wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 02:22 PM BST

PDB ID	:	3J7A
EMDB ID:	:	EMD-2660
Title	:	Cryo-EM structure of the Plasmodium falciparum 80S ribosome bound to the anti-protozoan drug emetine, small subunit
Authors	:	Wong, W.; Bai, X.C.; Brown, A.; Fernandez, I.S.; Hanssen, E.; Condron, M.; Tan, Y.H.; Baum, J.; Scheres, S.H.W.
Deposited on	:	2014-06-03
Resolution	:	3.20 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could
stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp

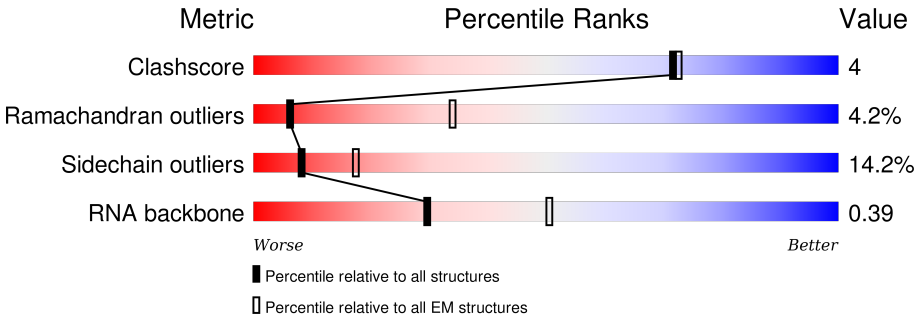
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	2092	45% 26% 5% 23%
2	B	262	53% 22% 5% 20%
3	C	263	55% 17% • 26%
4	D	221	56% 14% • 29%
5	E	189	71% 26% • •
6	F	261	71% 23% • •
7	G	272	65% 15% • 18%
8	H	306	50% 14% • 33%

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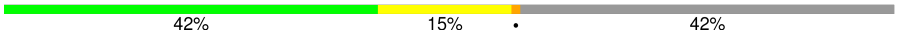
Mol	Chain	Length	Quality of chain
9	I	195	
10	J	194	
11	K	130	
12	L	218	
13	M	144	
14	N	118	
15	O	137	
16	P	151	
17	Q	145	
18	R	141	
19	S	156	
20	T	54	
21	U	151	
22	V	161	
23	W	137	
24	X	145	
25	Y	170	
26	Z	82	
27	1	133	
28	2	105	
29	3	107	
30	4	82	
31	5	67	
32	6	58	
33	7	74	

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 68866 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	1608	34277	15347	6109	11213	1608	0	0

- Molecule 2 is a protein called 40S ribosomal protein eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	210	1713	1097	301	303	12	0	0

- Molecule 3 is a protein called 40S ribosomal protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	195	1538	990	266	273	9	0	0

- Molecule 4 is a protein called 40S ribosomal protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	157	1228	782	225	214	7	0	0

- Molecule 5 is a protein called 40S ribosomal protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	185	1508	959	287	260	2	0	0

- Molecule 6 is a protein called 40S ribosomal protein eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	257	2061	1320	377	356	8	0	0

- Molecule 7 is a protein called 40S ribosomal protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	224	Total	C	N	O	S	0	0
			1757	1132	307	309	9		

- Molecule 8 is a protein called 40S ribosomal protein eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	204	Total	C	N	O	S	0	0
			1644	1042	313	283	6		

- Molecule 9 is a protein called 40S ribosomal protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	180	Total	C	N	O	S	0	0
			1424	893	263	258	10		

- Molecule 10 is a protein called 40S ribosomal protein eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	188	Total	C	N	O	S	0	0
			1528	982	264	278	4		

- Molecule 11 is a protein called 40S ribosomal protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	129	Total	C	N	O	S	0	0
			1037	665	189	178	5		

- Molecule 12 is a protein called 40S ribosomal protein eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	172	Total	C	N	O	S	0	0
			1392	878	266	244	4		

- Molecule 13 is a protein called 40S ribosomal protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	138	Total	C	N	O	S	0	0
			1098	704	200	193	1		

- Molecule 14 is a protein called 40S ribosomal protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	98	Total	C	N	O	S	0	0
			772	484	135	148	5		

- Molecule 15 is a protein called 40S ribosomal protein eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	79	Total	C	N	O	S	0	0
			686	450	116	118	2		

- Molecule 16 is a protein called 40S ribosomal protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	127	Total	C	N	O	S	0	0
			953	591	184	175	3		

- Molecule 17 is a protein called 40S ribosomal protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	144	Total	C	N	O	S	0	0
			1129	712	222	193	2		

- Molecule 18 is a protein called 40S ribosomal protein eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	98	Total	C	N	O	S	0	0
			746	474	123	145	4		

- Molecule 19 is a protein called 40S ribosomal protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	128	Total	C	N	O	S	0	0
			1042	655	204	179	4		

- Molecule 20 is a protein called 40S ribosomal protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	48	Total	C	N	O	S	0	0
			404	252	85	63	4		

- Molecule 21 is a protein called 40S ribosomal protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	149	Total	C	N	O	S	0	0
			1202	769	220	210	3		

- Molecule 22 is a protein called 40S ribosomal protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	146	Total	C	N	O	S	0	0
			1206	772	227	200	7		

- Molecule 23 is a protein called 40S ribosomal protein eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	95	Total	C	N	O	S	0	0
			785	498	149	135	3		

- Molecule 24 is a protein called 40S ribosomal protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	96	Total	C	N	O	S	0	0
			776	497	137	138	4		

- Molecule 25 is a protein called 40S ribosomal protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	154	Total	C	N	O	S	0	0
			1266	811	239	214	2		

- Molecule 26 is a protein called 40S ribosomal protein eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	72	Total	C	N	O	S	0	0
			556	346	102	104	4		

- Molecule 27 is a protein called 40S ribosomal protein eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	1	120	Total	C	N	O	S	0	0
			981	629	188	162	2		

- Molecule 28 is a protein called 40S ribosomal protein eS25.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	2	41	Total	C	N	O	0	0
			320	208	56	56		

- Molecule 29 is a protein called 40S ribosomal protein eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	3	95	Total	C	N	O	S	0	0
			781	478	169	128	6		

- Molecule 30 is a protein called 40S ribosomal protein eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	4	76	Total	C	N	O	S	0	0
			586	368	102	107	9		

- Molecule 31 is a protein called 40S ribosomal protein eS28.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	5	58	Total	C	N	O	0	0
			451	282	90	79		

- Molecule 32 is a protein called 40S ribosomal protein eS30.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	6	43	Total	C	N	O	0	0
			345	213	75	57		

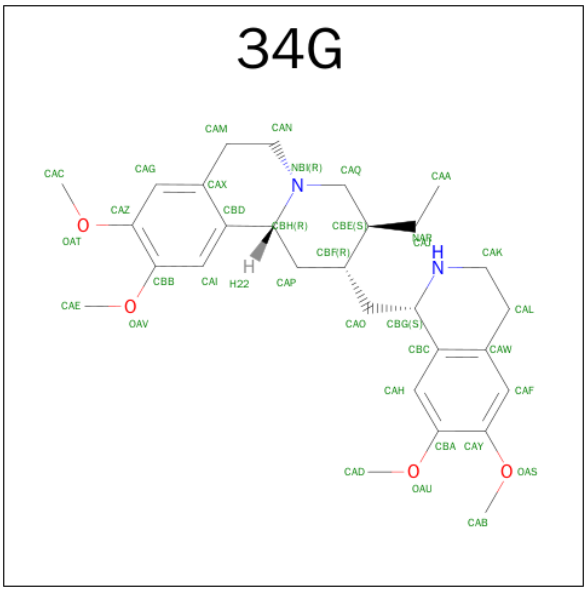
- Molecule 33 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	7	74	Total	C	N	O	P	0	0
			1571	702	275	521	73		

- Molecule 34 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
34	A	67	Total	Mg	0
			67	67	

- Molecule 35 is EMETINE (three-letter code: 34G) (formula: $C_{29}H_{40}N_2O_4$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
35	A	1	35	29	2	4	0

- Molecule 36 is ZINC ION (three-letter code: ZN) (formula: Zn).

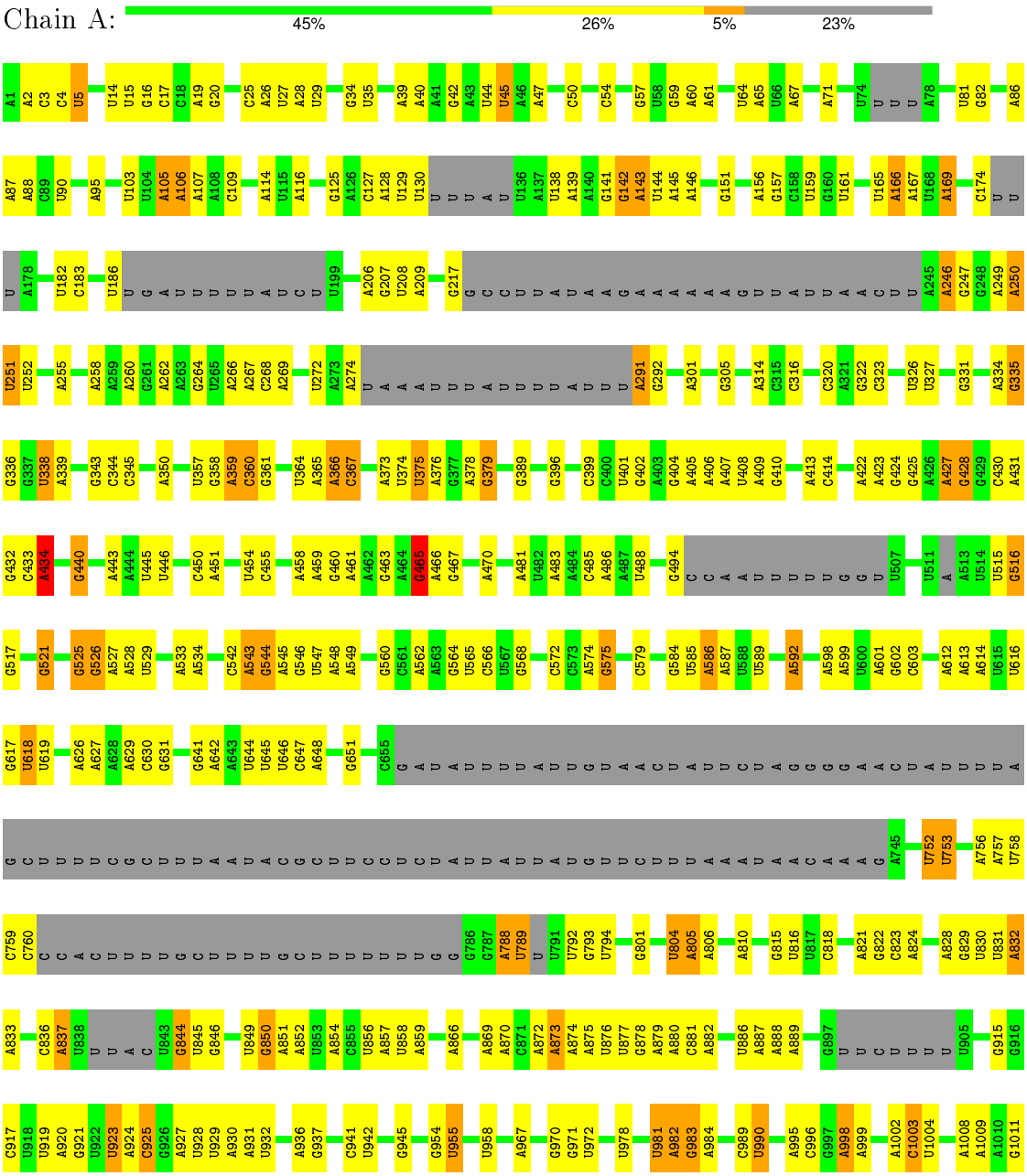
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
36	T	1	1	1	0

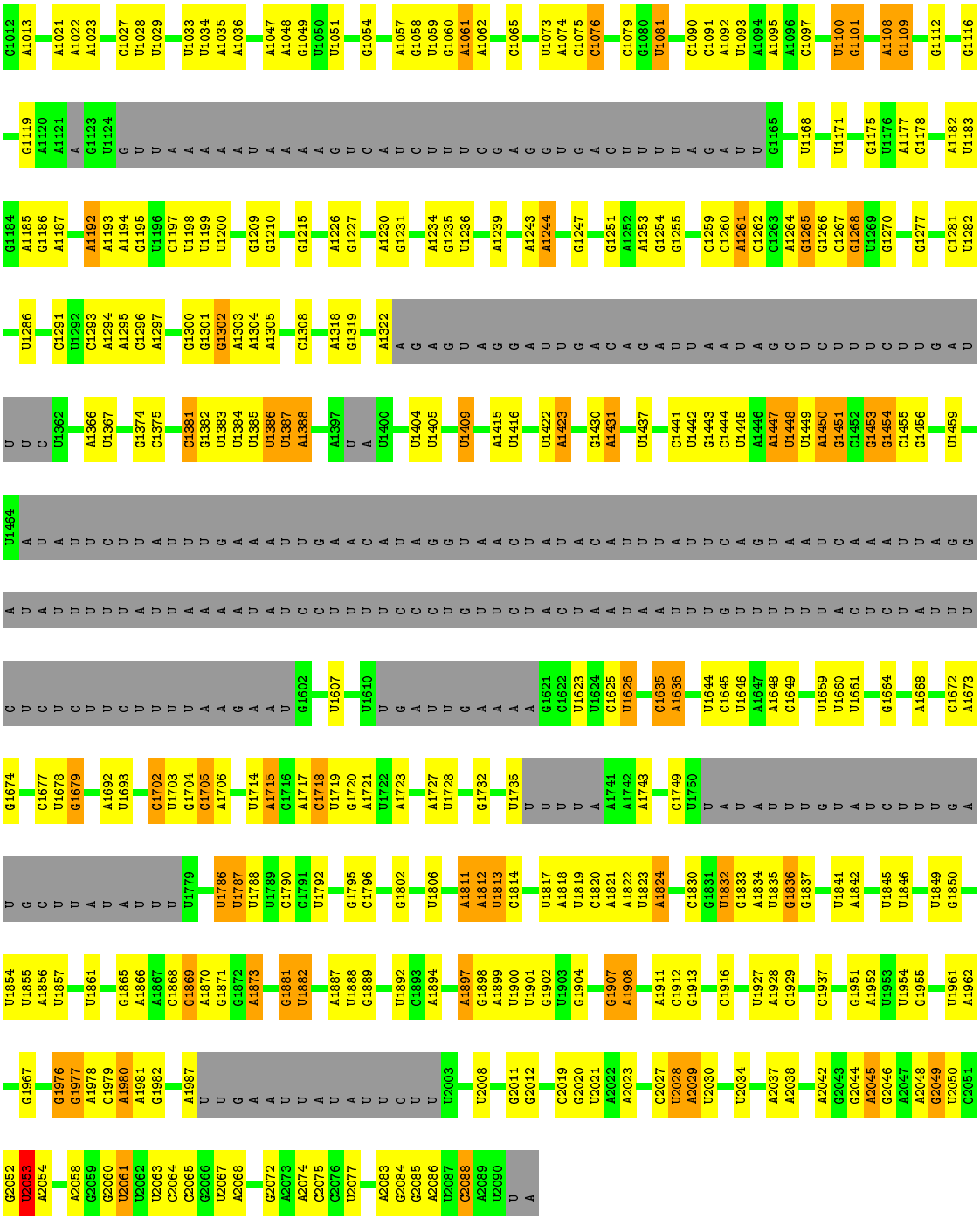
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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: 18S ribosomal RNA

