



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:43 PM GMT

PDB ID : 1UVI
Title : THE STRUCTURAL BASIS FOR RNA SPECIFICITY AND CA2 INHIBITION OF AN RNA-DEPENDENT RNA POLYMERASE PHI6P2 WITH 6NT RNA
Authors : Salgado, P.S.; Makeyev, E.V.; Butcher, S.; Bamford, D.; Stuart, D.I.; Grimes, J.M.
Deposited on : 2004-01-21
Resolution : 2.15 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

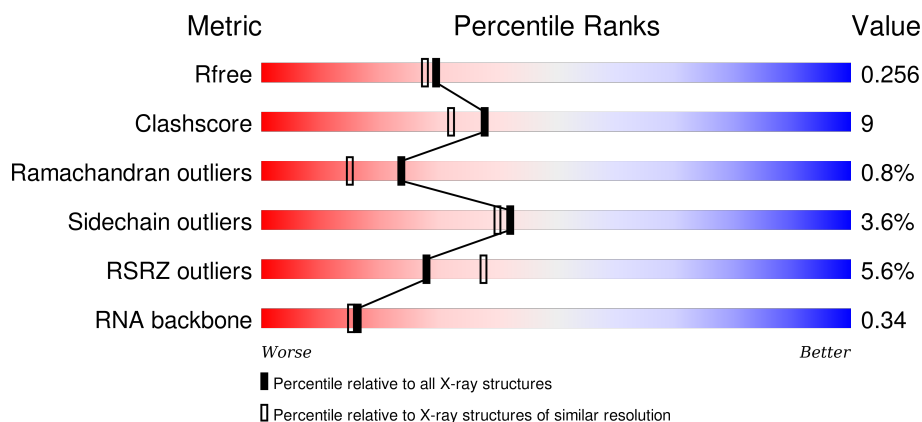
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)
RNA backbone	2183	1077 (2.80-1.52)

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	A	664	<div> <div>5%</div> <div>82%</div> <div>15%</div> <div>.</div> </div>
1	B	664	<div> <div>3%</div> <div>81%</div> <div>17%</div> <div>.</div> </div>
1	C	664	<div> <div>7%</div> <div>82%</div> <div>16%</div> <div>.</div> </div>
2	D	6	<div> <div>67%</div> <div>17%</div> <div>33%</div> <div>17%</div> <div>33%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain			
2	E	6	67%			
			17%	33%	17%	33%
2	F	6	67%			
			17%	33%	17%	33%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16447 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called RNA-DEPENDENT RNA POLYMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	664	Total	C	N	O	S	0	0	0
			5265	3342	914	977	32			
1	B	664	Total	C	N	O	S	0	0	0
			5265	3342	914	977	32			
1	C	664	Total	C	N	O	S	0	0	0
			5265	3342	914	977	32			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	456	MET	ILE	CONFLICT	UNP P11124
B	456	MET	ILE	CONFLICT	UNP P11124
C	456	MET	ILE	CONFLICT	UNP P11124

- Molecule 2 is a RNA chain called 5'-R(*UP*UP*UP*UP*CP*CP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	4	Total	C	N	O	P	0	0	0
			77	36	10	28	3			
2	E	4	Total	C	N	O	P	0	0	0
			77	36	10	28	3			
2	F	4	Total	C	N	O	P	0	0	0
			77	36	10	28	3			

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mn	0	0
			1	1		
3	A	1	Total	Mn	0	0
			1	1		

Continued on next page...

Continued from previous page...

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

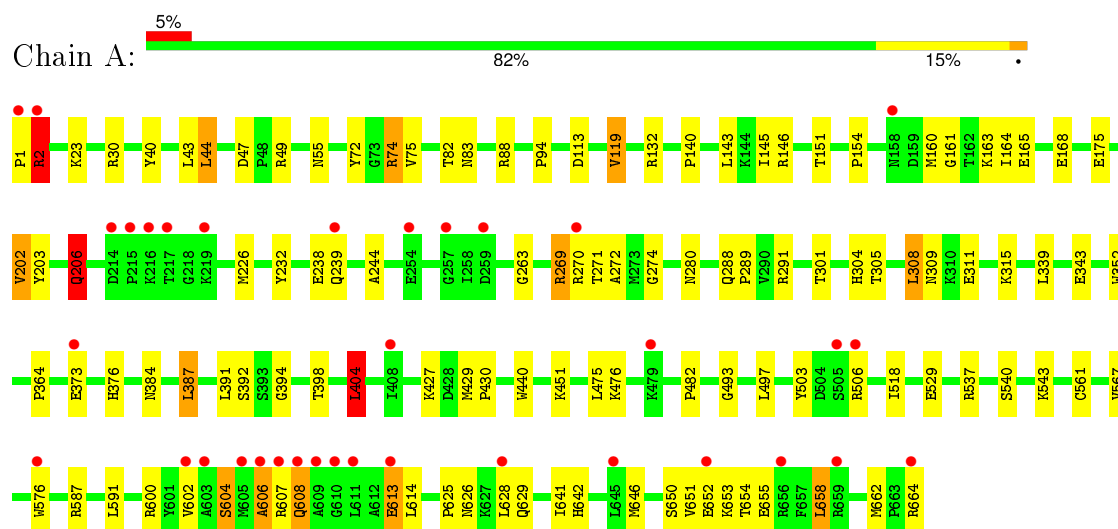
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	116	Total 116	O 116	0	0
4	B	192	Total 192	O 192	0	0
4	C	109	Total 109	O 109	0	0
4	D	1	Total 1	O 1	0	0

