



# Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 09:31 am BST

PDB ID : 2FZ2  
Title : Structure of Turnip Yellow Mosaic Virus at 100 K  
Authors : Larson, S.B.; Lucas, R.W.; McPherson, A.  
Deposited on : 2006-02-08  
Resolution : 2.90 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](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
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

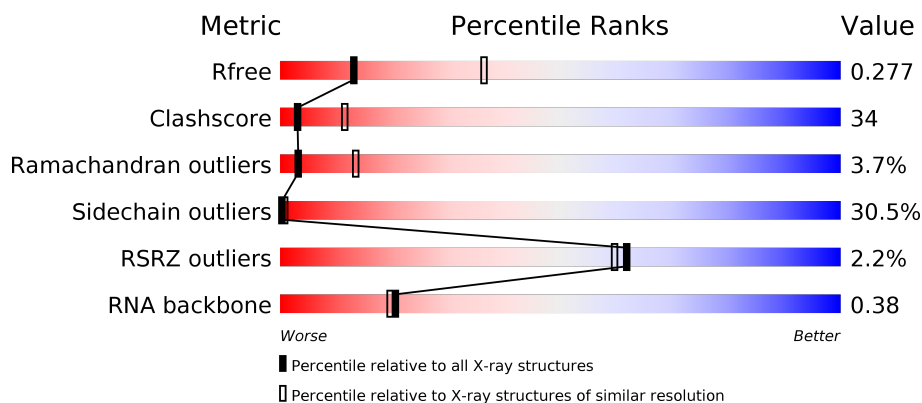
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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))
$R_{free}$	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (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  $\leq 5\%$ . 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	D	3	<div> <div>100%</div> <div> <div>33%</div> <div>67%</div> </div> </div>
2	A	189	<div> <div>3%</div> <div> <div>40%</div> <div>32%</div> <div>14%</div> <div>13%</div> </div> </div>
2	B	189	<div> <div>2%</div> <div> <div>39%</div> <div>44%</div> <div>15%</div> </div> </div>
2	C	189	<div> <div>0%</div> <div> <div>36%</div> <div>48%</div> <div>16%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4122 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 5'-R(\*CP\*CP\*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	3	Total	C	N	O	P	0	0	0
			57	27	9	19	2			

- Molecule 2 is a protein called Coat protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	164	Total	C	N	O	S	0	0	0
			1231	792	195	237	7			
2	B	189	Total	C	N	O	S	6	0	0
			1417	909	225	275	8			
2	C	189	Total	C	N	O	S	0	0	0
			1417	909	225	275	8			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	99	GLN	ASN	VARIANT	UNP P20125
A	123	GLN	ASN	VARIANT	UNP P20125
A	138	GLN	ASN	VARIANT	UNP P20125
B	99	GLN	ASN	VARIANT	UNP P20125
B	123	GLN	ASN	VARIANT	UNP P20125
B	138	GLN	ASN	VARIANT	UNP P20125
C	99	GLN	ASN	VARIANT	UNP P20125
C	123	GLN	ASN	VARIANT	UNP P20125
C	138	GLN	ASN	VARIANT	UNP P20125

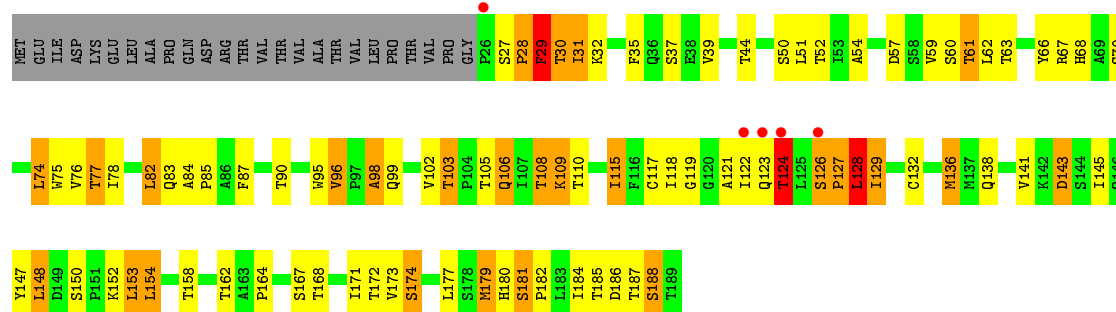
### 3 Residue-property plots [i](#)