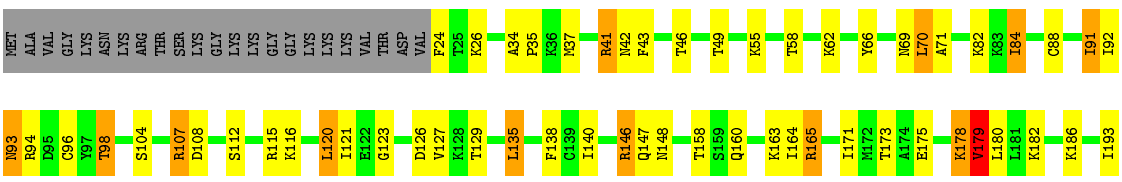
Chain A:





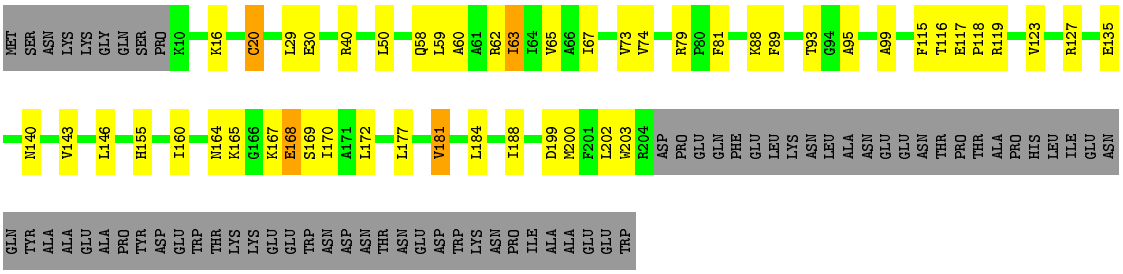
- Molecule 2: 40S ribosomal protein eS1

Chain B:



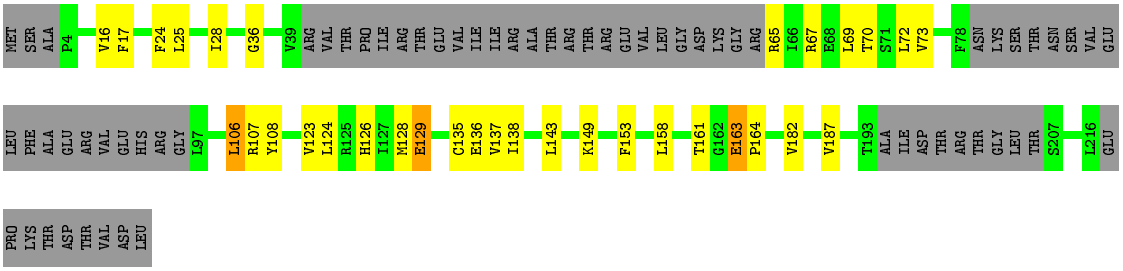
- Molecule 3: 40S ribosomal protein uS2

Chain C:



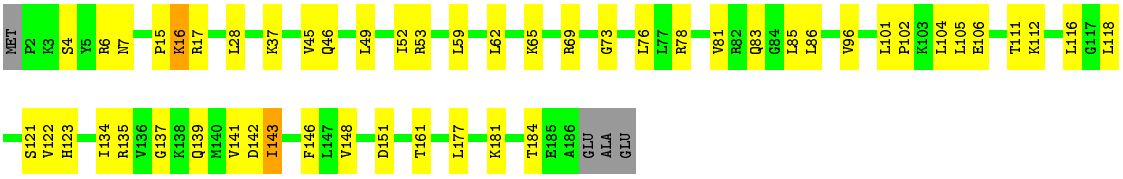
- Molecule 4: 40S ribosomal protein uS3

Chain D:



- Molecule 5: 40S ribosomal protein uS4

Chain E:

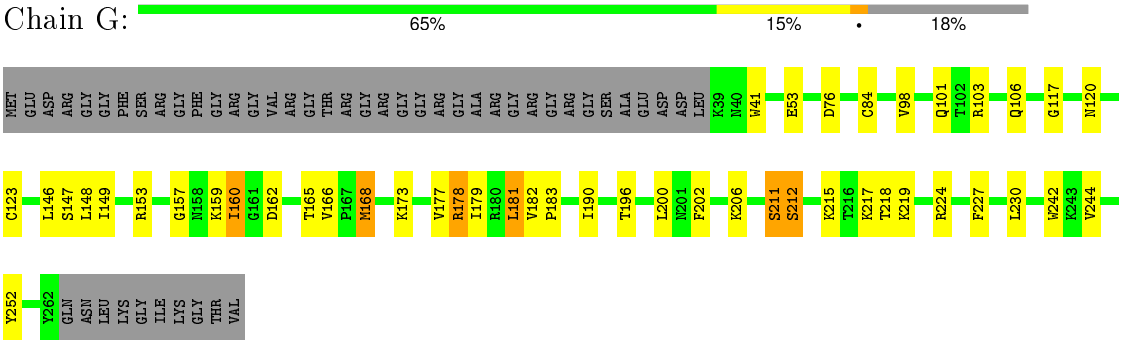


- Molecule 6: 40S ribosomal protein eS4

Chain F:

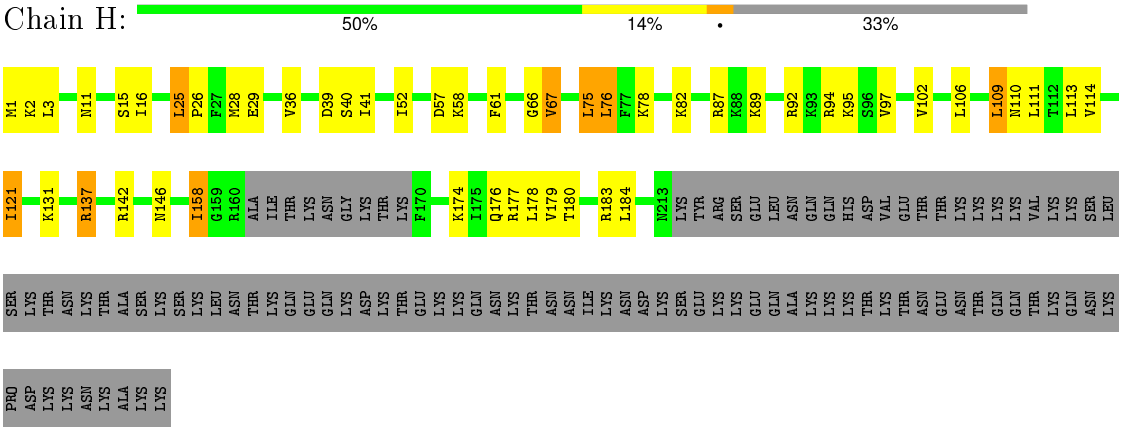
- Molecule 7: 40S ribosomal protein uS5

Chain G:



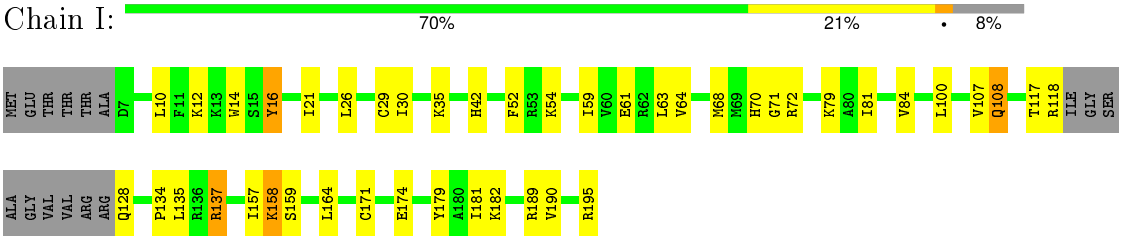
- Molecule 8: 40S ribosomal protein eS6

Chain H:



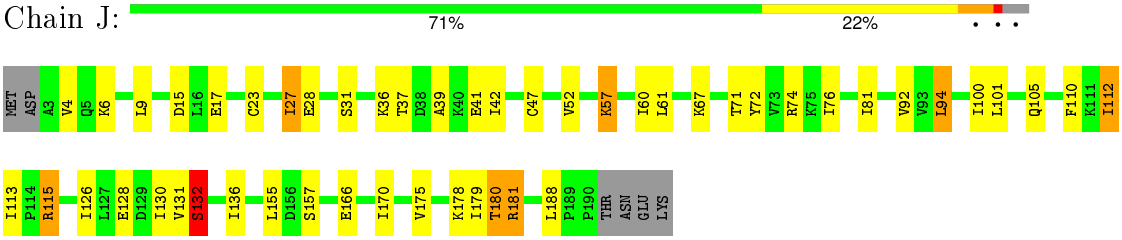
- Molecule 9: 40S ribosomal protein uS7

Chain I:



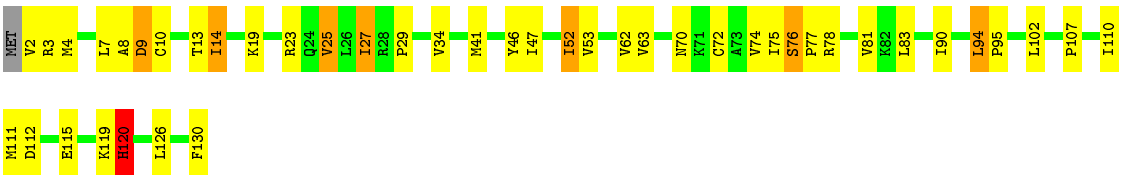
- Molecule 10: 40S ribosomal protein eS7

Chain J:



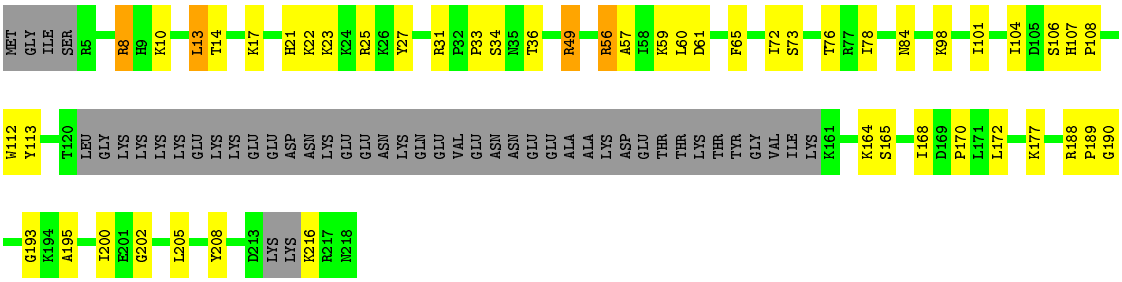
- Molecule 11: 40S ribosomal protein uS8

Chain K:



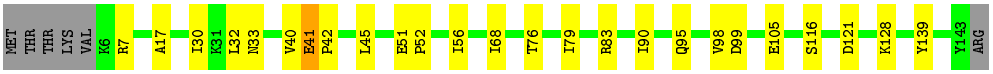
- Molecule 12: 40S ribosomal protein eS8

Chain L:



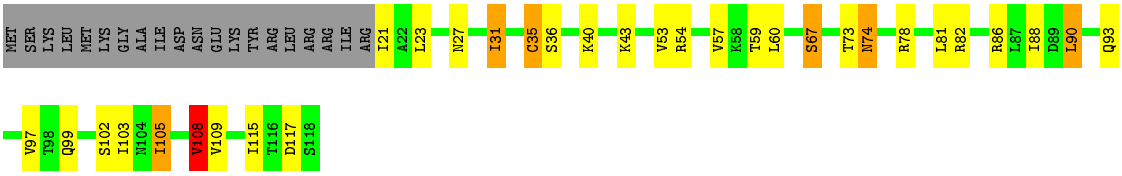
- Molecule 13: 40S ribosomal protein uS9

Chain M:



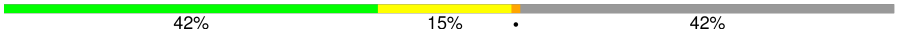
- Molecule 14: 40S ribosomal protein uS10

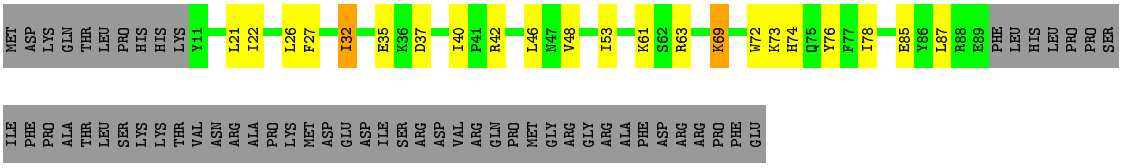
Chain N:



- Molecule 15: 40S ribosomal protein eS10

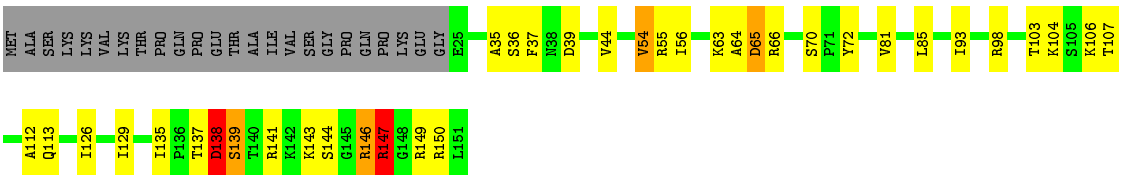
Chain O:





- Molecule 16: 40S ribosomal protein uS11

Chain P:

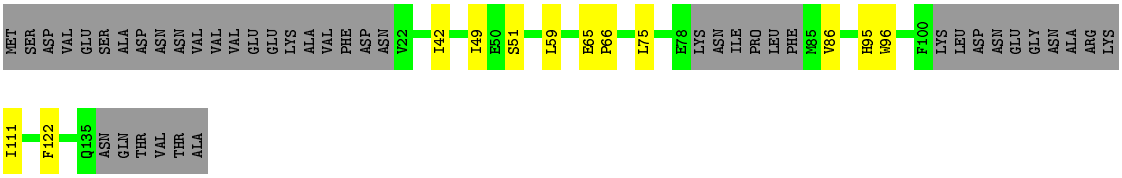


- Molecule 17: 40S ribosomal protein uS12

Chain Q:

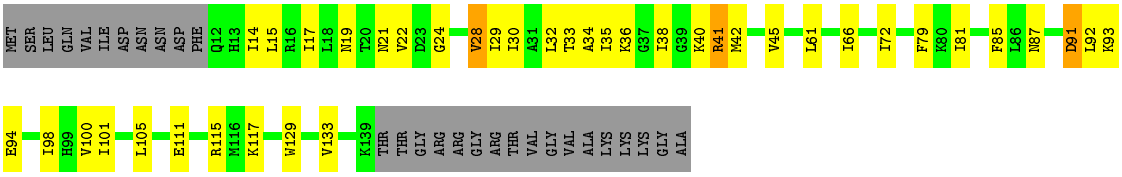
- Molecule 18: 40S ribosomal protein eS12

Chain R:



- Molecule 19: 40S ribosomal protein uS13

Chain S:

