



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:18 AM GMT

PDB ID : 2GIC
Title : Crystal Structure of a vesicular stomatitis virus nucleocapsid-RNA complex
Authors : Green, T.J.; Zhang, X.; Wertz, G.W.; Luo, M.
Deposited on : 2006-03-28
Resolution : 2.92 Å(reported)

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

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

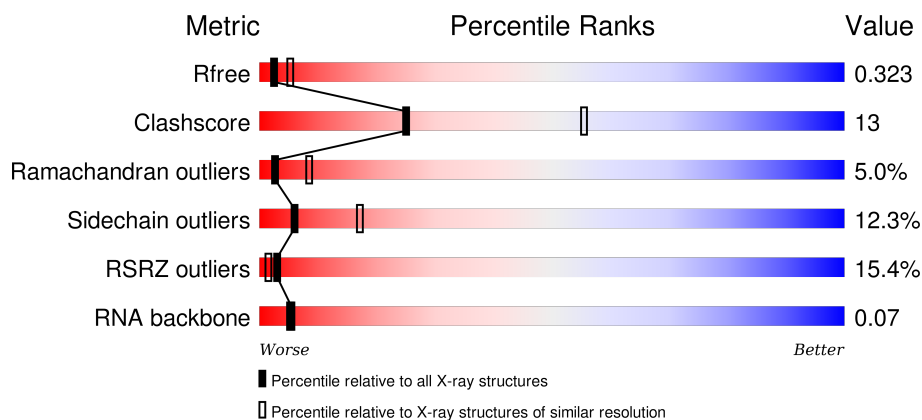
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.92 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}	91344	1643 (2.94-2.90)
Clashscore	102246	1871 (2.94-2.90)
Ramachandran outliers	100387	1824 (2.94-2.90)
Sidechain outliers	100360	1826 (2.94-2.90)
RSRZ outliers	91569	1650 (2.94-2.90)
RNA backbone	2183	1004 (3.30-2.54)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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>38%</div> <div> <div>9%</div> <div>29%</div> <div>51%</div> <div>11%</div> </div> </div>
2	A	422	<div> <div>15%</div> <div> <div>70%</div> <div>24%</div> <div>5%</div> </div> </div>
2	B	422	<div> <div>12%</div> <div> <div>67%</div> <div>25%</div> <div>7%</div> <div>•</div> </div> </div>
2	C	422	<div> <div>12%</div> <div> <div>68%</div> <div>23%</div> <div>6%</div> <div>••</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	D	422	<div><div></div><div>13%</div><div>70%</div><div>24%</div><div>5%</div></div>
2	E	422	<div><div></div><div>22%</div><div>68%</div><div>26%</div><div>5%</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17432 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

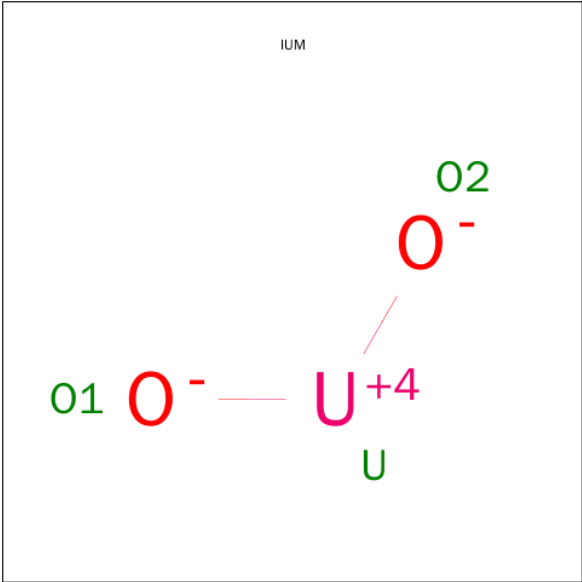
- Molecule 1 is a RNA chain called 45-MER.

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 Nucleocapsid protein.

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 URANYL (VI) ION (three-letter code: IUM) (formula: O₂U).



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

Continued on next page...

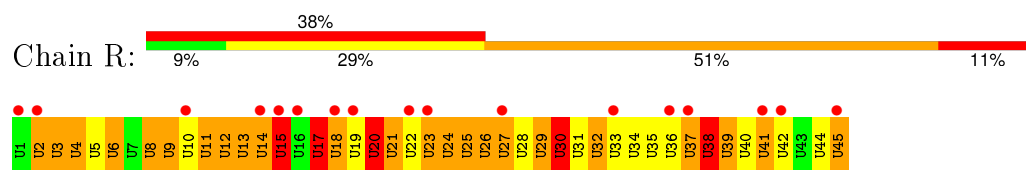
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total	U	0	0
			1	1		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

