



# Full wwPDB Geometry-Only Validation Report ⓘ

May 29, 2020 – 01:21 am BST

PDB ID : 2TMV  
Title : VISUALIZATION OF PROTEIN-NUCLEIC ACID INTERACTIONS IN A VIRUS. REFINED STRUCTURE OF INTACT TOBACCO MOSAIC VIRUS AT 2.9 ANGSTROMS RESOLUTION BY X-RAY FIBER DIFFRACTION  
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Deposited on : 1988-09-15  
Resolution : 2.90 Å(reported)

This is a Full wwPDB Geometry-Only Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

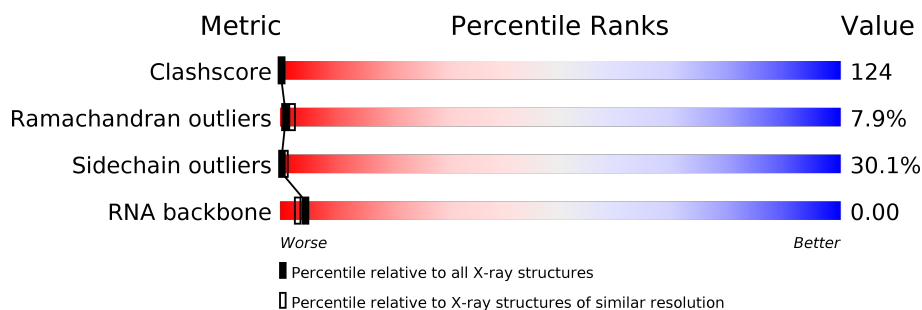
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*FIBER DIFFRACTION*

The reported resolution of this entry is 2.90 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))
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RNA backbone	3102	1007 (3.16-2.64)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	R	3	100%
2	P	158	16% 42% 31% 8% .

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 1354 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called RNA (5'-R(P\*GP\*AP\*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	R	3	Total	C	N	O	P	0	0	0
			67	30	15	19	3			

- Molecule 2 is a protein called TMV COAT PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	154	Total	C	N	O	S	0	0	0
			1212	762	211	238	1			

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	R	1	Total	Ca	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	R	14	Total	O	0	0
			14	14		
4	P	60	Total	O	0	0
			60	60		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

Note EDS was not executed.

- Molecule 1: RNA (5'-R(P\*GP\*AP\*A)-3')

Chain R:  100%

G1  
A2  
A3

- Molecule 2: TMV COAT PROTEIN

Chain P:  16% 42% 31% 8% .

S1 T2 T3 S3 T4 T5 T6 T7 S8 S9 F10 F11 F12 F13 S14 S15 A16 A17 A18 A19 D19 F20 F21 E22 E23 L23 L24 L25 L26 C27 T28 T29 A30 A31 L31 G32 G33 Q34 Q35 F35 Q36 T37 Q38 Q39 A40 A41 T42 T43 V44 Q45 R46 Q47 F48 S49 E50 V51 V52 V53 P54 S55 P56 Q57 V58 V60

R61 F62 P63 D64 S65 D66 K68 V69 R70 R71 Y72 N73 N74 V75 L76 D77 P78 L79 V80 T81 A82 L83 L84 G85 G86 F87 D88 T89 R90 R91 R92 R93 E94 E95 V96 E97 R98 Q99 A100 N101 P102 T103 T104 A105 E106 T107 L108 D109 A110 R113 V114 D115 D116 A117 T118 V119 A120 I121

R122 S123 A124 I125 N126 N127 L128 I129 V130 E131 R134 G135 T136 S138 Y139 N140 R141 S142 S143 F144 S147 S148 G149 L150 V151 W152 T153 S154 GLY PRO ALA THR

## 4 Model quality ⓘ

### 4.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	R	1.22	0/75	3.44	14/115 (12.2%)
2	P	0.83	0/1236	2.23	48/1689 (2.8%)
All	All	0.86	0/1311	2.33	62/1804 (3.4%)

There are no bond length outliers.