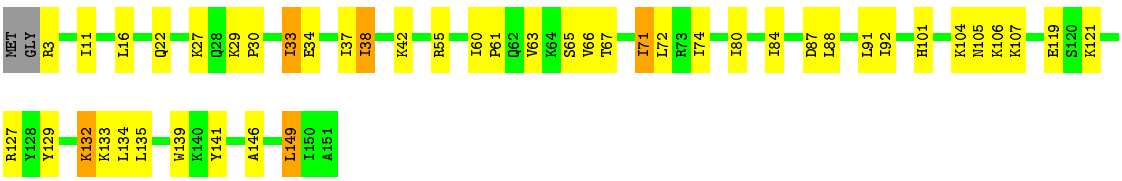


- Molecule 20: 40S ribosomal protein uS14

Chain T:

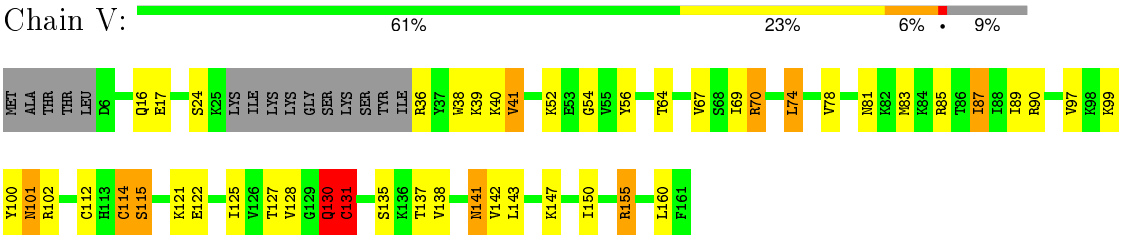
- Molecule 21: 40S ribosomal protein uS15

Chain U:



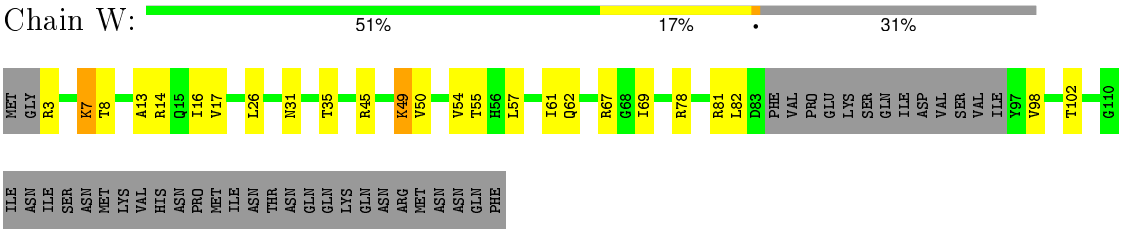
- Molecule 22: 40S ribosomal protein uS17

Chain V:



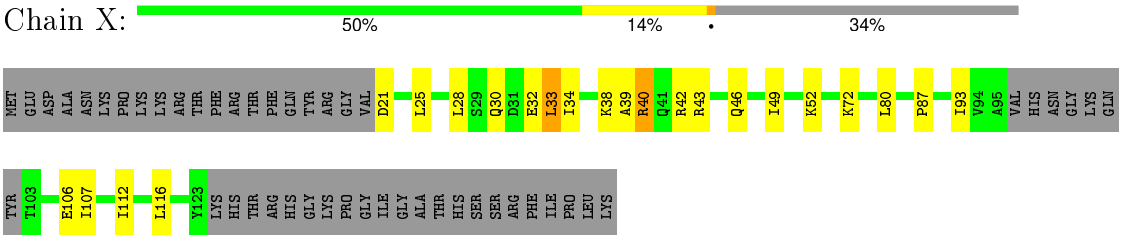
• Molecule 23: 40S ribosomal protein eS17

Chain W:



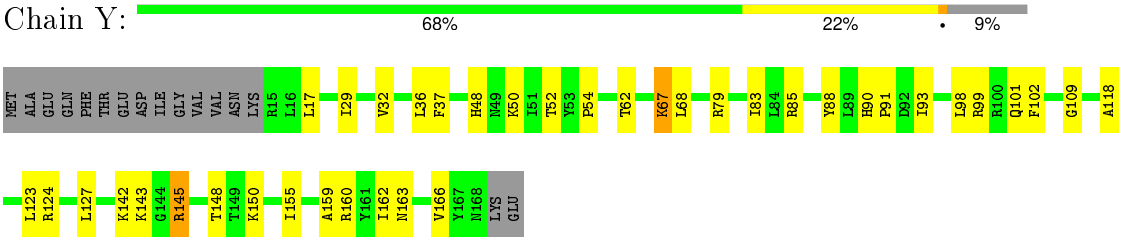
• Molecule 24: 40S ribosomal protein uS19

Chain X:



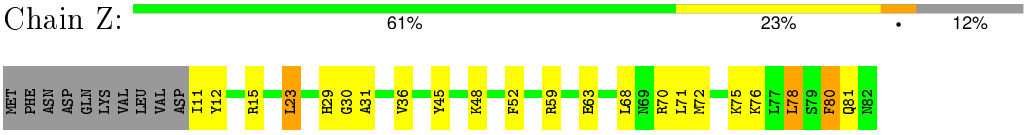
• Molecule 25: 40S ribosomal protein eS19

Chain Y:



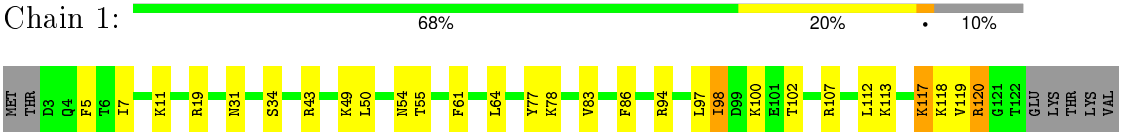
• Molecule 26: 40S ribosomal protein eS21

Chain Z:



• Molecule 27: 40S ribosomal protein eS24

Chain 1:



- Molecule 28: 40S ribosomal protein eS25

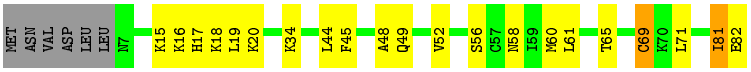
Chain 2:

- Molecule 29: 40S ribosomal protein eS26

Chain 3:

- Molecule 30: 40S ribosomal protein eS27

Chain 4:

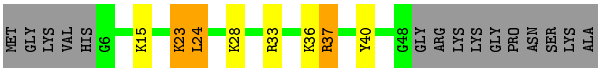


- Molecule 31: 40S ribosomal protein eS28

Chain 5:

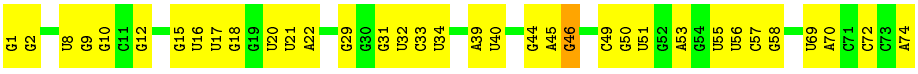
- Molecule 32: 40S ribosomal protein eS30

Chain 6:



- Molecule 33: tRNA

Chain 7:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	105247	Depositor
Resolution determination method	FSC 0.143 gold-standard	Depositor
CTF correction method	Each particle	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	20	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3800	Depositor
Magnification	78000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 34G, MG

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	#$\|Z\|>2$	RMSZ	#$\|Z\|>2$
1	A	0.35	3/38345 (0.0%)	0.75	16/59689 (0.0%)
10	J	0.45	0/1544	0.78	0/2064
11	K	0.51	0/1054	0.92	1/1411 (0.1%)
12	L	0.51	0/1416	0.82	1/1890 (0.1%)
13	M	0.45	0/1113	0.71	0/1487
14	N	0.45	0/780	0.81	0/1053
15	O	0.48	0/705	0.73	0/950
16	P	0.47	0/965	0.88	1/1295 (0.1%)
17	Q	0.47	0/1149	0.80	0/1532
18	R	0.47	0/754	0.66	0/1013
19	S	0.48	0/1058	0.82	0/1420
2	B	0.46	0/1737	0.81	0/2321
20	T	0.42	0/411	0.73	0/544
21	U	0.45	0/1223	0.87	0/1634
22	V	0.50	0/1233	0.79	1/1645 (0.1%)
23	W	0.47	0/792	0.86	0/1053
24	X	0.49	0/787	0.81	0/1050
25	Y	0.46	0/1294	0.86	1/1742 (0.1%)
26	Z	0.44	0/564	0.78	0/758
27	1	0.49	0/994	0.86	0/1317
28	2	0.48	0/323	0.67	0/435
29	3	0.48	0/793	0.90	0/1055
3	C	0.43	0/1569	0.79	0/2129
30	4	0.45	0/597	0.73	0/801
31	5	0.40	0/452	0.64	0/599
32	6	0.42	0/348	0.80	0/458
33	7	0.24	0/1754	0.72	0/2732
4	D	0.46	0/1240	0.79	1/1652 (0.1%)
5	E	0.47	0/1532	0.87	0/2048
6	F	0.47	0/2097	0.80	1/2819 (0.0%)
7	G	0.48	0/1799	0.78	0/2429
8	H	0.43	0/1661	0.77	0/2205

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >2	RMSZ	#|Z| >2
9	I	0.47	0/1443	0.86	0/1936
All	All	0.40	3/73526 (0.0%)	0.77	23/107166 (0.0%)

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
10	J	0	1
11	K	0	3
12	L	0	1
19	S	0	1
2	B	0	1
21	U	0	1
24	X	0	1
27	1	0	1
All	All	0	10

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	788	A	O3'-P	8.01	1.70	1.61
1	A	789	U	C1'-N1	6.93	1.59	1.48
1	A	788	A	C1'-N9	-5.21	1.39	1.46

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	788	A	P-O3'-C3'	-10.85	106.69	119.70
1	A	788	A	OP2-P-O3'	7.78	122.32	105.20
1	A	2053	U	C2'-C3'-O3'	7.76	126.57	109.50
1	A	850	G	C2'-C3'-O3'	7.72	126.49	109.50
1	A	1381	C	C2'-C3'-O3'	7.23	125.40	109.50
1	A	1386	U	C2'-C3'-O3'	7.17	125.28	109.50
1	A	525	G	C2'-C3'-O3'	6.75	124.50	113.70
1	A	291	A	C2'-C3'-O3'	6.43	123.98	113.70
1	A	465	G	C2'-C3'-O3'	6.32	123.81	113.70
1	A	246	A	C2'-C3'-O3'	6.21	123.63	113.70
25	Y	124	ARG	NE-CZ-NH2	5.80	123.20	120.30
1	A	338	U	O5'-P-OP1	-5.70	100.57	105.70
22	V	74	LEU	CA-CB-CG	5.58	128.14	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	788	A	O3'-P-O5'	-5.51	93.53	104.00
4	D	106	LEU	CA-CB-CG	5.48	127.90	115.30
12	L	56	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	A	844	G	C2'-C3'-O3'	5.35	122.26	113.70
16	P	147	ARG	NE-CZ-NH2	5.29	122.95	120.30
6	F	18	TRP	CA-CB-CG	5.28	123.72	113.70
1	A	1786	U	C2'-C3'-O3'	5.25	122.10	113.70
1	A	463	G	C2'-C3'-O3'	5.24	122.08	113.70
11	K	76	SER	C-N-CD	-5.09	109.40	120.60
1	A	434	A	C2'-C3'-O3'	5.04	121.76	113.70

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
27	1	118	LYS	Peptide
2	B	148	ASN	Peptide
10	J	132	SER	Peptide
11	K	27	ILE	Peptide
11	K	76	SER	Peptide
11	K	94	LEU	Peptide
12	L	164	LYS	Peptide
19	S	36	LYS	Peptide
21	U	104	LYS	Peptide
24	X	38	LYS	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	34277	0	17246	210	0
2	B	1713	0	1838	25	0
3	C	1538	0	1600	17	0
4	D	1228	0	1311	14	0
5	E	1508	0	1594	16	0
6	F	2061	0	2200	23	0
7	G	1757	0	1811	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	H	1644	0	1795	15	0
9	I	1424	0	1471	9	0
10	J	1528	0	1680	20	0
11	K	1037	0	1099	16	0
12	L	1392	0	1447	20	0
13	M	1098	0	1183	7	0
14	N	772	0	813	8	0
15	O	686	0	695	7	0
16	P	953	0	997	20	0
17	Q	1129	0	1196	12	0
18	R	746	0	754	2	0
19	S	1042	0	1095	23	0
20	T	404	0	416	5	0
21	U	1202	0	1299	19	0
22	V	1206	0	1239	16	0
23	W	785	0	858	6	0
24	X	776	0	832	9	0
25	Y	1266	0	1316	12	0
26	Z	556	0	558	7	0
27	1	981	0	1065	9	0
28	2	320	0	338	0	0
29	3	781	0	818	12	0
30	4	586	0	604	5	0
31	5	451	0	485	2	0
32	6	345	0	381	4	0
33	7	1571	0	797	3	0
34	A	67	0	0	0	0
35	A	35	0	40	2	0
36	T	1	0	0	0	0
All	All	68866	0	52871	522	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 4.

