Full wwPDB X-ray Structure Validation Report ⓘ

Jan 23, 2021 – 02:30 PM GMT

PDB ID	:	4WF9
Title	:	The crystal structure of the large ribosomal subunit of Staphylococcus aureus in complex with telithromycin
Authors	:	Eyal, Z.; Matzov, D.; Krupkin, M.; Wekselman, I.; Zimmerman, E.; Rozenberg, H.; Bashan, A.; Yonath, A.E.
Deposited on	:	2014-09-14
Resolution	:	3.43 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 following versions of software and data (see references ⓘ) were used in the production of this report:

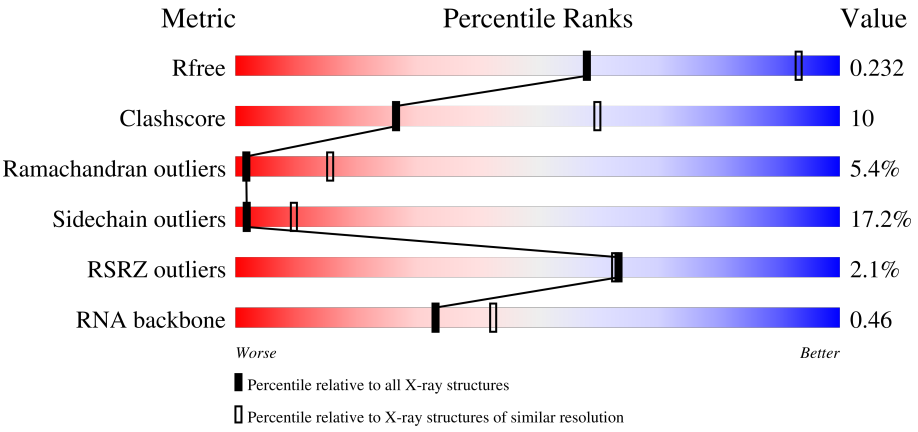
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.16
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.16

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.43 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}	130704	1486 (3.50-3.34)
Clashscore	141614	1572 (3.50-3.34)
Ramachandran outliers	138981	1534 (3.50-3.34)
Sidechain outliers	138945	1535 (3.50-3.34)
RSRZ outliers	127900	1395 (3.50-3.34)
RNA backbone	3102	1012 (3.88-2.96)

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 <=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	X	2923	51% 32% 9% • 7%
2	Y	114	49% 44% 5% •
3	A	277	6% 67% 26% • •
4	B	220	52% 36% 10% •

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Mol	Chain	Length	Quality of chain
5	C	207	60% 30% 7%
6	D	179	12% 78% 9% 11%
7	E	178	6% 55% 28% 5% 12%
8	G	145	3% 61% 28% 10%
9	H	122	2% 61% 31% 8%
10	I	146	3% 50% 32% 8% 10%
11	J	144	8% 60% 33% 5%
12	K	122	52% 34% 11%
13	L	119	% 66% 18% 7% 8%
14	M	116	47% 39% 9% 5%
15	N	118	61% 33%
16	O	102	52% 42% 6%
17	P	117	2% 59% 31% 6%
18	Q	91	8% 66% 27%
19	R	105	11% 63% 26% 8%
20	S	217	4% 56% 16% 5% 23%
21	T	94	3% 55% 21% 20%
22	V	69	68% 17% 6% 9%
23	W	59	2% 69% 22% 7%
24	Z	58	2% 43% 29% 5% 22%
25	2	45	7% 62% 31%
26	3	66	68% 21% 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	TEL	X	3001	X	-	-	-
28	MPD	X	3005	-	-	X	-
29	MG	X	3010	-	-	-	X
29	MG	X	3011	-	-	-	X
29	MG	X	3014	-	-	-	X
29	MG	X	3016	-	-	-	X
29	MG	X	3022	-	-	-	X
29	MG	X	3025	-	-	-	X
29	MG	X	3028	-	-	-	X
29	MG	X	3226	-	-	-	X
29	MG	X	3252	-	-	-	X
29	MG	X	3258	-	-	-	X
29	MG	X	3260	-	-	-	X
29	MG	X	3276	-	-	-	X
29	MG	X	3303	-	-	-	X
29	MG	X	3340	-	-	-	X
29	MG	X	3349	-	-	-	X
29	MG	X	3354	-	-	-	X
29	MG	X	3357	-	-	-	X
29	MG	X	3358	-	-	-	X
29	MG	X	3360	-	-	-	X
29	MG	Y	207	-	-	-	X
30	MN	X	3032	-	-	-	X
30	MN	X	3040	-	-	-	X
30	MN	X	3051	-	-	-	X
30	MN	X	3151	-	-	-	X
30	MN	X	3181	-	-	-	X
30	MN	X	3200	-	-	-	X
30	MN	X	3267	-	-	-	X
30	MN	X	3272	-	-	-	X
32	EOH	X	3367	-	-	-	X

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 81033 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	X	2712	58145	25958	10650	18825	2712	0	0	0

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	Y	114	2430	1086	436	794	114	0	0	0

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	269	1640	995	319	321	5	0	0	0

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	B	215	1566	980	291	290	5	0	0	0

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	C	200	1314	812	250	250	2	0	0	0

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	D	160	823	498	160	164	1	0	0	0

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	156	Total	C	N	O	S	0	0	0
			930	575	173	181	1			

- Molecule 8 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	G	145	Total	C	N	O	S	0	0	0
			1105	691	205	206	3			

- Molecule 9 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	H	122	Total	C	N	O	S	0	0	0
			877	542	166	165	4			

- Molecule 10 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	I	131	Total	C	N	O	S	0	0	0
			830	503	164	162	1			

- Molecule 11 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	141	Total	C	N	O	S	0	0	0
			1054	673	196	181	4			

- Molecule 12 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	119	Total	C	N	O	S	0	0	0
			900	554	174	171	1			

- Molecule 13 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	L	109	Total	C	N	O	0	0	0
			667	405	134	128			

- Molecule 14 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	M	110	Total	C	N	O	0	0	0
			834	526	167	141			

- Molecule 15 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	N	116	Total	C	N	O	S	0	0	0
			929	584	188	153	4			

- Molecule 16 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	O	102	Total	C	N	O	S	0	0	0
			756	481	138	136	1			

- Molecule 17 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	P	112	Total	C	N	O	S	0	0	0
			856	534	161	158	3			

- Molecule 18 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	Q	89	Total	C	N	O	S	0	0	0
			600	375	107	116	2			

- Molecule 19 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	R	101	Total	C	N	O	S	0	0	0
			609	373	111	124	1			

- Molecule 20 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	S	167	Total	C	N	O	S	0	0	0
			1082	680	192	208	2			

- Molecule 21 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	T	75	Total	C	N	O	0	0	0
			541	336	101	104			

- Molecule 22 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
22	V	63	Total	C	N	O	0	0	0
			416	256	75	85			

- Molecule 23 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	W	58	Total	C	N	O	S	0	0	0
			449	279	84	85	1			

- Molecule 24 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	Z	45	Total	C	N	O	S	0	0	0
			352	215	73	60	4			

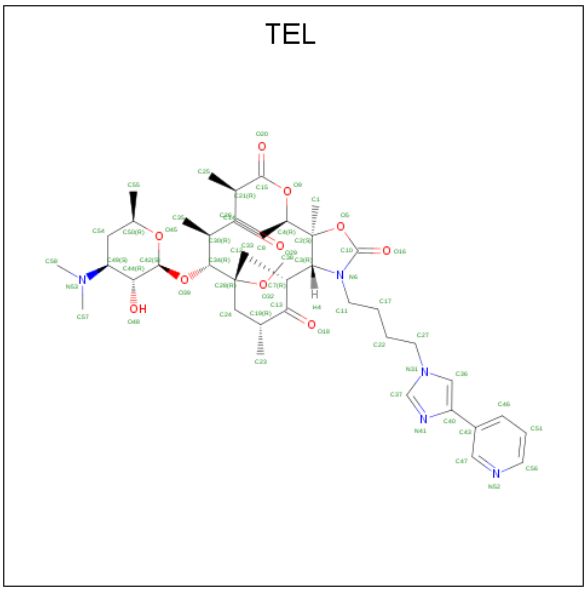
- Molecule 25 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	2	44	Total	C	N	O	S	0	0	0
			362	222	86	53	1			

- Molecule 26 is a protein called 50S ribosomal protein L35.

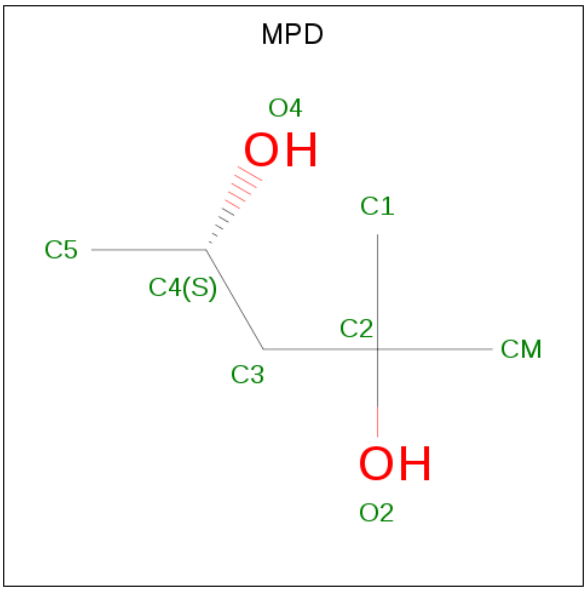
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	3	60	Total	C	N	O	S	0	0	0
			390	239	77	72	2			

- Molecule 27 is TELITHROMYCIN (three-letter code: TEL) (formula: $C_{43}H_{65}N_5O_{10}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	X	1	Total	C	N	O	0	0
			58	43	5	10		

- Molecule 28 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	X	1	Total	C	O	0	0
			8	6	2		
28	X	1	Total	C	O	0	0
			8	6	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	X	1	Total C O 8 6 2	0	0
28	X	1	Total C O 8 6 2	0	0
28	X	1	Total C O 8 6 2	0	0
28	X	1	Total C O 8 6 2	0	0
28	X	1	Total C O 8 6 2	0	0
28	X	1	Total C O 8 6 2	0	0

- Molecule 29 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	G	1	Total Mg 1 1	0	0
29	B	1	Total Mg 1 1	0	0
29	C	3	Total Mg 3 3	0	0
29	A	1	Total Mg 1 1	0	0
29	T	1	Total Mg 1 1	0	0
29	X	136	Total Mg 136 136	0	0
29	O	1	Total Mg 1 1	0	0
29	R	1	Total Mg 1 1	0	0
29	Y	4	Total Mg 4 4	0	0

- Molecule 30 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	X	221	Total Mn 221 221	0	0
30	I	2	Total Mn 2 2	0	0

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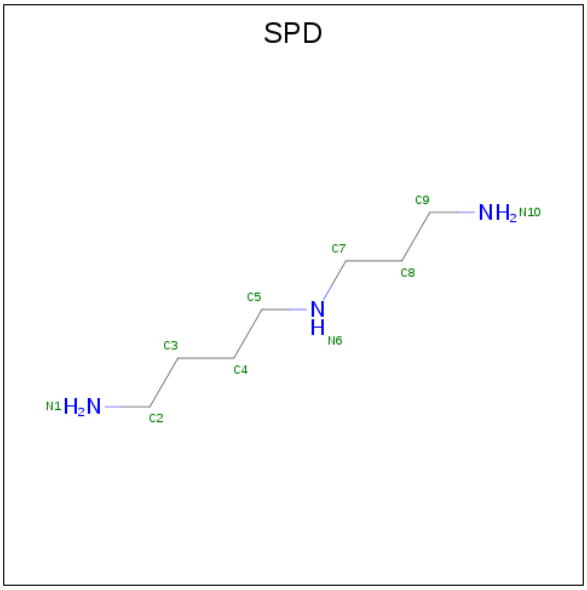
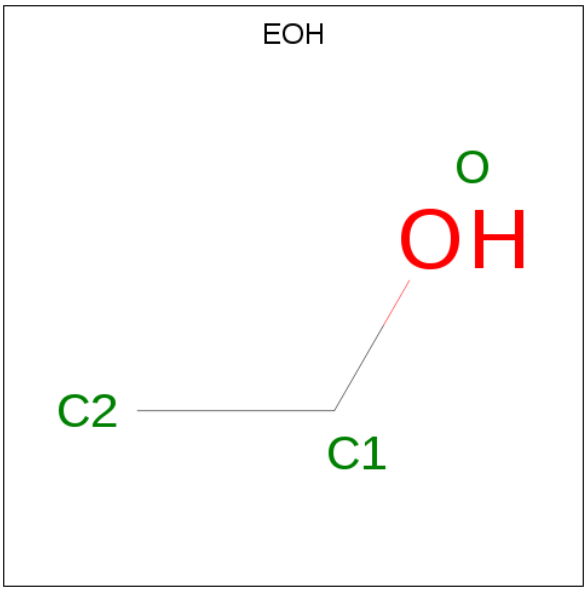
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	Y	6	Total Mn 6 6	0	0
30	J	1	Total Mn 1 1	0	0
30	M	1	Total Mn 1 1	0	0

- Molecule 31 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).



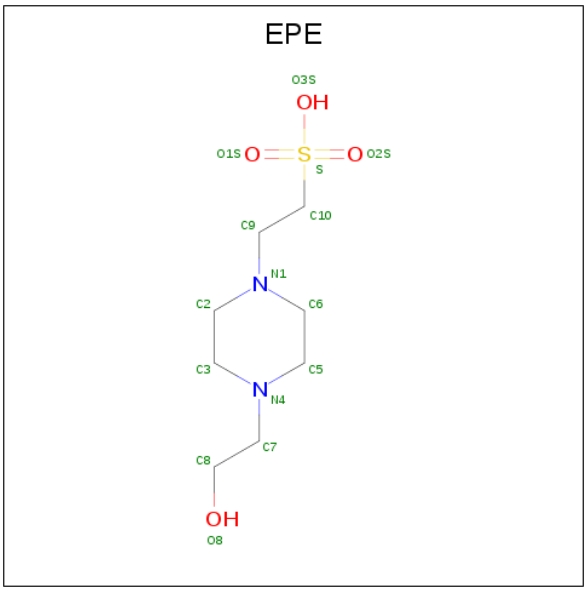
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	X	1	Total C N 10 7 3	0	0
31	X	1	Total C N 10 7 3	0	0
31	X	1	Total C N 10 7 3	0	0
31	X	1	Total C N 10 7 3	0	0
31	S	1	Total C N 10 7 3	0	0

- Molecule 32 is ETHANOL (three-letter code: EOH) (formula: C_2H_6O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	X	1	Total C O 3 2 1	0	0
32	X	1	Total C O 3 2 1	0	0
32	X	1	Total C O 3 2 1	0	0

- Molecule 33 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



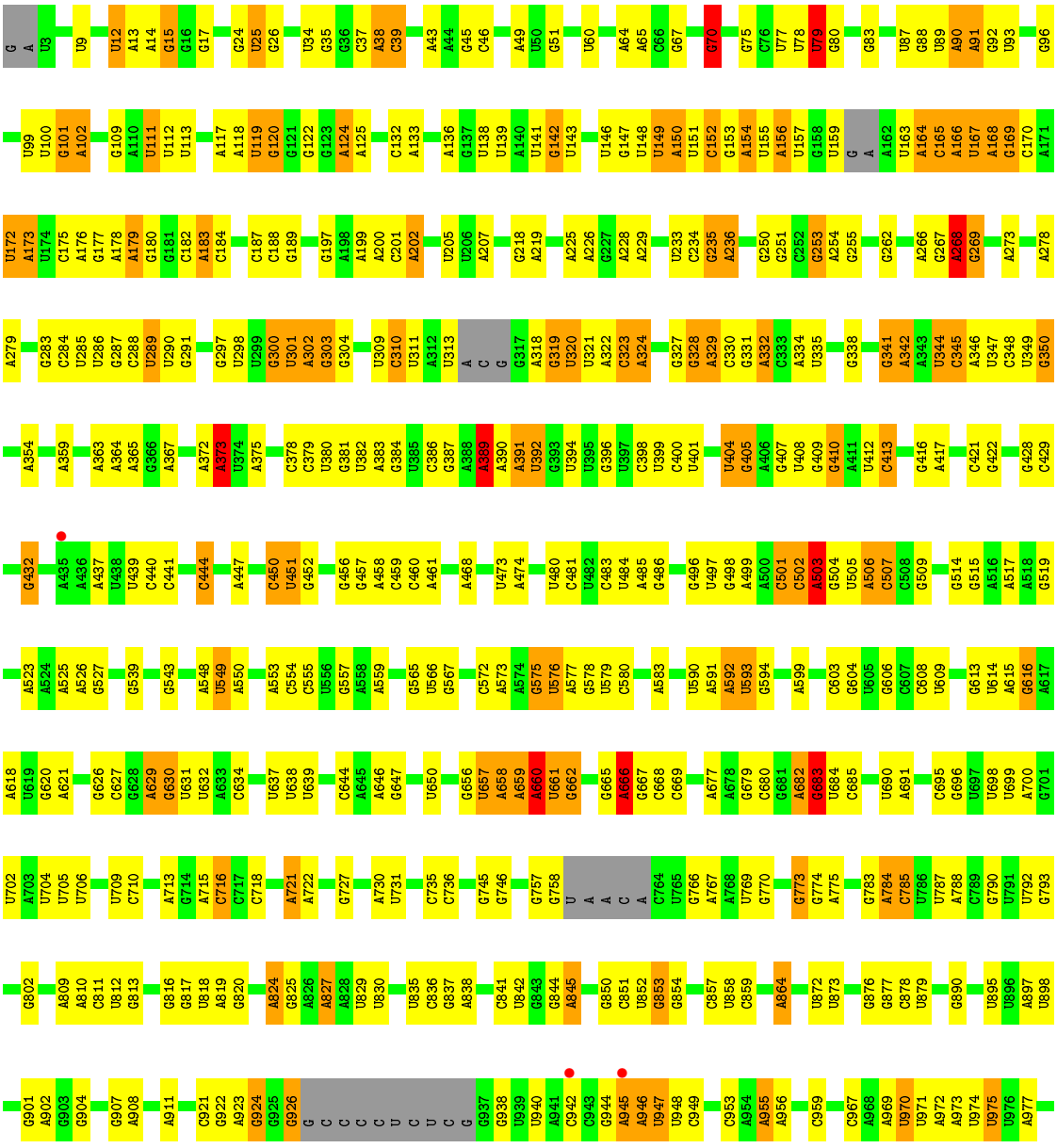
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
33	L	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

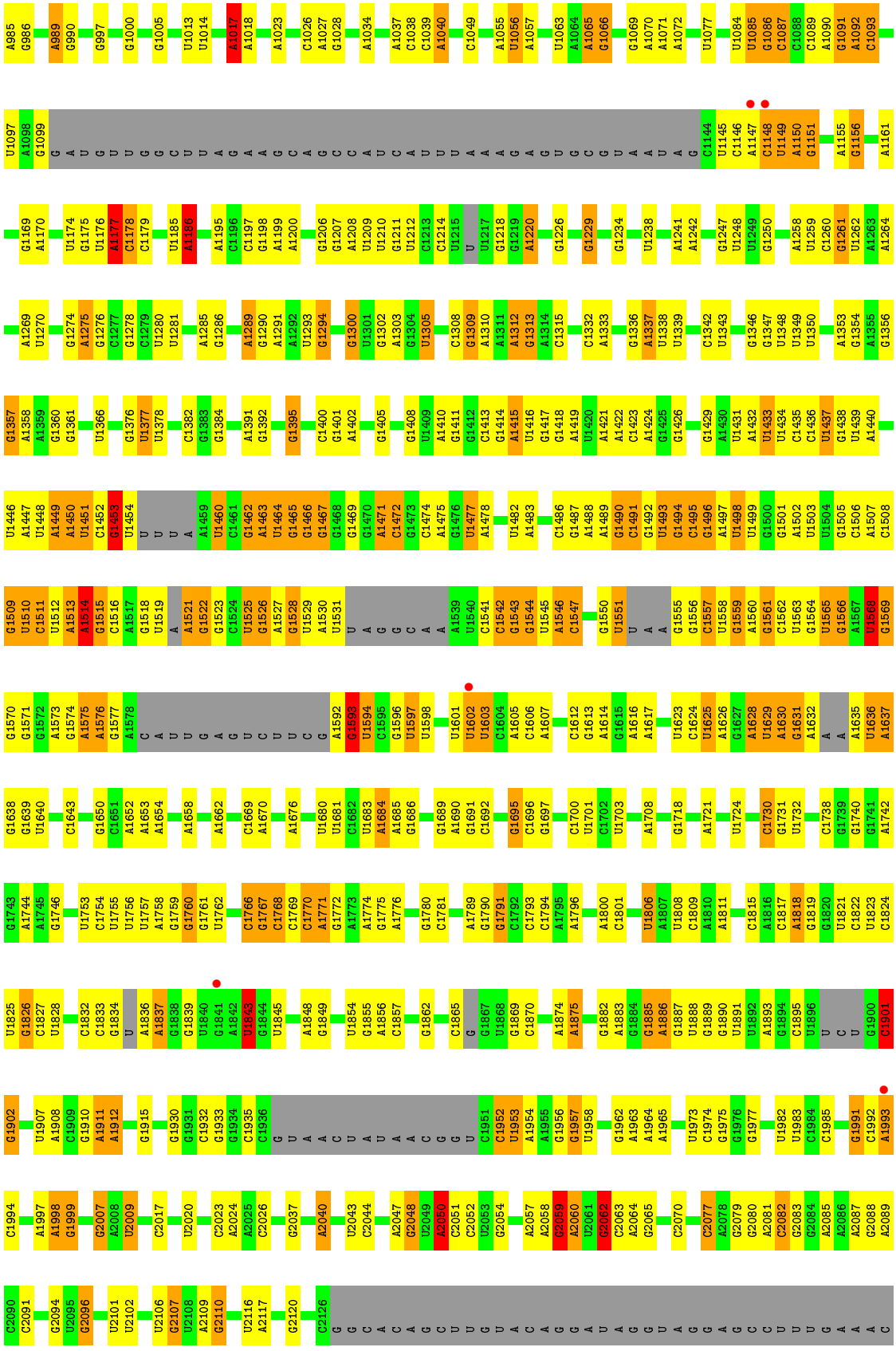
3 Residue-property plots (i)

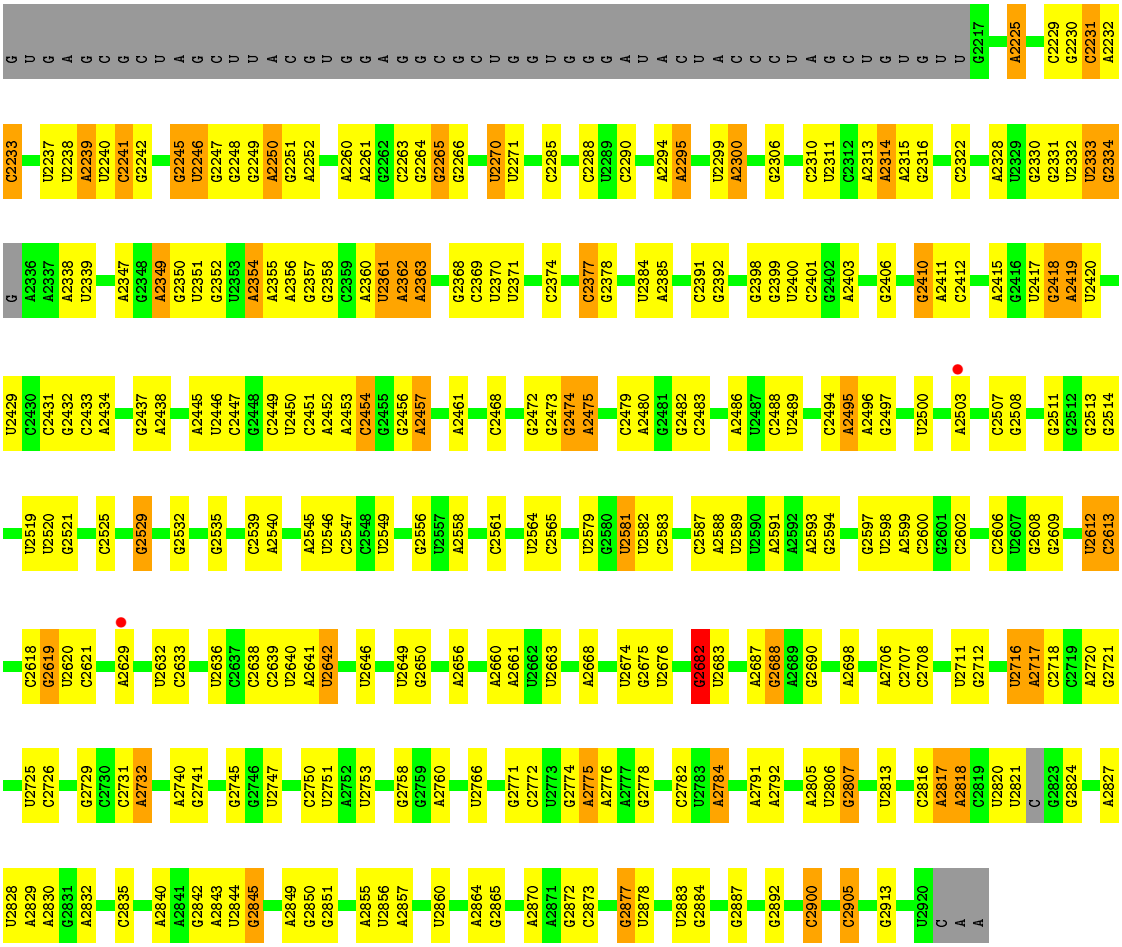
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 23S ribosomal RNA

Chain X:

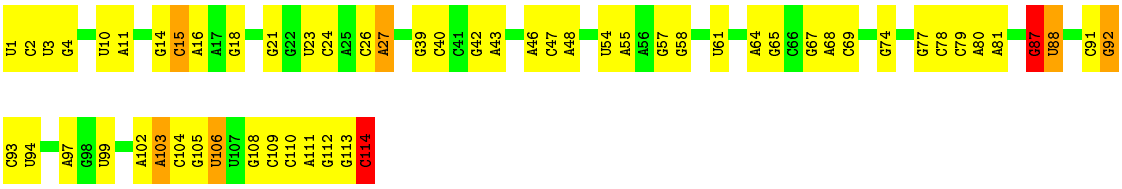






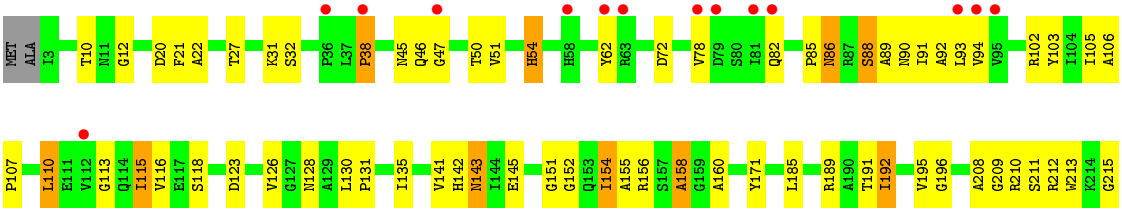
- Molecule 2: 5S ribosomal RNA

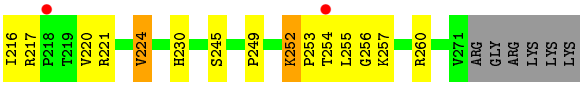
Chain Y:



- Molecule 3: 50S ribosomal protein L2

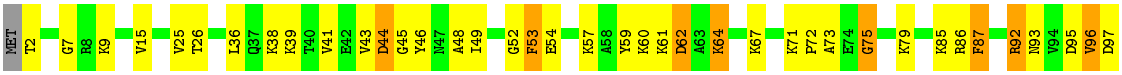
Chain A:

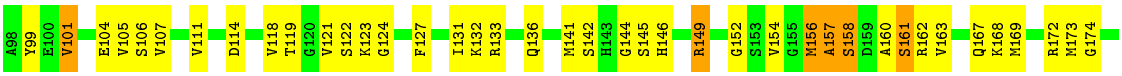


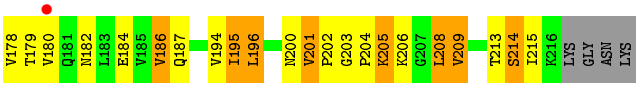


• Molecule 4: 50S ribosomal protein L3

Chain B:

