



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:36 AM GMT

PDB ID : 2XPJ  
Title : Crystal structure of Physalis Mottle Virus with intact ordered RNA  
Authors : Sagurthi, S.R.; Rajaram, V.; Savithri, H.S.; Murthy, M.R.N.  
Deposited on : 2010-08-26  
Resolution : 3.40 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  
<http://wwpdb.org/validation/2016/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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

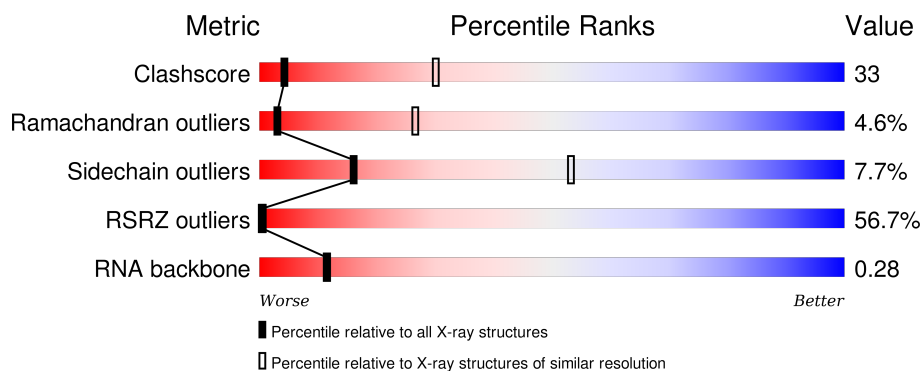
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 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	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)
RNA backbone	2183	1041 (4.00-2.80)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	188	<div> <div>47%</div> <div>43% 38% 6% • 12%</div> </div>
1	B	188	<div> <div>56%</div> <div>47% 43% 6% •</div> </div>
1	C	188	<div> <div>56%</div> <div>39% 50% 9% ••</div> </div>
2	D	3	<div> <div>100%</div> <div>67% 33%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4001 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.

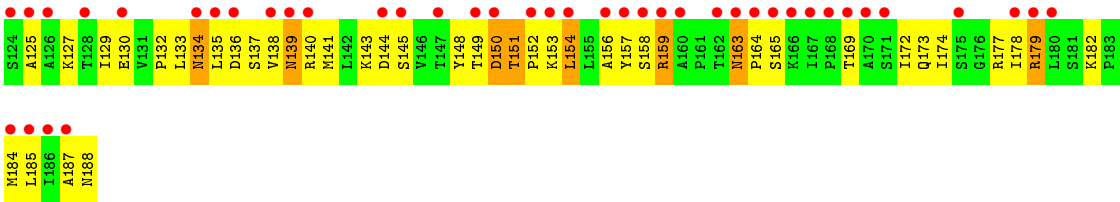
- Molecule 1 is a protein called COAT PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	165	Total	C	N	O	S	0	0	0
			1218	777	205	233	3			
1	B	180	Total	C	N	O	S	0	0	0
			1343	859	225	256	3			
1	C	185	Total	C	N	O	S	0	0	0
			1383	882	232	266	3			

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

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





• Molecule 2: 5'-R(CP\*CP\*CP)-3'



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	285.40Å 288.36Å 290.61Å 62.92° 65.30° 60.85°	Depositor
Resolution (Å)	30.00 – 3.40 29.99 – 3.40	Depositor EDS
% Data completeness (in resolution range)	69.1 (30.00-3.40) 61.3 (29.99-3.40)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.54 (at 3.39Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.308 , 0.311 (Not available) , (Not available)	Depositor DCC
$R_{free}$ test set	NotAvailable	DCC
Wilson B-factor (Å <sup>2</sup> )	58.5	Xtriage
Anisotropy	0.191	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , -10.0	EDS
Estimated twinning fraction	0.000 for -k,-h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtriage
Outliers	0 of 661310 reflections	Xtriage
$F_o, F_c$ correlation	0.16	EDS
Total number of atoms	4001	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.42	0/1245	0.72	1/1710 (0.1%)
1	B	0.41	0/1370	0.69	1/1876 (0.1%)
1	C	0.40	0/1412	0.73	0/1936
2	D	0.81	0/62	0.92	0/94
All	All	0.42	0/4089	0.72	2/5616 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	137	SER	N-CA-C	-5.32	96.63	111.00
1	A	54	LEU	N-CA-C	-5.00	97.50	111.00

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	1218	0	1233	83	0
1	B	1343	0	1400	94	0
1	C	1383	0	1435	101	0
2	D	57	0	35	1	0
All	All	4001	0	4103	269	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 33.

