



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:27 PM UTC

PDB ID : 1C04 / pdb_00001c04
Title : IDENTIFICATION OF KNOWN PROTEIN AND RNA STRUCTURES IN A
5 A MAP OF THE LARGE RIBOSOMAL SUBUNIT FROM HALOARCUA
MARISMORTUI
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Deposited on : 1999-07-14
Resolution : 5.00 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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
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

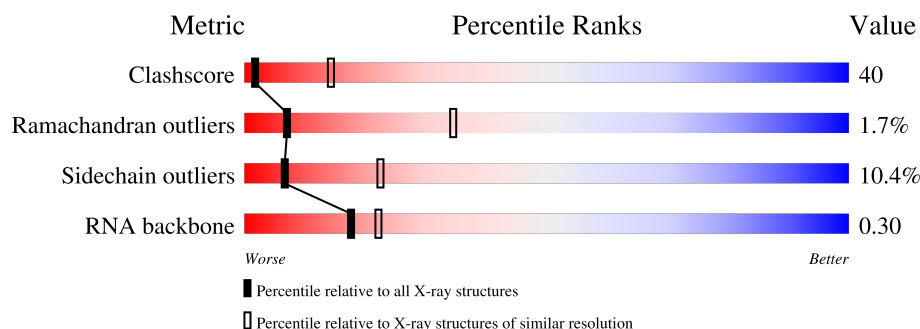
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.00 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	1040 (6.00-4.00)
Ramachandran outliers	187476	1015 (6.06-3.92)
Sidechain outliers	187428	1136 (6.10-3.90)
RNA backbone	3983	1045 (6.76-3.10)

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	E	58	
2	F	29	
3	A	137	
4	B	177	
5	C	67	
6	D	122	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5570 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 23S RRNA FRAGMENT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	58	Total	C	N	O	P	0	0	0
			1243	556	229	400	58			

- Molecule 2 is a RNA chain called 23S RRNA FRAGMENT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	29	Total	C	N	O	P	1	0	0
			621	278	118	197	28			

- Molecule 3 is a protein called RIBOSOMAL PROTEIN L2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	A	135	Total	C	N	O	S	Se	0	0	0
			1024	645	187	188	1	3			

- Molecule 4 is a protein called RIBOSOMAL PROTEIN L6.

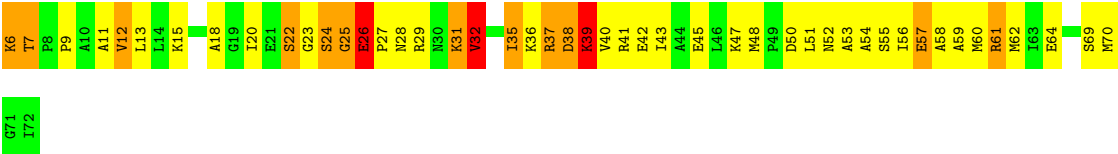
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	164	Total	C	N	O	S	0	0	0
			1251	787	225	237	2			

- Molecule 5 is a protein called RIBOSOMAL PROTEIN L11.

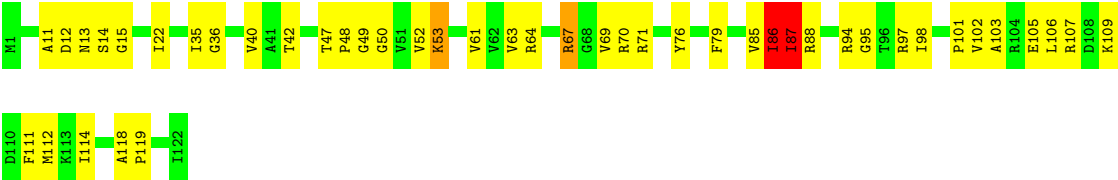
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	67	Total	C	N	O	S	0	0	0
			494	304	92	94	4			

- Molecule 6 is a protein called RIBOSOMAL PROTEIN L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	122	Total	C	N	O	S	0	0	0
			937	585	180	169	3			



● Molecule 6: RIBOSOMAL PROTEIN L14



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	212.00Å 301.40Å 576.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	60.00 – 5.00	Depositor
% Data completeness (in resolution range)	(Not available) (60.00-5.00)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5570	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

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	E	1.34	4/1392 (0.3%)	2.42	122/2168 (5.6%)
2	F	0.61	0/695	0.95	1/1083 (0.1%)
3	A	0.64	3/1034 (0.3%)	1.00	7/1388 (0.5%)
4	B	0.84	0/1270	1.09	8/1715 (0.5%)
5	C	0.70	0/497	1.25	6/663 (0.9%)
6	D	1.33	2/946 (0.2%)	1.57	8/1269 (0.6%)
All	All	1.01	9/5834 (0.2%)	1.60	152/8286 (1.8%)

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	E	0	4
6	D	0	1
All	All	0	5

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	86	ILE	C-N	-28.36	0.95	1.33
6	D	87	ILE	C-N	24.24	1.67	1.33
3	A	113	MSE	SE-CE	-6.99	1.74	1.95
3	A	116	MSE	SE-CE	-6.39	1.76	1.95
1	E	50	C	O3'-P	-6.26	1.51	1.61
3	A	182	MSE	SE-CE	-6.21	1.76	1.95
1	E	52	C	O3'-P	-5.66	1.52	1.61
1	E	50	C	C4'-C3'	-5.51	1.44	1.52
1	E	14	C	C4'-O4'	-5.04	1.38	1.45