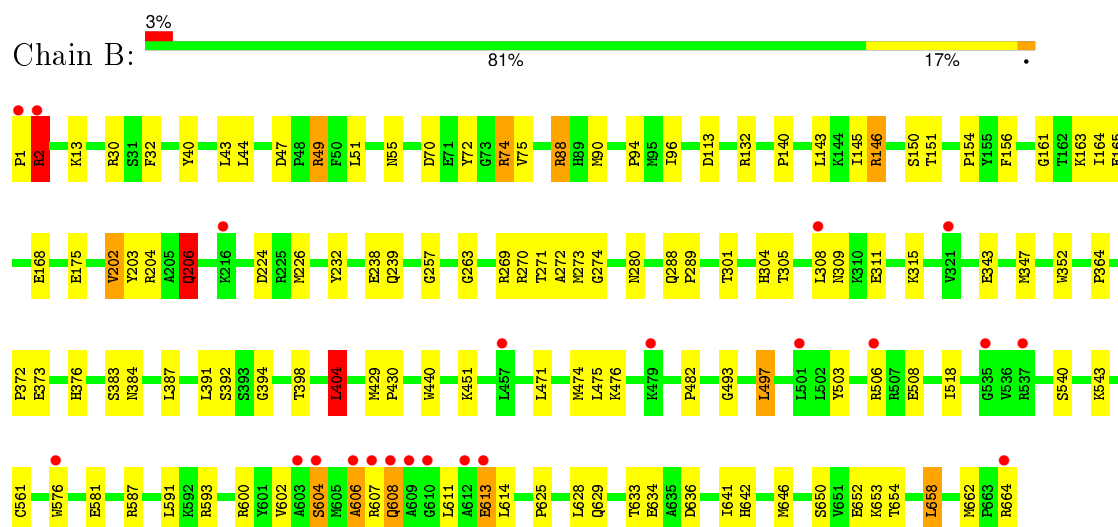
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

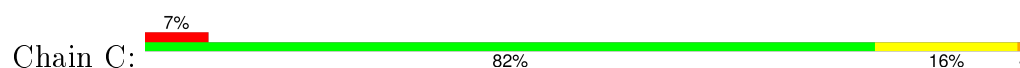
• Molecule 1: RNA-DEPENDENT RNA POLYMERASE

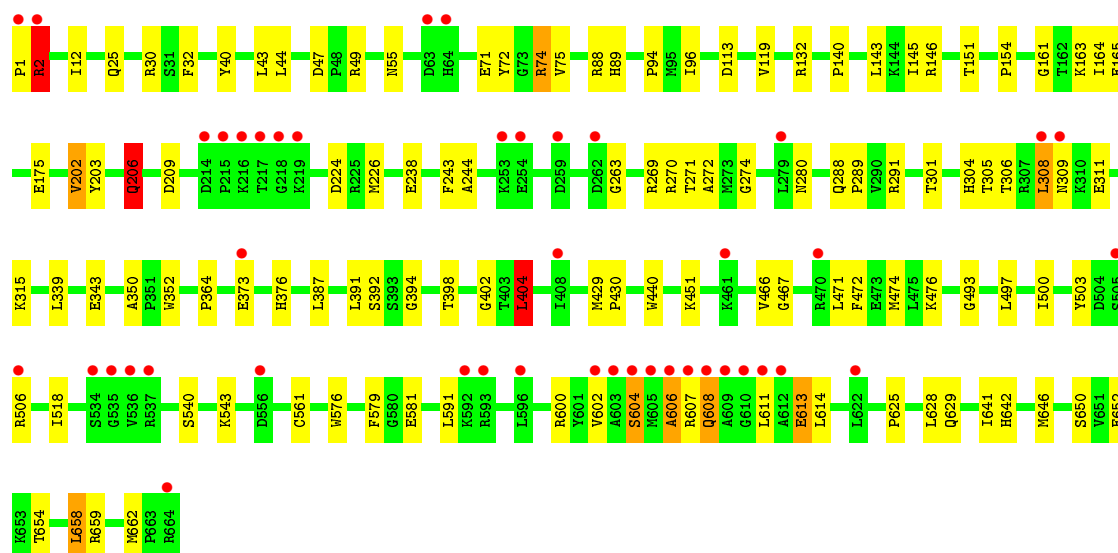


• Molecule 1: RNA-DEPENDENT RNA POLYMERASE

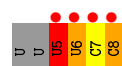


• Molecule 1: RNA-DEPENDENT RNA POLYMERASE

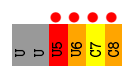




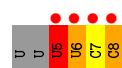
● Molecule 2: 5'-R(*UP*UP*UP*UP*CP*CP)-3'



● Molecule 2: 5'-R(*UP*UP*UP*UP*CP*CP)-3'



● Molecule 2: 5'-R(*UP*UP*UP*UP*CP*CP)-3'



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	105.13Å 93.71Å 140.74Å 90.00° 101.22° 90.00°	Depositor
Resolution (Å)	19.93 – 2.15 19.93 – 2.15	Depositor EDS
% Data completeness (in resolution range)	97.8 (19.93-2.15) 97.9 (19.93-2.15)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 2.15Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.230 , 0.256 0.230 , 0.256	Depositor DCC
R_{free} test set	7208 reflections (5.06%)	DCC
Wilson B-factor (Å ²)	27.7	Xtriage
Anisotropy	0.631	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 43.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 142480 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16447	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% 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: MN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.52	0/5396	0.69	2/7297 (0.0%)
1	B	0.53	0/5396	0.71	4/7297 (0.1%)
1	C	0.51	0/5396	0.70	2/7297 (0.0%)
2	D	0.44	0/84	0.89	0/128
2	E	0.62	0/84	1.08	0/128
2	F	0.52	0/84	0.90	0/128
All	All	0.52	0/16440	0.71	8/22275 (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
1	C	0	1
2	D	0	1
2	E	0	1
2	F	0	1
All	All	0	4