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

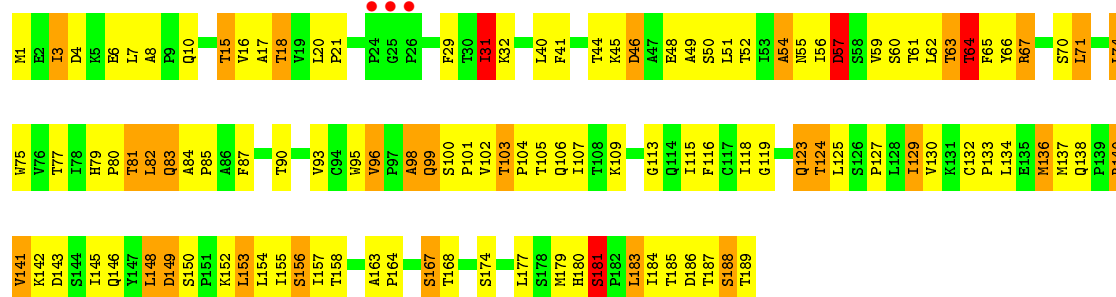
- Molecule 1: 5'-R(\*CP\*CP\*C)-3'



- Molecule 2: Coat protein

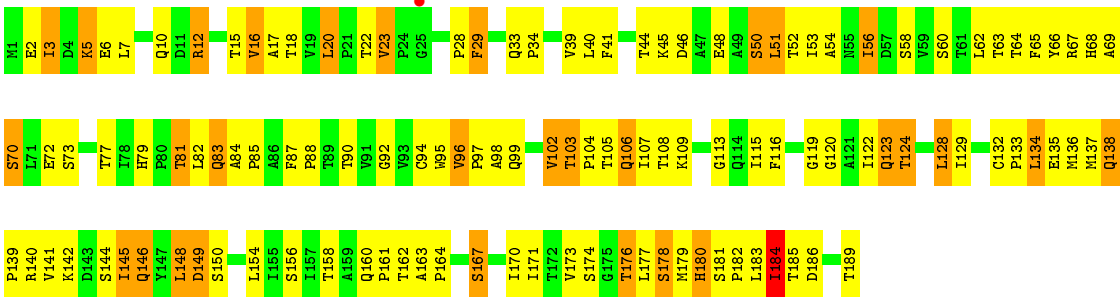


- Molecule 2: Coat protein



- Molecule 2: Coat protein





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	511.53Å 511.53Å 303.76Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	59.12 – 2.90 59.72 – 2.60	Depositor EDS
% Data completeness (in resolution range)	42.8 (59.12-2.90) 32.3 (59.72-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.62 (at 2.61Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.276 , 0.289 0.264 , 0.277	Depositor DCC
$R_{free}$ test set	10857 reflections (4.38%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.3	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 40.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.80	EDS
Total number of atoms	4122	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.70% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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

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	D	0.91	0/62	1.44	3/94 (3.2%)
2	A	0.58	0/1263	0.86	0/1735
2	B	0.57	0/1452	0.85	1/1997 (0.1%)
2	C	0.59	0/1452	0.85	0/1997
All	All	0.59	0/4229	0.86	4/5823 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1	C	O4'-C1'-N1	6.87	113.70	108.20
1	D	1	C	O5'-C5'-C4'	5.43	122.01	111.70
2	B	31	ILE	CB-CA-C	-5.27	101.06	111.60
1	D	1	C	O4'-C4'-C3'	-5.04	98.96	104.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	57	0	35	1	0
2	A	1231	0	1258	80	0
2	B	1417	0	1454	102	0
2	C	1417	0	1454	110	0
All	All	4122	0	4201	281	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 34.

