



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:34 PM UTC

PDB ID : 1DDL / pdb_00001ddl
Title : DESMODIUM YELLOW MOTTLE TYMOVIRUS
Authors : Larson, S.B.; Day, J.; Canady, M.A.; Greenwood, A.; McPherson, A.
Deposited on : 1999-11-10
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

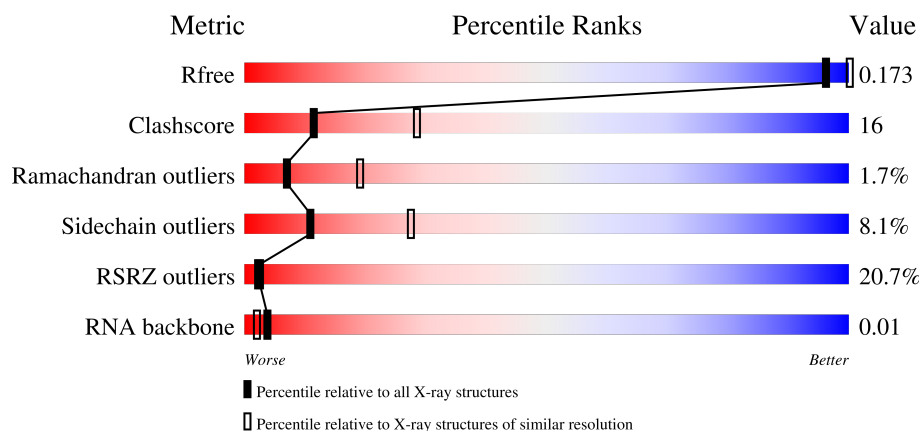
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)
RNA backbone	3983	1044 (2.90-2.50)

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 $\leq 5\%$. 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	7	100% 29% 29% 43%
2	E	2	100% 100%
3	A	188	22% 74% 22% .
3	B	188	18% 77% 18% 5% .

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Mol	Chain	Length	Quality of chain
3	C	188	17% 70% 18% 5% • 7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4670 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*UP*UP*UP*UP*UP*UP*U)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	7	Total	C	N	O	P	24	0	0
			141	63	14	57	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	2	Total	C	N	O	P	8	0	0
			41	18	4	17	2			

- Molecule 3 is a protein called DESMODIUM YELLOW MOTTLE VIRUS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	188	Total	C	N	O	S	0	5	0
			1436	916	234	282	4			
3	B	188	Total	C	N	O	S	0	8	0
			1450	927	236	283	4			
3	C	175	Total	C	N	O	S	0	2	0
			1317	845	212	257	3			

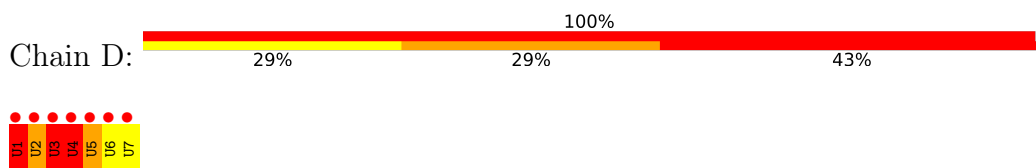
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	1	Total	O	0	0
			1	1		
4	A	106	Total	O	0	0
			106	106		
4	B	93	Total	O	0	0
			93	93		
4	C	85	Total	O	0	0
			85	85		

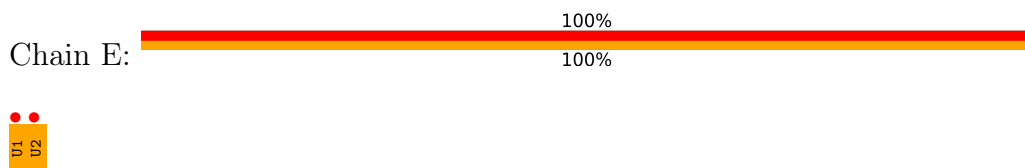
3 Residue-property plots

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 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.