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	206	GLN	N-CA-C	-7.57	90.57	111.00
1	A	206	GLN	N-CA-C	-7.43	90.94	111.00
1	B	206	GLN	N-CA-C	-7.24	91.46	111.00
1	B	88	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	B	49	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	B	404	LEU	CA-CB-CG	5.45	127.84	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	404	LEU	CA-CB-CG	5.12	127.08	115.30
1	C	404	LEU	CA-CB-CG	5.04	126.90	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	40	TYR	Sidechain
2	D	5	U	Sidechain
2	E	5	U	Sidechain
2	F	5	U	Sidechain

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	A	5265	0	5165	92	0
1	B	5265	0	5165	98	0
1	C	5265	0	5165	90	0
2	D	77	0	44	16	0
2	E	77	0	44	19	0
2	F	77	0	44	15	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	116	0	0	3	0
4	B	192	0	0	0	0
4	C	109	0	0	2	0
4	D	1	0	0	0	0
All	All	16447	0	15627	292	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 9.

All (292) 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:B:274:GLY:HA2	2:E:6:U:H1'	1.33	1.11
1:C:274:GLY:HA2	2:F:6:U:H1'	1.42	1.01
1:A:274:GLY:HA2	2:D:6:U:H1'	1.44	0.98
1:A:364:PRO:HA	1:A:387:LEU:HD22	1.56	0.87
1:C:301:THR:HG23	1:C:440:TRP:O	1.75	0.87
1:B:451:LYS:HE2	2:E:8:C:N4	1.90	0.86
1:A:30:ARG:HH12	2:D:5:U:H3	1.24	0.84
1:B:301:THR:HG23	1:B:440:TRP:O	1.79	0.83
1:A:308:LEU:H	1:A:308:LEU:HD22	1.44	0.83
1:A:301:THR:HG23	1:A:440:TRP:O	1.79	0.81
1:C:451:LYS:HE2	2:F:8:C:N4	1.95	0.81
1:C:308:LEU:H	1:C:308:LEU:HD22	1.46	0.80
1:C:629:GLN:HG2	2:F:7:C:C4	2.17	0.80
1:A:2:ARG:HD3	1:A:2:ARG:O	1.83	0.79
1:A:427:LYS:HE3	1:C:12:ILE:HG21	1.63	0.79
1:C:600:ARG:HB2	1:C:600:ARG:HH11	1.48	0.78
1:A:613:GLU:CD	1:A:613:GLU:H	1.87	0.78
1:C:364:PRO:HA	1:C:387:LEU:HD22	1.66	0.77
1:A:47:ASP:OD1	1:A:49:ARG:HD3	1.84	0.77
1:B:274:GLY:CA	2:E:6:U:H1'	2.13	0.76
1:B:364:PRO:HA	1:B:387:LEU:HD22	1.67	0.76
1:C:206:GLN:HG3	1:C:270:ARG:HD2	1.68	0.75
1:B:2:ARG:O	1:B:2:ARG:HD3	1.87	0.75
1:B:308:LEU:HD22	1:B:308:LEU:H	1.50	0.75
1:A:629:GLN:HG2	2:D:7:C:C4	2.22	0.74
1:A:451:LYS:HE2	2:D:8:C:N4	2.04	0.73
1:C:30:ARG:HH12	2:F:5:U:H3	1.37	0.72
1:C:613:GLU:H	1:C:613:GLU:CD	1.93	0.72
1:C:600:ARG:HB2	1:C:600:ARG:NH1	2.04	0.72
1:A:206:GLN:HG3	1:A:270:ARG:HD2	1.71	0.72
1:B:600:ARG:HB2	1:B:600:ARG:HH11	1.54	0.72
1:A:658:LEU:HB3	1:A:662:MET:CE	2.20	0.71
1:B:613:GLU:H	1:B:613:GLU:CD	1.94	0.71
1:C:140:PRO:HB3	1:C:658:LEU:HD23	1.73	0.71
1:A:600:ARG:HH11	1:A:600:ARG:HB2	1.57	0.70
2:E:5:U:O2'	2:E:6:U:OP1	2.06	0.70
1:B:206:GLN:HG3	1:B:270:ARG:HD2	1.73	0.69
1:C:301:THR:HG22	4:C:2083:HOH:O	1.93	0.69
1:C:47:ASP:OD1	1:C:49:ARG:HD3	1.92	0.69
1:C:274:GLY:CA	2:F:6:U:H1'	2.22	0.68
1:C:451:LYS:CE	2:F:8:C:N4	2.56	0.68
1:B:47:ASP:OD1	1:B:49:ARG:HD3	1.93	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:ASN:ND2	1:A:394:GLY:O	2.27	0.67
1:B:602:VAL:HG12	1:B:604:SER:HB3	1.77	0.67
2:D:5:U:O2'	2:D:6:U:OP1	2.12	0.66
1:C:600:ARG:CB	1:C:600:ARG:HH11	2.08	0.66
1:C:132:ARG:NH1	1:C:343:GLU:OE2	2.29	0.66
1:A:203:TYR:HE1	1:A:271:THR:HG22	1.60	0.66
1:A:291:ARG:HD3	2:D:8:C:H6	1.61	0.65
1:B:600:ARG:NH1	1:B:600:ARG:HB2	2.11	0.65
2:F:5:U:O2'	2:F:6:U:OP1	2.14	0.64
1:B:600:ARG:CB	1:B:600:ARG:HH11	2.10	0.64
1:C:140:PRO:CB	1:C:658:LEU:HD23	2.27	0.64
1:A:140:PRO:HB3	1:A:658:LEU:HD23	1.80	0.63
1:B:475:LEU:HD21	1:B:482:PRO:HG3	1.81	0.63
1:A:537:ARG:HD3	4:A:2095:HOH:O	1.98	0.63
1:A:274:GLY:CA	2:D:6:U:H1'	2.26	0.62