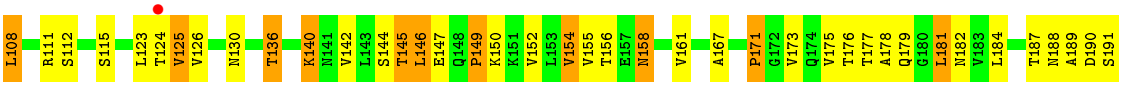


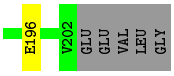




• Molecule 5: 50S ribosomal protein L4

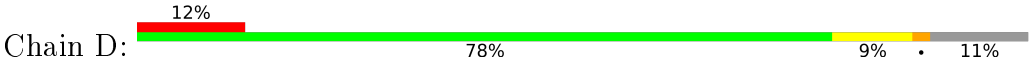
Chain C:

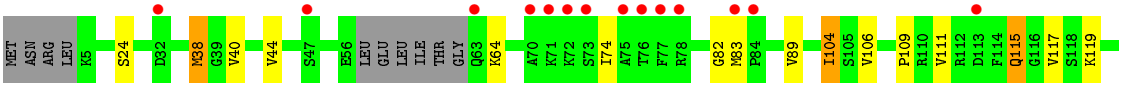


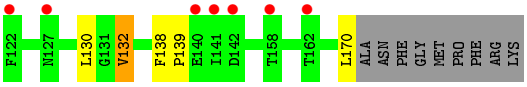


• Molecule 6: 50S ribosomal protein L5

Chain D:

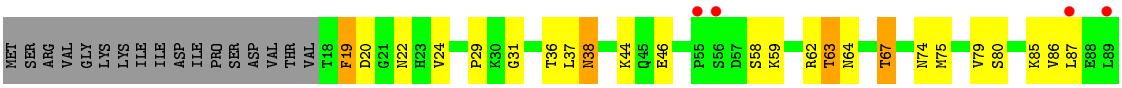


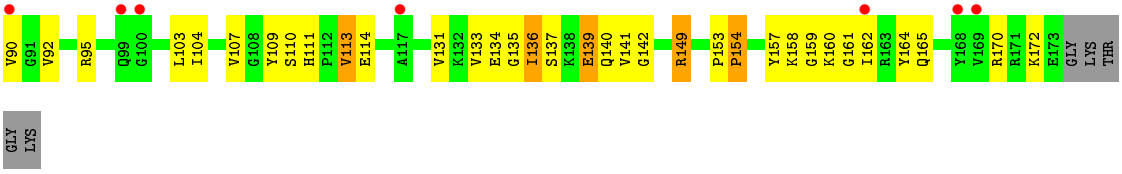




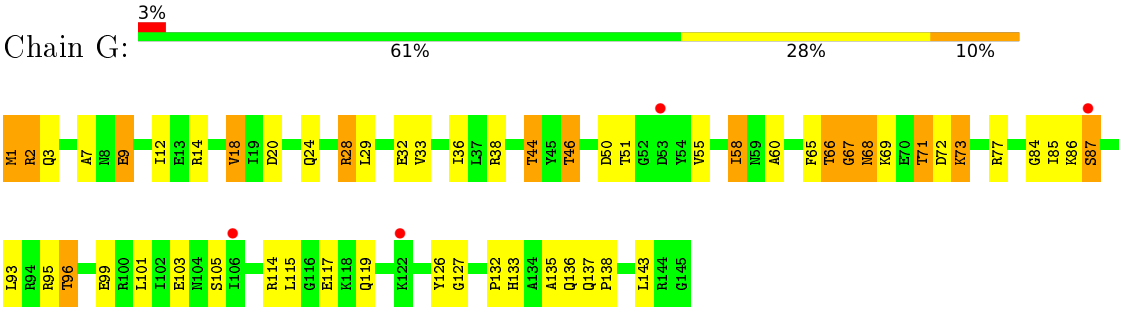
• Molecule 7: 50S ribosomal protein L6

Chain E:

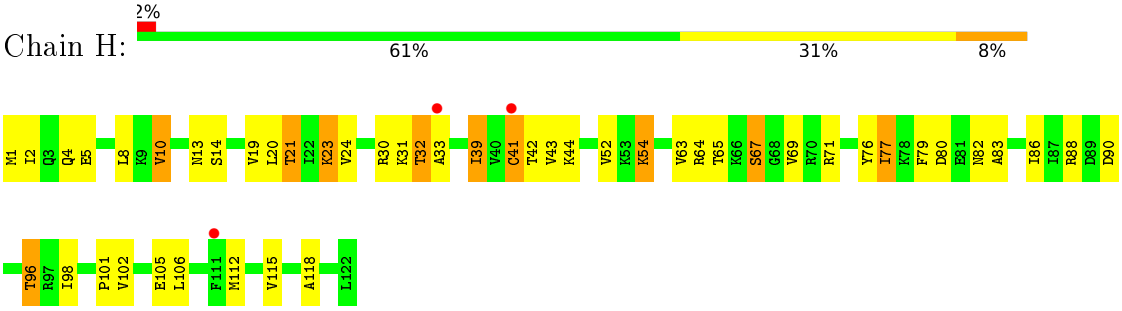




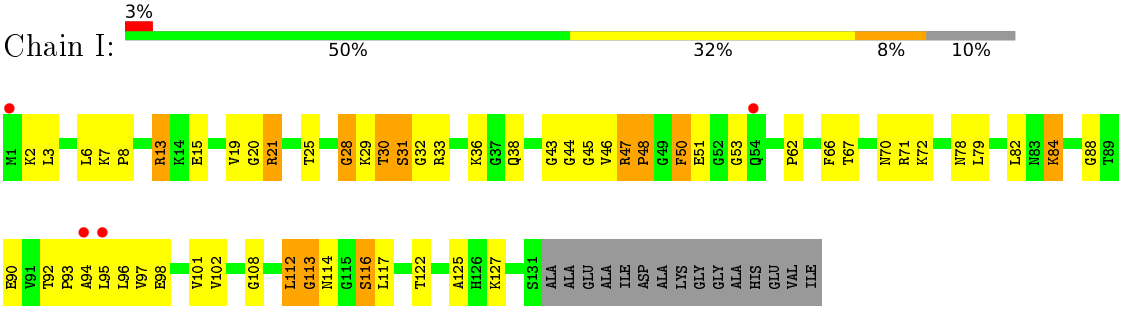
• Molecule 8: 50S ribosomal protein L13



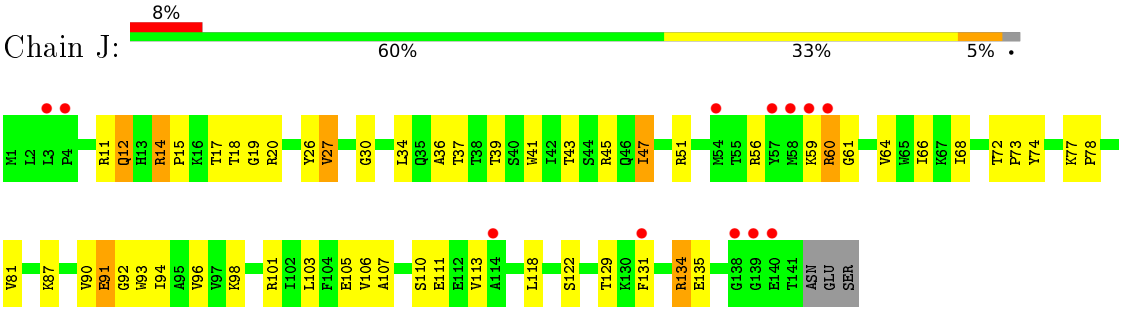
• Molecule 9: 50S ribosomal protein L14



• Molecule 10: 50S ribosomal protein L15

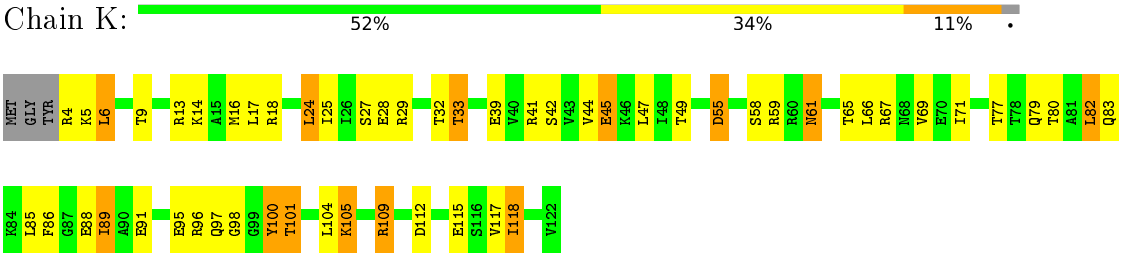


• Molecule 11: 50S ribosomal protein L16



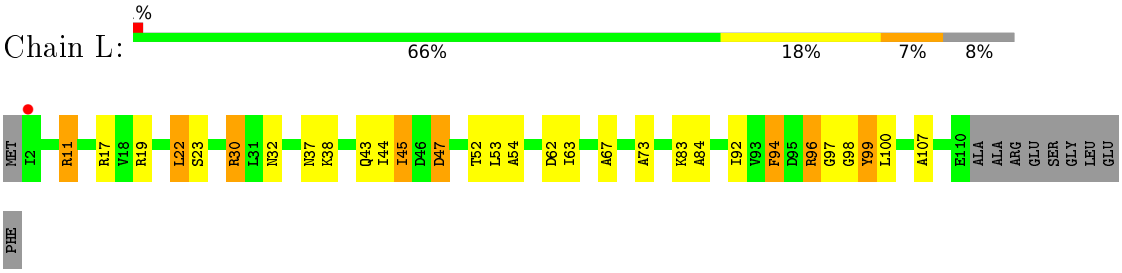
• Molecule 12: 50S ribosomal protein L17

Chain K:



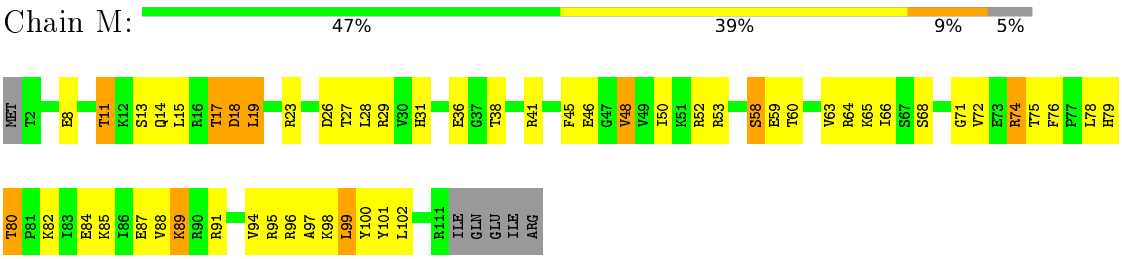
• Molecule 13: 50S ribosomal protein L18

Chain L:



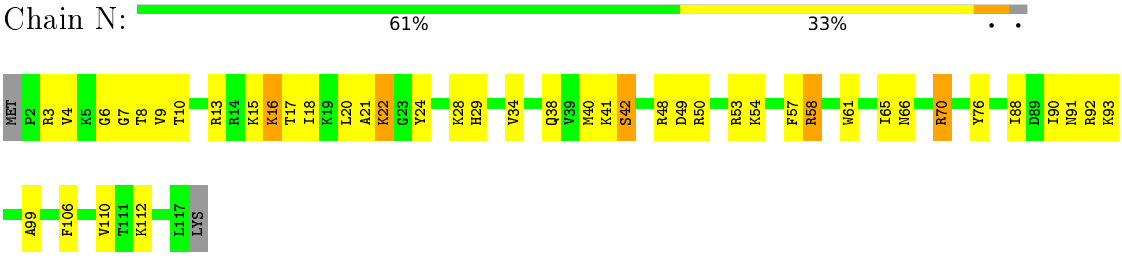
• Molecule 14: 50S ribosomal protein L19

Chain M:



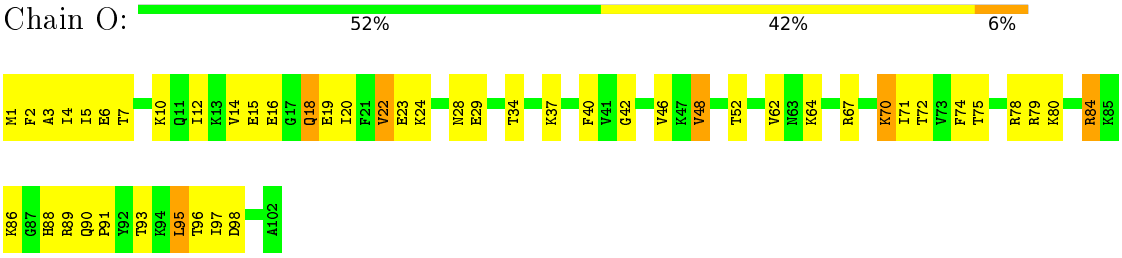
• Molecule 15: 50S ribosomal protein L20

Chain N:



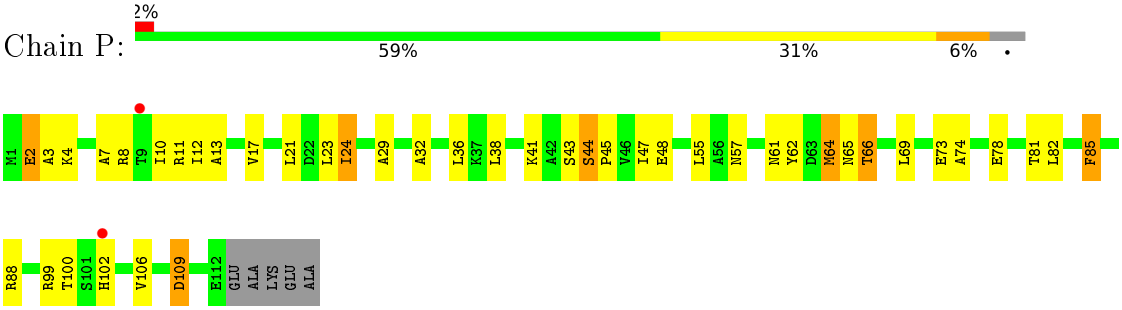
• Molecule 16: 50S ribosomal protein L21

Chain O:



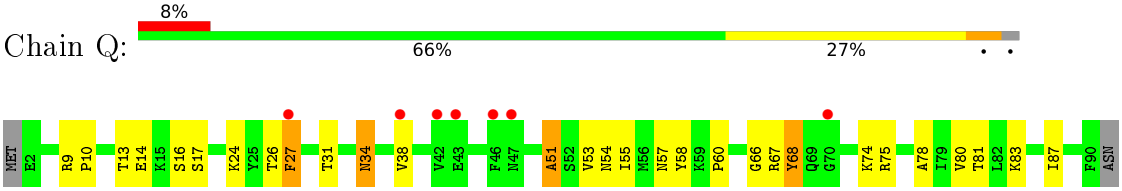
• Molecule 17: 50S ribosomal protein L22

Chain P:



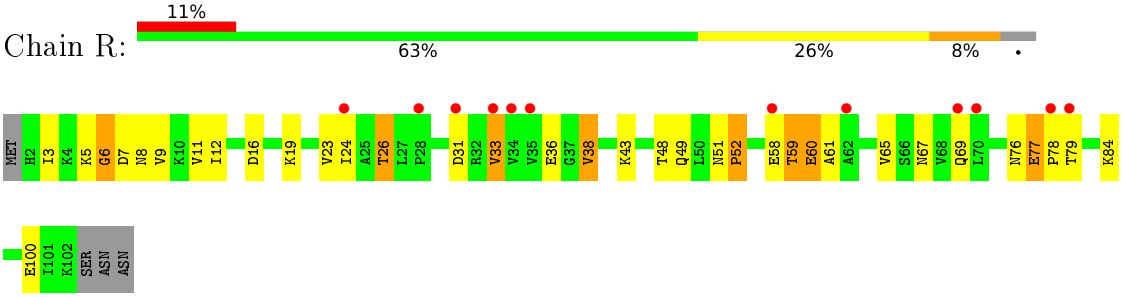
• Molecule 18: 50S ribosomal protein L23

Chain Q:



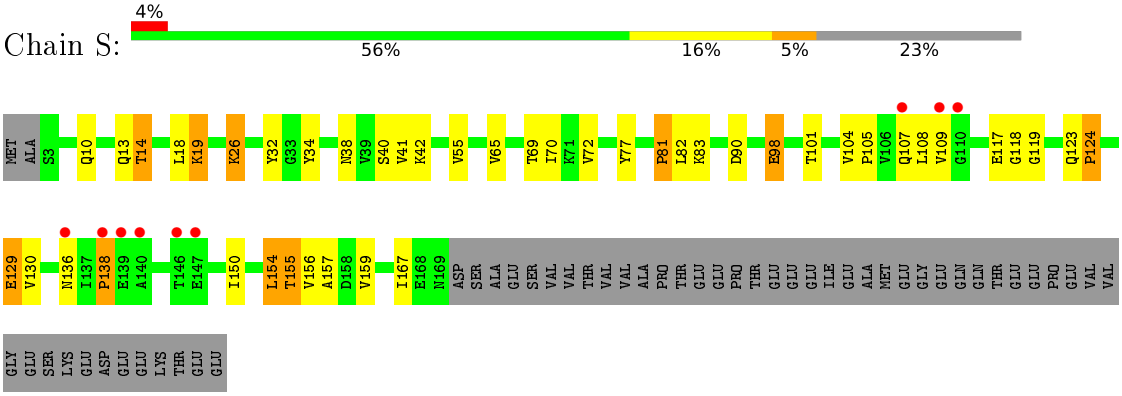
• Molecule 19: 50S ribosomal protein L24

Chain R:



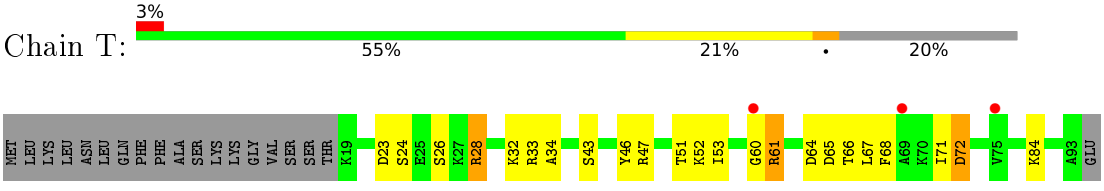
• Molecule 20: 50S ribosomal protein L25

Chain S:



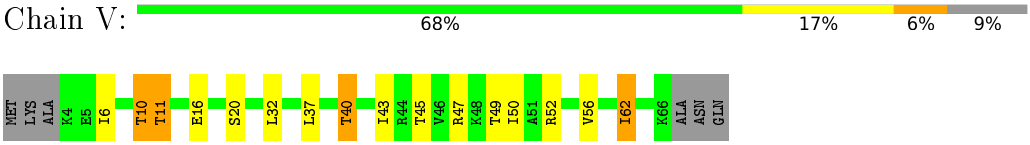
• Molecule 21: 50S ribosomal protein L27

Chain T:



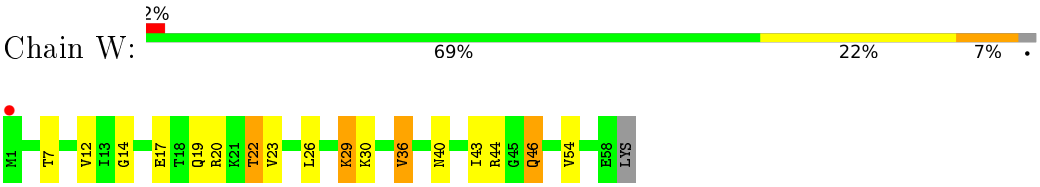
• Molecule 22: 50S ribosomal protein L29

Chain V:



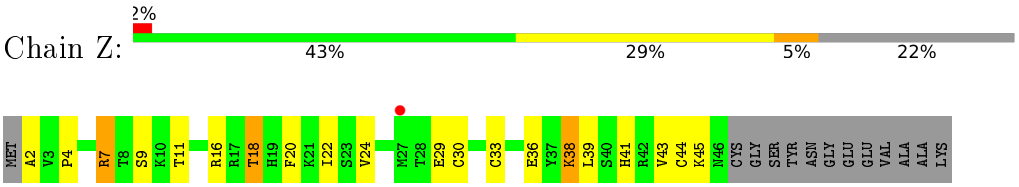
• Molecule 23: 50S ribosomal protein L30

Chain W:



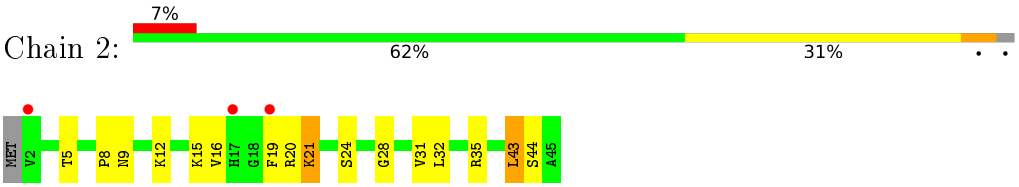
• Molecule 24: 50S ribosomal protein L32

Chain Z:



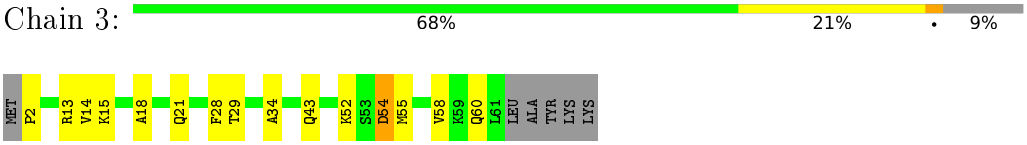
• Molecule 25: 50S ribosomal protein L34

Chain 2:



• Molecule 26: 50S ribosomal protein L35

Chain 3:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	282.66Å 282.66Å 877.08Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.19 – 3.43 50.19 – 3.43	Depositor EDS
% Data completeness (in resolution range)	97.4 (50.19-3.43) 97.4 (50.19-3.43)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.14 (at 3.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.192 , 0.232 0.192 , 0.232	Depositor DCC
R_{free} test set	13519 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	114.5	Xtriage
Anisotropy	0.215	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.22 , 76.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	81033	wwPDB-VP
Average B, all atoms (Å^2)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.30% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

Bond lengths and bond angles in the following residue types are not validated in this section: MG, MN, TEL, EOH, MPD, EPE, SPD

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	X	0.56	10/65105 (0.0%)	1.06	170/101500 (0.2%)
2	Y	0.52	1/2717 (0.0%)	1.06	14/4232 (0.3%)
3	A	0.35	0/1671	0.65	0/2304
4	B	0.51	0/1589	0.79	1/2139 (0.0%)
5	C	0.46	0/1332	0.72	0/1826
6	D	0.26	0/826	0.61	0/1147
7	E	0.51	0/941	0.79	0/1302
8	G	0.45	0/1127	0.68	0/1524
9	H	0.40	0/884	0.63	0/1195
10	I	0.56	0/838	0.91	1/1139 (0.1%)
11	J	0.43	0/1078	0.68	0/1457
12	K	0.44	0/903	0.71	0/1209
13	L	0.34	0/672	0.66	0/922
14	M	0.46	0/846	0.75	1/1139 (0.1%)
15	N	0.51	0/941	0.67	0/1248
16	O	0.46	0/766	0.68	0/1028
17	P	0.47	0/864	0.69	0/1164
18	Q	0.33	0/607	0.58	0/830
19	R	0.39	0/614	0.65	0/847
20	S	0.38	0/1094	0.64	1/1503 (0.1%)
21	T	0.44	0/547	0.63	0/733
22	V	0.36	0/417	0.53	0/571
23	W	0.47	0/451	0.66	0/607
24	Z	0.48	0/358	0.67	0/478
25	2	0.41	0/366	0.65	0/480
26	3	0.51	0/393	0.76	0/529
All	All	0.53	11/87947 (0.0%)	1.00	188/133053 (0.1%)

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
3	A	0	1
5	C	0	1
All	All	0	2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	2845	G	N9-C4	-7.38	1.32	1.38
1	X	2845	G	C2-N3	-5.96	1.27	1.32
1	X	350	G	N9-C4	5.89	1.42	1.38
1	X	2048	G	N9-C8	5.88	1.42	1.37
1	X	1065	A	N9-C4	-5.80	1.34	1.37
1	X	2048	G	N9-C4	-5.63	1.33	1.38
1	X	1289	A	N9-C4	-5.54	1.34	1.37
1	X	1065	A	N7-C5	-5.38	1.36	1.39
1	X	1065	A	N3-C4	-5.31	1.31	1.34
2	Y	92	G	N9-C4	-5.12	1.33	1.38
1	X	2059	G	N9-C8	-5.01	1.34	1.37