All (152) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	86	ILE	O-C-N	-19.80	97.81	122.57
6	D	87	ILE	CA-C-N	-19.16	84.95	121.54
6	D	87	ILE	C-N-CA	-19.16	84.95	121.54
6	D	86	ILE	CA-C-N	-18.67	88.37	121.97
6	D	86	ILE	C-N-CA	-18.67	88.37	121.97
1	E	50	C	C1'-C2'-O2'	17.73	135.00	108.40
1	E	20	A	N9-C1'-C2'	-17.01	88.48	114.00
1	E	53	A	C2'-C3'-O3'	-16.05	89.62	113.70
1	E	47	U	C4'-C3'-C2'	-15.18	87.42	102.60
1	E	53	A	O5'-P-OP2	-14.59	64.23	108.00
1	E	54	C	N1-C1'-C2'	13.90	132.85	112.00
1	E	50	C	O4'-C4'-C3'	-13.18	90.82	104.00
1	E	40	A	C1'-C2'-O2'	13.01	127.92	108.40
6	D	87	ILE	O-C-N	12.76	138.52	122.57
1	E	58	U	C2'-C3'-O3'	11.77	131.35	113.70
1	E	51	U	C1'-C2'-O2'	10.78	124.57	108.40
1	E	27	A	C1'-C2'-O2'	10.58	124.27	108.40
1	E	4	A	C1'-C2'-O2'	10.56	124.24	108.40
1	E	50	C	C3'-C2'-C1'	-10.55	90.75	101.30
1	E	24	G	C1'-C2'-O2'	10.39	123.98	108.40
1	E	42	C	C4'-C3'-C2'	-10.36	92.24	102.60
1	E	30	A	C4'-C3'-C2'	-10.36	92.24	102.60
1	E	19	A	N9-C1'-C2'	10.25	129.38	114.00
1	E	55	U	C1'-C2'-O2'	10.25	123.77	108.40
1	E	39	A	C1'-C2'-O2'	10.14	127.00	111.80
1	E	8	U	C1'-C2'-O2'	9.88	123.21	108.40
1	E	54	C	P-O3'-C3'	-9.80	105.50	120.20
1	E	56	G	C1'-C2'-O2'	9.80	123.09	108.40
1	E	6	G	C1'-C2'-O2'	9.72	122.98	108.40
1	E	43	G	C1'-C2'-O2'	9.71	122.96	108.40
1	E	58	U	O5'-P-OP2	-9.69	78.93	108.00
1	E	37	G	N9-C1'-C2'	9.54	126.31	112.00
1	E	41	G	C1'-C2'-O2'	9.44	122.57	108.40
1	E	41	G	C2'-C3'-O3'	9.41	127.81	113.70
1	E	50	C	C4'-C3'-C2'	9.39	111.99	102.60
1	E	54	C	P-O5'-C5'	-9.26	107.01	120.90
1	E	53	A	C4'-C3'-C2'	8.93	111.53	102.60
1	E	31	U	C2'-C3'-O3'	-8.91	100.34	113.70
1	E	24	G	N9-C1'-C2'	8.68	125.02	112.00
1	E	20	A	O4'-C1'-C2'	8.59	114.39	105.80
1	E	34	A	C1'-C2'-O2'	8.51	121.16	108.40
1	E	41	G	N9-C1'-C2'	8.49	124.74	112.00
1	E	54	C	C2'-C3'-O3'	8.48	126.42	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	45	A	C1'-C2'-O2'	8.41	121.02	108.40
5	C	26	GLU	N-CA-C	8.39	128.34	109.81
1	E	23	A	C1'-C2'-O2'	8.38	120.98	108.40
1	E	9	G	C1'-C2'-O2'	8.35	120.93	108.40
1	E	20	A	C1'-O4'-C4'	-8.26	101.44	109.70
1	E	25	C	C1'-C2'-O2'	8.14	120.61	108.40
1	E	9	G	N9-C1'-C2'	8.13	124.20	112.00
1	E	19	A	C1'-C2'-O2'	8.12	123.98	111.80
1	E	28	U	C1'-C2'-O2'	8.00	120.40	108.40
1	E	52	C	C4'-C3'-C2'	-7.62	94.97	102.60
1	E	19	A	C3'-C2'-C1'	-7.62	93.88	101.50
1	E	5	G	C3'-C2'-C1'	-7.61	93.69	101.30
1	E	14	C	C4'-C3'-C2'	-7.54	95.06	102.60
1	E	31	U	C1'-C2'-O2'	7.48	119.62	108.40
1	E	11	A	C1'-C2'-O2'	7.47	123.00	111.80
1	E	31	U	C4'-C3'-C2'	7.45	110.05	102.60
1	E	32	U	C1'-C2'-O2'	7.43	119.55	108.40
1	E	39	A	N9-C1'-C2'	-7.43	102.86	114.00
1	E	44	U	C1'-C2'-O2'	7.41	119.52	108.40
1	E	39	A	C3'-C2'-C1'	-7.40	94.10	101.50
1	E	15	U	C1'-C2'-O2'	7.14	119.12	108.40
1	E	16	U	C4'-C3'-C2'	-7.12	95.48	102.60
1	E	55	U	C2'-C3'-O3'	-7.09	103.06	113.70
1	E	53	A	C1'-C2'-O2'	7.04	118.96	108.40
1	E	11	A	N9-C1'-C2'	-7.00	103.50	114.00
1	E	31	U	O4'-C4'-C3'	-6.98	97.02	104.00
1	E	9	G	C4'-C3'-C2'	6.97	109.57	102.60
1	E	21	G	C4'-C3'-C2'	-6.96	95.64	102.60
5	C	25	GLY	N-CA-C	-6.95	96.70	113.18
1	E	7	A	N9-C1'-C2'	-6.94	101.59	112.00
1	E	18	G	C1'-C2'-O2'	6.91	118.76	108.40
1	E	50	C	P-O3'-C3'	-6.88	109.87	120.20
1	E	12	G	C1'-C2'-O2'	6.85	118.68	108.40
1	E	49	G	C2'-C3'-O3'	6.76	123.84	113.70
1	E	38	A	N9-C1'-C2'	6.70	124.04	114.00
1	E	57	G	C1'-C2'-O2'	6.68	118.42	108.40
1	E	12	G	N9-C1'-C2'	6.65	121.97	112.00
1	E	23	A	C2'-C3'-O3'	-6.64	103.74	113.70
1	E	39	A	O4'-C1'-C2'	6.63	112.43	105.80
1	E	9	G	O4'-C4'-C3'	-6.59	97.41	104.00
4	B	154	GLU	CA-C-N	6.56	127.08	119.47
4	B	154	GLU	C-N-CA	6.56	127.08	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	39	LYS	N-CA-C	6.48	119.31	111.40
1	E	54	C	C1'-C2'-O2'	6.41	118.02	108.40
1	E	17	A	C1'-C2'-O2'	6.37	117.96	108.40
1	E	33	U	C1'-C2'-O2'	6.36	117.94	108.40
1	E	38	A	C4'-C3'-C2'	6.33	108.94	102.60
6	D	40	VAL	N-CA-C	-6.33	99.31	108.36
1	E	10	U	N1-C1'-C2'	6.20	123.30	114.00
1	E	2	C	N1-C1'-C2'	-6.19	102.71	112.00
1	E	27	A	C1'-O4'-C4'	-6.17	103.73	109.90
1	E	55	U	N1-C1'-C2'	-6.11	102.83	112.00
1	E	21	G	C4'-C3'-O3'	-6.10	103.85	113.00
1	E	10	U	C1'-C2'-O2'	6.10	120.95	111.80
1	E	27	A	O4'-C1'-C2'	6.08	113.68	107.60
1	E	39	A	C1'-O4'-C4'	-6.02	103.68	109.70
1	E	55	U	C4'-C3'-C2'	6.02	108.62	102.60
3	A	104	ILE	N-CA-C	-6.02	101.78	109.30
1	E	22	C	C4'-C3'-C2'	-5.97	96.63	102.60
1	E	57	G	P-O3'-C3'	-5.92	111.32	120.20
1	E	42	C	C3'-C2'-C1'	-5.88	95.42	101.30
3	A	73	ILE	N-CA-C	5.88	112.91	107.56
1	E	8	U	O4'-C4'-C3'	-5.87	98.13	104.00
1	E	38	A	C1'-C2'-O2'	5.87	120.61	111.80
1	E	54	C	O4'-C1'-C2'	-5.84	101.76	107.60
1	E	27	A	P-O5'-C5'	-5.83	112.16	120.90
1	E	9	G	P-O3'-C3'	-5.82	111.47	120.20
4	B	155	PRO	N-CA-C	5.82	122.25	113.81
1	E	10	U	P-O5'-C5'	-5.80	112.20	120.90
1	E	20	A	C4'-C3'-O3'	5.73	117.99	109.40
1	E	53	A	N9-C1'-C2'	-5.68	103.47	112.00
1	E	50	C	C4'-C3'-O3'	-5.66	104.51	113.00
1	E	23	A	C4'-C3'-C2'	5.62	108.22	102.60
1	E	48	A	C2'-C3'-O3'	5.61	122.12	113.70
1	E	25	C	P-O5'-C5'	-5.60	112.50	120.90
1	E	53	A	OP1-P-OP2	5.59	136.37	119.60
1	E	58	U	C4'-C3'-C2'	-5.57	97.03	102.60
1	E	1	G	N9-C1'-C2'	-5.55	103.67	112.00
3	A	134	ILE	N-CA-C	5.51	113.89	107.89
5	C	22	SER	N-CA-C	5.50	117.16	108.96
1	E	44	U	P-O5'-C5'	-5.49	112.67	120.90
1	E	39	A	P-O5'-C5'	-5.49	112.67	120.90
4	B	101	LYS	N-CA-C	5.48	118.86	110.20
1	E	40	A	C3'-C2'-C1'	-5.44	95.86	101.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	35	ILE	N-CA-C	5.44	116.59	108.54
2	F	6	C	O4'-C4'-C3'	-5.39	98.61	104.00
1	E	51	U	O5'-P-OP2	5.38	124.14	108.00
5	C	31	LYS	N-CA-C	5.37	119.68	113.18
1	E	8	U	N1-C1'-C2'	5.37	120.05	112.00
6	D	112	MET	N-CA-C	5.34	117.10	111.28
1	E	11	A	C3'-C2'-C1'	-5.32	96.18	101.50
1	E	19	A	O5'-C5'-C4'	-5.28	103.78	111.70
4	B	100	LYS	N-CA-C	-5.24	106.84	113.18
1	E	42	C	N1-C1'-C2'	5.20	119.79	112.00
1	E	47	U	C1'-O4'-C4'	-5.17	104.73	109.90
4	B	74	MET	N-CA-C	-5.17	105.73	111.36
1	E	26	C	C5'-C4'-C3'	-5.15	108.27	116.00
1	E	11	A	O4'-C1'-C2'	5.14	110.94	105.80
3	A	134	ILE	CA-C-N	5.12	125.36	119.83
3	A	134	ILE	C-N-CA	5.12	125.36	119.83
4	B	152	PRO	CA-C-N	5.10	125.34	119.83
4	B	152	PRO	C-N-CA	5.10	125.34	119.83
1	E	51	U	OP1-P-OP2	-5.08	104.37	119.60
3	A	118	GLY	CA-C-N	5.07	124.85	119.28
3	A	118	GLY	C-N-CA	5.07	124.85	119.28
1	E	46	A	C2'-C3'-O3'	-5.06	106.11	113.70
1	E	19	A	P-O5'-C5'	-5.05	113.32	120.90
1	E	7	A	C5'-C4'-C3'	-5.01	108.48	116.00
1	E	48	A	C1'-C2'-O2'	5.01	115.91	108.40