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	46	ARG	NE-CZ-NH1	19.99	130.29	120.30
2	P	134	ARG	NE-CZ-NH2	-15.27	112.67	120.30
2	P	134	ARG	NE-CZ-NH1	14.03	127.32	120.30
1	R	1	G	P-O3'-C3'	13.39	135.76	119.70
1	R	2	A	P-O3'-C3'	11.95	134.04	119.70
2	P	66	ASP	CB-CG-OD1	11.23	128.41	118.30
2	P	71	ARG	NE-CZ-NH1	10.57	125.58	120.30
2	P	46	ARG	NE-CZ-NH2	-9.81	115.40	120.30
2	P	152	TRP	CA-CB-CG	9.27	131.31	113.70
2	P	41	ARG	NE-CZ-NH1	9.09	124.84	120.30
2	P	113	ARG	NE-CZ-NH1	8.66	124.63	120.30
2	P	64	ASP	CB-CG-OD1	8.47	125.93	118.30
2	P	134	ARG	CD-NE-CZ	-7.89	112.55	123.60
2	P	67	PHE	CA-CB-CG	7.57	132.06	113.90
2	P	91	ASN	N-CA-CB	7.53	124.16	110.60
2	P	19	ASP	CB-CG-OD1	7.48	125.03	118.30
1	R	2	A	N1-C2-N3	-7.32	125.64	129.30
1	R	2	A	P-O5'-C5'	-7.31	109.20	120.90
2	P	36	GLN	CB-CA-C	7.06	124.52	110.40
2	P	90	ARG	NE-CZ-NH2	6.91	123.75	120.30
2	P	138	SER	N-CA-C	-6.76	92.76	111.00
2	P	47	GLN	N-CA-CB	6.68	122.62	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	41	ARG	NE-CZ-NH2	-6.68	116.96	120.30
2	P	141	ARG	CD-NE-CZ	-6.43	114.59	123.60
2	P	92	ARG	NE-CZ-NH1	6.42	123.51	120.30
2	P	42	THR	N-CA-CB	6.30	122.28	110.30
2	P	67	PHE	CB-CA-C	6.29	122.98	110.40
1	R	2	A	O4'-C1'-N9	6.28	113.22	108.20
1	R	3	A	N1-C2-N3	-6.11	126.25	129.30
1	R	1	G	C5-C6-N1	6.00	114.50	111.50
2	P	88	ASP	CA-CB-CG	5.92	126.43	113.40
1	R	3	A	OP1-P-OP2	-5.87	110.79	119.60
2	P	64	ASP	CB-CG-OD2	-5.80	113.08	118.30
2	P	87	PHE	CA-CB-CG	5.78	127.77	113.90
2	P	92	ARG	N-CA-CB	5.73	120.92	110.60
2	P	33	ASN	CB-CA-C	5.69	121.77	110.40
2	P	88	ASP	CB-CG-OD1	5.66	123.40	118.30
2	P	97	GLU	CA-CB-CG	5.63	125.78	113.40
2	P	74	ALA	CB-CA-C	5.62	118.53	110.10
2	P	66	ASP	CA-CB-CG	5.60	125.72	113.40
2	P	79	LEU	CA-CB-CG	5.53	128.03	115.30
2	P	66	ASP	N-CA-CB	5.50	120.50	110.60
1	R	1	G	OP1-P-OP2	-5.50	111.35	119.60
2	P	42	THR	CA-CB-CG2	5.49	120.09	112.40
2	P	92	ARG	NE-CZ-NH2	-5.46	117.57	120.30
2	P	101	ASN	CB-CA-C	5.46	121.31	110.40
2	P	46	ARG	CD-NE-CZ	5.40	131.16	123.60
2	P	128	LEU	CB-CA-C	5.39	120.45	110.20
2	P	92	ARG	CA-CB-CG	5.36	125.20	113.40
1	R	1	G	C6-N1-C2	-5.32	121.91	125.10
2	P	97	GLU	N-CA-C	-5.31	96.67	111.00
1	R	1	G	O4'-C1'-N9	5.29	112.43	108.20
2	P	14	SER	CA-C-N	-5.28	105.57	117.20
2	P	61	ARG	NE-CZ-NH1	5.24	122.92	120.30
2	P	116	ASP	CB-CG-OD1	5.14	122.93	118.30
2	P	97	GLU	CA-C-N	5.13	128.50	117.20
1	R	3	A	C2'-C3'-O3'	5.11	121.88	113.70
1	R	2	A	C6-N1-C2	5.11	121.67	118.60
2	P	91	ASN	CA-CB-CG	5.08	124.57	113.40
2	P	17	TRP	CA-CB-CG	-5.06	104.08	113.70
2	P	17	TRP	CA-C-N	-5.05	106.09	117.20
1	R	2	A	OP1-P-OP2	-5.04	112.03	119.60

There are no chirality outliers.

There are no planarity outliers.

## 4.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	R	67	0	34	22	0
2	P	1212	0	1191	306	0
3	R	1	0	0	0	0
4	P	60	0	0	25	0
4	R	14	0	0	2	0
All	All	1354	0	1225	310	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 124.

