Full wwPDB X-ray Structure Validation Report ⓘ

Sep 12, 2023 – 04:13 PM EDT

PDB ID	:	4NIA
Title	:	Satellite Tobacco Mosaic Virus Refined at room temperature to 1.8 A Resolution using NCS Restraints
Authors	:	Larson, S.B.; Day, J.S.; McPherson, A.
Deposited on	:	2013-11-05
Resolution	:	1.82 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 ⓘ 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 ⓘ) were used in the production of this report:

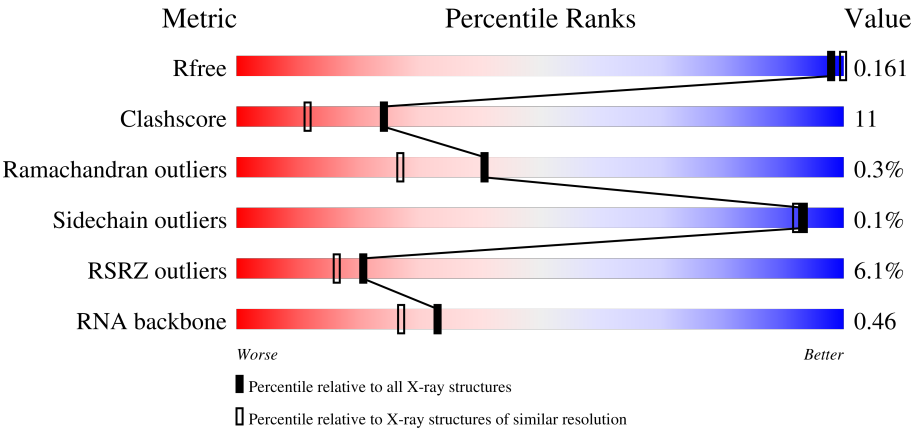
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 1.82 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.



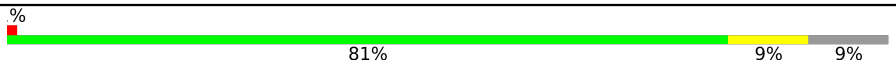
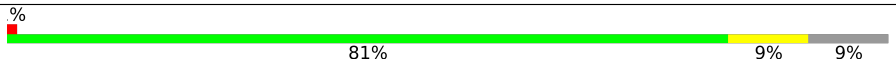
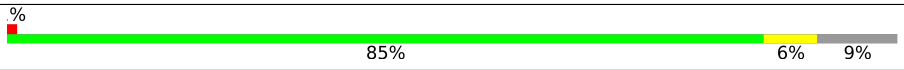
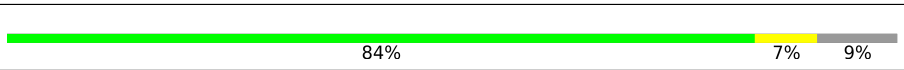
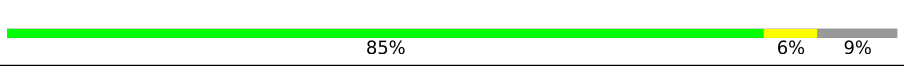
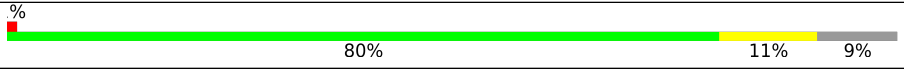
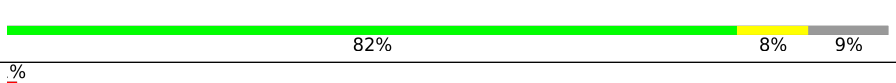
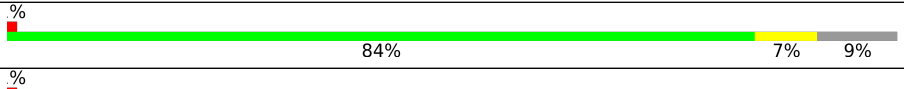
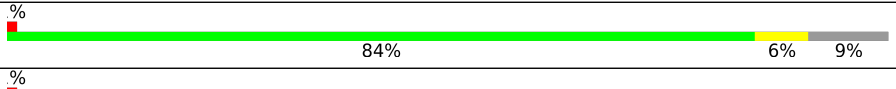
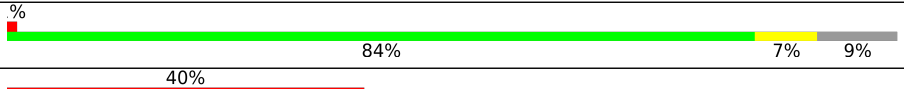
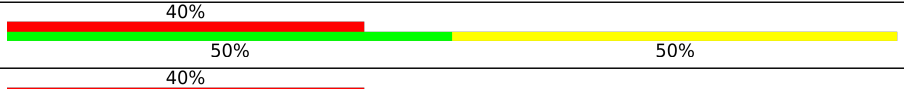
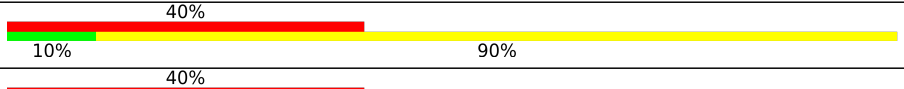
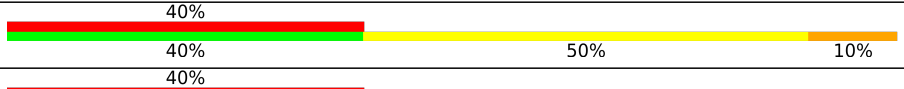
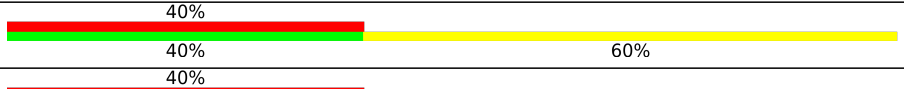
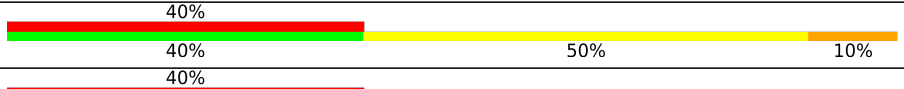
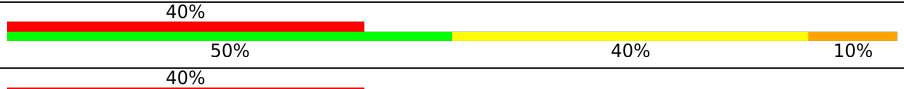
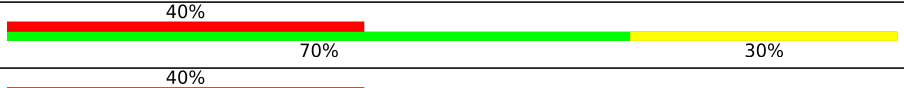
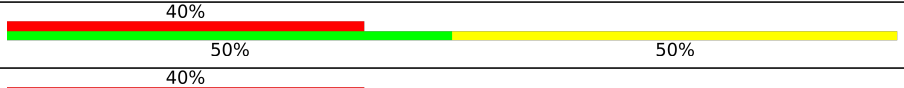
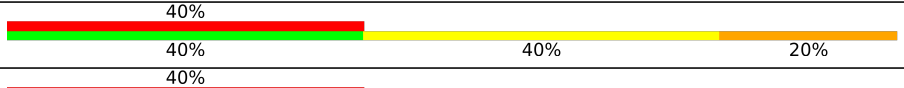
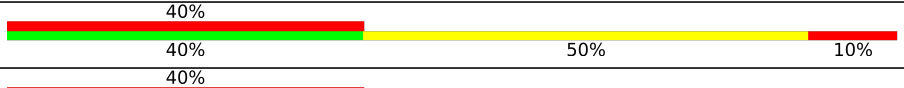
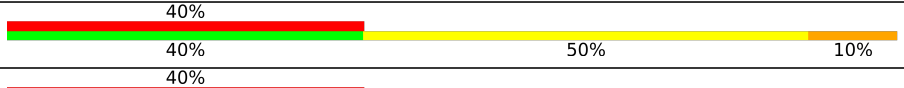
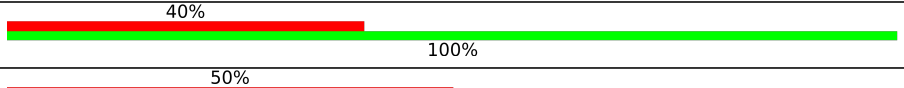
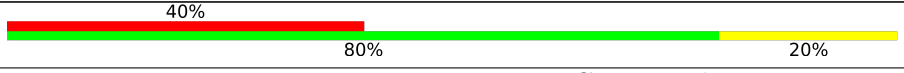
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	7484 (1.84-1.80)
Clashscore	141614	8401 (1.84-1.80)
Ramachandran outliers	138981	8290 (1.84-1.80)
Sidechain outliers	138945	8290 (1.84-1.80)
RSRZ outliers	127900	7371 (1.84-1.80)
RNA backbone	3102	1047 (2.40-1.24)

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	A	159	82% 8% 9%
1	B	159	86% 9%
1	C	159	83% 8% 9%
1	D	159	76% 14% 9%