1:B:202:VAL:HG22	1:B:272:ALA:HB3	1.80	0.62
1:C:202:VAL:HG22	1:C:272:ALA:HB3	1.81	0.62
1:C:2:ARG:O	1:C:2:ARG:HD3	1.99	0.62
1:C:175:GLU:HA	1:C:352:TRP:CE3	2.35	0.62
1:C:291:ARG:HD3	2:F:8:C:H6	1.65	0.61
4:A:2112:HOH:O	1:B:581:GLU:HG3	1.99	0.61
1:B:30:ARG:HH12	2:E:5:U:H3	1.47	0.61
1:C:602:VAL:HG12	1:C:604:SER:HB3	1.81	0.61
1:A:308:LEU:N	1:A:308:LEU:HD22	2.16	0.61
1:A:600:ARG:NH1	1:A:600:ARG:HB2	2.15	0.61
1:A:55:ASN:OD1	1:A:88:ARG:NH2	2.30	0.60
1:C:1:PRO:HD2	1:C:238:GLU:OE2	2.02	0.60
1:A:427:LYS:HE3	1:C:12:ILE:CG2	2.30	0.60
1:B:602:VAL:CG1	1:B:604:SER:HB3	2.32	0.60
1:A:88:ARG:HD3	1:A:263:GLY:O	2.02	0.60
1:C:1:PRO:HD2	1:C:238:GLU:OE1	2.01	0.60
1:C:30:ARG:O	1:C:376:HIS:HE1	1.85	0.60
1:C:658:LEU:HB3	1:C:662:MET:CE	2.32	0.60
1:C:145:ILE:HD12	1:C:164:ILE:HD13	1.84	0.60
1:A:203:TYR:CE1	1:A:271:THR:HG22	2.36	0.59
1:A:451:LYS:CE	2:D:8:C:N4	2.65	0.59
1:A:140:PRO:CB	1:A:658:LEU:HD23	2.32	0.59
1:C:602:VAL:CG1	1:C:604:SER:HB3	2.33	0.59
1:B:55:ASN:OD1	1:B:88:ARG:NH2	2.30	0.59
1:B:650:SER:HB2	1:B:652:GLU:OE1	2.03	0.59
1:A:602:VAL:HG12	1:A:604:SER:HB3	1.83	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:392:SER:O	1:B:398:THR:HG21	2.02	0.59
1:B:140:PRO:CB	1:B:658:LEU:HD23	2.33	0.58
1:C:74:ARG:HB3	1:C:503:TYR:CD2	2.37	0.58
1:B:140:PRO:HB3	1:B:658:LEU:HD23	1.84	0.58
1:B:280:ASN:ND2	1:B:394:GLY:O	2.31	0.58
1:C:88:ARG:HD3	1:C:263:GLY:O	2.04	0.58
1:C:72:TYR:CE1	1:C:476:LYS:HD3	2.37	0.58
1:B:652:GLU:CD	1:B:652:GLU:H	2.08	0.58
1:A:72:TYR:CE1	1:A:476:LYS:HD3	2.38	0.58
1:A:74:ARG:HB3	1:A:503:TYR:CD2	2.39	0.57
1:C:55:ASN:OD1	1:C:88:ARG:NH2	2.33	0.57
1:C:203:TYR:HE1	1:C:271:THR:HG22	1.70	0.57
1:B:72:TYR:CE1	1:B:476:LYS:HD3	2.40	0.57
1:B:308:LEU:HD22	1:B:308:LEU:N	2.17	0.56
1:A:30:ARG:O	1:A:376:HIS:HE1	1.89	0.56
1:A:658:LEU:HB3	1:A:662:MET:HE2	1.87	0.56
1:A:392:SER:O	1:A:398:THR:CG2	2.53	0.56
1:C:1:PRO:HD2	1:C:238:GLU:CD	2.26	0.56
1:A:202:VAL:HG22	1:A:272:ALA:HB3	1.85	0.56
1:C:652:GLU:CD	1:C:652:GLU:H	2.09	0.56
1:B:628:LEU:O	2:E:8:C:O2	2.24	0.56
2:D:8:C:O2	2:D:8:C:H3'	2.06	0.56
1:C:392:SER:O	1:C:398:THR:HG21	2.05	0.56
1:B:1:PRO:HD2	1:B:238:GLU:OE1	2.06	0.56
1:A:1:PRO:HD2	1:A:238:GLU:OE1	2.06	0.55
1:B:658:LEU:HB3	1:B:662:MET:CE	2.37	0.55
1:B:145:ILE:HD12	1:B:164:ILE:HD13	1.89	0.55
1:A:364:PRO:HA	1:A:387:LEU:CD2	2.33	0.55
1:A:30:ARG:NH1	2:D:5:U:H3	2.01	0.55
1:A:301:THR:HG22	4:A:2078:HOH:O	2.06	0.55
1:C:308:LEU:N	1:C:308:LEU:HD22	2.19	0.55
1:B:132:ARG:NH1	1:B:343:GLU:OE2	2.38	0.55
1:C:175:GLU:HA	1:C:352:TRP:CD2	2.42	0.54
1:C:642:HIS:CE1	1:C:646:MET:HG3	2.42	0.54
1:B:88:ARG:HD3	1:B:263:GLY:O	2.08	0.54
2:F:8:C:O2	2:F:8:C:H3'	2.07	0.54
1:A:119:VAL:O	1:C:25:GLN:HG3	2.08	0.54
1:A:608:GLN:HE22	1:B:593:ARG:CZ	2.21	0.54
2:E:8:C:H3'	2:E:8:C:O2	2.08	0.53
1:A:308:LEU:CD2	1:A:308:LEU:H	2.18	0.53
2:F:5:U:O4'	2:F:5:U:O2	2.25	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:600:ARG:HH11	1:A:600:ARG:CB	2.20	0.53
1:B:392:SER:O	1:B:398:THR:CG2	2.56	0.53
1:C:308:LEU:H	1:C:308:LEU:CD2	2.18	0.53
1:C:151:THR:CG2	1:C:163:LYS:HG2	2.39	0.53
1:A:291:ARG:HD3	2:D:8:C:C6	2.44	0.53
1:C:311:GLU:O	1:C:315:LYS:HB2	2.09	0.53
1:B:203:TYR:HE1	1:B:271:THR:HG22	1.73	0.53
1:B:151:THR:CG2	1:B:163:LYS:HG2	2.39	0.53
1:A:652:GLU:CD	1:A:652:GLU:H	2.12	0.52
1:C:280:ASN:ND2	1:C:394:GLY:O	2.33	0.52
1:B:175:GLU:HA	1:B:352:TRP:CD2	2.44	0.52
2:D:5:U:O4'	2:D:5:U:O2	2.24	0.52
1:C:614:LEU:HD21	1:C:641:ILE:HD11	1.92	0.52
1:B:1:PRO:HD2	1:B:238:GLU:OE2	2.08	0.52