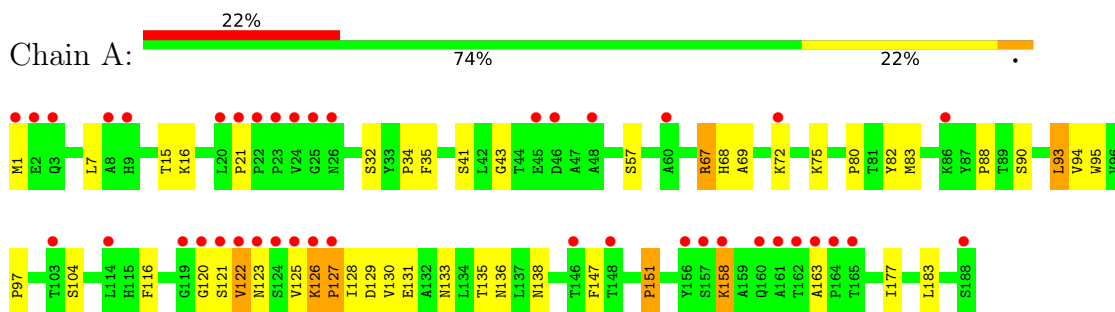
- Molecule 1: RNA (5'-R(P*UP*UP*UP*UP*UP*U)-3')



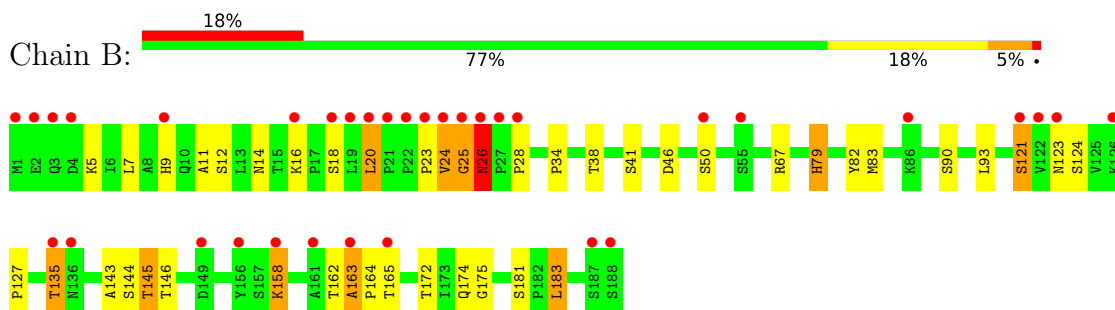
- Molecule 2: RNA (5'-R(P*UP*U)-3')



