



Full wwPDB Geometry-Only Validation Report ⓘ

Mar 17, 2026 – 06:21 PM UTC

PDB ID : 2TMV / pdb_00002tmv
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

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 : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

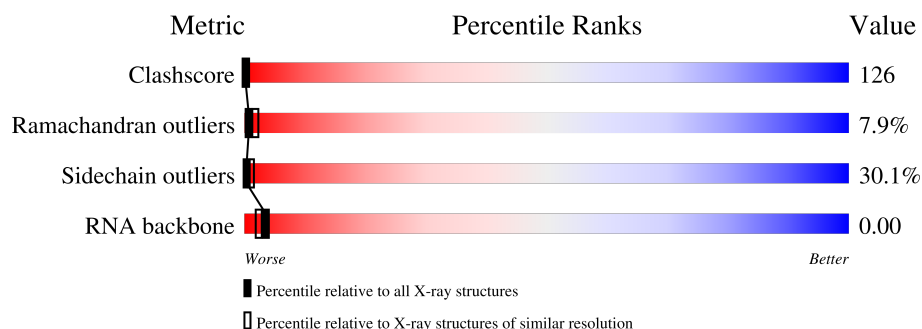
1 Overall quality at a glance

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	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RNA backbone	3983	1120 (3.10-2.70)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	R	3	100%
2	P	158	9% 39% 32% 17% .

2 Entry composition [i](#)

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 (CCD ID: 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, 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. 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.

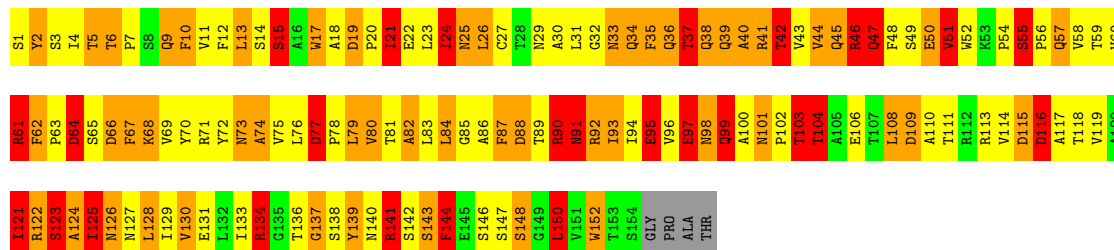
- Molecule 1: RNA (5'-R(P*GP*AP*A)-3')

Chain R:  100%

G1
A2
A3

- Molecule 2: TMV COAT PROTEIN

Chain P:  9% 39% 32% 17%



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	0.99	0/75	2.35	5/115 (4.3%)
2	P	1.04	0/1236	2.79	117/1689 (6.9%)
All	All	1.04	0/1311	2.77	122/1804 (6.8%)

There are no bond length outliers.