All (188) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	2845	G	N3-C4-N9	-15.55	116.67	126.00
1	X	2845	G	N3-C4-C5	13.97	135.58	128.60
1	X	2048	G	C5-N7-C8	-11.50	98.55	104.30
1	X	2048	G	N3-C4-C5	11.50	134.35	128.60
1	X	2048	G	C4-C5-N7	10.80	115.12	110.80
1	X	1065	A	C2-N3-C4	-10.55	105.32	110.60
1	X	2845	G	N3-C2-N2	-10.41	112.61	119.90
1	X	350	G	N3-C4-N9	10.25	132.15	126.00
1	X	2048	G	C2-N3-C4	-10.12	106.84	111.90
1	X	350	G	N3-C4-C5	-10.09	123.55	128.60
1	X	1843	U	C5-C6-N1	9.54	127.47	122.70
2	Y	93	C	N3-C2-O2	-9.23	115.44	121.90
1	X	1289	A	C5-N7-C8	-9.22	99.29	103.90
1	X	1305	U	N3-C2-O2	-8.89	115.97	122.20
1	X	1289	A	C2-N3-C4	-8.88	106.16	110.60
1	X	2048	G	N3-C4-N9	-8.84	120.70	126.00
1	X	2716	U	C5-C4-O4	8.72	131.13	125.90
1	X	2845	G	C8-N9-C1'	8.62	138.20	127.00
1	X	1806	U	C5-C6-N1	-8.60	118.40	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	350	G	C4-N9-C1'	8.32	137.31	126.50
1	X	2048	G	N7-C8-N9	8.11	117.16	113.10
1	X	2845	G	N1-C2-N2	8.05	123.44	116.20
2	Y	88	U	N3-C2-O2	-7.87	116.69	122.20
1	X	721	A	C2-N3-C4	-7.87	106.67	110.60
1	X	721	A	C5-N7-C8	-7.77	100.02	103.90
1	X	12	U	N1-C2-O2	7.56	128.09	122.80
1	X	2845	G	C2-N3-C4	-7.53	108.14	111.90
2	Y	93	C	N1-C2-O2	7.42	123.36	118.90
1	X	2845	G	C4-N9-C1'	-7.42	116.86	126.50
1	X	12	U	N3-C2-O2	-7.36	117.05	122.20
1	X	70	G	C4-N9-C1'	7.32	136.02	126.50
1	X	2716	U	N3-C4-O4	-7.32	114.28	119.40
1	X	350	G	C8-N9-C1'	-7.30	117.51	127.00
1	X	496	G	C6-C5-N7	-7.24	126.06	130.40
1	X	428	G	N3-C4-C5	-7.15	125.03	128.60
1	X	268	A	O4'-C1'-N9	7.14	113.92	108.20
1	X	1289	A	N7-C8-N9	7.08	117.34	113.80
1	X	12	U	C2-N1-C1'	7.06	126.18	117.70
1	X	721	A	C6-C5-N7	-7.02	127.38	132.30
1	X	323	C	C6-N1-C2	-6.97	117.51	120.30
2	Y	92	G	N3-C4-C5	6.96	132.08	128.60
1	X	660	A	P-O3'-C3'	6.92	128.01	119.70
1	X	323	C	C2-N1-C1'	6.90	126.39	118.80
14	M	99	LEU	CA-CB-CG	6.90	131.16	115.30
1	X	557	G	O4'-C1'-N9	6.88	113.70	108.20
1	X	1275	A	O4'-C1'-N9	6.83	113.66	108.20
1	X	1186	A	C2-N3-C4	-6.82	107.19	110.60
1	X	1289	A	N1-C6-N6	6.82	122.69	118.60
2	Y	88	U	N1-C2-O2	6.80	127.56	122.80
1	X	721	A	C4-C5-N7	6.76	114.08	110.70
1	X	721	A	N7-C8-N9	6.72	117.16	113.80
1	X	1065	A	N1-C2-N3	6.71	132.65	129.30
1	X	1065	A	C5-N7-C8	-6.71	100.55	103.90
1	X	1433	U	C2-N1-C1'	6.68	125.72	117.70
1	X	660	A	C8-N9-C4	6.59	108.44	105.80
1	X	1065	A	C8-N9-C4	-6.56	103.17	105.80
1	X	496	G	N1-C6-O6	6.56	123.83	119.90
1	X	2716	U	C5-C6-N1	-6.46	119.47	122.70
1	X	373	A	C2-N3-C4	-6.45	107.38	110.60
2	Y	114	C	C6-N1-C2	-6.44	117.72	120.30
1	X	1395	G	N1-C6-O6	-6.39	116.07	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	721	A	N1-C6-N6	6.37	122.42	118.60
1	X	1065	A	N7-C8-N9	6.33	116.96	113.80
1	X	70	G	C8-N9-C4	-6.28	103.89	106.40
1	X	1568	U	P-O3'-C3'	6.28	127.24	119.70
1	X	1395	G	N3-C4-C5	-6.27	125.47	128.60
1	X	1453	G	N3-C4-N9	-6.26	122.24	126.00
1	X	2716	U	C2-N1-C1'	-6.26	110.18	117.70
1	X	341	G	N3-C4-N9	6.24	129.74	126.00
1	X	1261	G	C6-C5-N7	-6.21	126.67	130.40
1	X	1305	U	N1-C2-O2	6.20	127.14	122.80
1	X	1065	A	N1-C6-N6	6.19	122.31	118.60
1	X	1065	A	C6-C5-N7	-6.18	127.97	132.30
1	X	1275	A	C5-N7-C8	-6.17	100.81	103.90
1	X	1289	A	C4-C5-N7	6.17	113.78	110.70
1	X	389	A	C8-N9-C4	-6.04	103.38	105.80
1	X	721	A	O4'-C1'-N9	6.04	113.04	108.20
1	X	1305	U	C5-C6-N1	-6.03	119.69	122.70
1	X	1294	G	C4-N9-C1'	6.02	134.33	126.50
1	X	2740	A	N1-C6-N6	5.99	122.19	118.60
4	B	144	GLY	N-CA-C	-5.96	98.20	113.10
1	X	1565	U	N3-C2-O2	-5.95	118.03	122.20
1	X	1453	G	C4-N9-C1'	-5.91	118.81	126.50
1	X	503	A	C5-N7-C8	-5.91	100.95	103.90
1	X	2535	G	N1-C6-O6	5.90	123.44	119.90
1	X	1065	A	C5-C6-N1	-5.89	114.75	117.70
1	X	341	G	N3-C4-C5	-5.86	125.67	128.60
1	X	373	A	N1-C2-N3	5.86	132.23	129.30
1	X	2845	G	N9-C4-C5	5.85	107.74	105.40
1	X	2740	A	C5-N7-C8	-5.83	100.98	103.90
1	X	1149	U	N1-C2-O2	5.80	126.86	122.80
1	X	1593	G	N3-C4-N9	5.80	129.48	126.00
2	Y	103	A	C6-N1-C2	5.80	122.08	118.60
1	X	1177	A	C8-N9-C4	-5.79	103.48	105.80
1	X	1566	G	N3-C4-N9	-5.78	122.53	126.00
1	X	1017	A	C8-N9-C4	-5.77	103.49	105.80
1	X	428	G	N3-C4-N9	5.76	129.46	126.00
1	X	79	U	C5-C6-N1	5.76	125.58	122.70
1	X	341	G	N7-C8-N9	5.76	115.98	113.10
1	X	1597	U	N1-C2-O2	5.74	126.82	122.80
1	X	389	A	N7-C8-N9	5.73	116.66	113.80
1	X	496	G	C4-C5-C6	5.70	122.22	118.80
1	X	1597	U	N3-C2-O2	-5.69	118.22	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	1514	A	N9-C4-C5	-5.68	103.53	105.80
1	X	1801	C	N3-C2-O2	-5.68	117.92	121.90
1	X	2062	G	C5-C6-N1	5.67	114.33	111.50
1	X	341	G	C4-N9-C1'	5.64	133.84	126.50
1	X	1305	U	C4-C5-C6	5.64	123.08	119.70
1	X	2816	C	C6-N1-C2	5.62	122.55	120.30
2	Y	93	C	C6-N1-C2	-5.61	118.06	120.30
1	X	1275	A	N7-C8-N9	5.60	116.60	113.80
1	X	2062	G	O5'-P-OP2	-5.57	100.68	105.70
1	X	2474	G	N1-C6-O6	5.56	123.24	119.90
1	X	43	A	O4'-C1'-N9	5.53	112.62	108.20
1	X	503	A	N7-C8-N9	5.53	116.56	113.80
1	X	1289	A	C6-C5-N7	-5.52	128.44	132.30
1	X	1593	G	N3-C4-C5	-5.49	125.85	128.60
1	X	350	G	O4'-C1'-N9	5.49	112.59	108.20
1	X	1177	A	N9-C4-C5	5.49	108.00	105.80
1	X	2740	A	C4-C5-N7	5.49	113.44	110.70
2	Y	92	G	N3-C4-N9	-5.48	122.71	126.00
1	X	1843	U	C4-C5-C6	-5.48	116.41	119.70
1	X	2529	G	C5-C6-O6	-5.47	125.32	128.60
1	X	323	C	C5-C6-N1	5.46	123.73	121.00
1	X	35	G	N3-C4-N9	-5.46	122.72	126.00
1	X	565	G	N1-C6-O6	5.46	123.18	119.90
1	X	1294	G	N3-C4-C5	-5.46	125.87	128.60
1	X	2583	C	C6-N1-C2	-5.45	118.12	120.30
1	X	341	G	C8-N9-C4	-5.45	104.22	106.40
1	X	2048	G	C8-N9-C4	-5.45	104.22	106.40
1	X	70	G	C8-N9-C1'	-5.44	119.92	127.00
1	X	350	G	C2-N3-C4	5.44	114.62	111.90
1	X	1453	G	C8-N9-C1'	5.43	134.06	127.00
1	X	113	U	C2-N1-C1'	5.43	124.22	117.70
1	X	2040	A	C4-C5-C6	5.43	119.71	117.00
1	X	1229	G	N1-C6-O6	5.42	123.15	119.90
1	X	1275	A	C6-C5-N7	-5.42	128.51	132.30
2	Y	106	U	N1-C2-O2	5.42	126.59	122.80
1	X	323	C	N1-C2-O2	5.41	122.15	118.90
1	X	565	G	C5-C6-O6	-5.41	125.35	128.60
1	X	2050	A	C8-N9-C4	-5.41	103.64	105.80
1	X	1357	G	C5-C6-O6	5.40	131.84	128.60
1	X	2682	G	O4'-C1'-N9	5.39	112.51	108.20
1	X	70	G	N7-C8-N9	5.38	115.79	113.10
1	X	1915	G	C4-N9-C1'	5.38	133.49	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	721	A	C8-N9-C4	-5.36	103.66	105.80
1	X	854	G	N3-C4-C5	-5.34	125.93	128.60
2	Y	106	U	N3-C2-O2	-5.33	118.47	122.20
1	X	1289	A	C5-C6-N1	-5.32	115.04	117.70
1	X	721	A	C5-C6-N1	-5.31	115.05	117.70
1	X	1360	G	C4-C5-N7	5.30	112.92	110.80
1	X	2619	G	C6-C5-N7	-5.29	127.22	130.40
1	X	496	G	C4-N9-C1'	5.28	133.36	126.50
1	X	1360	G	N1-C6-O6	5.24	123.05	119.90
1	X	2845	G	C5-N7-C8	-5.23	101.69	104.30
1	X	2473	G	C8-N9-C4	5.22	108.49	106.40
1	X	1915	G	N3-C4-N9	5.22	129.13	126.00
1	X	341	G	C2-N3-C4	5.19	114.49	111.90
2	Y	15	C	C6-N1-C2	5.18	122.37	120.30
1	X	853	G	C5-C6-N1	-5.17	108.92	111.50
20	S	154	LEU	CA-CB-CG	5.17	127.19	115.30
1	X	496	G	N3-C4-N9	5.17	129.10	126.00
2	Y	87	G	N3-C4-C5	5.16	131.18	128.60
1	X	428	G	C4-N9-C1'	5.16	133.20	126.50
1	X	1229	G	C4-C5-N7	5.16	112.86	110.80
10	I	53	GLY	N-CA-C	-5.15	100.23	113.10
1	X	666	A	C2-N3-C4	-5.14	108.03	110.60
2	Y	99	U	N3-C2-O2	-5.14	118.60	122.20
1	X	576	U	N3-C2-O2	-5.14	118.60	122.20
1	X	341	G	C4-C5-N7	5.13	112.85	110.80
1	X	2608	G	N1-C6-O6	-5.11	116.84	119.90
1	X	1186	A	N1-C2-N3	5.10	131.85	129.30
1	X	2063	C	C6-N1-C2	-5.09	118.26	120.30
1	X	683	G	N9-C4-C5	5.08	107.43	105.40
1	X	1361	G	C5-C6-O6	-5.08	125.55	128.60
1	X	1493	U	C2-N1-C1'	5.08	123.80	117.70
1	X	2040	A	N1-C6-N6	5.08	121.65	118.60
1	X	2081	A	C2-N3-C4	-5.06	108.07	110.60
1	X	2682	G	OP2-P-O3'	5.05	116.32	105.20
1	X	1801	C	N1-C2-O2	5.05	121.93	118.90
1	X	2062	G	O4'-C1'-N9	5.05	112.24	108.20
1	X	2845	G	C4-C5-C6	-5.05	115.77	118.80
1	X	1957	G	N3-C4-N9	5.04	129.03	126.00
1	X	1275	A	C4-C5-N7	5.04	113.22	110.70
1	X	1901	C	P-O3'-C3'	5.03	125.73	119.70
1	X	2091	C	C6-N1-C2	5.02	122.31	120.30
1	X	1565	U	N1-C2-O2	5.00	126.30	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	657	U	C2-N1-C1'	5.00	123.70	117.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	115	ILE	Peptide
5	C	140	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	X	58145	0	29245	725	1
2	Y	2430	0	1229	40	0
3	A	1640	0	1255	51	0
4	B	1566	0	1559	68	0
5	C	1314	0	1146	44	0
6	D	823	0	433	7	0
7	E	930	0	688	32	0
8	G	1105	0	1064	34	0
9	H	877	0	882	33	0
10	I	830	0	703	32	0
11	J	1054	0	1040	30	0
12	K	900	0	924	38	0
13	L	667	0	507	20	0
14	M	834	0	850	33	0
15	N	929	0	988	34	0
16	O	756	0	754	32	0
17	P	856	0	909	33	0
18	Q	600	0	500	22	0
19	R	609	0	484	17	0
20	S	1082	0	919	17	0
21	T	541	0	518	12	0
22	V	416	0	348	5	0
23	W	449	0	490	8	0
24	Z	352	0	358	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	2	362	0	398	12	0
26	3	390	0	346	4	0
27	X	58	0	65	13	0
28	X	64	0	112	15	0
29	A	1	0	0	0	0
29	B	1	0	0	0	0
29	C	3	0	0	0	0
29	G	1	0	0	0	0
29	O	1	0	0	0	0
29	R	1	0	0	0	0
29	T	1	0	0	0	0
29	X	136	0	0	0	0
29	Y	4	0	0	0	0
30	I	2	0	0	0	0
30	J	1	0	0	0	0
30	M	1	0	0	0	0
30	X	221	0	0	0	0
30	Y	6	0	0	0	0
31	S	10	0	19	1	0
31	X	40	0	76	5	0
32	X	9	0	18	0	0
33	L	15	0	17	0	0
All	All	81033	0	48844	1274	1

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 10.

