



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:13 PM UTC

PDB ID : 2Y9H / pdb_00002y9h
Title : Structure A of CRISPR endoribonuclease Cse3 bound to 19 nt RNA
Authors : Sashital, D.G.; Jinek, M.; Doudna, J.A.
Deposited on : 2011-02-14
Resolution : 2.50 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

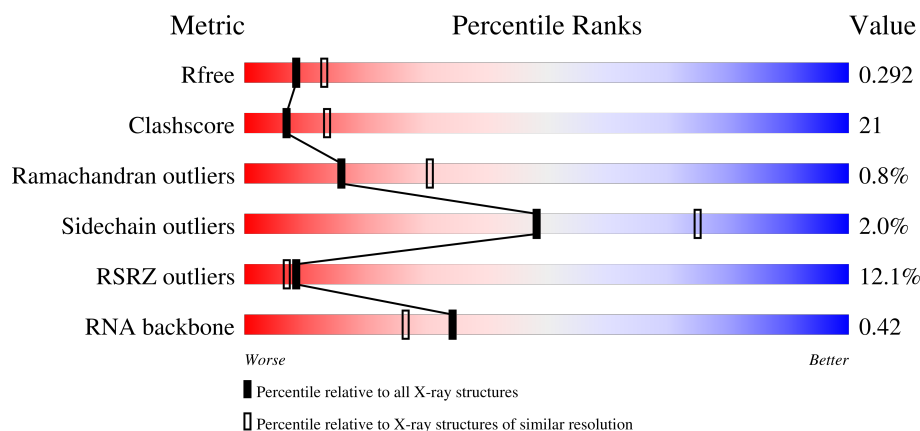
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)
RNA backbone	3983	1003 (2.78-2.22)

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	A	215	7% 59% 39% ..
1	C	215	7% 61% 33% ..
1	E	215	5% 53% 43% ..
1	G	215	4% 65% 26% 7%

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Mol	Chain	Length	Quality of chain
1	I	215	
1	K	215	
1	M	215	
1	O	215	
2	B	19	
2	D	19	
2	F	19	
2	H	19	
2	J	19	
2	L	19	
2	N	19	
2	P	19	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 15663 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 CSE3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	213	Total	C	N	O	S	0	0	0
			1685	1074	319	290	2			
1	C	211	Total	C	N	O	S	0	0	0
			1676	1069	317	288	2			
1	E	211	Total	C	N	O	S	0	0	0
			1668	1064	316	286	2			
1	G	199	Total	C	N	O	S	0	0	0
			1587	1017	300	268	2			
1	I	195	Total	C	N	O	S	0	0	0
			1545	992	289	262	2			
1	K	191	Total	C	N	O	S	0	0	0
			1519	975	282	260	2			
1	M	193	Total	C	N	O	S	0	0	0
			1528	982	284	260	2			
1	O	177	Total	C	N	O		0	0	0
			908	554	177	177				

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP Q53WG9
A	-2	THR	-	expression tag	UNP Q53WG9
A	-1	GLY	-	expression tag	UNP Q53WG9
A	0	ALA	-	expression tag	UNP Q53WG9
C	-3	GLY	-	expression tag	UNP Q53WG9
C	-2	THR	-	expression tag	UNP Q53WG9
C	-1	GLY	-	expression tag	UNP Q53WG9
C	0	ALA	-	expression tag	UNP Q53WG9
E	-3	GLY	-	expression tag	UNP Q53WG9
E	-2	THR	-	expression tag	UNP Q53WG9
E	-1	GLY	-	expression tag	UNP Q53WG9
E	0	ALA	-	expression tag	UNP Q53WG9
G	-3	GLY	-	expression tag	UNP Q53WG9

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-2	THR	-	expression tag	UNP Q53WG9
G	-1	GLY	-	expression tag	UNP Q53WG9
G	0	ALA	-	expression tag	UNP Q53WG9
I	-3	GLY	-	expression tag	UNP Q53WG9
I	-2	THR	-	expression tag	UNP Q53WG9
I	-1	GLY	-	expression tag	UNP Q53WG9
I	0	ALA	-	expression tag	UNP Q53WG9
K	-3	GLY	-	expression tag	UNP Q53WG9
K	-2	THR	-	expression tag	UNP Q53WG9
K	-1	GLY	-	expression tag	UNP Q53WG9
K	0	ALA	-	expression tag	UNP Q53WG9
M	-3	GLY	-	expression tag	UNP Q53WG9
M	-2	THR	-	expression tag	UNP Q53WG9
M	-1	GLY	-	expression tag	UNP Q53WG9
M	0	ALA	-	expression tag	UNP Q53WG9
O	-3	GLY	-	expression tag	UNP Q53WG9
O	-2	THR	-	expression tag	UNP Q53WG9
O	-1	GLY	-	expression tag	UNP Q53WG9
O	0	ALA	-	expression tag	UNP Q53WG9

- Molecule 2 is a RNA chain called 5'-R(*UP*CP*CP*CP*CP*AP*CP*GP*CP*GP*UP*GP*UP*GP *GP*GP*DGP*AP*UP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	19	Total	C	N	O	P	0	0	0
			385	171	69	127	18			
2	D	19	Total	C	N	O	P	0	0	0
			385	171	69	127	18			
2	F	19	Total	C	N	O	P	0	0	0
			385	171	69	127	18			
2	H	19	Total	C	N	O	P	0	0	0
			385	171	69	127	18			
2	J	19	Total	C	N	O	P	0	0	0
			385	171	69	127	18			
2	L	19	Total	C	N	O	P	0	0	0
			385	171	69	127	18			
2	N	18	Total	C	N	O	P	0	0	0
			381	171	69	124	17			
2	P	18	Total	C	N	O	P	0	0	0
			381	171	69	124	17			

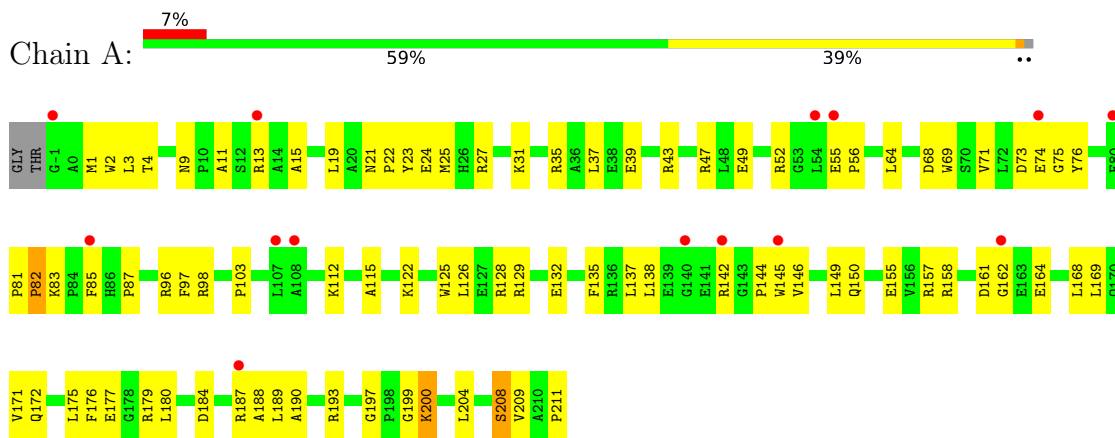
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	35	Total 35	O 35	0	0
3	B	13	Total 13	O 13	0	0
3	C	30	Total 30	O 30	0	0
3	D	19	Total 19	O 19	0	0
3	E	51	Total 51	O 51	0	0
3	F	25	Total 25	O 25	0	0
3	G	30	Total 30	O 30	0	0
3	H	13	Total 13	O 13	0	0
3	I	57	Total 57	O 57	0	0
3	J	24	Total 24	O 24	0	0
3	K	56	Total 56	O 56	0	0
3	L	20	Total 20	O 20	0	0
3	M	44	Total 44	O 44	0	0
3	N	23	Total 23	O 23	0	0
3	O	22	Total 22	O 22	0	0
3	P	13	Total 13	O 13	0	0

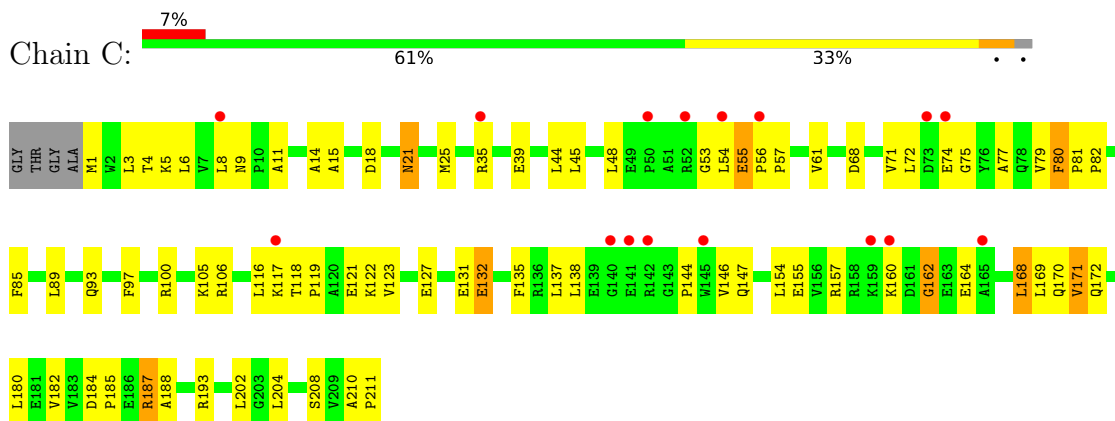
3 Residue-property plots [i](#)

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.