- Molecule 3: DESMODIUM YELLOW MOTTLE VIRUS

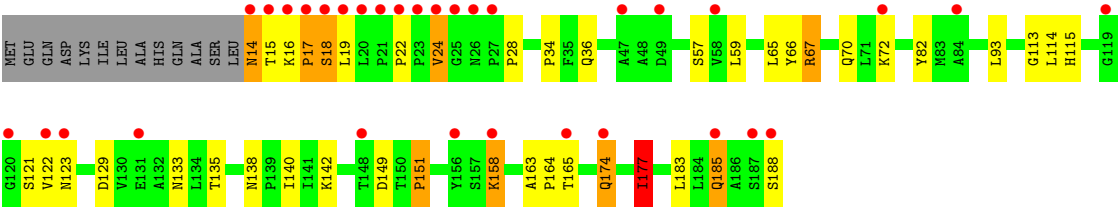


- Molecule 3: DESMODIUM YELLOW MOTTLE VIRUS



- Molecule 3: DESMODIUM YELLOW MOTTLE VIRUS





4 Data and refinement statistics

Property	Value	Source
Space group	P 42 3 2	Depositor
Cell constants a, b, c, α , β , γ	348.55Å 348.55Å 348.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.70 40.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	68.7 (40.00-2.70) 84.4 (40.00-2.70)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 2.69Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.151 , 0.159 0.167 , 0.173	Depositor DCC
R_{free} test set	17757 reflections (9.94%)	wwPDB-VP
Wilson B-factor (Å ²)	31.3	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 56.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.39	EDS
Total number of atoms	4670	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.46% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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	1.09	1/154 (0.6%)	1.58	5/234 (2.1%)
2	E	1.40	1/44 (2.3%)	1.30	0/64
3	A	0.71	2/1485 (0.1%)	1.20	7/2038 (0.3%)
3	B	0.72	3/1507 (0.2%)	1.20	7/2067 (0.3%)
3	C	0.71	2/1360 (0.1%)	1.24	7/1872 (0.4%)
All	All	0.74	9/4550 (0.2%)	1.23	26/6275 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	2
3	A	0	1
3	C	0	1
All	All	0	4

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1	U	OP3-P	7.19	1.62	1.48
1	D	1	U	OP3-P	6.83	1.62	1.48
3	A	34	PRO	CA-CB	-6.29	1.47	1.54
3	B	83	MET	CG-SD	-5.99	1.65	1.80
3	B	34	PRO	CA-CB	-5.86	1.47	1.54
3	B	127	PRO	CA-CB	-5.74	1.45	1.53
3	C	34	PRO	CA-CB	-5.47	1.46	1.54
3	A	80	PRO	CA-CB	-5.02	1.47	1.53
3	C	28	PRO	CA-CB	-5.01	1.49	1.54

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	4	U	C2'-C3'-O3'	8.36	122.03	109.50
1	D	1	U	C3'-C2'-O2'	7.31	121.67	110.70
3	B	121	SER	CA-C-N	6.82	132.02	120.29
3	B	121	SER	C-N-CA	6.82	132.02	120.29
3	C	177	ILE	CB-CA-C	-6.81	100.46	110.81
3	A	135	THR	N-CA-C	-6.33	105.59	113.38
3	C	123	ASN	CA-C-N	-6.20	112.35	122.65
3	C	123	ASN	C-N-CA	-6.20	112.35	122.65
3	C	22	PRO	N-CA-C	5.92	117.92	110.70
1	D	3	U	C2'-C3'-O3'	-5.84	104.93	113.70
3	B	79	HIS	CB-CA-C	-5.84	103.68	110.17
3	B	145	THR	CB-CA-C	-5.80	99.69	109.50
3	C	135	THR	N-CA-C	-5.79	106.20	113.72
3	B	135	THR	N-CA-C	-5.74	106.44	113.50
3	A	163	ALA	CA-C-N	5.56	126.02	120.52
3	A	163	ALA	C-N-CA	5.56	126.02	120.52
1	D	6	U	C2'-C3'-O3'	-5.31	105.73	113.70
3	A	43	GLY	N-CA-C	5.27	120.96	114.69
1	D	1	U	N1-C1'-C2'	-5.23	104.16	112.00
3	A	151	PRO	N-CA-C	5.22	119.29	111.14
3	A	21	PRO	CA-C-N	-5.14	115.96	119.66
3	A	21	PRO	C-N-CA	-5.14	115.96	119.66
3	C	140	ILE	CB-CA-C	-5.13	106.36	111.80
3	B	163	ALA	CA-C-N	5.09	125.56	120.52
3	B	163	ALA	C-N-CA	5.09	125.56	120.52
3	C	151	PRO	N-CA-C	5.07	118.84	111.03

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	67	ARG	Sidechain
3	C	67	ARG	Sidechain
1	D	1	U	Sidechain
1	D	3	U	Sidechain

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	141	0	71	37	0
2	E	41	0	21	18	0
3	A	1436	0	1442	46	0
3	B	1450	0	1464	56	0
3	C	1317	0	1333	46	0
4	A	106	0	0	7	0
4	B	93	0	0	4	0
4	C	85	0	0	1	0
4	E	1	0	0	0	0
All	All	4670	0	4331	140	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 16.