All (122) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	67	PHE	CA-CB-CG	18.26	132.06	113.80
2	P	87	PHE	CA-CB-CG	13.97	127.77	113.80
2	P	88	ASP	CA-CB-CG	13.83	126.43	112.60
2	P	66	ASP	CA-CB-CG	13.12	125.72	112.60
2	P	91	ASN	CA-CB-CG	11.97	124.57	112.60
2	P	64	ASP	CA-CB-CG	11.55	124.16	112.60
1	R	1	G	P-O3'-C3'	10.38	135.76	120.20
2	P	47	GLN	N-CA-C	-9.91	99.92	112.90
2	P	109	ASP	CA-CB-CG	9.54	122.14	112.60
2	P	62	PHE	O-C-N	9.35	129.88	121.18
2	P	152	TRP	CA-CB-CG	9.32	131.31	113.60
2	P	89	THR	N-CA-C	9.25	122.74	108.96
1	R	2	A	P-O3'-C3'	9.23	134.04	120.20
2	P	19	ASP	CA-CB-CG	9.09	121.69	112.60
2	P	138	SER	N-CA-C	-9.03	92.76	108.20
2	P	35	PHE	CA-CB-CG	-8.90	104.90	113.80
2	P	97	GLU	N-CA-C	-8.83	96.67	110.36
2	P	46	ARG	NE-CZ-NH1	8.79	130.29	121.50
2	P	134	ARG	CD-NE-CZ	-8.47	112.55	124.40
2	P	36	GLN	CB-CA-C	8.38	124.52	110.44
2	P	97	GLU	CA-C-O	-8.21	111.88	121.82
2	P	47	GLN	N-CA-CB	8.20	122.62	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	17	TRP	CA-C-O	8.10	129.69	120.54
2	P	89	THR	CA-C-O	8.09	130.11	121.45
2	P	111	THR	N-CA-C	-8.09	103.54	113.41
2	P	91	ASN	N-CA-CB	8.09	124.16	110.49
2	P	144	PHE	CA-CB-CG	8.08	121.88	113.80
1	R	2	A	P-O5'-C5'	-7.80	109.20	120.90
2	P	126	ASN	CA-C-O	-7.79	112.29	120.55
2	P	36	GLN	CA-C-O	7.78	127.82	119.34
2	P	80	VAL	N-CA-C	7.74	118.28	110.23
2	P	42	THR	N-CA-CB	7.72	122.28	110.39
2	P	101	ASN	CB-CA-C	7.60	121.31	109.15
2	P	4	ILE	N-CA-C	7.59	114.33	106.21
2	P	77	ASP	O-C-N	7.37	129.79	121.32
2	P	134	ARG	NE-CZ-NH2	-7.26	112.67	119.20
2	P	115	ASP	CA-C-O	7.19	128.25	120.20
2	P	86	ALA	N-CA-C	-7.14	104.71	113.50
2	P	128	LEU	N-CA-C	-7.09	103.24	110.97
2	P	126	ASN	OD1-CG-ND2	7.06	129.66	122.60
2	P	139	TYR	N-CA-C	7.02	120.73	109.79
2	P	141	ARG	CD-NE-CZ	-7.00	114.59	124.40
2	P	124	ALA	N-CA-C	-6.97	104.75	113.18
2	P	14	SER	CA-C-O	6.92	129.69	121.88
2	P	19	ASP	N-CA-C	-6.88	100.82	110.31
2	P	123	SER	N-CA-C	6.75	119.64	111.40
2	P	146	SER	CA-C-O	6.70	127.53	119.43
2	P	130	VAL	CA-C-N	6.69	129.72	120.63
2	P	130	VAL	C-N-CA	6.69	129.72	120.63
2	P	133	ILE	O-C-N	6.61	128.28	121.87
2	P	41	ARG	N-CA-C	-6.56	105.10	113.23
2	P	103	THR	CA-C-N	6.51	133.97	121.54
2	P	103	THR	C-N-CA	6.51	133.97	121.54
2	P	15	SER	N-CA-C	-6.36	101.83	110.68
2	P	57	GLN	OE1-CD-NE2	6.31	128.91	122.60
2	P	34	GLN	CB-CA-C	6.28	119.40	110.24
2	P	90	ARG	CA-C-N	6.28	133.53	121.54
2	P	90	ARG	C-N-CA	6.28	133.53	121.54
2	P	79	LEU	O-C-N	6.26	128.52	122.07
2	P	73	ASN	OD1-CG-ND2	6.25	128.85	122.60
2	P	68	LYS	CA-C-O	6.20	127.75	120.43