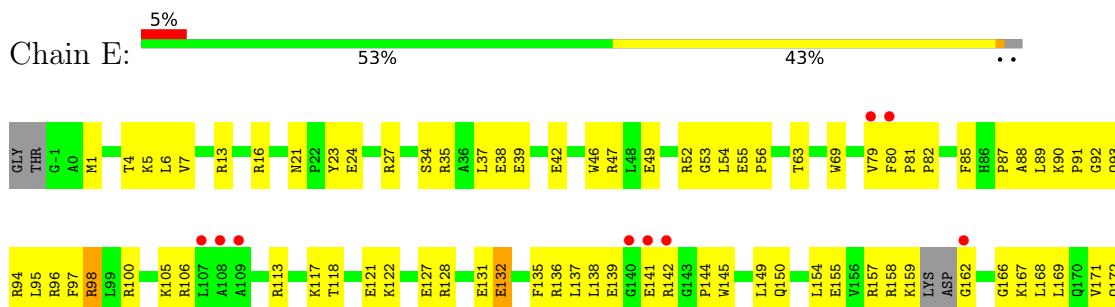
• Molecule 1: CSE3



• Molecule 1: CSE3

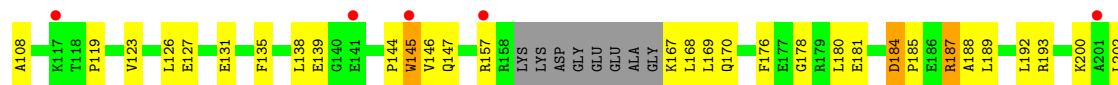


• Molecule 1: CSE3

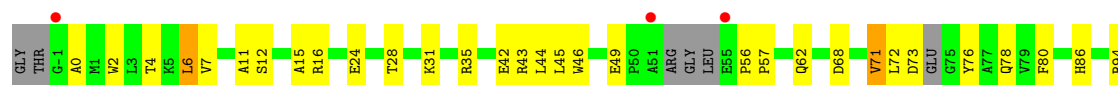




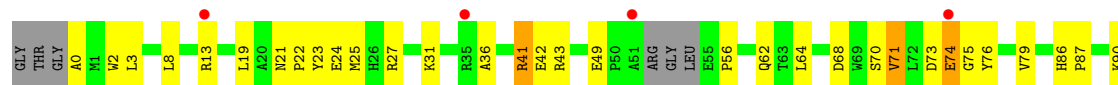
• Molecule 1: CSE3



• Molecule 1: CSE3

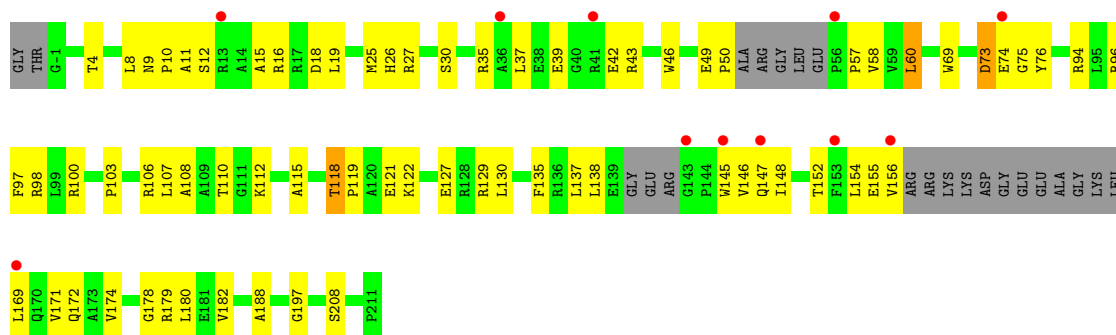


• Molecule 1: CSE3

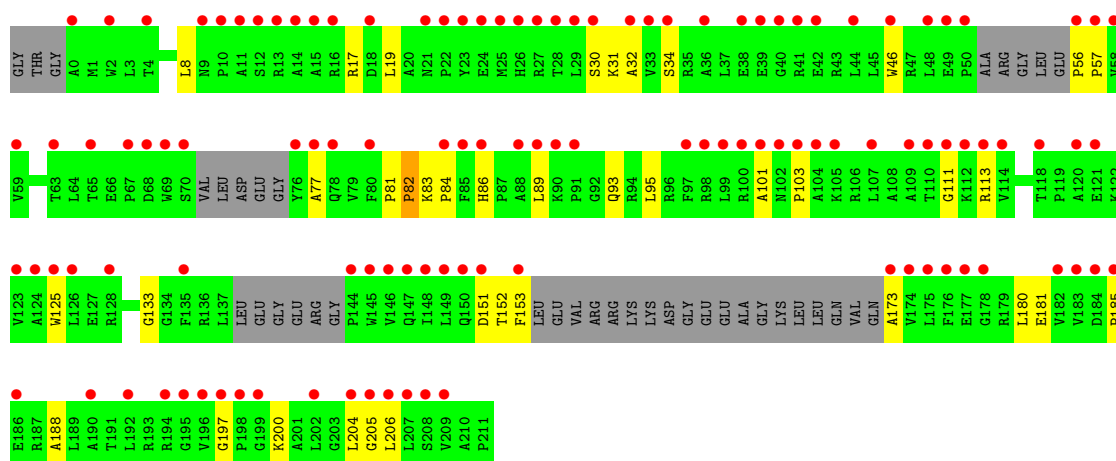


• Molecule 1: CSE3

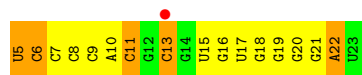
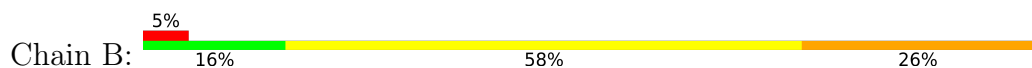




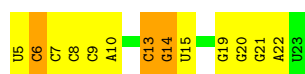
• Molecule 1: CSE3



• Molecule 2: 5'-R(*UP*CP*CP*CP*CP*AP*CP*GP*CP*GP*UP*GP*UP*GP*GP*GP*DGP*AP*UP)-3'



• Molecule 2: 5'-R(*UP*CP*CP*CP*CP*AP*CP*GP*CP*GP*UP*GP*UP*GP*GP*GP*DGP*AP*UP)-3'



• Molecule 2: 5'-R(*UP*CP*CP*CP*CP*AP*CP*GP*CP*GP*UP*GP*UP*GP*GP*GP*DGP*AP*UP)-3'

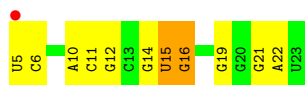




● Molecule 2: 5'-R(*UP*CP*CP*CP*CP*AP*CP*GP*CP*GP*UP*GP*UP*GP *GP*GP*DGP*AP*UP)-3'



● Molecule 2: 5'-R(*UP*CP*CP*CP*CP*AP*CP*GP*CP*GP*UP*GP*UP*GP *GP*GP*DGP*AP*UP)-3'



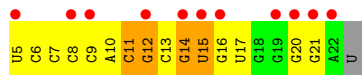
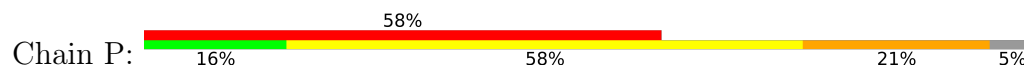
● Molecule 2: 5'-R(*UP*CP*CP*CP*CP*AP*CP*GP*CP*GP*UP*GP*UP*GP *GP*GP*DGP*AP*UP)-3'



● Molecule 2: 5'-R(*UP*CP*CP*CP*CP*AP*CP*GP*CP*GP*UP*GP*UP*GP *GP*GP*DGP*AP*UP)-3'



● Molecule 2: 5'-R(*UP*CP*CP*CP*CP*AP*CP*GP*CP*GP*UP*GP*UP*GP *GP*GP*DGP*AP*UP)-3'



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.86Å 149.81Å 87.26Å 90.00° 94.60° 90.00°	Depositor
Resolution (Å)	58.70 – 2.50 58.70 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (58.70-2.50) 99.9 (58.70-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 2.40Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.231 , 0.289 0.235 , 0.292	Depositor DCC
R_{free} test set	1994 reflections (2.33%)	wwPDB-VP
Wilson B-factor (Å ²)	37.4	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 69.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	15663	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 82.85 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.5178e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	A	0.58	1/1721 (0.1%)	0.92	0/2329
1	C	0.62	1/1712 (0.1%)	1.00	7/2317 (0.3%)
1	E	0.65	1/1703 (0.1%)	0.94	3/2304 (0.1%)
1	G	0.59	1/1621 (0.1%)	0.99	5/2194 (0.2%)
1	I	0.65	0/1577	0.97	4/2135 (0.2%)
1	K	0.64	1/1552 (0.1%)	0.95	4/2103 (0.2%)
1	M	0.53	0/1561	0.94	6/2115 (0.3%)
1	O	0.55	0/920	1.12	7/1285 (0.5%)
2	B	0.65	0/429	0.70	2/668 (0.3%)
2	D	0.62	0/429	0.57	0/668
2	F	0.74	1/429 (0.2%)	0.78	2/668 (0.3%)
2	H	0.60	0/429	0.65	1/668 (0.1%)
2	J	0.43	0/429	0.67	0/668
2	L	0.38	0/429	0.59	0/668
2	N	0.29	0/425	0.41	0/661
2	P	0.24	0/425	0.51	0/661
All	All	0.59	6/15791 (0.0%)	0.90	41/22112 (0.2%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	187	ARG	C-O	-7.19	1.15	1.24
1	G	187	ARG	C-O	-5.67	1.17	1.24
1	E	46	TRP	C-O	-5.25	1.17	1.23
1	K	56	PRO	CA-C	5.25	1.54	1.51
2	F	22	A	O5'-C5'	-5.15	1.35	1.42
1	A	208	SER	C-O	-5.10	1.17	1.23

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	184	ASP	CA-C-N	8.36	127.67	118.97
1	G	184	ASP	C-N-CA	8.36	127.67	118.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	22	A	O4'-C1'-C2'	-7.98	97.82	105.80
1	O	197	GLY	CA-C-N	7.83	128.28	119.83
1	O	197	GLY	C-N-CA	7.83	128.28	119.83
1	E	21	ASN	CA-C-N	6.91	126.72	119.05
1	E	21	ASN	C-N-CA	6.91	126.72	119.05
1	O	86	HIS	CA-C-N	6.86	128.41	119.84
1	O	86	HIS	C-N-CA	6.86	128.41	119.84
1	M	118	THR	CA-C-N	6.65	126.16	119.24
1	M	118	THR	C-N-CA	6.65	126.16	119.24
1	M	197	GLY	CA-C-N	6.62	127.16	120.14
1	M	197	GLY	C-N-CA	6.62	127.16	120.14
1	M	73	ASP	N-CA-C	-6.45	102.22	110.53
1	C	21	ASN	CA-C-N	6.41	126.90	119.47
1	C	21	ASN	C-N-CA	6.41	126.90	119.47
1	C	55	GLU	CA-C-N	6.38	126.95	120.38
1	C	55	GLU	C-N-CA	6.38	126.95	120.38
1	O	101	ALA	N-CA-C	6.17	115.58	108.49
1	O	77	ALA	N-CA-C	6.11	117.47	108.86
1	G	21	ASN	CA-C-N	5.98	127.32	119.84
1	G	21	ASN	C-N-CA	5.98	127.32	119.84
1	K	21	ASN	CA-C-N	5.56	125.22	119.05
1	K	21	ASN	C-N-CA	5.56	125.22	119.05
2	B	22	A	C5'-C4'-C3'	-5.46	107.02	115.20
1	K	41	ARG	N-CA-C	-5.45	105.25	112.94
1	C	132	GLU	N-CA-C	-5.41	106.18	112.89
2	F	22	A	C4'-C3'-C2'	-5.38	97.22	102.60
1	I	80	PHE	CA-C-N	5.38	125.92	120.38
1	I	80	PHE	C-N-CA	5.38	125.92	120.38
2	B	22	A	C3'-C2'-C1'	-5.37	96.14	101.50
1	K	104	ALA	N-CA-C	5.35	115.19	108.45
2	H	22	A	O3'-P-O5'	5.33	112.00	104.00
1	M	58	VAL	N-CA-C	5.33	115.52	107.80
1	C	184	ASP	CA-C-N	5.28	124.73	119.24
1	C	184	ASP	C-N-CA	5.28	124.73	119.24
1	E	132	GLU	N-CA-C	-5.23	105.64	112.23
1	O	111	GLY	N-CA-C	-5.21	108.64	115.47
1	I	101	ALA	N-CA-C	5.05	117.09	109.41
1	I	177	GLU	N-CA-C	-5.05	101.52	109.50
1	G	70	SER	N-CA-C	-5.01	106.42	112.54