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	D	86	ILE	Mainchain
1	E	19	A	Sidechain
1	E	37	G	Sidechain
1	E	45	A	Sidechain
1	E	48	A	Sidechain

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	E	1243	0	625	130	0
2	F	621	0	318	31	0
3	A	1024	0	1073	51	0
4	B	1251	0	1294	55	0
5	C	494	0	524	134	0
6	D	937	0	995	116	31
All	All	5570	0	4829	417	31

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 40.

All (417) 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)
6:D:79:PHE:CZ	6:D:103:ALA:HB2	1.33	1.58
6:D:79:PHE:CZ	6:D:103:ALA:CB	1.87	1.57
6:D:63:VAL:CB	6:D:106:LEU:HD21	1.34	1.55
6:D:87:ILE:C	6:D:88:ARG:N	1.67	1.52
6:D:63:VAL:HG12	6:D:106:LEU:CD2	1.38	1.51
1:E:31:U:C5'	5:C:53:ALA:HA	1.23	1.49
1:E:31:U:H5'	5:C:53:ALA:CA	1.38	1.48
1:E:9:G:N2	5:C:62:MET:HE2	1.32	1.45
4:B:29:LYS:CG	4:B:81:GLY:N	1.78	1.45
6:D:61:VAL:HG21	6:D:111:PHE:CE2	1.50	1.43
1:E:9:G:C1'	5:C:50:ASP:O	1.66	1.41
6:D:61:VAL:HG11	6:D:111:PHE:CE1	1.54	1.39
6:D:85:VAL:HG11	6:D:114:ILE:CD1	1.53	1.37
6:D:63:VAL:CG1	6:D:106:LEU:CD2	2.01	1.37
6:D:79:PHE:CE1	6:D:103:ALA:HB2	1.60	1.36
6:D:61:VAL:HG11	6:D:111:PHE:CZ	1.62	1.34
6:D:63:VAL:CA	6:D:106:LEU:HD21	1.58	1.33
1:E:9:G:H4'	5:C:50:ASP:CA	1.59	1.32
1:E:26:C:H4'	5:C:26:GLU:OE2	1.26	1.31
6:D:85:VAL:CG1	6:D:114:ILE:HD11	1.59	1.31
1:E:29:C:O2	5:C:62:MET:HG2	1.32	1.30
1:E:9:G:C4'	5:C:50:ASP:CB	2.02	1.28
4:B:32:LEU:CD2	4:B:136:ASP:HB2	1.64	1.28
1:E:9:G:C2'	5:C:50:ASP:HB3	1.36	1.27
4:B:29:LYS:HG3	4:B:81:GLY:CA	1.65	1.26
6:D:64:ARG:NH1	6:D:102:VAL:HG12	1.51	1.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:63:VAL:CG1	6:D:106:LEU:HD21	1.61	1.24
6:D:63:VAL:HB	6:D:106:LEU:CD1	1.65	1.24
1:E:26:C:H4'	5:C:26:GLU:CD	1.55	1.22
6:D:87:ILE:C	6:D:88:ARG:CA	2.11	1.21
6:D:63:VAL:CB	6:D:106:LEU:CD2	2.14	1.21
1:E:27:A:H1'	5:C:69:SER:CB	1.71	1.19
1:E:26:C:C4'	5:C:26:GLU:OE2	1.89	1.19
1:E:26:C:C4'	5:C:26:GLU:CD	2.06	1.19
6:D:35:ILE:HG21	6:D:105:GLU:CB	1.74	1.17
1:E:9:G:H4'	5:C:50:ASP:CB	1.61	1.16
6:D:63:VAL:CG1	6:D:106:LEU:HD22	1.71	1.15
4:B:29:LYS:HG3	4:B:81:GLY:N	0.83	1.15
6:D:61:VAL:CG1	6:D:111:PHE:CZ	2.29	1.14
1:E:9:G:H1'	5:C:50:ASP:O	1.44	1.13
4:B:32:LEU:HD21	4:B:136:ASP:HB2	1.29	1.13
1:E:9:G:O4'	5:C:50:ASP:O	1.63	1.12
1:E:9:G:H4'	5:C:50:ASP:HA	1.18	1.12
1:E:9:G:C2'	5:C:50:ASP:CB	2.25	1.10
6:D:61:VAL:CG1	6:D:111:PHE:CE1	2.35	1.10
4:B:76:GLU:HB3	4:B:82:TYR:OH	1.52	1.09
1:E:9:G:C4'	5:C:50:ASP:CA	2.28	1.09
6:D:87:ILE:CA	6:D:88:ARG:N	2.15	1.09
6:D:36:GLY:HA2	6:D:109:LYS:HG3	1.32	1.09
1:E:29:C:O2'	5:C:62:MET:HA	1.50	1.09
1:E:30:A:N3	5:C:62:MET:HE1	1.66	1.08
6:D:64:ARG:HH11	6:D:102:VAL:HA	1.10	1.08
1:E:9:G:O2'	5:C:50:ASP:CB	2.02	1.07
6:D:35:ILE:HG21	6:D:105:GLU:HB3	1.19	1.07
6:D:79:PHE:CE1	6:D:103:ALA:CB	2.26	1.07
6:D:36:GLY:CA	6:D:109:LYS:HG3	1.85	1.07
6:D:85:VAL:CG2	6:D:114:ILE:HD13	1.85	1.06
6:D:63:VAL:HB	6:D:106:LEU:HD11	1.08	1.06
6:D:61:VAL:CB	6:D:111:PHE:CZ	2.39	1.06
1:E:30:A:C4	5:C:62:MET:CE	2.39	1.05
6:D:64:ARG:HH12	6:D:102:VAL:HG12	0.92	1.05
6:D:86:ILE:HG22	6:D:87:ILE:N	1.69	1.05
1:E:31:U:C5'	5:C:53:ALA:CA	2.03	1.04
1:E:9:G:N2	5:C:62:MET:CE	2.19	1.04
6:D:85:VAL:HG21	6:D:114:ILE:HD13	1.06	1.03
4:B:32:LEU:CD2	4:B:136:ASP:CB	2.37	1.02
1:E:30:A:C4	5:C:62:MET:HE3	1.93	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:10:U:OP1	5:C:47:LYS:NZ	1.93	1.01
6:D:64:ARG:HH12	6:D:102:VAL:CG1	1.71	1.01
6:D:61:VAL:CG2	6:D:111:PHE:CE2	2.42	1.01
6:D:63:VAL:HA	6:D:106:LEU:HD21	1.38	1.01
4:B:80:LYS:C	4:B:81:GLY:N	2.18	1.01
6:D:61:VAL:HG21	6:D:111:PHE:CZ	1.98	0.99
6:D:85:VAL:HG21	6:D:114:ILE:CD1	1.91	0.99
1:E:9:G:O2'	5:C:50:ASP:HB2	1.60	0.99
4:B:32:LEU:HD21	4:B:136:ASP:CB	1.93	0.99
6:D:79:PHE:HZ	6:D:103:ALA:CB	1.65	0.99
6:D:87:ILE:C	6:D:88:ARG:C	2.30	0.98
6:D:79:PHE:CZ	6:D:103:ALA:HB1	1.94	0.98
6:D:63:VAL:HB	6:D:106:LEU:CG	1.94	0.98
6:D:63:VAL:CB	6:D:106:LEU:HD11	1.93	0.98
6:D:13:ASN:ND2	6:D:97:ARG:H	1.62	0.96
6:D:79:PHE:CZ	6:D:103:ALA:CA	2.48	0.96
1:E:9:G:C4'	5:C:50:ASP:HA	1.93	0.96
1:E:27:A:H1'	5:C:69:SER:HB2	1.45	0.95
5:C:36:LYS:HG3	5:C:37:ARG:H	1.32	0.95
6:D:64:ARG:NH1	6:D:102:VAL:CG1	2.30	0.95
1:E:27:A:H1'	5:C:69:SER:HB3	1.47	0.95
4:B:29:LYS:CG	4:B:81:GLY:CA	2.32	0.95
6:D:35:ILE:CG2	6:D:105:GLU:HB3	1.97	0.94
6:D:61:VAL:HG21	6:D:111:PHE:HE2	1.21	0.94
1:E:29:C:O2	5:C:62:MET:CG	2.16	0.94
1:E:31:U:O2'	5:C:52:ASN:HA	1.67	0.94
6:D:63:VAL:HB	6:D:106:LEU:HD21	1.47	0.93