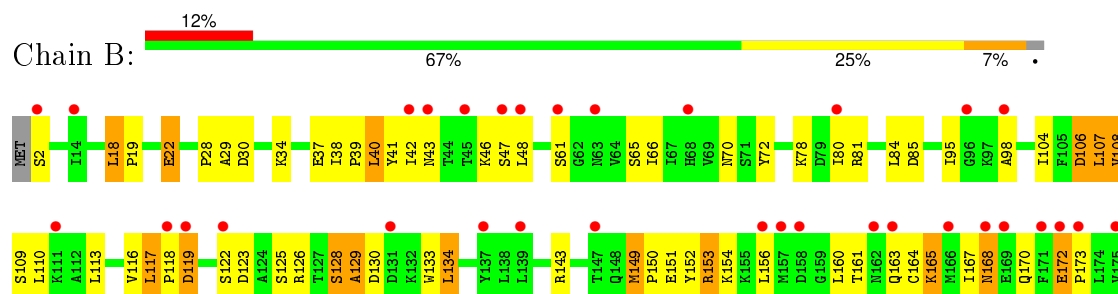
- Molecule 1: 45-MER

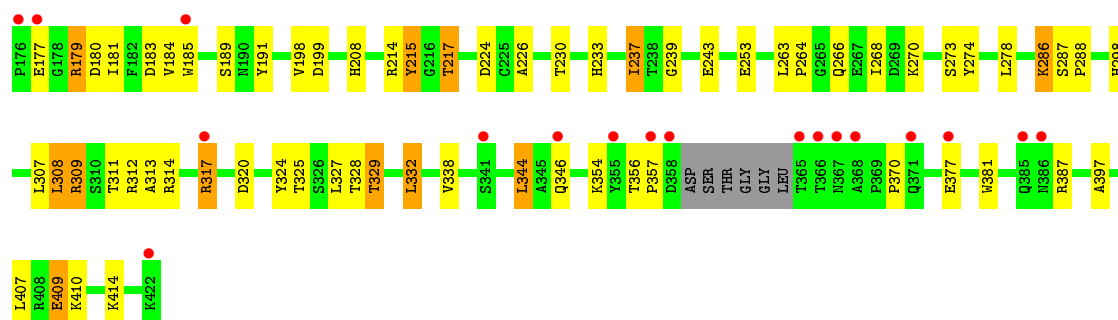


- Molecule 2: Nucleocapsid protein

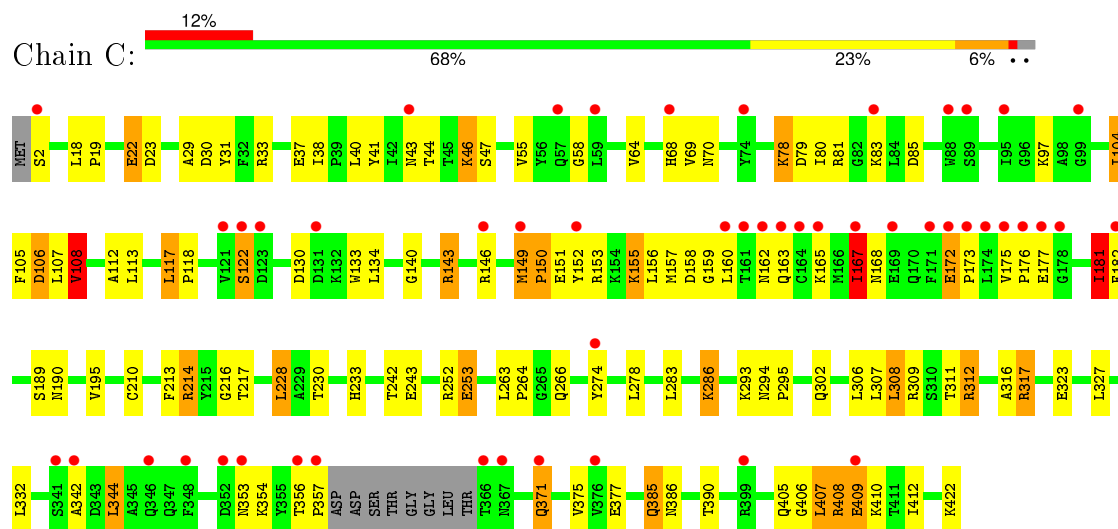


- Molecule 2: Nucleocapsid protein

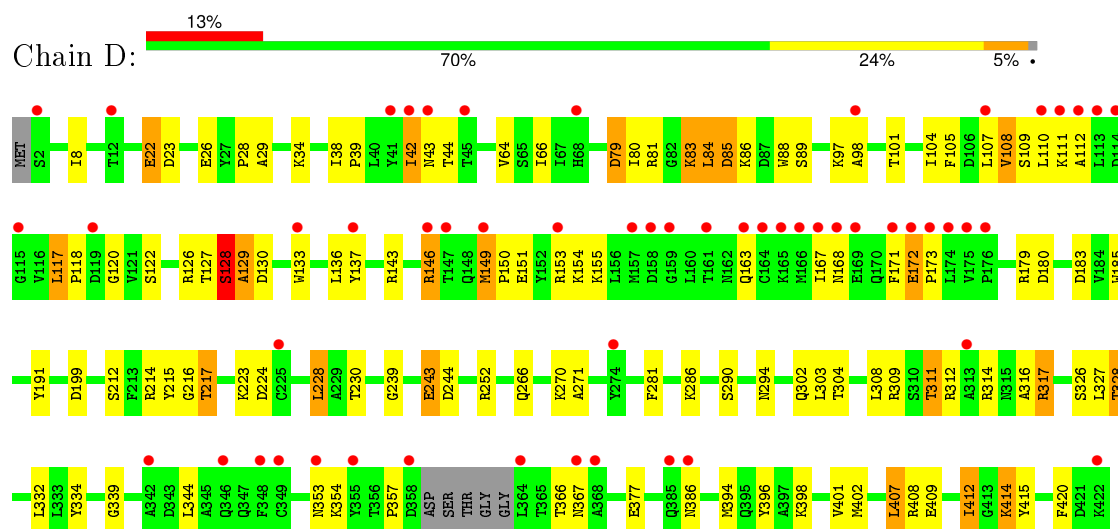




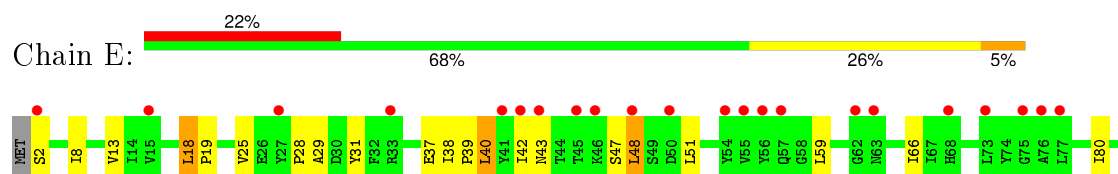
• Molecule 2: Nucleocapsid protein

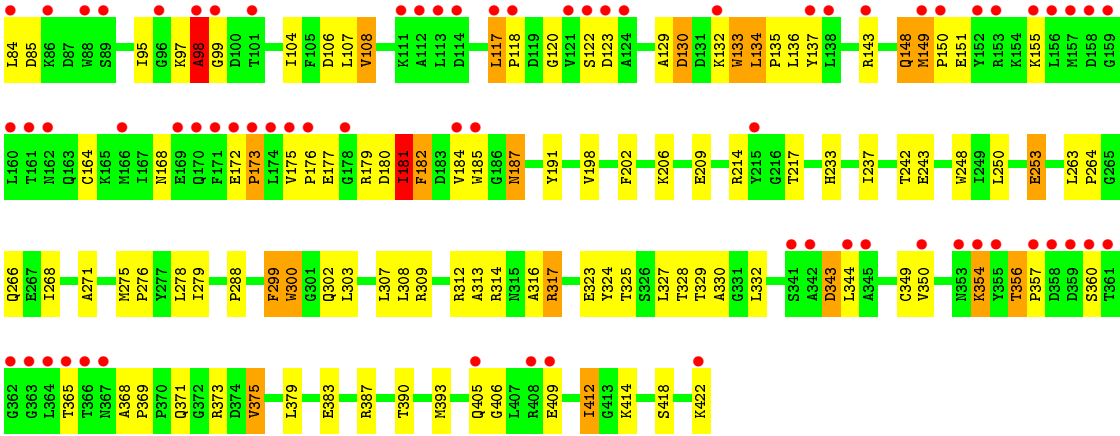


• Molecule 2: Nucleocapsid protein



• Molecule 2: Nucleocapsid protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	166.16 Å 236.32 Å 75.65 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.86 – 2.92 44.84 – 2.92	Depositor EDS
% Data completeness (in resolution range)	91.9 (44.86-2.92) 90.5 (44.84-2.92)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.95 (at 2.90 Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.255 , 0.306 0.270 , 0.323	Depositor DCC
R_{free} test set	3262 reflections (5.79%)	DCC
Wilson B-factor (Å ²)	73.1	Xtriage
Anisotropy	0.676	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 33.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	4 of 64651 reflections (0.006%)	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	17432	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.35% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 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	0.93	0/989	1.56	10/1526 (0.7%)
2	A	0.39	0/3403	0.54	0/4607
2	B	0.40	0/3365	0.55	0/4554
2	C	0.39	0/3350	0.56	0/4533
2	D	0.39	0/3373	0.56	0/4565
2	E	0.40	0/3403	0.54	0/4607
All	All	0.44	0/17883	0.66	10/24392 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
2	E	0	1
All	All	0	2

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	20	U	P-O3'-C3'	8.96	130.45	119.70
1	R	9	U	O4'-C1'-N1	6.62	113.50	108.20
1	R	9	U	O4'-C4'-C3'	-6.12	97.88	104.00
1	R	34	U	O4'-C1'-N1	5.87	112.90	108.20
1	R	15	U	C2-N1-C1'	5.75	124.61	117.70
1	R	17	U	P-O3'-C3'	5.33	126.10	119.70
1	R	32	U	C3'-C2'-C1'	5.22	105.68	101.50
1	R	37	U	O4'-C1'-N1	5.11	112.29	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	38	U	P-O3'-C3'	5.09	125.81	119.70
1	R	30	U	C4'-C3'-C2'	-5.07	97.53	102.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	106	ASP	Peptide
2	E	98	ALA	Peptide

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	62	0
2	A	3327	0	3287	87	0
2	B	3290	0	3253	105	0
2	C	3275	0	3242	81	0
2	D	3298	0	3264	75	0
2	E	3327	0	3287	92	0
3	A	4	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	2	0	0	0	0
3	E	3	0	0	0	0
All	All	17432	0	16784	435	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 13.

All (435) 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)
2:A:143:ARG:HD2	2:A:155:LYS:CE	1.44	1.45
2:A:143:ARG:CD	2:A:155:LYS:HE2	1.52	1.36