All (281) 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:B:81:THR:HG23	2:B:83:GLN:H	1.16	1.10
2:C:83:GLN:HA	2:C:83:GLN:HE21	1.23	1.00
2:C:102:VAL:HG12	2:C:106:GLN:HG3	1.43	0.98
2:B:153:LEU:HD13	2:B:155:ILE:HD11	1.46	0.97
2:C:81:THR:HG23	2:C:83:GLN:H	1.30	0.93
2:C:145:ILE:HD12	2:C:146:GLN:H	1.34	0.92
2:B:103:THR:H	2:B:106:GLN:HE21	1.14	0.91
2:C:160:GLN:HG3	2:C:161:PRO:HD2	1.52	0.90
2:B:103:THR:HG23	2:B:106:GLN:HG3	1.53	0.88
2:C:123:GLN:HE21	2:C:123:GLN:C	1.79	0.86
2:B:59:VAL:O	2:B:63:THR:HG23	1.76	0.85
2:A:129:ILE:HD13	2:A:129:ILE:H	1.41	0.84
2:C:138:GLN:HE21	2:C:138:GLN:C	1.80	0.84
2:A:30:THR:CG2	2:A:180:HIS:HB3	2.08	0.84
2:C:134:LEU:HD22	2:C:134:LEU:H	1.43	0.84
2:C:138:GLN:HE21	2:C:138:GLN:CA	1.92	0.83
2:A:102:VAL:HG13	2:A:106:GLN:HG3	1.61	0.82
2:B:81:THR:CG2	2:B:83:GLN:H	1.92	0.81
2:A:30:THR:HG23	2:A:180:HIS:HB3	1.61	0.81
2:C:184:ILE:HD12	2:C:184:ILE:H	1.47	0.80
2:B:18:THR:HB	2:C:20:LEU:HB3	1.61	0.79
2:C:88:PRO:HG3	2:C:120:GLY:HA3	1.63	0.79
2:A:124:THR:O	2:A:124:THR:HG23	1.83	0.79
2:C:15:THR:HG22	2:C:136:MET:HB2	1.64	0.78
2:A:98:ALA:HB3	2:A:148:LEU:O	1.84	0.77
2:A:29:PHE:HE2	2:A:181:SER:H	1.33	0.77
2:A:77:THR:HG23	2:A:129:ILE:HG22	1.66	0.76
2:C:119:GLY:H	2:C:124:THR:HB	1.50	0.76
2:A:78:ILE:HB	2:A:128:LEU:HD23	1.68	0.76
2:C:83:GLN:HA	2:C:83:GLN:NE2	2.01	0.74
2:B:153:LEU:CD1	2:B:155:ILE:HD11	2.16	0.74
2:A:84:ALA:HB3	2:A:85:PRO:HD3	1.69	0.74
2:B:16:VAL:HG22	2:B:17:ALA:N	2.03	0.73
2:C:66:TYR:O	2:C:142:LYS:HE2	1.89	0.73
2:C:81:THR:CG2	2:C:83:GLN:H	2.01	0.73
2:C:68:HIS:HB2	2:C:180:HIS:CE1	2.25	0.72
2:B:153:LEU:HD13	2:B:155:ILE:CD1	2.20	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:128:LEU:HD22	2:A:128:LEU:N	2.05	0.72
2:C:40:LEU:HD12	2:C:41:PHE:H	1.55	0.72
2:A:30:THR:HG22	2:A:179:MET:O	1.92	0.70
2:B:138:GLN:HB3	2:B:149:ASP:O	1.92	0.70
2:A:127:PRO:C	2:A:128:LEU:HD22	2.13	0.69
2:B:81:THR:HG23	2:B:82:LEU:N	2.08	0.69
2:A:90:THR:HB	2:A:158:THR:HB	1.75	0.69
2:A:126:SER:O	2:A:128:LEU:N	2.27	0.67
2:A:68:HIS:HD2	2:A:143:ASP:OD1	1.77	0.67
2:C:81:THR:HG23	2:C:82:LEU:N	2.08	0.67
2:C:77:THR:HB	2:C:79:HIS:CE1	2.30	0.67
2:B:102:VAL:HA	2:B:106:GLN:NE2	2.10	0.66
2:B:102:VAL:HG13	2:B:106:GLN:HB2	1.78	0.66
2:B:81:THR:HG21	2:B:167:SER:O	1.96	0.66
2:B:103:THR:H	2:B:106:GLN:NE2	1.92	0.66
2:B:77:THR:HB	2:B:79:HIS:CE1	2.30	0.66
2:C:145:ILE:HD12	2:C:146:GLN:N	2.09	0.65
2:A:103:THR:O	2:A:106:GLN:HG2	1.97	0.65
2:A:186:ASP:OD1	2:A:188:SER:HB3	1.96	0.65
2:B:74:LEU:HD22	2:B:75:TRP:N	2.10	0.65
2:B:71:LEU:HD13	2:B:177:LEU:CD2	2.27	0.64
2:B:81:THR:HG23	2:B:83:GLN:N	2.00	0.64
2:C:81:THR:HG21	2:C:167:SER:O	1.97	0.64
2:A:99:GLN:O	2:A:99:GLN:HG2	1.95	0.64
2:B:83:GLN:HA	2:B:83:GLN:HE21	1.62	0.64
2:B:15:THR:HB	2:C:182:PRO:HD2	1.80	0.64
2:C:40:LEU:HD12	2:C:41:PHE:N	2.12	0.64
2:C:96:VAL:HG22	2:C:97:PRO:HD2	1.80	0.63
2:C:161:PRO:HG2	2:C:162:THR:H	1.64	0.63
2:B:103:THR:N	2:B:106:GLN:HE21	1.92	0.62
2:B:20:LEU:HD12	2:B:20:LEU:O	1.98	0.62
2:B:74:LEU:HD22	2:B:75:TRP:H	1.63	0.62
2:C:99:GLN:OE1	2:C:149:ASP:HB3	1.99	0.62
2:B:61:THR:O	2:B:64:THR:HB	1.98	0.62