2:F:23:C:O2	2:F:23:C:H2'	1.66	0.92
1:E:26:C:O2'	5:C:69:SER:O	1.86	0.92
1:E:9:G:C2	5:C:62:MET:HE2	2.05	0.91
6:D:63:VAL:HG12	6:D:106:LEU:HD22	0.93	0.91
4:B:76:GLU:CB	4:B:82:TYR:OH	2.13	0.91
4:B:32:LEU:HD22	4:B:136:ASP:OD2	1.70	0.90
1:E:9:G:C4'	5:C:50:ASP:OD2	2.11	0.90
1:E:26:C:C2'	5:C:69:SER:O	2.20	0.89
4:B:32:LEU:HD22	4:B:136:ASP:HB2	1.53	0.89
6:D:63:VAL:HB	6:D:106:LEU:CD2	1.93	0.89
1:E:31:U:O2'	5:C:52:ASN:CA	2.18	0.88
6:D:87:ILE:HA	6:D:88:ARG:N	1.85	0.88
6:D:86:ILE:CG2	6:D:87:ILE:N	2.24	0.88
6:D:61:VAL:CG2	6:D:111:PHE:CZ	2.56	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:12:G:N2	5:C:69:SER:OG	2.07	0.87
4:B:29:LYS:HB3	4:B:81:GLY:HA2	1.55	0.87
1:E:9:G:O2'	5:C:50:ASP:HB3	1.69	0.87
6:D:63:VAL:HA	6:D:106:LEU:CD2	2.04	0.87
4:B:32:LEU:HD22	4:B:136:ASP:CB	2.03	0.87
5:C:48:MET:HE1	5:C:53:ALA:HB3	1.56	0.87
1:E:9:G:C1'	5:C:50:ASP:HB3	2.05	0.86
2:F:16:G:O2'	2:F:17:A:H5'	1.76	0.86
5:C:36:LYS:HG3	5:C:37:ARG:N	1.91	0.85
1:E:29:C:O2'	5:C:62:MET:CA	2.25	0.85
1:E:9:G:H22	5:C:62:MET:HE2	1.03	0.85
1:E:9:G:C1'	5:C:50:ASP:C	2.50	0.84
1:E:29:C:H2'	5:C:62:MET:CG	2.07	0.84
6:D:13:ASN:ND2	6:D:97:ARG:N	2.23	0.83
6:D:22:ILE:HD11	6:D:42:THR:HG23	1.59	0.83
1:E:30:A:N3	5:C:62:MET:CE	2.41	0.83
6:D:64:ARG:HH11	6:D:102:VAL:CA	1.90	0.83
1:E:11:A:O4'	1:E:20:A:H1'	1.79	0.82
1:E:9:G:C2	5:C:62:MET:CE	2.63	0.82
1:E:29:C:H2'	5:C:62:MET:HG2	1.59	0.82
4:B:32:LEU:HD22	4:B:136:ASP:CG	2.04	0.82
6:D:64:ARG:NH1	6:D:102:VAL:HA	1.93	0.81
1:E:31:U:C5'	5:C:53:ALA:C	2.54	0.81
2:F:12:A:H1'	2:F:20:A:N6	1.97	0.80
6:D:85:VAL:CG1	6:D:114:ILE:CD1	2.36	0.80
6:D:35:ILE:HG21	6:D:105:GLU:HB2	1.62	0.79
6:D:63:VAL:CB	6:D:106:LEU:CD1	2.55	0.79
4:B:32:LEU:HD21	4:B:136:ASP:CA	2.12	0.79
6:D:61:VAL:HG11	6:D:111:PHE:CD1	2.16	0.79
6:D:61:VAL:HB	6:D:111:PHE:CZ	2.16	0.79
2:F:21:A:H2'	2:F:22:C:C6	2.17	0.79
1:E:9:G:H1'	5:C:50:ASP:C	2.08	0.77
6:D:79:PHE:CE2	6:D:103:ALA:HB2	2.17	0.77
3:A:135:PRO:O	3:A:138:THR:HG23	1.84	0.77
4:B:29:LYS:CB	4:B:81:GLY:HA2	2.14	0.77
1:E:9:G:H5''	5:C:50:ASP:OD2	1.85	0.77
1:E:55:U:O2'	1:E:56:G:H5'	1.84	0.77
1:E:30:A:C4	5:C:62:MET:HE1	2.11	0.76
6:D:61:VAL:HB	6:D:111:PHE:HZ	1.51	0.76
1:E:9:G:C5'	5:C:50:ASP:OD2	2.34	0.76
5:C:36:LYS:CG	5:C:37:ARG:H	1.98	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:36:GLY:HA3	6:D:109:LYS:HG3	1.67	0.75
2:F:24:G:C2	2:F:25:C:C5	2.75	0.75
5:C:61:ARG:HG2	5:C:61:ARG:HH11	1.51	0.74
1:E:24:G:C2'	1:E:25:C:O5'	2.34	0.74
3:A:114:GLU:O	3:A:115:ILE:HD12	1.87	0.74
6:D:13:ASN:CG	6:D:97:ARG:H	1.96	0.74
2:F:21:A:H2'	2:F:22:C:H6	1.50	0.74
1:E:26:C:O4'	5:C:26:GLU:OE2	2.05	0.74
6:D:79:PHE:CZ	6:D:103:ALA:HA	2.22	0.74
2:F:24:G:C2	2:F:25:C:C6	2.76	0.73
3:A:166:LYS:NZ	3:A:166:LYS:HB3	2.01	0.73
1:E:12:G:N2	5:C:69:SER:CB	2.51	0.73
6:D:67:ARG:HH11	6:D:67:ARG:HG3	1.54	0.73
6:D:64:ARG:NH1	6:D:101:PRO:O	2.22	0.73
6:D:86:ILE:O	6:D:87:ILE:CG2	2.27	0.72
3:A:147:PRO:HD3	3:A:187:CYS:SG	2.29	0.72
5:C:13:LEU:HD13	5:C:43:ILE:HG23	1.72	0.72
3:A:61:TYR:CZ	3:A:85:ASN:HB2	2.26	0.71
6:D:79:PHE:CE1	6:D:103:ALA:HB1	2.18	0.71
4:B:30:GLY:HA3	4:B:135:ALA:CB	2.20	0.71
1:E:12:G:H22	5:C:69:SER:HB2	1.56	0.71
1:E:29:C:O2	5:C:62:MET:CE	2.38	0.71
6:D:87:ILE:C	6:D:88:ARG:O	2.33	0.71
6:D:36:GLY:HA3	6:D:109:LYS:CE	2.21	0.70
6:D:67:ARG:HH11	6:D:67:ARG:CG	2.03	0.70
4:B:29:LYS:O	4:B:135:ALA:HB2	1.90	0.70
5:C:28:ASN:HB3	5:C:29:ARG:NH1	2.06	0.70
3:A:174:ARG:NE	3:A:178:GLY:HA2	2.06	0.70
1:E:14:C:H2'	1:E:15:U:O4'	1.90	0.70
5:C:20:ILE:HD12	5:C:22:SER:O	1.91	0.70
6:D:36:GLY:HA3	6:D:109:LYS:HE2	1.74	0.69
6:D:63:VAL:CA	6:D:106:LEU:CD2	2.49	0.69
2:F:24:G:N3	2:F:25:C:C6	2.60	0.69
1:E:9:G:H2'	1:E:10:U:C6	2.27	0.69
5:C:55:SER:OG	5:C:57:GLU:HG2	1.93	0.69
2:F:23:C:O2	2:F:23:C:C2'	2.41	0.69
4:B:157:LYS:HA	4:B:157:LYS:HE2	1.75	0.68
1:E:24:G:H2'	1:E:25:C:O5'	1.92	0.68
4:B:32:LEU:HD11	4:B:136:ASP:HA	1.74	0.68
6:D:61:VAL:HG11	6:D:111:PHE:CE2	2.27	0.68
3:A:118:GLY:HA2	3:A:188:ARG:NH2	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:94:ASN:HD22	3:A:100:LYS:HG3	1.59	0.68
1:E:31:U:H5'	5:C:53:ALA:C	2.16	0.67
5:C:40:VAL:HG11	5:C:64:GLU:CG	2.24	0.67
4:B:30:GLY:HA3	4:B:135:ALA:HB2	1.77	0.67
1:E:29:C:C2	5:C:62:MET:HG2	2.24	0.67
4:B:29:LYS:CE	4:B:81:GLY:N	2.58	0.67
4:B:81:GLY:C	4:B:82:TYR:N	2.53	0.66
2:F:12:A:H1'	2:F:20:A:H61	1.59	0.66
3:A:166:LYS:HD2	3:A:171:VAL:HG22	1.76	0.66
6:D:52:VAL:HG22	6:D:94:ARG:NH1	2.10	0.65
1:E:11:A:H4'	1:E:21:G:OP2	1.96	0.65