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	A	1685	0	1762	103	0
1	C	1676	0	1754	73	1
1	E	1668	0	1744	98	0
1	G	1587	0	1667	52	0
1	I	1545	0	1615	46	0
1	K	1519	0	1582	64	0
1	M	1528	0	1597	70	0
1	O	908	0	513	18	0
2	B	385	0	196	27	0
2	D	385	0	196	23	0
2	F	385	0	196	21	0
2	H	385	0	196	14	0
2	J	385	0	196	18	0
2	L	385	0	196	15	0
2	N	381	0	197	18	0
2	P	381	0	197	19	0
3	A	35	0	0	3	0
3	B	13	0	0	3	0
3	C	30	0	0	1	1
3	D	19	0	0	0	0
3	E	51	0	0	7	2
3	F	25	0	0	3	0
3	G	30	0	0	4	0
3	H	13	0	0	2	0
3	I	57	0	0	5	0
3	J	24	0	0	2	0
3	K	56	0	0	3	0
3	L	20	0	0	1	0
3	M	44	0	0	2	0
3	N	23	0	0	5	0
3	O	22	0	0	2	0
3	P	13	0	0	0	0
All	All	15663	0	13804	611	2

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 21.

All (611) 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:K:74:GLU:HA	1:K:76:TYR:H	1.08	1.17
1:K:74:GLU:HG3	1:K:75:GLY:HA2	1.25	1.14
2:J:21:DG:C2'	2:J:22:A:H5'	1.92	0.99
1:A:83:LYS:HE2	2:F:9:C:OP1	1.63	0.97
1:A:145:TRP:CD1	1:A:179:ARG:HB2	2.00	0.95
1:A:83:LYS:HZ1	2:F:9:C:C5'	1.80	0.94
1:K:74:GLU:HA	1:K:76:TYR:N	1.82	0.94
1:M:74:GLU:H	1:M:76:TYR:H	0.99	0.94
1:M:74:GLU:HB2	1:M:75:GLY:HA3	1.49	0.94
2:B:9:C:H2'	2:B:10:A:H8	1.32	0.93
1:M:118:THR:HG23	1:M:121:GLU:H	1.34	0.93
2:L:15:U:H4'	2:L:16:G:OP2	1.66	0.92
2:L:5:U:O2'	2:L:6:C:OP2	1.86	0.92
2:H:15:U:O2'	2:H:16:G:OP2	1.86	0.92
1:C:1:MET:HE2	1:C:193:ARG:HH11	1.34	0.91
2:B:5:U:H2'	2:B:5:U:O2	1.66	0.90
2:N:6:C:H5'	3:N:2003:HOH:O	1.70	0.90
1:C:118:THR:HG23	1:C:121:GLU:H	1.37	0.90
1:M:73:ASP:O	1:M:76:TYR:HB3	1.71	0.90
1:M:74:GLU:H	1:M:76:TYR:N	1.71	0.88
1:C:168:LEU:HD12	1:C:169:LEU:N	1.89	0.88
1:C:144:PRO:HG3	1:E:158:ARG:HH12	1.39	0.87
1:I:95:LEU:O	1:I:179:ARG:HG2	1.74	0.87
1:C:56:PRO:HB2	1:C:57:PRO:HD2	1.55	0.87
1:E:117:LYS:HG2	1:E:121:GLU:OE1	1.75	0.86
1:M:74:GLU:N	1:M:76:TYR:H	1.74	0.86
1:G:1:MET:HE2	1:G:193:ARG:HH11	1.40	0.86
1:E:145:TRP:CD1	1:E:179:ARG:HB2	2.11	0.85
1:O:46:TRP:O	3:O:2007:HOH:O	1.95	0.84
1:E:47:ARG:HD3	3:E:2050:HOH:O	1.77	0.84
1:A:112:LYS:NZ	2:B:5:U:H5'	1.94	0.82
2:J:21:DG:H2''	2:J:22:A:H5'	1.62	0.82
1:A:145:TRP:NE1	1:A:179:ARG:HD2	1.93	0.82
1:C:131:GLU:OE2	1:E:155:GLU:OE2	1.98	0.81
2:L:5:U:O2'	2:L:6:C:H5'	1.81	0.80
1:A:83:LYS:NZ	2:F:9:C:C5'	2.44	0.79
1:M:74:GLU:CB	1:M:75:GLY:HA3	2.11	0.79
1:A:155:GLU:HG3	1:A:168:LEU:HD11	1.63	0.79
1:G:3:LEU:HD23	1:G:83:LYS:HE3	1.66	0.78
1:I:151:ASP:OD2	3:I:2044:HOH:O	2.01	0.78
2:P:14:G:C8	2:P:15:U:C5	2.72	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:88:ALA:HB3	1:E:93:GLN:HE22	1.47	0.77
1:E:52:ARG:O	1:E:55:GLU:HG3	1.83	0.77
1:A:168:LEU:HD22	1:G:139:GLU:HG3	1.66	0.77
1:I:118:THR:HG23	1:I:121:GLU:H	1.49	0.77
2:J:21:DG:H2'	2:J:22:A:H5'	1.66	0.76
2:F:5:U:H2'	2:F:5:U:O2	1.86	0.76
1:I:96:ARG:HG2	1:I:210:ALA:O	1.83	0.76
2:J:19:G:OP2	3:J:2014:HOH:O	2.03	0.76
2:P:14:G:H4'	2:P:15:U:OP1	1.85	0.76
1:K:74:GLU:HG3	1:K:75:GLY:CA	2.12	0.76
1:K:190:ALA:O	1:K:194:ARG:HG3	1.86	0.75
1:A:145:TRP:HD1	1:A:179:ARG:HB2	1.51	0.75
1:K:106:ARG:O	2:L:16:G:H5''	1.86	0.75
1:C:35:ARG:O	1:C:39:GLU:HG3	1.88	0.74
2:D:14:G:N3	1:E:27:ARG:HD2	2.02	0.74
1:E:96:ARG:HD3	1:E:211:PRO:HA	1.68	0.74
1:G:108:ALA:HB3	2:H:15:U:O2'	1.87	0.74
1:A:129:ARG:HD2	3:B:2009:HOH:O	1.87	0.74
2:N:22:A:O3'	3:N:2022:HOH:O	2.05	0.74
1:C:168:LEU:HD12	1:C:169:LEU:H	1.51	0.73
1:A:83:LYS:CE	2:F:9:C:OP1	2.36	0.73
2:J:12:G:C5	1:K:211:PRO:HG2	2.23	0.73
1:C:137:LEU:HD23	1:C:144:PRO:HB2	1.70	0.72
1:K:87:PRO:HG2	1:K:189:LEU:HD13	1.71	0.72
1:I:122:LYS:NZ	1:I:172:GLN:OE1	2.20	0.71
2:P:12:G:H4'	2:P:12:G:OP1	1.88	0.71
2:J:5:U:HO5'	2:J:5:U:H6	1.39	0.71
1:E:122:LYS:NZ	1:E:172:GLN:OE1	2.22	0.71
1:G:135:PHE:CZ	1:G:188:ALA:HB1	2.26	0.71
1:A:97:PHE:CD2	1:A:180:LEU:HD23	2.26	0.71
1:E:159:LYS:HE2	1:E:167:LYS:HB3	1.72	0.71
1:E:117:LYS:HG3	1:E:118:THR:HG23	1.73	0.70
1:M:73:ASP:HB3	1:M:74:GLU:HG2	1.73	0.70
1:C:144:PRO:CG	1:E:158:ARG:HH12	2.03	0.70
1:A:83:LYS:NZ	2:F:9:C:O5'	2.20	0.70
2:L:5:U:HO2'	2:L:6:C:P	2.13	0.70
1:A:83:LYS:NZ	2:F:9:C:H5''	2.07	0.70
1:E:87:PRO:HB2	1:E:89:LEU:HD13	1.74	0.70
1:A:1:MET:HB2	1:A:85:PHE:HB3	1.72	0.69
1:I:106:ARG:O	2:J:16:G:H5''	1.92	0.69
1:A:87:PRO:HG3	1:A:189:LEU:HD13	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:131:GLU:OE2	3:E:2026:HOH:O	2.10	0.68
1:I:73:ASP:OD1	1:I:76:TYR:HB2	1.93	0.68
2:N:14:G:O6	3:N:2012:HOH:O	2.10	0.68
1:E:49:GLU:O	3:E:2009:HOH:O	2.11	0.68
1:E:7:VAL:HG23	1:E:80:PHE:HE2	1.57	0.67
1:M:130:LEU:HD12	1:M:137:LEU:CD1	2.24	0.67
1:A:180:LEU:C	1:A:180:LEU:HD12	2.19	0.67
1:A:149:LEU:HD11	1:A:177:GLU:OE1	1.95	0.67
2:B:7:C:H2'	2:B:8:C:H6	1.59	0.67
2:F:5:U:H5'	3:F:2002:HOH:O	1.93	0.67
1:M:103:PRO:HG2	1:M:122:LYS:HG2	1.77	0.66
1:K:106:ARG:HG3	1:K:106:ARG:HH11	1.60	0.66
1:A:47:ARG:HD3	3:A:2035:HOH:O	1.95	0.66
1:C:21:ASN:OD1	1:C:21:ASN:C	2.38	0.66
1:C:3:LEU:HB2	1:C:85:PHE:HE2	1.60	0.66
1:A:55:GLU:HG2	1:A:56:PRO:HD2	1.78	0.66
2:F:19:G:OP2	3:F:2018:HOH:O	2.13	0.66
1:A:122:LYS:NZ	1:A:172:GLN:OE1	2.26	0.66
1:I:96:ARG:HD2	3:I:2057:HOH:O	1.95	0.66
2:D:5:U:H2'	2:D:6:C:C6	2.31	0.66
1:A:112:LYS:HZ1	2:B:5:U:H5'	1.58	0.65
1:E:93:GLN:HE21	1:E:95:LEU:HD21	1.61	0.65
1:G:2:TRP:CD1	3:G:2002:HOH:O	2.49	0.65
1:E:203:GLY:O	3:E:2049:HOH:O	2.13	0.65
1:A:161:ASP:OD1	1:A:162:GLY:N	2.28	0.65
1:C:127:GLU:O	1:C:131:GLU:HG3	1.97	0.65
2:D:5:U:H2'	2:D:6:C:H6	1.62	0.65
2:N:21:DG:H2'	2:N:22:A:C8	2.32	0.65
1:K:154:LEU:HB2	1:K:171:VAL:HG23	1.79	0.64
2:N:9:C:O2'	3:N:2006:HOH:O	2.14	0.64
1:A:112:LYS:HZ1	2:B:6:C:H5''	1.63	0.64
1:I:7:VAL:HB	1:I:78:GLN:HG2	1.79	0.64
1:C:202:LEU:HD11	2:D:22:A:N6	2.13	0.64
1:M:130:LEU:HD12	1:M:137:LEU:HD11	1.78	0.64
1:I:169:LEU:HB2	2:J:5:U:O2	1.97	0.64
1:K:144:PRO:N	3:K:2041:HOH:O	2.30	0.64
2:B:9:C:H2'	2:B:10:A:C8	2.24	0.63
2:H:15:U:H4'	2:H:16:G:O5'	1.98	0.63
1:C:160:LYS:C	1:C:162:GLY:N	2.55	0.63
1:E:162:GLY:N	3:E:2035:HOH:O	2.32	0.63
1:M:115:ALA:HB1	1:M:172:GLN:NE2	2.12	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:35:ARG:O	1:M:39:GLU:HG3	1.99	0.63
1:C:164:GLU:HG3	1:M:16:ARG:HD3	1.81	0.63
1:E:98:ARG:HH11	1:E:98:ARG:HB2	1.64	0.63
1:E:127:GLU:HG2	1:E:137:LEU:HD22	1.81	0.62
1:K:74:GLU:CA	1:K:76:TYR:H	1.99	0.62
1:M:50:PRO:HG2	1:M:98:ARG:HH12	1.63	0.62
1:A:64:LEU:HD13	1:A:193:ARG:NH2	2.15	0.62
1:E:149:LEU:HD11	1:E:177:GLU:OE1	1.99	0.62
1:I:184:ASP:OD2	1:I:187:ARG:HG2	1.99	0.62
1:G:8:LEU:O	1:G:10:PRO:HD3	2.00	0.62
1:O:151:ASP:HA	1:O:173:ALA:O	2.00	0.62
2:D:21:DG:C2'	2:D:22:A:H5'	2.30	0.61
1:C:118:THR:OG1	1:C:119:PRO:HD2	2.00	0.61
1:C:180:LEU:HD12	1:C:180:LEU:C	2.25	0.61
1:G:135:PHE:CE1	1:G:188:ALA:HB1	2.35	0.61