All (310) 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:P:87:PHE:CE2	2:P:121:ILE:HG23	1.80	1.17
2:P:96:VAL:HG13	2:P:100:ALA:HA	1.24	1.13
1:R:1:G:N2	2:P:115:ASP:HB3	1.63	1.11
2:P:79:LEU:HD11	2:P:131:GLU:HG3	1.26	1.11
2:P:18:ALA:HB3	2:P:69:VAL:HB	1.24	1.10
2:P:9:GLN:HG2	2:P:150:LEU:HD23	1.34	1.10
2:P:2:TYR:HB2	2:P:58:VAL:HG13	1.20	1.09
2:P:119:VAL:HG13	2:P:122:ARG:HH22	0.93	1.09
2:P:117:ALA:O	2:P:121:ILE:HG13	1.54	1.08
1:R:1:G:H21	2:P:115:ASP:HB3	1.17	1.07
2:P:67:PHE:O	2:P:68:LYS:HG2	1.54	1.07
2:P:48:PHE:HB2	4:P:205:HOH:O	1.56	1.05
2:P:90:ARG:HD2	2:P:114:VAL:HG13	1.37	1.05
2:P:87:PHE:HE2	2:P:121:ILE:HG23	0.91	1.04
2:P:64:ASP:HB3	2:P:141:ARG:HH12	1.19	1.03
2:P:96:VAL:HG12	2:P:97:GLU:O	1.62	1.00
2:P:119:VAL:HG13	2:P:122:ARG:NH2	1.79	0.97
2:P:119:VAL:CG1	2:P:122:ARG:HH22	1.77	0.96
2:P:82:ALA:HB2	4:P:197:HOH:O	1.66	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:119:VAL:O	2:P:123:SER:HB2	1.65	0.95
1:R:1:G:C5	2:P:119:VAL:HG22	2.04	0.93
2:P:6:THR:HG22	2:P:7:PRO:HD2	1.48	0.93
2:P:96:VAL:HG13	2:P:100:ALA:CA	1.96	0.93
2:P:23:LEU:HD22	4:P:202:HOH:O	1.68	0.92
2:P:40:ALA:O	2:P:44:VAL:HG23	1.70	0.91
2:P:2:TYR:HB2	2:P:58:VAL:CG1	2.01	0.91
2:P:119:VAL:HA	2:P:122:ARG:HH21	1.35	0.89
2:P:52:TRP:HE1	2:P:71:ARG:HB2	1.38	0.89
2:P:44:VAL:HA	2:P:47:GLN:HG3	1.52	0.89
2:P:55:SER:OG	2:P:56:PRO:HD3	1.73	0.89
2:P:13:LEU:HG	2:P:57:GLN:HA	1.54	0.88
2:P:148:SER:OG	2:P:150:LEU:HD11	1.73	0.88
2:P:80:VAL:HG12	2:P:84:LEU:HD12	1.56	0.88
2:P:79:LEU:CD1	2:P:131:GLU:HG3	2.03	0.88
2:P:130:VAL:HG12	2:P:134:ARG:NH1	1.88	0.87
1:R:2:A:H5'	2:P:119:VAL:CG1	2.05	0.86
2:P:95:GLU:O	2:P:95:GLU:HG3	1.74	0.86
2:P:35:PHE:CD2	2:P:121:ILE:HG21	2.11	0.86
2:P:2:TYR:CB	2:P:58:VAL:HG13	2.06	0.85
2:P:2:TYR:CE2	2:P:13:LEU:HD13	2.12	0.85
2:P:62:PHE:CZ	2:P:68:LYS:HG3	2.12	0.85
2:P:74:ALA:HB1	4:P:194:HOH:O	1.76	0.84
2:P:148:SER:HB2	2:P:150:LEU:HG	1.60	0.84
2:P:41:ARG:HH22	2:P:90:ARG:HG2	1.42	0.83
2:P:87:PHE:HE2	2:P:121:ILE:CG2	1.86	0.82
2:P:64:ASP:HB3	2:P:141:ARG:NH1	1.95	0.82
2:P:9:GLN:HG2	2:P:150:LEU:CD2	2.09	0.82
1:R:2:A:H5'	2:P:119:VAL:HG11	1.61	0.82
2:P:21:ILE:HD11	4:P:182:HOH:O	1.78	0.81
2:P:99:GLN:HG3	2:P:100:ALA:H	1.46	0.81
2:P:24:ILE:HG22	2:P:25:ASN:OD1	1.80	0.81
2:P:13:LEU:CG	2:P:57:GLN:HA	2.11	0.81
2:P:20:PRO:HB3	2:P:67:PHE:CE1	2.16	0.80
2:P:50:GLU:C	2:P:52:TRP:H	1.83	0.80
2:P:40:ALA:O	2:P:44:VAL:CG2	2.30	0.80
2:P:24:ILE:HA	4:P:212:HOH:O	1.80	0.79
2:P:41:ARG:NH2	2:P:90:ARG:HG2	1.97	0.79
1:R:3:A:C8	2:P:113:ARG:HB3	2.17	0.79
2:P:49:SER:O	2:P:52:TRP:HB2	1.81	0.79
