	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:81:ARG:O	2:D:201:PHE:HZ	2.02	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:E:44:THR:HA	2:E:111:LYS:HE2	2.01	0.43
2:E:143:ARG:HE	2:E:155:LYS:HE3	1.84	0.43
1:R:9:U:C3’	1:R:10:U:H5”	2.49	0.43
1:R:43:U:H2’	1:R:44:U:C6	2.54	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:40:LEU:C	2:C:40:LEU:HD22	2.39	0.43
2:C:302:GLN:HG2	2:C:316:ALA:HB2	2.00	0.43
1:R:20:U:H2’	1:R:21:U:C5’	2.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:245:VAL:O	2:B:249:ILE:HD12	2.19	0.43
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
2:A:243:GLU:O	2:A:247:THR:HG23	2.19	0.42
2:B:134:LEU:HD22	2:B:134:LEU:HA	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
1:R:5:U:C4'	2:D:317:ARG:NH2	2.81	0.42
2:A:42:ILE:HD12	2:A:42:ILE:O	2.19	0.42
2:B:212:SER:HA	2:B:215:TYR:CE2	2.54	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:179:ARG:O	2:C:161:THR: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
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:129:ALA:O	2:B:133:TRP:CD1	2.72	0.42
2:B:293:LYS:HD3	2:B:293:LYS:HA	1.83	0.42
2:C:78:LYS:HA	2:C:78:LYS:HZ2	1.85	0.42
2:C:78:LYS:HA	2:C:78:LYS:NZ	2.34	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
1:R:6:U:H3'	2:D:408:ARG:HH12	1.85	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
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
1:R:25:U:O2'	3:R:101:DV4:C19	2.68	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: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: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:66:ILE:HG23	2:D:67:ILE:HD12	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:303:LEU:CD2	2:D:328:THR:HA	2.50	0.42
2:E:40:LEU:HD22	2:E:42:ILE:CG1	2.50	0.42
1:R:38:U:C3'	1:R:39:U:H5"	2.46	0.41
2:A:41:TYR:O	2:A:190:ASN:ND2	2.53	0.41
2:A:166:MET:H	2:E:184:VAL:HG13	1.85	0.41
2:A:239:GLY:HA3	2:E:323:GLU:CD	2.40	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
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:D:314:ARG:HG2	2:D:314:ARG:H	1.67	0.41
2:E:293:LYS:HD2	2:E:293:LYS:HA	1.91	0.41
2:B:84:LEU:HD22	2:B:84:LEU:HA	1.95	0.41
2:C:33:ARG:O	2:C:33:ARG:HG3	2.19	0.41
2:E:42:ILE:HD13	2:E:74:TYR:HB2	2.03	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
1:R:19:U:OP2	2:C:218:ILE:HD12	2.21	0.41
2:A:328:THR:HG21	2:A:415:TYR:CE2	2.55	0.41
2:C:44:THR:HG22	2:C:71:SER:OG	2.19	0.41
2:C:111:LYS:HB3	2:C:111:LYS:HE3	1.79	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:1:U:H6	1:R:2:U:C6	2.38	0.41
2:A:18:LEU:H	2:A:18:LEU:HD23	1.85	0.41
2:A:166:MET:N	2:E:184:VAL:HG13	2.36	0.41
2:A:293:LYS:HA	2:A:293:LYS:HD3	1.87	0.41
2:A:369:PRO:HA	2:A:370:PRO:HD3	1.95	0.41
2:E:25:VAL:HG11	2:E:260:GLN:OE1	2.20	0.41
2:E:177:GLU:HG2	2:E:179:ARG:H	1.84	0.41
2:E:366:THR:C	2:E:368:ALA:H	2.23	0.41
2:A:302:GLN:HG2	2:A:316:ALA:CB	2.51	0.41
2:A:308:LEU:HD12	2:A:308:LEU:HA	1.81	0.41
2:C:149:MET:C	2:C:151:GLU:N	2.73	0.41
2:D:46:LYS:O	2:D:47:SER:O	2.39	0.41
2:D:369:PRO:HA	2:D:370:PRO:HD3	1.97	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:15:U:O2	1:R:15:U:C5'	2.68	0.41
1:R:26:U:H3'	2:B:143:ARG:NH2	2.35	0.41
1:R:31:U:H5'	1:R:32:U:OP1	2.20	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:278:LEU:H	2:A:278:LEU:HD23	1.85	0.41
2:A:336:TYR:CG	2:A:393:MET:HG2	2.55	0.41
2:B:48:LEU:HD22	2:B:48:LEU:N	2.35	0.41
2:B:184:VAL:CG1	2:C:165:LYS:HA	2.44	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:HD12	2:C:308:LEU:HA	1.85	0.41
2:D:410:LYS:HA	2:D:410:LYS:HD2	1.89	0.41
2:C:307:LEU:HD13	2:C:307:LEU:HA	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
1:R:14:U:P	2:C:317:ARG:NH2	2.93	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
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
1:R:5:U:O4'	2:D:317:ARG:NH2	2.48	0.40
1:R:31:U:O3'	2:A:317:ARG:NH2	2.54	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:OE1	2:C:169:GLU:HA	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
2:B:143:ARG:HB2	2:B:216:GLY:O	2.20	0.40
2:C:66:ILE:HD12	2:C:69:VAL:CG2	2.51	0.40
2:C:397:ALA:O	2:C:401:VAL:HG22	2.21	0.40
2:D:104:ILE:H	2:D:104:ILE:HG12	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 (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
2	A	419/421 (100%)	357 (85%)	41 (10%)	21 (5%)	2 18
2	B	411/421 (98%)	355 (86%)	41 (10%)	15 (4%)	3 25
2	C	409/421 (97%)	354 (87%)	39 (10%)	16 (4%)	3 24
2	D	412/421 (98%)	360 (87%)	34 (8%)	18 (4%)	2 21
2	E	419/421 (100%)	356 (85%)	46 (11%)	17 (4%)	3 23
All	All	2070/2105 (98%)	1782 (86%)	201 (10%)	87 (4%)	3 22