All (522) 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)
19:S:33:THR:O	19:S:38:ILE:HG12	1.15	1.32
1:A:759:C:O2	1:A:788:A:C2	1.84	1.30
19:S:35:ILE:O	19:S:38:ILE:CG1	1.76	1.30
1:A:759:C:C2	1:A:788:A:C2	2.30	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:35:ILE:O	19:S:38:ILE:HG13	0.91	1.09
19:S:33:THR:O	19:S:38:ILE:CG1	2.05	1.04
1:A:759:C:C2	1:A:788:A:H2	1.77	0.96
1:A:1447:A:O2'	1:A:1448:U:OP2	1.85	0.94
1:A:1448:U:O2'	1:A:1449:U:O5'	1.85	0.93
1:A:759:C:O2	1:A:788:A:H2	1.40	0.89
1:A:759:C:C2	1:A:788:A:N1	2.39	0.89
1:A:788:A:H2'	1:A:789:U:H6	1.41	0.85
1:A:2044:G:C2'	1:A:2045:A:H5'	2.07	0.84
1:A:1447:A:O2'	1:A:1448:U:P	2.36	0.84
1:A:2044:G:O2'	1:A:2045:A:H5'	1.79	0.81
1:A:759:C:N3	1:A:788:A:N1	2.28	0.81
4:D:106:LEU:HD22	4:D:123:VAL:HG21	1.61	0.79
1:A:1447:A:HO2'	1:A:1448:U:P	2.04	0.79
1:A:338:U:P	12:L:56:ARG:HH22	2.07	0.78
1:A:788:A:H2'	1:A:789:U:C6	2.19	0.78
1:A:1448:U:HO2'	1:A:1449:U:P	2.09	0.76
19:S:38:ILE:HG22	19:S:38:ILE:O	1.86	0.75
16:P:35:ALA:CB	16:P:112:ALA:HB2	2.20	0.71
16:P:35:ALA:HB2	16:P:112:ALA:HB2	1.71	0.71
4:D:135:CYS:SG	4:D:136:GLU:N	2.64	0.71
10:J:81:ILE:HD11	10:J:94:LEU:HD22	1.73	0.70
1:A:1387:U:O2'	1:A:1388:A:O4'	2.09	0.70
5:E:86:LEU:HD11	5:E:96:VAL:HG12	1.72	0.70
17:Q:102:VAL:HG22	17:Q:127:VAL:HG12	1.75	0.68
1:A:1836:G:C5	19:S:30:ILE:HG13	2.29	0.68
5:E:28:LEU:HD11	32:6:40:TYR:HA	1.76	0.68
1:A:2044:G:H2'	1:A:2045:A:H5'	1.77	0.67
25:Y:29:ILE:HG22	25:Y:159:ALA:HB2	1.76	0.66
12:L:200:ILE:HD11	12:L:208:TYR:CD2	2.30	0.66
12:L:36:THR:HG21	12:L:189:PRO:HB2	1.78	0.66
1:A:1033:U:OP1	21:U:132:LYS:NZ	2.29	0.65
26:Z:29:HIS:O	26:Z:31:ALA:N	2.31	0.64
1:A:981:U:OP1	1:A:982:A:O2'	2.13	0.64
18:R:49:ILE:HG21	18:R:75:LEU:HB3	1.80	0.63
10:J:61:LEU:HD11	10:J:175:VAL:HG23	1.81	0.62
1:A:64:U:O2'	1:A:166:A:N3	2.29	0.62
4:D:28:ILE:HD13	15:O:69:LYS:HD2	1.82	0.62
19:S:41:ARG:O	19:S:45:VAL:HG13	2.01	0.61
1:A:1061:A:O2'	1:A:2077:U:O2	2.17	0.61
1:A:1049:G:H4'	1:A:2068:A:H4'	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:23:CYS:O	10:J:27:ILE:HG23	2.01	0.61
16:P:113:GLN:HG2	29:3:45:VAL:HG12	1.82	0.60
13:M:45:LEU:HB3	13:M:79:ILE:HD13	1.81	0.60
1:A:1448:U:O2'	1:A:1449:U:H2'	2.02	0.60
1:A:1894:A:OP2	20:T:30:ARG:NH2	2.34	0.60
5:E:45:VAL:HG13	5:E:101:LEU:HD22	1.83	0.60
22:V:78:VAL:HG23	22:V:122:GLU:HA	1.84	0.59
1:A:1449:U:O2	1:A:1812:A:H5'	2.02	0.59
6:F:65:LEU:HD22	6:F:70:VAL:HG11	1.85	0.59
6:F:107:GLY:HA2	6:F:189:VAL:HG11	1.84	0.59
11:K:25:VAL:HG13	11:K:63:VAL:HG13	1.85	0.59
3:C:59:LEU:O	3:C:63:ILE:HG23	2.03	0.59
11:K:14:ILE:HG12	11:K:27:ILE:HD11	1.84	0.58
22:V:69:ILE:HD13	22:V:143:LEU:HD11	1.85	0.58
1:A:1907:G:O2'	1:A:1908:A:OP2	2.21	0.58
5:E:123:HIS:CE1	32:6:37:ARG:HD3	2.39	0.58
1:A:2027:C:C5	1:A:2028:U:C5	2.93	0.57
1:A:373:A:H2'	1:A:374:U:O4'	2.03	0.57
25:Y:32:VAL:HG21	25:Y:159:ALA:HB1	1.86	0.57
13:M:45:LEU:HD11	13:M:76:THR:HG22	1.86	0.57
21:U:55:ARG:NH1	30:4:49:GLN:OE1	2.38	0.57
1:A:1075:C:N3	35:A:2168:34G:H1	2.19	0.57
1:A:145:A:H2'	1:A:146:A:C8	2.40	0.57
2:B:58:THR:HG23	2:B:91:ILE:HG12	1.87	0.57
1:A:1048:A:N3	1:A:2067:U:O2'	2.37	0.57
5:E:45:VAL:HG11	5:E:105:LEU:HD21	1.87	0.57
1:A:1718:C:H2'	1:A:1832:U:O4	2.05	0.57
26:Z:52:PHE:CD1	26:Z:71:LEU:HD23	2.40	0.57
16:P:146:ARG:O	16:P:147:ARG:HG2	2.05	0.57
1:A:2029:A:H2'	1:A:2030:U:C6	2.40	0.57
1:A:1836:G:C4	19:S:30:ILE:HG13	2.40	0.56
1:A:334:A:H2'	1:A:335:G:O4'	2.05	0.56
11:K:8:ALA:CB	11:K:74:VAL:HG11	2.35	0.56
1:A:1967:G:O2'	1:A:2023:A:N6	2.38	0.56
1:A:106:A:OP2	1:A:314:A:N6	2.37	0.56
10:J:60:ILE:HB	10:J:92:VAL:HG12	1.86	0.56
1:A:142:G:O2'	1:A:143:A:H5'	2.05	0.56
24:X:30:GLN:O	24:X:34:ILE:HG23	2.06	0.56
1:A:1952:A:C2	1:A:2038:A:C2	2.94	0.56
25:Y:83:ILE:HD11	25:Y:123:LEU:CD1	2.36	0.56
1:A:1849:U:O4	24:X:40:ARG:NH2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:18:TRP:O	6:F:51:ARG:NH2	2.39	0.56
12:L:65:PHE:CD2	12:L:104:ILE:HD11	2.41	0.56
2:B:34:ALA:HB3	2:B:41:ARG:HA	1.89	0.55
1:A:1267:C:H2'	1:A:1268:G:O4'	2.06	0.55
1:A:1841:U:H2'	1:A:1842:A:O4'	2.07	0.55
1:A:598:A:H2'	1:A:599:A:C8	2.41	0.55
5:E:59:LEU:HD13	5:E:73:GLY:HA2	1.88	0.55
9:I:30:ILE:HD13	9:I:59:ILE:HD12	1.88	0.55
1:A:2028:U:H2'	1:A:2028:U:O2	2.06	0.55
15:O:27:PHE:HB2	15:O:87:LEU:HD23	1.88	0.55
6:F:86:LEU:HD13	6:F:103:TYR:CE2	2.42	0.55
1:A:1881:G:H1	1:A:1907:G:HO2'	1.45	0.55
23:W:98:VAL:HG12	23:W:102:THR:HG23	1.88	0.55
12:L:21:HIS:O	12:L:21:HIS:CG	2.60	0.55
29:3:50:GLN:O	29:3:53:ILE:HG22	2.07	0.54
1:A:543:A:C5	1:A:544:G:C8	2.95	0.54
1:A:521:G:N7	1:A:544:G:N2	2.56	0.54
1:A:366:A:H2'	1:A:367:C:H4'	1.88	0.54
19:S:33:THR:HB	19:S:38:ILE:HG23	1.90	0.54
1:A:2029:A:H2'	1:A:2030:U:O4'	2.08	0.54
2:B:88:CYS:SG	2:B:96:CYS:SG	3.04	0.54
1:A:2045:A:O2'	1:A:2046:G:H5'	2.07	0.54
17:Q:102:VAL:HG13	17:Q:124:VAL:HG23	1.90	0.54
26:Z:78:LEU:HD11	26:Z:80:PHE:CZ	2.43	0.54
2:B:204:ILE:HD13	2:B:204:ILE:C	2.28	0.54
3:C:89:PHE:O	3:C:93:THR:HG22	2.08	0.54
12:L:34:SER:HB2	12:L:56:ARG:HD2	1.90	0.53
3:C:164:ASN:HD22	3:C:170:ILE:HD11	1.73	0.53
12:L:65:PHE:CZ	12:L:78:ILE:HG21	2.43	0.53
2:B:164:ILE:HG13	2:B:204:ILE:HD12	1.91	0.53
1:A:1423:A:N6	3:C:135:GLU:OE2	2.42	0.53
1:A:338:U:P	12:L:56:ARG:NH2	2.79	0.53
21:U:33:ILE:HD11	21:U:63:VAL:HG12	1.91	0.53
35:A:2168:34G:CAE	35:A:2168:34G:H41	2.39	0.53
1:A:879:A:N1	1:A:925:C:O2	2.41	0.53
12:L:72:ILE:HD12	12:L:73:SER:N	2.23	0.53
12:L:76:THR:OG1	12:L:104:ILE:HG23	2.09	0.52
1:A:1387:U:O2'	1:A:1388:A:O5'	2.27	0.52
3:C:177:LEU:O	3:C:181:VAL:HG13	2.08	0.52
1:A:401:U:H2'	1:A:402:G:O4'	2.10	0.52
3:C:146:LEU:O	3:C:164:ASN:ND2	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:60:LEU:HD13	12:L:195:ALA:HB2	1.92	0.52
1:A:45:U:O2	1:A:440:G:H1'	2.10	0.52
1:A:647:C:O2	1:A:647:C:O4'	2.27	0.52
10:J:128:GLU:O	10:J:131:VAL:O	2.27	0.52
3:C:202:LEU:HD23	3:C:203:TRP:N	2.25	0.52
2:B:171:ILE:HD11	2:B:200:GLN:HG3	1.92	0.52
12:L:107:HIS:N	12:L:108:PRO:CD	2.73	0.52
2:B:66:TYR:HE1	2:B:88:CYS:SG	2.33	0.51
24:X:28:LEU:HD13	24:X:32:GLU:HB2	1.91	0.51
19:S:33:THR:O	19:S:38:ILE:HG23	2.09	0.51
11:K:14:ILE:CG1	11:K:27:ILE:HD11	2.40	0.51
33:7:1:G:N2	33:7:70:A:C2	2.79	0.51
5:E:106:GLU:HA	5:E:111:THR:HG21	1.91	0.51
1:A:413:A:H2'	1:A:414:C:C6	2.45	0.51
7:G:149:ILE:HD12	7:G:227:PHE:CZ	2.44	0.51
9:I:61:GLU:O	9:I:64:VAL:HG22	2.10	0.51
19:S:38:ILE:CG2	19:S:38:ILE:O	2.58	0.51
17:Q:96:ILE:HG22	17:Q:127:VAL:HG11	1.92	0.51
1:A:529:U:O2'	27:1:61:PHE:O	2.27	0.51
10:J:71:THR:HG23	10:J:72:TYR:CD2	2.45	0.51
10:J:36:LYS:HG2	10:J:37:THR:HG23	1.92	0.51
16:P:56:ILE:HG13	16:P:81:VAL:HG23	1.93	0.51
1:A:427:A:HO2'	1:A:428:G:P	2.34	0.51
6:F:228:ILE:HD11	6:F:236:ILE:HD11	1.92	0.51
2:B:178:LYS:O	2:B:179:VAL:HG13	2.10	0.51
1:A:1850:G:O6	24:X:43:ARG:NH2	2.44	0.51
33:7:15:G:C6	33:7:46:G:N2	2.79	0.51
1:A:1811:A:O2'	1:A:1813:U:OP2	2.24	0.51
11:K:83:LEU:HD22	11:K:120:HIS:O	2.12	0.50
1:A:932:U:O4'	1:A:932:U:O2	2.27	0.50
1:A:981:U:H4'	1:A:982:A:OP2	2.11	0.50
22:V:40:LYS:O	22:V:41:VAL:HG22	2.11	0.50
16:P:56:ILE:O	16:P:56:ILE:HG22	2.11	0.50
7:G:168:MET:SD	7:G:168:MET:N	2.84	0.50
1:A:455:C:OP1	6:F:29:PRO:O	2.30	0.50
12:L:57:ALA:HB2	12:L:193:GLY:HA2	1.94	0.50
27:1:97:LEU:HB3	27:1:98:ILE:HD13	1.94	0.50
2:B:175:GLU:HG3	2:B:193:ILE:HD12	1.93	0.50
3:C:168:GLU:HB3	3:C:202:LEU:HD11	1.94	0.50
1:A:433:C:H2'	1:A:434:A:O4'	2.11	0.50
22:V:128:VAL:HG12	22:V:142:VAL:HA	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:G:OP1	22:V:137:THR:HG22	2.12	0.50
1:A:1059:U:H2'	1:A:1060:G:O4'	2.12	0.49
6:F:186:GLY:O	6:F:188:SER:N	2.44	0.49
3:C:63:ILE:HG22	26:Z:36:VAL:HG22	1.94	0.49
1:A:2029:A:O2'	1:A:2030:U:H5'	2.12	0.49
6:F:45:VAL:HG23	6:F:80:CYS:O	2.11	0.49
20:T:27:ALA:HB1	20:T:38:ARG:HD2	1.94	0.49
19:S:29:ILE:O	19:S:33:THR:HG23	2.12	0.49
25:Y:162:ILE:O	25:Y:166:VAL:HG13	2.11	0.49
1:A:644:U:O2	10:J:115:ARG:NH2	2.44	0.49
11:K:78:ARG:CD	11:K:126:LEU:HD23	2.42	0.49
29:3:23:CYS:SG	29:3:74:CYS:HB3	2.52	0.49
22:V:99:LYS:HG2	22:V:100:TYR:CE2	2.48	0.49
2:B:34:ALA:HB2	2:B:43:PHE:CE2	2.46	0.49
7:G:168:MET:HB2	11:K:95:PRO:HB2	1.94	0.49
1:A:5:U:O2'	1:A:560:G:O3'	2.24	0.49
3:C:74:VAL:HG13	3:C:118:PRO:HB3	1.95	0.49
1:A:822:G:OP1	6:F:22:LYS:NZ	2.46	0.49
10:J:76:ILE:HD12	10:J:76:ILE:O	2.12	0.49
16:P:106:LYS:CE	16:P:135:ILE:HG22	2.43	0.49
1:A:1409:U:O2	1:A:1409:U:O4'	2.29	0.49
1:A:970:G:N1	1:A:971:G:C6	2.81	0.49
2:B:204:ILE:HD13	2:B:205:TYR:HB2	1.95	0.48
21:U:33:ILE:HG21	21:U:66:VAL:HG11	1.95	0.48
27:1:100:LYS:HB2	27:1:102:THR:HG23	1.95	0.48
1:A:1980:A:N6	1:A:2011:G:C6	2.81	0.48
1:A:1281:C:H2'	1:A:1282:U:O4'	2.14	0.48
1:A:1022:A:H2'	1:A:1023:A:C8	2.48	0.48
1:A:619:U:OP2	17:Q:5:LYS:HE3	2.12	0.48
1:A:1788:U:O4'	1:A:1788:U:O2	2.29	0.48
14:N:103:ILE:HG22	14:N:103:ILE:O	2.13	0.48
23:W:13:ALA:O	23:W:16:ILE:O	2.31	0.48
1:A:338:U:OP1	12:L:31:ARG:NE	2.45	0.48
1:A:999:A:OP1	29:3:32:LYS:NZ	2.42	0.48
1:A:1186:G:OP1	7:G:178:ARG:NH1	2.47	0.48
1:A:575:G:H4'	17:Q:90:ASP:HA	1.95	0.48
19:S:15:LEU:HD11	19:S:66:ILE:HD11	1.94	0.48
1:A:2053:U:O5'	1:A:2053:U:O2	2.31	0.48
16:P:138:ASP:CG	16:P:139:SER:N	2.67	0.48
1:A:1234:A:H2'	1:A:1235:G:O4'	2.14	0.48
1:A:1047:A:H2'	1:A:1048:A:O4'	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:142:ARG:O	8:H:146:ASN:N	2.46	0.48
1:A:1404:U:H2'	1:A:1405:U:O4'	2.13	0.48
27:1:119:VAL:O	27:1:119:VAL:HG13	2.13	0.48
24:X:21:ASP:O	24:X:25:LEU:HD13	2.13	0.48
16:P:36:SER:O	16:P:37:PHE:HB2	2.14	0.48
24:X:93:ILE:HG22	24:X:106:GLU:HA	1.94	0.48
10:J:39:ALA:HA	10:J:42:ILE:HG22	1.96	0.48
8:H:52:ILE:HD12	8:H:109:LEU:HD21	1.96	0.48
10:J:61:LEU:CD1	10:J:175:VAL:HG23	2.44	0.47
11:K:90:ILE:HG22	11:K:102:LEU:HG	1.95	0.47
20:T:28:ILE:HA	20:T:37:CYS:HA	1.96	0.47
1:A:301:A:H4'	6:F:130:LEU:HD21	1.94	0.47
26:Z:72:MET:HB2	26:Z:78:LEU:HD22	1.96	0.47
6:F:43:PRO:HG2	6:F:46:ILE:HG12	1.96	0.47
2:B:37:MET:HE3	2:B:231:LEU:HD21	1.96	0.47
8:H:57:ASP:HA	8:H:106:LEU:HA	1.95	0.47
1:A:2045:A:H2'	1:A:2046:G:O4'	2.14	0.47
8:H:57:ASP:OD1	8:H:61:PHE:N	2.47	0.47
4:D:124:LEU:HD11	4:D:153:PHE:HB3	1.97	0.47
2:B:120:LEU:HD12	2:B:120:LEU:C	2.35	0.47
1:A:1171:U:O2'	30:4:16:LYS:O	2.32	0.47
1:A:1635:C:H4'	23:W:49:LYS:HA	1.95	0.47
30:4:44:LEU:HD21	30:4:52:VAL:HG21	1.96	0.47
25:Y:163:ASN:O	25:Y:166:VAL:HG22	2.14	0.47
11:K:41:MET:HG2	11:K:46:TYR:HB2	1.96	0.47
1:A:1679:G:O2'	20:T:24:ASN:OD1	2.32	0.47
1:A:95:A:C6	1:A:404:G:C6	3.03	0.47
19:S:17:ILE:CG2	19:S:35:ILE:HD11	2.45	0.47
16:P:106:LYS:HE2	16:P:135:ILE:HG22	1.96	0.47
10:J:28:GLU:HB2	10:J:39:ALA:HB3	1.96	0.47
1:A:995:A:H2'	1:A:996:C:O4'	2.15	0.47
14:N:23:LEU:HB3	14:N:31:ILE:HD11	1.96	0.47
15:O:22:ILE:HD11	15:O:48:VAL:HG11	1.96	0.47
1:A:1100:U:H3'	1:A:1101:G:H5'	1.97	0.47
1:A:2088:C:N4	29:3:93:ARG:HD3	2.30	0.47
10:J:126:ILE:O	10:J:130:ILE:HG23	2.14	0.47
9:I:26:LEU:CD2	9:I:108:GLN:HA	2.45	0.47
1:A:114:A:O2'	22:V:70:ARG:NE	2.48	0.47
11:K:8:ALA:HB1	11:K:74:VAL:HG11	1.97	0.47
23:W:7:LYS:HE3	23:W:8:THR:HG23	1.97	0.47
1:A:54:C:O2'	1:A:465:G:N7	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:106:LEU:HD21	4:D:123:VAL:HG11	1.96	0.47
7:G:179:ILE:HD11	7:G:181:LEU:CD1	2.45	0.47
1:A:375:U:O2	1:A:375:U:O4'	2.32	0.47
1:A:1270:G:O2'	1:A:1873:A:N6	2.48	0.47
1:A:1388:A:N1	1:A:1430:G:O2'	2.36	0.46
1:A:19:A:H2'	1:A:20:G:O4'	2.15	0.46
14:N:108:VAL:HG12	14:N:109:VAL:HG23	1.95	0.46
1:A:161:U:O2	1:A:161:U:O4'	2.31	0.46
1:A:823:C:OP1	6:F:21:ASN:HB3	2.15	0.46
15:O:37:ASP:HB3	15:O:40:ILE:HD13	1.97	0.46
1:A:1857:U:O4'	1:A:1857:U:O2	2.31	0.46
2:B:171:ILE:HD11	2:B:200:GLN:CG	2.45	0.46
9:I:26:LEU:HD22	9:I:108:GLN:HG3	1.96	0.46
7:G:165:THR:HG23	7:G:166:VAL:O	2.16	0.46
25:Y:29:ILE:HG21	25:Y:155:ILE:CG2	2.46	0.46
21:U:129:TYR:CB	21:U:135:LEU:HD13	2.45	0.46
1:A:2063:U:H2'	1:A:2064:C:O4'	2.15	0.46
1:A:1704:G:N3	1:A:1704:G:H2'	2.31	0.46
1:A:818:C:H1'	5:E:143:ILE:HG13	1.96	0.46
13:M:98:VAL:HG12	13:M:99:ASP:H	1.81	0.46
1:A:1888:U:H2'	1:A:1889:G:H8	1.81	0.46
14:N:57:VAL:HG23	14:N:57:VAL:O	2.16	0.46
3:C:119:ARG:HD2	7:G:252:TYR:HB3	1.96	0.46
4:D:106:LEU:CD2	4:D:123:VAL:HG21	2.39	0.46
12:L:56:ARG:NH1	12:L:190:GLY:O	2.49	0.46
8:H:25:LEU:HB3	8:H:26:PRO:HD3	1.98	0.46
1:A:2061:U:O2	16:P:150:ARG:HD2	2.15	0.46
1:A:528:A:H2'	1:A:529:U:O4'	2.16	0.45
22:V:87:ILE:HD12	22:V:114:CYS:SG	2.55	0.45