1:M:100:ARG:HH22	1:M:152:THR:CG2	2.12	0.61
1:G:207:LEU:N	3:G:2030:HOH:O	2.18	0.61
1:G:202:LEU:HD11	2:H:22:A:N6	2.15	0.61
1:O:200:LYS:HA	1:O:204:LEU:O	1.99	0.61
2:P:12:G:H2'	2:P:13:C:C6	2.36	0.61
1:C:122:LYS:NZ	1:C:172:GLN:OE1	2.23	0.61
2:B:7:C:H2'	2:B:8:C:C6	2.35	0.61
2:L:5:U:O2'	2:L:6:C:P	2.56	0.61
2:B:5:U:O2	2:B:5:U:C2'	2.44	0.61
1:C:117:LYS:HB3	1:C:121:GLU:OE1	2.01	0.61
1:C:106:ARG:HG3	1:C:106:ARG:HH11	1.66	0.60
1:A:128:ARG:O	1:A:132:GLU:HG3	2.01	0.60
2:B:20:G:O2'	2:B:21:DG:H5'	2.01	0.60
1:K:22:PRO:HB2	1:K:202:LEU:CD2	2.31	0.60
2:P:14:G:H8	2:P:15:U:C5	2.16	0.60
1:A:52:ARG:HE	1:A:55:GLU:HB2	1.66	0.60
2:D:8:C:O2'	2:D:9:C:H5'	2.01	0.60
2:L:5:U:O2	2:L:6:C:H5''	2.01	0.60
1:E:87:PRO:HG2	1:E:189:LEU:HD13	1.83	0.60
1:A:83:LYS:CE	2:F:9:C:P	2.90	0.60
1:G:2:TRP:NE1	3:G:2002:HOH:O	2.33	0.60
1:A:158:ARG:NH1	1:G:144:PRO:HD3	2.17	0.59
1:E:158:ARG:O	1:E:159:LYS:CB	2.50	0.59
1:E:94:ARG:HG2	1:E:138:LEU:HD11	1.83	0.59
1:E:35:ARG:NH2	1:K:24:GLU:OE1	2.35	0.59
1:A:15:ALA:O	1:A:19:LEU:HG	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:ASP:HB3	1:A:164:GLU:O	2.02	0.59
1:G:119:PRO:O	1:G:123:VAL:HG23	2.02	0.59
2:J:5:U:H6	2:J:5:U:O5'	1.85	0.59
1:C:89:LEU:HB3	1:C:182:VAL:HG21	1.84	0.59
1:K:180:LEU:C	1:K:180:LEU:HD12	2.28	0.59
1:K:118:THR:HG23	1:K:121:GLU:OE1	2.01	0.59
2:J:15:U:H2'	2:J:15:U:O2	2.01	0.59
1:K:8:LEU:HD22	1:K:19:LEU:HD21	1.84	0.59
2:P:5:U:O2	2:P:5:U:H2'	2.02	0.58
1:C:56:PRO:CB	1:C:57:PRO:HD2	2.30	0.58
1:C:157:ARG:O	1:C:168:LEU:CD1	2.51	0.58
1:K:90:LYS:HB2	1:K:93:GLN:HB2	1.84	0.58
1:M:73:ASP:CB	1:M:74:GLU:HG2	2.33	0.58
1:A:87:PRO:CG	1:A:189:LEU:HD13	2.33	0.58
1:A:4:THR:HG21	1:A:69:TRP:CE2	2.39	0.58
2:D:14:G:C2	1:E:27:ARG:HD2	2.39	0.58
1:M:127:GLU:HA	1:M:137:LEU:HD13	1.86	0.58
1:A:145:TRP:HE1	1:A:179:ARG:HD2	1.65	0.58
1:E:118:THR:O	1:E:122:LYS:HG3	2.04	0.58
1:A:112:LYS:HE3	2:B:5:U:O5'	2.04	0.57
2:F:16:G:O2'	2:F:17:U:H5'	2.03	0.57
1:E:201:ALA:C	1:E:202:LEU:HD12	2.29	0.57
2:F:7:C:O2'	2:F:8:C:H5'	2.04	0.57
2:P:10:A:H2'	2:P:11:C:O4'	2.02	0.57
1:C:44:LEU:O	1:C:45:LEU:HD23	2.04	0.57
1:G:106:ARG:HH11	1:G:106:ARG:HG3	1.68	0.57
1:C:171:VAL:HG13	2:D:5:U:C5	2.40	0.57
1:C:202:LEU:HD11	2:D:22:A:H62	1.69	0.57
2:H:5:U:H1'	3:H:2001:HOH:O	2.04	0.57
1:A:112:LYS:NZ	2:B:6:C:H5''	2.20	0.57
1:C:118:THR:CG2	1:C:121:GLU:H	2.14	0.57
1:A:55:GLU:CG	1:A:56:PRO:HD2	2.35	0.57
2:P:8:C:H2'	2:P:9:C:H6	1.70	0.57
2:P:5:U:O2	2:P:5:U:C2'	2.53	0.56
1:E:35:ARG:O	1:E:39:GLU:HG3	2.05	0.56
1:C:100:ARG:HG2	1:C:204:LEU:CD2	2.36	0.56
1:E:4:THR:HG21	1:E:69:TRP:CE2	2.40	0.56
1:E:94:ARG:O	1:E:95:LEU:HD22	2.05	0.56
1:E:141:GLU:HG2	1:E:142:ARG:HA	1.86	0.56
1:G:157:ARG:HG3	1:G:169:LEU:HD12	1.86	0.56
1:I:118:THR:HG22	1:I:121:GLU:OE1	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:3:LEU:HD23	1:K:3:LEU:C	2.31	0.56
1:A:83:LYS:HZ3	2:F:9:C:H5''	1.69	0.56
1:I:147:GLN:N	1:I:147:GLN:CD	2.63	0.56
1:E:90:LYS:O	1:E:93:GLN:HB2	2.05	0.56
1:E:97:PHE:CD2	1:E:180:LEU:HD23	2.40	0.56
1:K:22:PRO:HB2	1:K:202:LEU:HD22	1.87	0.56
1:A:73:ASP:O	1:A:76:TYR:HB2	2.04	0.56
1:M:169:LEU:HB3	2:N:5:U:O2	2.06	0.56
1:G:1:MET:CE	1:G:189:LEU:HD11	2.36	0.55
1:K:145:TRP:CH2	2:N:14:G:P	3.00	0.55
1:I:0:ALA:HB2	1:I:86:HIS:CE1	2.40	0.55
2:D:14:G:H2'	2:D:14:G:OP1	2.06	0.55
2:D:14:G:H4'	2:D:15:U:OP2	2.07	0.55
1:C:157:ARG:O	1:C:168:LEU:HD12	2.07	0.55
1:O:89:LEU:O	1:O:185:PRO:HB3	2.06	0.55
1:G:180:LEU:C	1:G:180:LEU:HD12	2.32	0.55
1:M:25:MET:HG2	1:M:46:TRP:CH2	2.42	0.55
1:A:112:LYS:HZ2	2:B:5:U:H5'	1.70	0.54
1:A:187:ARG:HH11	1:A:190:ALA:HB3	1.71	0.54
2:L:7:C:H5''	3:L:2003:HOH:O	2.06	0.54
1:I:98:ARG:NH2	3:I:2045:HOH:O	2.36	0.54
1:M:112:LYS:HE2	2:N:6:C:OP2	2.07	0.54
1:A:155:GLU:OE2	1:G:131:GLU:OE2	2.25	0.54
1:E:158:ARG:O	1:E:159:LYS:HB3	2.06	0.54
1:M:138:LEU:HD12	1:M:179:ARG:HG3	1.89	0.54
1:C:9:ASN:HB3	1:C:75:GLY:O	2.08	0.54
1:E:206:LEU:HB3	3:E:2051:HOH:O	2.07	0.54
1:E:149:LEU:HD11	1:E:177:GLU:CD	2.33	0.54
1:I:118:THR:OG1	1:I:119:PRO:HD2	2.07	0.54
1:A:122:LYS:CE	1:A:172:GLN:OE1	2.56	0.54
1:M:138:LEU:C	1:M:145:TRP:HD1	2.16	0.54
1:E:122:LYS:HD3	1:E:174:VAL:HG21	1.90	0.54
2:B:10:A:H5'	3:B:2002:HOH:O	2.09	0.53
1:E:53:GLY:C	1:E:54:LEU:HD12	2.33	0.53
2:F:5:U:O2	2:F:5:U:C2'	2.56	0.53
1:M:18:ASP:HB3	1:M:25:MET:HA	1.90	0.53
2:J:5:U:H2'	2:J:6:C:H6	1.72	0.53
1:C:80:PHE:N	1:C:80:PHE:CD1	2.77	0.53
1:G:49:GLU:OE1	1:G:49:GLU:HA	2.08	0.53
1:K:184:ASP:OD2	1:K:187:ARG:HB2	2.08	0.53
2:B:19:G:N2	2:B:20:G:C4	2.76	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:GLU:HA	1:C:135:PHE:O	2.09	0.53
1:G:23:TYR:HE1	2:H:22:A:OP1	1.92	0.53
1:C:48:LEU:HD11	1:C:57:PRO:HB2	1.90	0.53
1:A:55:GLU:HG2	1:A:56:PRO:CD	2.39	0.53
2:F:5:U:C5'	3:F:2002:HOH:O	2.52	0.53
1:K:8:LEU:HD21	1:K:25:MET:HE1	1.91	0.53
1:C:132:GLU:O	1:E:16:ARG:HD2	2.09	0.53
1:C:160:LYS:O	1:C:164:GLU:O	2.27	0.52
2:D:7:C:O2'	2:D:8:C:H5'	2.08	0.52
1:E:159:LYS:HD3	1:E:169:LEU:HD11	1.91	0.52
1:K:135:PHE:CZ	1:K:188:ALA:HB1	2.44	0.52
1:M:74:GLU:HB2	1:M:75:GLY:CA	2.28	0.52
1:M:115:ALA:HB1	1:M:172:GLN:HE21	1.74	0.52
1:A:187:ARG:NH1	1:A:190:ALA:HB3	2.24	0.52
1:A:200:LYS:HA	1:A:204:LEU:O	2.09	0.52
1:K:145:TRP:HZ3	2:N:14:G:H5'	1.74	0.52
1:O:133:GLY:O	1:O:188:ALA:HA	2.09	0.52
1:C:169:LEU:HB3	2:D:5:U:O2	2.09	0.52
1:M:112:LYS:HE2	2:N:6:C:P	2.50	0.52
1:M:118:THR:HG22	1:M:121:GLU:OE1	2.09	0.52
1:E:52:ARG:HB3	1:E:55:GLU:OE2	2.09	0.52
1:E:94:ARG:C	1:E:95:LEU:HD22	2.34	0.52
1:A:1:MET:O	1:A:85:PHE:N	2.39	0.52
1:E:155:GLU:HG3	1:E:168:LEU:HD11	1.91	0.52
1:M:155:GLU:O	1:M:156:VAL:HB	2.10	0.52
2:B:18:G:H2'	2:B:19:G:H8	1.75	0.52
1:C:118:THR:HG22	1:C:121:GLU:HG3	1.92	0.52
1:G:21:ASN:OD1	1:G:21:ASN:C	2.52	0.52
1:I:49:GLU:OE1	1:I:49:GLU:HA	2.10	0.52
2:B:21:DG:C2'	2:B:22:A:O5'	2.58	0.52
1:C:135:PHE:CZ	1:C:188:ALA:HB1	2.45	0.52
1:G:5:LYS:NZ	3:G:2003:HOH:O	2.42	0.52
1:A:144:PRO:HB2	1:A:146:VAL:HG12	1.90	0.51
1:C:119:PRO:O	1:C:123:VAL:HG23	2.11	0.51
1:C:171:VAL:HG13	2:D:5:U:C4	2.45	0.51
1:E:42:GLU:OE2	1:E:63:THR:HB	2.10	0.51
2:D:9:C:H2'	2:D:10:A:C8	2.45	0.51
1:M:100:ARG:HH22	1:M:152:THR:HG23	1.75	0.51
1:E:128:ARG:O	1:E:132:GLU:HG3	2.10	0.51
1:M:57:PRO:HD2	3:M:2007:HOH:O	2.11	0.51
1:C:3:LEU:HB2	1:C:85:PHE:CE2	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:8:C:O2'	2:F:9:C:H5'	2.11	0.51
1:M:19:LEU:HD23	1:M:25:MET:HE1	1.93	0.51
1:O:103:PRO:HB3	1:O:125:TRP:CB	2.41	0.51
1:C:74:GLU:HG2	1:C:75:GLY:N	2.25	0.51
1:E:141:GLU:CG	1:E:142:ARG:HA	2.41	0.51
1:I:95:LEU:O	1:I:179:ARG:CG	2.55	0.51
1:C:144:PRO:HD3	1:E:158:ARG:NH1	2.24	0.51
1:C:55:GLU:HB2	1:C:56:PRO:HD2	1.93	0.51
1:E:145:TRP:HD1	1:E:179:ARG:N	2.08	0.51