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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 (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
2	A	362/362 (100%)	329 (91%)	33 (9%)	9 35
2	B	358/362 (99%)	317 (88%)	41 (12%)	5 24
2	C	356/362 (98%)	306 (86%)	50 (14%)	3 17
2	D	359/362 (99%)	314 (88%)	45 (12%)	4 21
2	E	362/362 (100%)	333 (92%)	29 (8%)	12 40
All	All	1797/1810 (99%)	1599 (89%)	198 (11%)	6 27

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Sometimes 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 monosaccharides 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	2.37	14 (45%)	30,50,50	3.48	16 (53%)

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	-	-	6/14/27/27	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	101	DV4	C16-N18	5.59	1.46	1.33
3	R	101	DV4	C02-N04	4.98	1.45	1.36
3	R	101	DV4	C22-N24	4.54	1.45	1.35
3	R	101	DV4	C08-N10	4.13	1.46	1.35
3	R	101	DV4	C30-N28	-3.98	1.32	1.38
3	R	101	DV4	O17-C16	-2.88	1.17	1.23
3	R	101	DV4	O23-C22	-2.80	1.17	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	101	DV4	O09-C08	-2.74	1.17	1.23
3	R	101	DV4	O03-C02	-2.48	1.17	1.23
3	R	101	DV4	C07-N32	-2.44	1.31	1.36
3	R	101	DV4	C11-N10	2.31	1.45	1.40
3	R	101	DV4	C15-N31	-2.20	1.31	1.34
3	R	101	DV4	C25-N24	2.12	1.45	1.41
3	R	101	DV4	C05-N04	2.11	1.45	1.41