18:R:95:HIS:NE2	18:R:111:ILE:HD13	2.32	0.45
1:A:2027:C:H2'	1:A:2028:U:H6	1.81	0.45
8:H:106:LEU:HD11	8:H:109:LEU:HD12	1.97	0.45
3:C:60:ALA:HB2	3:C:160:ILE:HD11	1.96	0.45
30:4:65:THR:HG22	30:4:69:CYS:HA	1.98	0.45
1:A:3:C:O2	5:E:17:ARG:NH2	2.47	0.45
6:F:125:LYS:HA	6:F:159:THR:HA	1.98	0.45
13:M:32:LEU:HD23	13:M:68:ILE:HB	1.99	0.45
9:I:171:CYS:HA	9:I:181:ILE:HD11	1.99	0.45
8:H:75:LEU:HD21	8:H:97:VAL:HG22	1.99	0.45
1:A:1447:A:HO2'	1:A:1450:A:N6	2.14	0.45
2:B:121:ILE:HD13	2:B:164:ILE:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:22:GLN:O	17:Q:23:ARG:C	2.54	0.45
12:L:25:ARG:O	12:L:27:TYR:N	2.48	0.45
21:U:129:TYR:HB3	21:U:135:LEU:HD13	1.98	0.45
1:A:1951:G:C6	1:A:2037:A:C6	3.05	0.45
1:A:1264:A:N6	1:A:1265:G:C6	2.85	0.45
1:A:1091:C:O2'	1:A:1226:A:N1	2.44	0.45
15:O:74:HIS:HB2	15:O:76:TYR:CE2	2.51	0.45
25:Y:83:ILE:HD11	25:Y:123:LEU:HD12	1.98	0.45
21:U:63:VAL:HG21	21:U:71:ILE:HB	1.99	0.45
1:A:1076:C:O3'	16:P:149:ARG:NH2	2.50	0.45
14:N:35:CYS:SG	14:N:36:SER:N	2.89	0.45
4:D:163:GLU:N	4:D:164:PRO:CD	2.80	0.45
2:B:70:LEU:HD12	2:B:84:ILE:HD11	1.99	0.45
25:Y:29:ILE:HG21	25:Y:155:ILE:HG23	1.99	0.45
1:A:1027:C:O2'	21:U:55:ARG:NH2	2.50	0.45
1:A:998:A:N7	16:P:137:THR:HG23	2.32	0.45
1:A:167:A:H5'	8:H:176:GLN:HG2	1.99	0.45
7:G:211:SER:OG	7:G:212:SER:N	2.49	0.45
1:A:1108:A:O2'	1:A:1109:G:OP2	2.29	0.45
7:G:117:GLY:HA3	7:G:202:PHE:HB3	1.98	0.45
1:A:1869:G:N3	1:A:1869:G:H2'	2.31	0.45
29:3:79:ILE:HG22	29:3:84:VAL:HG23	1.98	0.45
1:A:1626:U:O2'	1:A:1812:A:N1	2.45	0.44
5:E:6:ARG:NH1	6:F:23:MET:SD	2.89	0.44
1:A:525:G:C2'	1:A:526:G:O5'	2.65	0.44
19:S:33:THR:O	19:S:38:ILE:CG2	2.65	0.44
19:S:34:ALA:O	19:S:38:ILE:HD11	2.17	0.44
2:B:34:ALA:HB2	2:B:43:PHE:HE2	1.80	0.44
10:J:126:ILE:CD1	10:J:179:ILE:HG21	2.47	0.44
3:C:155:HIS:O	26:Z:59:ARG:NH1	2.50	0.44
32:6:23:LYS:O	32:6:24:LEU:CB	2.65	0.44
1:A:832:A:N3	1:A:832:A:C2'	2.80	0.44
1:A:1702:C:O2	1:A:1702:C:O4'	2.34	0.44
1:A:1215:G:O2'	1:A:1231:G:O6	2.33	0.44
1:A:1431:A:OP1	4:D:161:THR:HG21	2.17	0.44
4:D:126:HIS:O	4:D:129:GLU:HG3	2.17	0.44
2:B:69:ASN:O	2:B:71:ALA:N	2.51	0.44
1:A:2027:C:H2'	1:A:2028:U:C6	2.52	0.44
1:A:269:A:OP1	8:H:176:GLN:NE2	2.49	0.44
10:J:41:GLU:HB3	10:J:72:TYR:CD2	2.53	0.44
1:A:618:U:H5"	17:Q:15:LEU:HD22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1881:G:N1	1:A:1907:G:O2'	2.36	0.44
1:A:90:U:H4'	1:A:169:A:O4'	2.18	0.44
17:Q:92:CYS:HB3	17:Q:132:LEU:HD11	1.99	0.44
3:C:73:VAL:HG12	3:C:73:VAL:O	2.17	0.44
19:S:33:THR:O	19:S:38:ILE:CB	2.65	0.44
1:A:141:G:N7	8:H:177:ARG:NH2	2.65	0.44
19:S:100:VAL:HG13	19:S:105:LEU:HB2	2.00	0.44
4:D:137:VAL:HG22	4:D:187:VAL:HG23	2.00	0.44
8:H:158:ILE:H	8:H:158:ILE:HD13	1.82	0.44
1:A:1743:A:C2	1:A:1787:U:O4	2.71	0.44
2:B:160:GLN:HB3	2:B:204:ILE:HD11	1.98	0.44
9:I:64:VAL:HG12	9:I:84:VAL:HG11	2.00	0.44
22:V:38:TRP:CE2	22:V:52:LYS:HG2	2.53	0.44
10:J:81:ILE:CD1	10:J:94:LEU:HD22	2.46	0.43
12:L:101:ILE:HG13	12:L:200:ILE:HD12	2.00	0.43
1:A:2027:C:C4	1:A:2028:U:C5	3.06	0.43
1:A:1302:G:C2	1:A:1897:A:C2	3.06	0.43
13:M:41:GLU:HB3	13:M:42:PRO:HD3	2.00	0.43
1:A:65:A:C2	1:A:86:A:N7	2.86	0.43
1:A:810:A:C2	1:A:854:A:C2	3.06	0.43
22:V:78:VAL:HG12	22:V:89:ILE:HG22	2.01	0.43
5:E:49:LEU:HB2	5:E:104:LEU:CD1	2.48	0.43
1:A:378:A:C5	1:A:379:G:H1'	2.53	0.43
17:Q:102:VAL:HG22	17:Q:127:VAL:CG1	2.46	0.43
16:P:126:ILE:HG21	29:3:53:ILE:HD11	2.01	0.43
10:J:126:ILE:HD13	10:J:179:ILE:HG21	2.00	0.43
14:N:21:ILE:HB	14:N:88:ILE:HG23	1.99	0.43
2:B:179:VAL:HB	2:B:180:LEU:HG	2.01	0.43
1:A:28:A:H2'	1:A:29:U:O4'	2.17	0.43
22:V:130:GLN:O	22:V:131:CYS:CB	2.66	0.43
5:E:116:LEU:O	5:E:118:LEU:HD13	2.18	0.43
8:H:28:MET:HA	8:H:102:VAL:HG23	2.00	0.43
6:F:38:LEU:O	6:F:38:LEU:HD12	2.18	0.43
21:U:71:ILE:O	21:U:74:ILE:HG12	2.18	0.43
1:A:1108:A:N6	1:A:1192:A:C8	2.87	0.43
25:Y:90:HIS:CB	25:Y:93:ILE:HD11	2.49	0.43
21:U:30:PRO:O	21:U:34:GLU:HG2	2.18	0.43
1:A:1266:G:C6	1:A:1267:C:C4	3.06	0.43
5:E:121:SER:OG	5:E:122:VAL:N	2.51	0.43
1:A:1008:A:H2'	1:A:1009:A:C8	2.53	0.43
21:U:80:ILE:HG22	21:U:80:ILE:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:52:VAL:HG11	10:J:170:ILE:CG2	2.48	0.43
14:N:90:LEU:HD22	14:N:97:VAL:HG12	1.99	0.43
17:Q:102:VAL:HG12	17:Q:104:VAL:HG12	2.00	0.43
1:A:364:U:H2'	1:A:366:A:H5"	2.00	0.43
16:P:55:ARG:O	16:P:56:ILE:HD13	2.18	0.43
1:A:1704:G:C2	1:A:1705:C:C5	3.07	0.43
1:A:1821:A:H2'	1:A:1822:A:C8	2.53	0.43
14:N:59:THR:HG22	14:N:82:ARG:HB3	2.01	0.43
16:P:44:VAL:CG1	16:P:54:VAL:HG23	2.48	0.43
10:J:100:ILE:C	10:J:101:LEU:HD12	2.39	0.43
33:7:39:A:C2	33:7:40:U:C2	3.07	0.43
19:S:91:ASP:O	19:S:93:LYS:N	2.51	0.43
10:J:180:THR:O	10:J:180:THR:OG1	2.37	0.43
11:K:7:LEU:C	11:K:7:LEU:HD23	2.38	0.43
2:B:34:ALA:HB1	2:B:35:PRO:HD2	2.01	0.43
21:U:37:ILE:HD11	21:U:63:VAL:HG11	2.01	0.43
22:V:114:CYS:O	22:V:115:SER:OG	2.37	0.43
1:A:832:A:N3	1:A:832:A:H2'	2.33	0.43
21:U:92:ILE:HD11	21:U:139:TRP:HH2	1.84	0.43
6:F:47:LEU:HD11	6:F:101:LEU:HD21	2.00	0.43
1:A:1823:U:H3'	1:A:1824:A:H5"	2.01	0.43
8:H:2:LYS:O	8:H:3:LEU:HD12	2.19	0.43
6:F:18:TRP:CH2	6:F:42:ILE:HA	2.54	0.43
1:A:1100:U:H3'	1:A:1101:G:C5'	2.49	0.43
5:E:52:ILE:HG23	5:E:76:LEU:HD11	2.01	0.43
1:A:364:U:H2'	1:A:366:A:C5'	2.49	0.42
22:V:67:VAL:HG21	22:V:141:ASN:HD21	1.84	0.42
4:D:72:LEU:HD11	15:O:78:ILE:HD11	2.00	0.42
1:A:14:U:OP2	7:G:218:THR:HG21	2.18	0.42
24:X:28:LEU:HD12	24:X:33:LEU:HD22	2.01	0.42
1:A:109:C:H5"	1:A:389:G:O2'	2.18	0.42
6:F:138:ILE:HD12	6:F:146:SER:HB3	2.01	0.42
3:C:172:LEU:HD13	3:C:172:LEU:C	2.40	0.42
11:K:9:ASP:OD1	11:K:9:ASP:C	2.58	0.42
27:1:77:TYR:CG	27:1:83:VAL:HG22	2.54	0.42
19:S:42:MET:O	19:S:45:VAL:HG22	2.19	0.42
1:A:2049:G:C2	1:A:2050:U:C6	3.07	0.42
5:E:53:ARG:CZ	5:E:53:ARG:HB3	2.49	0.42
1:A:1448:U:OP2	1:A:1450:A:N6	2.45	0.42
6:F:183:VAL:HG11	6:F:188:SER:O	2.19	0.42
1:A:336:G:O2'	12:L:33:PRO:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:101:HIS:CE1	21:U:105:ASN:HD22	2.36	0.42
1:A:105:A:H5'	1:A:107:A:C4	2.55	0.42
31:5:9:VAL:HG13	31:5:25:VAL:HG13	2.00	0.42
13:M:56:ILE:HD13	13:M:90:ILE:HG21	2.01	0.42
1:A:2083:A:N7	29:3:34:LYS:NZ	2.67	0.42
3:C:184:LEU:O	26:Z:45:TYR:N	2.44	0.42
11:K:10:CYS:SG	11:K:27:ILE:HG23	2.60	0.42
1:A:167:A:OP2	8:H:137:ARG:NH1	2.52	0.42
9:I:135:LEU:HD23	31:5:47:PRO:HG2	2.00	0.42
9:I:134:PRO:O	9:I:137:ARG:HG2	2.20	0.42
1:A:804:U:H3'	1:A:805:A:H5'	2.01	0.42
1:A:1714:U:H2'	1:A:1715:A:O4'	2.19	0.42
15:O:26:LEU:HG	15:O:32:ILE:HD12	2.02	0.42
17:Q:96:ILE:CG2	17:Q:127:VAL:HG11	2.50	0.42
11:K:9:ASP:OD1	11:K:10:CYS:N	2.53	0.42
1:A:923:U:N3	1:A:925:C:O2	2.53	0.42
1:A:954:G:H2'	1:A:955:U:C6	2.55	0.42
23:W:31:ASN:O	23:W:35:THR:HG23	2.20	0.42
12:L:13:LEU:HD23	12:L:14:THR:N	2.34	0.42
1:A:1882:U:C5	1:A:1907:G:N2	2.88	0.42
1:A:1882:U:O4	1:A:1908:A:C2	2.73	0.42
1:A:1061:A:H2	1:A:1081:U:O4	2.02	0.42
1:A:250:A:H4'	1:A:251:U:OP1	2.19	0.42
19:S:28:VAL:HG12	19:S:61:LEU:HD11	2.02	0.42
25:Y:102:PHE:O	25:Y:118:ALA:HB2	2.19	0.42
2:B:140:ILE:HG23	2:B:213:ARG:HD3	2.00	0.42
1:A:485:C:O2	1:A:517:G:N2	2.53	0.42
1:A:1450:A:H2'	1:A:1451:G:O4'	2.20	0.42
1:A:1888:U:H2'	1:A:1889:G:C8	2.54	0.42
1:A:936:A:H2'	1:A:937:G:O4'	2.19	0.42
1:A:1447:A:HO2'	1:A:1450:A:H62	1.67	0.41
17:Q:102:VAL:CG2	17:Q:127:VAL:HG12	2.47	0.41
1:A:1679:G:N9	20:T:39:GLN:HG3	2.35	0.41
27:1:77:TYR:CD2	27:1:83:VAL:HG22	2.55	0.41
1:A:989:C:H2'	1:A:990:U:C6	2.55	0.41
25:Y:29:ILE:HD11	25:Y:88:TYR:HB3	2.02	0.41
1:A:525:G:H2'	1:A:526:G:O5'	2.20	0.41
1:A:87:A:OP1	27:1:120:ARG:NH2	2.53	0.41
21:U:55:ARG:HA	21:U:60:ILE:O	2.20	0.41
29:3:74:CYS:SG	29:3:75:VAL:N	2.92	0.41
2:B:123:GLY:HA2	2:B:165:ARG:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:38:ILE:HD12	21:U:42:LYS:HE2	2.03	0.41
27:1:5:PHE:O	27:1:43:ARG:NH1	2.48	0.41
1:A:981:U:O2'	1:A:982:A:P	2.78	0.41
1:A:1235:G:H2'	1:A:1236:U:O4'	2.20	0.41
25:Y:93:ILE:N	25:Y:93:ILE:HD12	2.36	0.41
3:C:62:ARG:HA	3:C:184:LEU:HD13	2.02	0.41
30:4:45:PHE:O	30:4:48:ALA:HB2	2.21	0.41
13:M:51:GLU:N	13:M:52:PRO:HD2	2.35	0.41
6:F:48:LEU:HA	6:F:48:LEU:HD13	1.98	0.41
4:D:28:ILE:HG21	4:D:69:LEU:HD21	2.02	0.41
21:U:71:ILE:C	21:U:71:ILE:HD13	2.41	0.41
22:V:114:CYS:HA	22:V:142:VAL:HG12	2.03	0.41
1:A:1108:A:O2'	1:A:1109:G:P	2.78	0.41
1:A:1821:A:C6	1:A:1822:A:C6	3.08	0.41
21:U:84:ILE:HD12	21:U:149:LEU:HD12	2.03	0.41
1:A:586:A:H2'	1:A:586:A:N3	2.35	0.41
8:H:76:LEU:HA	8:H:94:ARG:HA	2.01	0.41
1:A:338:U:OP1	12:L:56:ARG:NH2	2.53	0.41
16:P:64:ALA:O	16:P:66:ARG:N	2.54	0.41
5:E:83:GLN:CB	5:E:85:LEU:HD23	2.50	0.41
1:A:486:A:C2	1:A:516:G:C2	3.09	0.41
21:U:87:ASP:OD1	21:U:87:ASP:N	2.53	0.41
1:A:1243:A:H2'	1:A:1244:A:O4'	2.19	0.41
1:A:1185:A:H2'	1:A:1186:G:O4'	2.21	0.41
1:A:1261:A:H2'	1:A:1262:C:C6	2.56	0.41
1:A:752:U:O2'	1:A:753:U:O5'	2.36	0.41
1:A:542:C:H3'	1:A:543:A:H5"	2.03	0.41
29:3:23:CYS:SG	29:3:74:CYS:N	2.94	0.41
7:G:165:THR:OG1	7:G:183:PRO:HA	2.21	0.41
1:A:831:U:C3'	1:A:832:A:H5'	2.51	0.41
1:A:15:U:H2'	1:A:16:G:O4'	2.21	0.41
1:A:1453:G:C2'	1:A:1454:G:H5'	2.50	0.41
1:A:872:A:H2'	1:A:873:A:O4'	2.21	0.41
16:P:107:THR:HG23	29:3:42:ARG:NH1	2.36	0.41
6:F:86:LEU:HD13	6:F:103:TYR:CD2	2.55	0.41
16:P:36:SER:HG	16:P:39:ASP:H	1.67	0.41
4:D:24:PHE:HZ	4:D:72:LEU:HD13	1.86	0.41
22:V:135:SER:HB3	22:V:138:VAL:HG12	2.03	0.41
2:B:135:LEU:HD12	2:B:217:ILE:HG22	2.03	0.41
16:P:146:ARG:O	16:P:147:ARG:CG	2.69	0.40
22:V:112:CYS:SG	22:V:128:VAL:HG11	2.61	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:92:ILE:O	2:B:94:ARG:N	2.55	0.40
11:K:2:VAL:HG22	11:K:3:ARG:N	2.36	0.40
1:A:1277:G:N3	1:A:1296:C:O2'	2.43	0.40
1:A:1976:G:C6	1:A:1977:G:N1	2.89	0.40
1:A:981:U:O2	1:A:983:G:N1	2.54	0.40
19:S:45:VAL:HG11	19:S:85:PHE:CZ	2.56	0.40
4:D:70:THR:O	4:D:73:VAL:HG22	2.21	0.40
1:A:87:A:H2'	1:A:88:A:O4'	2.21	0.40
1:A:1636:A:N7	23:W:3:ARG:NH2	2.69	0.40
1:A:592:A:OP1	32:6:15:LYS:NZ	2.53	0.40
19:S:35:ILE:O	19:S:38:ILE:HG12	1.98	0.40
7:G:149:ILE:HD12	7:G:227:PHE:CE2	2.55	0.40
9:I:81:ILE:O	9:I:84:VAL:HG22	2.21	0.40
1:A:1253:A:O3'	29:3:85:ARG:NH2	2.54	0.40
1:A:1003:C:N4	1:A:1178:C:H4'	2.37	0.40
1:A:1900:U:H2'	1:A:1901:U:O4'	2.22	0.40
1:A:533:A:OP2	27:1:94:ARG:NH1	2.55	0.40
1:A:359:A:C6	1:A:360:C:C2	3.10	0.40
1:A:836:C:HO2'	1:A:837:A:C5'	2.33	0.40
6:F:158:ASP:HB2	6:F:173:LEU:O	2.21	0.40
11:K:119:LYS:O	11:K:120:HIS:HB2	2.22	0.40
24:X:93:ILE:HG22	24:X:106:GLU:CA	2.51	0.40
1:A:958:U:H4'	1:A:1058:G:OP1	2.21	0.40
6:F:69:ILE:HB	6:F:93:THR:HG22	2.03	0.40
1:A:1846:U:C5	24:X:39:ALA:HB3	2.57	0.40
1:A:1034:U:H3'	1:A:1034:U:O2	2.22	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 PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	208/262 (79%)	168 (81%)	28 (14%)	12 (6%)	2 17
3	C	193/263 (73%)	163 (84%)	22 (11%)	8 (4%)	3 27
4	D	149/221 (67%)	129 (87%)	17 (11%)	3 (2%)	9 48
5	E	183/189 (97%)	159 (87%)	19 (10%)	5 (3%)	6 39
6	F	255/261 (98%)	217 (85%)	31 (12%)	7 (3%)	6 39
7	G	222/272 (82%)	195 (88%)	20 (9%)	7 (3%)	5 33
8	H	200/306 (65%)	173 (86%)	19 (10%)	8 (4%)	4 27
9	I	176/195 (90%)	153 (87%)	14 (8%)	9 (5%)	2 20
10	J	186/194 (96%)	160 (86%)	17 (9%)	9 (5%)	3 22
11	K	127/130 (98%)	104 (82%)	16 (13%)	7 (6%)	2 18
12	L	166/218 (76%)	134 (81%)	23 (14%)	9 (5%)	2 19
13	M	136/144 (94%)	116 (85%)	13 (10%)	7 (5%)	2 20
14	N	96/118 (81%)	83 (86%)	8 (8%)	5 (5%)	2 19
15	O	77/137 (56%)	66 (86%)	10 (13%)	1 (1%)	15 59
16	P	125/151 (83%)	103 (82%)	18 (14%)	4 (3%)	5 33
17	Q	142/145 (98%)	128 (90%)	13 (9%)	1 (1%)	26 72
18	R	92/141 (65%)	73 (79%)	13 (14%)	6 (6%)	1 13
19	S	126/156 (81%)	100 (79%)	17 (14%)	9 (7%)	1 10
20	T	46/54 (85%)	43 (94%)	2 (4%)	1 (2%)	8 45
21	U	147/151 (97%)	133 (90%)	10 (7%)	4 (3%)	6 39
22	V	142/161 (88%)	123 (87%)	9 (6%)	10 (7%)	1 10
23	W	91/137 (66%)	80 (88%)	7 (8%)	4 (4%)	3 24
24	X	92/145 (63%)	82 (89%)	6 (6%)	4 (4%)	3 25
25	Y	152/170 (89%)	134 (88%)	12 (8%)	6 (4%)	4 28
26	Z	70/82 (85%)	62 (89%)	3 (4%)	5 (7%)	1 10
27	1	118/133 (89%)	104 (88%)	9 (8%)	5 (4%)	3 26
28	2	35/105 (33%)	30 (86%)	5 (14%)	0	100 100
29	3	93/107 (87%)	80 (86%)	10 (11%)	3 (3%)	5 33
30	4	74/82 (90%)	48 (65%)	21 (28%)	5 (7%)	1 11
31	5	54/67 (81%)	50 (93%)	4 (7%)	0	100 100
32	6	41/58 (71%)	34 (83%)	4 (10%)	3 (7%)	1 9
All	All	4014/4955 (81%)	3427 (85%)	420 (10%)	167 (4%)	6 26