1:A:44:LEU:HD11	1:B:257:GLY:HA3	1.89	0.52
1:C:224:ASP:HB3	1:C:226:MET:HE1	1.90	0.52
1:B:629:GLN:HG2	2:E:7:C:C4	2.45	0.52
1:B:311:GLU:O	1:B:315:LYS:HB2	2.09	0.52
1:A:151:THR:CG2	1:A:163:LYS:HG2	2.39	0.52
1:A:304:HIS:HA	1:A:309:ASN:ND2	2.24	0.52
1:A:75:VAL:HG12	1:A:493:GLY:HA2	1.91	0.52
1:B:164:ILE:O	1:B:168:GLU:HG3	2.10	0.52
1:B:74:ARG:HB3	1:B:503:TYR:CD2	2.45	0.52
1:C:203:TYR:CE1	1:C:271:THR:HG22	2.45	0.51
1:B:175:GLU:HA	1:B:352:TRP:CE3	2.45	0.51
1:C:506:ARG:HG3	1:C:506:ARG:HH11	1.75	0.51
1:C:392:SER:O	1:C:398:THR:CG2	2.58	0.51
1:B:30:ARG:O	1:B:376:HIS:HE1	1.94	0.51
1:A:175:GLU:HA	1:A:352:TRP:CE3	2.46	0.51
1:A:132:ARG:NH1	1:A:343:GLU:OE2	2.38	0.51
1:B:224:ASP:HB3	1:B:226:MET:CE	2.41	0.51
1:C:628:LEU:O	2:F:8:C:O2	2.29	0.50
1:B:650:SER:OG	1:B:653:LYS:HG3	2.12	0.50
1:B:1:PRO:HD2	1:B:238:GLU:CD	2.32	0.50
1:A:175:GLU:HA	1:A:352:TRP:CD2	2.46	0.50
1:A:288:GLN:HB3	1:A:289:PRO:HD3	1.93	0.50
1:B:471:LEU:HD12	1:B:474:MET:HE2	1.94	0.50
1:A:602:VAL:CG1	1:A:604:SER:HB3	2.42	0.50
1:A:650:SER:HB2	1:A:652:GLU:OE1	2.12	0.50
1:A:304:HIS:HA	1:A:309:ASN:HD21	1.77	0.50
1:A:392:SER:O	1:A:398:THR:HG21	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:5:U:O2	2:E:5:U:O4'	2.30	0.49
1:C:650:SER:HB2	1:C:652:GLU:OE1	2.12	0.49
1:C:161:GLY:O	1:C:165:GLU:HG3	2.13	0.49
1:C:543:LYS:O	1:C:625:PRO:HD2	2.12	0.49
1:C:304:HIS:HA	1:C:309:ASN:HD21	1.77	0.49
1:C:288:GLN:HB3	1:C:289:PRO:HD3	1.94	0.49
1:C:611:LEU:HD22	1:C:614:LEU:HD12	1.94	0.49
1:C:606:ALA:C	1:C:608:GLN:H	2.15	0.49
1:B:224:ASP:HB3	1:B:226:MET:HE1	1.95	0.49
1:A:664:ARG:HG3	1:A:664:ARG:O	2.12	0.49
1:B:161:GLY:O	1:B:165:GLU:HG3	2.12	0.49
1:A:311:GLU:O	1:A:315:LYS:HB2	2.12	0.49
1:C:226:MET:HE2	1:C:244:ALA:HA	1.95	0.48
1:B:308:LEU:CD2	1:B:308:LEU:H	2.22	0.48
1:A:145:ILE:HD12	1:A:164:ILE:HD13	1.94	0.48
1:B:606:ALA:C	1:B:608:GLN:H	2.17	0.48
1:B:204:ARG:HH12	2:E:7:C:N4	2.11	0.48
1:B:451:LYS:CE	2:E:8:C:N4	2.69	0.48
1:A:164:ILE:O	1:A:168:GLU:HG3	2.14	0.48
1:A:506:ARG:HG3	1:A:506:ARG:HH11	1.79	0.48
1:B:40:TYR:OH	1:B:587:ARG:NH2	2.46	0.48
1:A:429:MET:HB2	1:A:430:PRO:HD3	1.96	0.48
1:A:232:TYR:HA	1:A:239:GLN:O	2.13	0.48
1:C:339:LEU:HD23	1:C:339:LEU:C	2.34	0.47
1:B:506:ARG:HG3	1:B:506:ARG:HH11	1.79	0.47
1:C:291:ARG:HD3	2:F:8:C:C6	2.47	0.47
1:A:82:THR:HG23	1:A:83:ASN:O	2.14	0.47
1:A:658:LEU:HB3	1:A:662:MET:HE1	1.95	0.47
1:A:518:ILE:HB	1:A:561:CYS:SG	2.55	0.47
1:B:203:TYR:CE1	1:B:271:THR:HG22	2.50	0.47
1:B:75:VAL:HG12	1:B:493:GLY:HA2	1.97	0.47
1:C:146:ARG:NH2	1:C:540:SER:O	2.48	0.47
1:B:404:LEU:HD12	1:B:404:LEU:C	2.35	0.47
1:A:404:LEU:HD12	1:A:404:LEU:C	2.36	0.46
1:A:226:MET:HE2	1:A:244:ALA:HA	1.97	0.46
1:A:628:LEU:O	2:D:8:C:O2	2.33	0.46
1:A:606:ALA:C	1:A:608:GLN:H	2.18	0.46
1:B:633:THR:HG22	1:B:636:ASP:OD2	2.16	0.46
1:A:94:PRO:CB	1:A:269:ARG:HG3	2.46	0.46
2:E:8:C:C2'	2:E:8:C:O2	2.62	0.46
2:F:8:C:O2	2:F:8:C:C2'	2.64	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:304:HIS:HA	1:C:309:ASN:ND2	2.30	0.46
1:C:32:PHE:CZ	1:C:96:ILE:HD11	2.50	0.46
1:B:664:ARG:O	1:B:664:ARG:HG3	2.13	0.46
1:C:75:VAL:HG12	1:C:493:GLY:HA2	1.98	0.46
1:C:89:HIS:CE1	1:C:209:ASP:H	2.34	0.46
1:C:94:PRO:CB	1:C:269:ARG:HG3	2.45	0.46
1:C:429:MET:HB2	1:C:430:PRO:HD3	1.98	0.46
1:B:629:GLN:HA	2:E:8:C:O2	2.16	0.46
1:B:642:HIS:CE1	1:B:646:MET:HG3	2.51	0.45
1:C:305:THR:H	1:C:309:ASN:ND2	2.14	0.45
1:B:543:LYS:O	1:B:625:PRO:HD2	2.16	0.45
1:C:659:ARG:NH1	1:C:659:ARG:HB2	2.31	0.45