1:E:29:C:H2'	5:C:62:MET:HG3	1.79	0.65
4:B:29:LYS:CD	4:B:81:GLY:N	2.57	0.65
4:B:80:LYS:O	4:B:81:GLY:N	2.30	0.64
4:B:29:LYS:CD	4:B:81:GLY:CA	2.75	0.64
6:D:13:ASN:C	6:D:95:GLY:HA3	2.22	0.64
5:C:26:GLU:HG2	5:C:69:SER:O	1.97	0.64
6:D:79:PHE:HZ	6:D:103:ALA:CA	2.00	0.64
1:E:1:G:H2'	1:E:2:C:C6	2.33	0.64
3:A:114:GLU:C	3:A:115:ILE:HD12	2.23	0.64
4:B:29:LYS:HE2	4:B:81:GLY:HA3	1.79	0.63
3:A:159:THR:HB	3:A:176:ALA:CB	2.29	0.63
1:E:9:G:O4'	5:C:50:ASP:C	2.39	0.63
3:A:174:ARG:HE	3:A:178:GLY:HA2	1.61	0.63
3:A:108:ASN:O	3:A:110:LYS:HE2	1.98	0.62
2:F:12:A:C2	2:F:13:C:H1'	2.35	0.62
3:A:61:TYR:CE1	3:A:85:ASN:HB2	2.35	0.62
1:E:29:C:C2'	5:C:62:MET:HG2	2.29	0.62
1:E:13:G:O2'	5:C:70:MET:SD	2.58	0.62
2:F:20:A:H2'	2:F:21:A:C8	2.35	0.61
2:F:20:A:H2'	2:F:21:A:O4'	1.99	0.61
1:E:26:C:H2'	5:C:69:SER:O	1.99	0.61
6:D:85:VAL:CG2	6:D:114:ILE:CD1	2.63	0.61
2:F:12:A:C1'	2:F:20:A:N6	2.64	0.61
6:D:52:VAL:CG2	6:D:94:ARG:NH1	2.64	0.60
1:E:27:A:OP1	5:C:27:PRO:HD3	2.02	0.60
4:B:21:ASN:ND2	4:B:35:THR:HG23	2.17	0.60
1:E:12:G:N2	5:C:69:SER:HB2	2.15	0.59
3:A:104:ILE:HG13	3:A:156:ALA:HB2	1.85	0.59
2:F:21:A:C4	2:F:22:C:C5	2.91	0.59
6:D:87:ILE:C	6:D:88:ARG:HA	2.24	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:17:A:O2'	1:E:18:G:H5'	2.02	0.59
5:C:40:VAL:HG11	5:C:64:GLU:HG2	1.83	0.59
5:C:61:ARG:HG2	5:C:61:ARG:NH1	2.18	0.59
5:C:23:GLY:O	5:C:24:SER:HB2	2.01	0.59
1:E:31:U:O2	5:C:52:ASN:CB	2.48	0.59
1:E:29:C:C2'	5:C:62:MET:CG	2.80	0.58
4:B:29:LYS:CD	4:B:81:GLY:HA3	2.32	0.58
4:B:39:ASP:O	4:B:54:PRO:HD3	2.03	0.58
3:A:164:LEU:HD13	3:A:174:ARG:HB2	1.85	0.58
6:D:85:VAL:HG11	6:D:114:ILE:HD11	0.68	0.58
1:E:11:A:O4'	1:E:20:A:C1'	2.52	0.58
6:D:85:VAL:CB	6:D:114:ILE:CD1	2.82	0.57
4:B:29:LYS:HE2	4:B:81:GLY:CA	2.34	0.57
5:C:25:GLY:O	5:C:27:PRO:HD2	2.04	0.57
3:A:90:ILE:HD12	3:A:102:TYR:CD2	2.39	0.57
1:E:27:A:O2'	1:E:28:U:H5'	2.05	0.56
6:D:61:VAL:CB	6:D:111:PHE:HZ	2.05	0.56
3:A:107:LYS:HG2	3:A:108:ASN:ND2	2.21	0.56
3:A:118:GLY:HA2	3:A:188:ARG:HH22	1.70	0.56
3:A:153:LEU:C	3:A:154:VAL:HG23	2.30	0.56
6:D:11:ALA:O	6:D:98:ILE:HG23	2.05	0.56
6:D:79:PHE:HZ	6:D:103:ALA:HB1	1.47	0.56
1:E:55:U:O2'	1:E:56:G:C5'	2.53	0.55
3:A:154:VAL:HG12	3:A:194:VAL:HG11	1.88	0.55
2:F:16:G:C2'	2:F:17:A:H5'	2.36	0.55
1:E:11:A:OP1	5:C:6:LYS:CD	2.55	0.55
1:E:27:A:C1'	5:C:69:SER:CB	2.65	0.55
4:B:29:LYS:CB	4:B:81:GLY:CA	2.77	0.55
4:B:29:LYS:HE2	4:B:81:GLY:N	2.22	0.55
3:A:77:VAL:HG23	3:A:115:ILE:HD13	1.87	0.55
1:E:9:G:O2'	5:C:47:LYS:HE3	2.07	0.54
2:F:7:U:O2'	2:F:8:C:H5'	2.08	0.54
4:B:158:GLY:HA3	4:B:170:LEU:HD11	1.88	0.54
1:E:29:C:O2	5:C:62:MET:HE2	2.07	0.54
3:A:82:TYR:OH	3:A:87:SER:HA	2.08	0.54
6:D:12:ASP:HA	6:D:98:ILE:HD13	1.89	0.54
1:E:9:G:C2	5:C:62:MET:HE1	2.40	0.54
1:E:27:A:C1'	5:C:69:SER:HB3	2.29	0.54
1:E:24:G:O2'	1:E:25:C:O5'	2.26	0.53
3:A:160:SER:OG	3:A:193:GLU:HA	2.08	0.53
4:B:32:LEU:CD1	4:B:136:ASP:HA	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:174:ARG:CZ	3:A:178:GLY:HA2	2.39	0.53
5:C:40:VAL:HG11	5:C:64:GLU:HG3	1.89	0.53
6:D:64:ARG:NH1	6:D:102:VAL:CA	2.63	0.53
1:E:11:A:OP1	5:C:6:LYS:HD3	2.08	0.53
4:B:11:PRO:HG2	4:B:14:VAL:HG21	1.90	0.53
4:B:32:LEU:HD21	4:B:136:ASP:N	2.22	0.53
5:C:41:ARG:NH1	5:C:60:MET:SD	2.81	0.53
2:F:20:A:C4	2:F:21:A:C8	2.97	0.53
4:B:76:GLU:HG3	4:B:80:LYS:HD2	1.90	0.53
1:E:1:G:H2'	1:E:2:C:H6	1.73	0.52
1:E:54:C:H6	1:E:54:C:O5'	1.92	0.52
1:E:12:G:H22	5:C:69:SER:CB	2.16	0.52
1:E:31:U:O2	5:C:52:ASN:HB3	2.09	0.52
5:C:28:ASN:HB3	5:C:29:ARG:CZ	2.40	0.52
6:D:70:ARG:HG3	6:D:76:TYR:CE2	2.44	0.51
3:A:164:LEU:CD1	3:A:174:ARG:HB2	2.40	0.51
1:E:26:C:O2	5:C:69:SER:HB2	2.10	0.51
3:A:144:GLU:O	3:A:187:CYS:HB3	2.11	0.51
4:B:29:LYS:CE	4:B:81:GLY:HA3	2.40	0.51
6:D:79:PHE:HZ	6:D:103:ALA:HA	1.67	0.51
1:E:46:A:H8	1:E:46:A:O5'	1.94	0.51
4:B:25:VAL:HG12	4:B:78:VAL:HG21	1.93	0.51
6:D:64:ARG:HD3	6:D:102:VAL:HA	1.92	0.50
1:E:13:G:O2'	5:C:70:MET:CE	2.58	0.50
1:E:16:U:O2	1:E:19:A:H8	1.94	0.50
1:E:3:C:C2'	1:E:4:A:H5'	2.42	0.50
1:E:11:A:C2	1:E:20:A:C5	3.00	0.50
3:A:110:LYS:H	3:A:113:MSE:SE	2.45	0.50
3:A:162:GLN:O	3:A:164:LEU:HD12	2.12	0.49
5:C:38:ASP:O	5:C:42:GLU:HG3	2.12	0.49
5:C:26:GLU:CD	5:C:26:GLU:N	2.70	0.49
4:B:162:ARG:HG3	4:B:163:TYR:O	2.12	0.49
1:E:10:U:OP1	5:C:47:LYS:CE	2.59	0.48
1:E:13:G:O3'	5:C:11:ALA:HB1	1.62	0.48
1:E:27:A:H1'	5:C:69:SER:CA	2.41	0.48
1:E:10:U:P	5:C:7:THR:H	2.36	0.48
6:D:36:GLY:HA3	6:D:109:LYS:HZ3	1.79	0.48