1:K:145:TRP:HH2	2:N:14:G:P	2.33	0.51
1:M:135:PHE:CE1	1:M:182:VAL:HG22	2.46	0.51
1:O:95:LEU:N	1:O:180:LEU:O	2.40	0.51
1:C:160:LYS:C	1:C:162:GLY:H	2.19	0.50
1:E:91:PRO:C	1:E:93:GLN:H	2.19	0.50
1:K:0:ALA:HB2	1:K:86:HIS:CE1	2.46	0.50
1:K:123:VAL:HG13	1:K:146:VAL:HG11	1.92	0.50
1:K:100:ARG:NH1	3:K:2031:HOH:O	2.44	0.50
1:A:52:ARG:HG2	1:A:55:GLU:OE1	2.11	0.50
1:C:56:PRO:HB2	1:C:57:PRO:CD	2.35	0.50
1:E:93:GLN:NE2	1:E:95:LEU:HD21	2.26	0.50
1:K:36:ALA:HB2	1:K:41:ARG:NH2	2.26	0.50
1:A:52:ARG:HG2	1:A:55:GLU:HB3	1.93	0.50
1:E:7:VAL:HG23	1:E:80:PHE:CE2	2.43	0.50
1:G:2:TRP:O	1:G:62:GLN:HA	2.11	0.50
1:M:135:PHE:HE1	1:M:182:VAL:HG22	1.76	0.50
1:E:34:SER:O	1:E:38:GLU:HG3	2.12	0.50
1:M:106:ARG:NE	2:N:17:U:O4	2.42	0.50
2:L:6:C:H5'	2:L:6:C:H6	1.76	0.50
1:M:43:ARG:HG3	1:M:43:ARG:O	2.12	0.50
1:A:74:GLU:OE1	1:A:75:GLY:HA2	2.12	0.50
1:G:1:MET:HE1	1:G:189:LEU:HD11	1.93	0.50
1:K:103:PRO:HG2	1:K:122:LYS:HG2	1.94	0.49
1:C:97:PHE:HA	1:C:208:SER:O	2.12	0.49
1:I:31:LYS:HB3	1:I:71:VAL:HG21	1.93	0.49
1:A:96:ARG:NE	1:A:211:PRO:O	2.45	0.49
2:B:7:C:O2'	2:B:8:C:H5'	2.13	0.49
1:M:73:ASP:O	1:M:76:TYR:CB	2.51	0.49
1:C:4:THR:HG22	1:C:5:LYS:N	2.28	0.49
1:A:52:ARG:HG2	1:A:55:GLU:CB	2.42	0.49
1:A:129:ARG:NH2	1:A:197:GLY:H	2.10	0.49
2:D:13:C:H4'	2:D:14:G:OP1	2.05	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:136:ARG:O	1:E:180:LEU:HB2	2.13	0.49
1:A:35:ARG:O	1:A:39:GLU:HG3	2.13	0.49
1:A:122:LYS:HE2	1:A:172:GLN:OE1	2.11	0.49
2:H:15:U:O2'	2:H:16:G:P	2.70	0.49
1:I:24:GLU:OE1	1:I:24:GLU:HA	2.13	0.49
1:C:118:THR:HG22	1:C:121:GLU:CG	2.42	0.49
1:C:135:PHE:CE1	1:C:188:ALA:HB1	2.48	0.49
1:E:141:GLU:HA	1:E:142:ARG:C	2.38	0.49
1:G:3:LEU:HD23	1:G:83:LYS:CE	2.40	0.49
1:K:106:ARG:HG3	1:K:106:ARG:NH1	2.27	0.49
1:A:35:ARG:NH2	1:I:24:GLU:OE1	2.46	0.49
1:A:83:LYS:NZ	2:F:9:C:P	2.86	0.49
1:C:1:MET:N	3:C:2001:HOH:O	2.37	0.49
1:K:31:LYS:HB3	1:K:71:VAL:HG21	1.95	0.48
1:M:135:PHE:CD1	1:M:180:LEU:HD13	2.48	0.48
1:G:167:LYS:HD2	1:G:167:LYS:C	2.39	0.48
1:K:73:ASP:O	1:K:74:GLU:C	2.56	0.48
2:P:10:A:H2	2:P:17:U:O2	1.96	0.48
1:M:18:ASP:O	1:M:25:MET:HE2	2.13	0.48
1:A:24:GLU:O	1:A:27:ARG:N	2.47	0.48
1:C:1:MET:HE2	1:C:193:ARG:NH1	2.15	0.48
1:K:23:TYR:CE1	2:L:22:A:H5'	2.48	0.48
2:L:20:G:O2'	2:L:21:DG:H5'	2.13	0.48
1:M:97:PHE:HA	1:M:208:SER:O	2.14	0.48
1:E:149:LEU:HD12	1:E:177:GLU:HB2	1.96	0.48
2:J:21:DG:H2''	2:J:22:A:C5'	2.37	0.48
1:K:74:GLU:CG	1:K:75:GLY:HA2	2.19	0.48
1:E:5:LYS:O	1:E:80:PHE:HD2	1.96	0.48
1:E:7:VAL:CG1	1:E:56:PRO:HB2	2.44	0.48
1:E:135:PHE:CE1	1:E:188:ALA:HB1	2.48	0.48
2:J:12:G:C6	1:K:211:PRO:HG2	2.48	0.48
1:C:155:GLU:HA	1:C:170:GLN:HB3	1.95	0.48
2:J:5:U:H2'	2:J:6:C:C6	2.48	0.48
1:O:93:GLN:O	1:O:181:GLU:HA	2.14	0.48
1:C:81:PRO:O	1:C:82:PRO:C	2.57	0.48
1:G:168:LEU:HD13	1:G:170:GLN:HG3	1.96	0.48
2:J:14:G:N7	1:K:94:ARG:NH1	2.61	0.48
1:K:112:LYS:HD3	2:L:5:U:H3'	1.96	0.48
1:M:97:PHE:CD2	1:M:180:LEU:HD23	2.49	0.48
1:C:9:ASN:HD21	1:C:11:ALA:HB3	1.78	0.47
1:K:64:LEU:HD13	1:K:193:ARG:NH2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:15:U:HO2'	2:L:16:G:P	2.37	0.47
1:M:8:LEU:O	1:M:10:PRO:HD3	2.14	0.47
1:K:13:ARG:HD3	3:K:2005:HOH:O	2.14	0.47
1:K:68:ASP:O	1:K:71:VAL:HG13	2.15	0.47
1:M:49:GLU:OE2	1:M:60:LEU:HD22	2.15	0.47
1:A:83:LYS:HZ1	2:F:9:C:P	2.36	0.47
2:B:13:C:O2	2:B:13:C:O4'	2.30	0.47
1:M:127:GLU:HA	1:M:137:LEU:CD1	2.44	0.47
1:G:184:ASP:HA	1:G:185:PRO:HD3	1.74	0.47
1:K:145:TRP:HH2	2:N:14:G:O5'	1.97	0.47
1:G:126:LEU:HD22	1:G:176:PHE:CG	2.50	0.47
2:H:5:U:H2'	2:H:6:C:C6	2.49	0.47
1:M:127:GLU:HG3	1:M:137:LEU:HD13	1.97	0.47
1:C:68:ASP:OD2	1:C:71:VAL:HG13	2.15	0.47
1:M:15:ALA:O	1:M:19:LEU:HG	2.15	0.47
1:O:152:THR:O	1:O:153:PHE:C	2.57	0.47
1:A:68:ASP:O	1:A:71:VAL:HG22	2.15	0.47
1:I:118:THR:HG22	1:I:121:GLU:CG	2.45	0.47
1:K:22:PRO:HB2	1:K:202:LEU:HD23	1.97	0.47
2:J:5:U:O2'	2:J:6:C:H5'	2.15	0.47
1:A:145:TRP:CD1	1:A:179:ARG:CB	2.87	0.46
1:G:35:ARG:O	1:G:38:GLU:HB2	2.15	0.46
1:M:4:THR:HG21	1:M:69:TRP:NE1	2.30	0.46
1:O:81:PRO:HA	1:O:82:PRO:HD2	1.80	0.46
1:E:94:ARG:CG	1:E:138:LEU:HD11	2.45	0.46
1:I:106:ARG:HG3	1:I:106:ARG:HH11	1.80	0.46
1:I:169:LEU:HD12	1:I:169:LEU:C	2.40	0.46
1:K:36:ALA:HA	1:K:41:ARG:NH1	2.30	0.46
1:I:42:GLU:OE1	1:I:43:ARG:N	2.45	0.46
1:O:113:ARG:O	2:P:5:U:H5''	2.15	0.46
1:A:83:LYS:HZ2	2:F:10:A:P	2.37	0.46
1:C:146:VAL:HG22	1:C:147:GLN:N	2.31	0.46
1:C:160:LYS:O	1:C:162:GLY:N	2.48	0.46
2:D:13:C:C4'	2:D:14:G:OP1	2.63	0.46
1:E:145:TRP:CD1	1:E:145:TRP:O	2.68	0.46
1:E:6:LEU:CD2	1:E:79:VAL:HG23	2.46	0.46
1:E:158:ARG:HD2	1:E:166:GLY:O	2.16	0.46
1:I:12:SER:O	1:I:15:ALA:HB3	2.16	0.46
1:I:135:PHE:CZ	1:I:188:ALA:HB1	2.51	0.46
1:O:56:PRO:HA	1:O:57:PRO:HD2	1.86	0.46
2:B:20:G:H2'	2:B:21:DG:O4'	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:96:ARG:NH1	1:E:96:ARG:HB2	2.30	0.45
1:G:146:VAL:HG22	1:G:147:GLN:N	2.30	0.45
1:I:68:ASP:O	1:I:71:VAL:HG13	2.16	0.45
1:K:23:TYR:OH	1:K:27:ARG:HD2	2.16	0.45
1:M:94:ARG:HD3	1:M:138:LEU:HD11	1.98	0.45
1:O:30:SER:C	1:O:32:ALA:H	2.24	0.45
1:C:132:GLU:OE1	1:E:13:ARG:HD2	2.16	0.45
1:I:73:ASP:OD1	1:I:76:TYR:CB	2.62	0.45
1:O:200:LYS:CB	3:O:2020:HOH:O	2.64	0.45
1:A:171:VAL:HG22	1:A:172:GLN:N	2.30	0.45
1:E:196:VAL:O	1:E:205:GLY:HA2	2.17	0.45
1:I:177:GLU:CD	3:I:2045:HOH:O	2.59	0.45
2:P:7:C:C2	2:P:21:DG:N2	2.84	0.45
1:A:98:ARG:HG3	1:A:175:LEU:HD11	1.98	0.45
2:B:11:C:H2'	2:B:11:C:O2	2.16	0.45
2:F:5:U:H5'	2:F:6:C:OP2	2.16	0.45
1:A:81:PRO:HA	1:A:82:PRO:HD2	1.78	0.45
1:G:80:PHE:CD1	1:G:80:PHE:N	2.84	0.45
2:P:10:A:C2	2:P:17:U:O2	2.70	0.45
1:A:24:GLU:O	1:A:25:MET:C	2.59	0.45
1:A:162:GLY:C	1:A:164:GLU:H	2.24	0.45
2:D:9:C:H2'	2:D:10:A:H8	1.80	0.45
1:I:98:ARG:NH1	1:I:175:LEU:HD21	2.31	0.45
2:D:14:G:H3'	2:D:15:U:H5'	1.99	0.45
1:E:96:ARG:HB2	1:E:210:ALA:O	2.16	0.45
1:G:33:VAL:HG21	1:G:42:GLU:OE1	2.17	0.45
1:M:97:PHE:CD1	1:M:97:PHE:C	2.94	0.45
1:M:135:PHE:CZ	1:M:188:ALA:HB1	2.51	0.45
1:A:103:PRO:HA	1:A:125:TRP:CE2	2.52	0.45
1:A:157:ARG:HD3	2:B:22:A:O2'	2.17	0.45
1:G:9:ASN:HB3	1:G:75:GLY:O	2.16	0.45
1:G:83:LYS:HA	1:G:84:PRO:HD3	1.79	0.45
1:I:2:TRP:O	1:I:62:GLN:HA	2.17	0.45
1:I:35:ARG:HD2	1:I:35:ARG:HA	1.60	0.45
1:M:171:VAL:HG22	2:N:5:U:C4	2.51	0.45
1:A:64:LEU:N	1:A:64:LEU:HD23	2.32	0.45
1:I:44:LEU:HD23	1:I:45:LEU:N	2.32	0.45
1:A:135:PHE:CD1	1:A:180:LEU:HD13	2.52	0.44
1:E:23:TYR:HE2	1:E:27:ARG:NH2	2.15	0.44
1:E:106:ARG:O	2:F:16:G:H5''	2.16	0.44
2:P:12:G:H8	2:P:12:G:H5''	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:199:GLY:HA3	1:K:204:LEU:HD12	1.98	0.44
1:M:118:THR:HG22	1:M:121:GLU:CG	2.47	0.44
1:M:138:LEU:HD23	1:M:138:LEU:HA	1.76	0.44