All (140) 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:D:1:U:H2'	1:D:2:U:C4'	1.54	1.35
2:E:2:U:H1'	3:A:95:TRP:N	1.55	1.21
1:D:1:U:H2'	1:D:2:U:C5'	1.70	1.20
2:E:2:U:C1'	3:A:95:TRP:H	1.65	1.08
2:E:2:U:H1'	3:A:95:TRP:H	0.89	1.05
3:A:88:PRO:HG3	3:A:120:GLY:HA2	1.38	1.03
1:D:1:U:H2'	1:D:2:U:H4'	1.07	1.03
1:D:3:U:H4'	3:B:9[A]:HIS:HD2	1.18	1.03
1:D:1:U:C2'	1:D:2:U:H5'	1.88	1.02
1:D:1:U:C2'	1:D:2:U:H4'	1.88	1.01
1:D:1:U:H2'	1:D:2:U:H5'	1.43	1.00
1:D:3:U:H5''	3:B:11:ALA:HB2	1.48	0.95
2:E:2:U:HO2'	3:A:95:TRP:HD1	1.16	0.93
3:B:20:LEU:CD1	3:C:17:PRO:HG2	1.99	0.91
3:B:20:LEU:HD11	3:C:17:PRO:HG2	1.53	0.91
1:D:3:U:H5''	3:B:11:ALA:CB	2.01	0.90
1:D:3:U:C5'	3:B:11:ALA:HB2	2.01	0.89
1:D:1:U:C2'	1:D:2:U:C5'	2.49	0.89
1:D:1:U:O2'	3:C:114:LEU:CD2	2.21	0.88
2:E:2:U:HO2'	3:A:95:TRP:CD1	1.92	0.88
2:E:2:U:C1'	3:A:94:VAL:HG23	2.04	0.87
1:D:1:U:C2'	1:D:2:U:C4'	2.48	0.85
1:D:3:U:H4'	3:B:9[A]:HIS:CD2	2.09	0.84
3:B:28:PRO:HG2	3:C:16:LYS:HB2	1.58	0.83
2:E:2:U:C1'	3:A:94:VAL:CG2	2.58	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:25:GLY:O	3:B:26:ASN:HB2	1.78	0.82
2:E:1:U:H3'	3:A:133:ASN:HD22	1.46	0.81
3:B:123:ASN:CG	3:B:124:SER:H	1.89	0.80
1:D:1:U:O2'	3:C:114:LEU:HD21	1.79	0.80
3:A:72:LYS:CD	4:A:2182:HOH:O	2.30	0.79
3:C:66:TYR:O	3:C:142:LYS:HE2	1.83	0.79
3:A:88:PRO:HG3	3:A:120:GLY:CA	2.13	0.78
1:D:2:U:H5'	3:C:114:LEU:HD23	1.64	0.78
3:B:20:LEU:HD11	3:C:17:PRO:CG	2.14	0.77
3:A:122:VAL:HG23	3:A:123:ASN:N	1.99	0.76
3:C:65:LEU:CD2	3:C:185[B]:GLN:HE22	1.99	0.75
3:A:72:LYS:HD2	4:A:2182:HOH:O	1.87	0.74
3:B:5:LYS:HE2	3:C:129:ASP:OD1	1.90	0.71
3:B:143:ALA:HB1	3:C:18:SER:HB3	1.71	0.71
3:C:14:ASN:O	3:C:15:THR:HG22	1.91	0.70
1:D:1:U:O2'	3:C:114:LEU:HD23	1.91	0.70
2:E:2:U:OP2	3:A:133:ASN:HB2	1.93	0.69
2:E:2:U:O2'	3:A:95:TRP:CD1	2.45	0.69
3:A:93:LEU:HD11	3:A:130:VAL:HG21	1.73	0.68
2:E:2:U:O2'	3:A:95:TRP:HD1	1.77	0.68
3:C:17:PRO:O	3:C:18:SER:HB3	1.94	0.68
3:B:123:ASN:CG	3:B:124:SER:N	2.51	0.67
3:B:181:SER:HA	3:C:14:ASN:HB3	1.76	0.67