2:D:8:C:O2	2:D:8:C:C2'	2.65	0.45
1:B:51:LEU:HD22	1:B:90:MET:HE1	1.99	0.45
1:B:634:GLU:HB2	1:B:642:HIS:NE2	2.32	0.45
1:B:429:MET:HB2	1:B:430:PRO:HD3	1.98	0.44
1:A:301:THR:HG21	1:A:440:TRP:HA	2.00	0.44
1:B:288:GLN:HB3	1:B:289:PRO:HD3	2.00	0.44
1:C:305:THR:OG1	1:C:306:THR:N	2.51	0.44
1:C:466:VAL:HG13	1:C:467:GLY:N	2.33	0.44
1:C:518:ILE:HB	1:C:561:CYS:SG	2.57	0.44
1:A:642:HIS:CE1	1:A:646:MET:HG3	2.52	0.44
1:C:506:ARG:HG3	1:C:506:ARG:NH1	2.33	0.44
1:B:506:ARG:O	1:B:508:GLU:HG3	2.17	0.44
1:A:518:ILE:HG12	1:A:567:VAL:HG21	1.98	0.44
1:A:40:TYR:OH	1:A:587:ARG:NH2	2.50	0.44
1:A:650:SER:OG	1:A:653:LYS:HG3	2.17	0.44
1:A:161:GLY:O	1:A:165:GLU:HG3	2.18	0.44
1:A:475:LEU:HD21	1:A:482:PRO:HG3	2.00	0.44
1:A:339:LEU:C	1:A:339:LEU:HD23	2.38	0.44
1:B:150:SER:CB	2:E:5:U:H2'	2.48	0.44
1:A:1:PRO:HD2	1:A:238:GLU:CD	2.38	0.44
1:A:160:MET:O	1:A:164:ILE:HG12	2.18	0.44
1:B:94:PRO:CB	1:B:269:ARG:HG3	2.47	0.43
1:B:202:VAL:HG11	2:E:5:U:H5'	2.00	0.43
1:C:301:THR:HG21	1:C:440:TRP:HA	2.01	0.43
1:B:146:ARG:NH2	1:B:540:SER:O	2.51	0.43
1:B:451:LYS:HE2	2:E:8:C:H41	1.79	0.43
1:B:232:TYR:HA	1:B:239:GLN:O	2.18	0.43
1:A:305:THR:H	1:A:309:ASN:ND2	2.16	0.43
1:B:304:HIS:HA	1:B:309:ASN:HD21	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:ASP:OD1	1:B:74:ARG:HD2	2.19	0.43
1:A:529:GLU:HG2	1:A:529:GLU:O	2.19	0.42
1:A:651:VAL:O	1:A:655:GLU:HB2	2.19	0.42
1:B:32:PHE:CZ	1:B:96:ILE:HD11	2.54	0.42
1:B:70:ASP:OD2	1:B:74:ARG:HD3	2.19	0.42
1:B:305:THR:H	1:B:309:ASN:ND2	2.18	0.42
1:B:304:HIS:HA	1:B:309:ASN:ND2	2.35	0.42
1:B:143:LEU:H	1:B:654:THR:HG21	1.84	0.42
1:B:518:ILE:HB	1:B:561:CYS:SG	2.59	0.42
1:B:13:LYS:NZ	1:B:383:SER:OG	2.53	0.42
1:C:658:LEU:HB3	1:C:662:MET:HE1	2.01	0.42
1:C:579:PHE:O	1:C:581:GLU:HG2	2.19	0.42
1:C:224:ASP:HB3	1:C:226:MET:CE	2.50	0.42
1:B:611:LEU:HD22	1:B:614:LEU:HD12	2.02	0.42
1:C:89:HIS:HE1	1:C:209:ASP:H	1.67	0.42
2:F:8:C:O2	2:F:8:C:C3'	2.68	0.41
1:C:75:VAL:HG21	1:C:500:ILE:HG21	2.01	0.41
1:A:614:LEU:HD21	1:A:641:ILE:HD11	2.01	0.41
1:C:350:ALA:HB1	1:C:352:TRP:NE1	2.35	0.41
1:B:32:PHE:CD2	1:B:372:PRO:HG3	2.54	0.41
1:B:343:GLU:O	1:B:347:MET:HG3	2.21	0.41
1:B:497:LEU:HD12	1:B:497:LEU:HA	1.80	0.41
1:A:543:LYS:O	1:A:625:PRO:HD2	2.20	0.41
1:B:156:PHE:HB3	2:E:5:U:C5	2.55	0.41
2:D:5:U:O2'	2:D:6:U:P	2.78	0.41
2:E:8:C:C3'	2:E:8:C:O2	2.69	0.41
1:A:506:ARG:HG3	1:A:506:ARG:NH1	2.36	0.41
1:A:146:ARG:NH2	1:A:540:SER:O	2.54	0.41
2:D:8:C:O2	2:D:8:C:C3'	2.68	0.41
1:B:273:MET:O	1:B:394:GLY:HA3	2.21	0.41
1:C:243:PHE:CD1	1:C:243:PHE:N	2.88	0.41
1:B:204:ARG:HH12	2:E:7:C:H42	1.68	0.41
1:C:143:LEU:H	1:C:654:THR:HG21	1.86	0.41
1:A:143:LEU:H	1:A:654:THR:HG21	1.86	0.41
2:F:5:U:O2'	2:F:6:U:P	2.79	0.41
1:A:1:PRO:HD2	1:A:238:GLU:OE2	2.21	0.41
1:C:471:LEU:HD12	1:C:474:MET:HE2	2.02	0.41
1:A:23:LYS:HE2	1:A:23:LYS:HB3	1.83	0.40
1:B:301:THR:HG21	1:B:440:TRP:HA	2.03	0.40
1:C:206:GLN:CG	1:C:270:ARG:HD2	2.46	0.40
1:B:506:ARG:NH1	1:B:506:ARG:HG3	2.36	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:402:GLY:HA3	4:C:2077:HOH:O	2.22	0.40
1:B:72:TYR:HB2	1:B:74:ARG:HD2	2.03	0.40
1:C:404:LEU:HD12	1:C:404:LEU:C	2.42	0.40
1:B:641:ILE:HD13	1:B:641:ILE:HA	1.92	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	
1	A	662/664 (100%)	636 (96%)	21 (3%)	5 (1%)	24	15
1	B	662/664 (100%)	637 (96%)	20 (3%)	5 (1%)	24	15
1	C	662/664 (100%)	635 (96%)	22 (3%)	5 (1%)	24	15
All	All	1986/1992 (100%)	1908 (96%)	63 (3%)	15 (1%)	24	15