All (167) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	84	ILE
2	B	93	ASN
2	B	147	GLN
2	B	179	VAL
3	C	20	CYS
3	C	95	ALA
4	D	149	LYS
5	E	16	LYS
8	H	39	ASP
8	H	67	VAL
9	I	71	GLY
9	I	157	ILE
9	I	159	SER
10	J	57	LYS
10	J	132	SER
11	K	23	ARG
11	K	77	PRO
12	L	23	LYS
12	L	49	ARG
12	L	168	ILE
13	M	17	ALA
14	N	74	ASN
14	N	105	ILE
14	N	108	VAL
18	R	42	ILE
18	R	51	SER
18	R	65	GLU
18	R	66	PRO
18	R	86	VAL
19	S	133	VAL
21	U	146	ALA
22	V	41	VAL
25	Y	54	PRO
25	Y	67	LYS
25	Y	145	ARG
26	Z	30	GLY
30	4	19	LEU
30	4	81	ILE
32	6	24	LEU
3	C	199	ASP
5	E	134	ILE
5	E	137	GLY

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Mol	Chain	Res	Type
5	E	146	PHE
6	F	187	HIS
6	F	231	ASN
8	H	66	GLY
9	I	42	HIS
9	I	174	GLU
10	J	4	VAL
10	J	157	SER
10	J	181	ARG
11	K	120	HIS
12	L	22	LYS
12	L	165	SER
13	M	40	VAL
13	M	41	GLU
13	M	139	TYR
14	N	102	SER
16	P	138	ASP
19	S	14	ILE
19	S	92	LEU
19	S	94	GLU
19	S	101	ILE
22	V	16	GLN
22	V	24	SER
22	V	101	ASN
22	V	130	GLN
23	W	17	VAL
23	W	67	ARG
23	W	69	ILE
24	X	112	ILE
25	Y	91	PRO
25	Y	109	GLY
26	Z	75	LYS
27	1	64	LEU
27	1	117	LYS
29	3	11	SER
29	3	60	SER
2	B	107	ARG
3	C	115	PHE
5	E	15	PRO
6	F	3	LYS
6	F	185	ALA
6	F	195	ILE

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Mol	Chain	Res	Type
6	F	232	THR
7	G	120	ASN
7	G	148	LEU
8	H	110	ASN
9	I	70	HIS
9	I	158	LYS
10	J	105	GLN
10	J	112	ILE
11	K	4	MET
11	K	29	PRO
12	L	8	ARG
12	L	61	ASP
19	S	19	ASN
22	V	131	CYS
25	Y	142	LYS
27	1	34	SER
27	1	49	LYS
29	3	46	ASP
30	4	56	SER
2	B	82	LYS
3	C	30	GLU
3	C	99	ALA
7	G	162	ASP
8	H	179	VAL
9	I	16	TYR
9	I	68	MET
10	J	15	ASP
10	J	110	PHE
13	M	33	ASN
14	N	67	SER
15	O	35	GLU
16	P	139	SER
19	S	40	LYS
21	U	132	LYS
21	U	141	TYR
22	V	56	TYR
22	V	115	SER
26	Z	23	LEU
30	4	58	ASN
32	6	23	LYS
32	6	28	LYS
2	B	70	LEU