All (269) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:PRO:HA	1:A:186:ILE:HD11	1.38	1.05
1:A:81:PRO:HG3	1:A:119:LEU:HD22	1.41	0.98
1:B:11:GLN:HE22	1:B:96:TRP:H	0.98	0.96
1:A:94:LEU:HD21	1:A:172:ILE:HD13	1.49	0.95
1:B:11:GLN:NE2	1:B:96:TRP:H	1.66	0.94
1:A:186:ILE:HG22	1:A:187:ALA:H	1.28	0.93
1:C:11:GLN:HE22	1:C:96:TRP:H	1.00	0.93
1:B:140:ARG:HH11	1:B:140:ARG:HB3	1.35	0.91
1:B:64:THR:HG23	1:B:143:LYS:HD2	1.51	0.89
1:B:61:THR:HA	1:B:64:THR:HB	1.56	0.87
1:C:158:SER:O	1:C:159:ARG:HB2	1.74	0.86
1:A:186:ILE:HG22	1:A:187:ALA:N	1.92	0.85
1:B:71:GLN:HB3	1:B:141:MET:SD	2.18	0.84
1:A:90:LEU:H	1:A:90:LEU:HD23	1.42	0.83
1:B:55:GLN:HB2	1:B:151:THR:HG21	1.59	0.82
1:B:69:HIS:HB2	1:B:181:SER:HB2	1.63	0.80
1:B:137:SER:O	1:B:138:VAL:HG22	1.81	0.80
1:A:118:VAL:HB	1:A:123:ILE:CB	2.13	0.79
1:B:66:PRO:HG2	1:B:67:TYR:CE1	2.18	0.79
1:A:139:ASN:HD22	1:A:140:ARG:N	1.80	0.79
1:B:9:VAL:HG12	1:B:115:GLN:HE22	1.50	0.76
1:C:9:VAL:HG12	1:C:115:GLN:HE22	1.52	0.75
1:A:79:LEU:HD13	1:A:119:LEU:HD21	1.69	0.75
1:A:83:ASP:O	1:A:86:VAL:HG22	1.86	0.75
1:A:185:LEU:HD12	1:C:111:VAL:HG12	1.69	0.75
1:B:29:SER:HB2	1:B:30:PRO:HD2	1.67	0.74
1:A:187:ALA:O	1:A:188:ASN:HB2	1.88	0.72
1:B:40:ALA:HB1	1:B:52:VAL:HG21	1.69	0.72
1:C:102:PRO:O	1:C:103:ALA:HB3	1.88	0.72
1:B:11:GLN:HE22	1:B:96:TRP:N	1.82	0.72
1:B:139:ASN:HB2	1:B:150:ASP:CB	2.20	0.71
1:C:49:ALA:HB2	1:C:157:TYR:HD1	1.55	0.71
1:C:187:ALA:O	1:C:188:ASN:HB2	1.91	0.70
1:A:133:LEU:O	1:A:134:ASN:HB2	1.91	0.70
1:C:97:VAL:HG13	1:C:98:PRO:HD2	1.72	0.70
1:A:188:ASN:OD1	1:C:110:ARG:HD2	1.92	0.70
1:B:187:ALA:O	1:B:188:ASN:HB2	1.90	0.69
1:C:138:VAL:HG21	1:C:152:PRO:HB3	1.73	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:11:GLN:NE2	1:C:96:TRP:H	1.84	0.68
1:A:109:LEU:HD21	1:A:116:SER:HB2	1.76	0.68
1:B:4:SER:O	1:B:5:GLU:HG2	1.94	0.68
1:A:186:ILE:CG2	1:A:187:ALA:H	2.05	0.67
1:C:66:PRO:HG2	1:C:67:TYR:CE1	2.30	0.66
1:B:45:THR:HG22	1:B:165:SER:O	1.94	0.66
1:C:9:VAL:CG1	1:C:115:GLN:HE22	2.08	0.66
1:C:66:PRO:HG2	1:C:67:TYR:CD1	2.31	0.66
1:C:98:PRO:O	1:C:99:ALA:HB3	1.95	0.66
1:A:99:ALA:HB3	1:A:149:THR:O	1.95	0.66
1:C:139:ASN:HD22	1:C:140:ARG:N	1.94	0.66
1:C:64:THR:HG23	1:C:143:LYS:HE3	1.78	0.65
1:B:139:ASN:HB2	1:B:150:ASP:HB2	1.78	0.64
1:A:54:LEU:O	1:A:55:GLN:HB3	1.98	0.63
1:A:37:GLN:HG3	1:A:175:SER:HB3	1.80	0.63
1:A:54:LEU:HD12	1:A:54:LEU:N	2.14	0.63
1:C:134:ASN:ND2	1:C:136:ASP:H	1.97	0.63
1:A:95:ALA:HB2	1:A:108:ILE:HG23	1.79	0.63
1:B:55:GLN:CB	1:B:151:THR:HG21	2.30	0.62
1:B:64:THR:CG2	1:B:143:LYS:HD2	2.29	0.61
1:A:133:LEU:O	1:A:134:ASN:CB	2.49	0.61
1:B:138:VAL:HG21	1:B:152:PRO:HB3	1.82	0.60
1:B:37:GLN:HG3	1:B:175:SER:HB3	1.83	0.60
1:B:44:GLY:O	1:B:161:PRO:HG3	2.02	0.60
1:C:41:THR:HG21	1:C:50:ALA:HB3	1.83	0.60
1:C:103:ALA:HA	1:C:107:GLN:OE1	2.02	0.60
1:C:49:ALA:HB2	1:C:157:TYR:CD1	2.36	0.60
1:A:79:LEU:HD11	1:A:92:VAL:CG2	2.32	0.60
1:A:65:ALA:HB3	1:A:66:PRO:HD3	1.83	0.59
1:C:69:HIS:HB2	1:C:182:LYS:HD2	1.83	0.59