2	P	92	ARG	N-CA-CB	6.17	120.92	110.49
2	P	128	LEU	CB-CA-C	6.16	120.45	110.96
2	P	65	SER	CA-CB-OG	6.16	123.42	111.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	126	ASN	N-CA-C	6.11	117.94	111.28
2	P	130	VAL	O-C-N	6.07	128.00	121.94
2	P	104	THR	N-CA-C	6.06	123.71	110.80
2	P	116	ASP	O-C-N	5.97	128.45	122.12
2	P	37	THR	CB-CA-C	5.95	121.46	111.22
2	P	67	PHE	CA-C-O	-5.95	114.02	121.46
2	P	89	THR	CA-C-N	5.91	132.82	121.54
2	P	89	THR	C-N-CA	5.91	132.82	121.54
2	P	128	LEU	N-CA-CB	-5.87	101.33	109.91
2	P	25	ASN	CB-CA-C	5.86	120.08	110.88
2	P	33	ASN	CA-CB-CG	-5.85	106.75	112.60
2	P	97	GLU	CA-CB-CG	5.84	125.78	114.10
2	P	134	ARG	NE-CZ-NH1	5.82	127.32	121.50
2	P	86	ALA	CA-C-O	5.81	125.53	119.14
2	P	21	ILE	O-C-N	5.75	127.86	121.94
2	P	150	LEU	CB-CA-C	5.74	119.19	109.84
2	P	33	ASN	CB-CA-C	5.71	121.77	110.42
2	P	91	ASN	O-C-N	5.66	130.12	122.59
2	P	66	ASP	N-CA-CB	5.66	120.50	111.56
2	P	80	VAL	N-CA-CB	-5.66	104.68	110.62
2	P	51	VAL	CB-CA-C	5.66	120.57	111.29
2	P	79	LEU	CA-C-N	5.64	128.16	120.77
2	P	79	LEU	C-N-CA	5.64	128.16	120.77
2	P	42	THR	CA-CB-CG2	5.64	120.09	110.50
2	P	14	SER	CA-C-N	5.63	130.53	122.08
2	P	14	SER	C-N-CA	5.63	130.53	122.08
2	P	36	GLN	N-CA-C	-5.62	104.64	113.02
2	P	146	SER	N-CA-C	-5.58	106.32	113.02
2	P	11	VAL	CB-CA-C	5.56	120.78	112.16
2	P	24	ILE	CA-C-O	5.56	127.07	121.17
2	P	92	ARG	CA-CB-CG	5.55	125.20	114.10
2	P	95	GLU	CB-CA-C	-5.53	102.98	111.83
2	P	63	PRO	CA-C-N	5.51	132.06	121.54
2	P	63	PRO	C-N-CA	5.51	132.06	121.54
2	P	86	ALA	CA-C-N	5.47	130.71	121.14
2	P	86	ALA	C-N-CA	5.47	130.71	121.14
1	R	3	A	C2'-C3'-O3'	5.45	121.88	113.70
2	P	130	VAL	CB-CA-C	-5.44	104.92	111.88
2	P	125	ILE	CB-CG1-CD1	5.43	125.21	113.80
2	P	61	ARG	CA-C-O	-5.42	115.43	121.23
2	P	64	ASP	CA-C-N	5.37	133.44	122.55
2	P	64	ASP	C-N-CA	5.37	133.44	122.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	63	PRO	CA-C-O	5.35	127.42	121.43
2	P	82	ALA	O-C-N	5.31	129.66	122.59
2	P	57	GLN	CB-CG-CD	-5.26	103.66	112.60
2	P	34	GLN	OE1-CD-NE2	5.25	127.86	122.60
2	P	62	PHE	CA-CB-CG	5.25	119.05	113.80
2	P	99	GLN	CA-C-N	5.24	131.55	121.54
2	P	99	GLN	C-N-CA	5.24	131.55	121.54
2	P	109	ASP	O-C-N	5.23	127.95	122.20
1	R	3	A	P-O5'-C5'	-5.17	113.14	120.90
2	P	59	THR	CA-C-O	5.12	125.55	119.10
2	P	44	VAL	CB-CA-C	5.11	119.04	112.14
2	P	121	ILE	CB-CG1-CD1	5.10	124.51	113.80
2	P	67	PHE	CB-CA-C	5.09	122.98	112.44
2	P	90	ARG	NE-CZ-NH2	5.06	123.75	119.20
2	P	45	GLN	O-C-N	5.01	127.45	122.08
2	P	17	TRP	CA-CB-CG	-5.01	104.08	113.60