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	604	SER
1	A	608	GLN
1	B	604	SER
1	B	608	GLN
1	C	604	SER
1	C	608	GLN
1	A	2	ARG
1	B	2	ARG
1	C	2	ARG
1	C	606	ALA
1	A	606	ALA
1	A	607	ARG
1	B	606	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	607	ARG
1	C	607	ARG

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	
1	A	557/557 (100%)	535 (96%)	22 (4%)	39	36
1	B	557/557 (100%)	539 (97%)	18 (3%)	46	45
1	C	557/557 (100%)	537 (96%)	20 (4%)	42	40
All	All	1671/1671 (100%)	1611 (96%)	60 (4%)	42	40

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	43	LEU
1	A	44	LEU
1	A	74	ARG
1	A	113	ASP
1	A	119	VAL
1	A	154	PRO
1	A	202	VAL
1	A	206	GLN
1	A	269	ARG
1	A	308	LEU
1	A	373	GLU
1	A	384	ASN
1	A	387	LEU
1	A	391	LEU
1	A	404	LEU
1	A	497	LEU
1	A	576	TRP
1	A	591	LEU
1	A	613	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	626	ASN
1	A	658	LEU
1	B	2	ARG
1	B	43	LEU
1	B	44	LEU
1	B	74	ARG
1	B	113	ASP
1	B	146	ARG
1	B	154	PRO
1	B	202	VAL
1	B	206	GLN
1	B	373	GLU
1	B	384	ASN
1	B	391	LEU
1	B	404	LEU
1	B	497	LEU
1	B	576	TRP
1	B	591	LEU
1	B	613	GLU
1	B	658	LEU
1	C	2	ARG
1	C	43	LEU
1	C	44	LEU
1	C	71	GLU
1	C	74	ARG
1	C	113	ASP
1	C	119	VAL
1	C	154	PRO
1	C	202	VAL
1	C	206	GLN
1	C	308	LEU
1	C	373	GLU
1	C	391	LEU
1	C	404	LEU
1	C	472	PHE
1	C	497	LEU
1	C	576	TRP
1	C	591	LEU
1	C	613	GLU
1	C	658	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	89	HIS
1	A	191	GLN
1	A	239	GLN
1	A	309	ASN
1	A	376	HIS
1	A	469	HIS
1	A	608	GLN
1	A	629	GLN
1	B	26	GLN
1	B	191	GLN
1	B	309	ASN
1	B	376	HIS
1	B	384	ASN
1	B	629	GLN
1	C	26	GLN
1	C	191	GLN
1	C	239	GLN
1	C	309	ASN
1	C	376	HIS
1	C	629	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	D	4/6 (66%)	2 (50%)	1 (25%)
2	E	4/6 (66%)	2 (50%)	1 (25%)
2	F	4/6 (66%)	2 (50%)	1 (25%)
All	All	12/18 (66%)	6 (50%)	3 (25%)