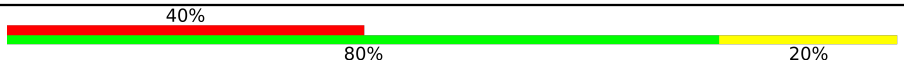
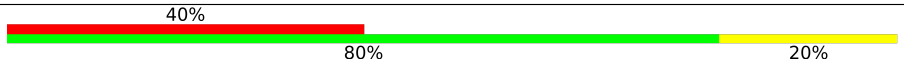
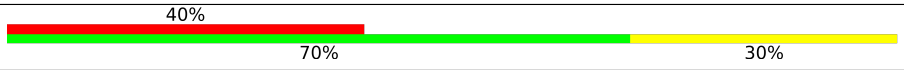
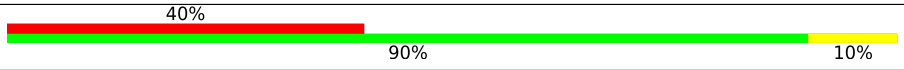
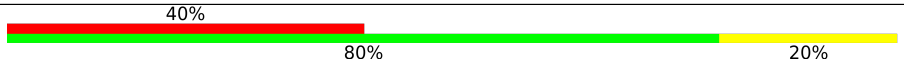
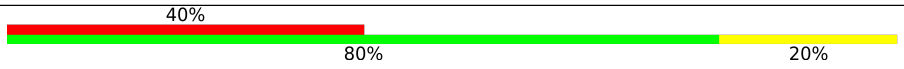
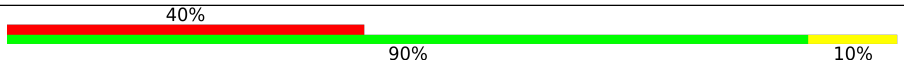
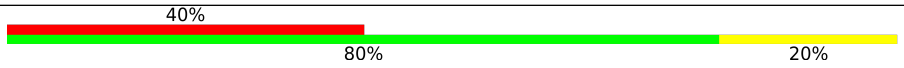
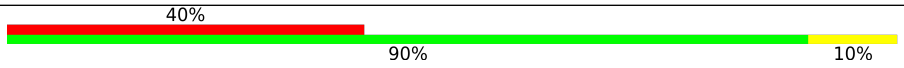
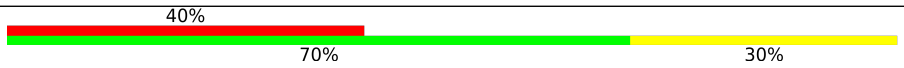
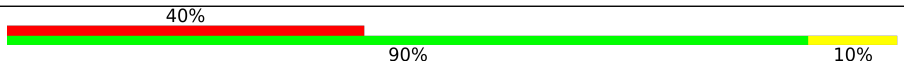
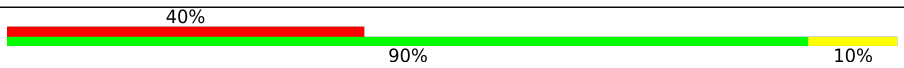
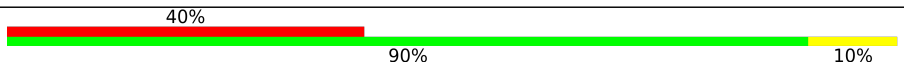
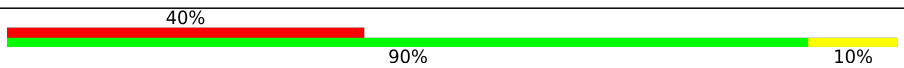
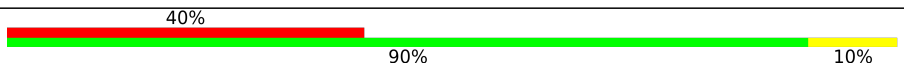
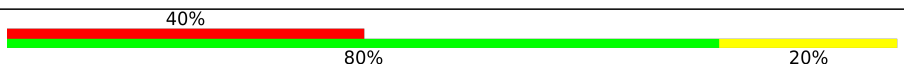
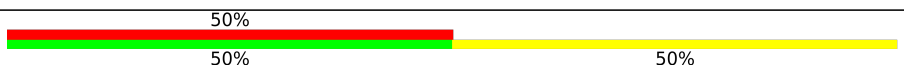
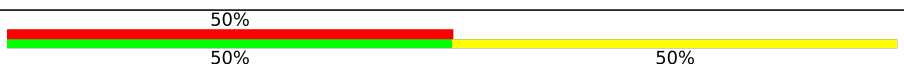
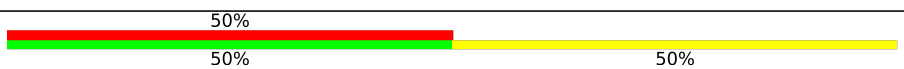
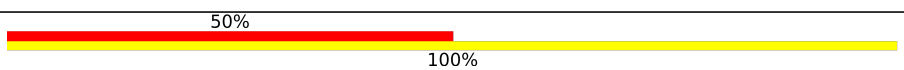
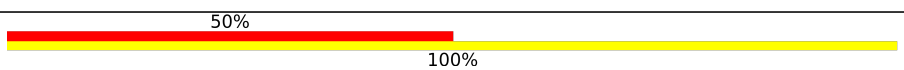
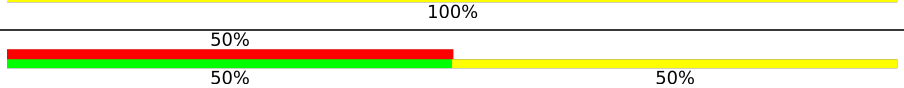
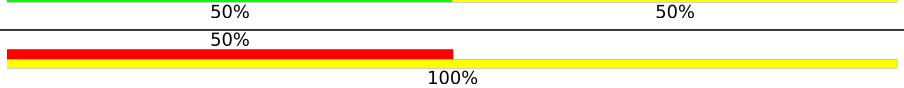
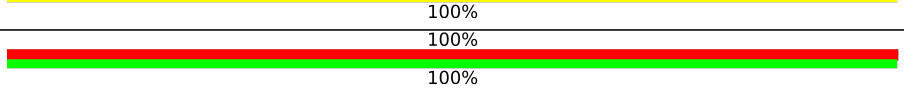
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	159	
1	F	159	
1	G	159	
1	H	159	
1	I	159	
1	J	159	
1	K	159	
1	L	159	
1	M	159	
1	N	159	
1	O	159	
2	P	10	
2	Q	10	
2	R	10	
2	S	10	
2	T	10	
2	U	10	
2	V	10	
2	W	10	
2	X	10	
2	Y	10	
2	Z	10	
2	a	10	
2	b	10	
2	c	10	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	d	10	
3	e	10	
3	f	10	
3	g	10	
3	h	10	
3	i	10	
3	j	10	
3	k	10	
3	l	10	
3	m	10	
3	n	10	
3	o	10	
3	p	10	
3	q	10	
3	r	10	
3	s	10	
4	1	2	
4	2	2	
4	3	2	
4	4	2	
4	5	2	
4	6	2	
4	7	2	
4	8	2	
4	t	2	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	u	2	50% 100%
4	v	2	50% 100%
4	w	2	100% 100%
4	x	2	50% 100%
4	y	2	100% 100%
4	z	2	100% 100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	SO4	E	201	-	-	-	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 28403 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 Coat protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	144	Total	C	N	O	S	0	19	0
			1224	778	212	226	8			
1	B	144	Total	C	N	O	S	0	17	0
			1201	761	209	222	9			
1	C	144	Total	C	N	O	S	0	19	0
			1226	779	213	225	9			
1	D	144	Total	C	N	O	S	0	22	0
			1244	793	215	228	8			
1	E	144	Total	C	N	O	S	0	19	0
			1215	770	211	226	8			
1	F	144	Total	C	N	O	S	0	19	0
			1225	775	214	228	8			
1	G	144	Total	C	N	O	S	0	18	0
			1208	764	212	224	8			
1	H	144	Total	C	N	O	S	0	20	0
			1222	775	213	225	9			
1	I	144	Total	C	N	O	S	0	16	0
			1196	754	208	225	9			
1	J	144	Total	C	N	O	S	0	19	0
			1216	773	209	225	9			
1	K	144	Total	C	N	O	S	0	20	0
			1221	772	213	227	9			
1	L	144	Total	C	N	O	S	0	18	0
			1206	762	210	225	9			
1	M	144	Total	C	N	O	S	0	15	0
			1186	751	207	220	8			
1	N	144	Total	C	N	O	S	0	19	0
			1220	774	213	224	9			
1	O	144	Total	C	N	O	S	0	20	0
			1221	776	212	224	9			

- Molecule 2 is a RNA chain called RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	10	Total	C	N	O	P	0	10	0
			221	100	50	61	10			
2	Q	10	Total	C	N	O	P	0	10	0
			221	100	50	61	10			
2	R	10	Total	C	N	O	P	0	10	0
			221	100	50	61	10			
2	S	10	Total	C	N	O	P	0	10	0
			221	100	50	61	10			
2	T	10	Total	C	N	O	P	0	10	0
			221	100	50	61	10			
2	U	10	Total	C	N	O	P	0	10	0
			221	100	50	61	10			
2	V	10	Total	C	N	O	P	0	10	0
			221	100	50	61	10			
2	W	10	Total	C	N	O	P	0	10	0
			221	100	50	61	10			
2	X	10	Total	C	N	O	P	0	10	0
			221	100	50	61	10			
2	Y	10	Total	C	N	O	P	0	10	0
			221	100	50	61	10			
2	Z	10	Total	C	N	O	P	0	10	0
			221	100	50	61	10			
2	a	10	Total	C	N	O	P	0	10	0
			221	100	50	61	10			
2	b	10	Total	C	N	O	P	0	10	0
			221	100	50	61	10			
2	c	10	Total	C	N	O	P	0	10	0
			221	100	50	61	10			
2	d	10	Total	C	N	O	P	0	10	0
			221	100	50	61	10			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	e	10	Total	C	N	O	P	0	10	0
			201	90	20	81	10			
3	f	10	Total	C	N	O	P	0	10	0
			201	90	20	81	10			
3	g	10	Total	C	N	O	P	0	10	0
			201	90	20	81	10			
3	h	10	Total	C	N	O	P	0	10	0
			201	90	20	81	10			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	i	10	Total	C	N	O	P	0	10	0
			201	90	20	81	10			
3	j	10	Total	C	N	O	P	0	10	0
			201	90	20	81	10			
3	k	10	Total	C	N	O	P	0	10	0
			201	90	20	81	10			
3	l	10	Total	C	N	O	P	0	10	0
			201	90	20	81	10			
3	m	10	Total	C	N	O	P	0	10	0
			201	90	20	81	10			
3	n	10	Total	C	N	O	P	0	10	0
			201	90	20	81	10			
3	o	10	Total	C	N	O	P	0	10	0
			201	90	20	81	10			
3	p	10	Total	C	N	O	P	0	10	0
			201	90	20	81	10			
3	q	10	Total	C	N	O	P	0	10	0
			201	90	20	81	10			
3	r	10	Total	C	N	O	P	0	10	0
			201	90	20	81	10			
3	s	10	Total	C	N	O	P	0	10	0
			201	90	20	81	10			

- Molecule 4 is a RNA chain called RNA (5'-R(P*UP*U)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	t	2	Total	C	N	O	P	0	2	0
			26	10	2	12	2			
4	u	2	Total	C	N	O	P	0	2	0
			26	10	2	12	2			
4	v	2	Total	C	N	O	P	0	2	0
			26	10	2	12	2			
4	w	2	Total	C	N	O	P	0	2	0
			26	10	2	12	2			
4	x	2	Total	C	N	O	P	0	2	0
			26	10	2	12	2			
4	y	2	Total	C	N	O	P	0	2	0
			26	10	2	12	2			
4	z	2	Total	C	N	O	P	0	2	0
			26	10	2	12	2			
4	1	2	Total	C	N	O	P	0	2	0
			26	10	2	12	2			

Continued on next page...

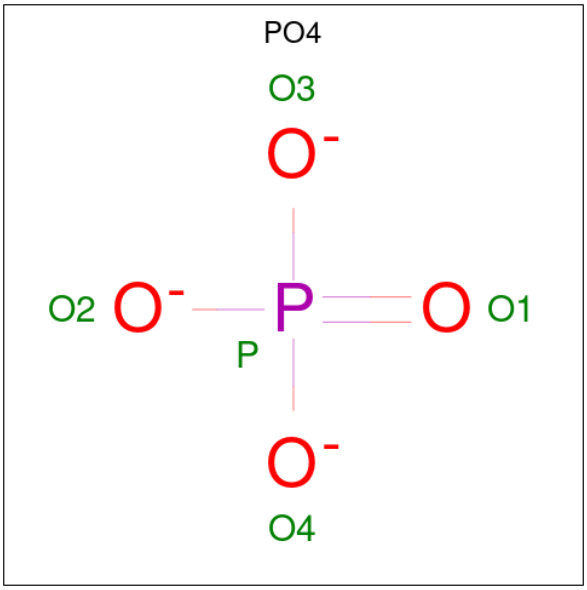
Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	2	2	Total	C	N	O	P	0	2	0
			26	10	2	12	2			
4	3	2	Total	C	N	O	P	0	2	0
			26	10	2	12	2			
4	4	2	Total	C	N	O	P	0	2	0
			26	10	2	12	2			
4	5	2	Total	C	N	O	P	0	2	0
			26	10	2	12	2			
4	6	2	Total	C	N	O	P	0	2	0
			26	10	2	12	2			
4	7	2	Total	C	N	O	P	0	2	0
			26	10	2	12	2			
4	8	2	Total	C	N	O	P	0	2	0
			26	10	2	12	2			

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

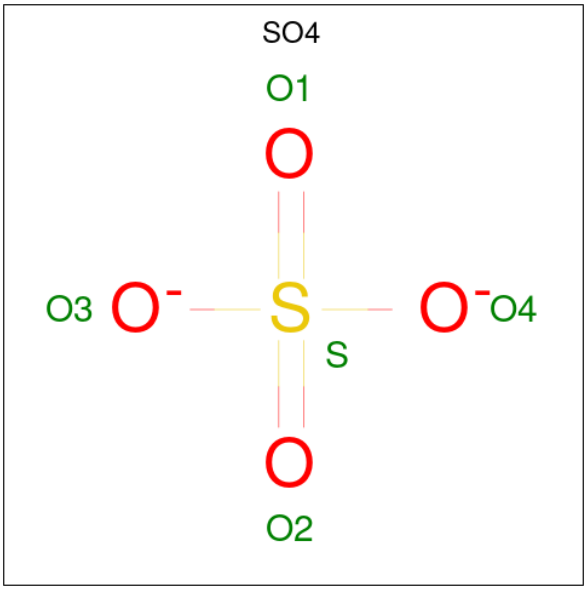
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	F	1	Total	Mg	0	0
			1	1		
5	K	1	Total	Mg	0	0
			1	1		