2:P:119:VAL:HA	2:P:122:ARG:NH2	1.97	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:121:ILE:O	2:P:125:ILE:HG13	1.84	0.78
2:P:61:ARG:HD2	2:P:152:TRP:CD1	2.20	0.77
2:P:139:TYR:HB3	2:P:143:SER:HB3	1.66	0.77
1:R:1:G:C4	2:P:119:VAL:CG2	2.67	0.77
2:P:77:ASP:HB3	2:P:78:PRO:HD3	1.67	0.77
2:P:55:SER:CB	2:P:56:PRO:HD3	2.14	0.77
2:P:2:TYR:CG	2:P:58:VAL:HA	2.19	0.77
2:P:45:GLN:O	2:P:48:PHE:HB3	1.85	0.77
2:P:2:TYR:H	2:P:58:VAL:HG13	1.51	0.76
2:P:130:VAL:CG1	2:P:134:ARG:NH1	2.49	0.76
2:P:73:ASN:HB3	2:P:76:LEU:HB2	1.67	0.76
2:P:75:VAL:HG12	2:P:131:GLU:OE2	1.85	0.76
1:R:1:G:H1'	4:R:8:HOH:O	1.85	0.76
2:P:34:GLN:O	2:P:37:THR:HG23	1.85	0.76
2:P:126:ASN:HA	2:P:129:ILE:HB	1.66	0.75
2:P:70:TYR:O	2:P:73:ASN:HB2	1.87	0.75
2:P:2:TYR:CE2	2:P:13:LEU:CD1	2.70	0.75
2:P:114:VAL:O	2:P:117:ALA:HB3	1.86	0.74
2:P:103:THR:C	2:P:106:GLU:HG2	2.07	0.74
1:R:3:A:C2	4:R:65:HOH:O	2.41	0.72
2:P:2:TYR:CD1	2:P:58:VAL:HA	2.24	0.72
2:P:12:PHE:CE1	2:P:148:SER:HA	2.23	0.72
2:P:128:LEU:O	2:P:131:GLU:HB2	1.89	0.72
2:P:130:VAL:HG12	4:P:209:HOH:O	1.89	0.72
2:P:130:VAL:CG1	4:P:209:HOH:O	2.38	0.72
2:P:13:LEU:CD1	2:P:57:GLN:HA	2.20	0.71
2:P:13:LEU:HD12	2:P:56:PRO:O	1.90	0.71
2:P:12:PHE:CD1	2:P:148:SER:HB3	2.25	0.71
2:P:17:TRP:CD1	2:P:56:PRO:HD2	2.25	0.71
2:P:48:PHE:CD1	4:P:205:HOH:O	2.44	0.71
2:P:70:TYR:CB	2:P:139:TYR:HE2	2.04	0.70
2:P:60:VAL:HG12	2:P:61:ARG:H	1.56	0.70
2:P:95:GLU:O	2:P:95:GLU:CG	2.37	0.70
1:R:1:G:C5	2:P:119:VAL:CG2	2.75	0.69
2:P:141:ARG:HG2	2:P:142:SER:N	2.07	0.69
2:P:90:ARG:HB2	2:P:114:VAL:HA	1.74	0.69
2:P:103:THR:HA	2:P:106:GLU:HG3	1.74	0.69
2:P:17:TRP:CZ2	2:P:144:PHE:HD1	2.11	0.69
1:R:1:G:H21	2:P:115:ASP:CB	1.99	0.69
2:P:124:ALA:HA	2:P:127:ASN:ND2	2.07	0.69
2:P:141:ARG:CG	2:P:142:SER:N	2.57	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:141:ARG:HG2	2:P:142:SER:H	1.58	0.68
1:R:1:G:C4	2:P:119:VAL:HG21	2.28	0.68
2:P:13:LEU:HD11	2:P:57:GLN:C	2.14	0.68
2:P:69:VAL:CG1	4:P:202:HOH:O	2.41	0.68
2:P:48:PHE:O	2:P:52:TRP:CE3	2.47	0.68
2:P:18:ALA:CB	4:P:202:HOH:O	2.42	0.68
2:P:148:SER:OG	2:P:150:LEU:CD1	2.41	0.67
2:P:144:PHE:O	2:P:147:SER:HB2	1.94	0.67
2:P:34:GLN:O	2:P:40:ALA:HB3	1.95	0.67
2:P:69:VAL:HG11	4:P:202:HOH:O	1.93	0.67
2:P:103:THR:HA	2:P:106:GLU:CG	2.24	0.66
2:P:6:THR:CG2	2:P:7:PRO:HD2	2.26	0.66
2:P:124:ALA:HA	2:P:127:ASN:HD22	1.60	0.65
2:P:17:TRP:CD1	2:P:56:PRO:CD	2.79	0.65
2:P:118:THR:O	2:P:121:ILE:N	2.30	0.65
1:R:1:G:C6	2:P:119:VAL:HG22	2.31	0.65
2:P:60:VAL:HG12	2:P:61:ARG:N	2.11	0.65
1:R:2:A:H5'	2:P:119:VAL:HG12	1.77	0.65
2:P:67:PHE:C	2:P:68:LYS:HG2	2.17	0.65
2:P:73:ASN:CG	2:P:76:LEU:HD12	2.17	0.65
2:P:79:LEU:HD11	2:P:131:GLU:CG	2.16	0.65