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:109:SER:O	2:B:110:LEU:HD23	1.31	1.22
2:D:107:LEU:O	2:D:108:VAL:HG22	1.42	1.18
2:B:107:LEU:N	2:B:107:LEU:HD23	1.56	1.16
2:B:37:GLU:HB2	2:B:108:VAL:CG2	1.76	1.14
2:B:117:LEU:HB2	2:B:118:PRO:HD3	1.30	1.11
2:C:143:ARG:HH11	2:C:155:LYS:HD3	1.17	1.08
1:R:22:U:H2'	2:B:317:ARG:HE	1.21	1.06
2:B:37:GLU:HB2	2:B:108:VAL:HG21	1.34	1.05
2:C:214:ARG:HA	2:C:217:THR:HG22	1.36	1.03
2:B:106:ASP:C	2:B:107:LEU:HD23	1.79	1.01
2:A:143:ARG:HD2	2:A:155:LYS:HE3	1.41	0.98
2:D:143:ARG:HE	2:D:155:LYS:HE3	1.27	0.96
2:A:117:LEU:HB3	2:A:118:PRO:HD3	1.46	0.94
2:E:133:TRP:CD1	2:E:134:LEU:N	2.36	0.94
2:D:117:LEU:HB2	2:D:118:PRO:HD3	1.48	0.93
2:B:172:GLU:HB3	2:B:173:PRO:HD3	1.49	0.93
2:B:107:LEU:N	2:B:107:LEU:CD2	2.31	0.92
2:E:129:ALA:HB1	2:E:133:TRP:HE1	1.33	0.91
2:A:143:ARG:HD2	2:A:155:LYS:HE2	0.92	0.90
2:B:37:GLU:HB2	2:B:108:VAL:HG22	1.56	0.88
2:D:214:ARG:HA	2:D:217:THR:HG22	1.54	0.88
2:B:320:ASP:HB3	2:C:312:ARG:NH2	1.89	0.88
2:B:109:SER:O	2:B:110:LEU:CD2	2.21	0.87
2:A:324:TYR:O	2:A:328:THR:HG23	1.76	0.86
2:D:146:ARG:HH11	2:D:223:LYS:HE2	1.40	0.85
2:C:117:LEU:HB2	2:C:118:PRO:HD3	1.59	0.85
2:B:107:LEU:HD13	2:B:274:TYR:OH	1.77	0.84
2:B:117:LEU:HB2	2:B:118:PRO:CD	2.07	0.83
2:C:2:SER:HB3	2:D:243:GLU:HG3	1.58	0.83
2:E:117:LEU:HB2	2:E:118:PRO:HD3	1.60	0.82
1:R:11:U:H3'	1:R:12:U:H5''	1.62	0.81
2:B:37:GLU:CB	2:B:108:VAL:HG21	2.09	0.81
2:A:143:ARG:CG	2:A:155:LYS:HE2	2.09	0.81
2:B:164:CYS:HA	2:B:168:ASN:H	1.46	0.81
2:D:83:LYS:HG3	2:D:101:THR:HG22	1.64	0.79
2:D:143:ARG:HE	2:D:155:LYS:CE	1.97	0.78
2:E:324:TYR:O	2:E:328:THR:HG23	1.84	0.78
2:B:106:ASP:C	2:B:107:LEU:CD2	2.53	0.77
2:A:323:GLU:OE1	2:B:239:GLY:HA3	1.84	0.77
2:C:143:ARG:NH1	2:C:155:LYS:HD3	1.97	0.77
2:D:107:LEU:O	2:D:108:VAL:CG2	2.30	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:253:GLU:CD	2:A:253:GLU:H	1.88	0.76
2:B:320:ASP:HB3	2:C:312:ARG:HH22	1.47	0.76
2:C:253:GLU:CD	2:C:253:GLU:H	1.89	0.76
2:A:215:TYR:N	2:A:215:TYR:HD2	1.83	0.75
2:D:143:ARG:NE	2:D:155:LYS:HE3	1.99	0.74
2:A:354:LYS:HD2	2:E:379:LEU:HB3	1.68	0.74
2:A:214:ARG:HA	2:A:217:THR:HG22	1.68	0.74
2:C:117:LEU:CB	2:C:118:PRO:HD3	2.17	0.74
2:A:215:TYR:CD2	2:A:215:TYR:N	2.55	0.74
2:E:133:TRP:O	2:E:136:LEU:N	2.20	0.74
2:D:107:LEU:C	2:D:108:VAL:HG22	2.06	0.74
2:D:146:ARG:HH11	2:D:223:LYS:CE	2.01	0.73
1:R:3:U:H2'	1:R:4:U:H4'	1.70	0.73
2:A:215:TYR:H	2:A:215:TYR:HD2	1.36	0.73
2:E:37:GLU:HB2	2:E:108:VAL:HG21	1.68	0.73
1:R:38:U:H3'	1:R:39:U:H5''	1.69	0.73
2:C:44:THR:OG1	2:C:46:LYS:HE3	1.90	0.71
2:C:172:GLU:H	2:C:173:PRO:HD2	1.55	0.71
2:E:129:ALA:HB1	2:E:133:TRP:NE1	2.04	0.71
2:E:133:TRP:HD1	2:E:133:TRP:H	1.35	0.71
2:A:399:ARG:HB3	2:E:422:LYS:NZ	2.06	0.70
1:R:23:U:H5'	2:B:317:ARG:HH21	1.56	0.70
2:B:214:ARG:HA	2:B:217:THR:HG22	1.74	0.70
1:R:44:U:H5''	2:E:143:ARG:NH2	2.07	0.70
1:R:15:U:C4	2:C:408:ARG:HD3	2.28	0.69
2:E:356:THR:HG23	2:E:357:PRO:HD3	1.72	0.69
2:C:214:ARG:HA	2:C:217:THR:CG2	2.20	0.68
2:C:37:GLU:HB2	2:C:108:VAL:HG21	1.76	0.68
1:R:23:U:H5'	2:B:317:ARG:NH2	2.09	0.68
2:E:253:GLU:CD	2:E:253:GLU:H	1.98	0.67
1:R:44:U:C2'	1:R:45:U:H5''	2.24	0.66
2:E:133:TRP:CG	2:E:134:LEU:N	2.64	0.66
2:C:172:GLU:H	2:C:173:PRO:CD	2.08	0.66
2:B:356:THR:HG23	2:B:357:PRO:HD3	1.77	0.66
1:R:12:U:OP2	2:C:286:LYS:NZ	2.28	0.66
2:E:354:LYS:HE3	2:E:356:THR:HA	1.76	0.66
1:R:29:U:OP1	2:A:286:LYS:NZ	2.25	0.65
2:A:399:ARG:HB3	2:E:422:LYS:HZ2	1.62	0.65
2:D:66:ILE:HD13	2:D:185:TRP:CD1	2.31	0.65
1:R:44:U:C3'	1:R:45:U:H5''	2.27	0.64
2:D:107:LEU:C	2:D:108:VAL:CG2	2.66	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:323:GLU:CD	2:D:239:GLY:HA3	2.18	0.64
2:A:364:LEU:HB3	2:A:368:ALA:HB2	1.80	0.64
1:R:13:U:H3'	2:C:317:ARG:HH21	1.62	0.64
2:D:28:PRO:HG2	2:D:266:GLN:HE21	1.62	0.64
2:C:233:HIS:CE1	2:C:312:ARG:HE	2.16	0.64
2:B:179:ARG:HA	2:B:183:ASP:CG	2.18	0.64
1:R:6:U:C6	1:R:6:U:H5''	2.32	0.63
2:E:40:LEU:HD22	2:E:42:ILE:HG13	1.80	0.63
2:E:379:LEU:O	2:E:383:GLU:HG2	1.99	0.63
1:R:6:U:O4'	2:D:149:MET:HG3	1.99	0.63
2:B:28:PRO:HG2	2:B:266:GLN:HE21	1.64	0.63
2:A:143:ARG:CD	2:A:155:LYS:CE	2.32	0.62
1:R:15:U:H5'	2:C:408:ARG:HH22	1.64	0.62
2:E:317:ARG:H	2:E:317:ARG:NE	1.97	0.62
2:B:325:THR:O	2:B:329:THR:HG22	2.00	0.62
1:R:15:U:H5''	2:C:408:ARG:HH12	1.64	0.62
1:R:2:U:H3'	1:R:3:U:H5''	1.79	0.62
2:C:79:ASP:C	2:C:81:ARG:H	2.03	0.62
2:A:253:GLU:O	2:A:257:GLU:HG3	2.00	0.62
2:A:42:ILE:HG21	2:A:70:ASN:HB3	1.80	0.62
1:R:44:U:H2'	1:R:45:U:H5''	1.82	0.61
2:D:29:ALA:H	2:D:266:GLN:HE22	1.47	0.61
2:E:104:ILE:HD11	2:E:198:VAL:HG22	1.81	0.61
2:E:133:TRP:HD1	2:E:134:LEU:H	1.42	0.61
2:C:143:ARG:HH11	2:C:155:LYS:CD	2.05	0.61
2:E:302:GLN:HG2	2:E:316:ALA:CB	2.31	0.61
1:R:44:U:OP2	2:E:155:LYS:NZ	2.33	0.61
1:R:41:U:O5'	2:E:317:ARG:NH2	2.34	0.60
1:R:17:U:H5''	2:C:143:ARG:HH12	1.65	0.60
2:B:149:MET:O	2:B:151:GLU:N	2.33	0.60
2:B:29:ALA:H	2:B:266:GLN:HE22	1.47	0.60
2:A:395:GLN:HA	2:A:395:GLN:HE21	1.65	0.60
2:C:149:MET:HB2	2:C:150:PRO:HD2	1.84	0.60
2:D:143:ARG:HD2	2:D:216:GLY:HA2	1.83	0.60
2:B:298:HIS:NE2	2:B:317:ARG:NH1	2.50	0.59
2:D:146:ARG:NH1	2:D:223:LYS:NZ	2.51	0.59
2:E:350:VAL:HG12	2:E:350:VAL:O	2.03	0.59
2:E:151:GLU:CD	2:E:155:LYS:HD2	2.22	0.58
2:E:97:LYS:O	2:E:98:ALA:C	2.40	0.58
2:D:89:SER:O	2:D:270:LYS:NZ	2.35	0.58
2:A:136:LEU:HD22	2:A:163:GLN:HE21	1.68	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:128:SER:OG	2:D:129:ALA:N	2.36	0.58
1:R:17:U:H3'	2:C:143:ARG:HH22	1.68	0.58
2:A:253:GLU:N	2:A:253:GLU:CD	2.56	0.58
2:A:317:ARG:CZ	2:A:317:ARG:H	2.16	0.58
2:B:230:THR:HG21	2:B:298:HIS:CE1	2.38	0.58
2:C:385:GLN:HG2	2:C:390:THR:HG22	1.84	0.58
1:R:3:U:H4'	2:D:224:ASP:HB3	1.86	0.58
2:B:233:HIS:CE1	2:B:312:ARG:HD2	2.39	0.58
1:R:17:U:H2'	1:R:18:U:H5''	1.85	0.58
2:D:303:LEU:HA	2:D:412:ILE:HD13	1.86	0.58
2:B:172:GLU:HB3	2:B:173:PRO:CD	2.29	0.58
2:B:106:ASP:O	2:B:107:LEU:HD22	2.05	0.57
2:D:38:ILE:O	2:D:38:ILE:HG13	2.04	0.57
2:D:407:LEU:HD13	2:D:414:LYS:HA	1.86	0.57
2:A:165:LYS:HA	2:E:184:VAL:HG22	1.86	0.57
2:C:155:LYS:HA	2:C:155:LYS:HE3	1.87	0.57
2:E:390:THR:OG1	2:E:393:MET:HG2	2.04	0.57
2:B:317:ARG:CZ	2:B:317:ARG:H	2.18	0.57
2:C:55:VAL:HG12	2:C:69:VAL:HG12	1.87	0.57
2:D:143:ARG:CD	2:D:216:GLY:HA2	2.35	0.56
1:R:20:U:OP1	2:B:286:LYS:NZ	2.30	0.56
2:B:104:ILE:HD11	2:B:198:VAL:HG22	1.87	0.56