All (1274) 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:X:2649:U:O2'	1:X:2845:G:N2	1.98	0.96
1:X:2231:C:HO2'	1:X:2232:A:H8	1.10	0.93
1:X:1886:A:N6	1:X:1910:G:O2'	2.06	0.89
1:X:721:A:H8	1:X:2096:G:H21	1.15	0.87
2:Y:18:G:H1	2:Y:61:U:H3	1.20	0.87
1:X:1518:G:H1	1:X:1562:C:H42	1.22	0.86
12:K:105:LYS:HA	12:K:117:VAL:HG12	1.58	0.86
1:X:1525:U:H2'	1:X:1526:G:H8	1.41	0.85
1:X:1862:G:H1	1:X:1957:G:H21	1.23	0.85
2:Y:79:C:H42	2:Y:92:G:H1	1.21	0.84
1:X:2361:U:H4'	13:L:17:ARG:HG2	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2775:A:H1'	7:E:67:THR:HG22	1.59	0.84
1:X:1515:G:H1	1:X:1565:U:H3	1.23	0.82
1:X:120:G:H4'	1:X:150:A:H5'	1.60	0.82
1:X:878:C:H1'	10:I:48:PRO:HB3	1.63	0.81
3:A:10:THR:HG22	3:A:12:GLY:H	1.47	0.80
1:X:1513:A:H3'	1:X:1514:A:H8	1.46	0.80
8:G:14:ARG:NH2	8:G:50:ASP:O	2.15	0.79
1:X:1528:G:N2	1:X:1547:C:N3	2.31	0.79
1:X:1575:A:H2'	1:X:1576:A:H5'	1.64	0.79
17:P:66:THR:HA	17:P:69:LEU:HD12	1.62	0.78
9:H:101:PRO:HD3	14:M:68:SER:HB2	1.65	0.78
1:X:1518:G:N2	1:X:1562:C:N3	2.30	0.77
28:X:3007:MPD:H52	5:C:61:GLY:HA2	1.65	0.77
1:X:650:U:H3	1:X:666:A:H2	1.33	0.77
13:L:96:ARG:HH11	13:L:96:ARG:HB3	1.48	0.77
1:X:1512:U:H2'	1:X:1513:A:C8	2.20	0.76
5:C:140:LYS:HA	5:C:142:VAL:HG12	1.67	0.76
15:N:7:GLY:O	15:N:9:VAL:N	2.17	0.76
1:X:1185:U:H2'	8:G:66:THR:HG21	1.67	0.76
20:S:105:PRO:HD2	20:S:124:PRO:HA	1.68	0.76
1:X:1563:U:H2'	1:X:1564:G:H8	1.51	0.76
13:L:19:ARG:NH1	13:L:22:LEU:O	2.19	0.76
5:C:111:ARG:O	5:C:115:SER:OG	2.03	0.76
19:R:12:ILE:H	19:R:67:ASN:HA	1.52	0.74
1:X:503:A:H2	1:X:517:A:H62	1.33	0.74
1:X:955:A:N7	11:J:15:PRO:HD2	2.03	0.74
1:X:1815:C:H5"	3:A:224:VAL:HG11	1.69	0.74
1:X:736:C:OP1	3:A:217:ARG:NH1	2.21	0.74
3:A:128:ASN:HA	3:A:191:THR:HG23	1.68	0.73
9:H:24:VAL:HG13	9:H:33:ALA:HB2	1.70	0.73
1:X:1063:U:H3	1:X:1186:A:H62	1.33	0.73
1:X:955:A:C5	11:J:15:PRO:HD2	2.24	0.73
20:S:81:PRO:O	20:S:83:LYS:N	2.22	0.73
1:X:459:C:HO2'	1:X:1907:U:HO2'	1.33	0.73
4:B:87:PHE:CD2	4:B:208:LEU:HG	2.24	0.73
1:X:83:G:H21	1:X:102:A:H2	1.34	0.72
1:X:132:C:H42	1:X:147:G:H1	1.36	0.72
5:C:108:LEU:O	5:C:112:SER:OG	2.06	0.72
1:X:1290:G:OP2	15:N:13:ARG:NH2	2.22	0.72
5:C:50:ALA:HB2	5:C:94:PRO:HD3	1.71	0.72
2:Y:80:A:H61	2:Y:91:C:H42	1.33	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:548:A:H5"	1:X:549:U:H5'	1.70	0.72
4:B:60:LYS:O	4:B:62:ASP:N	2.21	0.72
1:X:2905:C:H42	24:Z:39:LEU:HD11	1.54	0.72
1:X:1832:C:O2'	3:A:50:THR:O	2.06	0.72
1:X:1887:G:O6	1:X:1910:G:N2	2.16	0.72
1:X:1040:A:H4'	15:N:91:ASN:HD21	1.55	0.72
15:N:48:ARG:NH1	15:N:49:ASP:OD1	2.24	0.71
1:X:1039:C:OP2	15:N:54:LYS:NZ	2.22	0.71
9:H:1:MET:N	9:H:67:SER:OG	2.24	0.71
1:X:1174:U:O2	4:B:162:ARG:NH2	2.24	0.71
1:X:501:C:H3'	1:X:502:C:H5"	1.70	0.71
1:X:1491:C:O2	1:X:1509:G:N2	2.24	0.71
23:W:40:ASN:HB3	23:W:43:ILE:H	1.56	0.70
1:X:1683:U:H2'	1:X:1684:A:H5"	1.72	0.70
1:X:864:A:OP2	1:X:1226:G:N2	2.17	0.70
27:X:3001:TEL:H12	27:X:3001:TEL:H233	1.73	0.70
2:Y:77:G:H1	2:Y:94:U:H3	1.39	0.70
3:A:142:HIS:N	3:A:192:ILE:O	2.24	0.70
3:A:131:PRO:HA	3:A:189:ARG:HA	1.73	0.70
4:B:7:GLY:HA2	4:B:53:PHE:CZ	2.26	0.70
22:V:47:ARG:HA	22:V:50:ILE:HD12	1.72	0.70
24:Z:30:CYS:HB3	24:Z:33:CYS:HB3	1.73	0.70
3:A:209:GLY:HA2	3:A:212:ARG:HB2	1.73	0.70
17:P:4:LYS:HB2	17:P:106:VAL:HG22	1.73	0.70
1:X:1238:U:H1'	15:N:4:VAL:HG22	1.74	0.70
1:X:1440:A:HO2'	1:X:1514:A:HO2'	1.36	0.70
1:X:629:A:H62	1:X:1289:A:H2	1.37	0.69
1:X:2079:G:O2'	4:B:160:ALA:O	2.10	0.69
1:X:332:A:H61	1:X:394:U:H3	1.40	0.69
2:Y:65:G:O6	2:Y:105:G:N2	2.21	0.69
24:Z:44:CYS:SG	24:Z:45:LYS:N	2.66	0.69
1:X:329:A:H61	1:X:398:C:H42	1.39	0.69
19:R:59:THR:OG1	19:R:60:GLU:N	2.17	0.69
1:X:304:G:H1	1:X:413:C:H42	1.40	0.69
1:X:1037:A:OP1	15:N:50:ARG:NH1	2.27	0.68
1:X:15:G:H4'	24:Z:18:THR:HB	1.73	0.68
10:I:43:GLY:O	10:I:45:GLY:N	2.25	0.68
19:R:48:THR:OG1	19:R:49:GLN:N	2.27	0.68
1:X:1826:G:N2	1:X:1845:U:O2'	2.26	0.68
16:O:62:VAL:HA	16:O:95:LEU:HB3	1.74	0.68
1:X:1261:G:N2	1:X:1264:A:OP2	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:44:ILE:H	13:L:54:ALA:HB3	1.59	0.68
12:K:6:LEU:HA	12:K:13:ARG:HD3	1.75	0.67
1:X:1525:U:H2'	1:X:1526:G:C8	2.28	0.67
2:Y:15:C:H42	2:Y:105:G:N2	1.92	0.67
19:R:38:VAL:HG12	19:R:61:ALA:H	1.59	0.67
1:X:713:A:H2'	1:X:715:A:H62	1.58	0.67
1:X:2059:G:N7	28:X:3005:MPD:O2	2.22	0.67
4:B:44:ASP:O	4:B:46:TYR:N	2.26	0.66
1:X:1039:C:C5	8:G:1:MET:HA	2.31	0.66
8:G:12:ILE:HD11	8:G:51:THR:HA	1.77	0.66
9:H:98:ILE:HB	9:H:118:ALA:HB2	1.77	0.66
1:X:2642:U:C2	24:Z:4:PRO:HA	2.30	0.66
17:P:2:GLU:HA	17:P:64:MET:HE3	1.78	0.66
3:A:20:ASP:O	3:A:22:ALA:N	2.27	0.66
1:X:49:A:N7	1:X:119:U:H5	1.94	0.65
1:X:235:G:O2'	1:X:236:A:O5'	2.15	0.65
5:C:7:LEU:HD12	5:C:17:ILE:HD11	1.78	0.65
9:H:4:GLN:HG3	9:H:5:GLU:HG2	1.78	0.65
1:X:2758:G:OP1	4:B:182:ASN:ND2	2.28	0.65
1:X:1305:U:H5	1:X:2040:A:N7	1.94	0.65
1:X:1493:U:H5"	1:X:1575:A:N3	2.11	0.65
1:X:682:A:H4'	1:X:683:G:H5'	1.79	0.65
3:A:92:ALA:H	3:A:106:ALA:HB2	1.61	0.65
1:X:637:U:H2'	1:X:638:U:C6	2.32	0.65
1:X:2360:A:H5'	1:X:2362:A:H1'	1.79	0.65
1:X:2817:A:O2'	1:X:2818:A:OP2	2.12	0.65
1:X:1501:G:H22	1:X:2729:G:H22	1.45	0.64
7:E:136:ILE:HD12	7:E:137:SER:H	1.62	0.64
1:X:922:G:O6	1:X:942:C:N4	2.30	0.64
2:Y:21:G:H22	2:Y:58:G:H22	1.46	0.64
1:X:1448:U:H3'	1:X:1449:A:H5"	1.78	0.64
1:X:665:G:H4'	1:X:666:A:H5"	1.79	0.64
2:Y:21:G:H1	2:Y:58:G:H1	1.44	0.64
1:X:142:G:N2	1:X:1640:U:O3'	2.26	0.64
1:X:1466:G:H3'	1:X:1467:G:H5"	1.80	0.64
1:X:2322:C:H41	13:L:17:ARG:HH22	1.44	0.64
1:X:683:G:C6	1:X:696:G:C6	2.86	0.64
1:X:816:G:OP1	25:2:15:LYS:NZ	2.31	0.64
7:E:62:ARG:O	7:E:64:ASN:N	2.26	0.64
9:H:21:THR:HB	9:H:39:ILE:HD12	1.80	0.64
1:X:1465:G:H2'	1:X:1466:G:C8	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:65:A:N1	1:X:90:A:N6	2.46	0.63
1:X:2860:U:H5"	12:K:49:THR:HG21	1.80	0.63
1:X:2410:G:C6	1:X:2411:A:H2	2.16	0.63
1:X:2668:A:OP1	8:G:77:ARG:NH1	2.30	0.63
1:X:2495:A:HO2'	1:X:2496:A:H8	1.46	0.63
5:C:14:SER:OG	5:C:15:GLY:N	2.32	0.63
7:E:158:LYS:O	7:E:160:LYS:N	2.31	0.63
1:X:2082:C:N3	28:X:3005:MPD:HM2	2.14	0.63
16:O:4:ILE:HD13	16:O:40:PHE:HB3	1.79	0.63
1:X:572:C:O2	28:X:3009:MPD:O4	2.16	0.63
1:X:1463:A:H2	1:X:1625:U:H3	1.47	0.63
18:Q:9:ARG:O	18:Q:27:PHE:HB2	1.99	0.63
1:X:1384:G:H1	1:X:1643:C:H42	1.47	0.63
2:Y:69:C:H42	2:Y:102:A:H61	1.47	0.62
17:P:41:LYS:O	17:P:44:SER:OG	2.17	0.62
1:X:1440:A:O2'	1:X:1514:A:O2'	2.12	0.62
1:X:328:G:N2	1:X:329:A:N7	2.46	0.62
1:X:1843:U:H3'	1:X:1843:U:H6	1.64	0.62
1:X:827:A:C8	3:A:220:VAL:HG21	2.34	0.62
19:R:6:GLY:HA2	19:R:23:VAL:HG22	1.81	0.62
2:Y:64:A:N6	2:Y:104:C:H2'	2.15	0.62
1:X:1212:U:H3	1:X:1220:A:H61	1.46	0.62
1:X:460:C:H2'	1:X:461:A:C8	2.35	0.62
1:X:1563:U:H2'	1:X:1564:G:C8	2.35	0.62
27:X:3001:TEL:H242	27:X:3001:TEL:H3	1.81	0.62
1:X:1952:C:H4'	1:X:1953:U:OP1	2.00	0.61
1:X:2618:C:H2'	1:X:2619:G:C8	2.35	0.61
1:X:367:A:N6	1:X:381:G:O2'	2.33	0.61
5:C:78:ILE:HD12	5:C:79:ARG:HG2	1.82	0.61
11:J:90:VAL:HG12	11:J:91:GLU:H	1.65	0.61
3:A:78:VAL:HA	3:A:94:VAL:HG12	1.83	0.61
5:C:158:ASN:HA	5:C:161:VAL:HG22	1.81	0.61
1:X:1806:U:H5	1:X:1811:A:N7	1.98	0.61
2:Y:15:C:H42	2:Y:105:G:H21	1.49	0.61
1:X:1065:A:H62	1:X:1185:U:H3	1.49	0.61
1:X:2314:A:O2'	1:X:2315:A:O5'	2.17	0.61
1:X:323:C:H5'	1:X:324:A:OP2	2.01	0.61
3:A:91:ILE:HG22	3:A:105:ILE:HA	1.82	0.61
12:K:104:LEU:HB2	12:K:118:ILE:HG22	1.83	0.61
13:L:73:ALA:HB1	13:L:107:ALA:HB2	1.83	0.61
1:X:1089:C:O2	1:X:1091:G:N1	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1465:G:H2'	1:X:1466:G:H8	1.66	0.61
1:X:1492:G:N2	1:X:1508:C:N3	2.48	0.60
1:X:1512:U:H2'	1:X:1513:A:H8	1.66	0.60
8:G:18:VAL:HG22	8:G:138:PRO:HB2	1.83	0.60
20:S:157:ALA:HB3	20:S:159:VAL:HG23	1.82	0.60
1:X:1514:A:N6	1:X:1566:G:H1	2.00	0.60
11:J:30:GLY:O	11:J:134:ARG:NH2	2.34	0.60
27:X:3001:TEL:C38	27:X:3001:TEL:H221	2.32	0.60
1:X:1977:G:O6	31:X:3364:SPD:N6	2.35	0.60
3:A:86:ASN:OD1	3:A:86:ASN:N	2.34	0.60
4:B:9:LYS:HD3	4:B:203:GLY:O	2.02	0.60
10:I:112:LEU:H	10:I:112:LEU:HD23	1.66	0.60
1:X:2120:G:H21	1:X:2225:A:H62	1.49	0.60
1:X:2120:G:N3	1:X:2225:A:N6	2.50	0.60
4:B:2:THR:OG1	4:B:93:ASN:O	2.17	0.60
12:K:80:THR:HG22	12:K:82:LEU:H	1.66	0.60
27:X:3001:TEL:C15	27:X:3001:TEL:H222	2.32	0.60
4:B:141:MET:N	4:B:141:MET:SD	2.75	0.60
12:K:59:ARG:HA	12:K:86:PHE:CZ	2.37	0.60
1:X:1250:G:H21	1:X:1275:A:H2	1.49	0.60
1:X:1472:C:N4	1:X:1617:A:OP2	2.29	0.60
1:X:2707:C:H5'	4:B:202:PRO:HA	1.84	0.60
1:X:735:C:O2'	1:X:825:G:OP1	2.20	0.60
16:O:3:ALA:HB2	16:O:14:VAL:HG22	1.84	0.60
18:Q:10:PRO:HA	18:Q:27:PHE:HB3	1.83	0.60
1:X:1862:G:H1	1:X:1957:G:N2	1.96	0.59
1:X:505:U:H2'	1:X:506:A:H5"	1.83	0.59
1:X:895:U:O2'	23:W:22:THR:OG1	2.16	0.59
1:X:2007:G:O2'	1:X:2009:U:OP2	2.19	0.59
3:A:145:GLU:HA	3:A:152:GLY:HA2	1.84	0.59
2:Y:21:G:H22	2:Y:58:G:N2	2.01	0.59
1:X:1450:A:H61	1:X:1635:A:H62	1.51	0.59
27:X:3001:TEL:C24	27:X:3001:TEL:H3	2.33	0.59
1:X:2835:C:H1'	24:Z:39:LEU:HD23	1.83	0.59
3:A:89:ALA:HB1	3:A:196:GLY:HA3	1.84	0.59
5:C:177:THR:O	5:C:181:LEU:HB2	2.03	0.59
5:C:77:THR:HG22	5:C:79:ARG:H	1.68	0.59
8:G:33:VAL:HG13	8:G:55:VAL:HG11	1.84	0.59
12:K:27:SER:O	12:K:29:ARG:N	2.34	0.59
1:X:923:A:N6	1:X:926:G:N7	2.50	0.59
1:X:2313:A:H4'	1:X:2314:A:O4'	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:283:G:N2	1:X:289:U:O2	2.35	0.59
1:X:2082:C:C4	28:X:3005:MPD:HM2	2.36	0.59
2:Y:79:C:N4	2:Y:92:G:H1	1.98	0.59
4:B:201:VAL:HG12	4:B:202:PRO:HD2	1.85	0.59
12:K:80:THR:HB	12:K:83:GLN:HG3	1.84	0.59
1:X:404:U:O2'	1:X:405:G:O5'	2.19	0.59
4:B:64:LYS:H	4:B:64:LYS:HD2	1.68	0.59
4:B:38:LYS:HD2	4:B:96:VAL:O	2.02	0.59
9:H:63:VAL:HG12	9:H:106:LEU:HD11	1.83	0.59
16:O:16:GLU:HA	16:O:97:ILE:HB	1.83	0.59
1:X:1261:G:OP1	16:O:67:ARG:NH2	2.35	0.59
1:X:1091:G:H8	1:X:1091:G:H5"	1.68	0.58
1:X:787:U:H2'	1:X:788:A:C8	2.38	0.58
2:Y:78:C:H2'	2:Y:79:C:H5	1.68	0.58
1:X:1490:G:O2'	1:X:1491:C:O5'	2.14	0.58
10:I:28:GLY:H	10:I:30:THR:H	1.52	0.58
1:X:319:G:N7	1:X:400:C:N4	2.51	0.58
1:X:658:A:H3'	1:X:659:A:C5'	2.33	0.58
10:I:70:ASN:O	10:I:72:LYS:N	2.28	0.58
11:J:64:VAL:HG12	11:J:106:VAL:HG12	1.84	0.58
1:X:1724:U:N3	1:X:1791:G:OP2	2.34	0.58
1:X:499:A:N3	1:X:503:A:O2'	2.37	0.58
14:M:29:ARG:HD2	14:M:89:LYS:HZ3	1.68	0.58
1:X:1521:A:N1	1:X:1559:G:N2	2.52	0.58
7:E:109:TYR:O	7:E:111:HIS:N	2.34	0.58
1:X:132:C:N3	1:X:147:G:N2	2.47	0.58
1:X:83:G:H1	1:X:101:G:HO2'	1.48	0.58
1:X:1346:G:H4'	25:2:8:PRO:HG2	1.85	0.58
1:X:683:G:H2'	1:X:684:U:H6	1.68	0.58
1:X:946:A:O2'	1:X:947:U:O4'	2.21	0.58
12:K:109:ARG:HD3	12:K:112:ASP:OD1	2.04	0.58
1:X:1099:G:H1	1:X:1148:C:H42	1.49	0.58
1:X:437:A:O2'	1:X:456:G:OP1	2.13	0.58
1:X:498:G:H21	1:X:503:A:H8	1.52	0.58
1:X:683:G:H2'	1:X:684:U:C6	2.39	0.58
3:A:107:PRO:HA	3:A:195:VAL:HA	1.86	0.57
1:X:506:A:H2	1:X:515:G:H21	1.52	0.57
16:O:3:ALA:HB3	16:O:14:VAL:H	1.68	0.57
1:X:1494:G:C8	1:X:1495:C:H5	2.21	0.57
20:S:155:THR:OG1	20:S:155:THR:O	2.22	0.57
1:X:1452:C:O2	1:X:1631:G:N2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2558:A:H5"	7:E:157:TYR:CZ	2.39	0.57
1:X:422:G:H1	1:X:444:C:H42	1.52	0.57
1:X:1911:A:HO2'	1:X:1912:A:H8	1.51	0.57
1:X:2495:A:O2'	1:X:2496:A:H8	1.86	0.57
3:A:62:TYR:HA	3:A:86:ASN:HD21	1.69	0.57
1:X:450:C:H4'	1:X:451:U:H5'	1.86	0.57
25:2:16:VAL:H	25:2:21:LYS:HG3	1.69	0.57
5:C:149:PRO:HD2	5:C:187:THR:HA	1.86	0.57
1:X:817:G:H2'	1:X:818:U:H6	1.70	0.57
2:Y:74:G:H22	2:Y:97:A:H61	1.51	0.57
5:C:173:VAL:HG11	5:C:196:GLU:HG2	1.87	0.57
9:H:77:ILE:HG13	14:M:74:ARG:HG3	1.85	0.57
21:T:46:TYR:CZ	21:T:53:ILE:HD13	2.39	0.57
1:X:1185:U:OP2	8:G:66:THR:OG1	2.19	0.57
1:X:1185:U:H4'	1:X:1186:A:O4'	2.04	0.57
1:X:460:C:H2'	1:X:461:A:H8	1.68	0.57
1:X:1575:A:H2'	1:X:1576:A:C5'	2.34	0.57
19:R:5:LYS:O	19:R:7:ASP:N	2.38	0.57
1:X:1305:U:C5	1:X:2040:A:N7	2.73	0.57
2:Y:15:C:N4	2:Y:105:G:H21	2.02	0.57
1:X:124:A:H5'	25:2:20:ARG:HD3	1.87	0.56
7:E:104:ILE:N	7:E:113:VAL:O	2.38	0.56
1:X:100:U:H3'	1:X:101:G:H5'	1.86	0.56
1:X:2322:C:N4	13:L:17:ARG:HH22	2.02	0.56
1:X:2602:C:H5'	4:B:157:ALA:HB2	1.85	0.56
12:K:5:LYS:HB2	12:K:39:GLU:OE2	2.05	0.56
1:X:179:A:OP2	1:X:179:A:H8	1.88	0.56
1:X:1498:U:HO2'	1:X:1499:U:H5	1.54	0.56
1:X:1901:C:O2'	1:X:1902:G:O5'	2.19	0.56
1:X:1975:G:H1	1:X:1985:C:H42	1.54	0.56
1:X:2047:A:H5'	24:Z:9:SER:HB3	1.86	0.56
26:3:55:MET:HA	26:3:58:VAL:HG23	1.87	0.56
4:B:26:THR:HG21	4:B:201:VAL:HG23	1.87	0.56
9:H:20:LEU:HB3	9:H:42:THR:HG22	1.86	0.56
12:K:45:GLU:OE1	12:K:100:TYR:N	2.38	0.56
1:X:1528:G:H1	1:X:1547:C:H42	1.53	0.56
1:X:661:U:O2'	1:X:662:G:OP2	2.22	0.56
4:B:208:LEU:HD22	4:B:209:VAL:H	1.70	0.56
5:C:123:LEU:HD12	5:C:188:ASN:HB3	1.86	0.56
15:N:66:ASN:HA	15:N:76:TYR:HB2	1.86	0.56
1:X:2239:A:N7	1:X:2241:C:N4	2.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1302:G:OP1	24:Z:16:ARG:NH2	2.38	0.56
9:H:63:VAL:HB	9:H:102:VAL:HG22	1.87	0.56
12:K:79:GLN:NE2	12:K:88:GLU:OE1	2.25	0.56
5:C:102:PRO:HB2	5:C:105:MET:HG3	1.88	0.56
6:D:111:VAL:H	6:D:170:LEU:H	1.54	0.56
2:Y:87:G:H8	11:J:19:GLY:HA3	1.71	0.56
4:B:48:ALA:HB2	4:B:92:ARG:HG3	1.87	0.56
7:E:133:VAL:HG21	7:E:141:VAL:HG22	1.86	0.56
7:E:103:LEU:H	7:E:114:GLU:HA	1.71	0.56
7:E:133:VAL:HG11	7:E:141:VAL:HG13	1.87	0.56
1:X:1395:G:O2'	1:X:1410:A:N6	2.38	0.56
1:X:1315:C:OP1	12:K:32:THR:HG23	2.06	0.56
2:Y:1:U:O2'	2:Y:2:C:OP2	2.23	0.56
17:P:65:ASN:OD1	17:P:65:ASN:N	2.38	0.56
19:R:7:ASP:OD1	19:R:8:ASN:N	2.39	0.56
1:X:2856:U:H2'	1:X:2857:A:C8	2.41	0.56
4:B:121:VAL:O	4:B:122:SER:HB3	2.05	0.55
4:B:95:ASP:O	4:B:97:ASP:N	2.38	0.55
1:X:38:A:H1'	5:C:48:THR:O	2.07	0.55
1:X:341:G:H5'	1:X:342:A:OP1	2.05	0.55
1:X:785:C:H5'	1:X:1811:A:H3'	1.88	0.55
1:X:1511:C:H5'	1:X:1512:U:OP1	2.06	0.55
1:X:2581:U:H2'	1:X:2582:U:C6	2.41	0.55
1:X:658:A:H3'	1:X:659:A:H5"	1.89	0.55
1:X:1423:C:H2'	1:X:1424:A:C8	2.41	0.55
1:X:1730:C:H42	1:X:1746:G:H1	1.55	0.55
4:B:67:LYS:HA	4:B:86:ARG:NH2	2.21	0.55
5:C:103:LYS:HA	5:C:106:ARG:NE	2.21	0.55
11:J:110:SER:HB3	11:J:113:VAL:HB	1.87	0.55
25:2:43:LEU:HD23	25:2:44:SER:H	1.71	0.55
23:W:19:GLN:O	23:W:23:VAL:HG23	2.06	0.55
1:X:150:A:H61	1:X:179:A:H2	1.54	0.55
5:C:57:VAL:HB	5:C:79:ARG:HD2	1.88	0.55
9:H:44:LYS:O	9:H:54:LYS:NZ	2.37	0.55
17:P:23:LEU:HD11	24:Z:22:ILE:HD11	1.89	0.55
19:R:9:VAL:HG22	19:R:23:VAL:HG12	1.89	0.55
1:X:2331:G:H22	1:X:2339:U:H3	1.55	0.55
1:X:970:U:H3'	1:X:971:U:H5'	1.88	0.55
4:B:194:VAL:HG12	4:B:195:ILE:H	1.72	0.55
1:X:1092:A:HO2'	1:X:1093:C:H6	1.55	0.55
1:X:1247:G:O2'	1:X:1275:A:N6	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1463:A:H3'	1:X:1464:U:H5"	1.89	0.55
1:X:2026:C:H5"	1:X:2750:C:O2'	2.07	0.55
1:X:2294:A:H5"	1:X:2295:A:H5'	1.88	0.55
1:X:2772:C:O2'	7:E:142:GLY:HA3	2.06	0.55
10:I:70:ASN:C	10:I:72:LYS:H	2.10	0.55
12:K:47:LEU:HB3	12:K:85:LEU:HD21	1.89	0.55
1:X:1013:U:O3'	23:W:14:GLY:HA2	2.06	0.55
1:X:132:C:N4	1:X:147:G:H1	2.04	0.55
25:2:9:ASN:ND2	25:2:12:LYS:HB2	2.22	0.54
3:A:142:HIS:ND1	3:A:143:ASN:HB2	2.22	0.54
1:X:1289:A:OP1	15:N:13:ARG:NH1	2.40	0.54
16:O:2:PHE:CD2	16:O:42:GLY:HA3	2.42	0.54
1:X:1017:A:OP1	1:X:1017:A:H8	1.90	0.54
1:X:1793:C:H2'	1:X:1794:C:H6	1.72	0.54
1:X:1598:U:H4'	1:X:1768:C:H1'	1.88	0.54
1:X:2060:A:O2'	1:X:2062:G:OP2	2.25	0.54
1:X:2612:U:H5'	1:X:2613:C:OP1	2.07	0.54
1:X:549:U:C6	1:X:549:U:H5"	2.41	0.54
18:Q:51:ALA:HB2	18:Q:83:LYS:N	2.22	0.54
19:R:59:THR:HG1	19:R:60:GLU:H	1.53	0.54
5:C:49:HIS:O	5:C:49:HIS:ND1	2.36	0.54
1:X:2241:C:H2'	1:X:2242:G:O4'	2.07	0.54
3:A:142:HIS:CE1	3:A:143:ASN:HB2	2.43	0.54
1:X:323:C:H3'	1:X:324:A:C8	2.43	0.54
1:X:665:G:H4'	1:X:666:A:C5'	2.38	0.54
4:B:124:GLY:HA2	4:B:174:GLY:HA3	1.90	0.54
12:K:55:ASP:OD1	12:K:55:ASP:N	2.33	0.54
14:M:29:ARG:HB2	14:M:87:GLU:HB2	1.90	0.54
15:N:58:ARG:HA	15:N:61:TRP:CE3	2.43	0.54
15:N:91:ASN:OD1	15:N:92:ARG:N	2.40	0.54
16:O:62:VAL:HG22	16:O:95:LEU:HD23	1.90	0.54
1:X:2842:G:H2'	1:X:2843:A:H5"	1.90	0.54
4:B:73:ALA:O	4:B:75:GLY:N	2.38	0.54
22:V:45:THR:O	22:V:49:THR:HG23	2.08	0.54
10:I:116:SER:OG	10:I:117:LEU:N	2.40	0.53
18:Q:34:ASN:O	18:Q:38:VAL:HG23	2.07	0.53
1:X:788:A:O2'	1:X:1703:U:OP1	2.24	0.53
1:X:1766:C:H2'	1:X:1767:G:H5'	1.90	0.53
27:X:3001:TEL:H381	27:X:3001:TEL:H221	1.90	0.53
1:X:2807:G:N1	8:G:103:GLU:OE1	2.35	0.53
9:H:13:ASN:OD1	9:H:96:THR:N	2.35	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:109:ASP:OD1	17:P:109:ASP:N	2.40	0.53
1:X:1496:G:N7	1:X:1502:A:N1	2.56	0.53
3:A:89:ALA:HB2	3:A:158:ALA:HA	1.90	0.53
4:B:131:ILE:HD11	4:B:149:ARG:CZ	2.38	0.53
5:C:7:LEU:HG	5:C:124:THR:HG23	1.90	0.53
1:X:1353:A:H2'	1:X:1354:G:C8	2.43	0.53
1:X:1602:U:O2'	1:X:1603:U:OP1	2.15	0.53
1:X:2446:U:H2'	1:X:2447:C:C6	2.43	0.53
8:G:2:ARG:HG3	8:G:3:GLN:HG2	1.90	0.53
9:H:64:ARG:NH1	9:H:101:PRO:O	2.32	0.53
1:X:378:C:H2'	1:X:379:C:H6	1.73	0.53
7:E:109:TYR:C	7:E:111:HIS:H	2.12	0.53
12:K:115:GLU:OE2	24:Z:41:HIS:NE2	2.41	0.53
1:X:1895:C:H42	1:X:1901:C:H42	1.55	0.53
1:X:2079:G:H4'	4:B:156:MET:O	2.09	0.53
14:M:97:ALA:O	14:M:99:LEU:N	2.42	0.53
1:X:267:G:H2'	1:X:268:A:H5"	1.90	0.53
1:X:1395:G:OP2	1:X:1395:G:N2	2.37	0.53
2:Y:91:C:H2'	2:Y:92:G:C8	2.43	0.53
7:E:22:ASN:H	7:E:29:PRO:HG2	1.74	0.53
1:X:1086:G:HO2'	1:X:1087:C:H6	1.54	0.53
5:C:152:VAL:HG21	5:C:156:THR:H	1.74	0.53
16:O:12:ILE:HG22	16:O:14:VAL:HG12	1.90	0.53
1:X:1522:G:H1	1:X:1558:U:H3	1.56	0.53
1:X:1845:U:OP2	3:A:156:ARG:HD2	2.07	0.53
1:X:631:U:H2'	1:X:632:U:C6	2.44	0.53
9:H:80:ASP:OD2	14:M:64:ARG:NH2	2.42	0.53
1:X:986:G:H5"	10:I:32:GLY:HA2	1.91	0.53
18:Q:58:TYR:HB2	18:Q:75:ARG:HG2	1.90	0.53
1:X:1040:A:H4'	15:N:91:ASN:ND2	2.22	0.53
1:X:817:G:H2'	1:X:818:U:C6	2.44	0.53
2:Y:21:G:N2	2:Y:58:G:H22	2.04	0.53
1:X:1013:U:OP1	23:W:17:GLU:HG2	2.08	0.52
1:X:156:A:H61	1:X:172:U:H3	1.57	0.52
1:X:514:G:H21	28:X:3008:MPD:H53	1.74	0.52
1:X:1313:G:OP2	1:X:1689:G:O2'	2.22	0.52
3:A:230:HIS:CD2	3:A:249:PRO:HG3	2.44	0.52
5:C:178:ALA:O	5:C:182:ASN:ND2	2.35	0.52
8:G:68:ASN:N	8:G:68:ASN:OD1	2.43	0.52
1:X:1072:A:N6	1:X:1169:G:H2'	2.24	0.52
1:X:679:G:H2'	1:X:680:C:C6	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:19:VAL:HG12	9:H:43:VAL:HA	1.91	0.52
16:O:20:ILE:HD13	16:O:97:ILE:HD11	1.91	0.52
20:S:14:THR:HA	20:S:18:LEU:HD12	1.92	0.52
1:X:1415:A:O2'	1:X:1417:G:N7	2.32	0.52
1:X:2457:A:H2'	1:X:2457:A:N3	2.23	0.52
1:X:2549:U:O2'	1:X:2674:U:OP1	2.18	0.52
1:X:656:G:N2	1:X:661:U:O4	2.43	0.52
4:B:131:ILE:HD11	4:B:149:ARG:NH2	2.25	0.52
21:T:71:ILE:HG12	21:T:72:ASP:N	2.23	0.52
1:X:2370:U:H2'	1:X:2371:U:C6	2.44	0.52
24:Z:29:GLU:HA	24:Z:36:GLU:HG2	1.90	0.52
10:I:96:LEU:HD12	10:I:97:VAL:N	2.25	0.52
14:M:50:ILE:HG22	14:M:98:LYS:O	2.09	0.52
22:V:10:THR:OG1	22:V:11:THR:N	2.38	0.52
1:X:637:U:H2'	1:X:638:U:H6	1.75	0.52
1:X:1091:G:HO2'	1:X:1092:A:P	2.33	0.52
1:X:2043:U:H2'	1:X:2044:C:C6	2.44	0.52
1:X:2311:U:H3	1:X:2411:A:N6	2.07	0.52
1:X:318:A:C6	1:X:319:G:H1'	2.45	0.52
5:C:125:VAL:HG12	5:C:190:ASP:HA	1.92	0.52
1:X:1796:A:O2'	1:X:1985:C:OP1	2.26	0.52
1:X:2101:U:H2'	1:X:2102:U:C6	2.44	0.52
12:K:55:ASP:OD1	12:K:58:SER:OG	2.24	0.52
14:M:31:HIS:HD2	14:M:85:LYS:HD2	1.75	0.52
14:M:28:LEU:O	14:M:46:GLU:HA	2.10	0.52
1:X:2037:G:OP2	17:P:41:LYS:HE3	2.09	0.52
1:X:2419:A:H2	1:X:2451:C:H42	1.56	0.52
2:Y:78:C:H2'	2:Y:79:C:C5	2.44	0.52
3:A:210:ARG:HA	3:A:213:TRP:CE3	2.45	0.52
3:A:72:ASP:HA	3:A:118:SER:CB	2.40	0.52
14:M:80:THR:HG22	14:M:82:LYS:H	1.74	0.52
1:X:1207:G:OP1	16:O:24:LYS:NZ	2.42	0.52
1:X:2642:U:H1'	24:Z:4:PRO:HB3	1.92	0.52
1:X:1817:C:H2'	1:X:1818:A:C5	2.45	0.51
1:X:1823:U:H2'	1:X:1824:C:C6	2.45	0.51
1:X:2314:A:O2'	1:X:2315:A:H2'	2.10	0.51
1:X:2784:A:N1	7:E:67:THR:HG21	2.25	0.51
1:X:498:G:N2	1:X:503:A:H8	2.07	0.51
24:Z:39:LEU:O	24:Z:41:HIS:ND1	2.33	0.51
1:X:2077:C:H1'	4:B:169:MET:HE1	1.93	0.51
5:C:152:VAL:HG23	5:C:154:VAL:H	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:85:PHE:HD1	17:P:85:PHE:H	1.57	0.51
1:X:1300:G:OP2	17:P:99:ARG:NH2	2.40	0.51
20:S:10:GLN:NE2	20:S:41:VAL:O	2.44	0.51
6:D:64:LYS:HA	6:D:83:MET:HA	1.92	0.51
12:K:91:GLU:N	12:K:91:GLU:OE2	2.41	0.51
1:X:1526:G:N3	1:X:1526:G:H2'	2.25	0.51
3:A:78:VAL:HB	3:A:113:GLY:HA2	1.93	0.51
1:X:1023:A:H2'	1:X:1026:C:H42	1.75	0.51
1:X:1463:A:H2	1:X:1625:U:N3	2.09	0.51
5:C:124:THR:HA	5:C:189:ALA:O	2.10	0.51
1:X:1568:U:O2'	1:X:1569:G:OP2	2.29	0.51
1:X:1834:G:H21	1:X:1836:A:H3'	1.76	0.51
1:X:873:U:H4'	1:X:876:G:N1	2.25	0.51
11:J:59:LYS:O	11:J:61:GLY:N	2.43	0.51
1:X:1410:A:H2'	1:X:1411:G:O4'	2.10	0.51
1:X:1962:G:H1'	1:X:1991:G:N2	2.26	0.51
1:X:329:A:N6	1:X:398:C:H42	2.08	0.51
20:S:77:TYR:CZ	31:S:301:SPD:H91	2.46	0.51
1:X:1280:U:H2'	1:X:1281:U:C6	2.46	0.51
1:X:1506:C:C4	1:X:1507:A:C6	2.99	0.51
1:X:17:G:OP1	24:Z:11:THR:HG22	2.11	0.51
2:Y:67:G:H2'	2:Y:68:A:H8	1.75	0.51
13:L:44:ILE:O	13:L:53:LEU:N	2.41	0.51
1:X:1488:A:N1	1:X:1490:G:N1	2.58	0.51
1:X:2488:C:H2'	1:X:2489:U:C6	2.46	0.51
1:X:634:C:HO2'	26:3:2:PRO:N	2.09	0.51
1:X:713:A:H2'	1:X:715:A:N6	2.26	0.51
1:X:858:U:H2'	1:X:859:C:C6	2.46	0.51
4:B:111:VAL:O	4:B:114:ASP:HB2	2.11	0.50
5:C:136:THR:O	5:C:140:LYS:HD2	2.11	0.50
14:M:31:HIS:HB2	14:M:85:LYS:HB2	1.93	0.50
20:S:117:GLU:O	20:S:119:GLY:N	2.42	0.50
1:X:2051:C:H2'	1:X:2052:C:H6	1.76	0.50
1:X:2687:A:H2'	1:X:2688:G:O4'	2.11	0.50
7:E:38:ASN:N	7:E:38:ASN:OD1	2.43	0.50
9:H:24:VAL:CG1	9:H:33:ALA:HB2	2.40	0.50
9:H:64:ARG:HB2	9:H:83:ALA:HB3	1.93	0.50
18:Q:51:ALA:HB3	18:Q:81:THR:O	2.10	0.50
1:X:1275:A:OP1	31:X:3365:SPD:N1	2.44	0.50
1:X:1542:C:H3'	1:X:1543:G:H5"	1.93	0.50
1:X:684:U:H2'	1:X:685:C:C6	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:877:G:OP1	10:I:36:LYS:HB2	2.12	0.50
1:X:907:G:H2'	1:X:908:A:O4'	2.11	0.50
8:G:71:THR:O	8:G:73:LYS:N	2.42	0.50
15:N:38:GLN:O	15:N:42:SER:HB2	2.11	0.50
1:X:342:A:N1	1:X:365:A:O2'	2.35	0.50
9:H:88:ARG:O	9:H:90:ASP:N	2.44	0.50
1:X:1834:G:N2	1:X:1836:A:H3'	2.25	0.50
1:X:579:U:H5'	15:N:42:SER:OG	2.11	0.50
1:X:1513:A:H3'	1:X:1514:A:C8	2.37	0.50
4:B:194:VAL:HG12	4:B:195:ILE:N	2.26	0.50
1:X:1065:A:H3'	1:X:1065:A:C8	2.47	0.50
1:X:1241:A:H2'	1:X:1242:A:C8	2.47	0.50
1:X:1450:A:N6	1:X:1635:A:H62	2.09	0.50
1:X:1630:A:C2	1:X:1631:G:H2'	2.46	0.50
1:X:235:G:HO2'	1:X:236:A:P	2.34	0.50
1:X:811:C:N4	1:X:812:U:O4	2.44	0.50
1:X:956:A:H2'	11:J:11:ARG:NH2	2.27	0.50
16:O:70:LYS:HA	16:O:89:ARG:HG2	1.94	0.50
1:X:2116:U:H2'	1:X:2117:A:C8	2.46	0.50
8:G:93:LEU:HD12	8:G:93:LEU:N	2.27	0.50
9:H:112:MET:HA	9:H:115:VAL:HG12	1.94	0.50
1:X:1695:G:OP1	12:K:33:THR:HG21	2.11	0.50
18:Q:14:GLU:OE1	18:Q:14:GLU:N	2.43	0.50
20:S:107:GLN:HA	20:S:138:PRO:HD2	1.93	0.50
1:X:1708:A:H61	1:X:2023:C:H42	1.60	0.50
1:X:2354:A:H2'	1:X:2355:A:C8	2.47	0.50
1:X:268:A:O2'	1:X:269:G:H4'	2.12	0.50
16:O:42:GLY:HA2	16:O:46:VAL:HG12	1.94	0.49
20:S:32:TYR:HE1	20:S:90:ASP:HB3	1.77	0.49
1:X:1530:A:N1	1:X:1546:A:N6	2.60	0.49
1:X:278:A:H2'	1:X:279:A:C8	2.47	0.49
1:X:65:A:H1'	1:X:502:C:N4	2.27	0.49
1:X:974:U:H2'	1:X:975:U:O4'	2.12	0.49
10:I:15:GLU:OE1	10:I:15:GLU:N	2.45	0.49
11:J:27:VAL:HG12	11:J:105:GLU:OE2	2.13	0.49
17:P:8:ARG:HG2	17:P:102:HIS:CG	2.47	0.49
1:X:2047:A:P	24:Z:7:ARG:HH11	2.34	0.49
1:X:2355:A:H2'	1:X:2356:A:C8	2.48	0.49
1:X:2872:G:H2'	1:X:2873:C:O4'	2.12	0.49
1:X:460:C:O2	1:X:1891:U:O2'	2.27	0.49
1:X:638:U:H2'	1:X:639:U:C6	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:810:A:H2'	1:X:811:C:C6	2.47	0.49
3:A:105:ILE:O	3:A:107:PRO:HD3	2.12	0.49
9:H:102:VAL:HG13	9:H:106:LEU:HD12	1.95	0.49
1:X:706:U:H1'	10:I:13:ARG:HA	1.93	0.49
1:X:1843:U:H3'	1:X:1843:U:C6	2.45	0.49
1:X:2883:U:H2'	1:X:2884:G:H8	1.77	0.49
5:C:39:LEU:HD12	5:C:39:LEU:O	2.13	0.49
16:O:7:THR:OG1	16:O:22:VAL:HG21	2.12	0.49
1:X:2877:G:H5'	1:X:2878:U:OP2	2.11	0.49
1:X:302:A:HO2'	1:X:303:G:H8	1.60	0.49
1:X:349:U:H2'	1:X:350:G:O4'	2.13	0.49
4:B:133:ARG:HD2	4:B:173:MET:HB3	1.95	0.49
5:C:145:THR:HG22	5:C:146:LEU:H	1.76	0.49
8:G:77:ARG:N	8:G:87:SER:HA	2.28	0.49
1:X:1336:G:N1	1:X:1684:A:OP2	2.34	0.49
1:X:592:A:O2'	1:X:593:U:O5'	2.30	0.49
4:B:119:THR:HG23	4:B:179:THR:HG22	1.95	0.49
7:E:109:TYR:O	7:E:111:HIS:ND1	2.46	0.49
1:X:1482:U:H2'	1:X:1483:A:H8	1.77	0.49
1:X:1658:A:H61	17:P:88:ARG:H	1.59	0.49
1:X:1769:C:N4	1:X:1770:C:H41	2.10	0.49
1:X:2288:C:H1'	1:X:2415:A:N3	2.28	0.49
1:X:923:A:HO2'	1:X:924:G:H8	1.59	0.49
7:E:95:ARG:CB	7:E:104:ILE:HA	2.43	0.49
8:G:126:TYR:OH	8:G:133:HIS:NE2	2.44	0.49
1:X:1071:A:C6	1:X:1170:A:C4	3.01	0.49
1:X:1308:C:H5"	1:X:1309:G:O5'	2.13	0.49
1:X:1874:A:O2'	1:X:1875:A:N7	2.45	0.49
9:H:19:VAL:HB	9:H:41:CYS:SG	2.53	0.49
17:P:2:GLU:HG3	17:P:109:ASP:H	1.76	0.49
19:R:11:VAL:HG11	19:R:16:ASP:O	2.13	0.49
1:X:1289:A:H5"	15:N:13:ARG:HH12	1.77	0.49
1:X:1854:U:OP2	3:A:221:ARG:NH1	2.45	0.49
1:X:2682:G:O2'	1:X:2683:U:H5	1.96	0.49
1:X:660:A:H1'	1:X:661:U:O5'	2.11	0.49
2:Y:87:G:C8	11:J:19:GLY:HA3	2.48	0.49
4:B:205:LYS:O	4:B:206:LYS:HB2	2.13	0.49
2:Y:3:U:H3	2:Y:112:G:H1	1.61	0.49
4:B:53:PHE:CG	4:B:54:GLU:N	2.81	0.49
12:K:41:ARG:HB2	12:K:101:THR:HG21	1.95	0.49
1:X:1597:U:H2'	1:X:1598:U:O4'	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:37:C:H2'	1:X:38:A:C8	2.48	0.49
1:X:38:A:H2'	1:X:39:C:O4'	2.12	0.49
26:3:15:LYS:HD2	26:3:60:GLN:O	2.13	0.48
11:J:74:TYR:CE2	11:J:92:GLY:HA3	2.48	0.48
18:Q:67:ARG:HH11	18:Q:68:TYR:HE1	1.61	0.48
1:X:1377:U:OP2	18:Q:58:TYR:OH	2.30	0.48
1:X:1629:U:C2'	1:X:1630:A:H5'	2.42	0.48
1:X:1854:U:H2'	1:X:1855:G:O4'	2.13	0.48
1:X:1869:G:H2'	1:X:1870:C:C6	2.47	0.48
27:X:3001:TEL:C37	27:X:3001:TEL:H21	2.43	0.48
1:X:378:C:H2'	1:X:379:C:C6	2.47	0.48
1:X:505:U:C2'	1:X:506:A:H5"	2.43	0.48
17:P:36:LEU:HD11	17:P:47:ILE:HG22	1.95	0.48
1:X:1669:C:H2'	1:X:1670:A:O4'	2.13	0.48
1:X:363:A:H4'	1:X:365:A:N7	2.28	0.48
7:E:85:LYS:H	7:E:133:VAL:HG12	1.77	0.48
1:X:1206:G:N3	16:O:90:GLN:NE2	2.56	0.48
1:X:1462:G:H8	1:X:1626:A:H62	1.61	0.48
1:X:1700:C:H2'	1:X:1701:U:C6	2.49	0.48
1:X:989:A:C4	1:X:2475:A:C2	3.02	0.48
1:X:2717:A:OP1	12:K:4:ARG:NH2	2.35	0.48
1:X:484:U:H2'	1:X:485:A:C8	2.48	0.48
1:X:2646:U:H5'	4:B:163:VAL:O	2.14	0.48
19:R:11:VAL:HG12	19:R:19:LYS:O	2.13	0.48
1:X:2358:G:P	21:T:52:LYS:HZ3	2.36	0.48
1:X:373:A:H2	1:X:1248:U:HO2'	1.56	0.48
3:A:91:ILE:HD12	3:A:103:TYR:CD1	2.48	0.48
1:X:1289:A:OP1	15:N:10:THR:HG22	2.13	0.48
23:W:26:LEU:HG	23:W:46:GLN:HG2	1.94	0.48
1:X:2351:U:H3	1:X:2358:G:H1	1.61	0.48
1:X:2410:G:H8	1:X:2410:G:H5'	1.78	0.48
1:X:901:G:H2'	1:X:902:A:C8	2.49	0.48
4:B:208:LEU:HD22	4:B:209:VAL:N	2.28	0.48
10:I:21:ARG:HA	10:I:21:ARG:HD3	1.55	0.48
12:K:24:LEU:HD21	12:K:44:VAL:HG21	1.94	0.48
1:X:200:A:N6	1:X:2457:A:O2'	2.46	0.48
5:C:65:TRP:CZ2	5:C:75:GLN:HG3	2.48	0.48
1:X:967:C:O2'	21:T:34:ALA:HB2	2.13	0.48
1:X:2843:A:OP1	4:B:127:PHE:HB2	2.14	0.48
8:G:115:LEU:O	8:G:119:GLN:HG3	2.13	0.48
18:Q:16:SER:HB2	18:Q:26:THR:OG1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1522:G:H2'	1:X:1523:G:H8	1.79	0.48
1:X:2675:G:H2'	1:X:2676:U:C6	2.49	0.48
1:X:715:A:H4'	1:X:716:C:C5'	2.44	0.48
3:A:38:PRO:HD3	3:A:62:TYR:H	1.79	0.48
4:B:44:ASP:N	4:B:44:ASP:OD1	2.47	0.48
8:G:136:GLN:OE1	8:G:136:GLN:N	2.47	0.48
15:N:61:TRP:O	15:N:65:ILE:HG12	2.14	0.48
1:X:1770:C:O2'	1:X:1771:A:H5'	2.14	0.48
1:X:319:G:H3'	1:X:320:U:H5'	1.95	0.48