All (6) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	D	6	U
2	D	8	C
2	E	6	U
2	E	8	C
2	F	6	U
2	F	8	C

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	D	5	U
2	E	5	U
2	F	5	U

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - 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	A	664/664 (100%)	0.20	35 (5%)	30 40	17, 30, 52, 102	0
1	B	664/664 (100%)	0.22	22 (3%)	50 60	17, 28, 51, 102	0
1	C	664/664 (100%)	0.47	44 (6%)	22 30	18, 31, 53, 103	0
2	D	4/6 (66%)	3.16	4 (100%)	0 0	115, 116, 122, 128	0
2	E	4/6 (66%)	4.45	4 (100%)	0 0	115, 116, 123, 129	0
2	F	4/6 (66%)	3.88	4 (100%)	0 0	115, 116, 123, 129	0
All	All	2004/2010 (99%)	0.32	113 (5%)	28 38	17, 30, 53, 129	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	607	ARG	11.4
1	C	603	ALA	11.3
1	B	606	ALA	9.9
1	C	606	ALA	9.5
1	B	609	ALA	9.0
1	C	604	SER	8.8
1	C	608	GLN	8.6
1	C	609	ALA	8.5
1	A	606	ALA	8.4
1	C	664	ARG	7.9
1	C	610	GLY	7.0
1	C	612	ALA	6.9
1	B	608	GLN	6.7
1	A	605	MET	6.2
1	A	664	ARG	6.1
1	C	216	LYS	6.1
1	A	1	PRO	6.0
1	B	610	GLY	5.9
2	F	8	C	5.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	664	ARG	5.6
1	B	607	ARG	5.4
1	B	603	ALA	5.4
1	A	607	ARG	5.2
2	E	7	C	5.1
1	C	215	PRO	5.0
2	E	8	C	4.9
2	E	5	U	4.8
1	B	604	SER	4.8
1	C	537	ARG	4.7
1	B	1	PRO	4.7
2	D	5	U	4.7
1	C	1	PRO	4.5
1	C	611	LEU	4.4
1	C	2	ARG	4.4
1	A	609	ALA	4.3
1	B	576	TRP	4.3
1	B	537	ARG	4.2
1	A	217	THR	4.1
1	C	254	GLU	4.1
1	B	216	LYS	4.0
2	F	5	U	3.9
1	C	605	MET	3.9
1	B	612	ALA	3.8
1	A	216	LYS	3.8
1	A	610	GLY	3.8
1	C	470	ARG	3.7
1	C	506	ARG	3.7
1	A	254	GLU	3.6
1	C	505	SER	3.6
1	A	659	ARG	3.5
1	C	217	THR	3.5
1	C	63	ASP	3.5
1	A	576	TRP	3.5
1	C	596	LEU	3.3
2	F	7	C	3.3
1	C	535	GLY	3.3
1	C	556	ASP	3.3
1	C	259	ASP	3.2
1	C	592	LYS	3.1
1	B	613	GLU	3.1
1	A	506	ARG	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	8	C	3.1
1	B	2	ARG	3.0
1	A	652	GLU	3.0
1	A	215	PRO	3.0
1	A	270	ARG	3.0
2	E	6	U	2.9
1	A	505	SER	2.9
1	A	603	ALA	2.8
1	A	611	LEU	2.8
1	A	373	GLU	2.8
1	C	461	LYS	2.6
1	A	219	LYS	2.6
2	D	7	C	2.6
1	C	373	GLU	2.5
1	C	308	LEU	2.5
1	C	602	VAL	2.5
1	C	214	ASP	2.5
1	C	219	LYS	2.5
2	F	6	U	2.4
1	C	279	LEU	2.4
1	A	2	ARG	2.4
1	A	239	GLN	2.4
1	B	535	GLY	2.4
1	C	408	ILE	2.3
1	C	593	ARG	2.3
1	A	259	ASP	2.3
2	D	6	U	2.3
1	C	534	SER	2.3
1	C	536	VAL	2.3
1	A	214	ASP	2.3
1	B	321	VAL	2.2
1	A	645	LEU	2.2
1	B	457	LEU	2.2
1	B	479	LYS	2.2
1	C	309	ASN	2.2
1	A	656	ARG	2.2
1	A	613	GLU	2.2
1	C	262	ASP	2.1
1	A	602	VAL	2.1
1	A	408	ILE	2.1
1	B	308	LEU	2.1
1	A	158	ASN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	501	LEU	2.1
1	C	218	GLY	2.1
1	B	506	ARG	2.1
1	A	628	LEU	2.0
1	C	622	LEU	2.0
1	A	479	LYS	2.0
1	A	608	GLN	2.0
1	C	253	LYS	2.0
1	C	64	HIS	2.0
1	A	257	GLY	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(\AA^2)	Q<0.9
3	MN	A	1665	1/1	0.99	0.08	-1.31	29,29,29,29	0
3	MN	C	1665	1/1	0.99	0.05	-2.62	30,30,30,30	0
3	MN	B	1665	1/1	0.98	0.06	-3.53	26,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.