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total O P 21 20 1	0	1
6	H	1	Total O P 21 20 1	0	1
6	K	1	Total O P 21 20 1	0	1

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	E	1	Total O S 5 4 1	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	224	Total O 224 224	0	33
8	P	8	Total O 8 8	0	0
8	e	9	Total O 9 9	0	1
8	t	1	Total O 1 1	0	0
8	B	205	Total O 205 205	0	36
8	Q	11	Total O 11 11	0	2

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	f	2	Total O 2 2	0	0
8	C	204	Total O 204 204	0	29
8	R	13	Total O 13 13	0	1
8	g	3	Total O 3 3	0	0
8	v	1	Total O 1 1	0	0
8	D	203	Total O 203 203	0	42
8	S	12	Total O 12 12	0	1
8	h	5	Total O 5 5	0	0
8	E	201	Total O 201 201	0	31
8	T	5	Total O 5 5	0	0
8	i	9	Total O 9 9	0	0
8	F	209	Total O 209 209	0	37
8	U	9	Total O 9 9	0	1
8	j	9	Total O 9 9	0	1
8	G	205	Total O 205 205	0	29
8	V	16	Total O 16 16	0	0
8	k	5	Total O 5 5	0	2
8	H	215	Total O 215 215	0	33
8	W	12	Total O 12 12	0	2
8	l	3	Total O 3 3	0	1
8	1	1	Total O 1 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	I	213	Total O 213 213	0	35
8	X	14	Total O 14 14	0	2
8	m	5	Total O 5 5	0	0
8	J	212	Total O 212 212	0	28
8	Y	8	Total O 8 8	0	1
8	n	5	Total O 5 5	0	0
8	3	1	Total O 1 1	0	0
8	K	192	Total O 192 192	0	36
8	Z	11	Total O 11 11	0	1
8	o	10	Total O 10 10	0	1
8	L	226	Total O 226 226	0	40
8	a	11	Total O 11 11	0	0
8	p	8	Total O 8 8	0	2
8	M	203	Total O 203 203	0	24
8	b	11	Total O 11 11	0	0
8	q	2	Total O 2 2	0	1
8	N	206	Total O 206 206	0	28
8	c	10	Total O 10 10	0	0
8	r	6	Total O 6 6	0	1
8	O	209	Total O 209 209	0	38
8	d	6	Total O 6 6	0	2

Continued on next page...

Continued from previous page...

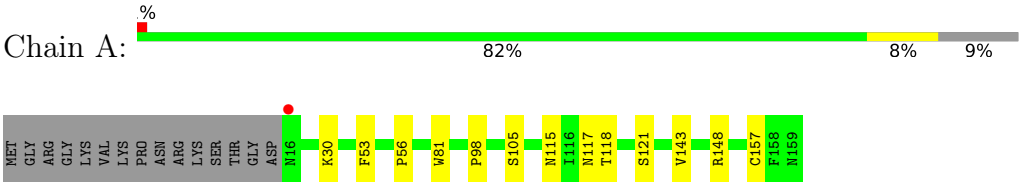
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	s	11	Total O 11 11	0	1
8	8	1	Total O 1 1	0	0

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.

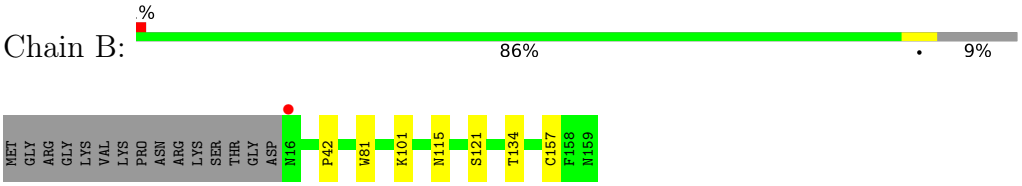
• Molecule 1: Coat protein

Chain A:



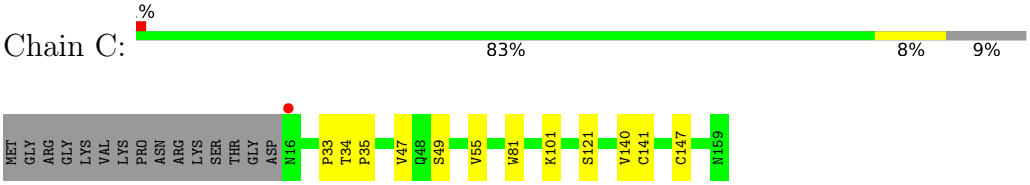
• Molecule 1: Coat protein

Chain B:



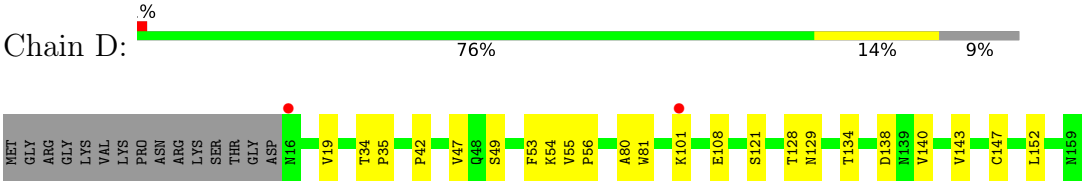
• Molecule 1: Coat protein

Chain C:



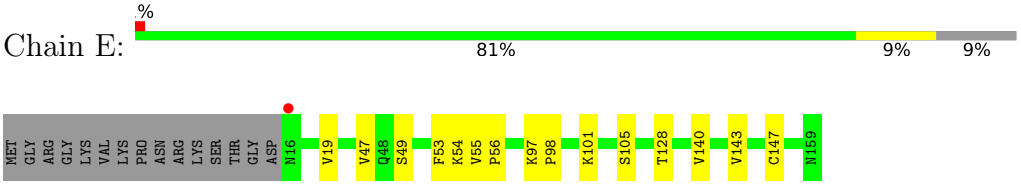
• Molecule 1: Coat protein

Chain D:



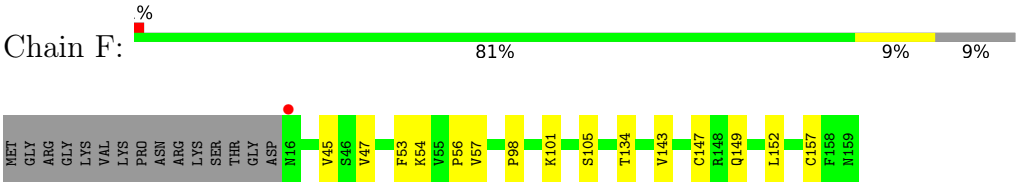
• Molecule 1: Coat protein

Chain E:



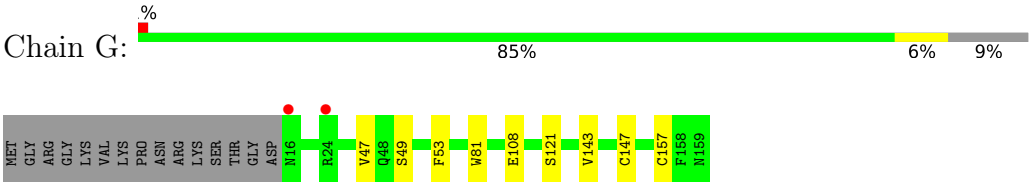
• Molecule 1: Coat protein

Chain F:



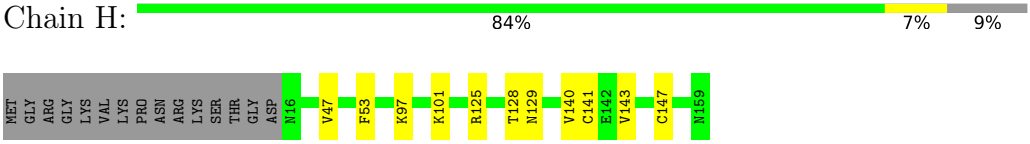
• Molecule 1: Coat protein

Chain G:



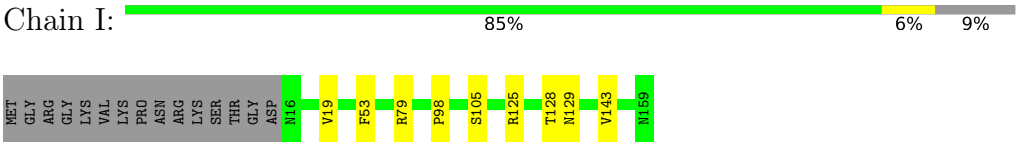
• Molecule 1: Coat protein

Chain H:



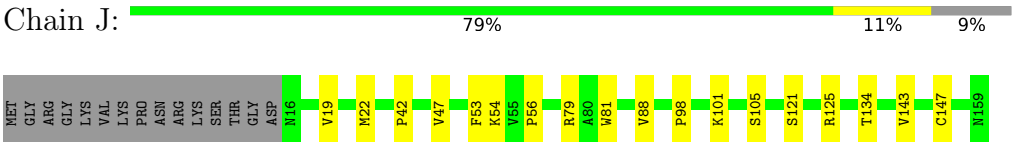
• Molecule 1: Coat protein

Chain I:



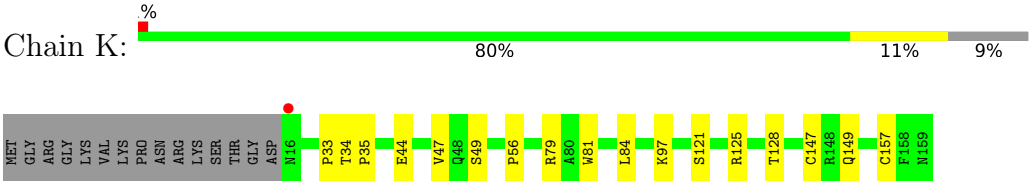
• Molecule 1: Coat protein

Chain J:



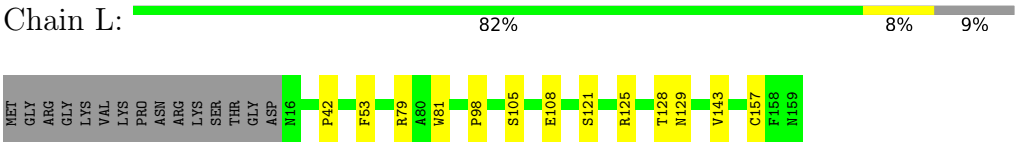
• Molecule 1: Coat protein

Chain K:



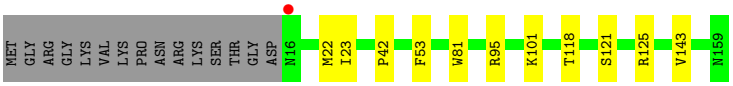
• Molecule 1: Coat protein

Chain L:



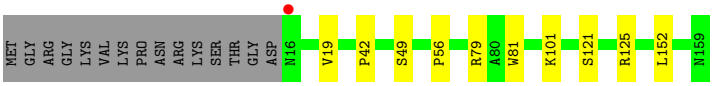
• Molecule 1: Coat protein

Chain M:



• Molecule 1: Coat protein

Chain N:

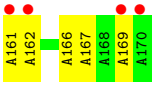


• Molecule 1: Coat protein

Chain O:

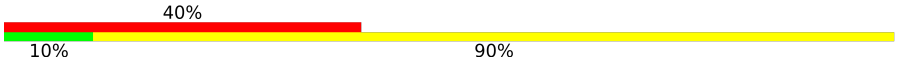
• Molecule 2: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')

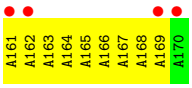
Chain P:



• Molecule 2: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')

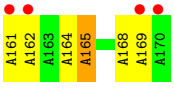
Chain Q:





• Molecule 2: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')