1:X:506:A:H3'	1:X:507:C:H6	1.79	0.48
1:X:613:G:H2'	1:X:2057:A:N7	2.28	0.48
2:Y:47:C:OP1	13:L:99:TYR:N	2.46	0.48
1:X:1014:U:OP1	23:W:20:ARG:NH2	2.47	0.48
1:X:2109:A:H2'	1:X:2110:G:O4'	2.14	0.48
1:X:273:A:OP2	1:X:297:G:N2	2.44	0.48
1:X:2864:A:H2'	1:X:2865:G:O4'	2.14	0.48
25:2:31:VAL:O	25:2:35:ARG:HG3	2.14	0.47
4:B:53:PHE:HB3	4:B:87:PHE:HB2	1.96	0.47
16:O:15:GLU:O	16:O:16:GLU:HB3	2.15	0.47
1:X:1601:U:O2	1:X:1602:U:H5	1.97	0.47
1:X:2632:U:H2'	1:X:2633:C:C6	2.49	0.47
2:Y:113:G:H5'	2:Y:114:C:OP2	2.14	0.47
1:X:2511:G:OP1	11:J:45:ARG:HD3	2.14	0.47
14:M:48:VAL:O	14:M:63:VAL:HA	2.14	0.47
16:O:6:GLU:OE2	16:O:37:LYS:HD2	2.14	0.47
1:X:1049:C:H1'	1:X:1056:U:C4	2.49	0.47
1:X:1983:U:H1'	1:X:2579:U:OP1	2.14	0.47
1:X:2900:C:H1'	12:K:98:GLY:O	2.14	0.47
27:X:3001:TEL:C1	27:X:3001:TEL:H233	2.42	0.47
4:B:160:ALA:C	4:B:162:ARG:H	2.17	0.47
7:E:31:GLY:O	7:E:79:VAL:HG21	2.15	0.47
9:H:30:ARG:NH1	9:H:32:THR:O	2.47	0.47
15:N:22:LYS:HA	15:N:22:LYS:HD3	1.40	0.47
17:P:29:ALA:HB1	17:P:55:LEU:HD11	1.96	0.47
1:X:1092:A:O2'	1:X:1093:C:H6	1.97	0.47
1:X:2059:G:N7	28:X:3005:MPD:H4	2.29	0.47
11:J:51:ARG:HG3	11:J:66:ILE:HD11	1.96	0.47
1:X:2708:C:O2'	28:X:3003:MPD:H51	2.15	0.47
1:X:344:U:HO2'	1:X:345:C:H6	1.59	0.47
3:A:85:PRO:HG2	3:A:86:ASN:OD1	2.15	0.47
8:G:66:THR:HG22	8:G:67:GLY:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2391:C:H5"	21:T:64:ASP:HB2	1.96	0.47
1:X:1781:C:H5	14:M:96:ARG:HH22	1.63	0.47
1:X:2377:C:H2'	1:X:2378:G:O4'	2.14	0.47
1:X:730:A:C8	1:X:819:A:C6	3.03	0.47
1:X:1208:A:H2'	1:X:1209:U:C6	2.50	0.47
1:X:1628:A:OP1	1:X:1628:A:H4'	2.14	0.47
2:Y:68:A:N1	2:Y:103:A:N1	2.62	0.47
7:E:133:VAL:HG22	7:E:135:GLY:H	1.80	0.47
17:P:73:GLU:HG2	17:P:106:VAL:HB	1.97	0.47
17:P:24:ILE:HD11	17:P:32:ALA:O	2.15	0.47
1:X:1490:G:H2'	1:X:1490:G:N3	2.29	0.47
1:X:1561:G:H1'	28:X:3002:MPD:H13	1.97	0.47
1:X:303:G:H2'	1:X:304:G:O4'	2.15	0.47
4:B:187:GLN:HB3	4:B:196:LEU:HD22	1.95	0.47
17:P:81:THR:HB	17:P:99:ARG:HA	1.97	0.47
1:X:1391:A:H2'	1:X:1392:G:O4'	2.15	0.47
1:X:1631:G:H1'	1:X:1632:A:N7	2.30	0.47
1:X:2706:A:H4'	4:B:178:VAL:HG11	1.97	0.47
1:X:334:A:H2'	1:X:335:U:C6	2.50	0.47
1:X:841:C:H2'	1:X:842:U:C6	2.49	0.47
4:B:132:LYS:HG2	4:B:173:MET:SD	2.55	0.47
14:M:26:ASP:HB2	14:M:91:ARG:HA	1.97	0.47
21:T:60:GLY:HA3	21:T:68:PHE:CZ	2.50	0.47
1:X:1312:A:N6	1:X:1333:A:H4'	2.29	0.47
1:X:1515:G:N2	1:X:1565:U:O2	2.46	0.47
1:X:1731:G:H1'	1:X:1746:G:N2	2.29	0.47
2:Y:4:G:C2	2:Y:112:G:C2	3.03	0.47
12:K:25:ILE:HG23	12:K:89:ILE:HD13	1.97	0.46
1:X:111:U:H5'	1:X:112:U:OP2	2.15	0.46
1:X:2620:U:H2'	1:X:2621:C:C6	2.51	0.46
1:X:45:G:H5"	1:X:46:C:O5'	2.15	0.46
8:G:1:MET:N	8:G:1:MET:SD	2.72	0.46
14:M:29:ARG:HH11	14:M:89:LYS:HZ3	1.63	0.46
1:X:1378:U:OP2	1:X:1431:U:O2'	2.31	0.46
1:X:1755:U:H3	1:X:1774:A:H61	1.62	0.46
1:X:1973:U:H2'	1:X:1974:C:C6	2.51	0.46
1:X:92:G:H2'	1:X:93:U:C6	2.50	0.46
1:X:774:G:OP1	3:A:10:THR:HG21	2.15	0.46
9:H:106:LEU:HD23	9:H:106:LEU:HA	1.69	0.46
10:I:84:LYS:NZ	10:I:84:LYS:HB3	2.30	0.46
10:I:66:PHE:HD2	10:I:96:LEU:HB2	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1353:A:H2'	1:X:1354:G:H8	1.80	0.46
1:X:1449:A:H4'	1:X:1449:A:OP1	2.15	0.46
1:X:151:U:H2'	1:X:152:C:O4'	2.15	0.46
1:X:1384:G:H1	1:X:1643:C:N4	2.12	0.46
1:X:168:A:H3'	1:X:169:G:H5'	1.96	0.46
1:X:1998:A:O2'	1:X:1999:G:OP1	2.32	0.46
1:X:345:C:H2'	1:X:346:A:C8	2.50	0.46
2:Y:14:G:C6	2:Y:67:G:C2	3.04	0.46
8:G:7:ALA:H	8:G:46:THR:HG21	1.80	0.46
14:M:29:ARG:HG3	14:M:89:LYS:HG3	1.96	0.46
20:S:136:ASN:O	20:S:138:PRO:HD3	2.14	0.46
1:X:1819:G:O2'	1:X:1857:C:OP1	2.33	0.46
1:X:331:G:C6	1:X:396:G:C6	3.03	0.46
1:X:502:C:H5	18:Q:68:TYR:CD1	2.33	0.46
1:X:718:C:H5"	5:C:81:PRO:HD2	1.96	0.46
1:X:852:U:H2'	1:X:853:G:H8	1.81	0.46
4:B:163:VAL:HG13	4:B:167:GLN:HG3	1.98	0.46
5:C:123:LEU:O	5:C:188:ASN:HA	2.15	0.46
10:I:20:GLY:O	10:I:21:ARG:HD3	2.15	0.46
10:I:7:LYS:HA	10:I:8:PRO:HD3	1.74	0.46
1:X:1450:A:H5"	1:X:1451:U:H5	1.81	0.46
1:X:1498:U:O2'	1:X:1499:U:H5	1.97	0.46
3:A:211:SER:O	3:A:216:ILE:HB	2.15	0.46
8:G:99:GLU:O	8:G:103:GLU:HB2	2.16	0.46
12:K:32:THR:HG22	12:K:33:THR:H	1.81	0.46
1:X:122:G:H4'	1:X:1413:C:H5'	1.97	0.46
1:X:2496:A:H1'	11:J:56:ARG:HH21	1.80	0.46
28:X:3003:MPD:H4	28:X:3003:MPD:H12	1.87	0.46
25:2:21:LYS:O	25:2:24:SER:OG	2.33	0.46
5:C:150:LYS:HA	5:C:188:ASN:OD1	2.15	0.46
8:G:65:PHE:HB3	8:G:69:LYS:HD2	1.97	0.46
10:I:19:VAL:HB	10:I:30:THR:HG23	1.97	0.46
17:P:7:ALA:HB1	17:P:10:ILE:HD11	1.97	0.46
17:P:36:LEU:HA	17:P:36:LEU:HD23	1.79	0.46
20:S:26:LYS:HG2	20:S:42:LYS:HD3	1.97	0.46
1:X:1275:A:OP2	31:X:3365:SPD:H81	2.15	0.46
1:X:2539:C:H2'	1:X:2540:A:O4'	2.15	0.46
1:X:709:U:H2'	1:X:710:C:H6	1.79	0.46
1:X:784:A:OP2	1:X:784:A:H8	1.99	0.46
3:A:252:LYS:HA	3:A:253:PRO:HD3	1.65	0.46
8:G:9:GLU:OE2	8:G:14:ARG:NH1	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:29:ARG:HD2	14:M:89:LYS:NZ	2.30	0.46
1:X:1436:C:OP1	18:Q:24:LYS:NZ	2.37	0.46
1:X:1775:G:H2'	1:X:1776:A:C8	2.51	0.46
1:X:1911:A:O2'	1:X:1912:A:H8	1.99	0.46
1:X:948:U:H2'	1:X:949:C:C6	2.51	0.46
1:X:1700:C:H2'	1:X:1701:U:H6	1.80	0.46
1:X:2085:A:C2	27:X:3001:TEL:H241	2.50	0.46
9:H:2:ILE:HG22	9:H:21:THR:HG21	1.96	0.46
1:X:1612:C:C4	1:X:1614:A:C2	3.04	0.46
1:X:167:U:H2'	1:X:168:A:H5"	1.97	0.46
1:X:2494:C:H2'	1:X:2495:A:O4'	2.16	0.46
1:X:483:C:H2'	1:X:484:U:C6	2.50	0.46
3:A:93:LEU:HD12	3:A:102:ARG:O	2.15	0.45
1:X:2403:A:C4	13:L:96:ARG:NH2	2.85	0.45
1:X:897:A:H2'	1:X:898:U:H6	1.79	0.45
7:E:154:PRO:HA	7:E:161:GLY:HA3	1.96	0.45
12:K:14:LYS:O	12:K:18:ARG:HG3	2.16	0.45
17:P:44:SER:N	17:P:45:PRO:HD2	2.32	0.45
1:X:1525:U:H3	1:X:1550:G:H1	1.64	0.45
1:X:1760:G:H1	1:X:1770:C:H42	1.64	0.45
1:X:1400:C:H1'	1:X:1837:A:H1'	1.98	0.45
1:X:2299:U:H5"	1:X:2300:A:OP1	2.16	0.45
1:X:946:A:C8	1:X:2328:A:H5"	2.52	0.45
1:X:329:A:N3	1:X:329:A:H2'	2.31	0.45
14:M:17:THR:O	14:M:19:LEU:N	2.45	0.45
15:N:112:LYS:HE3	16:O:48:VAL:HG11	1.99	0.45
1:X:1545:U:H2'	1:X:1546:A:C8	2.51	0.45
1:X:409:G:H2'	1:X:410:G:H1'	1.99	0.45
4:B:123:LYS:CD	4:B:204:PRO:HB3	2.46	0.45
1:X:1242:A:H4'	10:I:3:LEU:HD23	1.97	0.45
1:X:956:A:H2'	11:J:11:ARG:HH22	1.81	0.45
15:N:17:THR:O	15:N:20:LEU:HB2	2.17	0.45
15:N:28:LYS:HA	15:N:34:VAL:HG12	1.98	0.45
1:X:1063:U:H3	1:X:1186:A:N6	2.06	0.45
1:X:2311:U:H3	1:X:2411:A:H61	1.64	0.45
1:X:2480:A:N3	28:X:3005:MPD:H53	2.32	0.45
1:X:439:U:H2'	1:X:440:C:C6	2.52	0.45
1:X:90:A:O2'	1:X:91:A:O4'	2.34	0.45
1:X:945:A:HO2'	1:X:946:A:C5'	2.29	0.45
3:A:254:THR:O	3:A:256:GLY:N	2.50	0.45
5:C:78:ILE:HG22	5:C:83:TRP:CZ3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Q:60:PRO:HD3	18:Q:74:LYS:HB3	1.99	0.45
1:X:1895:C:H42	1:X:1901:C:N4	2.14	0.45
2:Y:91:C:H2'	2:Y:92:G:H8	1.81	0.45
1:X:1817:C:O2'	3:A:208:ALA:HB2	2.16	0.45
4:B:71:LYS:N	4:B:72:PRO:HD2	2.31	0.45
1:X:1229:G:OP1	10:I:31:SER:HA	2.17	0.45
14:M:45:PHE:CE1	14:M:65:LYS:HE2	2.52	0.45
1:X:609:U:O4	16:O:79:ARG:HD3	2.16	0.45
1:X:1492:G:N7	1:X:1493:U:C4	2.84	0.45
1:X:172:U:H3'	1:X:173:A:H8	1.82	0.45
1:X:2349:A:H2'	1:X:2350:G:O4'	2.16	0.45
1:X:250:G:H4'	1:X:432:G:C5	2.52	0.45
1:X:684:U:H2'	1:X:685:C:H6	1.81	0.45
3:A:62:TYR:HA	3:A:86:ASN:ND2	2.31	0.45
12:K:13:ARG:O	12:K:17:LEU:HD12	2.17	0.45
13:L:43:GLN:HA	13:L:54:ALA:HB3	1.99	0.45
1:X:1508:C:O2'	1:X:1509:G:H5'	2.16	0.45
1:X:329:A:H61	1:X:398:C:N4	2.09	0.45
4:B:39:LYS:HD3	4:B:46:TYR:OH	2.16	0.45
14:M:46:GLU:O	14:M:65:LYS:HD3	2.17	0.45
14:M:98:LYS:HA	14:M:98:LYS:HD3	1.72	0.45
1:X:1886:A:N6	1:X:1910:G:HO2'	2.13	0.45
1:X:2026:C:OP1	4:B:132:LYS:NZ	2.43	0.45
1:X:2507:C:H2'	1:X:2508:G:H5'	1.99	0.45
1:X:773:G:OP2	1:X:773:G:H8	2.00	0.45
1:X:2391:C:C5'	21:T:64:ASP:HB2	2.46	0.45
1:X:1395:G:C6	1:X:1408:G:N7	2.85	0.45
1:X:1565:U:H2'	1:X:1566:G:C8	2.52	0.45
1:X:603:C:H2'	1:X:604:G:O4'	2.16	0.45
1:X:878:C:H2'	1:X:879:U:C6	2.52	0.45
8:G:28:ARG:HG2	8:G:28:ARG:H	1.56	0.45
8:G:93:LEU:HB3	8:G:96:THR:OG1	2.16	0.45
10:I:108:GLY:HA2	10:I:127:LYS:CB	2.47	0.45
15:N:21:ALA:HB1	15:N:24:TYR:CD2	2.52	0.45
16:O:90:GLN:HA	16:O:91:PRO:HD3	1.75	0.45
1:X:1598:U:H4'	1:X:1768:C:O2	2.16	0.45
1:X:1683:U:C2'	1:X:1684:A:H5"	2.45	0.45
1:X:2106:U:H2'	1:X:2107:G:O4'	2.17	0.45
1:X:2400:U:H2'	1:X:2401:C:C6	2.52	0.45
7:E:139:GLU:HG2	7:E:140:GLN:N	2.32	0.44
9:H:4:GLN:CG	9:H:5:GLU:HG2	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:630:G:P	10:I:21:ARG:HH22	2.40	0.44
15:N:99:ALA:HB2	15:N:106:PHE:CD1	2.52	0.44
19:R:77:GLU:HA	19:R:78:PRO:HD3	1.66	0.44
1:X:1312:A:N1	1:X:1332:C:O2'	2.48	0.44
1:X:1629:U:H2'	1:X:1630:A:H5'	1.99	0.44
1:X:2496:A:H1'	11:J:56:ARG:NH2	2.33	0.44
1:X:2817:A:HO2'	1:X:2818:A:P	2.39	0.44
19:R:9:VAL:HG12	19:R:69:GLN:HB3	1.99	0.44
20:S:14:THR:HB	20:S:19:LYS:HZ1	1.83	0.44
1:X:1885:G:H1'	1:X:1911:A:H62	1.82	0.44
1:X:2232:A:H5'	1:X:2233:C:OP2	2.16	0.44
1:X:501:C:H3'	1:X:502:C:C5'	2.42	0.44
1:X:608:C:H2'	1:X:609:U:O4'	2.18	0.44
1:X:660:A:H62	5:C:101:MET:HB3	1.82	0.44
1:X:99:U:O2	1:X:101:G:N1	2.50	0.44
14:M:28:LEU:HD12	14:M:88:VAL:HA	1.99	0.44
15:N:16:LYS:O	15:N:20:LEU:HD23	2.17	0.44
15:N:40:MET:HG2	16:O:74:PHE:CE1	2.52	0.44
1:X:373:A:H2	1:X:1248:U:O2'	1.99	0.44
25:2:16:VAL:N	25:2:21:LYS:HG3	2.31	0.44
3:A:10:THR:HG22	3:A:12:GLY:N	2.24	0.44
7:E:86:VAL:HB	7:E:165:GLN:CB	2.48	0.44
8:G:32:GLU:O	8:G:36:ILE:HG12	2.18	0.44
12:K:32:THR:HG22	12:K:33:THR:N	2.32	0.44
13:L:30:ARG:HB3	13:L:45:ILE:HG13	1.98	0.44
1:X:1821:U:H2'	1:X:1822:C:C6	2.52	0.44
1:X:1833:C:H2'	1:X:1834:G:C8	2.52	0.44
1:X:2247:G:H2'	1:X:2248:G:C8	2.52	0.44
1:X:2851:G:N7	4:B:64:LYS:HG3	2.32	0.44
13:L:11:ARG:HG3	13:L:94:PHE:CD2	2.52	0.44
17:P:62:TYR:CD1	17:P:62:TYR:N	2.86	0.44
21:T:52:LYS:C	21:T:53:ILE:HD12	2.37	0.44
1:X:1211:G:H2'	1:X:1212:U:C6	2.52	0.44
1:X:146:U:H2'	1:X:147:G:O4'	2.17	0.44
1:X:1487:G:N2	1:X:1597:U:C2	2.86	0.44
1:X:1492:G:H1	1:X:1508:C:N4	2.15	0.44
1:X:745:G:O2'	1:X:1676:A:N3	2.45	0.44
18:Q:67:ARG:HD3	18:Q:68:TYR:CE1	2.53	0.44
1:X:1356:G:C5	1:X:1357:G:C6	3.06	0.44
1:X:183:A:H5'	1:X:481:C:H1'	2.00	0.44
1:X:1882:G:H2'	1:X:1883:A:H8	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:201:C:H2'	1:X:202:A:H5"	2.00	0.44
1:X:2418:G:C6	1:X:2454:C:H1'	2.53	0.44
1:X:2564:U:H2'	1:X:2565:C:C6	2.52	0.44
1:X:2774:G:O6	1:X:2782:C:H5"	2.18	0.44
1:X:953:C:P	11:J:101:ARG:HH22	2.40	0.44
1:X:2850:G:OP1	4:B:67:LYS:HG3	2.18	0.44
10:I:90:GLU:O	10:I:92:THR:HG23	2.18	0.44
12:K:47:LEU:HD13	12:K:66:LEU:HD12	2.00	0.44
1:X:1780:G:OP1	14:M:95:ARG:HD2	2.17	0.44
16:O:88:HIS:HE2	16:O:90:GLN:HB2	1.81	0.44
16:O:19:GLU:HA	16:O:96:THR:HA	1.99	0.44
1:X:1084:U:H2'	1:X:1085:U:O4'	2.17	0.44
1:X:1556:G:HO2'	1:X:1557:C:H6	1.65	0.44
1:X:1742:A:OP1	1:X:1742:A:H8	2.01	0.44
1:X:2331:G:N2	1:X:2339:U:H3	2.16	0.44
1:X:24:G:H2'	1:X:25:U:H6	1.82	0.44
1:X:2731:C:H2'	1:X:2732:A:O4'	2.17	0.44
1:X:660:A:N3	1:X:660:A:O4'	2.51	0.44
1:X:926:G:H22	1:X:940:U:H3	1.66	0.44
1:X:2717:A:H62	12:K:13:ARG:HD2	1.83	0.44
14:M:8:GLU:O	14:M:11:THR:HG22	2.18	0.44
14:M:58:SER:O	14:M:59:GLU:HB2	2.17	0.44
1:X:1150:A:C8	1:X:1151:G:H8	2.36	0.44
1:X:138:U:N3	1:X:141:U:OP2	2.43	0.44
1:X:2333:U:H3'	1:X:2334:G:H8	1.83	0.44
1:X:2587:C:C2	1:X:2588:A:C8	3.06	0.44
3:A:91:ILE:CG2	3:A:105:ILE:HA	2.45	0.44
6:D:38:MET:O	6:D:82:GLY:HA2	2.18	0.44
17:P:13:ALA:O	17:P:17:VAL:HG23	2.17	0.44
20:S:10:GLN:HG2	20:S:40:SER:O	2.17	0.44
1:X:1490:G:HO2'	1:X:1491:C:P	2.39	0.44
1:X:150:A:C6	1:X:151:U:C4	3.06	0.44
1:X:1555:G:H2'	1:X:1556:G:H8	1.82	0.44
1:X:155:U:H5'	1:X:156:A:OP2	2.17	0.44
1:X:165:C:O2'	1:X:166:A:OP1	2.32	0.44
1:X:2249:G:O3'	3:A:171:TYR:OH	2.34	0.44
1:X:379:C:C2	1:X:380:U:C5	3.06	0.44
4:B:2:THR:HA	4:B:213:THR:OG1	2.18	0.43
11:J:39:THR:HG23	11:J:98:LYS:HA	1.98	0.43
14:M:60:THR:HA	14:M:76:PHE:O	2.17	0.43
15:N:15:LYS:HE2	15:N:15:LYS:HB2	1.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1602:U:HO2'	1:X:1603:U:P	2.36	0.43
1:X:615:A:H5"	1:X:616:G:OP2	2.18	0.43
1:X:262:G:N2	1:X:666:A:H8	2.16	0.43
24:Z:38:LYS:HE2	24:Z:38:LYS:HB2	1.78	0.43
11:J:43:THR:HA	11:J:94:ILE:HD13	1.99	0.43
1:X:1286:G:C4	15:N:3:ARG:HG3	2.52	0.43
1:X:1992:C:H5"	1:X:1993:A:H2'	2.00	0.43
1:X:2064:A:C6	1:X:2065:G:C6	3.07	0.43
1:X:266:A:H2'	1:X:267:G:O4'	2.18	0.43
1:X:2844:U:H2'	1:X:2845:G:O4'	2.18	0.43
1:X:365:A:C5	1:X:383:A:C2	3.06	0.43
1:X:523:A:OP1	31:X:3365:SPD:H51	2.18	0.43
1:X:669:C:O2'	1:X:702:U:H5"	2.17	0.43
1:X:972:A:H2'	1:X:973:A:C8	2.53	0.43
1:X:2639:C:HO2'	24:Z:2:ALA:N	2.17	0.43
1:X:1701:U:OP2	4:B:149:ARG:HG3	2.17	0.43
4:B:79:LYS:HD3	4:B:79:LYS:HA	1.80	0.43
11:J:118:LEU:HD12	11:J:131:PHE:CE1	2.52	0.43
9:H:79:PHE:HD1	14:M:72:VAL:HG22	1.84	0.43
18:Q:53:VAL:HA	18:Q:80:VAL:HG12	1.99	0.43
1:X:1038:C:OP1	15:N:53:ARG:NH2	2.51	0.43
1:X:1336:G:H5"	1:X:1337:A:OP1	2.17	0.43
1:X:1565:U:H2'	1:X:1566:G:O4'	2.18	0.43
1:X:2249:G:O2'	1:X:2250:A:H5'	2.17	0.43
1:X:2263:C:H2'	1:X:2264:G:O4'	2.17	0.43
1:X:2482:G:H2'	1:X:2483:C:H6	1.83	0.43
3:A:145:GLU:CA	3:A:152:GLY:HA2	2.49	0.43
6:D:111:VAL:N	6:D:170:LEU:H	2.15	0.43
7:E:19:PHE:HB3	7:E:20:ASP:H	1.67	0.43
10:I:67:THR:CG2	10:I:93:PRO:HD2	2.48	0.43
15:N:91:ASN:OD1	15:N:93:LYS:N	2.48	0.43
1:X:1040:A:OP2	15:N:93:LYS:NZ	2.48	0.43
1:X:12:U:H2'	1:X:12:U:O2	2.17	0.43
1:X:1438:G:H2'	1:X:1439:U:C6	2.53	0.43
1:X:1843:U:C3'	1:X:1843:U:C6	3.01	0.43
1:X:2082:C:O2	28:X:3005:MPD:H11	2.18	0.43
1:X:650:U:N3	1:X:666:A:C2	2.77	0.43
5:C:104:LYS:HE2	5:C:104:LYS:HB3	1.68	0.43
8:G:44:THR:O	8:G:46:THR:HG22	2.19	0.43
17:P:57:ASN:HB2	17:P:61:ASN:ND2	2.34	0.43
21:T:47:ARG:HA	21:T:66:THR:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1887:G:H2'	1:X:1888:U:C6	2.53	0.43
1:X:187:C:H2'	1:X:188:C:C6	2.53	0.43
1:X:2051:C:H2'	1:X:2052:C:C6	2.53	0.43
4:B:26:THR:OG1	4:B:200:ASN:HA	2.19	0.43
8:G:84:GLY:O	8:G:86:LYS:N	2.49	0.43
12:K:66:LEU:HD23	12:K:67:ARG:O	2.19	0.43
18:Q:66:GLY:O	18:Q:68:TYR:N	2.46	0.43
19:R:51:ASN:HA	19:R:52:PRO:HD3	1.83	0.43
21:T:61:ARG:NH1	21:T:65:ASP:OD1	2.51	0.43
1:X:122:G:O3'	1:X:1413:C:H4'	2.17	0.43
1:X:1275:A:C8	1:X:1276:G:H1'	2.53	0.43
1:X:2314:A:HO2'	1:X:2315:A:P	2.41	0.43
1:X:2829:A:H2'	1:X:2830:A:C8	2.54	0.43
1:X:2606:C:O2'	4:B:146:HIS:O	2.28	0.43
7:E:133:VAL:HG22	7:E:135:GLY:N	2.34	0.43
17:P:3:ALA:HB2	17:P:62:TYR:CD2	2.54	0.43
17:P:36:LEU:HD13	17:P:48:GLU:HA	2.01	0.43
1:X:1522:G:H2'	1:X:1523:G:C8	2.53	0.43
1:X:1793:C:H2'	1:X:1794:C:C6	2.52	0.43
1:X:2660:A:H1'	4:B:72:PRO:HG3	1.99	0.43
1:X:87:U:H5"	1:X:88:G:H5'	2.00	0.43
6:D:138:PHE:HA	6:D:139:PRO:HD2	1.90	0.43
16:O:24:LYS:HA	16:O:93:THR:OG1	2.19	0.43
16:O:29:GLU:OE2	16:O:64:LYS:HA	2.18	0.43
1:X:1493:U:N3	1:X:1494:G:C6	2.87	0.43
1:X:1529:U:O4	1:X:1530:A:N6	2.51	0.43
1:X:2482:G:H2'	1:X:2483:C:C6	2.53	0.43
1:X:267:G:C2'	1:X:268:A:H5"	2.48	0.43
1:X:327:G:O2'	1:X:328:G:H8	2.01	0.43
1:X:347:U:H2'	1:X:348:C:C6	2.54	0.43
1:X:379:C:H2'	1:X:380:U:H6	1.81	0.43
1:X:704:U:H2'	1:X:705:U:O4'	2.18	0.43
1:X:972:A:H2'	1:X:973:A:H8	1.83	0.43
3:A:171:TYR:CD1	3:A:185:LEU:HA	2.54	0.43
12:K:95:GLU:H	12:K:95:GLU:HG2	1.56	0.43
17:P:24:ILE:HD12	17:P:24:ILE:HA	1.76	0.43
18:Q:24:LYS:HE3	18:Q:81:THR:HB	1.99	0.43
1:X:1543:G:N7	1:X:1544:G:C5	2.87	0.43
1:X:1845:U:H5"	3:A:156:ARG:HB2	2.01	0.43
1:X:2368:G:H2'	1:X:2369:C:H6	1.84	0.43
1:X:2856:U:H2'	1:X:2857:A:H8	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:R:26:THR:HB	19:R:33:VAL:HG12	2.01	0.43
1:X:1087:C:H42	1:X:1156:G:H1	1.65	0.43
1:X:1426:G:H1	1:X:1435:C:H42	1.67	0.43
1:X:1436:C:HO2'	1:X:1437:U:H6	1.64	0.43
1:X:1486:C:H2'	1:X:1487:G:C8	2.54	0.43
1:X:1460:U:H3	1:X:1628:A:H61	1.65	0.43
1:X:391:A:H2'	1:X:392:U:C6	2.54	0.43
1:X:615:A:N6	1:X:616:G:C6	2.87	0.43
7:E:87:LEU:HA	7:E:87:LEU:HD23	1.80	0.42
8:G:137:GLN:N	8:G:138:PRO:HD3	2.34	0.42
8:G:60:ALA:HB3	8:G:127:GLY:HA2	2.00	0.42
12:K:79:GLN:HB3	12:K:80:THR:H	1.55	0.42
16:O:3:ALA:HB1	16:O:5:ILE:HG23	2.00	0.42
1:X:2900:C:O2'	12:K:96:ARG:NH1	2.52	0.42
11:J:30:GLY:HA2	11:J:107:ALA:HB2	2.02	0.42
1:X:2717:A:N6	12:K:13:ARG:HD2	2.33	0.42
20:S:26:LYS:N	20:S:26:LYS:HD2	2.33	0.42
1:X:1477:U:H2'	1:X:1478:A:C8	2.54	0.42
1:X:1491:C:H1'	1:X:1492:G:N2	2.34	0.42
1:X:148:U:H2'	1:X:149:U:C6	2.54	0.42
1:X:2437:G:H2'	1:X:2438:A:O4'	2.18	0.42
1:X:660:A:H4'	1:X:661:U:OP1	2.19	0.42
7:E:162:ILE:HG13	7:E:162:ILE:H	1.63	0.42
8:G:20:ASP:HA	8:G:58:ILE:HG22	2.00	0.42
9:H:76:TYR:HB2	14:M:75:THR:CG2	2.49	0.42
14:M:26:ASP:CB	14:M:91:ARG:HA	2.50	0.42
1:X:1013:U:H2'	1:X:1014:U:C6	2.54	0.42
1:X:2270:U:H2'	1:X:2271:U:C6	2.54	0.42
1:X:2519:U:H2'	1:X:2520:U:C6	2.54	0.42
1:X:2609:G:H2'	1:X:2609:G:N3	2.35	0.42
2:Y:80:A:C4	2:Y:81:A:C8	3.07	0.42
1:X:2849:A:OP1	4:B:86:ARG:NH1	2.53	0.42
16:O:70:LYS:HG3	16:O:71:ILE:N	2.35	0.42
17:P:21:LEU:HD22	17:P:74:ALA:HB1	2.01	0.42
1:X:1234:G:N3	1:X:1264:A:H2	2.17	0.42
1:X:1269:A:H2'	1:X:1270:U:H6	1.84	0.42
1:X:1312:A:C6	1:X:1333:A:H4'	2.55	0.42
1:X:1465:G:H1	1:X:1624:C:H42	1.66	0.42
1:X:1510:U:H3	1:X:1571:G:H22	1.67	0.42
1:X:2358:G:O2'	1:X:2363:A:N1	2.46	0.42
1:X:2368:G:H2'	1:X:2369:C:C6	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2445:A:H2'	1:X:2446:U:O4'	2.19	0.42
1:X:2285:C:O2'	1:X:2453:A:H4'	2.19	0.42
3:A:160:ALA:HB3	3:A:195:VAL:HG23	2.02	0.42
5:C:29:ASN:CG	5:C:32:VAL:HG23	2.40	0.42
1:X:1177:A:H4'	1:X:1178:C:H5'	2.01	0.42
1:X:1696:C:H2'	1:X:1697:G:O4'	2.20	0.42
1:X:226:A:C6	1:X:468:A:C4	3.08	0.42
1:X:2479:C:C4	1:X:2480:A:C6	3.08	0.42
1:X:2725:U:H2'	1:X:2726:C:C6	2.55	0.42
27:X:3001:TEL:H30	27:X:3001:TEL:H242	1.61	0.42
1:X:89:U:H3'	1:X:90:A:H8	1.83	0.42
1:X:2599:A:N7	4:B:158:SER:HB3	2.35	0.42
7:E:62:ARG:C	7:E:64:ASN:H	2.20	0.42
1:X:1000:G:O3'	11:J:77:LYS:HD3	2.19	0.42
18:Q:51:ALA:HB2	18:Q:83:LYS:H	1.82	0.42
21:T:32:LYS:HA	21:T:32:LYS:HD3	1.89	0.42
1:X:1259:U:H2'	1:X:1260:C:C6	2.54	0.42
1:X:1848:A:H2'	1:X:1849:G:C8	2.54	0.42
1:X:2260:A:H2'	1:X:2261:A:C8	2.54	0.42
1:X:404:U:C2	1:X:405:G:C8	3.08	0.42
4:B:25:VAL:HG21	4:B:196:LEU:HB3	2.02	0.42
1:X:2330:G:H4'	6:D:115:GLN:H	1.85	0.42
10:I:47:ARG:HA	10:I:48:PRO:HD3	1.84	0.42
11:J:36:ALA:HB2	11:J:103:LEU:HD21	2.02	0.42
1:X:1474:C:H2'	1:X:1475:A:H8	1.84	0.42
1:X:1492:G:H1'	1:X:1593:G:N2	2.35	0.42
1:X:1885:G:H1'	1:X:1911:A:N6	2.35	0.42
1:X:2120:G:N2	1:X:2225:A:H62	2.14	0.42
1:X:2720:A:H2'	1:X:2721:G:H8	1.84	0.42
1:X:2827:A:H2'	1:X:2828:U:O4'	2.20	0.42
2:Y:15:C:H2'	2:Y:16:A:O4'	2.19	0.42
8:G:38:ARG:HA	8:G:119:GLN:OE1	2.20	0.42
12:K:58:SER:HA	12:K:61:ASN:HB2	2.01	0.42
13:L:96:ARG:O	13:L:98:GLY:N	2.52	0.42
1:X:187:C:H2'	1:X:188:C:H6	1.85	0.42
1:X:197:G:C2	1:X:205:U:H1'	2.55	0.42
1:X:268:A:N6	1:X:473:U:O2'	2.53	0.42
1:X:262:G:N2	1:X:666:A:C8	2.87	0.42
1:X:77:U:H2'	1:X:78:U:O4'	2.20	0.42
2:Y:109:C:H2'	2:Y:110:C:C6	2.55	0.42
2:Y:67:G:H2'	2:Y:68:A:C8	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:107:PRO:HD2	3:A:110:LEU:HD12	2.01	0.42
10:I:47:ARG:HB2	10:I:47:ARG:HE	1.65	0.42
16:O:78:ARG:O	16:O:80:LYS:HG2	2.20	0.42
17:P:57:ASN:O	17:P:61:ASN:HB2	2.19	0.42
20:S:98:GLU:HA	20:S:129:GLU:O	2.19	0.42
1:X:1378:U:P	1:X:1434:U:H3	2.42	0.42
1:X:1514:A:N6	1:X:1566:G:N1	2.66	0.42
1:X:2245:G:C6	1:X:2246:U:N3	2.88	0.42
1:X:2391:C:H2'	1:X:2392:G:O4'	2.20	0.42
28:X:3007:MPD:H12	28:X:3007:MPD:H4	1.94	0.42
1:X:309:U:O2'	1:X:310:C:H6	2.03	0.42
1:X:408:U:H2'	1:X:409:G:C8	2.55	0.42
1:X:440:C:H2'	1:X:441:C:H6	1.85	0.42
1:X:509:G:N7	28:X:3006:MPD:H32	2.35	0.42
1:X:523:A:OP2	31:X:3365:SPD:H42	2.19	0.42
1:X:262:G:H21	1:X:666:A:H8	1.64	0.42
1:X:695:C:H6	1:X:695:C:O5'	2.02	0.42
26:3:13:ARG:HA	26:3:21:GLN:O	2.20	0.42
11:J:47:ILE:HD11	11:J:68:ILE:HG13	2.01	0.42
12:K:109:ARG:NH1	12:K:112:ASP:OD2	2.52	0.42
15:N:66:ASN:OD1	15:N:70:ARG:NH1	2.51	0.42
15:N:7:GLY:O	15:N:9:VAL:HG22	2.19	0.42
16:O:18:GLN:O	16:O:97:ILE:HG12	2.19	0.42
16:O:86:LYS:HE3	16:O:86:LYS:HB3	1.89	0.42
19:R:69:GLN:H	19:R:69:GLN:HG2	1.64	0.42
22:V:40:THR:O	22:V:43:ILE:HG13	2.20	0.42
1:X:153:G:O2'	1:X:154:A:H5'	2.20	0.42
1:X:1550:G:O2'	1:X:1551:U:O5'	2.35	0.42
1:X:1561:G:H8	1:X:1562:C:C6	2.37	0.42
27:X:3001:TEL:H11	27:X:3001:TEL:H82	1.60	0.42
1:X:389:A:H2'	1:X:390:A:O4'	2.19	0.42
1:X:412:U:O2'	1:X:413:C:O4'	2.37	0.42
1:X:579:U:H2'	1:X:580:C:C6	2.55	0.42
11:J:34:LEU:HD11	11:J:129:THR:HB	2.01	0.41
15:N:106:PHE:O	15:N:110:VAL:HG23	2.20	0.41
19:R:26:THR:HA	19:R:33:VAL:HG12	2.02	0.41
1:X:2384:U:OP1	21:T:28:ARG:NH2	2.53	0.41
1:X:1209:U:H2'	1:X:1210:U:C6	2.55	0.41
1:X:1680:U:H2'	1:X:1681:U:C6	2.55	0.41
1:X:2232:A:H61	1:X:2246:U:H3	1.67	0.41
1:X:2883:U:H2'	1:X:2884:G:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:386:C:H2'	1:X:387:G:H8	1.85	0.41
4:B:7:GLY:HA2	4:B:53:PHE:CE2	2.55	0.41
10:I:29:LYS:O	10:I:30:THR:HB	2.21	0.41
18:Q:53:VAL:C	18:Q:54:ASN:HD22	2.24	0.41
20:S:104:VAL:HG12	20:S:124:PRO:HB3	2.02	0.41
22:V:62:ILE:HA	22:V:62:ILE:HD13	1.84	0.41
1:X:1833:C:H2'	1:X:1834:G:H8	1.84	0.41
1:X:26:G:H1'	1:X:559:A:N6	2.35	0.41
1:X:302:A:O2'	1:X:303:G:H8	2.02	0.41
1:X:548:A:C5'	1:X:549:U:H5'	2.44	0.41
1:X:609:U:H5	16:O:79:ARG:HG2	1.85	0.41
7:E:133:VAL:HG13	7:E:134:GLU:N	2.35	0.41
9:H:31:LYS:HB3	9:H:31:LYS:HE2	1.70	0.41
1:X:2385:A:N1	10:I:50:PHE:HZ	2.19	0.41
18:Q:57:ASN:O	18:Q:58:TYR:HD1	2.04	0.41
1:X:1825:U:OP1	3:A:260:ARG:N	2.53	0.41
1:X:2431:C:H2'	1:X:2432:G:O4'	2.21	0.41
1:X:301:U:H5"	1:X:302:A:OP2	2.20	0.41
1:X:620:G:C6	1:X:621:A:N6	2.88	0.41
1:X:769:U:H2'	1:X:770:G:O4'	2.20	0.41
4:B:154:VAL:HG21	4:B:169:MET:HE3	2.01	0.41
5:C:102:PRO:O	5:C:105:MET:HB2	2.21	0.41
9:H:71:ARG:HE	9:H:105:GLU:CD	2.21	0.41
13:L:19:ARG:HH12	13:L:23:SER:HA	1.85	0.41
14:M:66:ILE:HA	14:M:71:GLY:HA2	2.02	0.41
14:M:78:LEU:HB3	14:M:79:HIS:HD2	1.85	0.41
17:P:10:ILE:HG22	17:P:12:ILE:H	1.86	0.41
1:X:24:G:O2'	17:P:78:GLU:O	2.38	0.41
1:X:164:A:H1'	1:X:165:C:H5'	2.02	0.41
1:X:1685:A:C8	1:X:1686:G:C8	3.09	0.41
1:X:17:G:P	24:Z:11:THR:HG22	2.60	0.41
1:X:391:A:H2'	1:X:392:U:H6	1.86	0.41
1:X:660:A:N6	5:C:106:ARG:NE	2.68	0.41
1:X:125:A:N3	25:2:19:PHE:HB3	2.35	0.41
3:A:45:ASN:C	3:A:47:GLY:H	2.24	0.41
4:B:53:PHE:O	4:B:85:LYS:HD2	2.21	0.41
5:C:150:LYS:O	5:C:171:PRO:HD2	2.21	0.41
7:E:87:LEU:CD2	7:E:164:TYR:HA	2.51	0.41
16:O:84:ARG:HH21	16:O:84:ARG:HB3	1.85	0.41
1:X:1753:U:H2'	1:X:1754:C:C6	2.55	0.41
1:X:2350:G:O5'	1:X:2350:G:H8	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2650:G:O5'	1:X:2845:G:N2	2.53	0.41
1:X:302:A:N6	1:X:450:C:C2	2.88	0.41
1:X:363:A:H4'	1:X:365:A:C8	2.56	0.41
1:X:421:C:H2'	1:X:422:G:C8	2.56	0.41
1:X:668:C:H2'	1:X:669:C:C6	2.56	0.41
1:X:79:U:O2'	1:X:389:A:H8	2.04	0.41
2:Y:57:G:H3'	2:Y:58:G:H8	1.86	0.41
25:2:15:LYS:O	25:2:16:VAL:HB	2.21	0.41
25:2:28:GLY:O	25:2:32:LEU:HG	2.21	0.41
3:A:156:ARG:O	3:A:160:ALA:HB2	2.20	0.41
1:X:2842:G:O3'	4:B:172:ARG:NH2	2.54	0.41
1:X:2813:U:O2'	4:B:72:PRO:O	2.33	0.41
5:C:101:MET:HG3	5:C:102:PRO:HD2	2.01	0.41
1:X:1302:G:C6	1:X:1303:A:N6	2.89	0.41
1:X:1494:G:C8	1:X:1495:C:C5	3.05	0.41
1:X:165:C:HO2'	1:X:166:A:P	2.44	0.41
1:X:165:C:O2'	1:X:166:A:P	2.79	0.41
1:X:24:G:H2'	1:X:25:U:C6	2.56	0.41
1:X:2711:U:O4	28:X:3003:MPD:O4	2.38	0.41
27:X:3001:TEL:H382	27:X:3001:TEL:H331	1.71	0.41
24:Z:16:ARG:HH11	24:Z:16:ARG:HG2	1.85	0.41
5:C:96:SER:O	5:C:97:TYR:HB2	2.20	0.41
13:L:11:ARG:HG3	13:L:94:PHE:CE2	2.55	0.41
13:L:44:ILE:H	13:L:54:ALA:CB	2.32	0.41
1:X:1418:G:O6	1:X:1419:A:N6	2.54	0.41
1:X:1482:U:H2'	1:X:1483:A:C8	2.55	0.41
1:X:626:G:C6	1:X:627:C:C4	3.08	0.41
1:X:735:C:H1'	1:X:824:A:O3'	2.21	0.41
8:G:126:TYR:CE2	8:G:132:PRO:HD2	2.56	0.41
10:I:79:LEU:HA	10:I:108:GLY:H	1.85	0.41
18:Q:55:ILE:HG13	18:Q:78:ALA:HB2	2.02	0.41
1:X:1471:A:H1'	1:X:1472:C:C5	2.56	0.41
1:X:2314:A:H62	1:X:2371:U:H3	1.69	0.41
5:C:78:ILE:HG13	5:C:78:ILE:H	1.56	0.41
9:H:65:THR:HA	9:H:82:ASN:HA	2.02	0.41
11:J:11:ARG:C	11:J:12:GLN:HG2	2.41	0.41
1:X:1039:C:C5	15:N:57:PHE:CZ	3.09	0.41
1:X:1513:A:C3'	1:X:1514:A:H8	2.27	0.41
1:X:1518:G:H1	1:X:1562:C:N4	2.04	0.41
1:X:1488:A:C4	1:X:1596:G:N2	2.89	0.41
1:X:1630:A:H3'	1:X:1631:G:C5'	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2250:A:H2'	1:X:2251:G:O4'	2.21	0.41
1:X:383:A:H2'	1:X:384:G:O4'	2.21	0.41
3:A:154:ILE:HG22	3:A:155:ALA:N	2.36	0.41
3:A:54:HIS:HB2	3:A:215:GLY:O	2.21	0.41
4:B:154:VAL:HG13	4:B:163:VAL:HG22	2.03	0.41
4:B:67:LYS:HB3	4:B:67:LYS:HE2	1.86	0.41
9:H:10:VAL:HG11	9:H:86:ILE:HG13	2.03	0.41
14:M:96:ARG:HA	14:M:96:ARG:HD3	1.87	0.41
1:X:1376:G:OP1	18:Q:13:THR:HG21	2.21	0.41
1:X:1063:U:H2'	1:X:1065:A:H2	1.86	0.41
1:X:2356:A:H2'	1:X:2357:G:C8	2.55	0.41
1:X:2638:C:H1'	27:X:3001:TEL:H81	2.03	0.41
2:Y:4:G:H1	2:Y:111:A:H62	1.68	0.41
2:Y:26:C:H2'	2:Y:27:A:O4'	2.21	0.41
2:Y:48:A:OP2	13:L:67:ALA:HB3	2.20	0.41
10:I:66:PHE:CG	10:I:94:ALA:HB3	2.55	0.41
1:X:1889:G:O2'	1:X:1890:G:H5'	2.20	0.41
1:X:228:A:N6	1:X:234:C:H42	2.19	0.41
1:X:2520:U:H2'	1:X:2521:G:O4'	2.21	0.41
1:X:253:G:C6	1:X:254:A:C6	3.08	0.41
1:X:656:G:N2	1:X:659:A:H2'	2.36	0.41
1:X:70:G:H5"	1:X:112:U:H1'	2.03	0.41
7:E:149:ARG:O	7:E:153:PRO:HG3	2.21	0.40
11:J:73:PRO:HB3	11:J:93:TRP:CZ3	2.56	0.40
23:W:29:LYS:HB3	23:W:30:LYS:H	1.48	0.40
1:X:1072:A:N3	1:X:2513:G:O2'	2.40	0.40
1:X:1463:A:H5"	1:X:1465:G:O6	2.20	0.40
1:X:1636:U:O2'	1:X:1637:A:OP1	2.36	0.40
1:X:1806:U:C5	1:X:1811:A:N7	2.83	0.40
1:X:234:C:O2'	1:X:235:G:O4'	2.27	0.40
1:X:2597:G:H2'	1:X:2598:U:O4'	2.21	0.40
1:X:300:G:N2	1:X:302:A:N7	2.69	0.40
1:X:319:G:H3'	1:X:320:U:C5'	2.51	0.40
1:X:327:G:H2'	1:X:327:G:N3	2.35	0.40
5:C:8:LYS:O	5:C:125:VAL:HA	2.21	0.40
6:D:104:ILE:O	6:D:106:VAL:N	2.47	0.40
7:E:22:ASN:N	7:E:29:PRO:HG2	2.34	0.40
14:M:84:GLU:HG2	14:M:85:LYS:HG3	2.02	0.40
1:X:1170:A:OP1	1:X:1170:A:H8	2.03	0.40
1:X:1197:C:H2'	1:X:1198:G:O4'	2.20	0.40
1:X:2080:G:H4'	4:B:161:SER:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2102:U:C4	1:X:2265:G:C6	3.08	0.40
1:X:2717:A:H4'	1:X:2718:C:OP2	2.22	0.40
1:X:381:G:N2	1:X:382:U:H1'	2.36	0.40
1:X:404:U:HO2'	1:X:405:G:P	2.40	0.40
2:Y:46:A:H2'	2:Y:47:C:C6	2.56	0.40
24:Z:20:PHE:O	24:Z:20:PHE:CG	2.73	0.40
4:B:36:LEU:HD12	4:B:52:GLY:HA3	2.03	0.40
5:C:47:GLY:O	5:C:94:PRO:HA	2.21	0.40
10:I:66:PHE:HE2	10:I:113:GLY:HA3	1.86	0.40
11:J:78:PRO:HB2	11:J:81:VAL:HG21	2.03	0.40
13:L:30:ARG:O	13:L:44:ILE:HA	2.22	0.40
17:P:11:ARG:HG2	17:P:11:ARG:HH11	1.85	0.40
1:X:13:A:N3	1:X:15:G:C6	2.89	0.40
1:X:142:G:H5"	1:X:143:U:H5	1.86	0.40
1:X:575:G:N2	1:X:2050:A:OP1	2.54	0.40
8:G:7:ALA:HB2	8:G:44:THR:HG22	2.02	0.40
10:I:33:ARG:HE	10:I:33:ARG:HB2	1.52	0.40
1:X:1066:G:N2	1:X:1186:A:C2	2.89	0.40
1:X:1452:C:N3	1:X:1631:G:C2	2.90	0.40
1:X:1507:A:C5	1:X:1508:C:H5	2.40	0.40
1:X:1573:A:C2	1:X:1592:A:H8	2.40	0.40
1:X:1593:G:C8	1:X:1594:U:C4	3.09	0.40
1:X:659:A:O2'	1:X:660:A:OP2	2.33	0.40
1:X:844:G:C6	1:X:845:A:C6	3.09	0.40
9:H:23:LYS:HE3	9:H:23:LYS:HA	2.04	0.40
9:H:14:SER:O	9:H:52:VAL:HG22	2.21	0.40
11:J:14:ARG:NE	11:J:73:PRO:HD2	2.36	0.40
12:K:41:ARG:O	12:K:45:GLU:HG2	2.21	0.40
13:L:19:ARG:NH2	13:L:47:ASP:OD2	2.47	0.40
17:P:24:ILE:HG13	17:P:32:ALA:HB1	2.03	0.40
1:X:1269:A:H2'	1:X:1270:U:C6	2.57	0.40
1:X:2619:G:C6	1:X:2620:U:C4	3.10	0.40
2:Y:4:G:N3	2:Y:112:G:N2	2.70	0.40