2:F:12:A:H2'	2:F:13:C:O4'	2.13	0.48
4:B:98:GLN:HG3	4:B:103:VAL:HG21	1.96	0.48
1:E:31:U:C5'	5:C:54:ALA:N	2.77	0.48
3:A:121:ALA:HB3	3:A:129:LEU:HG	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:36:LYS:CG	5:C:37:ARG:N	2.59	0.48
3:A:151:GLY:O	3:A:155:ARG:NH1	2.44	0.47
6:D:36:GLY:HA3	6:D:109:LYS:CG	2.40	0.47
6:D:79:PHE:CE2	6:D:103:ALA:CA	2.95	0.47
6:D:79:PHE:CE2	6:D:103:ALA:HA	2.49	0.47
3:A:174:ARG:NH2	3:A:178:GLY:HA2	2.29	0.47
1:E:31:U:H5''	5:C:54:ALA:N	2.30	0.47
4:B:110:HIS:HB3	4:B:111:PRO:HD2	1.96	0.47
1:E:6:G:N2	1:E:52:C:C5	2.83	0.46
2:F:20:A:H2'	2:F:21:A:H8	1.80	0.46
1:E:11:A:OP1	5:C:6:LYS:CE	2.63	0.46
5:C:18:ALA:HB1	5:C:32:VAL:HG11	1.98	0.46
6:D:36:GLY:HA3	6:D:109:LYS:NZ	2.30	0.46
3:A:177:SER:OG	3:A:179:GLU:HB2	2.16	0.46
5:C:18:ALA:HB1	5:C:32:VAL:CG1	2.45	0.46
6:D:69:VAL:CG2	6:D:105:GLU:OE2	2.63	0.46
2:F:12:A:C2'	2:F:13:C:H5'	2.45	0.46
4:B:11:PRO:HG2	4:B:14:VAL:CG2	2.46	0.46
1:E:29:C:H2'	1:E:30:A:O4'	2.16	0.46
3:A:144:GLU:OE2	3:A:147:PRO:HA	2.16	0.46
4:B:32:LEU:CD2	4:B:136:ASP:CA	2.87	0.46
1:E:29:C:O2	5:C:62:MET:HE3	2.17	0.45
1:E:9:G:H4'	5:C:50:ASP:OD2	1.90	0.45
3:A:70:LYS:NZ	3:A:97:ASP:OD2	2.47	0.45
3:A:146:LYS:O	3:A:147:PRO:C	2.59	0.45
6:D:63:VAL:CG2	6:D:106:LEU:HD11	2.44	0.45
6:D:87:ILE:HB	6:D:88:ARG:O	2.15	0.45
1:E:3:C:O2'	1:E:4:A:H5'	2.15	0.45
3:A:61:TYR:CE2	3:A:85:ASN:HB2	2.51	0.45
3:A:82:TYR:CE2	3:A:84:PRO:HA	2.52	0.45
6:D:35:ILE:HD13	6:D:105:GLU:HB2	1.99	0.45
1:E:9:G:O4'	5:C:50:ASP:CA	2.65	0.45
1:E:29:C:C2	5:C:62:MET:HE3	2.51	0.45
6:D:64:ARG:CZ	6:D:101:PRO:O	2.64	0.45
6:D:67:ARG:HG3	6:D:67:ARG:NH1	2.28	0.45
1:E:31:U:H5''	5:C:53:ALA:C	2.38	0.44
4:B:153:PRO:HA	4:B:159:LYS:O	2.17	0.44
2:F:16:G:H2'	2:F:17:A:C8	2.53	0.44
2:F:20:A:H3'	2:F:21:A:H8	1.83	0.44
2:F:20:A:C6	2:F:21:A:C5	3.05	0.44
6:D:86:ILE:O	6:D:87:ILE:HG22	2.14	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:29:C:C2'	5:C:62:MET:HA	2.46	0.44
4:B:7:PRO:HB2	4:B:48:VAL:HB	2.00	0.44
4:B:26:LYS:HG2	4:B:31:GLU:HG3	2.00	0.44
1:E:53:A:OP2	1:E:53:A:H8	2.00	0.44
5:C:36:LYS:O	5:C:38:ASP:N	2.51	0.44
1:E:37:G:N2	1:E:40:A:C8	2.86	0.43
6:D:118:ALA:HA	6:D:119:PRO:HD3	1.85	0.43
1:E:30:A:O2'	5:C:53:ALA:HB2	2.18	0.43
4:B:21:ASN:ND2	4:B:35:THR:CG2	2.81	0.43
2:F:25:C:H2'	2:F:25:C:O2	2.17	0.43
3:A:83:ASP:OD2	3:A:86:ARG:HD2	2.18	0.43
1:E:14:C:H4'	5:C:23:GLY:N	2.33	0.43
5:C:41:ARG:O	5:C:45:GLU:HG3	2.18	0.43
6:D:36:GLY:CA	6:D:109:LYS:HE2	2.45	0.43
4:B:101:LYS:HE3	4:B:101:LYS:HB2	1.75	0.43
1:E:9:G:N1	5:C:62:MET:CE	2.82	0.43
4:B:34:ARG:HG2	4:B:34:ARG:HH11	1.84	0.43
1:E:9:G:C4'	5:C:50:ASP:HB3	1.63	0.43
5:C:15:LYS:HG3	5:C:70:MET:HE1	2.00	0.43
5:C:36:LYS:C	5:C:38:ASP:N	2.77	0.43
6:D:107:ARG:HG3	6:D:107:ARG:HH11	1.84	0.43
2:F:7:U:H2'	2:F:8:C:O4'	2.19	0.42
3:A:144:GLU:HG3	3:A:150:GLY:O	2.19	0.42
5:C:51:LEU:C	5:C:53:ALA:H	2.27	0.42
2:F:24:G:N3	2:F:25:C:C5	2.85	0.42
5:C:60:MET:O	5:C:61:ARG:C	2.62	0.42
1:E:9:G:C1'	5:C:50:ASP:CB	2.85	0.42
3:A:86:ARG:C	3:A:88:ALA:N	2.77	0.42
1:E:9:G:H2'	1:E:10:U:C5	2.54	0.42
1:E:15:U:OP1	5:C:22:SER:OG	2.21	0.42
5:C:36:LYS:HE3	5:C:37:ARG:HG3	2.02	0.42
6:D:22:ILE:HD11	6:D:42:THR:CG2	2.41	0.42
1:E:27:A:H2'	1:E:28:U:O4'	2.20	0.42
3:A:166:LYS:HB3	3:A:166:LYS:HZ1	1.81	0.42
3:A:124:LYS:O	3:A:125:ILE:C	2.62	0.42
6:D:71:ARG:HH21	6:D:105:GLU:CD	2.28	0.42
3:A:146:LYS:O	3:A:149:ARG:HB2	2.20	0.42
3:A:166:LYS:HB3	3:A:166:LYS:HZ2	1.84	0.42
1:E:29:C:O2'	5:C:62:MET:N	2.53	0.42
5:C:9:PRO:HD2	5:C:12:VAL:CG1	2.50	0.42
1:E:30:A:C4'	5:C:62:MET:HG3	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:32:U:C2'	1:E:33:U:O5'	2.67	0.41
2:F:9:A:O4'	2:F:11:U:C6	2.73	0.41
3:A:153:LEU:HD23	3:A:153:LEU:HA	1.91	0.41
5:C:35:ILE:O	5:C:39:LYS:HB2	2.20	0.41
3:A:106:PRO:HD2	3:A:109:LEU:HD22	2.02	0.41
2:F:26:A:H2'	2:F:27:C:C6	2.55	0.41
5:C:58:ALA:O	5:C:59:ALA:C	2.62	0.41
3:A:62:ARG:CD	3:A:62:ARG:H	2.34	0.41
1:E:43:G:C2'	1:E:48:A:H61	2.32	0.41
1:E:57:G:C6	1:E:58:U:N3	2.88	0.41
3:A:177:SER:C	3:A:179:GLU:H	2.27	0.41
2:F:6:C:H2'	2:F:7:U:H6	1.85	0.41
5:C:23:GLY:O	5:C:31:LYS:HG2	2.20	0.41
1:E:40:A:C2	1:E:41:G:C8	3.09	0.41
4:B:29:LYS:CG	4:B:81:GLY:HA2	2.26	0.41
4:B:82:TYR:HB3	4:B:137:LYS:HD3	2.02	0.41
3:A:83:ASP:OD1	3:A:83:ASP:C	2.64	0.41
3:A:129:LEU:HD12	3:A:129:LEU:N	2.36	0.41
2:F:27:C:C2'	2:F:28:C:H5'	2.51	0.40
6:D:64:ARG:NH1	6:D:102:VAL:CB	2.83	0.40
6:D:85:VAL:O	6:D:87:ILE:HG23	2.21	0.40
6:D:63:VAL:O	6:D:103:ALA:HB3	2.22	0.40