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	311	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	315	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 126.

All (315) 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
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:80:VAL:HG12	2:P:84:LEU:HD12	1.56	0.88
2:P:148:SER:OG	2:P:150:LEU:HD11	1.73	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:HG3	2:P:95:GLU:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:148:SER:HB2	2:P:150:LEU:HG	1.60	0.84
2:P:50:GLU:C	2:P:52:TRP:H	1.83	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: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:103:THR:C	2:P:106:GLU:HG2	2.07	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
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
1:R:1:G:C4	2:P:119:VAL:CG2	2.67	0.77
2:P:139:TYR:HB3	2:P:143:SER:HB3	1.66	0.77
2:P:77:ASP:HB3	2:P:78:PRO:HD3	1.67	0.77
2:P:2:TYR:CG	2:P:58:VAL:HA	2.19	0.77
2:P:55:SER:CB	2:P:56:PRO:HD3	2.14	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
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:13:LEU:HD11	2:P:57:GLN:C	2.14	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:12:PHE:CD1	2:P:148:SER:HB3	2.25	0.71
2:P:13:LEU:HD12	2:P:56:PRO:O	1.90	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:73:ASN:CG	2:P:76:LEU:HD12	2.17	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:67:PHE:C	2:P:68:LYS:HG2	2.17	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:17:TRP:CZ2	2:P:144:PHE:HD1	2.11	0.69
2:P:103:THR:HA	2:P:106:GLU:HG3	1.74	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:HG2	2:P:142:SER:H	1.58	0.68
2:P:141:ARG:CG	2:P:142:SER:N	2.57	0.68
1:R:1:G:C4	2:P:119:VAL:HG21	2.28	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:56:PRO:C	4:P:214:HOH:O	2.41	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
1:R:2:A:C5'	2:P:119:VAL:CG1	2.75	0.62
2:P:114:VAL:O	2:P:117:ALA:CB	2.48	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
2:P:50:GLU:C	2:P:52:TRP:N	2.55	0.61
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: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:67:PHE:C	2:P:68:LYS:CG	2.74	0.59
2:P:91:ASN:HB2	2:P:93:ILE:HG22	1.84	0.59
2:P:23:LEU:CD2	4:P:202:HOH:O	2.39	0.59
2:P:140:ASN:O	2:P:143:SER:N	2.36	0.59
2:P:44:VAL:HA	2:P:47:GLN:CG	2.30	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
1:R:3:A:H5''	1:R:3:A:N3	2.18	0.58
2:P:38:GLN:HA	2:P:41:ARG:HD3	1.84	0.58
2:P:90:ARG:CD	2:P:114:VAL:HG13	2.23	0.58
2:P:26:LEU:CD1	2:P:51:VAL:HG21	2.33	0.58
2:P:35:PHE:CD1	2:P:35:PHE:N	2.72	0.58
2:P:92:ARG:O	2:P:92:ARG:HG3	2.04	0.57
2:P:97:GLU:CB	2:P:100:ALA:O	2.53	0.57
2:P:131:GLU:HG2	4:P:209:HOH:O	2.04	0.57