2:C:123:GLN:HE21	2:C:124:THR:N	1.96	0.62
2:C:64:THR:O	2:C:65:PHE:HB2	1.98	0.62
2:A:184:ILE:HD12	2:A:184:ILE:H	1.65	0.62
2:B:138:GLN:HB3	2:B:149:ASP:C	2.21	0.61
2:B:66:TYR:O	2:B:142:LYS:HE2	2.01	0.61
2:B:95:TRP:CE2	2:B:132:CYS:HB2	2.36	0.61
2:C:138:GLN:HG3	2:C:149:ASP:OD2	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:163:ALA:HB1	2:B:164:PRO:HD2	1.83	0.61
2:B:154:LEU:C	2:B:155:ILE:HD12	2.20	0.61
2:C:92:GLY:HA2	2:C:115:ILE:HD13	1.83	0.60
2:A:30:THR:HG22	2:A:180:HIS:HB3	1.84	0.60
2:A:77:THR:CG2	2:A:129:ILE:HG22	2.31	0.60
2:B:103:THR:HG22	2:B:106:GLN:NE2	2.16	0.60
2:C:138:GLN:NE2	2:C:138:GLN:CA	2.62	0.60
2:B:32:LYS:HA	2:B:177:LEU:O	2.01	0.60
2:C:138:GLN:HB2	2:C:149:ASP:O	2.00	0.60
2:A:31:ILE:HD12	2:A:31:ILE:O	2.02	0.60
2:C:123:GLN:NE2	2:C:123:GLN:C	2.54	0.59
2:B:71:LEU:HD13	2:B:177:LEU:HD21	1.84	0.59
2:C:95:TRP:CE2	2:C:132:CYS:HB2	2.37	0.59
2:C:104:PRO:O	2:C:107:ILE:HG13	2.02	0.59
2:B:17:ALA:O	2:C:23:VAL:HG13	2.03	0.59
2:C:53:ILE:O	2:C:56:ILE:HG13	2.02	0.59
2:A:39:VAL:HG22	2:A:171:ILE:O	2.02	0.58
2:C:149:ASP:OD2	2:C:149:ASP:N	2.36	0.58
2:C:50:SER:HB3	2:C:154:LEU:CD2	2.32	0.58
2:B:3:ILE:H	2:B:3:ILE:HD12	1.68	0.58
2:B:90:THR:HB	2:B:158:THR:HB	1.85	0.58
2:A:67:ARG:HH12	2:C:17:ALA:HB2	1.68	0.58
2:B:16:VAL:CG2	2:B:17:ALA:N	2.66	0.58
2:A:35:PHE:O	2:A:174:SER:HB3	2.03	0.57
2:A:118:ILE:HD12	2:A:118:ILE:N	2.19	0.57
2:B:18:THR:OG1	2:C:144:SER:HB2	2.04	0.57
2:B:87:PHE:CD1	2:B:164:PRO:HB3	2.40	0.57
2:A:124:THR:O	2:A:124:THR:CG2	2.53	0.56
2:A:153:LEU:HD22	2:A:154:LEU:N	2.19	0.56
2:B:8:ALA:O	2:B:130:VAL:HG22	2.06	0.56
2:C:184:ILE:H	2:C:184:ILE:CD1	2.09	0.55
2:B:84:ALA:N	2:B:85:PRO:HD2	2.21	0.55
2:C:119:GLY:N	2:C:124:THR:HB	2.20	0.55
2:C:97:PRO:HD3	2:C:137:MET:HE1	1.89	0.55
2:C:83:GLN:HE21	2:C:83:GLN:CA	2.04	0.55
2:B:149:ASP:OD2	2:B:149:ASP:N	2.40	0.54
2:C:103:THR:O	2:C:106:GLN:HG2	2.07	0.54
2:A:127:PRO:O	2:A:128:LEU:O	2.25	0.54
2:A:185:THR:HG23	2:A:186:ASP:N	2.22	0.54
2:C:90:THR:HB	2:C:158:THR:HB	1.90	0.53
2:B:81:THR:CG2	2:B:168:THR:HA	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:32:LYS:HA	2:A:177:LEU:O	2.07	0.53
2:A:129:ILE:H	2:A:129:ILE:CD1	2.16	0.53
2:A:109:LYS:HB3	2:B:186:ASP:OD1	2.08	0.53
2:C:77:THR:HG23	2:C:129:ILE:CD1	2.39	0.53
2:C:33:GLN:HB3	2:C:62:LEU:HD13	1.91	0.52
2:B:20:LEU:HB3	2:C:20:LEU:HD11	1.90	0.52
2:C:50:SER:HB3	2:C:154:LEU:HD23	1.90	0.52
2:A:95:TRP:CE2	2:A:132:CYS:HB2	2.43	0.52
2:C:10:GLN:HE22	2:C:95:TRP:H	1.58	0.52
2:A:123:GLN:CD	2:A:123:GLN:O	2.47	0.52
2:B:98:ALA:HA	2:B:152:LYS:HB2	1.92	0.52
2:A:123:GLN:O	2:A:124:THR:HG22	2.10	0.51
2:A:28:PRO:O	2:A:29:PHE:HB3	2.11	0.51
2:A:29:PHE:C	2:A:29:PHE:CD2	2.84	0.51
2:B:185:THR:OG1	2:B:186:ASP:N	2.42	0.51
2:B:16:VAL:HG22	2:B:17:ALA:H	1.73	0.51
2:B:99:GLN:O	2:B:99:GLN:HG2	2.09	0.51
2:B:125:LEU:HD23	2:B:125:LEU:N	2.25	0.51
2:A:50:SER:C	2:A:51:LEU:HD23	2.31	0.51
2:C:87:PHE:CD1	2:C:164:PRO:HB3	2.46	0.51
2:C:77:THR:HG23	2:C:129:ILE:HD13	1.93	0.51
2:B:104:PRO:O	2:B:107:ILE:HG13	2.11	0.50
2:C:185:THR:OG1	2:C:186:ASP:N	2.44	0.50
2:C:69:ALA:O	2:C:141:VAL:HG22	2.11	0.50