1:B:94:LEU:HD22	1:B:154:LEU:HD11	1.84	0.59
1:C:7:VAL:HG21	1:C:127:LYS:HE3	1.85	0.59
1:B:104:THR:O	1:B:107:GLN:HG2	2.03	0.59
1:B:139:ASN:HB2	1:B:150:ASP:HB3	1.84	0.58
1:B:49:ALA:HB2	1:B:157:TYR:HD2	1.68	0.58
1:C:135:LEU:HD22	1:C:140:ARG:HG2	1.84	0.58
1:B:105:PRO:HB2	1:B:157:TYR:HB2	1.84	0.58
1:A:93:TYR:O	1:A:156:ALA:HA	2.03	0.58
1:C:61:THR:HG22	1:C:64:THR:HG21	1.85	0.57
1:B:46:ALA:O	1:B:48:THR:HG23	2.03	0.57
1:B:55:GLN:HB2	1:B:151:THR:CG2	2.30	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:TYR:CG	1:A:180:LEU:HB3	2.40	0.57
1:A:110:ARG:HD3	1:B:188:ASN:OD1	2.05	0.57
1:B:95:ALA:HB2	1:B:108:ILE:HG23	1.87	0.57
1:C:84:LEU:HB3	1:C:169:THR:HG22	1.87	0.57
1:A:139:ASN:HD22	1:A:140:ARG:H	1.50	0.56
1:A:54:LEU:HD12	1:A:54:LEU:H	1.71	0.56
1:C:71:GLN:HB3	1:C:141:MET:SD	2.45	0.56
1:C:32:ILE:HG13	1:C:33:VAL:N	2.21	0.56
1:C:55:GLN:HG3	1:C:151:THR:HG21	1.87	0.56
1:B:61:THR:HG23	1:B:64:THR:CG2	2.35	0.56
1:C:11:GLN:HE22	1:C:96:TRP:N	1.85	0.56
1:A:134:ASN:HB3	1:A:137:SER:OG	2.06	0.56
1:A:184:MET:O	1:A:186:ILE:HG13	2.06	0.55
1:C:94:LEU:HD21	1:C:172:ILE:HD13	1.88	0.55
1:C:93:TYR:O	1:C:156:ALA:HA	2.07	0.55
1:A:94:LEU:HD21	1:A:172:ILE:CD1	2.30	0.55
1:A:51:GLN:HE21	1:A:153:LYS:NZ	2.05	0.55
1:A:104:THR:HB	1:A:107:GLN:HG3	1.87	0.55
1:B:100:ASN:OD1	1:B:149:THR:HB	2.06	0.55
1:A:45:THR:HG22	1:A:166:LYS:HA	1.87	0.55
1:C:134:ASN:HD22	1:C:135:LEU:N	2.05	0.55
1:C:102:PRO:O	1:C:103:ALA:CB	2.54	0.54
1:B:45:THR:HG22	1:B:166:LYS:HA	1.90	0.54
1:A:90:LEU:N	1:A:90:LEU:HD23	2.19	0.53
1:C:76:LYS:HD2	1:C:130:GLU:OE1	2.07	0.53
1:C:64:THR:HG23	1:C:143:LYS:CE	2.39	0.53
1:C:95:ALA:HB2	1:C:108:ILE:HG23	1.89	0.53
1:A:165:SER:C	1:A:167:ILE:H	2.11	0.53
1:A:71:GLN:HE21	1:A:140:ARG:HD3	1.73	0.53
1:B:66:PRO:HG2	1:B:67:TYR:CD1	2.43	0.53
1:B:11:GLN:NE2	1:B:96:TRP:N	2.48	0.53
1:C:100:ASN:HD22	1:C:100:ASN:H	1.56	0.53
1:B:21:LEU:O	1:B:23:GLN:HG3	2.09	0.53
1:A:54:LEU:O	1:A:55:GLN:CB	2.57	0.53
1:A:24:PRO:HD3	1:B:22:SER:HB2	1.89	0.53
1:A:91:THR:HG23	1:A:91:THR:O	2.09	0.53
1:C:139:ASN:HD22	1:C:139:ASN:C	2.10	0.53
1:C:187:ALA:O	1:C:188:ASN:CB	2.57	0.52
1:C:74:GLU:HA	1:C:135:LEU:HD11	1.91	0.52
1:B:4:SER:O	1:B:5:GLU:CB	2.57	0.52
1:A:54:LEU:CD1	1:A:54:LEU:H	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78:ILE:O	1:C:172:ILE:HA	2.09	0.52
1:A:57:ALA:O	1:A:61:THR:HG23	2.10	0.52
1:C:14:ILE:HG13	1:C:14:ILE:O	2.09	0.52
1:C:61:THR:HA	1:C:64:THR:HB	1.90	0.51
1:C:20:ILE:HG22	1:C:21:LEU:O	2.09	0.51
1:B:133:LEU:HD11	1:B:152:PRO:HB2	1.92	0.51
1:C:51:GLN:HB3	1:C:153:LYS:HE2	1.92	0.51
1:A:158:SER:O	1:A:159:ARG:HG2	2.11	0.51
1:C:65:ALA:HB3	1:C:66:PRO:HD3	1.92	0.51
1:C:83:ASP:O	1:C:86:VAL:HG23	2.11	0.51
1:B:151:THR:HG23	1:B:152:PRO:HD2	1.93	0.51
1:A:55:GLN:O	1:A:55:GLN:HG2	2.11	0.51
1:B:80:THR:CG2	1:B:128:THR:HG23	2.41	0.51
1:B:64:THR:HG22	1:B:65:ALA:N	2.25	0.50
1:B:133:LEU:HD11	1:B:152:PRO:CB	2.41	0.50
1:B:49:ALA:HB1	1:B:105:PRO:CG	2.41	0.50