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	R	101	DV4	C15-C16-N18	13.88	129.39	115.60
3	R	101	DV4	O09-C08-N10	-5.81	110.43	123.71
3	R	101	DV4	C01-C02-N04	4.53	121.63	114.98
3	R	101	DV4	O17-C16-N18	-3.74	115.15	122.61
3	R	101	DV4	C05-N04-C02	-3.72	121.23	127.99
3	R	101	DV4	C07-C08-N10	3.52	137.23	117.76
3	R	101	DV4	C21-C22-N24	3.37	120.53	114.59
3	R	101	DV4	C11-N10-C08	3.26	137.09	128.07
3	R	101	DV4	C25-N24-C22	-2.84	122.52	127.50
3	R	101	DV4	O23-C22-C21	-2.78	116.93	122.02
3	R	101	DV4	C20-C21-C22	-2.59	106.00	113.26
3	R	101	DV4	C06-C05-C34	-2.38	104.89	106.05
3	R	101	DV4	C14-N13-C15	2.18	129.47	126.39
3	R	101	DV4	O03-C02-N04	-2.13	120.24	123.04
3	R	101	DV4	O03-C02-C01	-2.12	118.13	122.06
3	R	101	DV4	C34-N32-C07	2.04	110.82	108.65

There are no chirality outliers.

All (6) torsion outliers are listed below:

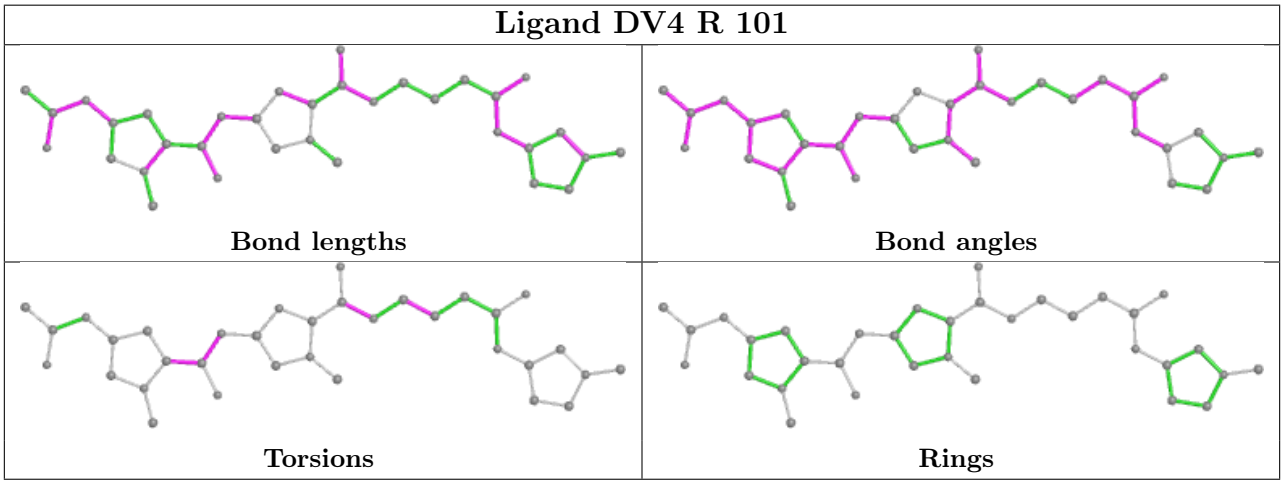
Mol	Chain	Res	Type	Atoms
3	R	101	DV4	C06-C07-C08-O09
3	R	101	DV4	C07-C08-N10-C11
3	R	101	DV4	O09-C08-N10-C11
3	R	101	DV4	C15-C16-N18-C19
3	R	101	DV4	O17-C16-N18-C19
3	R	101	DV4	N18-C19-C20-C21