2:C:143:ARG:HG2	2:C:216:GLY:HA2	1.87	0.56
1:R:24:U:H5'	1:R:24:U:H6	1.70	0.56
2:E:278:LEU:HD12	2:E:279:ILE:HG12	1.87	0.56
2:C:302:GLN:HG2	2:C:316:ALA:CB	2.35	0.56
2:A:17:LYS:HG3	2:B:268:ILE:HD11	1.87	0.56
2:C:155:LYS:O	2:C:155:LYS:HG3	2.05	0.56
2:A:187:ASN:N	2:A:187:ASN:HD22	2.02	0.56
2:B:38:ILE:HD11	2:B:107:LEU:HD12	1.87	0.56
2:A:342:ALA:N	2:E:387:ARG:HH12	2.04	0.56
2:C:157:MET:HG3	2:C:158:ASP:H	1.71	0.56
2:B:37:GLU:OE2	2:B:108:VAL:HG11	2.06	0.56
2:B:226:ALA:O	2:B:230:THR:HG23	2.06	0.56
2:B:253:GLU:H	2:B:253:GLU:CD	2.09	0.56
2:C:41:TYR:HB2	2:C:190:ASN:HD21	1.69	0.56
2:D:212:SER:O	2:D:215:TYR:HD1	1.90	0.55
2:E:133:TRP:N	2:E:133:TRP:CD1	2.67	0.55
2:C:253:GLU:CD	2:C:253:GLU:N	2.60	0.55
1:R:3:U:C2'	1:R:4:U:H4'	2.36	0.55
2:C:149:MET:O	2:C:151:GLU:N	2.38	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:336:TYR:O	2:A:340:SER:HB2	2.07	0.55
2:A:233:HIS:CE1	2:A:312:ARG:HD2	2.42	0.55
2:A:130:ASP:CG	2:A:131:ASP:H	2.09	0.55
1:R:22:U:H2'	2:B:317:ARG:NE	2.06	0.55
2:E:202:PHE:HB2	2:E:214:ARG:HD3	1.89	0.55
2:B:106:ASP:O	2:B:107:LEU:CD2	2.54	0.55
2:D:136:LEU:HD22	2:D:163:GLN:HG3	1.89	0.54
2:D:328:THR:HG21	2:D:415:TYR:HE1	1.71	0.54
2:B:356:THR:CG2	2:B:357:PRO:HD3	2.37	0.54
2:E:130:ASP:C	2:E:132:LYS:H	2.10	0.54
2:C:146:ARG:HD3	2:C:146:ARG:O	2.08	0.54
1:R:18:U:H4'	1:R:18:U:OP1	2.08	0.54
2:A:257:GLU:OE1	2:A:295:PRO:HD2	2.08	0.54
2:B:118:PRO:O	2:B:119:ASP:HB2	2.08	0.53
2:B:324:TYR:O	2:B:328:THR:HG22	2.07	0.53
2:E:268:ILE:HG22	2:E:275:MET:HG3	1.89	0.53
2:A:117:LEU:HB3	2:A:118:PRO:CD	2.29	0.53
1:R:6:U:H6	1:R:6:U:H5''	1.72	0.53
2:B:317:ARG:NH1	2:B:317:ARG:H	2.06	0.53
2:A:149:MET:O	2:A:151:GLU:N	2.41	0.53
2:E:97:LYS:O	2:E:99:GLY:N	2.42	0.53
2:D:179:ARG:HA	2:D:183:ASP:CG	2.29	0.53
1:R:30:U:H2'	1:R:31:U:O4'	2.09	0.53
2:C:29:ALA:H	2:C:266:GLN:HE22	1.57	0.53
2:A:302:GLN:HG2	2:A:316:ALA:CB	2.39	0.53
2:E:149:MET:O	2:E:151:GLU:N	2.38	0.53
2:C:38:ILE:O	2:C:38:ILE:HG13	2.08	0.53
2:E:133:TRP:O	2:E:134:LEU:C	2.48	0.52
2:C:210:CYS:HB3	2:C:213:PHE:CE1	2.44	0.52
2:E:129:ALA:O	2:E:133:TRP:CD1	2.62	0.52
1:R:41:U:C4	2:E:312:ARG:HG3	2.44	0.52
2:A:23:ASP:HB2	2:A:286:LYS:NZ	2.24	0.52
2:A:149:MET:C	2:A:151:GLU:H	2.13	0.52
2:B:66:ILE:HD13	2:B:185:TRP:CD1	2.44	0.52
2:D:304:THR:HG21	2:D:334:TYR:CD2	2.45	0.52
1:R:14:U:H5''	2:C:317:ARG:HH22	1.74	0.52
2:E:151:GLU:OE2	2:E:155:LYS:HD2	2.09	0.52
2:B:320:ASP:CB	2:C:312:ARG:HH22	2.22	0.52
2:D:43:ASN:HB2	2:D:112:ALA:N	2.25	0.52
1:R:4:U:OP2	2:D:290:SER:HB2	2.10	0.52
2:D:107:LEU:HD11	2:D:281:PHE:CZ	2.45	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:317:ARG:H	2:D:317:ARG:NE	2.08	0.52
2:A:298:HIS:NE2	2:A:317:ARG:NH1	2.58	0.51
1:R:4:U:C6	2:D:317:ARG:HG3	2.44	0.51
2:E:233:HIS:O	2:E:237:ILE:HG12	2.11	0.51
2:A:29:ALA:H	2:A:266:GLN:HE22	1.57	0.51
1:R:8:U:P	2:D:155:LYS:NZ	2.83	0.51
2:D:105:PHE:C	2:D:107:LEU:H	2.14	0.51
1:R:26:U:H5''	2:B:143:ARG:HH21	1.76	0.51
2:D:149:MET:O	2:D:151:GLU:N	2.44	0.51
2:B:104:ILE:HD11	2:B:198:VAL:HA	1.92	0.51
2:B:66:ILE:HD13	2:B:185:TRP:CG	2.46	0.51
2:D:107:LEU:CD1	2:D:281:PHE:CZ	2.93	0.51
2:A:143:ARG:HG3	2:A:155:LYS:HE2	1.92	0.51
1:R:23:U:C5'	2:B:317:ARG:NH2	2.74	0.50
2:C:133:TRP:HB3	2:C:167:ILE:HD12	1.92	0.50
1:R:44:U:H5''	2:E:143:ARG:HH22	1.76	0.50
2:B:270:LYS:HE3	2:B:273:SER:HB2	1.93	0.50
2:B:160:LEU:HD12	2:B:161:THR:HG23	1.94	0.50
2:D:146:ARG:NH1	2:D:223:LYS:CE	2.74	0.50
2:E:343:ASP:OD2	2:E:373:ARG:NH2	2.45	0.50
2:A:166:MET:C	2:A:167:ILE:HG13	2.32	0.50
2:A:143:ARG:HD3	2:A:219:VAL:HG11	1.94	0.50
2:D:117:LEU:HB2	2:D:118:PRO:CD	2.32	0.50
1:R:13:U:H3'	2:C:317:ARG:NH2	2.25	0.50
2:B:65:SER:HB2	2:B:117:LEU:HD11	1.94	0.50
2:A:324:TYR:HD1	2:B:237:ILE:HD11	1.76	0.50
2:D:133:TRP:HB3	2:D:167:ILE:HD13	1.94	0.50
2:A:214:ARG:HA	2:A:217:THR:CG2	2.38	0.49
2:E:253:GLU:CD	2:E:253:GLU:N	2.65	0.49
2:C:149:MET:C	2:C:151:GLU:H	2.14	0.49
2:A:106:ASP:C	2:A:107:LEU:HD12	2.33	0.49
2:C:106:ASP:C	2:C:107:LEU:HD12	2.33	0.49
2:A:143:ARG:HH11	2:A:155:LYS:HE3	1.77	0.49
2:D:328:THR:HG21	2:D:415:TYR:CE1	2.46	0.49
2:E:66:ILE:HD13	2:E:185:TRP:CD1	2.47	0.49
2:A:77:LEU:C	2:A:79:ASP:H	2.16	0.49
2:A:136:LEU:HD21	2:A:162:ASN:HD22	1.77	0.49
2:B:38:ILE:O	2:B:38:ILE:HG13	2.13	0.48
2:B:109:SER:C	2:B:110:LEU:HD23	2.24	0.48
2:A:320:ASP:HA	2:A:324:TYR:OH	2.14	0.48
2:A:338:VAL:HG13	2:A:373:ARG:NH1	2.28	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:107:LEU:CD1	2:B:274:TYR:HE2	2.26	0.48
2:B:107:LEU:HD23	2:B:107:LEU:H	1.66	0.48
2:D:172:GLU:HB3	2:D:173:PRO:HD3	1.96	0.48
1:R:6:U:H3'	2:D:408:ARG:HH22	1.79	0.48
2:D:109:SER:O	2:D:110:LEU:HD23	2.14	0.47
2:C:117:LEU:CB	2:C:118:PRO:CD	2.90	0.47
2:E:29:ALA:H	2:E:266:GLN:HE22	1.62	0.47
2:A:210:CYS:HB3	2:A:213:PHE:CE1	2.49	0.47
1:R:4:U:H3'	2:D:317:ARG:NE	2.28	0.47
2:C:43:ASN:CG	2:C:112:ALA:HB3	2.35	0.47
2:C:342:ALA:HB1	2:C:344:LEU:HD23	1.96	0.47
1:R:27:U:O2'	1:R:29:U:OP2	2.32	0.47
2:D:149:MET:C	2:D:151:GLU:H	2.18	0.47
2:A:166:MET:H	2:E:184:VAL:HG13	1.80	0.47
2:B:149:MET:C	2:B:151:GLU:H	2.18	0.47
1:R:2:U:OP1	2:D:286:LYS:NZ	2.34	0.47
2:A:414:LYS:HA	2:A:414:LYS:HE3	1.95	0.47
2:B:107:LEU:CD1	2:B:274:TYR:CE2	2.98	0.47
2:B:172:GLU:CB	2:B:173:PRO:HD3	2.33	0.47
2:A:81:ARG:HD2	2:A:208:HIS:HE2	1.80	0.47
2:B:66:ILE:O	2:B:70:ASN:ND2	2.48	0.47
2:C:19:PRO:HD3	2:D:228:LEU:HD22	1.97	0.47
2:B:184:VAL:HG13	2:C:165:LYS:HA	1.96	0.47
2:B:107:LEU:HD13	2:B:274:TYR:CZ	2.50	0.46
2:E:117:LEU:CB	2:E:118:PRO:HD3	2.36	0.46
2:E:250:LEU:HD22	2:E:379:LEU:HD21	1.98	0.46
2:A:42:ILE:CG2	2:A:70:ASN:HB3	2.45	0.46
2:E:368:ALA:HB1	2:E:369:PRO:HD2	1.96	0.46
2:B:41:TYR:HA	2:B:110:LEU:O	2.15	0.46
2:E:325:THR:O	2:E:329:THR:HG22	2.15	0.46
2:B:332:LEU:HD21	2:B:397:ALA:HB2	1.98	0.46
2:D:66:ILE:HD11	2:D:191:TYR:HB2	1.97	0.46
2:A:268:ILE:HG22	2:A:275:MET:SD	2.56	0.46
2:D:84:LEU:HD11	2:D:88:TRP:HB2	1.96	0.46
2:A:419:GLU:OE1	2:B:309:ARG:NH1	2.48	0.46
1:R:23:U:C5'	2:B:317:ARG:HH21	2.26	0.46
2:B:409:GLU:OE2	2:B:409:GLU:N	2.48	0.46
2:D:339:GLY:HA3	2:D:396:TYR:OH	2.16	0.46
1:R:8:U:OP1	2:D:154:LYS:NZ	2.46	0.46
2:B:199:ASP:OD1	2:B:214:ARG:HD2	2.16	0.46
2:B:152:TYR:HD1	2:B:153:ARG:H	1.63	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:199:ASP:OD1	2:D:217:THR:HG23	2.16	0.46
2:E:130:ASP:O	2:E:132:LYS:N	2.49	0.46