1:B:4:SER:O	1:B:5:GLU:CG	2.58	0.50
1:B:93:TYR:O	1:B:156:ALA:HA	2.11	0.50
1:C:90:LEU:HD21	1:C:119:LEU:HB2	1.93	0.50
1:C:98:PRO:O	1:C:99:ALA:CB	2.60	0.50
1:C:100:ASN:HB3	1:C:149:THR:O	2.12	0.49
1:C:100:ASN:HD22	1:C:100:ASN:N	2.09	0.49
1:C:134:ASN:HD22	1:C:134:ASN:C	2.13	0.49
1:A:37:GLN:HE21	1:A:175:SER:HB3	1.77	0.49
1:A:104:THR:CG2	1:A:105:PRO:HD2	2.43	0.49
1:C:178:ILE:HG22	1:C:179:ARG:N	2.28	0.48
1:B:29:SER:HB3	1:B:182:LYS:NZ	2.29	0.48
1:B:78:ILE:O	1:B:172:ILE:HA	2.13	0.48
1:B:14:ILE:HD12	1:B:14:ILE:O	2.13	0.48
1:A:58:ASP:HB2	1:A:59:PRO:HD3	1.95	0.48
1:C:41:THR:HG21	1:C:50:ALA:CB	2.42	0.48
1:B:6:VAL:HG23	1:B:128:THR:O	2.13	0.48
1:A:139:ASN:C	1:A:139:ASN:HD22	2.17	0.48
1:C:134:ASN:O	1:C:137:SER:HB3	2.14	0.48
1:C:4:SER:O	1:C:5:GLU:HB2	2.14	0.48
1:C:97:VAL:HG12	1:C:99:ALA:H	1.79	0.48
1:A:158:SER:C	1:A:159:ARG:HG2	2.34	0.48
1:C:52:VAL:CG1	1:C:154:LEU:HB3	2.44	0.48
1:C:139:ASN:ND2	1:C:141:MET:H	2.12	0.47
1:B:54:LEU:HD12	1:B:152:PRO:CG	2.45	0.47
1:A:45:THR:HG22	1:A:166:LYS:CA	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:64:THR:HG23	1:C:143:LYS:HD2	1.97	0.47
1:B:140:ARG:HB3	1:B:140:ARG:NH1	2.18	0.47
1:C:104:THR:O	1:C:107:GLN:HG3	2.15	0.47
1:C:65:ALA:HB3	1:C:66:PRO:CD	2.43	0.47
1:A:67:TYR:CD2	1:A:180:LEU:HB3	2.50	0.47
1:C:4:SER:O	1:C:5:GLU:CB	2.62	0.47
1:C:52:VAL:HG13	1:C:154:LEU:HB3	1.95	0.47
1:A:100:ASN:N	1:A:100:ASN:OD1	2.48	0.47
1:A:119:LEU:H	1:A:123:ILE:CB	2.28	0.47
1:B:137:SER:C	1:B:138:VAL:HG13	2.35	0.47
1:A:40:ALA:HB1	1:A:52:VAL:HG21	1.97	0.47
1:C:134:ASN:C	1:C:134:ASN:ND2	2.68	0.46
1:A:79:LEU:HD11	1:A:92:VAL:HG22	1.95	0.46
1:A:54:LEU:N	1:A:54:LEU:CD1	2.77	0.46
1:A:70:ALA:O	1:A:141:MET:O	2.34	0.46
1:C:99:ALA:HA	1:C:153:LYS:HD2	1.98	0.46
1:B:47:GLU:HB2	1:B:160:ALA:HB2	1.98	0.46
1:A:186:ILE:CG2	1:A:187:ALA:N	2.63	0.46
1:A:140:ARG:H	1:A:140:ARG:HG3	1.43	0.46
1:A:158:SER:O	1:A:159:ARG:O	2.34	0.46
1:B:39:GLU:HA	1:B:173:GLN:HA	1.98	0.46
1:A:112:TYR:HB3	1:B:185:LEU:HD22	1.98	0.46
1:A:159:ARG:HH11	1:A:159:ARG:HB3	1.81	0.46
1:B:133:LEU:HD23	1:B:133:LEU:C	2.37	0.46
1:C:134:ASN:HB3	1:C:137:SER:HB2	1.98	0.46
1:A:67:TYR:CD1	1:A:67:TYR:N	2.84	0.46
1:A:159:ARG:NH1	1:A:159:ARG:HB3	2.31	0.46
1:B:187:ALA:O	1:B:188:ASN:CB	2.61	0.45
1:B:79:LEU:CD2	1:B:119:LEU:HD11	2.46	0.45
1:B:65:ALA:HB3	1:B:66:PRO:HD3	1.98	0.45
1:B:100:ASN:OD1	1:B:149:THR:O	2.34	0.45
1:B:109:LEU:HD21	1:B:116:SER:HB2	1.99	0.45
1:C:23:GLN:NE2	1:C:23:GLN:N	2.65	0.45
1:A:183:PRO:HG2	1:C:14:ILE:HD12	1.97	0.45
1:A:68:ARG:HD3	1:C:150:ASP:HB3	1.98	0.45
1:A:90:LEU:CD2	1:A:90:LEU:H	2.22	0.45
1:A:111:VAL:HG12	1:A:112:TYR:N	2.31	0.45
1:B:186:ILE:HG12	1:B:187:ALA:N	2.32	0.45
1:C:54:LEU:HD12	1:C:152:PRO:HG2	1.99	0.45
1:C:24:PRO:HB2	1:C:26:THR:HG23	1.98	0.45
1:C:76:LYS:HA	1:C:132:PRO:HA	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:ASN:N	1:C:164:PRO:HD3	2.31	0.44
1:C:37:GLN:HA	1:C:174:ILE:O	2.17	0.44
1:A:125:ALA:O	1:A:126:ALA:HB3	2.17	0.44