2:D:20:G:H2'	2:D:21:DG:O4'	2.17	0.44
1:E:7:VAL:HG13	1:E:56:PRO:HB2	2.00	0.44
1:E:127:GLU:CG	1:E:137:LEU:HD22	2.48	0.44
1:K:91:PRO:HD3	1:K:185:PRO:CG	2.48	0.44
2:D:5:U:C2'	2:D:6:C:O5'	2.65	0.44
1:E:98:ARG:HB2	1:E:98:ARG:NH1	2.32	0.44
1:O:205:GLY:O	1:O:206:LEU:C	2.60	0.44
1:A:97:PHE:HA	1:A:208:SER:O	2.18	0.44
1:K:97:PHE:CD2	1:K:180:LEU:HD23	2.53	0.44
1:C:56:PRO:CB	1:C:57:PRO:CD	2.96	0.44
1:I:146:VAL:HG13	1:I:146:VAL:O	2.17	0.44
1:K:42:GLU:OE1	1:K:43:ARG:N	2.46	0.44
1:K:147:GLN:N	1:K:147:GLN:CD	2.76	0.44
1:A:115:ALA:HB1	1:A:172:GLN:NE2	2.33	0.43
1:E:1:MET:HB2	1:E:85:PHE:CE2	2.53	0.43
1:E:23:TYR:CE2	1:E:27:ARG:NH2	2.85	0.43
1:E:37:LEU:HD23	1:E:37:LEU:HA	1.84	0.43
1:I:97:PHE:HA	1:I:208:SER:O	2.17	0.43
1:K:147:GLN:HB3	2:N:15:U:O4'	2.18	0.43
1:G:192:LEU:HD23	1:G:207:LEU:HD23	2.00	0.43
1:I:44:LEU:HD22	1:I:46:TRP:HD1	1.83	0.43
1:A:31:LYS:O	1:A:31:LYS:HG2	2.18	0.43
1:A:74:GLU:HA	1:A:76:TYR:H	1.83	0.43
1:C:44:LEU:HD11	1:C:61:VAL:HG13	2.01	0.43
1:A:52:ARG:O	1:A:52:ARG:HG3	2.17	0.43
1:A:103:PRO:HA	1:A:125:TRP:CD2	2.54	0.43
1:C:89:LEU:O	1:C:185:PRO:HB3	2.19	0.43
1:E:145:TRP:CD1	1:E:179:ARG:CB	2.92	0.43
1:I:180:LEU:C	1:I:180:LEU:HD12	2.43	0.43
2:J:5:U:H1'	3:J:2001:HOH:O	2.18	0.43
1:M:129:ARG:NH1	3:M:2030:HOH:O	2.29	0.43
1:A:150:GLN:HG2	1:A:175:LEU:HB3	2.00	0.43
2:D:14:G:N2	1:E:24:GLU:OE1	2.33	0.43
1:A:73:ASP:O	1:A:76:TYR:CB	2.67	0.43
2:P:20:G:H2'	2:P:21:DG:O4'	2.17	0.43
2:B:9:C:O4'	3:B:2003:HOH:O	2.21	0.43
1:C:6:LEU:HD22	1:C:79:VAL:HG22	2.01	0.43
1:C:18:ASP:HB3	1:C:25:MET:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:33:VAL:HG22	1:G:36:ALA:HB3	1.99	0.43
1:M:96:ARG:HG2	1:M:179:ARG:HE	1.83	0.43
1:A:3:LEU:HD13	1:A:3:LEU:HA	1.88	0.43
1:A:126:LEU:HD22	1:A:176:PHE:CD1	2.54	0.43
2:H:10:A:H2'	2:H:11:C:O4'	2.19	0.43
1:K:145:TRP:CH2	2:N:14:G:O5'	2.72	0.43
1:K:200:LYS:HA	1:K:204:LEU:O	2.18	0.43
1:M:130:LEU:HD12	1:M:137:LEU:HD12	1.99	0.43
1:G:1:MET:HE1	1:G:189:LEU:CD1	2.49	0.43
1:A:13:ARG:HG2	2:H:18:G:H5'	2.00	0.43
1:A:21:ASN:HA	1:A:22:PRO:HD3	1.90	0.43
1:I:95:LEU:HD13	1:I:95:LEU:HA	1.69	0.43
2:P:7:C:H2'	2:P:8:C:C6	2.54	0.43
2:B:17:U:H2'	2:B:18:G:C8	2.54	0.42
1:E:138:LEU:O	1:E:145:TRP:HB3	2.19	0.42
1:E:158:ARG:O	1:E:159:LYS:HG2	2.19	0.42
2:H:19:G:O2'	2:H:20:G:H5'	2.19	0.42
2:L:15:U:O2'	2:L:16:G:P	2.77	0.42
1:O:17:ARG:C	1:O:19:LEU:H	2.27	0.42
1:A:4:THR:HG21	1:A:69:TRP:NE1	2.33	0.42
1:A:155:GLU:OE2	1:G:127:GLU:OE2	2.36	0.42
1:C:14:ALA:O	1:C:15:ALA:C	2.59	0.42
2:D:19:G:C2'	2:D:20:G:H5'	2.49	0.42
1:G:184:ASP:OD1	1:G:184:ASP:C	2.63	0.42
2:N:8:C:H1'	3:N:2005:HOH:O	2.19	0.42
1:G:193:ARG:HH11	1:G:193:ARG:HG2	1.83	0.42
1:I:28:THR:CG2	1:I:72:LEU:HD21	2.49	0.42
1:K:149:LEU:CD2	1:M:108:ALA:HB3	2.49	0.42
1:M:148:ILE:HG23	1:M:174:VAL:HG13	2.01	0.42
1:A:184:ASP:C	1:A:184:ASP:OD1	2.61	0.42
1:I:11:ALA:O	1:I:16:ARG:NH1	2.52	0.42
1:A:97:PHE:CD1	1:A:97:PHE:C	2.97	0.42
1:E:105:LYS:O	1:E:113:ARG:HA	2.20	0.42
1:G:1:MET:HE2	1:G:193:ARG:HG2	2.02	0.42
1:I:100:ARG:NH2	1:I:154:LEU:HD21	2.35	0.42
1:K:2:TRP:O	1:K:62:GLN:HA	2.19	0.42
2:P:12:G:C5'	2:P:12:G:C8	3.03	0.42
1:E:145:TRP:HE1	1:E:179:ARG:HG3	1.83	0.42
2:H:5:U:C1'	3:H:2001:HOH:O	2.67	0.42
1:M:100:ARG:HH21	1:M:154:LEU:HD21	1.83	0.42
1:E:150:GLN:HG2	1:E:175:LEU:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:24:GLU:OE1	1:G:24:GLU:HA	2.19	0.42
1:E:52:ARG:HD2	1:E:52:ARG:HA	1.57	0.42
2:H:5:U:O2'	2:H:6:C:O5'	2.34	0.42
1:K:68:ASP:OD1	1:K:70:SER:OG	2.36	0.42
1:O:83:LYS:HA	1:O:84:PRO:HD2	1.91	0.42
2:P:14:G:C4'	2:P:15:U:OP1	2.62	0.42
1:A:169:LEU:HD22	2:B:5:U:O2'	2.19	0.42
1:E:135:PHE:CZ	1:E:188:ALA:HB1	2.54	0.42
1:E:154:LEU:HB2	1:E:171:VAL:HG12	2.00	0.42
1:G:131:GLU:HA	1:G:135:PHE:O	2.20	0.42
1:M:37:LEU:HD23	1:M:42:GLU:HB3	2.01	0.42
1:G:33:VAL:HG22	1:G:33:VAL:O	2.20	0.42
1:G:127:GLU:OE2	1:G:131:GLU:OE2	2.38	0.42
1:I:190:ALA:O	1:I:194:ARG:HG3	2.19	0.42
1:G:145:TRP:O	1:G:178:GLY:HA3	2.20	0.41
1:C:8:LEU:HA	1:C:77:ALA:HB2	2.00	0.41
1:C:105:LYS:HE2	1:C:116:LEU:CD2	2.50	0.41
1:E:97:PHE:HB3	1:E:209:VAL:HG12	2.02	0.41
1:E:157:ARG:HD2	3:E:2034:HOH:O	2.19	0.41
1:G:138:LEU:HD21	1:G:181:GLU:HB2	2.01	0.41
1:K:23:TYR:CD1	2:L:22:A:H5'	2.55	0.41
1:M:146:VAL:HG22	1:M:147:GLN:N	2.34	0.41
1:A:179:ARG:NH1	3:A:2027:HOH:O	2.53	0.41
1:A:31:LYS:O	1:A:71:VAL:HG21	2.20	0.41
1:C:210:ALA:HA	1:C:211:PRO:HD3	1.87	0.41
1:E:97:PHE:CE2	1:E:180:LEU:HD23	2.56	0.41
1:G:106:ARG:HG3	1:G:106:ARG:NH1	2.34	0.41
1:M:107:LEU:HB2	1:M:110:THR:OG1	2.21	0.41
1:A:135:PHE:CZ	1:A:188:ALA:HB1	2.55	0.41
1:I:4:THR:HG22	1:I:6:LEU:HD12	2.03	0.41
1:K:194:ARG:O	1:K:200:LYS:HE2	2.21	0.41
2:B:9:C:O2'	2:B:10:A:H5'	2.21	0.41
1:C:53:GLY:C	1:C:55:GLU:H	2.29	0.41
1:K:119:PRO:O	1:K:123:VAL:HG23	2.21	0.41
1:M:26:HIS:O	1:M:30:SER:OG	2.34	0.41
1:A:137:LEU:HD12	1:A:137:LEU:HA	1.76	0.41
1:A:142:ARG:NH2	3:A:2023:HOH:O	2.54	0.41
1:A:168:LEU:HG	1:A:169:LEU:N	2.35	0.41
1:E:81:PRO:HA	1:E:82:PRO:HD2	1.92	0.41
1:E:85:PHE:CD1	1:E:85:PHE:C	2.99	0.41
1:E:97:PHE:CD1	1:E:97:PHE:C	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:43:ARG:NH1	1:G:200:LYS:HD3	2.36	0.41
1:I:56:PRO:HA	1:I:57:PRO:HD3	1.84	0.41
1:K:91:PRO:HD3	1:K:185:PRO:HG3	2.02	0.41
1:M:9:ASN:OD1	1:M:11:ALA:HB3	2.21	0.41
2:P:9:C:O2	2:P:9:C:H2'	2.21	0.41
1:A:23:TYR:CE2	1:A:27:ARG:NH1	2.89	0.41
1:A:43:ARG:O	1:A:43:ARG:HG3	2.19	0.41
1:C:89:LEU:HA	1:C:93:GLN:OE1	2.21	0.41
1:E:35:ARG:NH2	1:K:27:ARG:HB3	2.36	0.41
1:I:98:ARG:NE	3:I:2045:HOH:O	2.53	0.41
1:K:155:GLU:HG2	1:K:170:GLN:OE1	2.21	0.41
1:M:27:ARG:HH11	1:M:27:ARG:HG3	1.86	0.41
1:M:180:LEU:C	1:M:180:LEU:HD12	2.46	0.41
1:A:9:ASN:OD1	1:A:11:ALA:HB3	2.20	0.40
1:E:100:ARG:HG2	1:E:204:LEU:CD2	2.51	0.40
1:G:167:LYS:C	1:G:167:LYS:CD	2.94	0.40
1:M:118:THR:HG22	1:M:121:GLU:CD	2.46	0.40
2:N:21:DG:H2'	2:N:22:A:H8	1.84	0.40
1:O:81:PRO:O	1:O:82:PRO:C	2.64	0.40
2:B:19:G:C2	2:B:20:G:C4	3.09	0.40
1:E:145:TRP:HD1	1:E:179:ARG:H	1.67	0.40
1:K:49:GLU:OE1	1:K:49:GLU:HA	2.21	0.40
1:M:145:TRP:O	1:M:178:GLY:HA3	2.22	0.40
1:A:199:GLY:O	1:A:200:LYS:C	2.65	0.40
1:E:139:GLU:OE1	1:E:144:PRO:HA	2.21	0.40
1:G:200:LYS:HA	1:G:204:LEU:O	2.22	0.40
1:M:12:SER:HB3	1:M:15:ALA:HB3	2.02	0.40
1:M:118:THR:OG1	1:M:119:PRO:HD2	2.20	0.40
1:A:2:TRP:C	1:A:3:LEU:HD22	2.46	0.40
1:A:49:GLU:OE1	1:A:49:GLU:HA	2.21	0.40
1:C:80:PHE:HD1	1:C:80:PHE:H	1.69	0.40
2:H:15:U:HO2'	2:H:16:G:P	2.39	0.40
1:A:96:ARG:O	1:A:209:VAL:HA	2.20	0.40
1:A:189:LEU:O	1:A:190:ALA:C	2.62	0.40
1:C:100:ARG:NH2	1:C:154:LEU:HD13	2.36	0.40
1:E:96:ARG:HH11	1:E:210:ALA:C	2.29	0.40
2:J:10:A:H2'	2:J:11:C:O4'	2.22	0.40