2:C:293:LYS:C	2:C:295:PRO:HD3	2.36	0.46
2:B:317:ARG:O	2:B:317:ARG:HG2	2.16	0.46
2:C:79:ASP:C	2:C:81:ARG:N	2.68	0.46
2:B:72:TYR:CE1	2:B:134:LEU:HD12	2.51	0.46
2:D:317:ARG:H	2:D:317:ARG:CD	2.28	0.45
2:B:133:TRP:HB3	2:B:167:ILE:HG21	1.99	0.45
2:A:43:ASN:ND2	2:A:45:THR:OG1	2.48	0.45
2:E:175:VAL:HB	2:E:176:PRO:HD2	1.98	0.45
2:B:81:ARG:HD3	2:B:208:HIS:HE2	1.82	0.45
2:C:172:GLU:N	2:C:173:PRO:HD2	2.27	0.45
2:A:374:ASP:O	2:A:378:TRP:HD1	1.98	0.45
2:E:263:LEU:HA	2:E:264:PRO:HD3	1.83	0.45
1:R:11:U:H3'	1:R:12:U:C5'	2.42	0.45
2:B:18:LEU:HD21	2:C:242:THR:HG22	1.97	0.45
2:E:129:ALA:O	2:E:133:TRP:HD1	1.99	0.45
2:C:31:TYR:CD2	2:C:283:LEU:HA	2.51	0.45
2:B:37:GLU:CG	2:B:108:VAL:HG21	2.46	0.45
2:E:233:HIS:HB2	2:E:312:ARG:CZ	2.47	0.45
2:A:354:LYS:HE3	2:A:356:THR:HA	1.99	0.45
1:R:31:U:H3'	2:A:317:ARG:NE	2.30	0.45
2:C:41:TYR:HB2	2:C:190:ASN:ND2	2.31	0.45
2:B:81:ARG:HD3	2:B:208:HIS:CE1	2.52	0.45
2:B:128:SER:O	2:B:130:ASP:N	2.49	0.45
2:C:140:GLY:HA2	2:C:216:GLY:HA3	1.97	0.45
2:E:299:PHE:HE1	2:E:328:THR:HG22	1.82	0.45
2:B:253:GLU:CD	2:B:253:GLU:N	2.70	0.45
2:A:228:LEU:HD12	2:E:19:PRO:HD3	1.98	0.45
2:C:104:ILE:HD12	2:C:104:ILE:N	2.32	0.45
2:D:146:ARG:NH1	2:D:223:LYS:HE2	2.20	0.45
2:B:152:TYR:HD1	2:B:153:ARG:N	2.14	0.45
2:B:287:SER:HA	2:B:288:PRO:HD3	1.88	0.45
2:C:68:HIS:HE1	2:C:117:LEU:H	1.66	0.44
2:B:66:ILE:HD11	2:B:191:TYR:HB2	1.99	0.44
1:R:14:U:C5'	2:C:317:ARG:HH22	2.30	0.44
2:B:308:LEU:O	2:B:309:ARG:HB2	2.16	0.44
2:C:405:GLN:O	2:C:407:LEU:HG	2.16	0.44
2:B:38:ILE:H	2:B:108:VAL:HG23	1.82	0.44
2:C:317:ARG:NH1	2:C:317:ARG:H	2.16	0.44
2:B:123:ASP:C	2:B:125:SER:H	2.21	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:417:LYS:HE2	2:A:421:ASP:OD2	2.18	0.44
2:B:128:SER:O	2:B:129:ALA:C	2.56	0.44
2:D:117:LEU:CB	2:D:118:PRO:HD3	2.34	0.44
1:R:2:U:H3'	1:R:3:U:C5'	2.46	0.44
2:B:346:GLN:O	2:E:8:ILE:HD11	2.18	0.44
2:E:48:LEU:HA	2:E:51:LEU:HD12	2.00	0.44
2:C:306:LEU:HD22	2:C:412:ILE:HD12	1.99	0.44
2:A:122:SER:OG	2:A:123:ASP:N	2.50	0.43
2:B:215:TYR:N	2:B:215:TYR:CD2	2.86	0.43
2:E:172:GLU:H	2:E:173:PRO:CD	2.31	0.43
2:C:308:LEU:O	2:C:309:ARG:HB2	2.17	0.43
2:D:28:PRO:HG2	2:D:266:GLN:NE2	2.31	0.43
2:E:172:GLU:H	2:E:173:PRO:HD2	1.84	0.43
2:E:149:MET:C	2:E:151:GLU:H	2.21	0.43
2:E:148:GLN:HG2	2:E:179:ARG:HD2	2.00	0.43
2:D:214:ARG:HA	2:D:217:THR:CG2	2.37	0.43
1:R:14:U:O5'	2:C:317:ARG:NH2	2.51	0.43
2:D:302:GLN:HG2	2:D:316:ALA:CB	2.48	0.43
2:C:263:LEU:HA	2:C:264:PRO:HD3	1.84	0.43
2:E:66:ILE:HD11	2:E:191:TYR:HB2	2.00	0.43
2:E:172:GLU:N	2:E:173:PRO:CD	2.81	0.43
2:A:227:ALA:HA	2:A:230:THR:HG23	2.01	0.43
2:E:28:PRO:O	2:E:31:TYR:HB3	2.19	0.43
1:R:17:U:C5'	2:C:155:LYS:HZ3	2.32	0.43
2:E:233:HIS:HB2	2:E:312:ARG:NH1	2.34	0.43
2:E:59:LEU:HD11	2:E:137:TYR:CE2	2.53	0.43
2:A:228:LEU:HD23	2:A:289:TYR:HB3	2.00	0.43
2:E:303:LEU:HA	2:E:412:ILE:HD13	2.00	0.43
2:E:25:VAL:HG11	2:E:288:PRO:HA	2.01	0.43
2:A:288:PRO:HG2	2:A:289:TYR:CE2	2.53	0.43
2:E:181:ILE:HB	2:E:182:PHE:H	1.72	0.43
2:D:85:ASP:OD1	2:D:86:LYS:HE3	2.19	0.42
2:C:107:LEU:HD23	2:C:274:TYR:HE2	1.84	0.42
2:E:38:ILE:HA	2:E:39:PRO:HD3	1.84	0.42
2:A:408:ARG:HG2	2:A:408:ARG:H	1.65	0.42
2:A:212:SER:O	2:A:215:TYR:CD2	2.72	0.42
2:D:303:LEU:HD22	2:D:328:THR:HG22	2.01	0.42
1:R:12:U:P	2:C:286:LYS:HZ3	2.43	0.42
2:E:38:ILE:HD11	2:E:107:LEU:HB3	2.01	0.42
2:E:248:TRP:CD1	2:E:375:VAL:HG22	2.55	0.42
2:E:302:GLN:HG3	2:E:313:ALA:HB1	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:137:TYR:OH	2:D:173:PRO:HD3	2.20	0.42
2:B:152:TYR:CD1	2:B:153:ARG:N	2.88	0.42
2:B:19:PRO:HD3	2:C:228:LEU:HD22	2.02	0.42
2:B:263:LEU:HA	2:B:264:PRO:HD3	1.82	0.42
2:A:344:LEU:HD21	2:E:330:ALA:HB2	2.01	0.42
2:A:199:ASP:OD1	2:A:217:THR:HG23	2.19	0.42
1:R:21:U:H4'	2:B:224:ASP:CG	2.40	0.42
2:C:105:PHE:C	2:C:107:LEU:H	2.22	0.42
2:B:81:ARG:HD3	2:B:208:HIS:NE2	2.34	0.42
2:A:181:ILE:N	2:A:183:ASP:OD1	2.53	0.42
2:E:409:GLU:HA	2:E:414:LYS:HD2	2.01	0.42
2:A:239:GLY:HA3	2:E:323:GLU:CD	2.40	0.42
1:R:27:U:H4'	1:R:29:U:C5	2.54	0.42
2:E:172:GLU:N	2:E:173:PRO:HD2	2.34	0.42
2:C:78:LYS:HD3	2:C:78:LYS:HA	1.81	0.42
2:D:398:LYS:O	2:D:402:MET:HG2	2.20	0.41
2:C:409:GLU:O	2:C:410:LYS:HB2	2.19	0.41
1:R:23:U:H2'	1:R:25:U:H5''	2.02	0.41
2:A:172:GLU:CB	2:A:173:PRO:HD3	2.50	0.41
2:B:40:LEU:HD13	2:B:42:ILE:HD11	2.02	0.41
2:A:342:ALA:H	2:E:387:ARG:HH12	1.68	0.41
2:D:43:ASN:ND2	2:D:111:LYS:HD3	2.35	0.41
1:R:8:U:P	2:D:155:LYS:HZ1	2.42	0.41
2:D:290:SER:O	2:D:294:ASN:ND2	2.50	0.41
2:A:342:ALA:HB2	2:E:329:THR:HG21	2.02	0.41
2:D:79:ASP:HB2	2:D:81:ARG:HG3	2.02	0.41
2:A:381:TRP:O	2:A:384:ASP:HB2	2.20	0.41
2:B:370:PRO:HD3	2:B:381:TRP:CG	2.56	0.41
1:R:31:U:H2'	2:A:317:ARG:HE	1.84	0.41
2:E:275:MET:HB3	2:E:276:PRO:HD3	2.01	0.41
2:E:187:ASN:HD22	2:E:187:ASN:HA	1.70	0.41
2:E:214:ARG:HA	2:E:217:THR:OG1	2.21	0.41
2:E:130:ASP:C	2:E:132:LYS:N	2.73	0.41
2:C:293:LYS:HA	2:C:293:LYS:HD2	1.91	0.41
2:C:175:VAL:O	2:C:181:ILE:HG12	2.20	0.41
2:A:97:LYS:O	2:A:98:ALA:C	2.59	0.41
2:E:133:TRP:O	2:E:135:PRO:N	2.54	0.41
2:C:294:ASN:N	2:C:295:PRO:HD3	2.36	0.41
2:B:128:SER:C	2:B:130:ASP:N	2.70	0.41
2:A:199:ASP:OD1	2:A:214:ARG:NE	2.52	0.41
2:A:149:MET:C	2:A:151:GLU:N	2.75	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:401:VAL:HG23	2:A:421:ASP:HB2	2.03	0.41
2:A:243:GLU:HG3	2:E:2:SER:HB3	2.02	0.41
2:A:128:SER:C	2:A:130:ASP:H	2.23	0.41
2:D:311:THR:O	2:D:314:ARG:HG2	2.21	0.41
2:E:299:PHE:O	2:E:300:TRP:C	2.59	0.40
2:B:81:ARG:HB3	2:B:208:HIS:HE2	1.87	0.40
2:E:18:LEU:HB2	2:E:19:PRO:HD2	2.03	0.40
2:B:38:ILE:HA	2:B:39:PRO:HD3	1.88	0.40
2:B:28:PRO:HG2	2:B:266:GLN:NE2	2.34	0.40
2:E:302:GLN:HG3	2:E:313:ALA:CB	2.51	0.40
2:C:181:ILE:HB	2:C:182:PHE:H	1.51	0.40
2:D:401:VAL:HG21	2:D:420:PHE:HB2	2.03	0.40
2:B:313:ALA:O	2:B:314:ARG:C	2.58	0.40
1:R:35:U:OP2	2:A:155:LYS:NZ	2.41	0.40
1:R:13:U:H5'	1:R:14:U:OP2	2.21	0.40
2:A:395:GLN:HA	2:A:395:GLN:NE2	2.35	0.40
2:D:43:ASN:HD22	2:D:111:LYS:HD3	1.85	0.40
2:D:38:ILE:HA	2:D:39:PRO:HD3	1.91	0.40
1:R:20:U:H2'	1:R:21:U:O4'	2.21	0.40
2:C:356:THR:N	2:C:357:PRO:HD3	2.36	0.40
2:C:22:GLU:HB3	2:C:23:ASP:H	1.55	0.40
2:B:118:PRO:O	2:B:119:ASP:CB	2.70	0.40
2:C:58:GLY:HA3	2:C:64:VAL:HB	2.03	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	419/422 (99%)	354 (84%)	46 (11%)	19 (4%)	3	11
2	B	411/422 (97%)	344 (84%)	45 (11%)	22 (5%)	2	7