2:A:59:VAL:HG12	2:A:60:SER:N	2.25	0.50
2:B:83:GLN:NE2	2:B:83:GLN:HA	2.27	0.50
2:C:29:PHE:HD1	2:C:29:PHE:H	1.56	0.50
2:B:31:ILE:O	2:B:31:ILE:HD12	2.12	0.50
2:C:51:LEU:HD23	2:C:51:LEU:O	2.12	0.50
2:B:66:TYR:N	2:B:66:TYR:CD1	2.80	0.50
2:A:68:HIS:HE1	2:C:16:VAL:O	1.95	0.50
2:C:15:THR:CG2	2:C:136:MET:HB2	2.37	0.49
2:A:76:VAL:O	2:A:129:ILE:HA	2.12	0.49
2:C:29:PHE:CD1	2:C:29:PHE:N	2.77	0.49
2:A:59:VAL:C	2:A:61:THR:N	2.65	0.49
2:B:16:VAL:CG2	2:B:17:ALA:H	2.25	0.49
2:C:163:ALA:HB1	2:C:164:PRO:HD2	1.94	0.49
2:B:124:THR:C	2:B:125:LEU:HD23	2.32	0.49
2:B:15:THR:O	2:B:15:THR:HG23	2.13	0.49
2:C:103:THR:HG23	2:C:106:GLN:CD	2.33	0.49
2:C:138:GLN:HB2	2:C:149:ASP:C	2.33	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:81:THR:HG23	2:C:83:GLN:N	2.13	0.49
2:A:117:CYS:C	2:A:118:ILE:HD12	2.33	0.49
2:A:82:LEU:HD23	2:A:83:GLN:N	2.27	0.49
2:A:103:THR:OG1	2:A:105:THR:HG23	2.13	0.49
2:A:87:PHE:CG	2:A:164:PRO:HB3	2.47	0.49
2:A:128:LEU:N	2:A:128:LEU:CD2	2.76	0.48
2:C:17:ALA:HB1	2:C:138:GLN:HG2	1.95	0.48
2:A:129:ILE:HD13	2:A:129:ILE:N	2.20	0.48
2:A:29:PHE:HZ	2:A:182:PRO:HD3	1.76	0.48
2:B:15:THR:CG2	2:B:136:MET:HG3	2.42	0.48
2:C:63:THR:O	2:C:64:THR:C	2.51	0.48
2:C:95:TRP:CD1	2:C:132:CYS:HA	2.48	0.48
2:A:108:THR:HG23	2:A:115:ILE:HD12	1.96	0.48
2:A:103:THR:HG23	2:A:106:GLN:CD	2.34	0.48
2:A:59:VAL:C	2:A:61:THR:H	2.17	0.48
2:B:4:ASP:O	2:B:127:PRO:HD2	2.14	0.48
2:C:12:ARG:HB3	2:C:136:MET:CE	2.44	0.48
2:C:34:PRO:HA	2:C:176:THR:HA	1.95	0.48
2:A:68:HIS:CD2	2:A:143:ASP:OD1	2.62	0.47
2:B:155:ILE:N	2:B:155:ILE:HD12	2.29	0.47
2:B:77:THR:HG23	2:B:129:ILE:HG22	1.95	0.47
2:B:80:PRO:HG2	2:B:125:LEU:O	2.14	0.47
2:B:71:LEU:HD13	2:B:177:LEU:HD23	1.96	0.47
2:B:96:VAL:HG13	2:B:100:SER:HB3	1.94	0.47
2:C:69:ALA:HA	2:C:178:SER:O	2.15	0.47
2:C:68:HIS:CG	2:C:180:HIS:HE1	2.32	0.47
2:A:143:ASP:HB2	2:A:147:TYR:HE1	1.79	0.47
2:B:81:THR:HG22	2:B:168:THR:HA	1.95	0.47
2:C:84:ALA:N	2:C:85:PRO:CD	2.78	0.47
2:B:59:VAL:O	2:B:60:SER:C	2.51	0.47
2:B:54:ALA:HA	2:B:141:VAL:HG12	1.96	0.47
2:B:6:GLU:C	2:B:7:LEU:HD23	2.35	0.47
2:C:123:GLN:NE2	2:C:123:GLN:CA	2.78	0.47
2:B:46:ASP:N	2:B:46:ASP:OD2	2.48	0.47
2:B:48:GLU:HB3	2:B:104:PRO:HG2	1.96	0.47
2:B:186:ASP:OD1	2:B:188:SER:HB3	2.16	0.46
2:C:64:THR:O	2:C:65:PHE:CB	2.63	0.46
2:A:66:TYR:CD1	2:A:66:TYR:N	2.84	0.46
2:A:87:PHE:CD1	2:A:164:PRO:HB3	2.50	0.46
2:A:29:PHE:CG	2:A:29:PHE:O	2.68	0.46
2:B:99:GLN:HB3	2:B:148:LEU:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:160:GLN:CG	2:C:161:PRO:HD2	2.37	0.46
2:C:134:LEU:CD2	2:C:134:LEU:H	2.20	0.45
2:A:82:LEU:O	2:A:85:PRO:HD2	2.17	0.45
2:B:153:LEU:HD22	2:B:155:ILE:CD1	2.46	0.45
2:B:54:ALA:HA	2:B:141:VAL:CG1	2.46	0.45
2:A:28:PRO:O	2:A:29:PHE:CB	2.64	0.45
2:B:102:VAL:HA	2:B:106:GLN:HE22	1.80	0.45
2:B:20:LEU:HD12	2:B:20:LEU:C	2.35	0.45
2:B:180:HIS:HD2	2:B:181:SER:HB2	1.82	0.45
2:C:103:THR:HG23	2:C:106:GLN:NE2	2.31	0.45
2:C:128:LEU:C	2:C:129:ILE:HG12	2.37	0.45
2:A:54:ALA:HB2	2:A:141:VAL:HB	1.98	0.45
2:C:12:ARG:HB3	2:C:136:MET:HE3	1.98	0.45
2:C:82:LEU:HD23	2:C:82:LEU:H	1.82	0.45