2:P:15:SER:OG	2:P:54:PRO:HD3	1.97	0.65
2:P:70:TYR:HB2	2:P:139:TYR:CE2	2.32	0.65
2:P:68:LYS:O	2:P:139:TYR:N	2.30	0.64
2:P:55:SER:CB	2:P:56:PRO:CD	2.75	0.64
2:P:91:ASN:HD21	2:P:114:VAL:HG23	1.61	0.63
2:P:23:LEU:HD12	2:P:51:VAL:HG22	1.79	0.63
2:P:70:TYR:HB2	2:P:139:TYR:HE2	1.61	0.63
2:P:13:LEU:HD21	2:P:58:VAL:HG23	1.81	0.63
2:P:20:PRO:HB3	2:P:67:PHE:HE1	1.62	0.63
2:P:23:LEU:HD12	2:P:51:VAL:CG2	2.29	0.63
2:P:67:PHE:HB2	2:P:139:TYR:O	1.97	0.62
2:P:114:VAL:O	2:P:117:ALA:CB	2.48	0.62
1:R:2:A:C5'	2:P:119:VAL:CG1	2.75	0.62
2:P:2:TYR:H	2:P:58:VAL:CG1	2.12	0.62
2:P:90:ARG:CB	2:P:114:VAL:HA	2.30	0.62
2:P:19:ASP:OD2	2:P:22:GLU:HB2	1.99	0.62
2:P:34:GLN:HB3	2:P:37:THR:CG2	2.29	0.62
2:P:20:PRO:HG3	2:P:67:PHE:CE1	2.35	0.61
2:P:44:VAL:CA	2:P:47:GLN:HG3	2.27	0.61
2:P:76:LEU:O	2:P:80:VAL:HG23	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:48:PHE:O	2:P:52:TRP:CZ3	2.54	0.60
2:P:77:ASP:O	2:P:80:VAL:HB	2.02	0.60
2:P:50:GLU:C	2:P:52:TRP:N	2.55	0.60
2:P:55:SER:OG	2:P:56:PRO:CD	2.49	0.60
2:P:62:PHE:CE1	2:P:68:LYS:HG3	2.36	0.60
2:P:48:PHE:HD1	4:P:205:HOH:O	1.80	0.59
2:P:91:ASN:HB2	2:P:93:ILE:HG22	1.84	0.59
2:P:140:ASN:O	2:P:143:SER:N	2.36	0.59
2:P:23:LEU:CD2	4:P:202:HOH:O	2.39	0.59
2:P:44:VAL:HA	2:P:47:GLN:CG	2.30	0.59
2:P:56:PRO:C	4:P:214:HOH:O	2.41	0.59
2:P:77:ASP:HB3	2:P:78:PRO:CD	2.33	0.59
1:R:3:A:H8	2:P:113:ARG:HB3	1.64	0.58
2:P:90:ARG:CD	2:P:114:VAL:HG13	2.23	0.58
2:P:38:GLN:HA	2:P:41:ARG:HD3	1.84	0.58
1:R:3:A:H5"	1:R:3:A:N3	2.18	0.58
2:P:26:LEU:CD1	2:P:51:VAL:HG21	2.33	0.58
2:P:35:PHE:N	2:P:35:PHE:CD1	2.72	0.58
2:P:131:GLU:HG2	4:P:209:HOH:O	2.04	0.57
2:P:92:ARG:HG3	2:P:92:ARG:O	2.04	0.57
2:P:97:GLU:CB	2:P:100:ALA:O	2.53	0.57
2:P:13:LEU:HD11	2:P:57:GLN:HA	1.86	0.57
2:P:67:PHE:O	2:P:68:LYS:CG	2.42	0.57
2:P:127:ASN:O	2:P:130:VAL:HB	2.04	0.57
2:P:9:GLN:O	2:P:12:PHE:HB2	2.05	0.57
2:P:12:PHE:CG	2:P:148:SER:HB3	2.40	0.57
1:R:1:G:N2	2:P:115:ASP:CB	2.53	0.56
2:P:77:ASP:CB	2:P:78:PRO:HD3	2.35	0.56
2:P:79:LEU:O	2:P:82:ALA:HB3	2.05	0.56
2:P:60:VAL:CG1	2:P:61:ARG:H	2.19	0.56
2:P:27:CYS:HB2	4:P:212:HOH:O	2.06	0.56
2:P:148:SER:HB2	2:P:150:LEU:CG	2.33	0.55
2:P:91:ASN:ND2	2:P:114:VAL:CG2	2.69	0.55
2:P:118:THR:HA	2:P:121:ILE:HD12	1.88	0.55
1:R:2:A:C5'	2:P:119:VAL:HG11	2.34	0.55
2:P:17:TRP:CZ2	2:P:144:PHE:CD1	2.94	0.55
2:P:90:ARG:HH21	2:P:92:ARG:HA	1.72	0.55
2:P:67:PHE:C	2:P:68:LYS:CG	2.74	0.55
2:P:70:TYR:CB	2:P:139:TYR:CE2	2.89	0.55
2:P:47:GLN:O	2:P:51:VAL:HB	2.07	0.54
2:P:2:TYR:N	2:P:58:VAL:HG13	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:1:G:H22	2:P:115:ASP:HB3	1.64	0.54