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Mol	Chain	Res	Type
2	B	116	LYS
2	B	138	PHE
2	B	146	ARG
2	B	209	ASN
3	C	116	THR
3	C	143	VAL
4	D	143	LEU
6	F	30	LYS
7	G	212	SER
7	G	215	LYS
8	H	16	ILE
13	M	30	ILE
13	M	116	SER
16	P	65	ASP
18	R	122	PHE
19	S	28	VAL
20	T	9	PRO
21	U	61	PRO
22	V	155	ARG
23	W	26	LEU
24	X	49	ILE
24	X	87	PRO
24	X	116	LEU
26	Z	80	PHE
27	1	31	ASN
2	B	98	THR
7	G	157	GLY
16	P	144	SER
22	V	54	GLY
26	Z	81	GLN
30	4	69	CYS
8	H	25	LEU
11	K	52	ILE
11	K	107	PRO
12	L	170	PRO
17	Q	88	PRO
7	G	160	ILE
8	H	121	ILE
4	D	36	GLY
12	L	202	GLY
19	S	24	GLY

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 PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	195/238 (82%)	158 (81%)	37 (19%)	2 10
3	C	167/227 (74%)	144 (86%)	23 (14%)	4 21
4	D	132/188 (70%)	119 (90%)	13 (10%)	10 38
5	E	160/167 (96%)	137 (86%)	23 (14%)	4 19
6	F	233/237 (98%)	194 (83%)	39 (17%)	3 13
7	G	191/222 (86%)	160 (84%)	31 (16%)	3 14
8	H	181/279 (65%)	151 (83%)	30 (17%)	3 13
9	I	154/165 (93%)	128 (83%)	26 (17%)	2 13
10	J	177/183 (97%)	156 (88%)	21 (12%)	6 28
11	K	115/116 (99%)	94 (82%)	21 (18%)	2 10
12	L	152/193 (79%)	136 (90%)	16 (10%)	8 35
13	M	116/122 (95%)	110 (95%)	6 (5%)	29 69
14	N	91/109 (84%)	70 (77%)	21 (23%)	1 4
15	O	76/129 (59%)	65 (86%)	11 (14%)	4 19
16	P	99/119 (83%)	83 (84%)	16 (16%)	3 14
17	Q	120/121 (99%)	106 (88%)	14 (12%)	7 30
18	R	83/121 (69%)	81 (98%)	2 (2%)	57 86
19	S	113/136 (83%)	99 (88%)	14 (12%)	6 27
20	T	43/48 (90%)	38 (88%)	5 (12%)	7 30
21	U	132/133 (99%)	110 (83%)	22 (17%)	3 13
22	V	131/144 (91%)	106 (81%)	25 (19%)	2 10
23	W	86/127 (68%)	73 (85%)	13 (15%)	3 17
24	X	88/130 (68%)	80 (91%)	8 (9%)	12 42
25	Y	137/151 (91%)	117 (85%)	20 (15%)	4 19
26	Z	60/70 (86%)	50 (83%)	10 (17%)	3 13
27	1	103/115 (90%)	89 (86%)	14 (14%)	5 22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
28	2	35/88 (40%)	30 (86%)	5 (14%)	4 19
29	3	87/98 (89%)	76 (87%)	11 (13%)	5 26
30	4	70/76 (92%)	60 (86%)	10 (14%)	4 19
31	5	46/54 (85%)	42 (91%)	4 (9%)	13 45
32	6	36/47 (77%)	33 (92%)	3 (8%)	14 49
All	All	3609/4353 (83%)	3095 (86%)	514 (14%)	8 19

All (514) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	24	PHE
2	B	26	LYS
2	B	41	ARG
2	B	42	ASN
2	B	46	THR
2	B	49	THR
2	B	55	LYS
2	B	62	LYS
2	B	91	ILE
2	B	93	ASN
2	B	98	THR
2	B	104	SER
2	B	107	ARG
2	B	108	ASP
2	B	112	SER
2	B	115	ARG
2	B	120	LEU
2	B	126	ASP
2	B	127	VAL
2	B	129	THR
2	B	135	LEU
2	B	146	ARG
2	B	158	THR
2	B	163	LYS
2	B	165	ARG
2	B	173	THR
2	B	178	LYS
2	B	179	VAL
2	B	182	LYS
2	B	186	LYS

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Mol	Chain	Res	Type
2	B	199	LYS
2	B	203	LYS
2	B	204	ILE
2	B	218	LEU
2	B	219	LYS
2	B	222	LYS
2	B	233	THR
3	C	16	LYS
3	C	20	CYS
3	C	29	LEU
3	C	40	ARG
3	C	50	LEU
3	C	58	GLN
3	C	63	ILE
3	C	65	VAL
3	C	67	ILE
3	C	79	ARG
3	C	81	PHE
3	C	88	LYS
3	C	117	GLU
3	C	123	VAL
3	C	127	ARG
3	C	140	ASN
3	C	165	LYS
3	C	167	LYS
3	C	168	GLU
3	C	169	SER
3	C	181	VAL
3	C	188	ILE
3	C	200	MET
4	D	16	VAL
4	D	17	PHE
4	D	25	LEU
4	D	65	ARG
4	D	67	ARG
4	D	107	ARG
4	D	108	TYR
4	D	128	MET
4	D	129	GLU
4	D	138	ILE
4	D	158	LEU
4	D	163	GLU

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Mol	Chain	Res	Type
4	D	182	VAL
5	E	4	SER
5	E	7	ASN
5	E	16	LYS
5	E	37	LYS
5	E	46	GLN
5	E	62	LEU
5	E	65	LYS
5	E	69	ARG
5	E	78	ARG
5	E	81	VAL
5	E	102	PRO
5	E	112	LYS
5	E	135	ARG
5	E	139	GLN
5	E	141	VAL
5	E	142	ASP
5	E	143	ILE
5	E	148	VAL
5	E	151	ASP
5	E	161	THR
5	E	177	LEU
5	E	181	LYS
5	E	184	THR
6	F	3	LYS
6	F	5	ILE
6	F	9	LEU
6	F	18	TRP
6	F	38	LEU
6	F	39	LEU
6	F	44	LEU
6	F	59	ASP
6	F	65	LEU
6	F	72	VAL
6	F	75	LYS
6	F	77	ARG
6	F	92	ILE
6	F	93	THR
6	F	94	LYS
6	F	102	LEU
6	F	114	ILE
6	F	118	GLU

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Mol	Chain	Res	Type
6	F	122	LYS
6	F	130	LEU
6	F	132	ARG
6	F	138	ILE
6	F	153	ASP
6	F	159	THR
6	F	161	ARG
6	F	166	THR
6	F	168	LYS
6	F	169	VAL
6	F	173	LEU
6	F	180	LEU
6	F	181	VAL
6	F	184	THR
6	F	191	ARG
6	F	204	THR
6	F	220	THR
6	F	231	ASN
6	F	252	ARG
6	F	254	ASN
6	F	255	ARG
7	G	41	TRP
7	G	53	GLU
7	G	76	ASP
7	G	84	CYS
7	G	98	VAL
7	G	101	GLN
7	G	103	ARG
7	G	106	GLN
7	G	123	CYS
7	G	146	LEU
7	G	147	SER
7	G	153	ARG
7	G	159	LYS
7	G	160	ILE
7	G	168	MET
7	G	173	LYS
7	G	177	VAL
7	G	178	ARG
7	G	181	LEU
7	G	182	VAL
7	G	190	ILE

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Mol	Chain	Res	Type
7	G	196	THR
7	G	200	LEU
7	G	206	LYS
7	G	211	SER
7	G	217	LYS
7	G	219	LYS
7	G	224	ARG
7	G	230	LEU
7	G	242	TRP
7	G	244	VAL
8	H	1	MET
8	H	11	ASN
8	H	15	SER
8	H	29	GLU
8	H	36	VAL
8	H	40	SER
8	H	41	ILE
8	H	58	LYS
8	H	67	VAL
8	H	75	LEU
8	H	76	LEU
8	H	78	LYS
8	H	82	LYS
8	H	87	ARG
8	H	89	LYS
8	H	92	ARG
8	H	95	LYS
8	H	109	LEU
8	H	111	LEU
8	H	113	LEU
8	H	114	VAL
8	H	121	ILE
8	H	131	LYS
8	H	137	ARG
8	H	158	ILE
8	H	174	LYS
8	H	178	LEU
8	H	180	THR
8	H	183	ARG
8	H	184	LEU
9	I	10	LEU
9	I	12	LYS

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Mol	Chain	Res	Type
9	I	14	TRP
9	I	16	TYR
9	I	21	ILE
9	I	29	CYS
9	I	35	LYS
9	I	52	PHE
9	I	54	LYS
9	I	63	LEU
9	I	72	ARG
9	I	79	LYS
9	I	100	LEU
9	I	107	VAL
9	I	108	GLN
9	I	117	THR
9	I	118	ARG
9	I	128	GLN
9	I	137	ARG
9	I	158	LYS
9	I	164	LEU
9	I	179	TYR
9	I	182	LYS
9	I	189	ARG
9	I	190	VAL
9	I	195	ARG
10	J	6	LYS
10	J	9	LEU
10	J	17	GLU
10	J	27	ILE
10	J	31	SER
10	J	47	CYS
10	J	57	LYS
10	J	67	LYS
10	J	74	ARG
10	J	94	LEU
10	J	112	ILE
10	J	113	ILE
10	J	115	ARG
10	J	132	SER
10	J	136	ILE
10	J	155	LEU
10	J	166	GLU
10	J	178	LYS

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Mol	Chain	Res	Type
10	J	180	THR
10	J	181	ARG
10	J	188	LEU
11	K	9	ASP
11	K	13	THR
11	K	14	ILE
11	K	19	LYS
11	K	25	VAL
11	K	34	VAL
11	K	47	ILE
11	K	52	ILE
11	K	53	VAL
11	K	62	VAL
11	K	70	ASN
11	K	72	CYS
11	K	75	ILE
11	K	81	VAL
11	K	94	LEU
11	K	110	ILE
11	K	111	MET
11	K	112	ASP
11	K	115	GLU
11	K	120	HIS
11	K	130	PHE
12	L	8	ARG
12	L	10	LYS
12	L	13	LEU
12	L	17	LYS
12	L	49	ARG
12	L	59	LYS
12	L	84	ASN
12	L	98	LYS
12	L	106	SER
12	L	112	TRP
12	L	113	TYR
12	L	172	LEU
12	L	177	LYS
12	L	188	ARG
12	L	205	LEU
12	L	216	LYS
13	M	7	ARG
13	M	83	ARG

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Mol	Chain	Res	Type
13	M	95	GLN
13	M	105	GLU
13	M	121	ASP
13	M	128	LYS
14	N	27	ASN
14	N	31	ILE
14	N	35	CYS
14	N	40	LYS
14	N	43	LYS
14	N	53	VAL
14	N	54	ARG
14	N	60	LEU
14	N	67	SER
14	N	73	THR
14	N	74	ASN
14	N	78	ARG
14	N	81	LEU
14	N	86	ARG
14	N	90	LEU
14	N	93	GLN
14	N	99	GLN
14	N	105	ILE
14	N	108	VAL
14	N	115	ILE
14	N	117	ASP
15	O	21	LEU
15	O	32	ILE
15	O	42	ARG
15	O	46	LEU
15	O	53	ILE
15	O	61	LYS
15	O	63	ARG
15	O	69	LYS
15	O	72	TRP
15	O	73	LYS
15	O	85	GLU
16	P	54	VAL
16	P	63	LYS
16	P	65	ASP
16	P	70	SER
16	P	72	TYR
16	P	85	LEU

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Mol	Chain	Res	Type
16	P	93	ILE
16	P	98	ARG
16	P	103	THR
16	P	104	LYS
16	P	129	ILE
16	P	138	ASP
16	P	141	ARG
16	P	143	LYS
16	P	146	ARG
16	P	147	ARG
17	Q	5	LYS
17	Q	9	LEU
17	Q	19	ARG
17	Q	84	THR
17	Q	93	LEU
17	Q	94	ASN
17	Q	96	ILE
17	Q	97	ASP
17	Q	104	VAL
17	Q	107	PHE
17	Q	116	ASP
17	Q	126	LYS
17	Q	132	LEU
17	Q	135	LEU
18	R	59	LEU
18	R	96	TRP
19	S	21	ASN
19	S	22	VAL
19	S	32	LEU
19	S	41	ARG
19	S	72	ILE
19	S	79	PHE
19	S	81	ILE
19	S	87	ASN
19	S	91	ASP
19	S	98	ILE
19	S	111	GLU
19	S	115	ARG
19	S	117	LYS
19	S	129	TRP
20	T	17	ARG
20	T	28	ILE

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Mol	Chain	Res	Type
20	T	30	ARG
20	T	38	ARG
20	T	39	GLN
21	U	3	ARG
21	U	11	ILE
21	U	16	LEU
21	U	22	GLN
21	U	27	LYS
21	U	29	LYS
21	U	33	ILE
21	U	38	ILE
21	U	65	SER
21	U	67	THR
21	U	71	ILE
21	U	72	LEU
21	U	88	LEU
21	U	91	LEU
21	U	106	LYS
21	U	107	LYS
21	U	119	GLU
21	U	121	LYS
21	U	127	ARG
21	U	133	LYS
21	U	134	LEU
21	U	149	LEU
22	V	17	GLU
22	V	36	ARG
22	V	39	LYS
22	V	64	THR
22	V	70	ARG
22	V	74	LEU
22	V	81	ASN
22	V	83	MET
22	V	85	ARG
22	V	87	ILE
22	V	90	ARG
22	V	97	VAL
22	V	101	ASN
22	V	102	ARG
22	V	114	CYS
22	V	121	LYS
22	V	125	ILE

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Mol	Chain	Res	Type
22	V	127	THR
22	V	130	GLN
22	V	131	CYS
22	V	141	ASN
22	V	147	LYS
22	V	150	ILE
22	V	155	ARG
22	V	160	LEU
23	W	7	LYS
23	W	14	ARG
23	W	45	ARG
23	W	49	LYS
23	W	50	VAL
23	W	54	VAL
23	W	55	THR
23	W	57	LEU
23	W	61	ILE
23	W	62	GLN
23	W	78	ARG
23	W	81	ARG
23	W	82	LEU
24	X	33	LEU
24	X	40	ARG
24	X	42	ARG
24	X	46	GLN
24	X	52	LYS
24	X	72	LYS
24	X	80	LEU
24	X	107	ILE
25	Y	17	LEU
25	Y	36	LEU
25	Y	37	PHE
25	Y	48	HIS
25	Y	50	LYS
25	Y	52	THR
25	Y	62	THR
25	Y	67	LYS
25	Y	68	LEU
25	Y	79	ARG
25	Y	85	ARG
25	Y	98	LEU
25	Y	99	ARG

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Mol	Chain	Res	Type
25	Y	101	GLN
25	Y	127	LEU
25	Y	143	LYS
25	Y	145	ARG
25	Y	148	THR
25	Y	150	LYS
25	Y	160	ARG
26	Z	11	ILE
26	Z	12	TYR
26	Z	15	ARG
26	Z	23	LEU
26	Z	48	LYS
26	Z	63	GLU
26	Z	68	LEU
26	Z	70	ARG
26	Z	76	LYS
26	Z	78	LEU
27	1	7	ILE
27	1	11	LYS
27	1	19	ARG
27	1	50	LEU
27	1	54	ASN
27	1	55	THR
27	1	78	LYS
27	1	86	PHE
27	1	98	ILE
27	1	107	ARG
27	1	112	LEU
27	1	113	LYS
27	1	117	LYS
27	1	120	ARG
28	2	36	LEU
28	2	41	PHE
28	2	70	VAL
28	2	97	SER
28	2	98	GLN
29	3	5	ARG
29	3	10	ARG
29	3	26	CYS
29	3	38	ARG
29	3	50	GLN
29	3	62	PHE