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	R	45/45 (100%)	0.77	6 (13%) 3 5	104, 149, 197, 237	0
2	A	421/421 (100%)	0.56	45 (10%) 6 8	56, 112, 185, 250	0
2	B	415/421 (98%)	0.40	29 (6%) 16 18	54, 107, 170, 314	0
2	C	413/421 (98%)	0.43	30 (7%) 15 17	53, 110, 178, 258	0
2	D	416/421 (98%)	0.42	24 (5%) 23 23	58, 116, 180, 225	0
2	E	421/421 (100%)	0.72	53 (12%) 3 5	63, 125, 197, 246	0
All	All	2131/2150 (99%)	0.51	187 (8%) 10 12	53, 115, 185, 314	0

All (187) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	361	THR	15.0
2	E	2	SER	11.8
2	C	2	SER	10.7
2	E	366	THR	10.1
2	E	176	PRO	7.3
2	A	360	SER	7.2
2	C	357	PRO	6.7
2	C	101	THR	6.7
2	B	172	GLU	6.6
2	E	118	PRO	6.2
2	B	117	LEU	6.2
2	B	177	GLU	5.4
2	E	367	ASN	5.4
2	C	274	TYR	5.3
2	A	364	LEU	5.3
2	C	173	PRO	5.2
2	E	365	THR	5.1
2	C	213	PHE	5.1
2	D	113	LEU	5.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	E	173	PRO	4.9
2	A	120	GLY	4.9
2	E	153	ARG	4.9
2	E	72	TYR	4.6
2	C	174	LEU	4.5
2	D	39	PRO	4.5
2	A	363	GLY	4.5
2	B	176	PRO	4.4
2	E	113	LEU	4.4
2	E	101	THR	4.4
2	D	112	ALA	4.4
2	A	121	VAL	4.3
2	E	360	SER	4.3
2	E	141	LEU	4.2
2	E	22	GLU	4.1
2	E	175	VAL	4.1
2	C	356	THR	4.1
2	C	163	GLN	4.1
2	D	166	MET	4.1
2	C	100	ASP	4.0
2	D	2	SER	3.9
2	A	166	MET	3.9
2	A	2	SER	3.9
2	D	114	ASP	3.8
2	A	114	ASP	3.8
2	E	119	ASP	3.8
2	E	105	PHE	3.7
2	D	131	ASP	3.7
2	C	95	ILE	3.7
2	E	363	GLY	3.7
2	E	361	THR	3.7
2	A	407	LEU	3.7
2	A	108	VAL	3.7
2	A	102	ILE	3.6
2	B	274	TYR	3.6
2	C	27	TYR	3.6
2	E	68	HIS	3.6
2	E	362	GLY	3.6
2	A	365	THR	3.5
2	A	172	GLU	3.4
2	C	169	GLU	3.4
2	B	367	ASN	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	68	HIS	3.4
2	C	83	LYS	3.4
2	E	69	VAL	3.4
2	C	172	GLU	3.4
2	D	274	TYR	3.3
2	D	63	ASN	3.3
2	A	113	LEU	3.3
2	C	88	TRP	3.2
2	B	43	ASN	3.2
2	D	40	LEU	3.2
2	A	269	ASP	3.2
2	D	95	ILE	3.1
2	A	310	SER	3.1
2	D	171	PHE	3.1
2	D	38	ILE	3.1
2	A	366	THR	3.1
2	C	133	TRP	3.0