All (1) 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)
1:X:136:A:OP1	1:X:1453:G:N2[12_554]	2.19	0.01

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	A	267/277 (96%)	211 (79%)	34 (13%)	22 (8%)	1 8
4	B	213/220 (97%)	179 (84%)	18 (8%)	16 (8%)	1 9
5	C	198/207 (96%)	166 (84%)	20 (10%)	12 (6%)	1 13
6	D	156/179 (87%)	114 (73%)	30 (19%)	12 (8%)	1 9
7	E	154/178 (86%)	112 (73%)	29 (19%)	13 (8%)	1 8
8	G	143/145 (99%)	126 (88%)	13 (9%)	4 (3%)	5 30
9	H	120/122 (98%)	108 (90%)	12 (10%)	0	100 100
10	I	129/146 (88%)	89 (69%)	25 (19%)	15 (12%)	0 4
11	J	139/144 (96%)	119 (86%)	15 (11%)	5 (4%)	3 25
12	K	117/122 (96%)	99 (85%)	13 (11%)	5 (4%)	2 21
13	L	107/119 (90%)	88 (82%)	10 (9%)	9 (8%)	1 8
14	M	108/116 (93%)	94 (87%)	9 (8%)	5 (5%)	2 19
15	N	114/118 (97%)	107 (94%)	5 (4%)	2 (2%)	8 38
16	O	100/102 (98%)	90 (90%)	9 (9%)	1 (1%)	15 51
17	P	110/117 (94%)	104 (94%)	6 (6%)	0	100 100
18	Q	87/91 (96%)	76 (87%)	10 (12%)	1 (1%)	14 49
19	R	99/105 (94%)	72 (73%)	21 (21%)	6 (6%)	1 13
20	S	165/217 (76%)	129 (78%)	19 (12%)	17 (10%)	0 6
21	T	73/94 (78%)	66 (90%)	6 (8%)	1 (1%)	11 43
22	V	61/69 (88%)	57 (93%)	1 (2%)	3 (5%)	2 18
23	W	56/59 (95%)	51 (91%)	4 (7%)	1 (2%)	8 38
24	Z	43/58 (74%)	40 (93%)	3 (7%)	0	100 100
25	2	42/45 (93%)	39 (93%)	3 (7%)	0	100 100
26	3	58/66 (88%)	47 (81%)	6 (10%)	5 (9%)	1 8
All	All	2859/3116 (92%)	2383 (83%)	321 (11%)	155 (5%)	2 16