1:B:140:ARG:CB	1:B:140:ARG:HH11	2.16	0.44
1:A:76:LYS:HD2	1:A:130:GLU:OE1	2.17	0.44
1:B:79:LEU:HD23	1:B:172:ILE:HG22	1.99	0.44
1:C:45:THR:HG22	1:C:165:SER:O	2.17	0.44
1:A:165:SER:O	1:A:167:ILE:N	2.51	0.44
1:A:118:VAL:O	1:A:119:LEU:O	2.36	0.44
1:A:134:ASN:O	1:A:135:LEU:HB2	2.17	0.44
1:C:97:VAL:HG13	1:C:98:PRO:CD	2.46	0.44
1:B:41:THR:HG22	1:B:172:ILE:HG12	1.99	0.44
1:A:104:THR:HG22	1:A:105:PRO:HD2	1.99	0.44
1:C:46:ALA:O	1:C:48:THR:HG23	2.18	0.44
1:A:131:VAL:HA	1:A:132:PRO:HD3	1.78	0.43
1:B:90:LEU:N	1:B:90:LEU:HD23	2.33	0.43
1:C:54:LEU:HD12	1:C:152:PRO:CG	2.48	0.43
1:B:80:THR:HG22	1:B:128:THR:HG23	1.99	0.43
1:A:55:GLN:HG3	1:A:142:LEU:O	2.19	0.43
1:B:137:SER:O	1:B:138:VAL:CG2	2.59	0.43
1:B:9:VAL:HG12	1:B:115:GLN:NE2	2.25	0.43
1:C:83:ASP:OD2	1:C:84:LEU:HD12	2.19	0.43
1:A:51:GLN:HE21	1:A:153:LYS:CE	2.31	0.43
1:B:181:SER:HB3	1:B:182:LYS:H	1.64	0.43
1:C:7:VAL:HG21	1:C:127:LYS:CE	2.48	0.43
1:C:21:LEU:HD23	1:C:148:TYR:OH	2.18	0.43
1:C:90:LEU:HD23	1:C:90:LEU:N	2.34	0.43
1:C:89:PRO:HG3	1:C:121:GLY:N	2.33	0.43
1:B:54:LEU:HD12	1:B:152:PRO:HG2	2.01	0.42
1:B:61:THR:HG23	1:B:64:THR:HG22	2.00	0.42
1:C:85:ALA:O	1:C:120:GLY:HA3	2.20	0.42
1:B:94:LEU:CD2	1:B:154:LEU:HD11	2.49	0.42
1:C:144:ASP:OD2	1:C:145:SER:N	2.44	0.42
1:C:79:LEU:HB3	1:C:129:ILE:HB	2.00	0.42
1:C:39:GLU:HG3	1:C:173:GLN:HE21	1.83	0.42
1:C:4:SER:OG	1:C:5:GLU:N	2.48	0.42
1:A:186:ILE:O	1:C:111:VAL:HA	2.20	0.42
1:B:79:LEU:HD22	1:B:119:LEU:HD11	2.00	0.42
1:B:20:ILE:C	1:C:21:LEU:HD12	2.40	0.42
1:B:159:ARG:HB2	1:B:159:ARG:CZ	2.50	0.42
1:B:59:PRO:O	1:B:63:LEU:HD13	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:PHE:HE1	1:B:172:ILE:HG23	1.85	0.42
1:B:6:VAL:HG22	1:B:7:VAL:N	2.35	0.41
1:C:90:LEU:CD2	1:C:119:LEU:HB2	2.49	0.41
1:B:76:LYS:HA	1:B:132:PRO:HA	2.01	0.41
1:B:137:SER:O	1:B:138:VAL:HG13	2.20	0.41
2:D:3:C:H3'	2:D:3:C:H6	1.85	0.41
1:A:78:ILE:O	1:A:172:ILE:HA	2.19	0.41
1:B:186:ILE:CG1	1:B:187:ALA:N	2.83	0.41
1:B:72:ILE:HD11	1:B:142:LEU:HD21	2.03	0.41
1:C:184:MET:HG3	1:C:185:LEU:N	2.35	0.41
1:B:139:ASN:O	1:B:152:PRO:HD3	2.20	0.41
1:B:54:LEU:HB2	1:B:152:PRO:HG2	2.02	0.41
1:B:34:LEU:HA	1:B:35:PRO:HD3	1.86	0.41
1:B:181:SER:O	1:B:182:LYS:C	2.58	0.41
1:C:79:LEU:HD13	1:C:172:ILE:HG12	2.02	0.41
1:C:73:VAL:HB	1:C:177:ARG:O	2.21	0.41
1:A:111:VAL:CG1	1:A:112:TYR:N	2.83	0.41
1:B:4:SER:O	1:B:5:GLU:HB3	2.20	0.40
1:C:76:LYS:HE3	1:C:78:ILE:HD11	2.02	0.40
1:C:40:ALA:O	1:C:41:THR:HG23	2.22	0.40
1:A:61:THR:HA	1:A:64:THR:OG1	2.21	0.40
1:C:120:GLY:H	1:C:125:ALA:HB1	1.86	0.40
1:A:63:LEU:O	1:A:66:PRO:HD2	2.22	0.40
1:B:111:VAL:CG1	1:C:185:LEU:HD22	2.52	0.40
1:B:61:THR:HG23	1:B:64:THR:HG21	2.03	0.40
1:C:157:TYR:CG	1:C:158:SER:N	2.89	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	
1	A	163/188 (87%)	125 (77%)	26 (16%)	12 (7%)	1	14
1	B	176/188 (94%)	156 (89%)	15 (8%)	5 (3%)	6	41
1	C	183/188 (97%)	161 (88%)	15 (8%)	7 (4%)	4	32
All	All	522/564 (93%)	442 (85%)	56 (11%)	24 (5%)	3	26