2:P:38:GLN:NE2	2:P:38:GLN:C	2.61	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:97:GLU:O	2:P:98:ASN:C	2.48	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:1:SER:N	2:P:152:TRP:CZ3	2.67	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:32:GLY:O	2:P:33:ASN:CG	2.48	0.56
2:P:60:VAL:CG1	2:P:61:ARG:H	2.19	0.56
2:P:97:GLU:H	2:P:100:ALA:C	2.14	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:25:ASN:O	2:P:29:ASN:CG	2.49	0.55
2:P:91:ASN:ND2	2:P:114:VAL:CG2	2.69	0.55
1:R:2:A:C5'	2:P:119:VAL:HG11	2.34	0.55
2:P:118:THR:HA	2:P:121:ILE:HD12	1.88	0.55
2:P:38:GLN:C	2:P:38:GLN:HE21	2.14	0.55
2:P:81:THR:C	2:P:83:LEU:N	2.57	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:128:LEU:O	2:P:129:ILE:C	2.49	0.55
2:P:70:TYR:CB	2:P:139:TYR:CE2	2.89	0.55
2:P:144:PHE:C	2:P:144:PHE:CD2	2.86	0.54
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
1:R:1:G:H22	2:P:115:ASP:HB3	1.64	0.54
2:P:81:THR:O	2:P:82:ALA:C	2.51	0.54
2:P:82:ALA:CB	4:P:197:HOH:O	2.37	0.54
2:P:128:LEU:O	2:P:131:GLU:N	2.41	0.54
2:P:72:TYR:HA	2:P:77:ASP:HB2	1.89	0.53
2:P:39:GLN:O	2:P:42:THR:N	2.29	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:34:GLN:C	2:P:37:THR:HG23	2.34	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:85:GLY:HA2	2:P:88:ASP:OD1	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:48:PHE:CE2	2:P:52:TRP:CH2	2.98	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: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:94:ILE:HA	4:P:162:HOH:O	2.12	0.50
2:P:58:VAL:C	2:P:60:VAL:H	2.17	0.50
2:P:48:PHE:C	2:P:48:PHE:CD2	2.89	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: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:7:PRO:C	2:P:9:GLN:H	2.22	0.48
2:P:48:PHE:O	2:P:51:VAL:HG12	2.13	0.48
2:P:118:THR:O	2:P:119:VAL:C	2.57	0.48
2:P:34:GLN:C	2:P:36:GLN:H	2.22	0.48
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:137:GLY:N	4:P:171:HOH:O	2.46	0.47
2:P:73:ASN:O	2:P:75:VAL:N	2.47	0.47
2:P:87:PHE:CE2	2:P:121:ILE:CG2	2.73	0.47
2:P:119:VAL:CG1	2:P:122:ARG:NH2	2.58	0.47
2:P:1:SER:C	2:P:152:TRP:CZ3	2.92	0.47
2:P:97:GLU:N	2:P:100:ALA:O	2.44	0.47
2:P:18:ALA:CB	2:P:69:VAL:HB	2.17	0.47
2:P:125:ILE:HG22	2:P:129:ILE:HD12	1.97	0.47
2:P:26:LEU:HD13	2:P:51:VAL:HG21	1.97	0.47
2:P:44:VAL:HG22	2:P:47:GLN:OE1	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:103:THR:CA	2:P:106:GLU:HG2	2.45	0.47
2:P:1:SER:C	2:P:152:TRP:HZ3	2.23	0.47
2:P:17:TRP:CE3	2:P:68:LYS:HB3	2.49	0.47
2:P:83:LEU:HD23	2:P:124:ALA:HB3	1.96	0.47
2:P:24:ILE:HG22	2:P:25:ASN:N	2.29	0.46
2:P:109:ASP:HB3	2:P:110:ALA:H	1.58	0.46
1:R:1:G:H8	1:R:1:G:H5"	1.80	0.46
2:P:26:LEU:HD12	2:P:51:VAL:HG21	1.96	0.46
2:P:123:SER:O	2:P:127:ASN:ND2	2.48	0.46
2:P:17:TRP:HD1	2:P:56:PRO:HD2	1.79	0.46
2:P:48:PHE:CZ	2:P:80:VAL:HG13	2.50	0.46
2:P:35:PHE:C	2:P:36:GLN:HG2	2.41	0.46
2:P:90:ARG:HG3	2:P:91:ASN:H	1.81	0.46
2:P:104:THR:O	2:P:108:LEU:HB3	2.16	0.46