2:E:2:U:H4'	3:A:95:TRP:HB2	1.77	0.66
1:D:3:U:C5'	3:B:11:ALA:CA	2.74	0.66
3:B:20:LEU:HD12	3:C:17:PRO:HG2	1.75	0.65
1:D:3:U:C5'	3:B:11:ALA:CB	2.69	0.64
3:B:67:ARG:HG3	3:B:183:LEU:HB2	1.80	0.64
3:C:65:LEU:HD22	3:C:185[B]:GLN:HE22	1.63	0.64
1:D:3:U:H5'	3:B:11:ALA:CA	2.28	0.63
3:A:97:PRO:HG2	3:B:183:LEU:HD13	1.79	0.63
3:A:57[B]:SER:HB3	4:A:2113:HOH:O	2.00	0.62
1:D:1:U:O2'	1:D:2:U:H5'	1.98	0.62
3:A:128:ILE:HD12	3:A:128:ILE:H	1.65	0.62
3:B:144:SER:OG	3:C:17:PRO:HA	2.00	0.61
3:A:1:MET:HG2	3:A:1:MET:O	1.99	0.61
1:D:1:U:C2'	1:D:2:U:O3'	2.49	0.60
3:C:93:LEU:HD12	3:C:93:LEU:C	2.27	0.60
3:B:181:SER:HA	3:C:14:ASN:CB	2.32	0.60
3:B:93:LEU:C	3:B:93:LEU:HD12	2.26	0.60
3:B:123:ASN:ND2	3:B:124:SER:H	1.99	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:131:GLU:HG2	4:A:2184:HOH:O	2.00	0.60
3:B:162:THR:HB	4:B:2266:HOH:O	2.01	0.60
3:A:83:MET:HA	3:A:83:MET:HE2	1.84	0.59
1:D:2:U:OP1	3:C:115:HIS:N	2.22	0.58
1:D:3:U:C5'	3:B:11:ALA:HA	2.33	0.58
1:D:3:U:H5''	3:B:11:ALA:CA	2.33	0.58
3:A:122:VAL:HG23	3:A:123:ASN:OD1	2.04	0.57
1:D:5:U:H5'	3:B:14:ASN:HB2	1.88	0.56
3:B:18:SER:HB3	4:B:2263:HOH:O	2.06	0.56
3:B:20:LEU:CD1	3:C:17:PRO:CG	2.75	0.56
3:A:126:LYS:O	3:A:127:PRO:O	2.25	0.55
3:A:69:ALA:HB1	3:A:177:ILE:HD11	1.88	0.55
3:B:38:THR:HA	3:B:172:THR:HG22	1.88	0.55
1:D:3:U:H5'	3:B:11:ALA:N	2.21	0.55
2:E:2:U:OP2	3:A:133:ASN:CB	2.54	0.55
3:B:163:ALA:HB1	3:B:164:PRO:HD2	1.89	0.54
3:A:158:LYS:HG2	4:A:2128:HOH:O	2.07	0.54
3:C:14:ASN:N	3:C:14:ASN:ND2	2.55	0.54
3:C:14:ASN:O	3:C:15:THR:CG2	2.56	0.53
3:A:138:ASN:O	3:A:151:PRO:HD3	2.07	0.53
1:D:3:U:P	3:B:11:ALA:HB2	2.49	0.53
2:E:2:U:OP1	3:A:136:ASN:ND2	2.35	0.53
3:B:143:ALA:HB1	3:C:18:SER:CB	2.39	0.53
3:B:23:PRO:O	3:B:24:VAL:C	2.52	0.53
1:D:3:U:H5'	3:B:11:ALA:HA	1.92	0.52
3:C:158:LYS:HE2	4:C:2331:HOH:O	2.09	0.52
3:B:181:SER:OG	3:C:16:LYS:HB3	2.10	0.51
4:B:2618:HOH:O	3:C:133:ASN:HB2	2.09	0.51
3:C:65:LEU:HD23	3:C:185[B]:GLN:HE22	1.74	0.51
1:D:1:U:C1'	1:D:2:U:O3'	2.60	0.50
3:B:46:ASP:OD2	3:B:158:LYS:HE2	2.11	0.50