Chain R:

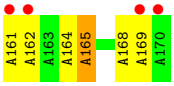


• Molecule 2: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')

Chain S:

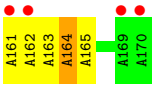
• Molecule 2: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')

Chain T:



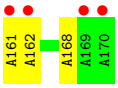
• Molecule 2: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')

Chain U:



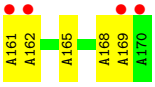
• Molecule 2: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')

Chain V:



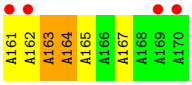
• Molecule 2: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')

Chain W:



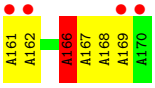
• Molecule 2: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')

Chain X:



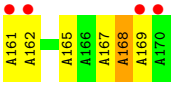
• Molecule 2: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')

Chain Y:



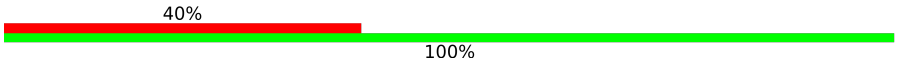
• Molecule 2: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')

Chain Z:



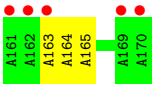
• Molecule 2: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')

Chain a:



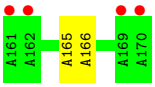
• Molecule 2: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')

Chain b:



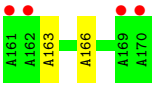
• Molecule 2: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')

Chain c:



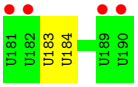
• Molecule 2: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')

Chain d:



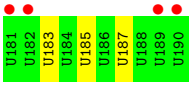
• Molecule 3: RNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3')

Chain e:



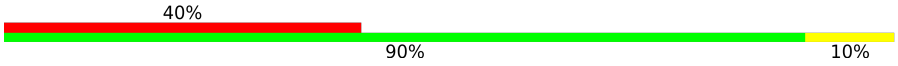
• Molecule 3: RNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3')

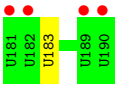
Chain f:



• Molecule 3: RNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3')

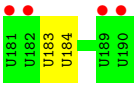
Chain g:





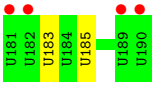
• Molecule 3: RNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3')

Chain h:



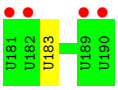
• Molecule 3: RNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3')

Chain i:



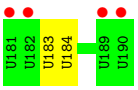
• Molecule 3: RNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3')

Chain j:



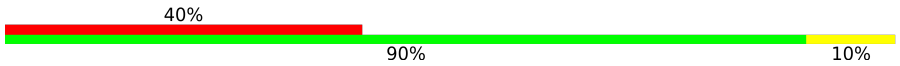
• Molecule 3: RNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3')

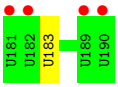
Chain k:



• Molecule 3: RNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3')

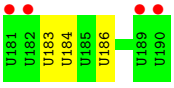
Chain l:





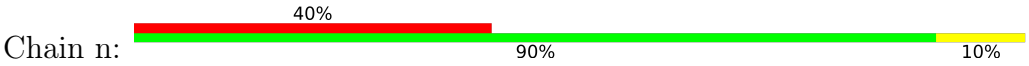
• Molecule 3: RNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3')

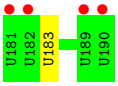
Chain m:



• Molecule 3: RNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3')

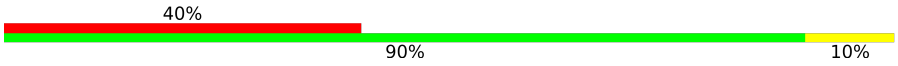
Chain n:

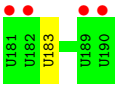




• Molecule 3: RNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3')

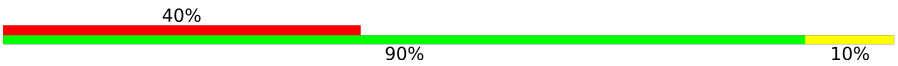
Chain o:

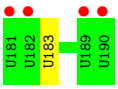




• Molecule 3: RNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3')

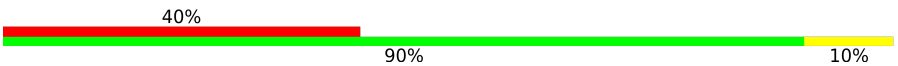
Chain p:

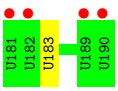




• Molecule 3: RNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3')

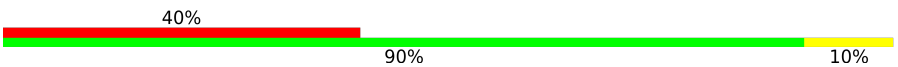
Chain q:

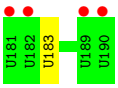




• Molecule 3: RNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3')

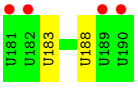
Chain r:





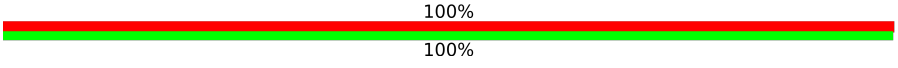
• Molecule 3: RNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3')

Chain s:



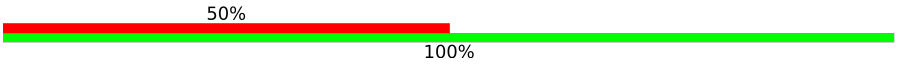
• Molecule 4: RNA (5'-R(P*UP*U)-3')

Chain t:



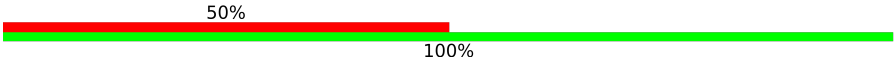
• Molecule 4: RNA (5'-R(P*UP*U)-3')

Chain u:



• Molecule 4: RNA (5'-R(P*UP*U)-3')

Chain v:

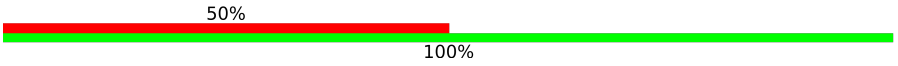


• Molecule 4: RNA (5'-R(P*UP*U)-3')

Chain w:

• Molecule 4: RNA (5'-R(P*UP*U)-3')

Chain x:

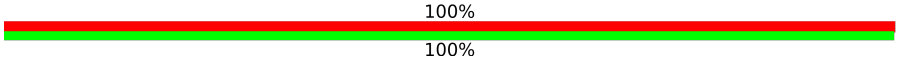


• Molecule 4: RNA (5'-R(P*UP*U)-3')

Chain y:

• Molecule 4: RNA (5'-R(P*UP*U)-3')

Chain z:



• Molecule 4: RNA (5'-R(P*UP*U)-3')

Chain 1:

• Molecule 4: RNA (5'-R(P*UP*U)-3')

Chain 2:

• Molecule 4: RNA (5'-R(P*UP*U)-3')

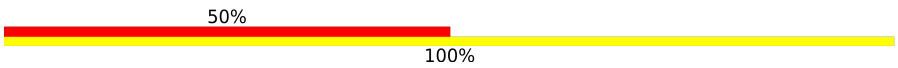
Chain 3:

• Molecule 4: RNA (5'-R(P*UP*U)-3')

Chain 4:

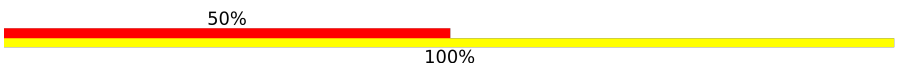
• Molecule 4: RNA (5'-R(P*UP*U)-3')

Chain 5:



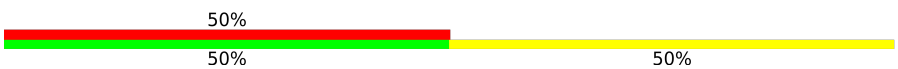
• Molecule 4: RNA (5'-R(P*UP*U)-3')

Chain 6:



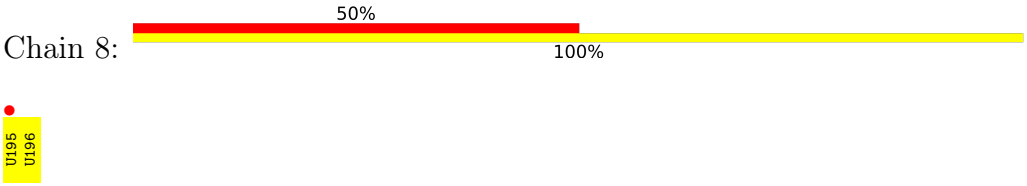
• Molecule 4: RNA (5'-R(P*UP*U)-3')

Chain 7:



• Molecule 4: RNA (5'-R(P*UP*U)-3')

Chain 8:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	174.27Å 191.77Å 202.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	87.04 – 1.82 63.67 – 1.82	Depositor EDS
% Data completeness (in resolution range)	89.5 (87.04-1.82) 89.6 (63.67-1.82)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.91 (at 1.82Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.123 , 0.156 0.131 , 0.161	Depositor DCC
R_{free} test set	3984 reflections (1.48%)	wwPDB-VP
Wilson B-factor (Å^2)	15.1	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 63.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	28403	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.18% 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: PO4, MG, SO4

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	0.55	0/1301	0.68	0/1767
1	B	0.54	0/1269	0.70	0/1725
1	C	0.55	0/1291	0.71	0/1755
1	D	0.54	0/1324	0.71	0/1800
1	E	0.54	0/1282	0.69	0/1745
1	F	0.55	0/1292	0.70	0/1757
1	G	0.55	0/1276	0.67	0/1735
1	H	0.54	0/1292	0.67	0/1756
1	I	0.57	0/1266	0.70	0/1721
1	J	0.54	0/1288	0.71	0/1752
1	K	0.55	0/1301	0.69	0/1768
1	L	0.54	0/1276	0.68	0/1734
1	M	0.58	0/1252	0.70	1/1702 (0.1%)
1	N	0.55	0/1294	0.70	0/1757
1	O	0.53	0/1299	0.69	0/1766
2	P	0.45	0/250	1.17	0/386
2	Q	0.45	0/250	1.13	1/386 (0.3%)
2	R	0.45	0/250	1.09	0/386
2	S	0.43	0/250	1.07	0/386
2	T	0.42	0/250	1.04	0/386
2	U	0.47	0/250	1.07	0/386
2	V	0.42	0/250	1.07	0/386
2	W	0.46	0/250	1.16	0/386
2	X	0.43	0/250	1.02	0/386
2	Y	0.46	0/250	1.18	1/386 (0.3%)
2	Z	0.43	0/250	1.14	1/386 (0.3%)
2	a	0.46	0/250	1.18	0/386
2	b	0.49	0/250	1.29	3/386 (0.8%)
2	c	0.48	0/250	1.22	2/386 (0.5%)
2	d	0.47	0/250	1.15	0/386
3	e	0.53	0/220	1.13	0/336
3	f	0.51	0/220	1.14	2/336 (0.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
3	g	0.56	0/220	1.12	0/336
3	h	0.53	0/220	1.14	0/336
3	i	0.54	0/220	1.08	1/336 (0.3%)
3	j	0.54	0/220	1.09	0/336
3	k	0.55	0/220	1.15	0/336
3	l	0.51	0/220	1.04	0/336
3	m	0.50	0/220	1.01	0/336
3	n	0.55	0/220	1.01	0/336
3	o	0.53	0/220	1.09	0/336
3	p	0.55	0/220	0.97	0/336
3	q	0.49	0/220	1.07	0/336
3	r	0.53	0/220	1.08	0/336
3	s	0.48	0/220	1.11	0/336
4	1	0.49	0/27	0.85	0/38
4	2	0.52	0/27	0.89	0/38
4	3	0.46	0/27	0.84	0/38
4	4	0.45	0/27	0.82	0/38
4	5	0.45	0/27	0.70	0/38
4	6	0.52	0/27	0.83	0/38
4	7	0.49	0/27	0.80	0/38
4	8	0.46	0/27	0.88	0/38
4	t	0.47	0/27	0.92	0/38
4	u	0.50	0/27	0.82	0/38
4	v	0.49	0/27	0.80	0/38
4	w	0.47	0/27	0.85	0/38
4	x	0.42	0/27	0.81	0/38
4	y	0.52	0/27	0.79	0/38
4	z	0.49	0/27	0.89	0/38
All	All	0.53	0/26758	0.84	12/37640 (0.0%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	b	164[B]	A	N1-C6-N6	7.90	123.34	118.60
2	b	165[B]	A	C4'-C3'-C2'	-5.63	96.97	102.60
2	Z	168[B]	A	C4'-C3'-C2'	-5.41	97.19	102.60
3	f	185[B]	U	C4'-C3'-C2'	-5.40	97.20	102.60
2	Y	166[A]	A	C3'-C2'-C1'	-5.35	97.22	101.50
2	Q	164[A]	A	O4'-C1'-N9	5.13	112.31	108.20
2	c	165[B]	A	N1-C6-N6	5.13	121.68	118.60
1	M	95	ARG	NE-CZ-NH2	-5.11	117.75	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	f	187[B]	U	C4'-C3'-C2'	-5.08	97.52	102.60
3	i	185[A]	U	C3'-C2'-C1'	-5.04	97.47	101.50
2	c	166[B]	A	O4'-C1'-N9	5.04	112.23	108.20
2	b	164[B]	A	N9-C4-C5	-5.02	103.79	105.80