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Mol	Chain	Res	Type
29	3	64	LEU
29	3	74	CYS
29	3	79	ILE
29	3	88	SER
29	3	93	ARG
30	4	15	LYS
30	4	17	HIS
30	4	18	LYS
30	4	20	LYS
30	4	34	LYS
30	4	60	MET
30	4	61	LEU
30	4	71	LEU
30	4	81	ILE
30	4	82	GLU
31	5	23	ILE
31	5	24	GLN
31	5	48	VAL
31	5	52	ASP
32	6	33	ARG
32	6	36	LYS
32	6	37	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	81	HIS
3	C	23	HIS
4	D	102	GLN
6	F	116	ASN
9	I	42	HIS
9	I	48	GLN
9	I	194	ASN
11	K	24	GLN
11	K	64	ASN
12	L	21	HIS
17	Q	94	ASN
21	U	101	HIS
23	W	31	ASN
27	1	52	ASN
27	1	54	ASN
30	4	7	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1586/2092 (75%)	474 (29%)	71 (4%)
33	7	73/74 (98%)	30 (41%)	3 (4%)
All	All	1659/2166 (76%)	504 (30%)	74 (4%)

All (504) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	A
1	A	4	C
1	A	5	U
1	A	17	C
1	A	25	C
1	A	26	A
1	A	27	U
1	A	34	G
1	A	35	U
1	A	40	A
1	A	42	G
1	A	44	U
1	A	45	U
1	A	47	A
1	A	50	C
1	A	57	G
1	A	59	G
1	A	60	A
1	A	61	A
1	A	67	A
1	A	71	A
1	A	81	U
1	A	82	G
1	A	103	U
1	A	106	A
1	A	116	A
1	A	125	G
1	A	127	C
1	A	128	A
1	A	129	U
1	A	130	U
1	A	138	U
1	A	139	A
1	A	142	G

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Mol	Chain	Res	Type
1	A	143	A
1	A	144	U
1	A	151	G
1	A	157	G
1	A	159	U
1	A	165	U
1	A	166	A
1	A	169	A
1	A	174	C
1	A	182	U
1	A	183	C
1	A	186	U
1	A	206	A
1	A	207	G
1	A	208	U
1	A	209	A
1	A	217	G
1	A	247	G
1	A	249	A
1	A	250	A
1	A	251	U
1	A	252	U
1	A	255	A
1	A	258	A
1	A	260	A
1	A	262	A
1	A	264	G
1	A	266	A
1	A	267	A
1	A	268	C
1	A	272	U
1	A	274	A
1	A	292	G
1	A	305	G
1	A	316	C
1	A	320	C
1	A	322	G
1	A	323	C
1	A	326	U
1	A	327	U
1	A	335	G
1	A	339	A

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Mol	Chain	Res	Type
1	A	343	G
1	A	344	C
1	A	345	C
1	A	350	A
1	A	357	U
1	A	358	G
1	A	359	A
1	A	360	C
1	A	361	G
1	A	365	A
1	A	366	A
1	A	367	C
1	A	375	U
1	A	376	A
1	A	379	G
1	A	396	G
1	A	399	C
1	A	405	A
1	A	406	A
1	A	407	A
1	A	408	U
1	A	409	A
1	A	410	G
1	A	422	A
1	A	423	A
1	A	424	G
1	A	425	G
1	A	428	G
1	A	430	C
1	A	431	A
1	A	432	G
1	A	434	A
1	A	440	G
1	A	443	A
1	A	445	U
1	A	446	U
1	A	450	C
1	A	451	A
1	A	454	U
1	A	458	A
1	A	459	A
1	A	460	G

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Mol	Chain	Res	Type
1	A	461	A
1	A	465	G
1	A	466	A
1	A	467	G
1	A	470	A
1	A	481	A
1	A	483	A
1	A	488	U
1	A	494	G
1	A	515	U
1	A	516	G
1	A	521	G
1	A	526	G
1	A	527	A
1	A	534	A
1	A	543	A
1	A	545	A
1	A	546	G
1	A	547	U
1	A	548	A
1	A	549	A
1	A	562	A
1	A	564	G
1	A	565	U
1	A	566	C
1	A	568	G
1	A	572	C
1	A	574	A
1	A	575	G
1	A	579	C
1	A	584	G
1	A	585	U
1	A	586	A
1	A	587	A
1	A	589	U
1	A	592	A
1	A	601	A
1	A	602	G
1	A	603	C
1	A	612	A
1	A	613	A
1	A	616	U

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Mol	Chain	Res	Type
1	A	617	G
1	A	618	U
1	A	626	A
1	A	627	A
1	A	629	A
1	A	630	C
1	A	631	G
1	A	641	G
1	A	642	A
1	A	645	U
1	A	646	U
1	A	648	A
1	A	651	G
1	A	753	U
1	A	756	A
1	A	757	A
1	A	758	U
1	A	760	C
1	A	792	U
1	A	793	G
1	A	794	U
1	A	801	G
1	A	804	U
1	A	805	A
1	A	806	A
1	A	815	G
1	A	816	U
1	A	821	A
1	A	824	A
1	A	828	A
1	A	829	G
1	A	830	U
1	A	832	A
1	A	833	A
1	A	837	A
1	A	845	U
1	A	846	G
1	A	849	U
1	A	851	A
1	A	852	A
1	A	856	U
1	A	857	A

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Mol	Chain	Res	Type
1	A	858	U
1	A	859	A
1	A	866	A
1	A	869	A
1	A	870	A
1	A	873	A
1	A	874	A
1	A	875	A
1	A	876	U
1	A	877	U
1	A	878	G
1	A	880	A
1	A	881	C
1	A	882	A
1	A	886	U
1	A	887	A
1	A	888	A
1	A	889	A
1	A	915	G
1	A	917	C
1	A	920	A
1	A	921	G
1	A	923	U
1	A	924	A
1	A	925	C
1	A	927	A
1	A	928	U
1	A	929	U
1	A	930	A
1	A	931	A
1	A	941	C
1	A	942	U
1	A	945	G
1	A	955	U
1	A	967	A
1	A	972	U
1	A	978	U
1	A	981	U
1	A	982	A
1	A	983	G
1	A	984	A
1	A	990	U

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Mol	Chain	Res	Type
1	A	998	A
1	A	1002	A
1	A	1003	C
1	A	1004	U
1	A	1011	G
1	A	1013	A
1	A	1021	A
1	A	1029	U
1	A	1035	A
1	A	1036	A
1	A	1051	U
1	A	1054	G
1	A	1057	A
1	A	1061	A
1	A	1062	A
1	A	1065	C
1	A	1073	U
1	A	1074	A
1	A	1076	C
1	A	1079	C
1	A	1081	U
1	A	1090	C
1	A	1092	A
1	A	1093	U
1	A	1095	A
1	A	1097	C
1	A	1101	G
1	A	1108	A
1	A	1109	G
1	A	1112	G
1	A	1116	G
1	A	1119	G
1	A	1168	U
1	A	1175	G
1	A	1177	A
1	A	1183	U
1	A	1187	A
1	A	1192	A
1	A	1193	A
1	A	1194	A
1	A	1195	G
1	A	1197	C

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Mol	Chain	Res	Type
1	A	1198	U
1	A	1199	U
1	A	1200	U
1	A	1209	G
1	A	1210	G
1	A	1227	G
1	A	1230	A
1	A	1239	A
1	A	1244	A
1	A	1247	G
1	A	1251	G
1	A	1254	G
1	A	1255	G
1	A	1259	C
1	A	1260	C
1	A	1261	A
1	A	1265	G
1	A	1268	G
1	A	1286	U
1	A	1291	C
1	A	1293	C
1	A	1294	A
1	A	1295	A
1	A	1297	A
1	A	1300	G
1	A	1301	G
1	A	1302	G
1	A	1303	A
1	A	1304	A
1	A	1305	A
1	A	1308	C
1	A	1318	A
1	A	1319	G
1	A	1322	A
1	A	1366	A
1	A	1367	U
1	A	1374	G
1	A	1375	C
1	A	1382	G
1	A	1383	U
1	A	1384	U
1	A	1385	U

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Mol	Chain	Res	Type
1	A	1386	U
1	A	1387	U
1	A	1388	A
1	A	1409	U
1	A	1415	A
1	A	1416	U
1	A	1422	U
1	A	1423	A
1	A	1431	A
1	A	1437	U
1	A	1441	C
1	A	1442	U
1	A	1443	G
1	A	1444	C
1	A	1445	U
1	A	1448	U
1	A	1450	A
1	A	1451	G
1	A	1453	G
1	A	1454	G
1	A	1456	G
1	A	1459	U
1	A	1607	U
1	A	1623	U
1	A	1625	C
1	A	1626	U
1	A	1635	C
1	A	1636	A
1	A	1644	U
1	A	1645	C
1	A	1646	U
1	A	1648	A
1	A	1649	C
1	A	1659	U
1	A	1660	U
1	A	1661	U
1	A	1664	G
1	A	1668	A
1	A	1673	A
1	A	1674	G
1	A	1677	C
1	A	1678	U

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Mol	Chain	Res	Type
1	A	1679	G
1	A	1692	A
1	A	1693	U
1	A	1702	C
1	A	1705	C
1	A	1706	A
1	A	1715	A
1	A	1717	A
1	A	1718	C
1	A	1719	U
1	A	1720	G
1	A	1721	A
1	A	1723	A
1	A	1727	A
1	A	1728	U
1	A	1732	G
1	A	1735	U
1	A	1749	C
1	A	1787	U
1	A	1790	C
1	A	1792	U
1	A	1795	G
1	A	1796	C
1	A	1802	G
1	A	1806	U
1	A	1811	A
1	A	1812	A
1	A	1813	U
1	A	1814	C
1	A	1817	U
1	A	1818	A
1	A	1819	U
1	A	1820	C
1	A	1824	A
1	A	1830	C
1	A	1832	U
1	A	1833	G
1	A	1834	A
1	A	1835	U
1	A	1836	G
1	A	1837	G
1	A	1845	U

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Mol	Chain	Res	Type
1	A	1854	U
1	A	1856	A
1	A	1861	U
1	A	1866	A
1	A	1868	C
1	A	1870	A
1	A	1871	G
1	A	1873	A
1	A	1881	G
1	A	1882	U
1	A	1887	A
1	A	1892	U
1	A	1898	G
1	A	1899	A
1	A	1902	G
1	A	1904	G
1	A	1907	G
1	A	1908	A
1	A	1911	A
1	A	1913	G
1	A	1916	C
1	A	1927	U
1	A	1928	A
1	A	1929	C
1	A	1937	C
1	A	1954	U
1	A	1955	G
1	A	1961	U
1	A	1962	A
1	A	1976	G
1	A	1977	G
1	A	1978	A
1	A	1979	C
1	A	1980	A
1	A	1981	A
1	A	1982	G
1	A	1987	A
1	A	2008	U
1	A	2012	G
1	A	2019	C
1	A	2020	G
1	A	2021	U

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Mol	Chain	Res	Type
1	A	2028	U
1	A	2029	A
1	A	2034	U
1	A	2042	A
1	A	2045	A
1	A	2048	A
1	A	2049	G
1	A	2052	G
1	A	2054	A
1	A	2058	A
1	A	2060	G
1	A	2061	U
1	A	2065	C
1	A	2072	G
1	A	2074	A
1	A	2075	C
1	A	2084	G
1	A	2085	G
1	A	2086	A
1	A	2088	C
33	7	2	G
33	7	8	U
33	7	9	G
33	7	10	G
33	7	12	G
33	7	16	U
33	7	17	U
33	7	18	G
33	7	20	U
33	7	21	U
33	7	22	A
33	7	29	G
33	7	31	G
33	7	32	U
33	7	33	C
33	7	34	U
33	7	44	G
33	7	45	A
33	7	46	G
33	7	49	C
33	7	50	G
33	7	51	U

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Mol	Chain	Res	Type
33	7	53	A
33	7	55	U
33	7	56	U
33	7	57	C
33	7	58	G
33	7	69	U
33	7	72	C
33	7	74	A

All (74) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	25	C
1	A	39	A
1	A	44	U
1	A	60	A
1	A	105	A
1	A	116	A
1	A	127	C
1	A	138	U
1	A	142	G
1	A	156	A
1	A	206	A
1	A	246	A
1	A	250	A
1	A	251	U
1	A	267	A
1	A	291	A
1	A	358	G
1	A	406	A
1	A	423	A
1	A	427	A
1	A	431	A
1	A	544	G
1	A	546	G
1	A	614	A
1	A	752	U
1	A	793	G
1	A	805	A
1	A	815	G
1	A	844	G
1	A	850	G

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Mol	Chain	Res	Type
1	A	858	U
1	A	877	U
1	A	919	U
1	A	923	U
1	A	930	A
1	A	981	U
1	A	983	G
1	A	1028	U
1	A	1100	U
1	A	1182	A
1	A	1183	U
1	A	1209	G
1	A	1259	C
1	A	1318	A
1	A	1381	C
1	A	1386	U
1	A	1423	A
1	A	1447	A
1	A	1448	U
1	A	1455	C
1	A	1645	C
1	A	1660	U
1	A	1672	C
1	A	1673	A
1	A	1692	A
1	A	1703	U
1	A	1786	U
1	A	1813	U
1	A	1818	A
1	A	1819	U
1	A	1834	A
1	A	1855	U
1	A	1865	G
1	A	1869	G
1	A	1870	A
1	A	1897	A
1	A	1898	G
1	A	1912	C
1	A	1976	G
1	A	1977	G
1	A	2053	U
33	7	9	G

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Mol	Chain	Res	Type
33	7	17	U
33	7	20	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 69 ligands modelled in this entry, 68 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
35	34G	A	2168	-	38,39,39	2.84	9 (23%)	51,56,56	1.97	9 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	34G	A	2168	-	-	0/14/49/49	0/5/5/5

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	A	2168	34G	CBC-CBG	-9.31	1.43	1.52
35	A	2168	34G	CAM-CAX	-7.61	1.38	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	A	2168	34G	CBD-CBH	-7.50	1.43	1.52
35	A	2168	34G	CAL-CAW	-5.58	1.41	1.51
35	A	2168	34G	CAP-CBH	-5.01	1.48	1.53
35	A	2168	34G	CBH-NBI	2.03	1.50	1.47
35	A	2168	34G	CAQ-NBI	2.60	1.51	1.47
35	A	2168	34G	CAK-CAL	3.35	1.58	1.50
35	A	2168	34G	CAO-CBG	3.72	1.58	1.54

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	A	2168	34G	CAW-CBC-CBG	-7.74	113.78	121.78
35	A	2168	34G	CBF-CAP-CBH	-4.98	102.90	111.53
35	A	2168	34G	CAP-CBF-CBE	-3.91	104.18	110.59
35	A	2168	34G	CAE-OAV-CBB	-2.58	113.76	117.53
35	A	2168	34G	CAC-OAT-CAZ	-2.02	114.57	117.53
35	A	2168	34G	CAH-CBC-CBG	2.22	126.62	120.92
35	A	2168	34G	OAS-CAY-CBA	2.25	118.45	115.41
35	A	2168	34G	CBD-CBH-NBI	3.22	116.68	111.71
35	A	2168	34G	CAQ-NBI-CBH	4.59	117.45	110.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	A	2168	34G	2	0

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.