3:B:123:ASN:OD1	3:B:124:SER:O	2.29	0.50
3:A:126:LYS:O	3:A:127:PRO:C	2.54	0.49
3:A:128:ILE:HD12	3:A:128:ILE:N	2.26	0.49
3:B:20:LEU:HD11	3:C:17:PRO:CB	2.43	0.49
3:A:72:LYS:HD3	4:A:2182:HOH:O	2.05	0.49
1:D:1:U:C3'	1:D:2:U:H5'	2.43	0.49
3:B:20:LEU:HG	3:C:17:PRO:HB2	1.96	0.48
3:B:135:THR:CG2	3:C:24:VAL:HG21	2.44	0.48
1:D:2:U:H5''	3:C:113:GLY:O	2.14	0.47
1:D:3:U:H5''	3:B:11:ALA:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:183:LEU:HD12	3:B:183:LEU:C	2.40	0.46
3:A:147:PHE:CZ	3:B:20:LEU:HD23	2.50	0.46
3:B:20:LEU:CD1	3:C:17:PRO:CB	2.93	0.46
2:E:2:U:C1'	3:A:94:VAL:HG22	2.44	0.46
3:C:59:LEU:HA	3:C:59:LEU:HD23	1.74	0.45
3:C:36:GLN:OE1	3:C:174:GLN:NE2	2.49	0.44
3:A:67:ARG:HG3	3:A:183:LEU:HB2	1.99	0.44
3:A:68:HIS:HD2	3:B:18:SER:OG	2.00	0.44
3:C:14:ASN:C	3:C:15:THR:HG22	2.43	0.44
3:C:138:ASN:O	3:C:151:PRO:HD3	2.17	0.43
2:E:2:U:C1'	3:A:95:TRP:N	2.43	0.43
3:A:183:LEU:HA	4:A:2105:HOH:O	2.17	0.43
3:B:181:SER:OG	3:C:14:ASN:HB2	2.19	0.43
2:E:1:U:H2'	2:E:2:U:OP2	2.19	0.42
3:B:135:THR:HG21	3:C:24:VAL:HG21	2.01	0.42
1:D:4:U:H5''	3:B:12:SER:O	2.19	0.42
3:C:177:ILE:HD13	3:C:177:ILE:HG21	1.78	0.42
1:D:1:U:H2'	1:D:2:U:C3'	2.36	0.42
3:A:116:PHE:CE2	3:A:128:ILE:HG21	2.54	0.42
3:C:67:ARG:HG2	3:C:183:LEU:HB2	2.02	0.42
3:C:163:ALA:HB1	3:C:164:PRO:HD2	2.01	0.42
2:E:2:U:O4'	3:A:94:VAL:CG2	2.68	0.42
3:A:147:PHE:CZ	3:B:20:LEU:CD2	3.02	0.42
3:A:15:THR:HG23	3:A:15:THR:O	2.19	0.41
3:A:75:LYS:HE3	3:A:129:ASP:OD2	2.20	0.41
1:D:1:U:O2'	1:D:2:U:O3'	2.39	0.41
3:C:149:ASP:OD2	3:C:149:ASP:N	2.53	0.41
3:C:16:LYS:N	3:C:17:PRO:HD3	2.36	0.41
3:B:145:THR:HG22	3:B:146:THR:N	2.35	0.41
3:B:174:GLN:HG2	3:B:175:GLY:N	2.36	0.41
4:B:2223:HOH:O	3:C:67:ARG:HB3	2.22	0.40
1:D:3:U:OP2	3:B:11:ALA:HB2	2.21	0.40
3:A:35:PHE:CD1	3:A:35:PHE:C	2.99	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	190/188 (101%)	179 (94%)	9 (5%)	2 (1%)	11	29
3	B	193/188 (103%)	178 (92%)	11 (6%)	4 (2%)	5	15
3	C	175/188 (93%)	168 (96%)	4 (2%)	3 (2%)	7	19
All	All	558/564 (99%)	525 (94%)	24 (4%)	9 (2%)	7	20