All (155) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	27	THR
3	A	51	VAL
3	A	126	VAL
3	A	141	VAL
3	A	154	ILE
3	A	158	ALA
3	A	192	ILE
4	B	61	LYS
4	B	101	VAL
4	B	145	SER
4	B	157	ALA
4	B	205	LYS
5	C	126	VAL
5	C	154	VAL
5	C	158	ASN
5	C	184	LEU
6	D	44	VAL
6	D	74	ILE
6	D	104	ILE
6	D	117	VAL
7	E	24	VAL
7	E	46	GLU
10	I	46	VAL
10	I	48	PRO
10	I	62	PRO
10	I	71	ARG
10	I	101	VAL
10	I	116	SER
12	K	69	VAL
13	L	100	LEU
14	M	89	LYS
14	M	101	TYR
15	N	8	THR
20	S	34	TYR
26	3	18	ALA
26	3	43	GLN
26	3	54	ASP
3	A	82	GLN
3	A	88	SER
3	A	257	LYS
4	B	45	GLY
4	B	87	PHE

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Mol	Chain	Res	Type
5	C	175	VAL
6	D	40	VAL
6	D	119	LYS
6	D	132	VAL
7	E	58	SER
7	E	159	GLY
8	G	135	ALA
10	I	44	GLY
11	J	91	GLU
11	J	135	GLU
12	K	71	ILE
12	K	97	GLN
13	L	37	ASN
14	M	36	GLU
19	R	6	GLY
20	S	14	THR
20	S	38	ASN
20	S	81	PRO
20	S	82	LEU
20	S	130	VAL
22	V	11	THR
26	3	28	PHE
3	A	21	PHE
4	B	186	VAL
5	C	67	GLN
5	C	130	ASN
5	C	171	PRO
5	C	191	SER
6	D	115	GLN
6	D	130	LEU
7	E	63	THR
7	E	110	SER
7	E	154	PRO
8	G	87	SER
10	I	13	ARG
10	I	30	THR
10	I	113	GLY
10	I	125	ALA
11	J	20	ARG
11	J	60	ARG
13	L	62	ASP
13	L	83	LYS

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Mol	Chain	Res	Type
14	M	18	ASP
14	M	38	THR
15	N	6	GLY
16	O	52	THR
19	R	36	GLU
19	R	58	GLU
20	S	109	VAL
22	V	10	THR
3	A	32	SER
3	A	38	PRO
3	A	130	LEU
3	A	245	SER
3	A	252	LYS
4	B	53	PHE
4	B	59	TYR
4	B	195	ILE
5	C	149	PRO
5	C	167	ALA
6	D	89	VAL
6	D	109	PRO
7	E	59	LYS
7	E	170	ARG
7	E	172	LYS
10	I	28	GLY
10	I	88	GLY
11	J	17	THR
12	K	28	GLU
13	L	32	ASN
13	L	38	LYS
19	R	76	ASN
19	R	77	GLU
20	S	13	GLN
20	S	98	GLU
20	S	150	ILE
20	S	167	ILE
21	T	84	LYS
23	W	36	VAL
3	A	31	LYS
3	A	135	ILE
3	A	255	LEU
4	B	99	TYR
4	B	152	GLY

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Mol	Chain	Res	Type
6	D	38	MET
7	E	90	VAL
10	I	51	GLU
13	L	63	ILE
13	L	84	ALA
19	R	52	PRO
20	S	124	PRO
20	S	129	GLU
20	S	138	PRO
4	B	214	SER
7	E	38	ASN
7	E	107	VAL
12	K	77	THR
18	Q	51	ALA
20	S	156	VAL
22	V	6	ILE
26	3	34	ALA
3	A	224	VAL
8	G	67	GLY
20	S	65	VAL
8	G	85	ILE
13	L	97	GLY
4	B	75	GLY
4	B	96	VAL
10	I	102	VAL
20	S	118	GLY
3	A	115	ILE
3	A	151	GLY
5	C	155	VAL

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	A	109/224 (49%)	100 (92%)	9 (8%)	11 39
4	B	156/177 (88%)	125 (80%)	31 (20%)	1 5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	C	103/169 (61%)	86 (84%)	17 (16%)	2 11
6	D	14/158 (9%)	12 (86%)	2 (14%)	3 17
7	E	56/155 (36%)	41 (73%)	15 (27%)	0 2
8	G	110/123 (89%)	88 (80%)	22 (20%)	1 5
9	H	89/100 (89%)	77 (86%)	12 (14%)	4 19
10	I	61/112 (54%)	45 (74%)	16 (26%)	0 2
11	J	99/119 (83%)	84 (85%)	15 (15%)	3 15
12	K	89/102 (87%)	72 (81%)	17 (19%)	1 6
13	L	36/95 (38%)	26 (72%)	10 (28%)	0 2
14	M	82/102 (80%)	63 (77%)	19 (23%)	1 3
15	N	92/98 (94%)	82 (89%)	10 (11%)	6 28
16	O	72/86 (84%)	58 (81%)	14 (19%)	1 6
17	P	90/94 (96%)	79 (88%)	11 (12%)	5 22
18	Q	46/82 (56%)	40 (87%)	6 (13%)	4 20
19	R	43/90 (48%)	30 (70%)	13 (30%)	0 2
20	S	84/190 (44%)	73 (87%)	11 (13%)	4 20
21	T	50/75 (67%)	40 (80%)	10 (20%)	1 5
22	V	33/62 (53%)	25 (76%)	8 (24%)	0 3
23	W	52/53 (98%)	44 (85%)	8 (15%)	2 14
24	Z	39/51 (76%)	34 (87%)	5 (13%)	4 20
25	2	37/40 (92%)	34 (92%)	3 (8%)	11 41
26	3	30/57 (53%)	26 (87%)	4 (13%)	4 19
All	All	1672/2614 (64%)	1384 (83%)	288 (17%)	2 10

All (288) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	46	GLN
3	A	54	HIS
3	A	86	ASN
3	A	88	SER
3	A	90	ASN
3	A	110	LEU
3	A	116	VAL

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Mol	Chain	Res	Type
3	A	123	ASP
3	A	143	ASN
4	B	15	VAL
4	B	41	VAL
4	B	43	VAL
4	B	44	ASP
4	B	49	ILE
4	B	57	LYS
4	B	62	ASP
4	B	64	LYS
4	B	92	ARG
4	B	101	VAL
4	B	104	GLU
4	B	105	VAL
4	B	106	SER
4	B	107	VAL
4	B	118	VAL
4	B	136	GLN
4	B	142	SER
4	B	149	ARG
4	B	156	MET
4	B	158	SER
4	B	161	SER
4	B	168	LYS
4	B	180	VAL
4	B	184	GLU
4	B	186	VAL
4	B	196	LEU
4	B	201	VAL
4	B	208	LEU
4	B	209	VAL
4	B	214	SER
4	B	215	ILE
5	C	5	ASP
5	C	10	ASP
5	C	39	LEU
5	C	51	VAL
5	C	57	VAL
5	C	70	THR
5	C	105	MET
5	C	108	LEU
5	C	125	VAL

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Mol	Chain	Res	Type
5	C	136	THR
5	C	144	SER
5	C	145	THR
5	C	146	LEU
5	C	147	GLU
5	C	176	THR
5	C	179	GLN
5	C	181	LEU
6	D	24	SER
6	D	132	VAL
7	E	19	PHE
7	E	36	THR
7	E	37	LEU
7	E	44	LYS
7	E	63	THR
7	E	67	THR
7	E	74	ASN
7	E	75	MET
7	E	80	SER
7	E	92	VAL
7	E	113	VAL
7	E	131	VAL
7	E	136	ILE
7	E	139	GLU
7	E	149	ARG
8	G	1	MET
8	G	2	ARG
8	G	9	GLU
8	G	18	VAL
8	G	24	GLN
8	G	28	ARG
8	G	29	LEU
8	G	44	THR
8	G	46	THR
8	G	58	ILE
8	G	66	THR
8	G	68	ASN
8	G	71	THR
8	G	72	ASP
8	G	73	LYS
8	G	95	ARG
8	G	96	THR

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Mol	Chain	Res	Type
8	G	101	LEU
8	G	105	SER
8	G	114	ARG
8	G	117	GLU
8	G	143	LEU
9	H	8	LEU
9	H	10	VAL
9	H	21	THR
9	H	23	LYS
9	H	32	THR
9	H	39	ILE
9	H	41	CYS
9	H	54	LYS
9	H	67	SER
9	H	69	VAL
9	H	77	ILE
9	H	96	THR
10	I	2	LYS
10	I	6	LEU
10	I	21	ARG
10	I	25	THR
10	I	31	SER
10	I	38	GLN
10	I	47	ARG
10	I	50	PHE
10	I	78	ASN
10	I	82	LEU
10	I	84	LYS
10	I	95	LEU
10	I	98	GLU
10	I	112	LEU
10	I	114	ASN
10	I	122	THR
11	J	12	GLN
11	J	14	ARG
11	J	18	THR
11	J	26	TYR
11	J	27	VAL
11	J	37	THR
11	J	41	TRP
11	J	47	ILE
11	J	60	ARG

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Mol	Chain	Res	Type
11	J	72	THR
11	J	87	LYS
11	J	96	VAL
11	J	111	GLU
11	J	122	SER
11	J	134	ARG
12	K	6	LEU
12	K	9	THR
12	K	16	MET
12	K	24	LEU
12	K	33	THR
12	K	42	SER
12	K	45	GLU
12	K	55	ASP
12	K	61	ASN
12	K	65	THR
12	K	82	LEU
12	K	89	ILE
12	K	100	TYR
12	K	101	THR
12	K	105	LYS
12	K	109	ARG
12	K	118	ILE
13	L	11	ARG
13	L	22	LEU
13	L	30	ARG
13	L	45	ILE
13	L	47	ASP
13	L	52	THR
13	L	92	ILE
13	L	94	PHE
13	L	96	ARG
13	L	99	TYR
14	M	11	THR
14	M	13	SER
14	M	14	GLN
14	M	15	LEU
14	M	17	THR
14	M	18	ASP
14	M	19	LEU
14	M	23	ARG
14	M	27	THR

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Mol	Chain	Res	Type
14	M	41	ARG
14	M	48	VAL
14	M	52	ARG
14	M	53	ARG
14	M	58	SER
14	M	74	ARG
14	M	80	THR
14	M	94	VAL
14	M	100	TYR
14	M	102	LEU
15	N	16	LYS
15	N	18	ILE
15	N	22	LYS
15	N	29	HIS
15	N	41	LYS
15	N	42	SER
15	N	58	ARG
15	N	70	ARG
15	N	88	ILE
15	N	90	ILE
16	O	1	MET
16	O	10	LYS
16	O	18	GLN
16	O	22	VAL
16	O	23	GLU
16	O	28	ASN
16	O	34	THR
16	O	48	VAL
16	O	70	LYS
16	O	72	THR
16	O	75	THR
16	O	84	ARG
16	O	95	LEU
16	O	98	ASP
17	P	2	GLU
17	P	24	ILE
17	P	38	LEU
17	P	43	SER
17	P	44	SER
17	P	64	MET
17	P	66	THR
17	P	82	LEU

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Mol	Chain	Res	Type
17	P	85	PHE
17	P	100	THR
17	P	109	ASP
18	Q	17	SER
18	Q	27	PHE
18	Q	31	THR
18	Q	34	ASN
18	Q	68	TYR
18	Q	87	ILE
19	R	3	ILE
19	R	24	ILE
19	R	26	THR
19	R	31	ASP
19	R	33	VAL
19	R	38	VAL
19	R	43	LYS
19	R	59	THR
19	R	60	GLU
19	R	65	VAL
19	R	79	THR
19	R	84	LYS
19	R	100	GLU
20	S	19	LYS
20	S	26	LYS
20	S	55	VAL
20	S	69	THR
20	S	70	ILE
20	S	72	VAL
20	S	101	THR
20	S	108	LEU
20	S	123	GLN
20	S	154	LEU
20	S	155	THR
21	T	23	ASP
21	T	24	SER
21	T	26	SER
21	T	28	ARG
21	T	33	ARG
21	T	43	SER
21	T	51	THR
21	T	61	ARG
21	T	67	LEU

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Mol	Chain	Res	Type
21	T	72	ASP
22	V	16	GLU
22	V	20	SER
22	V	32	LEU
22	V	37	LEU
22	V	40	THR
22	V	52	ARG
22	V	56	VAL
22	V	62	ILE
23	W	7	THR
23	W	12	VAL
23	W	22	THR
23	W	29	LYS
23	W	36	VAL
23	W	44	ARG
23	W	46	GLN
23	W	54	VAL
24	Z	7	ARG
24	Z	18	THR
24	Z	24	VAL
24	Z	38	LYS
24	Z	43	VAL
25	2	5	THR
25	2	21	LYS
25	2	43	LEU
26	3	14	VAL
26	3	29	THR
26	3	52	LYS
26	3	54	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	53	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	2693/2923 (92%)	619 (22%)	28 (1%)
2	Y	113/114 (99%)	16 (14%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	2806/3037 (92%)	635 (22%)	28 (0%)

All (635) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	X	9	U
1	X	14	A
1	X	15	G
1	X	25	U
1	X	34	U
1	X	39	C
1	X	51	G
1	X	60	U
1	X	64	A
1	X	67	G
1	X	70	G
1	X	75	G
1	X	79	U
1	X	80	G
1	X	90	A
1	X	91	A
1	X	96	G
1	X	101	G
1	X	102	A
1	X	109	G
1	X	111	U
1	X	117	A
1	X	118	A
1	X	119	U
1	X	120	G
1	X	124	A
1	X	133	A
1	X	139	U
1	X	142	G
1	X	150	A
1	X	152	C
1	X	154	A
1	X	156	A
1	X	157	U
1	X	159	U
1	X	163	U
1	X	164	A

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Mol	Chain	Res	Type
1	X	165	C
1	X	166	A
1	X	167	U
1	X	168	A
1	X	169	G
1	X	170	C
1	X	172	U
1	X	173	A
1	X	175	C
1	X	176	A
1	X	177	G
1	X	178	A
1	X	179	A
1	X	180	G
1	X	182	C
1	X	183	A
1	X	184	C
1	X	189	G
1	X	199	A
1	X	202	A
1	X	207	A
1	X	218	G
1	X	219	A
1	X	225	A
1	X	229	A
1	X	233	U
1	X	235	G
1	X	236	A
1	X	251	G
1	X	253	G
1	X	255	G
1	X	268	A
1	X	269	G
1	X	284	C
1	X	285	U
1	X	286	U
1	X	287	G
1	X	288	C
1	X	289	U
1	X	290	U
1	X	291	G
1	X	298	U

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Mol	Chain	Res	Type
1	X	300	G
1	X	301	U
1	X	302	A
1	X	303	G
1	X	310	C
1	X	311	U
1	X	313	U
1	X	319	G
1	X	320	U
1	X	321	U
1	X	322	A
1	X	324	A
1	X	328	G
1	X	329	A
1	X	330	C
1	X	332	A
1	X	338	G
1	X	342	A
1	X	344	U
1	X	345	C
1	X	354	A
1	X	359	A
1	X	364	A
1	X	372	A
1	X	373	A
1	X	375	A
1	X	389	A
1	X	391	A
1	X	392	U
1	X	399	U
1	X	401	U
1	X	404	U
1	X	405	G
1	X	407	G
1	X	410	G
1	X	413	C
1	X	416	G
1	X	417	A
1	X	429	C
1	X	432	G
1	X	444	C
1	X	447	A

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Mol	Chain	Res	Type
1	X	450	C
1	X	451	U
1	X	452	G
1	X	457	G
1	X	458	A
1	X	474	A
1	X	480	U
1	X	486	G
1	X	497	U
1	X	501	C
1	X	502	C
1	X	503	A
1	X	504	G
1	X	506	A
1	X	507	C
1	X	519	G
1	X	526	A
1	X	527	G
1	X	539	G
1	X	543	G
1	X	549	U
1	X	550	A
1	X	553	A
1	X	554	C
1	X	555	C
1	X	566	U
1	X	567	G
1	X	573	A
1	X	575	G
1	X	576	U
1	X	577	A
1	X	578	G
1	X	583	A
1	X	590	U
1	X	591	A
1	X	592	A
1	X	593	U
1	X	594	G
1	X	599	A
1	X	606	G
1	X	616	G
1	X	618	A

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Mol	Chain	Res	Type
1	X	629	A
1	X	630	G
1	X	644	C
1	X	646	A
1	X	647	G
1	X	657	U
1	X	658	A
1	X	659	A
1	X	660	A
1	X	661	U
1	X	662	G
1	X	666	A
1	X	667	G
1	X	677	A
1	X	682	A
1	X	683	G
1	X	690	U
1	X	691	A
1	X	698	U
1	X	699	U
1	X	700	A
1	X	716	C
1	X	722	A
1	X	727	G
1	X	731	U
1	X	746	G
1	X	757	G
1	X	758	G
1	X	766	G
1	X	767	A
1	X	773	G
1	X	775	A
1	X	783	G
1	X	784	A
1	X	785	C
1	X	790	G
1	X	792	U
1	X	793	G
1	X	802	G
1	X	809	A
1	X	813	G
1	X	820	G

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Mol	Chain	Res	Type
1	X	824	A
1	X	827	A
1	X	829	U
1	X	830	U
1	X	835	U
1	X	836	C
1	X	837	G
1	X	838	A
1	X	845	A
1	X	850	G
1	X	851	C
1	X	857	C
1	X	864	A
1	X	872	U
1	X	890	G
1	X	904	G
1	X	911	A
1	X	921	C
1	X	924	G
1	X	926	G
1	X	938	G
1	X	944	G
1	X	945	A
1	X	946	A
1	X	947	U
1	X	955	A
1	X	959	C
1	X	970	U
1	X	975	U
1	X	977	A
1	X	985	A
1	X	989	A
1	X	990	G
1	X	997	G
1	X	1005	G
1	X	1017	A
1	X	1018	A
1	X	1027	A
1	X	1034	A
1	X	1040	A
1	X	1055	A
1	X	1056	U

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Mol	Chain	Res	Type
1	X	1057	A
1	X	1066	G
1	X	1069	G
1	X	1070	A
1	X	1077	U
1	X	1085	U
1	X	1086	G
1	X	1087	C
1	X	1090	A
1	X	1091	G
1	X	1092	A
1	X	1093	C
1	X	1097	U
1	X	1145	U
1	X	1146	C
1	X	1147	A
1	X	1148	C
1	X	1149	U
1	X	1150	A
1	X	1151	G
1	X	1155	A
1	X	1156	G
1	X	1161	A
1	X	1175	G
1	X	1176	U
1	X	1177	A
1	X	1178	C
1	X	1179	C
1	X	1186	A
1	X	1195	A
1	X	1199	A
1	X	1200	A
1	X	1214	C
1	X	1218	G
1	X	1220	A
1	X	1258	A
1	X	1262	U
1	X	1274	G
1	X	1278	G
1	X	1285	A
1	X	1291	A
1	X	1293	U

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Mol	Chain	Res	Type
1	X	1294	G
1	X	1300	G
1	X	1309	G
1	X	1310	A
1	X	1312	A
1	X	1313	G
1	X	1337	A
1	X	1338	U
1	X	1339	U
1	X	1342	C
1	X	1343	U
1	X	1347	G
1	X	1348	U
1	X	1349	U
1	X	1350	U
1	X	1358	A
1	X	1366	U
1	X	1377	U
1	X	1382	C
1	X	1401	G
1	X	1402	A
1	X	1405	G
1	X	1414	G
1	X	1415	A
1	X	1416	U
1	X	1421	A
1	X	1422	A
1	X	1429	G
1	X	1432	A
1	X	1433	U
1	X	1437	U
1	X	1446	U
1	X	1447	A
1	X	1449	A
1	X	1450	A
1	X	1451	U
1	X	1453	G
1	X	1454	U
1	X	1460	U
1	X	1462	G
1	X	1463	A
1	X	1464	U

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Mol	Chain	Res	Type
1	X	1465	G
1	X	1466	G
1	X	1467	G
1	X	1469	G
1	X	1471	A
1	X	1472	C
1	X	1477	U
1	X	1489	A
1	X	1490	G
1	X	1491	C
1	X	1494	G
1	X	1495	C
1	X	1496	G
1	X	1497	A
1	X	1498	U
1	X	1503	U
1	X	1505	G
1	X	1509	G
1	X	1510	U
1	X	1511	C
1	X	1513	A
1	X	1514	A
1	X	1515	G
1	X	1516	C
1	X	1519	U
1	X	1522	G
1	X	1525	U
1	X	1526	G
1	X	1527	A
1	X	1528	G
1	X	1531	U
1	X	1541	C
1	X	1542	C
1	X	1543	G
1	X	1544	G
1	X	1546	A
1	X	1547	C
1	X	1551	U
1	X	1557	C
1	X	1559	G
1	X	1560	A
1	X	1561	G

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Mol	Chain	Res	Type
1	X	1568	U
1	X	1569	G
1	X	1570	G
1	X	1574	G
1	X	1575	A
1	X	1576	A
1	X	1577	G
1	X	1593	G
1	X	1594	U
1	X	1603	U
1	X	1605	A
1	X	1606	C
1	X	1607	A
1	X	1613	G
1	X	1616	A
1	X	1623	U
1	X	1625	U
1	X	1628	A
1	X	1629	U
1	X	1630	A
1	X	1631	G
1	X	1636	U
1	X	1637	A
1	X	1638	G
1	X	1639	G
1	X	1650	G
1	X	1652	A
1	X	1653	A
1	X	1654	A
1	X	1662	A
1	X	1684	A
1	X	1690	A
1	X	1691	G
1	X	1692	C
1	X	1695	G
1	X	1718	G
1	X	1721	A
1	X	1730	C
1	X	1732	U
1	X	1738	C
1	X	1740	G
1	X	1744	A

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Mol	Chain	Res	Type
1	X	1756	U
1	X	1757	U
1	X	1758	A
1	X	1759	G
1	X	1760	G
1	X	1761	G
1	X	1762	U
1	X	1766	C
1	X	1767	G
1	X	1768	C
1	X	1770	C
1	X	1771	A
1	X	1772	G
1	X	1789	A
1	X	1790	G
1	X	1791	G
1	X	1800	A
1	X	1808	U
1	X	1809	C
1	X	1818	A
1	X	1826	G
1	X	1827	C
1	X	1828	U
1	X	1837	A
1	X	1839	G
1	X	1843	U
1	X	1856	A
1	X	1865	C
1	X	1875	A
1	X	1886	A
1	X	1893	A
1	X	1902	G
1	X	1908	A
1	X	1911	A
1	X	1912	A
1	X	1930	G
1	X	1932	C
1	X	1933	G
1	X	1935	C
1	X	1952	C
1	X	1953	U
1	X	1954	A

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Mol	Chain	Res	Type
1	X	1956	G
1	X	1958	U
1	X	1963	A
1	X	1964	A
1	X	1965	A
1	X	1982	U
1	X	1991	G
1	X	1993	A
1	X	1994	C
1	X	1997	A
1	X	1998	A
1	X	1999	G
1	X	2007	G
1	X	2009	U
1	X	2017	C
1	X	2020	U
1	X	2024	A
1	X	2048	G
1	X	2050	A
1	X	2054	G
1	X	2058	A
1	X	2059	G
1	X	2060	A
1	X	2070	C
1	X	2077	C
1	X	2082	C
1	X	2083	G
1	X	2087	A
1	X	2088	G
1	X	2089	A
1	X	2094	G
1	X	2096	G
1	X	2107	G
1	X	2110	G
1	X	2225	A
1	X	2229	C
1	X	2230	G
1	X	2231	C
1	X	2233	C
1	X	2237	U
1	X	2238	U
1	X	2239	A

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Mol	Chain	Res	Type
1	X	2240	U
1	X	2241	C
1	X	2245	G
1	X	2246	U
1	X	2250	A
1	X	2252	A
1	X	2265	G
1	X	2266	G
1	X	2270	U
1	X	2290	C
1	X	2295	A
1	X	2300	A
1	X	2306	G
1	X	2310	C
1	X	2314	A
1	X	2316	G
1	X	2332	U
1	X	2333	U
1	X	2334	G
1	X	2338	A
1	X	2347	A
1	X	2349	A
1	X	2352	G
1	X	2354	A
1	X	2361	U
1	X	2362	A
1	X	2363	A
1	X	2374	C
1	X	2377	C
1	X	2398	G
1	X	2399	G
1	X	2406	G
1	X	2410	G
1	X	2412	C
1	X	2417	U
1	X	2418	G
1	X	2419	A
1	X	2420	U
1	X	2429	U
1	X	2433	C
1	X	2434	A
1	X	2450	U