All (2) 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)
3:C:2021:HOH:O	3:E:2020:HOH:O[2_445]	2.01	0.19
1:C:155:GLU:OE2	3:E:2026:HOH:O[2_445]	2.16	0.04

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	
1	A	211/215 (98%)	198 (94%)	12 (6%)	1 (0%)	24	43
1	C	209/215 (97%)	194 (93%)	14 (7%)	1 (0%)	24	43
1	E	207/215 (96%)	196 (95%)	10 (5%)	1 (0%)	24	43
1	G	193/215 (90%)	185 (96%)	5 (3%)	3 (2%)	7	14
1	I	185/215 (86%)	175 (95%)	10 (5%)	0	100	100
1	K	183/215 (85%)	174 (95%)	7 (4%)	2 (1%)	11	22
1	M	185/215 (86%)	174 (94%)	11 (6%)	0	100	100
1	O	167/215 (78%)	139 (83%)	24 (14%)	4 (2%)	4	8
All	All	1540/1720 (90%)	1435 (93%)	93 (6%)	12 (1%)	16	31

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	33	VAL
1	K	145	TRP
1	O	8	LEU
1	O	31	LYS
1	O	34	SER
1	G	73	ASP
1	G	145	TRP
1	K	74	GLU
1	A	82	PRO
1	C	162	GLY
1	O	82	PRO

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Mol	Chain	Res	Type
1	E	92	GLY

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	172/173 (99%)	169 (98%)	3 (2%)	53	78
1	C	172/173 (99%)	165 (96%)	7 (4%)	27	53
1	E	170/173 (98%)	168 (99%)	2 (1%)	63	83
1	G	164/173 (95%)	161 (98%)	3 (2%)	51	77
1	I	159/173 (92%)	155 (98%)	4 (2%)	42	69
1	K	157/173 (91%)	154 (98%)	3 (2%)	50	76
1	M	158/173 (91%)	157 (99%)	1 (1%)	78	91
1	O	17/173 (10%)	17 (100%)	0	100	100
All	All	1169/1384 (84%)	1146 (98%)	23 (2%)	48	75

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	LEU
1	A	138	LEU
1	A	200	LYS
1	C	54	LEU
1	C	72	LEU
1	C	80	PHE
1	C	138	LEU
1	C	168	LEU
1	C	171	VAL
1	C	187	ARG
1	E	98	ARG
1	E	202	LEU
1	G	46	TRP
1	G	79	VAL