2:P:128:LEU:O	2:P:131:GLU:N	2.41	0.54
2:P:82:ALA:CB	4:P:197:HOH:O	2.37	0.54
2:P:72:TYR:HA	2:P:77:ASP:HB2	1.89	0.53
2:P:38:GLN:NE2	2:P:38:GLN:C	2.61	0.53
2:P:39:GLN:O	2:P:42:THR:N	2.29	0.53
2:P:81:THR:C	2:P:83:LEU:N	2.57	0.53
2:P:13:LEU:HD11	2:P:57:GLN:CA	2.39	0.53
2:P:81:THR:O	2:P:83:LEU:N	2.42	0.53
2:P:126:ASN:O	2:P:130:VAL:HG23	2.08	0.53
2:P:61:ARG:HD2	2:P:152:TRP:NE1	2.23	0.53
2:P:38:GLN:O	2:P:41:ARG:HG2	2.09	0.53
2:P:97:GLU:O	2:P:98:ASN:C	2.48	0.53
2:P:85:GLY:HA2	2:P:88:ASP:OD1	2.08	0.52
2:P:85:GLY:CA	2:P:88:ASP:OD1	2.57	0.52
2:P:94:ILE:HG22	2:P:96:VAL:CG2	2.40	0.52
2:P:94:ILE:HG22	2:P:96:VAL:HG23	1.92	0.52
2:P:97:GLU:HB2	2:P:101:ASN:OD1	2.10	0.52
2:P:123:SER:HA	4:P:216:HOH:O	2.10	0.52
2:P:91:ASN:HD21	2:P:114:VAL:CG2	2.23	0.52
2:P:119:VAL:CA	2:P:122:ARG:NH2	2.69	0.52
2:P:43:VAL:O	2:P:47:GLN:HG3	2.10	0.51
2:P:70:TYR:HB3	2:P:139:TYR:HE2	1.75	0.51
2:P:114:VAL:O	2:P:117:ALA:N	2.42	0.51
2:P:130:VAL:HB	4:P:209:HOH:O	2.11	0.51
2:P:32:GLY:O	2:P:33:ASN:CG	2.48	0.51
2:P:48:PHE:CE2	2:P:52:TRP:CH2	2.98	0.51
2:P:97:GLU:H	2:P:100:ALA:C	2.14	0.51
2:P:77:ASP:CB	2:P:78:PRO:CD	2.88	0.51
2:P:91:ASN:ND2	2:P:110:ALA:O	2.42	0.51
2:P:25:ASN:O	2:P:29:ASN:CG	2.49	0.51
2:P:38:GLN:HE21	2:P:38:GLN:C	2.14	0.50
2:P:44:VAL:O	2:P:48:PHE:N	2.45	0.50
2:P:103:THR:HA	2:P:106:GLU:HG2	1.93	0.50
2:P:128:LEU:O	2:P:129:ILE:C	2.49	0.50
2:P:94:ILE:HA	4:P:162:HOH:O	2.12	0.50
2:P:144:PHE:CD2	2:P:144:PHE:C	2.86	0.50
2:P:2:TYR:HB2	2:P:58:VAL:CB	2.40	0.50
2:P:20:PRO:CB	2:P:67:PHE:CE1	2.91	0.50
2:P:23:LEU:CD1	2:P:51:VAL:HG22	2.42	0.49
2:P:81:THR:O	2:P:82:ALA:C	2.51	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:48:PHE:O	2:P:48:PHE:CD2	2.65	0.49
2:P:62:PHE:CE2	2:P:141:ARG:N	2.81	0.48
1:R:2:A:C5'	2:P:119:VAL:HG12	2.40	0.48
2:P:24:ILE:HG22	2:P:25:ASN:N	2.29	0.48
2:P:48:PHE:O	2:P:51:VAL:HG12	2.13	0.48
2:P:34:GLN:C	2:P:37:THR:HG23	2.34	0.48
2:P:137:GLY:N	4:P:171:HOH:O	2.46	0.47
2:P:13:LEU:CD2	2:P:58:VAL:HG23	2.44	0.47
2:P:94:ILE:O	2:P:96:VAL:HG23	2.14	0.47
2:P:73:ASN:O	2:P:75:VAL:N	2.47	0.47
2:P:119:VAL:CG1	2:P:122:ARG:NH2	2.58	0.47
2:P:87:PHE:CE2	2:P:121:ILE:CG2	2.73	0.47
2:P:97:GLU:N	2:P:100:ALA:O	2.44	0.47
2:P:125:ILE:HG22	2:P:129:ILE:HD12	1.97	0.47
2:P:1:SER:N	2:P:152:TRP:CZ3	2.67	0.47
2:P:18:ALA:CB	2:P:69:VAL:HB	2.17	0.47
2:P:44:VAL:HG22	2:P:47:GLN:OE1	2.15	0.47
2:P:26:LEU:HD13	2:P:51:VAL:HG21	1.97	0.47
2:P:103:THR:CA	2:P:106:GLU:HG2	2.45	0.47
2:P:83:LEU:HD23	2:P:124:ALA:HB3	1.96	0.47
2:P:17:TRP:CE3	2:P:68:LYS:HB3	2.49	0.47
2:P:109:ASP:HB3	2:P:110:ALA:H	1.58	0.46
2:P:123:SER:O	2:P:127:ASN:ND2	2.48	0.46
2:P:26:LEU:HD12	2:P:51:VAL:HG21	1.96	0.46