2	E	99	GLY	3.0
2	B	133	TRP	3.0
2	B	68	HIS	3.0
2	A	105	PHE	3.0
2	B	173	PRO	3.0
2	C	28	PRO	3.0
2	B	121	VAL	2.9
2	D	27	TYR	2.9
2	B	174	LEU	2.9
2	E	120	GLY	2.8
2	E	332	LEU	2.8
2	E	422	LYS	2.8
2	A	367	ASN	2.8
2	E	117	LEU	2.8
2	D	172	GLU	2.8
2	B	175	VAL	2.8
2	B	124	ALA	2.8
2	E	185	TRP	2.8
2	E	272	ASP	2.8
2	A	152	TYR	2.8
2	B	37	GLU	2.7
2	E	40	LEU	2.7
2	A	118	PRO	2.7
2	A	97	LYS	2.7
2	A	362	GLY	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	A	348	PHE	2.7
2	B	97	LYS	2.7
2	A	233	HIS	2.7
2	A	122	SER	2.6
2	E	174	LEU	2.6
2	D	364	LEU	2.6
2	A	14	ILE	2.6
2	E	172	GLU	2.6
2	B	145	GLY	2.5
2	B	88	TRP	2.5
2	E	84	LEU	2.5
2	D	14	ILE	2.5
2	D	60	LYS	2.5
2	A	164	CYS	2.5
2	A	99	GLY	2.5
1	R	41	U	2.4
2	E	89	SER	2.4
2	C	146	ARG	2.4
2	E	42	ILE	2.4
2	A	68	HIS	2.4
2	B	125	SER	2.4
2	E	267	GLU	2.4
2	A	213	PHE	2.4
2	C	57	GLN	2.4
2	E	57	GLN	2.4
2	E	121	VAL	2.4
2	E	45	THR	2.4
2	C	18	LEU	2.4
2	B	185	TRP	2.3
2	D	137	TYR	2.3
2	A	15	VAL	2.3
2	A	117	LEU	2.3
2	A	95	ILE	2.3
2	E	138	LEU	2.3
2	E	152	TYR	2.3
2	A	173	PRO	2.3
2	A	242	THR	2.3
2	A	60	LYS	2.3
2	A	246	THR	2.3
2	C	82	GLY	2.3
2	A	405	GLN	2.3
2	E	160	LEU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	20	ALA	2.2
2	D	346	GLN	2.2
2	A	278	LEU	2.2
1	R	43	U	2.2
2	B	39	PRO	2.2
2	A	16	PRO	2.2
2	D	310	SER	2.2
2	B	366	THR	2.2
2	C	143	ARG	2.2
2	D	185	TRP	2.2
2	B	116	VAL	2.2
2	C	102	ILE	2.2
2	E	358	ASP	2.2
2	C	210	CYS	2.2
2	C	348	PHE	2.2
2	B	357	PRO	2.2
2	E	321	ASP	2.2
2	A	356	THR	2.2
2	B	104	ILE	2.2
2	C	3	VAL	2.2
2	E	409	GLU	2.2
2	B	156	LEU	2.2
2	B	167	ILE	2.2
2	E	114	ASP	2.2
2	E	73	LEU	2.1
2	A	357	PRO	2.1
2	B	118	PRO	2.1
2	C	355	TYR	2.1
1	R	4	U	2.1
2	E	140	GLY	2.1
1	R	37	U	2.1
2	B	407	LEU	2.1
2	A	174	LEU	2.1
2	E	144	VAL	2.1
2	E	191	TYR	2.1
2	E	71	SER	2.1
2	C	176	PRO	2.1
1	R	27	U	2.1
2	E	88	TRP	2.0
2	E	268	ILE	2.0
2	C	233	HIS	2.0
1	R	45	U	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)