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	409/422 (97%)	340 (83%)	49 (12%)	20 (5%)	3	9
2	D	412/422 (98%)	343 (83%)	48 (12%)	21 (5%)	2	8
2	E	419/422 (99%)	349 (83%)	48 (12%)	22 (5%)	2	7
All	All	2070/2110 (98%)	1730 (84%)	236 (11%)	104 (5%)	3	8

All (104) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	47	SER
2	A	98	ALA
2	A	113	LEU
2	A	172	GLU
2	B	98	ALA
2	B	117	LEU
2	B	122	SER
2	B	128	SER
2	B	150	PRO
2	B	168	ASN
2	C	113	LEU
2	C	117	LEU
2	C	122	SER
2	C	172	GLU
2	C	181	ILE
2	D	98	ALA
2	D	122	SER
2	D	357	PRO
2	E	98	ALA
2	A	150	PRO
2	A	181	ILE
2	A	344	LEU
2	B	22	GLU
2	B	47	SER
2	B	119	ASP
2	B	129	ALA
2	B	172	GLU
2	B	177	GLU
2	B	344	LEU
2	C	130	ASP
2	C	150	PRO
2	C	344	LEU
2	C	371	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	120	GLY
2	D	130	ASP
2	D	168	ASN
2	D	344	LEU
2	D	366	THR
2	D	386	ASN
2	E	47	SER
2	E	120	GLY
2	E	122	SER
2	E	177	GLU
2	E	343	ASP
2	E	344	LEU
2	E	360	SER
2	E	371	GLN
2	E	406	GLY
2	A	22	GLU
2	A	176	PRO
2	A	180	ASP
2	A	386	ASN
2	B	43	ASN
2	B	61	SER
2	B	113	LEU
2	B	170	GLN
2	B	180	ASP
2	D	79	ASP
2	D	127	THR
2	D	150	PRO
2	D	172	GLU
2	D	180	ASP
2	E	150	PRO
2	E	299	PHE
2	E	300	TRP
2	A	117	LEU
2	A	122	SER
2	A	130	ASP
2	B	165	LYS
2	C	22	GLU
2	C	168	ASN
2	C	176	PRO
2	C	386	ASN
2	C	406	GLY
2	D	22	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	129	ALA
2	E	108	VAL
2	E	164	CYS
2	E	168	ASN
2	E	365	THR
2	A	128	SER
2	A	360	SER
2	C	47	SER
2	C	83	LYS
2	C	108	VAL
2	C	159	GLY
2	D	117	LEU
2	D	128	SER
2	D	271	ALA
2	E	173	PRO
2	E	271	ALA
2	B	179	ARG
2	B	309	ARG
2	C	167	ILE
2	E	80	ILE
2	E	117	LEU
2	A	121	VAL
2	A	264	PRO
2	C	80	ILE
2	E	181	ILE
2	B	80	ILE
2	D	42	ILE
2	D	80	ILE
2	A	108	VAL