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	127	PRO
3	B	24	VAL
3	B	26	ASN
3	A	121	SER
3	C	17	PRO
3	B	121	SER
3	C	18	SER
3	B	25	GLY
3	C	24	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	166/161 (103%)	154 (93%)	12 (7%)	13	32
3	B	168/161 (104%)	154 (92%)	14 (8%)	10	26
3	C	152/161 (94%)	137 (90%)	15 (10%)	7	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	486/483 (101%)	445 (92%)	41 (8%)	11	26

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

Mol	Chain	Res	Type
3	A	7	LEU
3	A	16	LYS
3	A	32	SER
3	A	41	SER
3	A	82	TYR
3	A	90	SER
3	A	93	LEU
3	A	104	SER
3	A	122	VAL
3	A	125	VAL
3	A	126	LYS
3	A	158	LYS
3	B	7[A]	LEU
3	B	7[B]	LEU
3	B	16	LYS
3	B	20	LEU
3	B	26	ASN
3	B	41	SER
3	B	50[A]	SER
3	B	50[B]	SER
3	B	79	HIS
3	B	82	TYR
3	B	90	SER
3	B	158	LYS
3	B	165	THR
3	B	183	LEU
3	C	14	ASN
3	C	19	LEU
3	C	57	SER
3	C	70	GLN
3	C	72	LYS
3	C	82	TYR
3	C	121	SER
3	C	122	VAL
3	C	158	LYS
3	C	165	THR
3	C	174	GLN

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Mol	Chain	Res	Type
3	C	177	ILE
3	C	185[A]	GLN
3	C	185[B]	GLN
3	C	188	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	3	GLN
3	A	68	HIS
3	A	115	HIS
3	A	174	GLN
3	B	26	ASN
3	B	136	ASN
3	B	174	GLN
3	C	14	ASN
3	C	70	GLN
3	C	174	GLN
3	C	176	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	D	6/7 (85%)	5 (83%)	1 (16%)
2	E	1/2 (50%)	1 (100%)	0
All	All	7/9 (77%)	6 (85%)	1 (14%)

All (6) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	D	2	U
1	D	3	U
1	D	4	U
1	D	5	U
1	D	7	U
2	E	2	U

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	D	4	U

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 oligosaccharides 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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	D	7/7 (100%)	12.68	7 (100%) 0 0	14, 53, 74, 131	7 (100%)
2	E	2/2 (100%)	10.96	2 (100%) 0 0	62, 62, 62, 184	2 (100%)
3	A	188/188 (100%)	1.64	41 (21%) 2 2	8, 19, 88, 113	5 (2%)
3	B	188/188 (100%)	1.40	34 (18%) 3 3	6, 16, 68, 151	9 (4%)
3	C	175/188 (93%)	1.59	32 (18%) 3 3	7, 16, 115, 190	2 (1%)
All	All	560/573 (97%)	1.72	116 (20%) 2 2	6, 18, 96, 190	25 (4%)