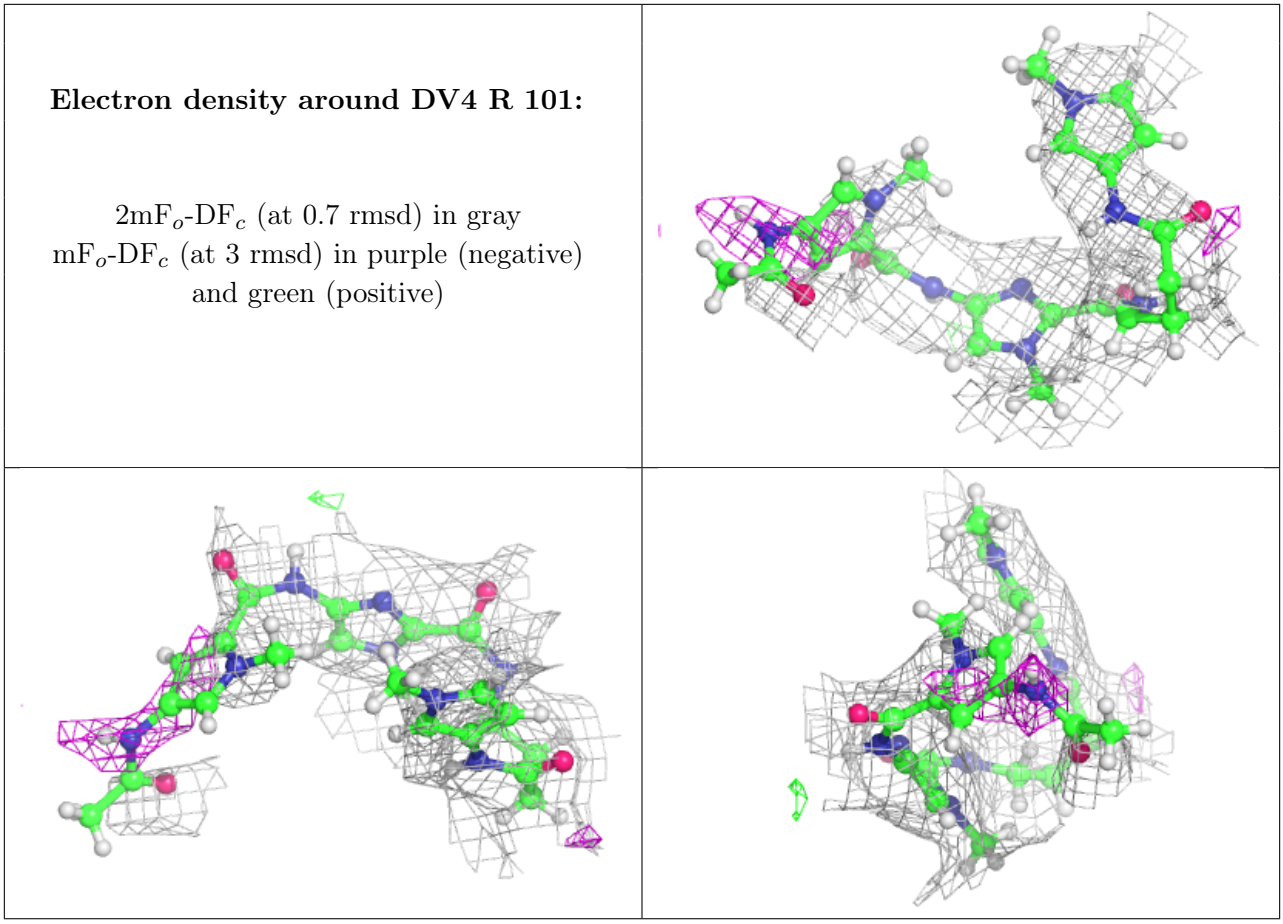
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	DV4	R	101	34/34	0.69	0.32	78,121,148,163	0
4	IUM	D	502	1/3	0.73	0.25	131,131,131,131	0
4	IUM	A	502	1/3	0.81	0.22	104,104,104,104	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	503	1/3	0.87	0.15	169,169,169,169	0
4	IUM	E	502	1/3	0.89	0.14	203,203,203,203	0
4	IUM	A	505	1/3	0.91	0.19	125,125,125,125	0
4	IUM	D	501	1/3	0.92	0.21	150,150,150,150	0
4	IUM	E	501	1/3	0.94	0.17	144,144,144,144	0
4	IUM	B	503	1/3	0.94	0.14	194,194,194,194	0
4	IUM	B	501	1/3	0.96	0.21	164,164,164,164	0
4	IUM	C	501	1/3	0.97	0.16	146,146,146,146	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	0.15	144,144,144,144	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around DV4 R 101:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers

There are no such residues in this entry.