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	30	PRO
1	A	119	LEU
1	A	159	ARG
1	B	5	GLU
1	B	138	VAL
1	C	159	ARG
1	A	134	ASN
1	C	5	GLU
1	C	114	GLY
1	A	56	THR
1	A	122	ALA
1	A	164	PRO
1	A	55	GLN
1	C	89	PRO
1	C	102	PRO
1	C	103	ALA
1	A	125	ALA
1	A	128	THR
1	B	182	LYS
1	C	57	ALA
1	A	166	LYS
1	B	65	ALA
1	B	89	PRO
1	A	168	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	132/159 (83%)	124 (94%)	8 (6%)	23	63
1	B	151/159 (95%)	144 (95%)	7 (5%)	33	72
1	C	156/159 (98%)	137 (88%)	19 (12%)	6	28
All	All	439/477 (92%)	405 (92%)	34 (8%)	16	53

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	PRO
1	A	79	LEU
1	A	107	GLN
1	A	134	ASN
1	A	139	ASN
1	A	140	ARG
1	A	151	THR
1	A	154	LEU
1	B	23	GLN
1	B	42	THR
1	B	64	THR
1	B	71	GLN
1	B	79	LEU
1	B	140	ARG
1	B	149	THR
1	C	5	GLU
1	C	23	GLN
1	C	25	ASN
1	C	26	THR
1	C	55	GLN
1	C	64	THR
1	C	87	SER
1	C	88	ASN
1	C	100	ASN
1	C	106	THR
1	C	107	GLN
1	C	133	LEU
1	C	134	ASN
1	C	139	ASN
1	C	150	ASP
1	C	151	THR
1	C	154	LEU
1	C	163	ASN
1	C	179	ARG