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	362/363 (100%)	323 (89%)	39 (11%)	8	23
2	B	358/363 (99%)	311 (87%)	47 (13%)	5	15

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	356/363 (98%)	303 (85%)	53 (15%)	4	11
2	D	359/363 (99%)	315 (88%)	44 (12%)	6	17
2	E	362/363 (100%)	324 (90%)	38 (10%)	8	25
All	All	1797/1815 (99%)	1576 (88%)	221 (12%)	6	17

All (221) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	18	LEU
2	A	22	GLU
2	A	40	LEU
2	A	87	ASP
2	A	116	VAL
2	A	134	LEU
2	A	143	ARG
2	A	153	ARG
2	A	156	LEU
2	A	157	MET
2	A	160	LEU
2	A	177	GLU
2	A	181	ILE
2	A	183	ASP
2	A	187	ASN
2	A	195	VAL
2	A	215	TYR
2	A	217	THR
2	A	228	LEU
2	A	230	THR
2	A	237	ILE
2	A	243	GLU
2	A	252	ARG
2	A	253	GLU
2	A	275	MET
2	A	307	LEU
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	344	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	353	ASN
2	A	359	ASP
2	A	395	GLN
2	A	405	GLN
2	A	408	ARG
2	A	414	LYS
2	B	2	SER
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	48	LEU
2	B	78	LYS
2	B	84	LEU
2	B	85	ASP
2	B	95	ILE
2	B	107	LEU
2	B	108	VAL
2	B	116	VAL
2	B	126	ARG
2	B	134	LEU
2	B	149	MET
2	B	153	ARG
2	B	154	LYS
2	B	156	LEU
2	B	163	GLN
2	B	165	LYS
2	B	181	ILE
2	B	189	SER
2	B	215	TYR
2	B	217	THR
2	B	237	ILE
2	B	243	GLU
2	B	278	LEU
2	B	286	LYS
2	B	307	LEU
2	B	308	LEU
2	B	311	THR
2	B	317	ARG
2	B	327	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	329	THR
2	B	332	LEU
2	B	338	VAL
2	B	344	LEU
2	B	354	LYS
2	B	377	GLU
2	B	387	ARG
2	B	407	LEU
2	B	409	GLU
2	B	410	LYS
2	B	414	LYS
2	C	18	LEU
2	C	30	ASP
2	C	33	ARG
2	C	40	LEU
2	C	46	LYS
2	C	70	ASN
2	C	78	LYS
2	C	85	ASP
2	C	97	LYS
2	C	104	ILE
2	C	106	ASP
2	C	108	VAL
2	C	122	SER
2	C	134	LEU
2	C	143	ARG
2	C	149	MET
2	C	152	TYR
2	C	153	ARG
2	C	155	LYS
2	C	156	LEU
2	C	160	LEU
2	C	162	ASN
2	C	163	GLN
2	C	167	ILE
2	C	177	GLU
2	C	181	ILE
2	C	189	SER
2	C	195	VAL
2	C	214	ARG
2	C	228	LEU
2	C	230	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	243	GLU
2	C	252	ARG
2	C	253	GLU
2	C	278	LEU
2	C	286	LYS
2	C	307	LEU
2	C	308	LEU
2	C	311	THR
2	C	312	ARG
2	C	317	ARG
2	C	327	LEU
2	C	332	LEU
2	C	353	ASN
2	C	354	LYS
2	C	371	GLN
2	C	375	VAL
2	C	377	GLU
2	C	385	GLN
2	C	407	LEU
2	C	408	ARG
2	C	409	GLU
2	C	422	LYS
2	D	8	ILE
2	D	22	GLU
2	D	23	ASP
2	D	26	GLU
2	D	34	LYS
2	D	42	ILE
2	D	44	THR
2	D	64	VAL
2	D	83	LYS
2	D	84	LEU
2	D	85	ASP
2	D	97	LYS
2	D	104	ILE
2	D	108	VAL
2	D	126	ARG
2	D	128	SER
2	D	146	ARG
2	D	149	MET
2	D	153	ARG
2	D	171	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	217	THR
2	D	228	LEU
2	D	230	THR
2	D	243	GLU
2	D	244	ASP
2	D	252	ARG
2	D	308	LEU
2	D	309	ARG
2	D	311	THR
2	D	312	ARG
2	D	317	ARG
2	D	326	SER
2	D	327	LEU
2	D	328	THR
2	D	332	LEU
2	D	353	ASN
2	D	354	LYS
2	D	367	ASN
2	D	377	GLU
2	D	394	MET
2	D	407	LEU
2	D	409	GLU
2	D	412	ILE
2	D	414	LYS
2	E	13	VAL
2	E	18	LEU
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	106	ASP
2	E	123	ASP
2	E	130	ASP
2	E	133	TRP
2	E	134	LEU
2	E	148	GLN
2	E	149	MET
2	E	180	ASP
2	E	181	ILE
2	E	182	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	187	ASN
2	E	206	LYS
2	E	209	GLU
2	E	242	THR
2	E	243	GLU
2	E	253	GLU
2	E	307	LEU
2	E	308	LEU
2	E	309	ARG
2	E	314	ARG
2	E	317	ARG
2	E	327	LEU
2	E	332	LEU
2	E	349	CYS
2	E	354	LYS
2	E	356	THR
2	E	375	VAL
2	E	405	GLN
2	E	412	ILE
2	E	418	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	43	ASN
2	A	68	HIS
2	A	70	ASN
2	A	162	ASN
2	A	163	GLN
2	A	187	ASN
2	A	260	GLN
2	A	266	GLN
2	A	347	GLN
2	A	395	GLN
2	B	70	ASN
2	B	163	GLN
2	B	266	GLN
2	B	347	GLN
2	B	385	GLN
2	C	63	ASN
2	C	68	HIS
2	C	70	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	168	ASN
2	C	266	GLN
2	D	43	ASN
2	D	57	GLN
2	D	63	ASN
2	D	68	HIS
2	D	70	ASN
2	D	163	GLN
2	D	203	HIS
2	D	266	GLN
2	D	347	GLN
2	D	371	GLN
2	D	395	GLN
2	E	70	ASN
2	E	187	ASN
2	E	266	GLN
2	E	315	ASN
2	E	347	GLN
2	E	395	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	R	44/45 (97%)	35 (79%)	8 (18%)

All (35) 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	8	U
1	R	9	U
1	R	10	U
1	R	11	U
1	R	12	U
1	R	13	U
1	R	14	U
1	R	15	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	26	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	40	U
1	R	41	U
1	R	42	U
1	R	45	U

All (8) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	R	4	U
1	R	5	U
1	R	6	U
1	R	12	U
1	R	14	U
1	R	20	U
1	R	32	U
1	R	39	U

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 15 are modelled with single atom - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	R	45/45 (100%)	1.88	17 (37%) 0 0	29, 44, 53, 58	0
2	A	421/422 (99%)	0.96	63 (14%) 3 2	23, 27, 35, 40	0
2	B	415/422 (98%)	0.89	51 (12%) 5 3	23, 27, 33, 42	0
2	C	413/422 (97%)	0.84	50 (12%) 6 3	23, 27, 33, 39	0
2	D	416/422 (98%)	0.94	55 (13%) 4 2	23, 27, 34, 43	0
2	E	421/422 (99%)	1.18	92 (21%) 1 1	23, 27, 36, 45	0
All	All	2131/2155 (98%)	0.98	328 (15%) 3 1	23, 27, 37, 58	0