1:R:1:G:H8	1:R:1:G:H5''	1.80	0.46
2:P:48:PHE:CZ	2:P:80:VAL:HG13	2.50	0.46
2:P:17:TRP:HD1	2:P:56:PRO:HD2	1.79	0.46
2:P:104:THR:O	2:P:108:LEU:HB3	2.16	0.46
2:P:58:VAL:C	2:P:60:VAL:H	2.17	0.46
2:P:90:ARG:HG3	2:P:91:ASN:H	1.81	0.46
2:P:61:ARG:HG2	2:P:62:PHE:N	2.31	0.46
2:P:143:SER:O	2:P:147:SER:OG	2.34	0.45
2:P:139:TYR:N	2:P:139:TYR:CD2	2.84	0.45
2:P:80:VAL:O	2:P:83:LEU:HB2	2.16	0.45
2:P:48:PHE:CD2	2:P:48:PHE:C	2.89	0.45
2:P:140:ASN:O	2:P:143:SER:CB	2.64	0.45
2:P:27:CYS:O	2:P:30:ALA:HB3	2.16	0.45
2:P:58:VAL:O	2:P:152:TRP:CZ3	2.70	0.45
2:P:20:PRO:CG	2:P:67:PHE:CE1	2.99	0.44
2:P:36:GLN:NE2	2:P:118:THR:OG1	2.37	0.44
2:P:130:VAL:HG12	2:P:134:ARG:CZ	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:97:GLU:HB3	2:P:100:ALA:O	2.17	0.44
2:P:64:ASP:CB	2:P:141:ARG:NH1	2.76	0.44
2:P:5:THR:N	2:P:9:GLN:HE22	2.15	0.44
2:P:46:ARG:HG3	2:P:46:ARG:HH11	1.82	0.44
2:P:91:ASN:ND2	2:P:114:VAL:HG22	2.32	0.44
2:P:99:GLN:HG3	2:P:100:ALA:N	2.24	0.44
2:P:110:ALA:HB3	2:P:113:ARG:HD3	2.00	0.44
2:P:56:PRO:CA	4:P:214:HOH:O	2.66	0.43
2:P:118:THR:O	2:P:119:VAL:C	2.57	0.43
2:P:17:TRP:NE1	2:P:56:PRO:CG	2.81	0.43
2:P:7:PRO:C	2:P:9:GLN:H	2.22	0.43
2:P:13:LEU:CD1	2:P:56:PRO:O	2.61	0.43
2:P:113:ARG:O	2:P:116:ASP:HB2	2.18	0.43
2:P:94:ILE:HG22	2:P:94:ILE:O	2.19	0.43
2:P:134:ARG:NH1	4:P:209:HOH:O	2.51	0.43
2:P:25:ASN:O	2:P:29:ASN:CB	2.67	0.43
2:P:26:LEU:O	2:P:30:ALA:N	2.48	0.42
2:P:25:ASN:O	2:P:29:ASN:ND2	2.52	0.42
2:P:1:SER:C	2:P:152:TRP:CZ3	2.92	0.42
2:P:148:SER:CB	2:P:150:LEU:HD11	2.49	0.42
2:P:1:SER:C	2:P:152:TRP:HZ3	2.23	0.42
2:P:34:GLN:C	2:P:36:GLN:H	2.22	0.42
2:P:83:LEU:HD12	2:P:128:LEU:CD1	2.49	0.42
2:P:17:TRP:CE3	2:P:68:LYS:CB	3.03	0.42
2:P:141:ARG:C	2:P:143:SER:N	2.73	0.41
2:P:35:PHE:C	2:P:36:GLN:HG2	2.41	0.41
2:P:90:ARG:HD2	2:P:114:VAL:CG1	2.28	0.41
2:P:73:ASN:C	2:P:75:VAL:N	2.74	0.41
2:P:140:ASN:O	2:P:143:SER:CA	2.69	0.41
2:P:101:ASN:O	2:P:104:THR:OG1	2.30	0.41
2:P:62:PHE:CD2	2:P:141:ARG:HA	2.55	0.41
2:P:38:GLN:NE2	2:P:38:GLN:O	2.54	0.41
2:P:108:LEU:C	2:P:108:LEU:HD13	2.41	0.41
2:P:37:THR:C	2:P:39:GLN:N	2.72	0.41
2:P:94:ILE:CG2	2:P:96:VAL:CG2	2.99	0.41
2:P:76:LEU:O	2:P:77:ASP:C	2.60	0.40
2:P:126:ASN:O	2:P:129:ILE:N	2.54	0.40
2:P:130:VAL:CB	4:P:209:HOH:O	2.64	0.40
2:P:80:VAL:CG1	2:P:84:LEU:HD12	2.37	0.40
2:P:87:PHE:CD2	2:P:121:ILE:HG12	2.56	0.40
2:P:31:LEU:HG	2:P:125:ILE:HG21	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:2:TYR:CZ	2:P:13:LEU:CD1	3.05	0.40
2:P:2:TYR:CE2	2:P:150:LEU:HD22	2.56	0.40
2:P:25:ASN:O	2:P:29:ASN:HB2	2.22	0.40
2:P:62:PHE:CD2	2:P:141:ARG:CA	3.04	0.40