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	A	1224	0	1272	13	0
1	B	1201	0	1236	5	0
1	C	1226	0	1263	11	0
1	D	1244	0	1290	20	0
1	E	1215	0	1241	14	0
1	F	1225	0	1250	11	0
1	G	1208	0	1241	8	0
1	H	1222	0	1260	12	0
1	I	1196	0	1217	7	0
1	J	1216	0	1251	14	0
1	K	1221	0	1246	16	0
1	L	1206	0	1233	9	0
1	M	1186	0	1220	15	0
1	N	1220	0	1261	10	0
1	O	1221	0	1264	10	0
2	P	221	0	94	7	0
2	Q	221	0	111	6	0
2	R	221	0	111	8	0
2	S	221	0	111	3	0
2	T	221	0	95	6	0
2	U	221	0	93	5	0
2	V	221	0	111	4	0
2	W	221	0	111	3	0
2	X	221	0	111	8	0
2	Y	221	0	94	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Z	221	0	93	7	0
2	a	221	0	111	0	0
2	b	221	0	111	0	0
2	c	221	0	111	0	0
2	d	221	0	95	0	0
3	e	201	0	83	0	0
3	f	201	0	101	0	0
3	g	201	0	101	0	0
3	h	201	0	101	0	0
3	i	201	0	83	0	0
3	j	201	0	85	0	0
3	k	201	0	101	0	0
3	l	201	0	101	0	0
3	m	201	0	101	0	0
3	n	201	0	85	0	0
3	o	201	0	82	0	0
3	p	201	0	101	0	0
3	q	201	0	101	0	0
3	r	201	0	101	0	0
3	s	201	0	84	0	0
4	1	26	0	10	1	0
4	2	26	0	10	1	0
4	3	26	0	10	2	0
4	4	26	0	10	3	0
4	5	26	0	10	2	0
4	6	26	0	10	5	0
4	7	26	0	10	2	0
4	8	26	0	10	6	0
4	t	26	0	10	0	0
4	u	26	0	10	0	0
4	v	26	0	10	0	0
4	w	26	0	10	0	0
4	x	26	0	10	0	0
4	y	26	0	10	0	0
4	z	26	0	10	0	0
5	A	1	0	0	0	0
5	F	1	0	0	0	0
5	K	1	0	0	0	0
6	C	21	0	0	0	0
6	H	21	0	0	0	0
6	K	21	0	0	0	0
7	E	5	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	1	1	0	0	0	0
8	3	1	0	0	0	0
8	8	1	0	0	0	0
8	A	224	0	0	2	0
8	B	205	0	0	0	0
8	C	204	0	0	5	0
8	D	203	0	0	7	0
8	E	201	0	0	3	0
8	F	209	0	0	3	0
8	G	205	0	0	6	0
8	H	215	0	0	6	0
8	I	213	0	0	1	0
8	J	212	0	0	4	0
8	K	192	0	0	5	0
8	L	226	0	0	2	0
8	M	203	0	0	6	0
8	N	206	0	0	8	0
8	O	209	0	0	3	0
8	P	8	0	0	0	0
8	Q	11	0	0	0	0
8	R	13	0	0	0	0
8	S	12	0	0	0	0
8	T	5	0	0	0	0
8	U	9	0	0	0	0
8	V	16	0	0	1	0
8	W	12	0	0	0	0
8	X	14	0	0	0	0
8	Y	8	0	0	0	0
8	Z	11	0	0	0	0
8	a	11	0	0	0	0
8	b	11	0	0	0	0
8	c	10	0	0	0	0
8	d	6	0	0	0	0
8	e	9	0	0	0	0
8	f	2	0	0	0	0
8	g	3	0	0	0	0
8	h	5	0	0	0	0
8	i	9	0	0	0	0
8	j	9	0	0	0	0
8	k	5	0	0	0	0
8	l	3	0	0	0	0
8	m	5	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	n	5	0	0	0	0
8	o	10	0	0	0	0
8	p	8	0	0	0	0
8	q	2	0	0	0	0
8	r	6	0	0	0	0
8	s	11	0	0	0	0
8	t	1	0	0	0	0
8	v	1	0	0	0	0
All	All	28403	0	21869	228	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 11.