All (328) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	2	SER	13.4
2	A	2	SER	11.6
2	A	361	THR	9.8
2	E	101	THR	8.1
2	D	166	MET	8.1
2	A	362	GLY	7.4
2	C	163	GLN	7.3
2	A	367	ASN	6.7
2	C	169	GLU	6.5
2	E	118	PRO	6.4
2	B	163	GLN	6.3
2	D	164	CYS	6.3
2	D	113	LEU	6.2
2	A	363	GLY	6.2
2	B	176	PRO	6.1
2	E	152	TYR	6.0
2	E	159	GLY	6.0
2	E	362	GLY	5.9
2	E	175	VAL	5.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	158	ASP	5.9
2	E	114	ASP	5.9
2	C	173	PRO	5.8
2	B	2	SER	5.7
2	B	169	GLU	5.6
2	D	174	LEU	5.6
2	D	2	SER	5.5
2	B	122	SER	5.4
2	B	175	VAL	5.4
2	B	166	MET	5.3
2	E	367	ASN	5.3
2	C	174	LEU	5.2
2	E	42	ILE	5.2
2	A	366	THR	5.2
2	C	175	VAL	5.2
2	E	117	LEU	5.1
2	B	43	ASN	5.0
2	E	98	ALA	4.9
2	E	43	ASN	4.9
2	A	83	LYS	4.9
2	B	172	GLU	4.8
2	D	368	ALA	4.8
2	E	157	MET	4.8
2	E	365	THR	4.8
2	A	353	ASN	4.8
2	E	174	LEU	4.8
1	R	19	U	4.8
2	B	386	ASN	4.7
2	A	164	CYS	4.7
2	E	162	ASN	4.7
2	B	367	ASN	4.7
2	E	158	ASP	4.6
2	D	41	TYR	4.6
2	C	131	ASP	4.6
2	B	365	THR	4.6
2	A	118	PRO	4.5
2	A	358	ASP	4.5
2	C	2	SER	4.4
2	D	111	LYS	4.4
2	D	112	ALA	4.4
2	A	160	LEU	4.4
2	C	162	ASN	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	E	161	THR	4.3
2	A	365	THR	4.3
2	B	162	ASN	4.3
2	D	42	ILE	4.3
2	A	364	LEU	4.3
2	E	361	THR	4.3
2	B	358	ASP	4.3
2	B	377	GLU	4.3
2	E	169	GLU	4.3
2	C	99	GLY	4.3
2	E	75	GLY	4.2
2	B	173	PRO	4.2
2	E	149	MET	4.2
2	B	147	THR	4.2
2	D	157	MET	4.2
2	E	166	MET	4.2
2	A	357	PRO	4.1
2	B	171	PHE	4.1
2	D	68	HIS	4.1
2	D	158	ASP	4.1
2	B	118	PRO	4.1
1	R	37	U	4.0
2	A	172	GLU	4.0
2	B	98	ALA	4.0
2	C	167	ILE	4.0
2	C	353	ASN	4.0
2	D	43	ASN	3.9
2	E	96	GLY	3.9
2	A	152	TYR	3.9
2	C	89	SER	3.9
2	C	178	GLY	3.9
2	E	171	PHE	3.9
2	C	43	ASN	3.9
2	D	176	PRO	3.8
2	B	119	ASP	3.8
2	E	160	LEU	3.8
2	A	166	MET	3.8
2	D	367	ASN	3.8
2	D	149	MET	3.8
2	A	117	LEU	3.7
2	E	156	LEU	3.7
1	R	42	U	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	A	82	GLY	3.6
2	E	341	SER	3.6
2	C	164	CYS	3.6
2	A	97	LYS	3.6
2	C	366	THR	3.6
2	E	185	TRP	3.6
2	A	42	ILE	3.6
2	C	74	TYR	3.6
2	C	83	LYS	3.5
2	D	167	ILE	3.5
2	A	165	LYS	3.5
2	E	363	GLY	3.5
2	D	165	LYS	3.5
2	E	124	ALA	3.5
2	D	163	GLN	3.4
2	C	161	THR	3.4
2	C	177	GLU	3.4
2	E	55	VAL	3.4
2	D	364	LEU	3.4
2	D	172	GLU	3.4
2	E	122	SER	3.4
2	D	137	TYR	3.4
2	E	176	PRO	3.4
2	E	155	LYS	3.4
2	C	346	GLN	3.4
2	E	170	GLN	3.4
2	D	12	THR	3.3
2	A	169	GLU	3.3
2	E	172	GLU	3.3
2	B	366	THR	3.3
2	C	123	ASP	3.3
2	D	119	ASP	3.3
2	A	149	MET	3.3
2	C	88	TRP	3.3
1	R	18	U	3.2
2	E	422	LYS	3.2
2	C	357	PRO	3.2
2	E	132	LYS	3.2
2	E	359	ASP	3.2
2	D	355	TYR	3.2
2	A	233	HIS	3.2
2	A	360	SER	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	A	213	PHE	3.2
2	B	156	LEU	3.1
2	D	313	ALA	3.1
2	D	114	ASP	3.1
2	C	59	LEU	3.1
2	D	169	GLU	3.1
2	B	61	SER	3.0
2	A	163	GLN	3.0
2	E	86	LYS	3.0
2	E	405	GLN	3.0
2	C	356	THR	3.0
2	E	113	LEU	3.0
2	D	171	PHE	3.0
2	E	88	TRP	3.0
2	A	102	ILE	3.0
2	B	185	TRP	3.0
2	C	274	TYR	3.0
2	D	161	THR	2.9
2	D	133	TRP	2.9
2	E	345	ALA	2.9
2	D	115	GLY	2.9
2	E	73	LEU	2.9
1	R	14	U	2.9
2	A	171	PHE	2.9
2	C	57	GLN	2.9
2	E	360	SER	2.9
2	C	352	ASP	2.9
2	C	171	PHE	2.9
1	R	33	U	2.9
2	A	45	THR	2.9
2	E	342	ALA	2.9
2	A	104	ILE	2.9
2	E	112	ALA	2.9
2	B	357	PRO	2.9
2	E	150	PRO	2.9
2	E	121	VAL	2.8
2	B	14	ILE	2.8
2	B	68	HIS	2.8
2	A	43	ASN	2.8
2	E	366	THR	2.8
2	E	50	ASP	2.8
2	D	146	ARG	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	107	LEU	2.8
2	A	314	ARG	2.8
2	E	355	TYR	2.8
2	D	422	LYS	2.8
2	B	177	GLU	2.8
2	E	358	ASP	2.7
2	E	354	LYS	2.7
2	E	99	GLY	2.7
2	E	344	LEU	2.7
2	C	160	LEU	2.7
2	C	149	MET	2.7
2	A	175	VAL	2.7
1	R	27	U	2.7
2	A	168	ASN	2.7
1	R	36	U	2.7
2	E	409	GLU	2.6
2	E	408	ARG	2.6
2	D	168	ASN	2.6
2	E	57	GLN	2.6
1	R	1	U	2.6
2	C	176	PRO	2.6
2	B	63	ASN	2.6
2	E	77	LEU	2.6
2	D	386	ASN	2.6
2	E	27	TYR	2.6
2	D	110	LEU	2.5
2	B	42	ILE	2.5
2	C	342	ALA	2.5
2	C	122	SER	2.5
1	R	23	U	2.5
2	C	152	TYR	2.5
2	E	84	LEU	2.5
2	A	101	THR	2.5
2	E	123	ASP	2.5
2	A	173	PRO	2.5
2	C	399	ARG	2.5
2	E	48	LEU	2.5
2	D	385	GLN	2.5
1	R	45	U	2.5
2	E	153	ARG	2.5
2	A	342	ALA	2.5
2	E	41	TYR	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	342	ALA	2.5
2	A	174	LEU	2.4
2	C	341	SER	2.4
2	C	371	GLN	2.4
2	A	87	ASP	2.4
2	A	201	PHE	2.4
2	D	353	ASN	2.4
2	B	371	GLN	2.4
1	R	41	U	2.4
2	A	352	ASP	2.4
2	B	131	ASP	2.4
2	A	157	MET	2.4
2	E	89	SER	2.4
2	D	274	TYR	2.4
2	C	172	GLU	2.4
2	E	350	VAL	2.4
2	B	96	GLY	2.4
2	E	68	HIS	2.4
2	D	358	ASP	2.4
2	D	349	CYS	2.4
2	E	54	TYR	2.4
1	R	15	U	2.3
2	B	346	GLN	2.3
2	E	62	GLY	2.3
2	D	348	PHE	2.3
2	A	65	SER	2.3
2	E	33	ARG	2.3
2	A	155	LYS	2.3
1	R	16	U	2.3
2	E	143	ARG	2.3
2	A	162	ASN	2.3
2	B	137	TYR	2.3
2	A	16	PRO	2.3
2	A	422	LYS	2.3
2	B	341	SER	2.3
2	A	274	TYR	2.2
2	C	182	PHE	2.2
2	C	376	VAL	2.2
2	A	84	LEU	2.2
2	E	76	ALA	2.2
2	D	45	THR	2.2
2	E	357	PRO	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	E	178	GLY	2.2
2	B	422	LYS	2.2
2	B	80	ILE	2.2
2	D	159	GLY	2.2
1	R	10	U	2.2
2	C	409	GLU	2.2
2	E	111	LYS	2.2
2	D	147	THR	2.2
2	C	348	PHE	2.2
1	R	22	U	2.2
2	C	146	ARG	2.2
2	A	235	CYS	2.2
2	C	367	ASN	2.2
2	C	95	ILE	2.2
2	C	165	LYS	2.2
2	D	175	VAL	2.2
2	D	346	GLN	2.2
2	B	317	ARG	2.1
2	B	157	MET	2.1
2	E	15	VAL	2.1
2	B	355	TYR	2.1
2	C	121	VAL	2.1
2	E	63	ASN	2.1
2	E	215	TYR	2.1
2	B	47	SER	2.1
2	B	111	LYS	2.1
2	E	46	LYS	2.1
2	B	385	GLN	2.1
2	A	44	THR	2.1
2	A	13	VAL	2.1
2	B	368	ALA	2.1
2	D	153	ARG	2.1
2	E	364	LEU	2.1
2	A	74	TYR	2.1
2	A	122	SER	2.1
2	B	48	LEU	2.1
2	E	45	THR	2.1
2	E	137	TYR	2.1
2	A	371	GLN	2.1
2	E	138	LEU	2.1
2	D	225	CYS	2.1
2	E	353	ASN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	139	LEU	2.1
2	A	359	ASP	2.0
2	C	68	HIS	2.0
2	A	355	TYR	2.0
2	A	55	VAL	2.0
2	E	184	VAL	2.0
2	E	173	PRO	2.0
2	A	158	ASP	2.0
1	R	2	U	2.0
2	A	376	VAL	2.0
2	D	98	ALA	2.0
2	D	173	PRO	2.0
2	B	168	ASN	2.0
2	E	56	TYR	2.0
2	B	45	THR	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	IUM	B	423	1/3	0.93	0.10	-1.35	129,129,129,129	0
3	IUM	A	424	1/3	0.99	0.14	-1.72	21,21,21,21	0
3	IUM	C	424	1/3	0.99	0.14	-1.97	22,22,22,22	0
3	IUM	E	424	1/3	0.99	0.14	-2.65	21,21,21,21	0
3	IUM	E	423	1/3	0.94	0.06	-3.12	107,107,107,107	0
3	IUM	B	424	1/3	0.99	0.12	-3.37	15,15,15,15	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	IUM	D	424	1/3	0.99	0.12	-5.04	17,17,17,17	0
3	IUM	A	423	1/3	0.95	0.09	-	92,92,92,92	0
3	IUM	C	423	1/3	0.97	0.11	-	54,54,54,54	0
3	IUM	B	425	1/3	0.96	0.04	-	184,184,184,184	0
3	IUM	E	425	1/3	0.79	0.07	-	192,192,192,192	0
3	IUM	A	425	1/3	0.97	0.03	-	129,129,129,129	0
3	IUM	C	425	1/3	0.94	0.05	-	123,123,123,123	0
3	IUM	A	426	1/3	0.95	0.14	-	114,114,114,114	0
3	IUM	D	423	1/3	0.85	0.09	-	120,120,120,120	0

6.5 Other polymers [i](#)

There are no such residues in this entry.