2:A:61:THR:HG22	2:A:62:LEU:N	2.32	0.44
2:B:67:ARG:HG2	2:B:183:LEU:HB2	1.99	0.44
2:C:3:ILE:O	2:C:5:LYS:N	2.50	0.44
2:A:37:SER:O	2:A:172:THR:HA	2.17	0.44
2:B:31:ILE:H	2:B:31:ILE:HD12	1.82	0.44
2:B:20:LEU:HA	2:B:21:PRO:HD3	1.71	0.44
2:B:56:ILE:O	2:B:57:ASP:C	2.55	0.44
2:C:136:MET:HE2	2:C:136:MET:HB3	1.71	0.44
2:C:2:GLU:C	2:C:3:ILE:HG13	2.37	0.44
2:C:58:SER:O	2:C:62:LEU:HG	2.17	0.44
2:C:39:VAL:HB	2:C:171:ILE:HG22	2.00	0.43
2:A:31:ILE:CD1	2:A:179:MET:HG3	2.48	0.43
2:B:95:TRP:CZ3	2:B:153:LEU:HG	2.53	0.43
2:B:20:LEU:O	2:B:140:ARG:NH2	2.52	0.43
2:A:59:VAL:O	2:A:63:THR:HG23	2.18	0.43
2:B:102:VAL:HG12	2:B:103:THR:N	2.34	0.43
2:C:123:GLN:HG3	2:C:123:GLN:O	2.19	0.43
2:B:18:THR:HG22	2:C:22:THR:HA	2.01	0.43
2:B:133:PRO:HB2	2:B:136:MET:HE3	2.00	0.43
2:B:95:TRP:CH2	2:B:153:LEU:HG	2.53	0.43
2:B:115:ILE:HD12	2:B:115:ILE:C	2.39	0.42
2:A:59:VAL:HG22	2:A:177:LEU:HD11	2.02	0.42
2:B:82:LEU:HD23	2:B:82:LEU:H	1.84	0.42
2:B:83:GLN:CA	2:B:83:GLN:HE21	2.27	0.42
2:B:87:PHE:CG	2:B:164:PRO:HB3	2.55	0.42
2:A:129:ILE:N	2:A:129:ILE:CD1	2.80	0.42
2:C:73:SER:OG	2:C:176:THR:HG23	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:156:SER:O	2:B:157:ILE:HD13	2.19	0.42
2:B:63:THR:O	2:B:65:PHE:N	2.53	0.42
2:C:145:ILE:CD1	2:C:146:GLN:H	2.18	0.42
2:C:56:ILE:H	2:C:56:ILE:HG13	1.44	0.42
2:A:124:THR:OG1	2:A:127:PRO:HD3	2.19	0.42
2:B:119:GLY:O	2:B:123:GLN:HG2	2.20	0.42
2:C:87:PHE:CG	2:C:164:PRO:HB3	2.54	0.42
2:C:10:GLN:HE22	2:C:94:CYS:HA	1.84	0.42
2:A:119:GLY:C	2:A:121:ALA:H	2.23	0.42
2:A:188:SER:HB2	2:C:109:LYS:HD2	2.02	0.42
2:C:133:PRO:HA	2:C:135:GLU:OE1	2.20	0.42
2:B:40:LEU:HD12	2:B:41:PHE:H	1.84	0.42
2:B:51:LEU:CD1	2:B:51:LEU:N	2.82	0.42
2:C:138:GLN:HE21	2:C:138:GLN:HA	1.78	0.41
2:C:33:GLN:HA	2:C:34:PRO:HD3	1.94	0.41
2:A:118:ILE:O	2:A:118:ILE:HG22	2.20	0.41
2:A:138:GLN:NE2	2:A:138:GLN:HA	2.35	0.41
2:C:92:GLY:CA	2:C:115:ILE:HD13	2.49	0.41
2:A:154:LEU:HA	2:A:154:LEU:HD12	1.79	0.41
2:C:138:GLN:HE21	2:C:139:PRO:N	2.18	0.41
2:C:138:GLN:NE2	2:C:138:GLN:HA	2.33	0.41
2:A:136:MET:HE3	2:A:136:MET:HB2	2.00	0.41
2:A:27:SER:OG	2:A:28:PRO:HD2	2.20	0.41
2:A:59:VAL:O	2:A:61:THR:N	2.53	0.41
2:C:122:ILE:HG13	2:C:122:ILE:O	2.21	0.41
2:A:68:HIS:ND1	2:A:180:HIS:CE1	2.89	0.41
2:A:96:VAL:HG12	2:A:152:LYS:HB3	2.02	0.41
1:D:2:C:H1'	2:C:12:ARG:HD3	2.02	0.41
2:C:28:PRO:HG2	2:C:180:HIS:CD2	2.55	0.41
2:C:98:ALA:HB3	2:C:148:LEU:O	2.21	0.41
2:C:70:SER:OG	2:C:140:ARG:HG2	2.20	0.41
2:A:74:LEU:HG	2:A:75:TRP:N	2.36	0.40
2:C:17:ALA:CB	2:C:138:GLN:HG2	2.51	0.40
2:B:81:THR:HG21	2:B:168:THR:HA	2.03	0.40
2:B:49:ALA:HB3	2:B:155:ILE:HB	2.04	0.40
2:B:153:LEU:HD22	2:B:155:ILE:HD12	2.02	0.40
2:B:67:ARG:HG3	2:B:181:SER:O	2.21	0.40
2:B:146:GLN:O	2:C:145:ILE:HD13	2.21	0.40
2:C:115:ILE:HD13	2:C:115:ILE:HA	1.85	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	162/189 (86%)	136 (84%)	18 (11%)	8 (5%)	<b>2</b>	<b>8</b>
2	B	187/189 (99%)	160 (86%)	19 (10%)	8 (4%)	<b>2</b>	<b>10</b>
2	C	187/189 (99%)	163 (87%)	20 (11%)	4 (2%)	<b>7</b>	<b>26</b>
All	All	536/567 (94%)	459 (86%)	57 (11%)	20 (4%)	<b>3</b>	<b>13</b>