All (228) 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:Z:161[B]:A:O2'	2:Z:162[B]:A:H5'	1.41	1.20
2:T:161[A]:A:O2'	2:T:162[A]:A:H5'	1.46	1.12
2:P:161[A]:A:O2'	2:P:162[A]:A:H5'	1.54	1.07
2:V:161[A]:A:O2'	2:V:162[A]:A:H5'	1.58	1.04
2:Z:161[B]:A:O2'	2:Z:162[B]:A:C5'	2.07	1.01
2:W:161[B]:A:O2'	2:W:162[B]:A:H5'	1.62	0.99
2:R:161[A]:A:O2'	2:R:162[A]:A:H5'	1.63	0.99
2:X:161[A]:A:O2'	2:X:162[A]:A:H5'	1.60	0.98
1:A:157[B]:CYS:SG	1:J:19:VAL:HG11	2.07	0.94
2:U:161[B]:A:O2'	2:U:162[B]:A:H5'	1.67	0.94
2:Q:161[A]:A:O2'	2:Q:162[A]:A:H5'	1.69	0.93
2:S:161[A]:A:O2'	2:S:162[A]:A:H5'	1.70	0.91
2:T:161[A]:A:O2'	2:T:162[A]:A:C5'	2.18	0.91
2:V:161[A]:A:O2'	2:V:162[A]:A:C5'	2.22	0.86
2:R:161[A]:A:O2'	2:R:162[A]:A:C5'	2.24	0.85
2:W:161[B]:A:O2'	2:W:162[B]:A:C5'	2.28	0.82
1:J:101[B]:LYS:HE2	8:J:358[B]:HOH:O	1.80	0.81
2:X:161[A]:A:O2'	2:X:162[A]:A:C5'	2.28	0.81
2:P:161[A]:A:O2'	2:P:162[A]:A:C5'	2.29	0.79
1:A:157[B]:CYS:SG	1:J:19:VAL:CG1	2.70	0.79
2:Y:161[A]:A:O2'	2:Y:162[A]:A:H5'	1.83	0.78
2:Q:161[A]:A:O2'	2:Q:162[A]:A:C5'	2.31	0.78
2:U:161[B]:A:O2'	2:U:162[B]:A:C5'	2.33	0.77
1:H:97[B]:LYS:HE2	8:H:386:HOH:O	1.85	0.77
1:B:157[B]:CYS:SG	1:N:19:VAL:HG11	2.26	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:161[A]:A:O2'	2:S:162[A]:A:C5'	2.34	0.75
1:N:56[B]:PRO:HG3	8:N:321:HOH:O	1.87	0.74
1:O:101[B]:LYS:HE2	8:O:401[B]:HOH:O	1.90	0.70
2:Y:161[A]:A:O2'	2:Y:162[A]:A:C5'	2.41	0.68
1:I:125:ARG:HD2	4:2:195[B]:U:OP3	1.95	0.67
1:D:19:VAL:HG11	1:G:157[B]:CYS:SG	2.34	0.67
2:X:164[A]:A:O2'	2:X:165[A]:A:H5'	1.95	0.67
1:K:49[A]:SER:HB3	8:K:386:HOH:O	1.95	0.67
2:R:164[A]:A:C2'	2:R:165[A]:A:H5'	2.24	0.66
1:E:19:VAL:HG11	1:K:157[B]:CYS:SG	2.35	0.66
1:D:101[B]:LYS:HD2	8:D:397[B]:HOH:O	1.95	0.66
1:I:19:VAL:HG11	1:L:157[B]:CYS:SG	2.36	0.65
2:T:164[A]:A:C2'	2:T:165[A]:A:H5'	2.28	0.64
2:Y:169[A]:A:H5"	4:4:195[A]:U:H5"	1.79	0.64
1:F:57:VAL:HG11	1:F:134[B]:THR:HG23	1.80	0.63
1:F:157[B]:CYS:SG	1:O:19:VAL:HG11	2.38	0.63
2:Q:168[A]:A:O2'	2:Q:169[A]:A:H5'	1.99	0.63
1:M:118[B]:THR:HG21	8:N:306[B]:HOH:O	1.98	0.63
1:H:101[B]:LYS:HD3	8:H:508[B]:HOH:O	1.97	0.62
1:N:49[B]:SER:HB2	8:N:279:HOH:O	1.99	0.62
1:O:125:ARG:HD2	4:8:195[A]:U:OP3	1.99	0.61
1:J:125:ARG:HD2	4:3:195[B]:U:OP3	2.00	0.61
1:M:125:ARG:HD2	4:6:195[A]:U:OP3	2.01	0.60
1:N:125:ARG:HD2	4:7:195[A]:U:OP3	2.01	0.60
1:B:101[B]:LYS:HZ2	1:B:134:THR:HG22	1.65	0.60
1:E:101[B]:LYS:HE3	8:G:206[B]:HOH:O	2.00	0.60
1:D:101[B]:LYS:CD	8:D:397[B]:HOH:O	2.49	0.59
1:E:101[B]:LYS:CE	8:G:206[B]:HOH:O	2.50	0.59
8:L:382[A]:HOH:O	4:5:196[A]:U:C5'	2.51	0.59
1:F:54:LYS:O	1:F:56[B]:PRO:HD3	2.02	0.59
2:R:164[A]:A:O2'	2:R:165[A]:A:H5'	2.03	0.58
2:P:169[A]:A:H5"	4:8:195[A]:U:C5'	2.33	0.58
1:E:54:LYS:O	1:E:56[B]:PRO:HD3	2.02	0.58
2:T:164[A]:A:H2'	2:T:165[A]:A:H5'	1.85	0.58
2:R:164[A]:A:H2'	2:R:165[A]:A:H5'	1.86	0.57
1:B:157[B]:CYS:SG	1:N:19:VAL:CG1	2.92	0.57
8:J:270:HOH:O	1:K:128[B]:THR:HG22	2.03	0.57
2:P:169[A]:A:H5"	4:8:195[A]:U:H5"	1.87	0.57
2:T:168[A]:A:O2'	2:T:169[A]:A:H5'	2.04	0.56
2:X:164[A]:A:C2'	2:X:165[A]:A:H5'	2.35	0.56
1:E:53:PHE:HB3	1:E:143[B]:VAL:CG1	2.35	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:101[B]:LYS:NZ	8:D:397[B]:HOH:O	2.37	0.56
1:H:101[B]:LYS:CD	8:H:508[B]:HOH:O	2.53	0.56
1:L:125:ARG:HD2	4:5:195[A]:U:OP3	2.04	0.56
1:J:54:LYS:O	1:J:56[B]:PRO:HD3	2.05	0.55
1:K:34:THR:N	1:K:35[B]:PRO:HD3	2.21	0.55
1:K:125:ARG:HD2	4:4:195[A]:U:OP3	2.07	0.55
1:A:53:PHE:HB3	1:A:143[B]:VAL:CG1	2.37	0.55
1:D:49[B]:SER:HB3	8:D:279:HOH:O	2.07	0.55
1:D:54:LYS:O	1:D:56[B]:PRO:HD3	2.06	0.55
1:C:101[B]:LYS:HD2	8:C:492[B]:HOH:O	2.07	0.55
1:M:101[B]:LYS:HE3	8:M:398[B]:HOH:O	2.06	0.55
1:M:118[B]:THR:CG2	8:N:306[B]:HOH:O	2.55	0.54
1:H:53:PHE:HB3	1:H:143[B]:VAL:CG1	2.38	0.53
2:Y:169[A]:A:H5"	4:4:195[A]:U:C5'	2.38	0.53
1:L:79[A]:ARG:NH2	8:L:360:HOH:O	2.38	0.53
1:D:19:VAL:CG1	1:G:157[B]:CYS:SG	2.96	0.53
1:D:49[A]:SER:HB2	8:D:279:HOH:O	2.08	0.53
1:H:97[B]:LYS:CE	8:H:386:HOH:O	2.50	0.53
2:X:163[A]:A:C2'	2:X:164[A]:A:H5'	2.39	0.53
1:I:19:VAL:CG1	1:L:157[B]:CYS:SG	2.97	0.53
2:Y:168[A]:A:C2'	2:Y:169[A]:A:H5'	2.38	0.53
1:F:101[B]:LYS:NZ	8:F:500[B]:HOH:O	2.41	0.53
1:H:125:ARG:HD2	4:1:195[A]:U:OP3	2.08	0.53
1:C:81:TRP:CD1	1:C:121:SER:HB3	2.44	0.52
2:Q:165[A]:A:O5'	2:Q:165[A]:A:H8	1.92	0.52
1:D:81:TRP:CD1	1:D:121:SER:HB3	2.45	0.52
1:M:101[B]:LYS:CE	8:M:398[B]:HOH:O	2.58	0.52
1:L:81:TRP:CD1	1:L:121:SER:HB3	2.44	0.52
8:M:382[A]:HOH:O	4:6:196[A]:U:C5'	2.57	0.52
1:E:101[B]:LYS:HD3	8:G:206[B]:HOH:O	2.09	0.51
1:N:49[A]:SER:HB3	8:N:279:HOH:O	2.10	0.51
2:Q:168[A]:A:C2'	2:Q:169[A]:A:H5'	2.40	0.51
2:U:163[B]:A:C2'	2:U:164[B]:A:H5'	2.40	0.51
1:N:79[B]:ARG:HD2	8:N:267:HOH:O	2.10	0.51
8:O:207:HOH:O	4:8:196[A]:U:C5'	2.58	0.51
2:P:169[A]:A:H5"	4:8:195[A]:U:O5'	2.11	0.51
1:J:53:PHE:HB3	1:J:143[B]:VAL:CG1	2.41	0.51
1:M:101[B]:LYS:HD3	8:M:398[B]:HOH:O	2.12	0.50
1:A:56[B]:PRO:HG3	8:A:416:HOH:O	2.11	0.50
1:E:128[B]:THR:HG22	8:F:381:HOH:O	2.11	0.50
1:A:148:ARG:HD2	8:A:485:HOH:O	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:140[B]:VAL:HG13	1:C:141:CYS:N	2.26	0.50
1:C:49[B]:SER:HB2	8:C:379:HOH:O	2.12	0.49
1:C:47[B]:VAL:CG2	1:C:147:CYS:O	2.60	0.49
1:E:47[B]:VAL:CG2	1:E:147:CYS:O	2.61	0.49
2:P:166[A]:A:O2'	2:P:167[A]:A:H5'	2.12	0.49
1:H:101[B]:LYS:CE	8:H:508[B]:HOH:O	2.61	0.49
1:E:101[B]:LYS:CD	8:G:206[B]:HOH:O	2.59	0.49
1:O:81:TRP:CD1	1:O:121:SER:HB3	2.48	0.49
1:C:55:VAL:HB	1:C:140[B]:VAL:CG1	2.43	0.48
1:J:81:TRP:CD1	1:J:121:SER:HB3	2.47	0.48
1:A:30:LYS:HB2	1:J:22[B]:MET:SD	2.54	0.48
1:M:101[B]:LYS:CD	8:M:398[B]:HOH:O	2.60	0.48
1:F:98:PRO:HD2	1:F:105[B]:SER:OG	2.14	0.48
2:R:168[A]:A:C2'	2:R:169[A]:A:H5'	2.44	0.48
1:C:101[B]:LYS:CD	8:C:492[B]:HOH:O	2.60	0.47
2:R:168[A]:A:O2'	2:R:169[A]:A:H5'	2.13	0.47
1:G:81:TRP:CD1	1:G:121:SER:HB3	2.49	0.47
1:A:98:PRO:HD2	1:A:105[B]:SER:OG	2.15	0.47
2:Y:168[A]:A:O2'	2:Y:169[A]:A:H5'	2.14	0.47
2:T:168[A]:A:C2'	2:T:169[A]:A:H5'	2.45	0.47
1:G:53:PHE:HB3	1:G:143[B]:VAL:CG1	2.44	0.47
1:H:101[B]:LYS:HE3	8:H:508[B]:HOH:O	2.15	0.47
1:E:97[A]:LYS:HE3	8:E:384:HOH:O	2.15	0.47
1:F:53:PHE:HB3	1:F:143[B]:VAL:HG13	1.97	0.47
1:K:56[B]:PRO:HG3	8:K:419:HOH:O	2.15	0.47
1:A:81:TRP:CD1	1:A:121:SER:HB3	2.50	0.47
1:D:80:ALA:HB2	1:D:152[B]:LEU:CD1	2.44	0.46
2:S:168[A]:A:O2'	2:S:169[A]:A:H5'	2.15	0.46
2:U:163[B]:A:O2'	2:U:164[B]:A:H5'	2.15	0.46
1:K:97[B]:LYS:NZ	8:K:462:HOH:O	2.47	0.46
1:J:47[B]:VAL:CG2	1:J:147:CYS:O	2.64	0.46
1:M:125:ARG:CD	4:6:195[A]:U:OP3	2.64	0.46
1:E:19:VAL:CG1	1:K:157[B]:CYS:SG	3.02	0.46
1:F:45:VAL:O	1:F:149[B]:GLN:HG3	2.16	0.46
1:F:47[B]:VAL:CG2	1:F:147:CYS:O	2.64	0.46
2:V:161[A]:A:HO2'	2:V:162[A]:A:C5'	2.27	0.46
1:H:47[B]:VAL:CG2	1:H:147:CYS:O	2.63	0.46
1:H:128[B]:THR:HG23	1:H:129:ASN:N	2.31	0.46
1:D:101[D]:LYS:HE3	8:D:273:HOH:O	2.16	0.46
1:E:49[A]:SER:HB3	8:E:379:HOH:O	2.15	0.45
1:I:53:PHE:HB3	1:I:143[B]:VAL:CG1	2.46	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:44:GLU:HB3	1:K:149[B]:GLN:HE21	1.81	0.45
1:D:34:THR:N	1:D:35[B]:PRO:HD3	2.31	0.45
2:X:164[A]:A:H2'	2:X:165[A]:A:H5'	1.97	0.45
1:O:53:PHE:HB3	1:O:143[B]:VAL:CG1	2.46	0.45
1:C:101[B]:LYS:NZ	8:C:492[B]:HOH:O	2.49	0.45
1:D:53:PHE:HB3	1:D:143[B]:VAL:CG1	2.46	0.45
1:J:101[B]:LYS:HZ3	1:J:134:THR:HG22	1.81	0.45
1:C:34:THR:N	1:C:35[B]:PRO:HD3	2.32	0.45
1:F:157[B]:CYS:SG	1:O:19:VAL:CG1	3.05	0.44
1:K:33:PRO:C	1:K:35[B]:PRO:HD3	2.37	0.44
1:M:101[A]:LYS:HG2	8:M:271:HOH:O	2.17	0.44
1:G:49[B]:SER:HB2	8:G:284[B]:HOH:O	2.18	0.44
8:N:341:HOH:O	1:O:108:GLU:HG3	2.18	0.44
1:D:101[C]:LYS:HZ2	1:D:134:THR:HG22	1.81	0.44
1:E:98:PRO:HD2	1:E:105[B]:SER:OG	2.18	0.44
1:I:98:PRO:HD2	1:I:105[B]:SER:OG	2.17	0.44
2:R:161[A]:A:C2'	2:R:162[A]:A:O5'	2.65	0.44
1:A:115:ASN:HB3	1:A:118[B]:THR:CG2	2.47	0.44
1:M:53:PHE:HB3	1:M:143[B]:VAL:CG1	2.47	0.44
1:F:53:PHE:HB3	1:F:143[B]:VAL:CG1	2.48	0.44
1:K:84:LEU:HD11	1:K:149[A]:GLN:HE21	1.82	0.44
2:Z:161[B]:A:C2'	2:Z:162[B]:A:O5'	2.66	0.44
1:O:56[B]:PRO:HG3	8:O:333:HOH:O	2.16	0.44
1:G:49[A]:SER:HB3	8:G:262[A]:HOH:O	2.18	0.43
2:W:168[B]:A:O2'	2:W:169[B]:A:H5'	2.18	0.43
2:X:161[A]:A:HO2'	2:X:162[A]:A:C5'	2.29	0.43
1:B:81:TRP:CD1	1:B:121:SER:HB3	2.53	0.43
1:K:47[B]:VAL:CG2	1:K:147:CYS:O	2.67	0.43
1:L:128[B]:THR:HG23	1:L:129:ASN:N	2.33	0.43
1:K:81:TRP:CD1	1:K:121:SER:HB3	2.53	0.43
1:N:101[B]:LYS:HD2	8:N:392[B]:HOH:O	2.17	0.43
1:M:125:ARG:HG3	4:6:195[A]:U:OP3	2.19	0.43
1:N:81:TRP:CD1	1:N:121:SER:HB3	2.53	0.43
1:D:47[B]:VAL:HG23	1:D:147:CYS:O	2.19	0.43
1:D:101[D]:LYS:HE3	1:D:138:ASP:OD2	2.19	0.43
2:U:164[B]:A:H2'	2:U:165[B]:A:H8	1.83	0.43
1:M:53:PHE:HB3	1:M:143[B]:VAL:HG12	2.00	0.43
1:E:55:VAL:O	1:E:140[B]:VAL:HG12	2.19	0.43
1:L:98:PRO:HD2	1:L:105[B]:SER:OG	2.18	0.43
8:C:440:HOH:O	1:D:108:GLU:HG3	2.18	0.42
1:F:101[B]:LYS:HD2	8:F:500[B]:HOH:O	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:166[A]:A:C2'	2:Y:167[A]:A:H5'	2.48	0.42
1:A:157[B]:CYS:SG	1:J:19:VAL:HG13	2.55	0.42
1:C:55:VAL:HB	1:C:140[B]:VAL:HG12	2.01	0.42
1:I:128[B]:THR:HG23	1:I:129:ASN:N	2.35	0.42
2:Z:168[B]:A:C2'	2:Z:169[B]:A:H5'	2.50	0.42
1:J:88[B]:VAL:HG22	8:J:395[B]:HOH:O	2.20	0.42
8:J:408:HOH:O	1:L:108:GLU:HG3	2.19	0.42
1:J:79[B]:ARG:NH2	2:Z:169[B]:A:OP1	2.52	0.42
2:P:169[A]:A:C5'	4:8:195[A]:U:O5'	2.68	0.42
1:K:149[B]:GLN:NE2	8:K:374:HOH:O	2.49	0.42
1:M:125:ARG:CG	4:6:195[A]:U:OP3	2.68	0.42
2:V:168[A]:A:N7	8:V:207:HOH:O	2.37	0.42
2:Q:166[A]:A:O2'	2:Q:167[A]:A:H5'	2.20	0.41
8:E:496:HOH:O	1:G:108:GLU:HG3	2.20	0.41
4:3:195[B]:U:H5"	2:Z:169[B]:A:H5"	2.02	0.41
1:G:47[B]:VAL:CG2	1:G:147:CYS:O	2.69	0.41
4:7:195[A]:U:H6	4:7:195[A]:U:H5'	1.86	0.41
2:Y:166[A]:A:H2'	2:Y:167[A]:A:H5'	2.02	0.41
1:M:22[B]:MET:HG2	1:M:23:ILE:N	2.36	0.41
2:X:163[A]:A:H2'	2:X:164[A]:A:H5'	2.02	0.41
1:L:53:PHE:HB3	1:L:143[B]:VAL:CG1	2.51	0.41
1:C:33:PRO:C	1:C:35[B]:PRO:HD3	2.41	0.41
1:J:98:PRO:HD2	1:J:105[B]:SER:OG	2.20	0.41
1:D:55:VAL:O	1:D:140[B]:VAL:HG12	2.21	0.41
1:K:79[A]:ARG:NH2	8:K:444:HOH:O	2.46	0.41
1:M:81:TRP:CD1	1:M:121:SER:HB3	2.55	0.41
1:H:140[B]:VAL:HG13	1:H:141:CYS:N	2.36	0.41
1:A:117:ASN:O	1:B:115:ASN:HA	2.21	0.40
1:D:56[B]:PRO:HG3	8:D:320:HOH:O	2.20	0.40
1:O:47[B]:VAL:CG2	1:O:147:CYS:O	2.69	0.40
1:I:79[B]:ARG:HD2	8:I:354[B]:HOH:O	2.21	0.40
2:Z:161[B]:A:O2'	2:Z:162[B]:A:O5'	2.38	0.40
1:H:53:PHE:HB3	1:H:143[B]:VAL:HG13	2.03	0.40
1:A:53:PHE:HB3	1:A:143[B]:VAL:HG13	2.03	0.40
1:D:128[B]:THR:HG23	1:D:129:ASN:N	2.37	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	163/159 (102%)	158 (97%)	5 (3%)	0	100	100
1	B	159/159 (100%)	154 (97%)	4 (2%)	1 (1%)	25	12
1	C	162/159 (102%)	156 (96%)	6 (4%)	0	100	100
1	D	166/159 (104%)	161 (97%)	4 (2%)	1 (1%)	25	12
1	E	161/159 (101%)	156 (97%)	5 (3%)	0	100	100
1	F	162/159 (102%)	157 (97%)	5 (3%)	0	100	100
1	G	160/159 (101%)	155 (97%)	5 (3%)	0	100	100
1	H	162/159 (102%)	156 (96%)	6 (4%)	0	100	100
1	I	159/159 (100%)	154 (97%)	5 (3%)	0	100	100
1	J	162/159 (102%)	157 (97%)	4 (2%)	1 (1%)	25	12
1	K	163/159 (102%)	158 (97%)	5 (3%)	0	100	100
1	L	160/159 (101%)	155 (97%)	4 (2%)	1 (1%)	25	12
1	M	157/159 (99%)	151 (96%)	5 (3%)	1 (1%)	25	12
1	N	162/159 (102%)	157 (97%)	4 (2%)	1 (1%)	25	12
1	O	163/159 (102%)	157 (96%)	6 (4%)	0	100	100
All	All	2421/2385 (102%)	2342 (97%)	73 (3%)	6 (0%)	41	33