2:P:61:ARG:HG2	2:P:62:PHE:N	2.31	0.46
2:P:108:LEU:HD13	2:P:108:LEU:C	2.41	0.45
2:P:141:ARG:C	2:P:143:SER:N	2.73	0.45
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:76:LEU:O	2:P:77:ASP:C	2.60	0.45
2:P:37:THR:C	2:P:39:GLN:N	2.72	0.45
2:P:27:CYS:O	2:P:30:ALA:HB3	2.16	0.45
2:P:140:ASN:O	2:P:143:SER:CB	2.64	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:75:VAL:HG12	2:P:131:GLU:CD	2.42	0.44
2:P:97:GLU:HB3	2:P:100:ALA:O	2.17	0.44
2:P:130:VAL:HG12	2:P:134:ARG:CZ	2.46	0.44
2:P:5:THR:N	2:P:9:GLN:HE22	2.15	0.44
2:P:64:ASP:CB	2:P:141:ARG:NH1	2.76	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:110:ALA:HB3	2:P:113:ARG:HD3	2.00	0.44
2:P:58:VAL:C	2:P:60:VAL:N	2.73	0.43
2:P:73:ASN:C	2:P:75:VAL:N	2.74	0.43
2:P:17:TRP:NE1	2:P:56:PRO:CG	2.81	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:25:ASN:O	2:P:29:ASN:CB	2.67	0.43
2:P:134:ARG:NH1	4:P:209:HOH:O	2.51	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:148:SER:CB	2:P:150:LEU:HD11	2.49	0.42
2:P:56:PRO:CA	4:P:214:HOH:O	2.66	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:26:LEU:C	2:P:26:LEU:HD23	2.45	0.41
2:P:90:ARG:HD2	2:P:114:VAL:CG1	2.28	0.41
2:P:140:ASN:O	2:P:143:SER:CA	2.69	0.41
2:P:38:GLN:NE2	2:P:38:GLN:O	2.54	0.41
2:P:62:PHE:CD2	2:P:141:ARG:HA	2.55	0.41
2:P:101:ASN:O	2:P:104:THR:OG1	2.30	0.41
2:P:94:ILE:CG2	2:P:96:VAL:CG2	2.99	0.41
2:P:108:LEU:C	2:P:108:LEU:CD1	2.94	0.40
2:P:10:PHE:C	2:P:12:PHE:N	2.78	0.40
2:P:48:PHE:C	2:P:51:VAL:HG12	2.46	0.40
2:P:80:VAL:CG1	2:P:84:LEU:HD12	2.37	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:2:TYR:CE2	2:P:150:LEU:HD22	2.56	0.40
2:P:2:TYR:CZ	2:P:13:LEU:CD1	3.05	0.40
2:P:25:ASN:O	2:P:29:ASN:HB2	2.22	0.40
2:P:31:LEU:HG	2:P:125:ILE:HG21	2.02	0.40
2:P:62:PHE:CD2	2:P:141:ARG:CA	3.04	0.40
2:P:87:PHE:CD2	2:P:121:ILE:HG12	2.56	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%)	1 2

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%)	0 1

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	13	LEU
2	P	15	SER
2	P	21	ILE

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Mol	Chain	Res	Type
2	P	24	ILE
2	P	26	LEU
2	P	37	THR
2	P	38	GLN
2	P	39	GLN
2	P	42	THR
2	P	46	ARG
2	P	47	GLN
2	P	50	GLU
2	P	55	SER
2	P	61	ARG
2	P	64	ASP
2	P	66	ASP
2	P	84	LEU
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
2	P	108	LEU
2	P	116	ASP
2	P	122	ARG
2	P	123	SER
2	P	134	ARG
2	P	136	THR
2	P	141	ARG
2	P	143	SER
2	P	144	PHE
2	P	148	SER
2	P	150	LEU

Sometimes 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 ⓘ

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

4.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

4.6 Ligand geometry ⓘ

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 ⓘ

There are no such residues in this entry.

4.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.