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

Mol	Chain	Res	Type
1	A	37	GLN
1	A	51	GLN
1	A	71	GLN
1	A	134	ASN
1	A	139	ASN
1	A	173	GLN
1	B	11	GLN
1	B	23	GLN
1	B	37	GLN
1	B	55	GLN
1	B	71	GLN
1	B	115	GLN
1	B	163	ASN
1	C	11	GLN
1	C	37	GLN
1	C	100	ASN
1	C	115	GLN
1	C	134	ASN
1	C	139	ASN
1	C	163	ASN
1	C	173	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	D	2/3 (66%)	1 (50%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	D	3	C

There are no RNA pucker outliers to report.

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

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 [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<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	A	165/188 (87%)	2.72	89 (53%) <b>0</b> <b>0</b>	42, 55, 96, 100	0
1	B	180/188 (95%)	2.86	105 (58%) <b>0</b> <b>0</b>	41, 52, 71, 96	0
1	C	185/188 (98%)	2.78	105 (56%) <b>0</b> <b>0</b>	39, 52, 70, 81	0
2	D	3/3 (100%)	5.28	3 (100%) <b>0</b> <b>0</b>	82, 82, 92, 97	0
All	All	533/567 (94%)	2.80	302 (56%) <b>0</b> <b>0</b>	39, 53, 82, 100	0

All (302) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	22	SER	15.0
1	C	18	GLY	11.4
1	B	23	GLN	10.9
1	A	25	ASN	10.0
1	B	167	ILE	9.8
1	A	188	ASN	9.4
1	A	124	SER	8.6
1	C	106	THR	8.3
1	A	30	PRO	7.9
1	B	166	LYS	7.9
1	B	82	THR	7.8
2	D	1	C	7.5
1	C	105	PRO	7.5
1	B	104	THR	7.4
1	B	188	ASN	7.3
1	B	45	THR	7.2
1	A	99	ALA	7.1
1	B	161	PRO	7.1
1	C	30	PRO	6.8
1	A	26	THR	6.8
1	C	4	SER	6.8

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Mol	Chain	Res	Type	RSRZ
1	A	24	PRO	6.7
1	C	13	SER	6.7
1	A	160	ALA	6.7
1	C	51	GLN	6.7
1	C	135	LEU	6.7
1	C	64	THR	6.6
1	C	136	ASP	6.6
1	A	162	THR	6.3
1	A	134	ASN	6.3
1	B	5	GLU	6.3
1	B	71	GLN	6.2
1	B	103	ALA	6.2
1	B	129	ILE	6.2
1	C	26	THR	6.1
1	C	134	ASN	6.1
1	C	59	PRO	6.0
1	B	165	SER	6.0
1	C	47	GLU	5.9
1	C	163	ASN	5.8
1	C	50	ALA	5.8
1	C	104	THR	5.8
1	A	103	ALA	5.8
1	C	158	SER	5.7
1	C	60	ILE	5.7
1	B	42	THR	5.6
1	B	107	GLN	5.6
1	A	128	THR	5.6
1	B	116	SER	5.6
1	B	162	THR	5.5
1	C	87	SER	5.5
1	A	56	THR	5.4
1	C	156	ALA	5.4
1	B	52	VAL	5.4
1	A	139	ASN	5.4
1	B	80	THR	5.3
1	C	185	LEU	5.3
1	C	138	VAL	5.3
1	A	58	ASP	5.3
1	C	12	ALA	5.2
1	B	105	PRO	5.2
1	A	82	THR	5.2
1	C	27	GLU	5.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	142	LEU	5.2
1	A	69	HIS	5.1
1	B	70	ALA	5.1
1	C	5	GLU	5.0
1	B	21	LEU	5.0
1	B	81	PRO	5.0
1	B	101	SER	4.9
1	B	144	ASP	4.9
1	A	125	ALA	4.9
1	B	85	ALA	4.9
1	A	126	ALA	4.9
1	A	113	GLY	4.8
1	C	44	GLY	4.8
1	A	177	ARG	4.8
1	A	136	ASP	4.7
1	B	4	SER	4.7
1	C	145	SER	4.7
1	A	161	PRO	4.7
1	B	87	SER	4.6
1	B	91	THR	4.6
1	C	39	GLU	4.6
1	B	10	LYS	4.5
1	A	64	THR	4.5
1	C	162	THR	4.5
1	C	28	GLN	4.4
1	B	106	THR	4.4
1	A	168	PRO	4.4
1	C	165	SER	4.4
1	A	140	ARG	4.4
2	D	3	C	4.4
1	B	95	ALA	4.4
1	A	29	SER	4.4
1	A	40	ALA	4.4
1	A	115	GLN	4.4
1	A	122	ALA	4.3
1	A	137	SER	4.3
1	C	24	PRO	4.3
1	B	53	SER	4.3
1	C	124	SER	4.2
1	B	32	ILE	4.2
1	A	145	SER	4.2
1	C	29	SER	4.2