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Mol	Chain	Res	Type
1	G	187	ARG
1	I	6	LEU
1	I	71	VAL
1	I	94	ARG
1	I	168	LEU
1	K	71	VAL
1	K	79	VAL
1	K	154	LEU
1	M	60	LEU

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

Mol	Chain	Res	Type
1	C	26	HIS
1	E	102	ASN
1	G	147	GLN
1	I	86	HIS
1	I	147	GLN
1	I	150	GLN
1	M	93	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	16/19 (84%)	5 (31%)	1 (6%)
2	D	15/19 (78%)	3 (20%)	1 (6%)
2	F	15/19 (78%)	6 (40%)	1 (6%)
2	H	15/19 (78%)	6 (40%)	1 (6%)
2	J	15/19 (78%)	2 (13%)	1 (6%)
2	L	16/19 (84%)	6 (37%)	2 (12%)
2	N	15/19 (78%)	3 (20%)	0
2	P	15/19 (78%)	5 (33%)	2 (13%)
All	All	122/152 (80%)	36 (29%)	9 (7%)

All (36) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	6	C
2	B	11	C
2	B	13	C

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Mol	Chain	Res	Type
2	B	15	U
2	B	16	G
2	D	6	C
2	D	13	C
2	D	14	G
2	F	6	C
2	F	11	C
2	F	12	G
2	F	14	G
2	F	15	U
2	F	16	G
2	H	6	C
2	H	11	C
2	H	12	G
2	H	14	G
2	H	15	U
2	H	16	G
2	J	15	U
2	J	16	G
2	L	6	C
2	L	7	C
2	L	8	C
2	L	13	C
2	L	15	U
2	L	16	G
2	N	11	C
2	N	15	U
2	N	16	G
2	P	6	C
2	P	11	C
2	P	12	G
2	P	15	U
2	P	16	G

All (9) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	5	U
2	D	13	C
2	F	14	G
2	H	15	U
2	J	15	U

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Mol	Chain	Res	Type
2	L	5	U
2	L	15	U
2	P	12	G
2	P	14	G

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	A	213/215 (99%)	0.39	14 (6%) 24 21	23, 41, 78, 118	0
1	C	211/215 (98%)	0.34	16 (7%) 20 17	21, 41, 82, 115	0
1	E	211/215 (98%)	0.36	11 (5%) 33 29	18, 41, 76, 112	0
1	G	199/215 (92%)	0.25	9 (4%) 38 33	21, 41, 64, 95	0
1	I	195/215 (90%)	-0.03	9 (4%) 37 33	12, 32, 64, 98	0
1	K	191/215 (88%)	0.03	10 (5%) 33 29	15, 35, 63, 99	0
1	M	193/215 (89%)	0.47	11 (5%) 29 26	27, 47, 78, 109	0
1	O	177/215 (82%)	2.59	117 (66%) 0 0	63, 85, 116, 132	0
2	B	19/19 (100%)	0.07	1 (5%) 32 28	43, 57, 104, 110	0
2	D	19/19 (100%)	-0.25	0 100 100	36, 52, 68, 69	0
2	F	19/19 (100%)	-0.25	0 100 100	34, 42, 58, 74	0
2	H	19/19 (100%)	-0.10	0 100 100	41, 55, 72, 84	0
2	J	19/19 (100%)	-0.25	1 (5%) 32 28	25, 37, 104, 118	0
2	L	19/19 (100%)	0.05	0 100 100	28, 46, 88, 148	0
2	N	18/19 (94%)	0.11	1 (5%) 30 26	41, 57, 87, 99	0
2	P	18/19 (94%)	2.44	11 (61%) 0 0	116, 128, 162, 176	0
All	All	1740/1872 (92%)	0.50	211 (12%) 8 7	12, 43, 95, 176	0

All (211) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	23	TYR	5.8
1	O	28	THR	5.6
1	O	114	VAL	5.6
1	O	29	LEU	5.6
1	O	89	LEU	5.5

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Mol	Chain	Res	Type	RSRZ
1	O	112	LYS	5.5
1	M	156	VAL	5.2
1	O	85	PHE	5.0
1	O	125	TRP	5.0
1	O	205	GLY	5.0
1	O	173	ALA	4.8
1	O	113	ARG	4.7
1	O	25	MET	4.7
1	O	26	HIS	4.5
1	E	108	ALA	4.5
1	I	168	LEU	4.5
1	O	174	VAL	4.5
1	O	0	ALA	4.5
1	O	97	PHE	4.4
1	O	208	SER	4.3
1	O	176	PHE	4.2
1	O	195	GLY	4.2
1	O	101	ALA	4.2
1	O	63	THR	4.1
1	O	15	ALA	4.0
1	O	33	VAL	4.0
2	P	14	G	4.0
1	C	73	ASP	3.9
1	O	111	GLY	3.9
1	O	199	GLY	3.9
1	E	80	PHE	3.8
1	O	58	VAL	3.8
1	O	150	GLN	3.8
1	O	67	PRO	3.8
1	O	30	SER	3.7
1	A	142	ARG	3.7
1	O	175	LEU	3.7
1	O	147	GLN	3.7
1	O	46	TRP	3.7
1	O	110	THR	3.7
1	O	196	VAL	3.7
1	O	59	VAL	3.7
2	P	21	DG	3.7
1	O	198	PRO	3.7
1	O	98	ARG	3.7
1	O	16	ARG	3.6
1	O	86	HIS	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	80	PHE	3.6
1	E	211	PRO	3.6
2	P	20	G	3.6
1	O	148	ILE	3.6
1	O	184	ASP	3.6
1	G	157	ARG	3.5
1	O	194	ARG	3.5
1	O	144	PRO	3.5
2	P	22	A	3.5
1	O	39	GLU	3.5
1	O	42	GLU	3.4
1	I	145	TRP	3.4
1	O	9	ASN	3.4
1	M	145	TRP	3.4
1	O	182	VAL	3.4
1	O	135	PHE	3.4
1	O	36	ALA	3.4
1	O	34	SER	3.3
1	O	126	LEU	3.3
1	O	209	VAL	3.3
1	M	56	PRO	3.2
1	M	169	LEU	3.2
1	K	111	GLY	3.2
1	O	151	ASP	3.2
2	B	13	C	3.2
1	O	197	GLY	3.2
2	P	5	U	3.2
1	O	49	GLU	3.1
1	A	54	LEU	3.1
1	O	40	GLY	3.1
1	E	210	ALA	3.1
1	O	88	ALA	3.1
1	O	84	PRO	3.1
1	O	99	LEU	3.1
1	O	2	TRP	3.1
1	C	145	TRP	3.1
1	O	38	GLU	3.0
1	O	186	GLU	3.0
1	O	183	VAL	3.0
1	O	68	ASP	3.0
1	O	80	PHE	3.0
1	O	14	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	O	50	PRO	2.9
1	C	160	LYS	2.9
1	E	162	GLY	2.9
1	O	4	THR	2.9
1	K	113	ARG	2.9
1	O	32	ALA	2.9
1	E	107	LEU	2.9
1	K	171	VAL	2.9
1	I	110	THR	2.9
1	C	8	LEU	2.9
1	K	108	ALA	2.9
1	G	145	TRP	2.9
1	O	21	ASN	2.8
1	O	100	ARG	2.8
2	J	5	U	2.8
2	P	15	U	2.8
2	P	8	C	2.8
1	O	207	LEU	2.8
1	O	105	LYS	2.8
1	O	178	GLY	2.8
1	E	141	GLU	2.8
1	O	27	ARG	2.8
1	O	91	PRO	2.8
1	I	169	LEU	2.8
1	C	142	ARG	2.8
1	M	143	GLY	2.8
1	A	108	ALA	2.8
1	K	74	GLU	2.8
1	O	90	LYS	2.8
1	O	153	PHE	2.8
1	A	85	PHE	2.7
1	O	206	LEU	2.7
1	A	162	GLY	2.7
1	A	145	TRP	2.7
1	O	192	LEU	2.7
1	K	51	ALA	2.7
1	G	141	GLU	2.7
1	G	56	PRO	2.7
2	P	9	C	2.7
1	K	35	ARG	2.7
1	O	65	THR	2.7
1	O	69	TRP	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	142	ARG	2.6
1	O	41	ARG	2.6
1	O	48	LEU	2.6
1	O	70	SER	2.6
1	A	-1	GLY	2.6
1	A	107	LEU	2.6
1	C	159	LYS	2.6
1	O	202	LEU	2.6
1	I	111	GLY	2.6
2	N	5	U	2.6
1	M	153	PHE	2.5
1	O	177	GLU	2.5
1	C	54	LEU	2.5
1	G	13	ARG	2.5
1	M	41	ARG	2.5
1	O	76	TYR	2.5
1	A	74	GLU	2.5
1	O	123	VAL	2.5
1	O	121	GLU	2.5
1	O	149	LEU	2.5
1	O	56	PRO	2.5
1	A	13	ARG	2.5
1	C	35	ARG	2.5
1	O	185	PRO	2.4
1	I	55	GLU	2.4
1	O	12	SER	2.4
1	O	146	VAL	2.4
1	O	104	ALA	2.4
1	K	112	LYS	2.4
1	K	13	ARG	2.4
1	O	24	GLU	2.4
1	M	147	GLN	2.4
1	O	18	ASP	2.4
2	P	16	G	2.4
1	I	51	ALA	2.4
1	O	103	PRO	2.3
1	M	13	ARG	2.3
2	P	19	G	2.3
1	O	118	THR	2.3
1	O	128	ARG	2.3
1	E	79	VAL	2.3
1	M	36	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	O	22	PRO	2.3
1	O	190	ALA	2.3
1	K	110	THR	2.3
1	C	117	LYS	2.3
1	O	102	ASN	2.2
1	A	187	ARG	2.2
1	O	124	ALA	2.2
1	O	107	LEU	2.2
1	M	74	GLU	2.2
1	C	52	ARG	2.2
1	G	117	LYS	2.2
1	O	120	ALA	2.2
1	I	95	LEU	2.2
1	O	13	ARG	2.2
1	O	145	TRP	2.2
1	G	23	TYR	2.1
1	O	57	PRO	2.1
1	O	11	ALA	2.1
1	A	55	GLU	2.1
1	C	74	GLU	2.1
2	P	12	G	2.1
1	O	10	PRO	2.1
1	G	104	ALA	2.1
1	G	201	ALA	2.1
1	O	77	ALA	2.1
1	C	141	GLU	2.1
1	O	78	GLN	2.0
1	C	165	ALA	2.0
1	O	109	ALA	2.0
1	O	204	LEU	2.0
1	E	140	GLY	2.0
1	E	109	ALA	2.0
1	O	44	LEU	2.0
1	A	140	GLY	2.0
1	C	140	GLY	2.0
1	I	-1	GLY	2.0
1	C	50	PRO	2.0
1	C	56	PRO	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 [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.