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	42	PRO
1	J	42	PRO
1	N	42	PRO
1	D	42	PRO
1	L	42	PRO
1	M	42	PRO

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	
1	A	149/140 (106%)	149 (100%)	0	100	100
1	B	145/140 (104%)	145 (100%)	0	100	100
1	C	148/140 (106%)	148 (100%)	0	100	100
1	D	152/140 (109%)	152 (100%)	0	100	100
1	E	147/140 (105%)	147 (100%)	0	100	100
1	F	148/140 (106%)	147 (99%)	1 (1%)	84	80
1	G	146/140 (104%)	146 (100%)	0	100	100
1	H	148/140 (106%)	148 (100%)	0	100	100
1	I	145/140 (104%)	145 (100%)	0	100	100
1	J	148/140 (106%)	148 (100%)	0	100	100
1	K	149/140 (106%)	149 (100%)	0	100	100
1	L	146/140 (104%)	146 (100%)	0	100	100
1	M	143/140 (102%)	143 (100%)	0	100	100
1	N	148/140 (106%)	147 (99%)	1 (1%)	84	80
1	O	149/140 (106%)	149 (100%)	0	100	100
All	All	2211/2100 (105%)	2209 (100%)	2 (0%)	93	92

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	152	LEU
1	N	152	LEU

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

Mol	Chain	Res	Type
1	M	18	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	P	9/10 (90%)	0	0
2	Q	9/10 (90%)	1 (11%)	0
2	R	9/10 (90%)	1 (11%)	0
2	S	9/10 (90%)	2 (22%)	0
2	T	9/10 (90%)	1 (11%)	0
2	U	9/10 (90%)	1 (11%)	0
2	V	9/10 (90%)	0	0
2	W	9/10 (90%)	1 (11%)	0
2	X	9/10 (90%)	3 (33%)	0
2	Y	9/10 (90%)	1 (11%)	0
2	Z	9/10 (90%)	2 (22%)	0
2	a	9/10 (90%)	0	0
2	b	9/10 (90%)	1 (11%)	0
2	c	9/10 (90%)	0	0
2	d	9/10 (90%)	2 (22%)	0
3	e	9/10 (90%)	2 (22%)	0
3	f	9/10 (90%)	1 (11%)	0
3	g	9/10 (90%)	1 (11%)	0
3	h	9/10 (90%)	2 (22%)	0
3	i	9/10 (90%)	1 (11%)	0
3	j	9/10 (90%)	1 (11%)	0
3	k	9/10 (90%)	2 (22%)	0
3	l	9/10 (90%)	1 (11%)	0
3	m	9/10 (90%)	3 (33%)	0
3	n	9/10 (90%)	1 (11%)	0
3	o	9/10 (90%)	1 (11%)	0
3	p	9/10 (90%)	1 (11%)	0
3	q	9/10 (90%)	1 (11%)	0
3	r	9/10 (90%)	1 (11%)	0
3	s	9/10 (90%)	2 (22%)	0
4	1	0/2	-	-
4	2	0/2	-	-
4	3	0/2	-	-
4	4	0/2	-	-
4	5	0/2	-	-
4	6	0/2	-	-
4	7	0/2	-	-
4	8	0/2	-	-
4	t	0/2	-	-
4	u	0/2	-	-
4	v	0/2	-	-

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	w	0/2	-	-
4	x	0/2	-	-
4	y	0/2	-	-
4	z	0/2	-	-
All	All	270/330 (81%)	37 (13%)	0

All (37) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	e	183[A]	U
3	e	184[A]	U
2	Q	163[A]	A
3	f	183[B]	U
2	R	165[A]	A
3	g	183[A]	U
2	S	165[A]	A
2	S	167[A]	A
3	h	183[A]	U
3	h	184[A]	U
2	T	165[A]	A
3	i	183[A]	U
2	U	164[B]	A
3	j	183[B]	U
3	k	183[B]	U
3	k	184[B]	U
2	W	165[B]	A
3	l	183[B]	U
2	X	163[A]	A
2	X	164[A]	A
2	X	167[A]	A
3	m	183[A]	U
3	m	184[A]	U
3	m	186[A]	U
2	Y	166[A]	A
3	n	183[A]	U
2	Z	165[B]	A
2	Z	167[B]	A
3	o	183[B]	U
3	p	183[B]	U
2	b	163[B]	A
3	q	183[B]	U
3	r	183[B]	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	d	163[B]	A
2	d	166[B]	A
3	s	183[B]	U
3	s	188[B]	U

There are no RNA pucker outliers to report.

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 19 ligands modelled in this entry, 3 are monoatomic - leaving 16 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	$\#\|Z\| > 2$
6	PO4	K	201[D]	5	4,4,4	0.90	0	6,6,6	0.53	0
6	PO4	H	201[A]	5	4,4,4	0.96	0	6,6,6	0.51	0
7	SO4	E	201	-	4,4,4	0.14	0	6,6,6	0.06	0
6	PO4	C	201[A]	5	4,4,4	0.96	0	6,6,6	0.48	0
6	PO4	H	201[E]	5	4,4,4	1.02	0	6,6,6	0.35	0
6	PO4	C	201[E]	5	4,4,4	0.97	0	6,6,6	0.41	0
6	PO4	H	201[C]	5	4,4,4	1.01	0	6,6,6	0.25	0
6	PO4	K	201[A]	5	4,4,4	0.87	0	6,6,6	0.59	0
6	PO4	C	201[C]	5	4,4,4	0.95	0	6,6,6	0.70	0
6	PO4	H	201[B]	5	4,4,4	0.98	0	6,6,6	0.50	0
6	PO4	K	201[B]	5	4,4,4	1.02	0	6,6,6	0.40	0
6	PO4	C	201[B]	5	4,4,4	0.91	0	6,6,6	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	PO4	K	201[C]	5	4,4,4	0.97	0	6,6,6	0.31	0
6	PO4	K	201[E]	5	4,4,4	0.91	0	6,6,6	0.45	0
6	PO4	H	201[D]	5	4,4,4	1.01	0	6,6,6	0.64	0
6	PO4	C	201[D]	5	4,4,4	0.97	0	6,6,6	0.43	0

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, 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	A	144/159 (90%)	-0.29	1 (0%) 87 86	15, 18, 31, 78	0
1	B	144/159 (90%)	-0.69	1 (0%) 87 86	15, 20, 34, 79	0
1	C	144/159 (90%)	-0.64	1 (0%) 87 86	15, 20, 34, 77	0
1	D	144/159 (90%)	-0.31	2 (1%) 75 72	14, 18, 32, 78	0
1	E	144/159 (90%)	-0.67	1 (0%) 87 86	15, 19, 32, 77	0
1	F	144/159 (90%)	-0.39	1 (0%) 87 86	14, 19, 32, 77	0
1	G	144/159 (90%)	-0.60	2 (1%) 75 72	14, 19, 32, 77	0
1	H	144/159 (90%)	-0.70	0 100 100	15, 19, 33, 77	0
1	I	144/159 (90%)	-0.32	0 100 100	13, 18, 31, 77	0
1	J	144/159 (90%)	-0.65	0 100 100	14, 19, 34, 77	0
1	K	144/159 (90%)	-0.18	1 (0%) 87 86	14, 18, 32, 79	0
1	L	144/159 (90%)	-0.73	0 100 100	15, 20, 33, 77	0
1	M	144/159 (90%)	-0.64	1 (0%) 87 86	14, 19, 32, 78	0
1	N	144/159 (90%)	-0.20	1 (0%) 87 86	14, 19, 32, 78	0
1	O	144/159 (90%)	-0.68	1 (0%) 87 86	14, 19, 33, 77	0
2	P	10/10 (100%)	2.39	4 (40%) 0 0	30, 46, 184, 215	10 (100%)
2	Q	10/10 (100%)	3.09	4 (40%) 0 0	32, 46, 186, 195	10 (100%)
2	R	10/10 (100%)	2.25	4 (40%) 0 0	41, 57, 189, 194	10 (100%)
2	S	10/10 (100%)	2.92	4 (40%) 0 0	42, 54, 190, 194	10 (100%)
2	T	10/10 (100%)	2.47	4 (40%) 0 0	41, 53, 180, 189	10 (100%)
2	U	10/10 (100%)	2.44	4 (40%) 0 0	51, 69, 205, 213	10 (100%)
2	V	10/10 (100%)	2.54	4 (40%) 0 0	40, 50, 196, 215	10 (100%)
2	W	10/10 (100%)	2.24	4 (40%) 0 0	34, 48, 184, 187	10 (100%)
2	X	10/10 (100%)	2.79	4 (40%) 0 0	45, 59, 196, 198	10 (100%)