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	28	PRO
2	A	29	PHE
2	A	98	ALA
2	A	124	THR
2	A	126	SER
2	A	127	PRO
2	A	128	LEU
2	B	64	THR
2	B	113	GLY
2	B	15	THR
2	B	57	ASP
2	B	98	ALA
2	C	113	GLY
2	A	181	SER
2	B	54	ALA
2	C	54	ALA
2	C	181	SER
2	B	101	PRO
2	C	184	ILE
2	B	181	SER

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	145/167 (87%)	108 (74%)	37 (26%)	0	1
2	B	167/167 (100%)	112 (67%)	55 (33%)	0	0
2	C	167/167 (100%)	113 (68%)	54 (32%)	0	0
All	All	479/501 (96%)	333 (70%)	146 (30%)	0	1

All (146) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	29	PHE
2	A	30	THR
2	A	31	ILE
2	A	44	THR
2	A	52	THR
2	A	57	ASP
2	A	61	THR
2	A	70	SER
2	A	74	LEU
2	A	77	THR
2	A	82	LEU
2	A	96	VAL
2	A	103	THR
2	A	106	GLN
2	A	108	THR
2	A	109	LYS
2	A	110	THR
2	A	115	ILE
2	A	122	ILE
2	A	124	THR
2	A	128	LEU
2	A	129	ILE
2	A	136	MET
2	A	143	ASP
2	A	145	ILE
2	A	148	LEU