All (31) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:15:GLY:CA	6:D:48:PRO:CG[3_655]	0.17	2.03
6:D:49:GLY:CA	6:D:52:VAL:O[3_655]	0.35	1.85
6:D:47:THR:CB	6:D:47:THR:CB[3_655]	0.69	1.51
6:D:47:THR:CA	6:D:47:THR:OG1[3_655]	0.70	1.50
6:D:47:THR:CA	6:D:47:THR:CB[3_655]	0.96	1.24
6:D:47:THR:C	6:D:47:THR:OG1[3_655]	1.02	1.18
6:D:49:GLY:CA	6:D:52:VAL:C[3_655]	1.08	1.12
6:D:49:GLY:N	6:D:52:VAL:O[3_655]	1.26	0.94
6:D:49:GLY:O	6:D:53:LYS:CA[3_655]	1.29	0.91
6:D:15:GLY:CA	6:D:48:PRO:CB[3_655]	1.43	0.77
6:D:47:THR:O	6:D:47:THR:O[3_655]	1.49	0.71
6:D:49:GLY:C	6:D:52:VAL:O[3_655]	1.50	0.70
6:D:15:GLY:N	6:D:48:PRO:CG[3_655]	1.55	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:15:GLY:C	6:D:48:PRO:CG[3_655]	1.57	0.63
6:D:50:GLY:O	6:D:53:LYS:CD[3_655]	1.68	0.52
6:D:15:GLY:CA	6:D:48:PRO:CD[3_655]	1.70	0.50
6:D:47:THR:CB	6:D:47:THR:CG2[3_655]	1.73	0.47
6:D:47:THR:OG1	6:D:48:PRO:N[3_655]	1.77	0.43
6:D:47:THR:N	6:D:47:THR:OG1[3_655]	1.94	0.26
6:D:14:SER:O	6:D:48:PRO:CB[3_655]	1.96	0.24
6:D:47:THR:CB	6:D:47:THR:OG1[3_655]	1.98	0.22
6:D:49:GLY:CA	6:D:53:LYS:N[3_655]	2.03	0.17
6:D:47:THR:CG2	6:D:47:THR:CG2[3_655]	2.06	0.14
6:D:47:THR:N	6:D:47:THR:CB[3_655]	2.08	0.12
6:D:49:GLY:C	6:D:53:LYS:CA[3_655]	2.11	0.09
6:D:47:THR:CA	6:D:47:THR:CA[3_655]	2.13	0.07
6:D:49:GLY:N	6:D:52:VAL:C[3_655]	2.13	0.07
6:D:49:GLY:O	6:D:53:LYS:C[3_655]	2.13	0.07
6:D:47:THR:O	6:D:47:THR:OG1[3_655]	2.14	0.06
6:D:50:GLY:O	6:D:53:LYS:NZ[3_655]	2.15	0.05
6:D:15:GLY:N	6:D:48:PRO:CB[3_655]	2.17	0.03