There are no symmetry-related clashes.

## 4.3 Torsion angles [i](#)

### 4.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	P	152/158 (96%)	98 (64%)	42 (28%)	12 (8%)	<a href="#">1</a> <a href="#">2</a>

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	P	93	ILE
2	P	121	ILE
2	P	137	GLY
2	P	74	ALA
2	P	40	ALA
2	P	55	SER
2	P	91	ASN
2	P	102	PRO
2	P	104	THR
2	P	77	ASP
2	P	125	ILE
2	P	51	VAL

### 4.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	P	136/138 (99%)	95 (70%)	41 (30%)	<b>0</b> <b>1</b>

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	P	2	TYR
2	P	3	SER
2	P	5	THR
2	P	6	THR
2	P	9	GLN
2	P	10	PHE
2	P	15	SER
2	P	21	ILE
2	P	24	ILE
2	P	26	LEU
2	P	37	THR
2	P	38	GLN
2	P	39	GLN
2	P	41	ARG
2	P	42	THR
2	P	46	ARG
2	P	47	GLN
2	P	50	GLU
2	P	52	TRP
2	P	55	SER
2	P	61	ARG
2	P	64	ASP
2	P	66	ASP
2	P	90	ARG
2	P	91	ASN
2	P	95	GLU
2	P	97	GLU
2	P	98	ASN
2	P	99	GLN
2	P	103	THR

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Mol	Chain	Res	Type
2	P	108	LEU
2	P	115	ASP
2	P	116	ASP
2	P	122	ARG
2	P	123	SER
2	P	136	THR
2	P	141	ARG
2	P	143	SER
2	P	144	PHE
2	P	148	SER
2	P	150	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	P	9	GLN
2	P	38	GLN
2	P	91	ASN
2	P	127	ASN

#### 4.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	R	3/3 (100%)	2 (66%)	2 (66%)

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	R	2	A
1	R	3	A

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	R	1	G
1	R	2	A

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

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

#### 4.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

#### 4.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is 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.

#### 4.7 Other polymers [i](#)

There are no such residues in this entry.

#### 4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.