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Mol	Chain	Res	Type
2	A	150	SER
2	A	153	LEU
2	A	154	LEU
2	A	162	THR
2	A	167	SER
2	A	168	THR
2	A	173	VAL
2	A	174	SER
2	A	179	MET
2	A	187	THR
2	A	188	SER
2	B	1	MET
2	B	3	ILE
2	B	10	GLN
2	B	18	THR
2	B	29	PHE
2	B	31	ILE
2	B	44	THR
2	B	45	LYS
2	B	46	ASP
2	B	50	SER
2	B	52	THR
2	B	55	ASN
2	B	57	ASP
2	B	62	LEU
2	B	63	THR
2	B	64	THR
2	B	67	ARG
2	B	70	SER
2	B	71	LEU
2	B	74	LEU
2	B	81	THR
2	B	82	LEU
2	B	83	GLN
2	B	93	VAL
2	B	96	VAL
2	B	99	GLN
2	B	103	THR
2	B	105	THR
2	B	109	LYS
2	B	116	PHE
2	B	118	ILE

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Mol	Chain	Res	Type
2	B	123	GLN
2	B	124	THR
2	B	129	ILE
2	B	134	LEU
2	B	136	MET
2	B	137	MET
2	B	140	ARG
2	B	141	VAL
2	B	143	ASP
2	B	145	ILE
2	B	148	LEU
2	B	149	ASP
2	B	150	SER
2	B	153	LEU
2	B	156	SER
2	B	167	SER
2	B	174	SER
2	B	179	MET
2	B	181	SER
2	B	183	LEU
2	B	184	ILE
2	B	187	THR
2	B	188	SER
2	B	189	THR
2	C	3	ILE
2	C	5	LYS
2	C	6	GLU
2	C	7	LEU
2	C	12	ARG
2	C	16	VAL
2	C	18	THR
2	C	20	LEU
2	C	23	VAL
2	C	29	PHE
2	C	44	THR
2	C	45	LYS
2	C	46	ASP
2	C	48	GLU
2	C	50	SER
2	C	51	LEU
2	C	52	THR
2	C	56	ILE

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Mol	Chain	Res	Type
2	C	60	SER
2	C	67	ARG
2	C	70	SER
2	C	72	GLU
2	C	81	THR
2	C	83	GLN
2	C	96	VAL
2	C	102	VAL
2	C	103	THR
2	C	105	THR
2	C	106	GLN
2	C	108	THR
2	C	116	PHE
2	C	123	GLN
2	C	124	THR
2	C	128	LEU
2	C	134	LEU
2	C	138	GLN
2	C	145	ILE
2	C	146	GLN
2	C	148	LEU
2	C	149	ASP
2	C	150	SER
2	C	156	SER
2	C	167	SER
2	C	170	ILE
2	C	173	VAL
2	C	174	SER
2	C	176	THR
2	C	177	LEU
2	C	178	SER
2	C	179	MET
2	C	180	HIS
2	C	183	LEU
2	C	184	ILE
2	C	189	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	33	GLN
2	A	55	ASN

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Mol	Chain	Res	Type
2	A	68	HIS
2	A	180	HIS
2	B	33	GLN
2	B	79	HIS
2	B	83	GLN
2	B	106	GLN
2	B	114	GLN
2	B	180	HIS
2	C	10	GLN
2	C	55	ASN
2	C	79	HIS
2	C	83	GLN
2	C	106	GLN
2	C	123	GLN
2	C	138	GLN
2	C	180	HIS

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	D	2/3 (66%)	0	0

There are no RNA backbone outliers to report.

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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	D	3/3 (100%)	3.80	3 (100%) 0 0	183, 183, 183, 190	0
2	A	164/189 (86%)	-0.08	5 (3%) 50 45	7, 21, 100, 162	0
2	B	189/189 (100%)	-0.11	3 (1%) 72 71	9, 21, 61, 99	1 (0%)
2	C	189/189 (100%)	-0.29	1 (0%) 91 91	9, 22, 51, 75	0
All	All	545/570 (95%)	-0.14	12 (2%) 62 59	7, 22, 69, 190	1 (0%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	26	PRO	12.8
2	A	123	GLN	8.4
2	B	24	PRO	5.3
2	B	25	GLY	5.1
1	D	1	C	4.7
2	A	124	THR	4.4
1	D	2	C	4.2
2	A	122	ILE	3.4
2	A	126	SER	3.2
1	D	3	C	2.6
2	C	25	GLY	2.3
2	B	26	PRO	2.2

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.