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	
3	A	133/137 (97%)	124 (93%)	7 (5%)	2 (2%)	8	38
4	B	159/177 (90%)	156 (98%)	3 (2%)	0	100	100
5	C	65/67 (97%)	49 (75%)	12 (18%)	4 (6%)	1	12
6	D	120/122 (98%)	114 (95%)	4 (3%)	2 (2%)	7	34
All	All	477/503 (95%)	443 (93%)	26 (6%)	8 (2%)	7	34

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	C	26	GLU
6	D	87	ILE
5	C	24	SER
5	C	32	VAL
6	D	86	ILE
3	A	161	ALA
5	C	37	ARG
3	A	154	VAL

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	
3	A	107/105 (102%)	85 (79%)	22 (21%)	1	7
4	B	137/147 (93%)	130 (95%)	7 (5%)	21	43
5	C	51/51 (100%)	41 (80%)	10 (20%)	1	8
6	D	101/101 (100%)	99 (98%)	2 (2%)	48	66
All	All	396/404 (98%)	355 (90%)	41 (10%)	7	22

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

Mol	Chain	Res	Type
3	A	60	GLN
3	A	62	ARG
3	A	70	LYS
3	A	85	ASN
3	A	86	ARG
3	A	100	LYS
3	A	110	LYS
3	A	111	VAL
3	A	113	MSE
3	A	116	MSE
3	A	120	ASP
3	A	124	LYS
3	A	129	LEU
3	A	149	ARG

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Mol	Chain	Res	Type
3	A	154	VAL
3	A	155	ARG
3	A	160	SER
3	A	166	LYS
3	A	167	GLU
3	A	184	LEU
3	A	188	ARG
3	A	194	VAL
4	B	9	GLU
4	B	38	PRO
4	B	45	GLU
4	B	117	GLU
4	B	157	LYS
4	B	169	ARG
4	B	170	LEU
5	C	6	LYS
5	C	7	THR
5	C	12	VAL
5	C	26	GLU
5	C	32	VAL
5	C	38	ASP
5	C	39	LYS
5	C	56	ILE
5	C	57	GLU
5	C	61	ARG
6	D	53	LYS
6	D	67	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	94	ASN
3	A	108	ASN
3	A	127	ASN
3	A	152	GLN
4	B	146	ASN
6	D	3	GLN
6	D	56	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	E	57/58 (98%)	18 (31%)	2 (3%)
2	F	28/29 (96%)	5 (17%)	0
All	All	85/87 (97%)	23 (27%)	2 (2%)

All (23) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	E	6	G
1	E	7	A
1	E	13	G
1	E	16	U
1	E	19	A
1	E	20	A
1	E	21	G
1	E	22	C
1	E	24	G
1	E	25	C
1	E	27	A
1	E	31	U
1	E	38	A
1	E	40	A
1	E	45	A
1	E	49	G
1	E	53	A
1	E	54	C
2	F	6	C
2	F	10	G
2	F	17	A
2	F	18	G
2	F	25	C

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	E	20	A
1	E	53	A

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 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	B	2
6	D	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	81:GLY	C	82:TYR	N	2.53
1	B	80:LYS	C	81:GLY	N	2.18
1	D	87:ILE	C	88:ARG	N	1.67
1	D	86:ILE	C	87:ILE	N	0.95

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.