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
2	Y	10/10 (100%)	2.26	4 (40%)	0	0	30, 48, 174, 185	10 (100%)
2	Z	10/10 (100%)	2.44	4 (40%)	0	0	40, 64, 204, 215	10 (100%)
2	a	10/10 (100%)	2.61	4 (40%)	0	0	24, 45, 181, 208	10 (100%)
2	b	10/10 (100%)	3.09	5 (50%)	0	0	24, 50, 188, 191	10 (100%)
2	c	10/10 (100%)	2.35	4 (40%)	0	0	27, 47, 177, 191	10 (100%)
2	d	10/10 (100%)	2.94	4 (40%)	0	0	50, 68, 204, 218	10 (100%)
3	e	10/10 (100%)	2.53	4 (40%)	0	0	18, 106, 208, 223	10 (100%)
3	f	10/10 (100%)	2.34	4 (40%)	0	0	19, 131, 215, 217	10 (100%)
3	g	10/10 (100%)	2.01	4 (40%)	0	0	20, 111, 227, 244	10 (100%)
3	h	10/10 (100%)	1.50	4 (40%)	0	0	16, 109, 217, 229	10 (100%)
3	i	10/10 (100%)	1.86	4 (40%)	0	0	14, 101, 208, 223	10 (100%)
3	j	10/10 (100%)	1.94	4 (40%)	0	0	15, 120, 203, 214	10 (100%)
3	k	10/10 (100%)	1.98	4 (40%)	0	0	20, 121, 193, 205	10 (100%)
3	l	10/10 (100%)	2.14	4 (40%)	0	0	16, 127, 218, 227	10 (100%)
3	m	10/10 (100%)	2.32	4 (40%)	0	0	41, 135, 233, 255	10 (100%)
3	n	10/10 (100%)	2.15	4 (40%)	0	0	17, 102, 206, 222	10 (100%)
3	o	10/10 (100%)	1.75	4 (40%)	0	0	19, 129, 215, 217	10 (100%)
3	p	10/10 (100%)	1.80	4 (40%)	0	0	21, 139, 231, 232	10 (100%)
3	q	10/10 (100%)	2.07	4 (40%)	0	0	17, 127, 211, 227	10 (100%)
3	r	10/10 (100%)	1.80	4 (40%)	0	0	19, 128, 229, 232	10 (100%)
3	s	10/10 (100%)	1.94	4 (40%)	0	0	18, 137, 207, 245	10 (100%)
4	1	2/2 (100%)	3.34	1 (50%)	0	0	58, 58, 58, 96	2 (100%)
4	2	2/2 (100%)	4.59	1 (50%)	0	0	61, 61, 61, 102	2 (100%)
4	3	2/2 (100%)	2.29	1 (50%)	0	0	58, 58, 58, 90	2 (100%)
4	4	2/2 (100%)	3.32	1 (50%)	0	0	60, 60, 60, 97	2 (100%)
4	5	2/2 (100%)	3.59	1 (50%)	0	0	57, 57, 57, 98	2 (100%)
4	6	2/2 (100%)	3.24	1 (50%)	0	0	58, 58, 58, 92	2 (100%)
4	7	2/2 (100%)	3.07	1 (50%)	0	0	54, 54, 54, 96	2 (100%)
4	8	2/2 (100%)	3.42	1 (50%)	0	0	59, 59, 59, 99	2 (100%)
4	t	2/2 (100%)	4.31	2 (100%)	0	0	60, 60, 60, 93	2 (100%)
4	u	2/2 (100%)	3.15	1 (50%)	0	0	60, 60, 60, 95	2 (100%)

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å^2)	Q<0.9
4	v	2/2 (100%)	3.28	1 (50%)	0	65, 65, 65, 100	2 (100%)
4	w	2/2 (100%)	3.98	2 (100%)	0	59, 59, 59, 91	2 (100%)
4	x	2/2 (100%)	4.23	1 (50%)	0	62, 62, 62, 100	2 (100%)
4	y	2/2 (100%)	4.39	2 (100%)	0	65, 65, 65, 94	2 (100%)
4	z	2/2 (100%)	4.91	2 (100%)	0	62, 62, 62, 98	2 (100%)
All	All	2490/2715 (91%)	-0.12	153 (6%)	21	13, 20, 137, 255	330 (13%)

All (153) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	d	170[B]	A	11.7
2	b	170[B]	A	11.3
2	Q	170[A]	A	10.6
2	a	161[A]	A	10.1
2	Z	170[B]	A	9.4
3	f	190[B]	U	9.2
2	S	161[A]	A	9.2
3	e	190[A]	U	9.1
2	U	161[B]	A	8.9
2	T	170[A]	A	8.7
2	P	161[A]	A	8.7
2	S	170[A]	A	8.5
3	m	190[A]	U	8.5
2	b	161[B]	A	8.4
3	n	190[A]	U	8.2
2	X	170[A]	A	8.1
3	e	181[A]	U	8.1
2	Q	161[A]	A	7.9
2	W	161[B]	A	7.9
2	V	170[A]	A	7.6
2	c	170[B]	A	7.6
2	V	161[A]	A	7.6
3	g	190[A]	U	7.5
2	X	161[A]	A	7.5
2	d	161[B]	A	7.4
2	Y	161[A]	A	7.3
2	Z	161[B]	A	7.3
3	n	181[A]	U	7.3
3	q	190[B]	U	7.2
3	s	181[B]	U	7.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	2	195[B]	U	7.2
4	z	195[A]	U	7.1
3	l	181[B]	U	7.1
2	R	170[A]	A	7.0
2	W	170[B]	A	7.0
2	c	161[B]	A	6.9
2	R	161[A]	A	6.8
3	j	190[B]	U	6.8
4	x	195[B]	U	6.8
3	i	181[A]	U	6.7
2	U	170[B]	A	6.6
2	a	170[A]	A	6.5
2	T	161[A]	A	6.5
3	m	181[A]	U	6.4
4	y	195[A]	U	6.4
4	5	195[A]	U	6.3
3	o	181[B]	U	6.3
3	l	190[B]	U	6.3
3	p	181[B]	U	6.1
3	k	190[B]	U	6.1
3	r	190[B]	U	6.0
4	t	195[B]	U	6.0
3	f	181[B]	U	5.9
3	h	181[A]	U	5.9
2	X	162[A]	A	5.9
3	k	181[B]	U	5.8
4	8	195[A]	U	5.8
3	p	190[B]	U	5.8
3	j	181[B]	U	5.7
3	i	190[A]	U	5.7
2	X	169[A]	A	5.6
3	r	181[B]	U	5.6
2	R	162[A]	A	5.5
2	V	162[A]	A	5.5
2	Q	162[A]	A	5.5
2	Y	162[A]	A	5.5
4	v	195[B]	U	5.5
2	S	162[A]	A	5.5
2	Y	170[A]	A	5.4
2	P	170[A]	A	5.3
2	S	169[A]	A	5.2
4	4	195[A]	U	5.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	6	195[A]	U	5.2
3	g	181[A]	U	5.1
4	w	195[B]	U	5.1
2	U	162[B]	A	5.0
3	q	181[B]	U	4.9
4	7	195[A]	U	4.9
2	a	162[A]	A	4.9
2	d	162[B]	A	4.9
2	Q	169[A]	A	4.9
4	1	195[A]	U	4.7
2	W	162[B]	A	4.7
2	T	169[A]	A	4.7
2	Z	169[B]	A	4.7
3	h	190[A]	U	4.7
3	o	182[B]	U	4.7
4	u	195[A]	U	4.6
3	r	182[B]	U	4.6
2	c	169[B]	A	4.5
2	P	162[A]	A	4.5
2	b	162[B]	A	4.5
3	k	182[B]	U	4.5
3	s	190[B]	U	4.4
2	c	162[B]	A	4.4
4	3	195[B]	U	4.3
3	i	182[A]	U	4.3
2	b	169[B]	A	4.3
3	l	182[B]	U	4.2
3	q	189[B]	U	4.2
2	a	169[A]	A	4.2
3	l	189[B]	U	4.2
2	T	162[A]	A	4.1
3	g	189[A]	U	4.1
2	P	169[A]	A	4.1
3	q	182[B]	U	4.0
3	j	189[B]	U	4.0
1	D	16	ASN	3.9
2	d	169[B]	A	3.9
3	o	190[B]	U	3.9
1	F	16	ASN	3.8
2	U	169[B]	A	3.8
3	f	189[B]	U	3.7
3	e	189[A]	U	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	e	182[A]	U	3.7
3	p	182[B]	U	3.7
2	W	169[B]	A	3.7
1	M	16	ASN	3.6
2	Y	169[A]	A	3.6
2	Z	162[B]	A	3.6
3	n	189[A]	U	3.6
2	V	169[A]	A	3.5
3	f	182[B]	U	3.5
3	m	189[A]	U	3.4
3	j	182[B]	U	3.4
3	s	182[B]	U	3.3
3	s	189[B]	U	3.2
2	R	169[A]	A	3.2
1	B	16	ASN	3.2
3	g	182[A]	U	3.1
1	G	16	ASN	3.1
3	n	182[A]	U	3.1
1	C	16	ASN	2.9
3	k	189[B]	U	2.9
3	h	182[A]	U	2.9
4	w	196[B]	U	2.9
3	m	182[A]	U	2.8
3	p	189[B]	U	2.8
1	K	16	ASN	2.8
4	z	196[A]	U	2.7
3	i	189[A]	U	2.7
4	t	196[B]	U	2.6
1	G	24	ARG	2.5
3	o	189[B]	U	2.5
3	h	189[A]	U	2.5
4	y	196[A]	U	2.4
1	O	16	ASN	2.2
3	r	189[B]	U	2.2
1	N	16	ASN	2.1
1	E	16	ASN	2.1
2	b	163[B]	A	2.0
1	A	16	ASN	2.0
1	D	101[A]	LYS	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
7	SO4	E	201	5/5	0.69	0.52	144,152,154,157	0
5	MG	A	201	1/1	0.91	0.37	63,63,63,63	0
5	MG	K	202	1/1	0.96	0.38	64,64,64,64	0
5	MG	F	201	1/1	0.96	0.24	57,57,57,57	0
6	PO4	C	201[B]	5/5	1.00	0.17	7,10,15,23	4
6	PO4	C	201[C]	5/5	1.00	0.17	8,12,13,15	4
6	PO4	C	201[D]	5/5	1.00	0.17	4,10,21,23	4
6	PO4	C	201[E]	5/5	1.00	0.17	12,15,17,30	4
6	PO4	H	201[A]	5/5	1.00	0.22	6,11,14,19	4
6	PO4	H	201[B]	5/5	1.00	0.22	8,9,16,26	4
6	PO4	H	201[C]	5/5	1.00	0.22	4,10,15,19	4
6	PO4	H	201[D]	5/5	1.00	0.22	7,12,14,18	4
6	PO4	H	201[E]	5/5	1.00	0.22	6,12,14,19	4
6	PO4	K	201[A]	5/5	1.00	0.20	7,10,13,18	4
6	PO4	K	201[B]	5/5	1.00	0.20	4,9,16,18	4
6	PO4	K	201[C]	5/5	1.00	0.20	6,13,14,29	4
6	PO4	K	201[D]	5/5	1.00	0.20	10,11,15,30	4
6	PO4	K	201[E]	5/5	1.00	0.20	4,6,13,19	4
6	PO4	C	201[A]	5/5	1.00	0.17	4,9,21,23	4

6.5 Other polymers (i)

There are no such residues in this entry.