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Mol	Chain	Res	Type	RSRZ
1	C	119	LEU	4.2
1	B	156	ALA	4.1
1	C	186	ILE	4.1
1	A	141	MET	4.1
1	A	184	MET	4.1
1	A	53	SER	4.1
1	B	183	PRO	4.1
1	B	163	ASN	4.0
1	A	83	ASP	4.0
1	C	139	ASN	4.0
1	B	37	GLN	4.0
2	D	2	C	3.9
1	C	187	ALA	3.9
1	B	41	THR	3.9
1	B	92	VAL	3.9
1	A	49	ALA	3.8
1	A	45	THR	3.8
1	C	11	GLN	3.8
1	C	52	VAL	3.8
1	C	17	PRO	3.8
1	A	170	ALA	3.8
1	C	53	SER	3.8
1	B	130	GLU	3.8
1	C	159	ARG	3.7
1	C	179	ARG	3.7
1	B	31	ALA	3.7
1	C	93	TYR	3.7
1	B	59	PRO	3.7
1	B	187	ALA	3.7
1	B	72	ILE	3.6
1	A	164	PRO	3.6
1	C	157	TYR	3.6
1	B	88	ASN	3.6
1	B	172	ILE	3.6
1	C	118	VAL	3.6
1	B	124	SER	3.6
1	C	88	ASN	3.5
1	B	93	TYR	3.5
1	C	168	PRO	3.5
1	A	84	LEU	3.5
1	A	71	GLN	3.5
1	C	45	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	138	VAL	3.5
1	C	58	ASP	3.4
1	C	167	ILE	3.4
1	A	149	THR	3.4
1	A	173	GLN	3.4
1	B	160	ALA	3.4
1	B	137	SER	3.4
1	A	31	ALA	3.4
1	B	128	THR	3.4
1	A	41	THR	3.4
1	C	56	THR	3.4
1	A	33	VAL	3.3
1	B	18	GLY	3.3
1	A	104	THR	3.3
1	C	166	LYS	3.3
1	A	102	PRO	3.3
1	A	59	PRO	3.3
1	C	42	THR	3.3
1	C	126	ALA	3.3
1	B	67	TYR	3.3
1	C	180	LEU	3.2
1	C	175	SER	3.2
1	C	184	MET	3.2
1	C	32	ILE	3.2
1	B	75	CYS	3.2
1	C	41	THR	3.2
1	B	78	ILE	3.2
1	B	173	GLN	3.2
1	B	134	ASN	3.1
1	B	13	SER	3.1
1	C	38	PHE	3.1
1	B	79	LEU	3.1
1	B	149	THR	3.1
1	C	107	GLN	3.1
1	B	170	ALA	3.1
1	C	63	LEU	3.0
1	A	46	ALA	3.0
1	A	183	PRO	3.0
1	A	121	GLY	3.0
1	B	151	THR	3.0
1	A	131	VAL	3.0
1	C	92	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	160	ALA	3.0
1	A	153	LYS	2.9
1	A	167	ILE	2.9
1	B	164	PRO	2.9
1	A	119	LEU	2.9
1	A	182	LYS	2.9
1	A	187	ALA	2.9
1	C	74	GLU	2.9
1	C	80	THR	2.9
1	B	111	VAL	2.9
1	A	100	ASN	2.9
1	A	174	ILE	2.9
1	A	159	ARG	2.9
1	B	176	GLY	2.9
1	C	169	THR	2.9
1	C	19	SER	2.9
1	A	135	LEU	2.9
1	B	135	LEU	2.9
1	C	170	ALA	2.8
1	C	89	PRO	2.8
1	B	177	ARG	2.8
1	B	102	PRO	2.8
1	A	171	SER	2.8
1	A	35	PRO	2.8
1	B	30	PRO	2.8
1	C	115	GLN	2.8
1	A	60	ILE	2.8
1	A	120	GLY	2.7
1	B	77	ALA	2.7
1	C	154	LEU	2.7
1	B	169	THR	2.7
1	A	42	THR	2.7
1	C	171	SER	2.7
1	C	69	HIS	2.7
1	B	84	LEU	2.7
1	B	150	ASP	2.7
1	B	138	VAL	2.7
1	B	86	VAL	2.7
1	C	164	PRO	2.7
1	C	128	THR	2.7
1	A	39	GLU	2.6
1	C	79	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	43	PHE	2.6
1	A	181	SER	2.6
1	C	22	SER	2.6
1	C	40	ALA	2.6
1	A	118	VAL	2.6
1	B	136	ASP	2.6
1	C	73	VAL	2.6
1	A	112	TYR	2.6
1	B	6	VAL	2.5
1	A	157	TYR	2.5
1	B	159	ARG	2.5
1	A	61	THR	2.5
1	C	149	THR	2.5
1	C	144	ASP	2.5
1	B	115	GLN	2.5
1	A	65	ALA	2.5
1	A	146	VAL	2.5
1	C	147	THR	2.5
1	B	168	PRO	2.5
1	A	129	ILE	2.5
1	B	171	SER	2.5
1	B	55	GLN	2.4
1	C	100	ASN	2.4
1	B	143	LYS	2.4
1	B	51	GLN	2.4
1	B	56	THR	2.4
1	C	116	SER	2.4
1	B	47	GLU	2.4
1	B	14	ILE	2.4
1	C	46	ALA	2.4
1	A	68	ARG	2.4
1	B	12	ALA	2.4
1	A	166	LYS	2.3
1	C	120	GLY	2.3
1	C	10	LYS	2.3
1	A	52	VAL	2.3
1	A	105	PRO	2.3
1	A	133	LEU	2.3
1	C	140	ARG	2.3
1	C	112	TYR	2.3
1	C	81	PRO	2.3
1	A	93	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	101	SER	2.3
1	B	127	LYS	2.3
1	B	19	SER	2.3
1	C	122	ALA	2.3
1	B	58	ASP	2.2
1	C	83	ASP	2.2
1	B	11	GLN	2.2
1	A	123	ILE	2.2
1	B	62	LYS	2.2
1	C	178	ILE	2.2
1	B	175	SER	2.2
1	B	66	PRO	2.2
1	B	154	LEU	2.2
1	C	130	GLU	2.2
1	C	152	PRO	2.2
1	C	125	ALA	2.1
1	C	153	LYS	2.1
1	B	147	THR	2.1
1	B	179	ARG	2.1
1	C	150	ASP	2.1
1	A	132	PRO	2.1
1	A	57	ALA	2.1
1	C	114	GLY	2.1
1	A	94	LEU	2.1
1	B	125	ALA	2.0
1	C	70	ALA	2.0
1	B	152	PRO	2.0
1	B	186	ILE	2.0
1	B	145	SER	2.0

## 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 ⓘ

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.