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	B	25	GLY	16.2
2	E	1	U	15.8
1	D	1	U	15.5
3	B	23	PRO	14.5
1	D	2	U	14.3
1	D	3	U	13.6
1	D	4	U	12.7
1	D	7	U	12.7
3	B	22	PRO	11.7
1	D	6	U	11.4
3	C	15	THR	10.9
3	C	24	VAL	10.7
3	A	1	MET	10.6
3	B	24	VAL	10.5
3	B	26	ASN	10.4
3	C	17	PRO	9.9
3	C	19	LEU	9.9
3	C	16	LYS	9.8
3	C	14	ASN	9.7
3	C	23	PRO	9.4

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Mol	Chain	Res	Type	RSRZ
3	C	22	PRO	9.2
3	A	121	SER	9.1
3	A	23	PRO	9.0
3	C	18	SER	8.9
3	C	21	PRO	8.8
3	C	20	LEU	8.6
3	B	1	MET	8.5
3	A	126	LYS	8.5
1	D	5	U	8.4
3	B	21	PRO	8.4
3	C	25	GLY	8.3
3	A	122	VAL	7.7
3	C	26	ASN	7.0
3	A	24	VAL	7.0
3	A	26	ASN	7.0
3	B	188[A]	SER	6.9
3	A	25	GLY	6.8
3	C	188	SER	6.6
3	A	22	PRO	6.4
3	A	125	VAL	6.3
3	A	2	GLU	6.2
3	A	188[A]	SER	6.2
2	E	2	U	6.1
3	B	2	GLU	5.9
3	A	3	GLN	5.8
3	B	27	PRO	5.5
3	A	123	ASN	5.5
3	B	20	LEU	5.4
3	A	124	SER	5.3
3	A	120	GLY	4.9
3	B	3	GLN	4.5
3	A	21	PRO	4.5
3	B	121	SER	4.2
3	C	123	ASN	4.0
3	A	86	LYS	3.9
3	A	163	ALA	3.7
3	C	122	VAL	3.7
3	A	158	LYS	3.6
3	C	185[A]	GLN	3.6
3	A	9[A]	HIS	3.5
3	C	27	PRO	3.4
3	B	9[A]	HIS	3.4

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Mol	Chain	Res	Type	RSRZ
3	B	18	SER	3.3
3	A	165	THR	3.3
3	A	156	TYR	3.2
3	A	161	ALA	3.1
3	B	165	THR	3.0
3	B	19	LEU	3.0
3	B	156	TYR	2.9
3	C	47	ALA	2.9
3	B	158	LYS	2.8
3	B	86	LYS	2.8
3	C	72	LYS	2.7
3	A	160	GLN	2.7
3	A	127	PRO	2.7
3	C	148	THR	2.7
3	A	45	GLU	2.6
3	A	162	THR	2.6
3	B	4	ASP	2.6
3	B	126	LYS	2.6
3	B	28	PRO	2.6
3	A	20	LEU	2.6
3	C	158	LYS	2.5
3	B	136	ASN	2.5
3	A	103	THR	2.5
3	A	114	LEU	2.5
3	A	8	ALA	2.4
3	A	119	GLY	2.4
3	B	149	ASP	2.4
3	A	164	PRO	2.4
3	C	120	GLY	2.4
3	C	174	GLN	2.4
3	A	48	ALA	2.4
3	C	165	THR	2.3
3	A	46	ASP	2.3
3	C	187	SER	2.3
3	C	156	TYR	2.3
3	A	148	THR	2.3
3	A	72	LYS	2.3
3	C	131	GLU	2.3
3	B	55	SER	2.3
3	C	49	ASP	2.3
3	A	146	THR	2.3
3	B	16	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
3	B	187[A]	SER	2.3
3	C	84	ALA	2.3
3	C	58	VAL	2.3
3	B	135	THR	2.2
3	C	119	GLY	2.2
3	B	122	VAL	2.2
3	A	60	ALA	2.1
3	A	157	SER	2.1
3	B	161	ALA	2.0
3	B	163	ALA	2.0
3	B	50[A]	SER	2.0
3	B	123	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.