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Mol	Chain	Res	Type
1	X	2452	A
1	X	2454	C
1	X	2456	G
1	X	2457	A
1	X	2461	A
1	X	2468	C
1	X	2472	G
1	X	2475	A
1	X	2486	A
1	X	2495	A
1	X	2497	G
1	X	2500	U
1	X	2503	A
1	X	2514	G
1	X	2525	C
1	X	2529	G
1	X	2532	G
1	X	2545	A
1	X	2546	U
1	X	2547	C
1	X	2556	G
1	X	2561	C
1	X	2581	U
1	X	2589	U
1	X	2591	A
1	X	2593	A
1	X	2594	G
1	X	2600	C
1	X	2612	U
1	X	2613	C
1	X	2629	A
1	X	2636	U
1	X	2640	U
1	X	2641	A
1	X	2642	U
1	X	2656	A
1	X	2661	A
1	X	2663	U
1	X	2682	G
1	X	2688	G
1	X	2690	G
1	X	2698	A

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Mol	Chain	Res	Type
1	X	2712	G
1	X	2716	U
1	X	2717	A
1	X	2732	A
1	X	2741	G
1	X	2745	G
1	X	2747	U
1	X	2751	U
1	X	2753	U
1	X	2760	A
1	X	2766	U
1	X	2771	G
1	X	2775	A
1	X	2776	A
1	X	2778	G
1	X	2784	A
1	X	2791	A
1	X	2792	A
1	X	2805	A
1	X	2806	U
1	X	2807	G
1	X	2817	A
1	X	2818	A
1	X	2820	U
1	X	2821	U
1	X	2824	G
1	X	2832	A
1	X	2840	A
1	X	2855	A
1	X	2870	A
1	X	2877	G
1	X	2887	G
1	X	2892	G
1	X	2900	C
1	X	2905	C
1	X	2913	G
2	Y	10	U
2	Y	11	A
2	Y	23	U
2	Y	24	C
2	Y	27	A
2	Y	39	G

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Mol	Chain	Res	Type
2	Y	40	C
2	Y	42	G
2	Y	43	A
2	Y	54	U
2	Y	55	A
2	Y	87	G
2	Y	88	U
2	Y	106	U
2	Y	108	G
2	Y	114	C

All (28) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	X	38	A
1	X	90	A
1	X	149	U
1	X	165	C
1	X	235	G
1	X	285	U
1	X	525	A
1	X	614	U
1	X	660	A
1	X	872	U
1	X	944	G
1	X	969	A
1	X	1028	G
1	X	1091	G
1	X	1490	G
1	X	1510	U
1	X	1521	A
1	X	1568	U
1	X	1576	A
1	X	1602	U
1	X	1629	U
1	X	1636	U
1	X	1885	G
1	X	1901	C
1	X	1952	C
1	X	2062	G
1	X	2449	C
1	X	2474	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 398 ligands modelled in this entry, 380 are monoatomic - leaving 18 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	$\#\|Z\| > 2$
31	SPD	X	3364	-	9,9,9	0.24	0	8,8,8	0.30	0
28	MPD	X	3006	-	7,7,7	0.73	0	9,10,10	0.49	0
28	MPD	X	3009	-	7,7,7	0.51	0	9,10,10	0.24	0
28	MPD	X	3007	-	7,7,7	0.58	0	9,10,10	0.11	0
28	MPD	X	3002	-	7,7,7	0.76	0	9,10,10	0.45	0
33	EPE	L	201	-	15,15,15	0.77	1 (6%)	18,20,20	0.58	0
31	SPD	X	3363	-	9,9,9	0.17	0	8,8,8	0.18	0
28	MPD	X	3003	-	7,7,7	0.58	0	9,10,10	0.26	0
32	EOH	X	3368	-	2,2,2	0.53	0	1,1,1	0.65	0
32	EOH	X	3366	-	2,2,2	0.58	0	1,1,1	0.62	0
31	SPD	S	301	-	9,9,9	0.19	0	8,8,8	0.42	0
28	MPD	X	3004	-	7,7,7	0.57	0	9,10,10	0.20	0
28	MPD	X	3005	-	7,7,7	0.81	0	9,10,10	1.13	0
31	SPD	X	3365	-	9,9,9	0.30	0	8,8,8	0.46	0
28	MPD	X	3008	-	7,7,7	0.84	0	9,10,10	0.28	0
31	SPD	X	3362	-	9,9,9	0.17	0	8,8,8	0.24	0
32	EOH	X	3367	-	2,2,2	0.48	0	1,1,1	0.75	0
27	TEL	X	3001	-	59,62,62	0.62	1 (1%)	77,92,92	1.69	11 (14%)

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
31	SPD	X	3364	-	-	4/7/7/7	-
28	MPD	X	3006	-	-	1/5/5/5	-
28	MPD	X	3009	-	-	4/5/5/5	-
28	MPD	X	3007	-	-	0/5/5/5	-
28	MPD	X	3002	-	-	1/5/5/5	-
27	TEL	X	3001	-	1/1/19/19	28/73/108/108	0/4/5/5
31	SPD	X	3363	-	-	2/7/7/7	-
28	MPD	X	3003	-	-	1/5/5/5	-
33	EPE	L	201	-	-	3/9/19/19	0/1/1/1
28	MPD	X	3004	-	-	1/5/5/5	-
28	MPD	X	3005	-	-	4/5/5/5	-
31	SPD	X	3365	-	-	5/7/7/7	-
28	MPD	X	3008	-	-	3/5/5/5	-
31	SPD	X	3362	-	-	3/7/7/7	-
31	SPD	S	301	-	-	2/7/7/7	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	X	3001	TEL	C21-C26	3.16	1.57	1.52
33	L	201	EPE	C10-S	-2.76	1.73	1.77

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	X	3001	TEL	O5-C2-C4	-6.85	90.45	105.63
27	X	3001	TEL	O5-C2-C3	-5.54	97.55	103.16
27	X	3001	TEL	C2-O5-C10	-4.57	105.67	109.29
27	X	3001	TEL	O32-C28-C24	4.21	114.97	105.71
27	X	3001	TEL	O9-C4-C2	3.34	113.02	105.48
27	X	3001	TEL	O29-C26-C21	-3.28	114.52	120.68
27	X	3001	TEL	O48-C44-C49	2.82	114.80	109.77
27	X	3001	TEL	C25-C21-C26	2.80	117.09	111.63
27	X	3001	TEL	O29-C26-C30	-2.48	117.08	120.60
27	X	3001	TEL	C40-C36-N31	-2.47	105.32	107.91
27	X	3001	TEL	O32-C28-C33	-2.20	102.79	110.75

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
27	X	3001	TEL	C21

All (62) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
28	X	3008	MPD	C1-C2-C3-C4
28	X	3008	MPD	O2-C2-C3-C4
33	L	201	EPE	C9-C10-S-O1S
28	X	3009	MPD	C2-C3-C4-O4
27	X	3001	TEL	C1-C2-C4-O9
27	X	3001	TEL	O5-C2-C4-O9
27	X	3001	TEL	C2-C3-C7-C13
27	X	3001	TEL	N6-C3-C7-C13
27	X	3001	TEL	O18-C13-C19-C23
27	X	3001	TEL	O32-C28-C34-C30
27	X	3001	TEL	C26-C30-C34-C28
27	X	3001	TEL	C35-C30-C34-C28
31	X	3362	SPD	C8-C7-N6-C5
27	X	3001	TEL	O45-C42-O39-C34
33	L	201	EPE	C9-C10-S-O3S
31	X	3363	SPD	C4-C5-N6-C7
31	X	3362	SPD	C4-C5-N6-C7
27	X	3001	TEL	C19-C13-C7-C3
31	X	3365	SPD	C3-C4-C5-N6
27	X	3001	TEL	N6-C3-C7-C12
27	X	3001	TEL	C2-C3-C7-C12
31	X	3365	SPD	C4-C5-N6-C7
27	X	3001	TEL	C54-C49-N53-C58
31	X	3364	SPD	C3-C4-C5-N6
31	X	3362	SPD	C2-C3-C4-C5
31	X	3364	SPD	C2-C3-C4-C5
27	X	3001	TEL	O5-C2-C4-C8
28	X	3009	MPD	O2-C2-C3-C4
27	X	3001	TEL	O9-C4-C8-C14
31	X	3365	SPD	C8-C7-N6-C5
27	X	3001	TEL	C19-C13-C7-C12
27	X	3001	TEL	C2-C4-C8-C14
27	X	3001	TEL	C24-C28-C34-C30
27	X	3001	TEL	C24-C28-C34-O39
28	X	3005	MPD	C2-C3-C4-C5
28	X	3006	MPD	C2-C3-C4-C5
28	X	3003	MPD	C2-C3-C4-C5
27	X	3001	TEL	C1-C2-C4-C8

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Mol	Chain	Res	Type	Atoms
27	X	3001	TEL	C36-C40-C43-C47
27	X	3001	TEL	O18-C13-C7-C3
27	X	3001	TEL	O18-C13-C7-C12
33	L	201	EPE	C9-C10-S-O2S
28	X	3008	MPD	CM-C2-C3-C4
28	X	3005	MPD	CM-C2-C3-C4
28	X	3009	MPD	C1-C2-C3-C4
28	X	3009	MPD	CM-C2-C3-C4
27	X	3001	TEL	C26-C30-C34-O39
28	X	3004	MPD	C1-C2-C3-C4
27	X	3001	TEL	C17-C22-C27-N31
31	S	301	SPD	C4-C5-N6-C7
27	X	3001	TEL	C7-C13-C19-C23
31	X	3364	SPD	C4-C5-N6-C7
31	X	3364	SPD	C8-C7-N6-C5
28	X	3002	MPD	O2-C2-C3-C4
28	X	3005	MPD	O2-C2-C3-C4
31	X	3365	SPD	C2-C3-C4-C5
31	S	301	SPD	C8-C7-N6-C5
31	X	3365	SPD	N1-C2-C3-C4
27	X	3001	TEL	C33-C28-C34-O39
31	X	3363	SPD	N1-C2-C3-C4
28	X	3005	MPD	C2-C3-C4-O4
27	X	3001	TEL	O18-C13-C19-C24

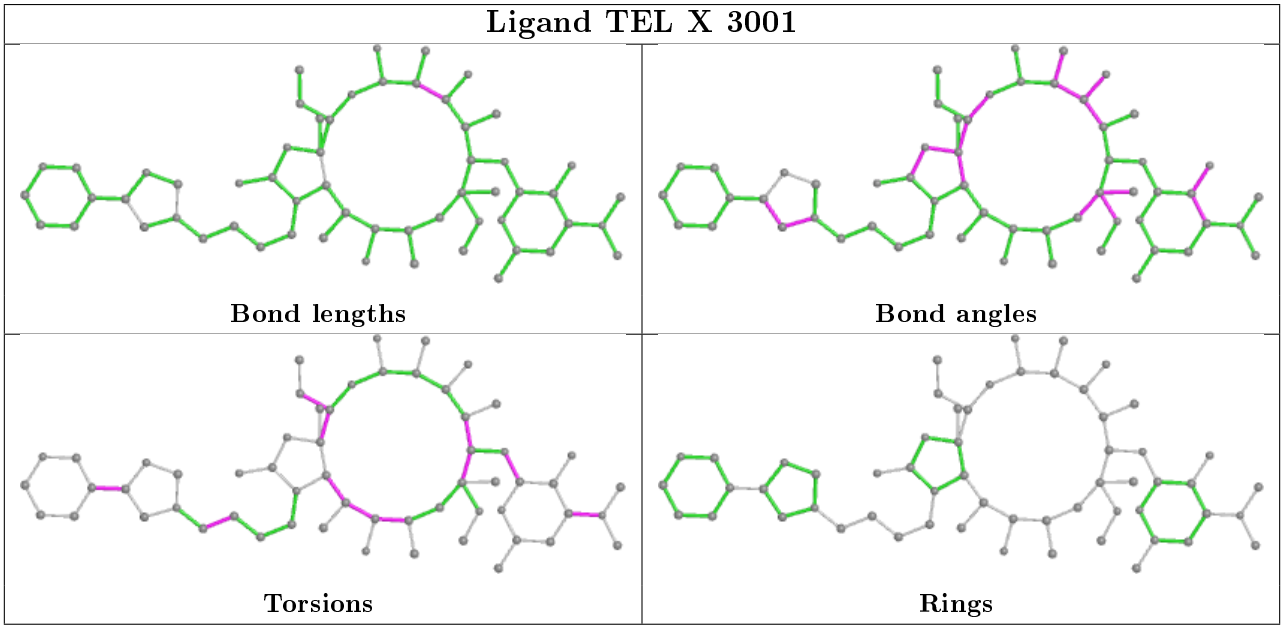
There are no ring outliers.

11 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	X	3364	SPD	1	0
28	X	3006	MPD	1	0
28	X	3009	MPD	1	0
28	X	3007	MPD	2	0
28	X	3002	MPD	1	0
28	X	3003	MPD	3	0
31	S	301	SPD	1	0
28	X	3005	MPD	6	0
31	X	3365	SPD	4	0
28	X	3008	MPD	1	0
27	X	3001	TEL	13	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	X	2712/2923 (92%)	-0.40	10 (0%) 92 91	27, 74, 174, 288	0
2	Y	114/114 (100%)	-0.53	0 100 100	48, 98, 151, 203	0
3	A	269/277 (97%)	-0.03	16 (5%) 22 24	56, 101, 146, 177	0
4	B	215/220 (97%)	-0.18	1 (0%) 91 90	34, 49, 101, 155	0
5	C	200/207 (96%)	-0.29	1 (0%) 91 90	40, 65, 112, 165	0
6	D	160/179 (89%)	0.27	21 (13%) 3 5	88, 155, 209, 263	0
7	E	156/178 (87%)	-0.19	11 (7%) 16 19	71, 131, 190, 205	0
8	G	145/145 (100%)	0.16	4 (2%) 53 52	36, 51, 83, 115	0
9	H	122/122 (100%)	-0.13	3 (2%) 57 56	57, 75, 116, 154	0
10	I	131/146 (89%)	-0.12	4 (3%) 49 48	22, 78, 139, 210	0
11	J	141/144 (97%)	0.55	12 (8%) 10 13	43, 73, 162, 258	0
12	K	119/122 (97%)	-0.26	0 100 100	31, 57, 129, 169	0
13	L	109/119 (91%)	-0.54	1 (0%) 84 83	55, 96, 149, 205	0
14	M	110/116 (94%)	-0.26	0 100 100	46, 69, 127, 189	0
15	N	116/118 (98%)	-0.38	0 100 100	18, 45, 80, 106	0
16	O	102/102 (100%)	-0.46	0 100 100	23, 60, 93, 179	0
17	P	112/117 (95%)	0.20	2 (1%) 68 67	37, 50, 116, 177	0
18	Q	89/91 (97%)	0.28	7 (7%) 12 16	63, 93, 138, 173	0
19	R	101/105 (96%)	0.33	12 (11%) 4 6	54, 98, 196, 218	0
20	S	167/217 (76%)	-0.29	9 (5%) 25 27	48, 83, 170, 292	0
21	T	75/94 (79%)	0.45	3 (4%) 38 38	44, 65, 106, 134	0
22	V	63/69 (91%)	-0.10	0 100 100	82, 107, 145, 185	0
23	W	58/59 (98%)	0.16	1 (1%) 70 69	26, 52, 98, 195	0
24	Z	45/58 (77%)	-0.18	1 (2%) 62 61	29, 60, 157, 181	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
25	2	44/45 (97%)	0.42	3 (6%) 17 20	59, 67, 97, 140	0
26	3	60/66 (90%)	-0.08	0 100 100	35, 57, 91, 96	0
All	All	5735/6153 (93%)	-0.23	122 (2%) 63 63	18, 75, 168, 292	0

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	D	83	MET	5.8
23	W	1	MET	5.8
20	S	146	THR	5.7
11	J	139	GLY	5.7
3	A	94	VAL	5.6
6	D	141	ILE	4.8
20	S	147	GLU	4.6
3	A	38	PRO	4.4
19	R	31	ASP	4.3
11	J	58	MET	4.1
6	D	113	ASP	4.1
20	S	109	VAL	4.1
6	D	142	ASP	3.9
7	E	100	GLY	3.9
6	D	127	ASN	3.7
18	Q	47	ASN	3.6
11	J	114	ALA	3.6
3	A	112	VAL	3.5
6	D	71	LYS	3.5
19	R	62	ALA	3.5
6	D	77	PHE	3.5
9	H	41	CYS	3.4
6	D	72	LYS	3.4
1	X	2629	A	3.4
20	S	140	ALA	3.4
3	A	78	VAL	3.3
11	J	140	GLU	3.3
3	A	79	ASP	3.3
11	J	138	GLY	3.3
3	A	36	PRO	3.3
8	G	87	SER	3.2
9	H	111	PHE	3.2
19	R	34	VAL	3.1
21	T	60	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
7	E	55	PRO	3.1
6	D	63	GLN	3.1
6	D	162	THR	3.1
7	E	168	TYR	3.0
11	J	57	TYR	3.0
1	X	1147	A	3.0
19	R	69	GLN	3.0
3	A	93	LEU	3.0
18	Q	38	VAL	3.0
25	2	19	PHE	3.0
13	L	2	ILE	3.0
11	J	4	PRO	3.0
7	E	117	ALA	3.0
6	D	70	ALA	3.0
10	I	1	MET	3.0
18	Q	70	GLY	3.0
6	D	122	PHE	3.0
20	S	139	GLU	2.9
20	S	138	PRO	2.9
11	J	54	MET	2.8
1	X	2503	A	2.8
19	R	28	PRO	2.8
6	D	76	THR	2.8
19	R	24	ILE	2.8
19	R	79	THR	2.8
19	R	78	PRO	2.8
7	E	162	ILE	2.8
6	D	78	ARG	2.7
7	E	169	VAL	2.7
3	A	58	HIS	2.7
20	S	107	GLN	2.7
6	D	84	PRO	2.6
24	Z	27	MET	2.6
10	I	95	LEU	2.6
6	D	75	ALA	2.6
1	X	1993	A	2.6
11	J	59	LYS	2.6
19	R	33	VAL	2.5
3	A	62	TYR	2.5
20	S	110	GLY	2.5
3	A	81	ILE	2.5
25	2	17	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
11	J	3	LEU	2.5
18	Q	46	PHE	2.5
1	X	942	C	2.5
1	X	1148	C	2.4
20	S	136	ASN	2.4
17	P	9	THR	2.4
19	R	58	GLU	2.4
17	P	102	HIS	2.4
4	B	180	VAL	2.4
6	D	32	ASP	2.3
18	Q	42	VAL	2.3
3	A	95	VAL	2.3
8	G	53	ASP	2.3
9	H	33	ALA	2.3
7	E	89	LEU	2.3
7	E	56	SER	2.3
3	A	254	THR	2.3
7	E	99	GLN	2.3
25	2	2	VAL	2.3
1	X	1602	U	2.3
1	X	1841	G	2.3
19	R	70	LEU	2.2
3	A	82	GLN	2.2
10	I	94	ALA	2.2
18	Q	27	PHE	2.2
21	T	75	VAL	2.2
21	T	69	ALA	2.2
3	A	63	ARG	2.2
6	D	158	THR	2.2
10	I	54	GLN	2.2
7	E	87	LEU	2.1
6	D	47	SER	2.1
1	X	945	A	2.1
6	D	140	GLU	2.1
8	G	106	ILE	2.1
8	G	122	LYS	2.1
11	J	60	ARG	2.1
6	D	73	SER	2.1
19	R	35	VAL	2.1
1	X	435	A	2.1
18	Q	43	GLU	2.0
3	A	47	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
3	A	218	PRO	2.0
11	J	131	PHE	2.0
7	E	90	VAL	2.0
5	C	124	THR	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
30	MN	X	3151	1/1	0.35	0.56	135,135,135,135	0
29	MG	X	3010	1/1	0.47	0.51	84,84,84,84	0
29	MG	X	3354	1/1	0.51	0.49	59,59,59,59	0
30	MN	X	3180	1/1	0.52	0.23	121,121,121,121	0
30	MN	X	3200	1/1	0.53	0.64	161,161,161,161	0
29	MG	X	3303	1/1	0.53	0.73	63,63,63,63	0
29	MG	X	3252	1/1	0.54	0.53	45,45,45,45	0
29	MG	T	101	1/1	0.55	0.36	44,44,44,44	0
30	MN	X	3040	1/1	0.56	0.55	100,100,100,100	0
29	MG	X	3260	1/1	0.56	0.54	64,64,64,64	0
30	MN	X	3218	1/1	0.58	0.22	128,128,128,128	0
30	MN	X	3272	1/1	0.58	0.52	156,156,156,156	0
30	MN	X	3036	1/1	0.59	0.34	96,96,96,96	0
29	MG	X	3226	1/1	0.60	0.45	64,64,64,64	0
29	MG	X	3335	1/1	0.60	0.28	81,81,81,81	0
29	MG	X	3316	1/1	0.62	0.12	38,38,38,38	0
31	SPD	S	301	10/10	0.63	0.39	67,67,67,67	0
29	MG	X	3022	1/1	0.65	1.09	62,62,62,62	0
32	EOH	X	3367	3/3	0.66	0.70	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
29	MG	X	3340	1/1	0.67	0.43	55,55,55,55	0
29	MG	X	3258	1/1	0.68	0.66	73,73,73,73	0
30	MN	X	3171	1/1	0.69	0.19	82,82,82,82	0
29	MG	X	3325	1/1	0.69	0.34	49,49,49,49	0
29	MG	X	3028	1/1	0.69	1.50	66,66,66,66	0
30	MN	X	3042	1/1	0.69	0.17	161,161,161,161	0
30	MN	X	3209	1/1	0.71	0.26	122,122,122,122	0
29	MG	X	3025	1/1	0.71	0.47	16,16,16,16	1
29	MG	Y	207	1/1	0.71	0.41	51,51,51,51	0
29	MG	X	3358	1/1	0.72	0.57	59,59,59,59	0
30	MN	X	3267	1/1	0.73	0.57	140,140,140,140	0
30	MN	X	3332	1/1	0.73	0.14	122,122,122,122	0
31	SPD	X	3364	10/10	0.74	0.26	80,80,80,80	0
30	MN	X	3051	1/1	0.74	0.58	120,120,120,120	0
29	MG	X	3349	1/1	0.74	0.73	74,74,74,74	0
30	MN	X	3181	1/1	0.75	0.52	121,121,121,121	0
29	MG	X	3357	1/1	0.75	0.40	51,51,51,51	0
30	MN	X	3032	1/1	0.76	0.46	122,122,122,122	0
30	MN	Y	205	1/1	0.76	0.24	132,132,132,132	0
29	MG	X	3360	1/1	0.76	1.35	78,78,78,78	0
29	MG	X	3014	1/1	0.76	0.41	26,26,26,26	1
30	MN	X	3182	1/1	0.76	0.24	117,117,117,117	0
29	MG	X	3276	1/1	0.77	0.66	51,51,51,51	0
30	MN	M	201	1/1	0.77	0.20	105,105,105,105	0
29	MG	X	3016	1/1	0.77	1.24	12,12,12,12	1
29	MG	X	3011	1/1	0.77	0.77	50,50,50,50	0
29	MG	X	3253	1/1	0.78	0.19	65,65,65,65	0
30	MN	X	3046	1/1	0.78	0.37	97,97,97,97	0
29	MG	X	3031	1/1	0.78	0.19	45,45,45,45	0
29	MG	X	3327	1/1	0.79	0.38	48,48,48,48	0
30	MN	X	3041	1/1	0.80	0.36	127,127,127,127	0
29	MG	X	3255	1/1	0.80	0.42	59,59,59,59	0
30	MN	X	3361	1/1	0.80	0.23	158,158,158,158	0
30	MN	X	3146	1/1	0.80	0.30	124,124,124,124	0
32	EOH	X	3368	3/3	0.81	0.71	55,55,55,55	0
29	MG	X	3273	1/1	0.81	0.26	78,78,78,78	0
29	MG	X	3308	1/1	0.81	0.51	44,44,44,44	0
29	MG	X	3274	1/1	0.81	0.96	44,44,44,44	0
30	MN	X	3205	1/1	0.81	0.10	141,141,141,141	0
30	MN	X	3247	1/1	0.81	0.18	104,104,104,104	0
29	MG	X	3020	1/1	0.81	0.97	40,40,40,40	0
30	MN	X	3058	1/1	0.81	0.49	113,113,113,113	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
30	MN	X	3175	1/1	0.81	0.07	111,111,111,111	0
30	MN	X	3092	1/1	0.81	0.56	103,103,103,103	0
30	MN	X	3152	1/1	0.81	0.37	104,104,104,104	0
29	MG	X	3018	1/1	0.81	1.05	42,42,42,42	0
30	MN	X	3037	1/1	0.81	0.58	131,131,131,131	0
30	MN	J	201	1/1	0.82	0.11	103,103,103,103	0
29	MG	B	301	1/1	0.82	0.35	46,46,46,46	0
29	MG	X	3235	1/1	0.82	0.63	62,62,62,62	0
29	MG	X	3282	1/1	0.82	0.41	43,43,43,43	0
30	MN	X	3091	1/1	0.83	0.27	78,78,78,78	0
29	MG	X	3030	1/1	0.83	0.38	48,48,48,48	0
29	MG	X	3339	1/1	0.83	0.38	66,66,66,66	0
30	MN	X	3170	1/1	0.83	0.39	70,70,70,70	0
31	SPD	X	3363	10/10	0.83	0.33	75,75,75,75	0
30	MN	X	3246	1/1	0.83	0.21	104,104,104,104	0
29	MG	X	3353	1/1	0.83	0.39	39,39,39,39	0
29	MG	X	3297	1/1	0.83	0.74	44,44,44,44	0
29	MG	C	301	1/1	0.83	0.13	31,31,31,31	0
29	MG	X	3249	1/1	0.83	0.28	59,59,59,59	0
29	MG	X	3259	1/1	0.84	1.00	63,63,63,63	0
30	MN	X	3220	1/1	0.84	0.92	153,153,153,153	0
30	MN	X	3033	1/1	0.84	0.28	106,106,106,106	0
30	MN	X	3101	1/1	0.84	0.26	83,83,83,83	0
30	MN	X	3185	1/1	0.84	0.32	112,112,112,112	0
30	MN	X	3094	1/1	0.85	0.57	94,94,94,94	0
29	MG	X	3347	1/1	0.85	0.41	37,37,37,37	0
29	MG	X	3231	1/1	0.85	0.67	64,64,64,64	0
29	MG	X	3348	1/1	0.85	0.57	46,46,46,46	0
29	MG	X	3275	1/1	0.85	0.63	29,29,29,29	0
29	MG	X	3191	1/1	0.85	0.84	79,79,79,79	0
30	MN	Y	208	1/1	0.85	0.57	173,173,173,173	0
29	MG	X	3024	1/1	0.85	0.42	31,31,31,31	1
29	MG	X	3343	1/1	0.85	1.28	53,53,53,53	0
29	MG	X	3230	1/1	0.85	0.28	71,71,71,71	0
30	MN	X	3206	1/1	0.85	0.51	133,133,133,133	0
30	MN	X	3065	1/1	0.86	0.40	76,76,76,76	0
30	MN	X	3271	1/1	0.86	0.21	140,140,140,140	0
30	MN	X	3237	1/1	0.86	0.50	87,87,87,87	0
30	MN	X	3117	1/1	0.86	0.28	67,67,67,67	0
30	MN	X	3084	1/1	0.86	0.21	72,72,72,72	0
29	MG	X	3315	1/1	0.86	0.37	60,60,60,60	0
29	MG	X	3229	1/1	0.86	1.16	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
30	MN	X	3144	1/1	0.86	0.40	127,127,127,127	0
30	MN	X	3164	1/1	0.86	0.12	103,103,103,103	0
29	MG	Y	206	1/1	0.87	0.48	45,45,45,45	0
30	MN	X	3198	1/1	0.87	1.22	162,162,162,162	0
30	MN	X	3183	1/1	0.87	0.29	128,128,128,128	0
29	MG	X	3224	1/1	0.87	1.04	70,70,70,70	0
29	MG	X	3324	1/1	0.87	0.27	55,55,55,55	0
30	MN	X	3112	1/1	0.87	0.35	77,77,77,77	0
30	MN	X	3265	1/1	0.87	0.36	148,148,148,148	0
30	MN	X	3135	1/1	0.87	0.15	99,99,99,99	0
29	MG	X	3301	1/1	0.87	0.15	30,30,30,30	0
30	MN	X	3266	1/1	0.88	0.37	147,147,147,147	0
29	MG	X	3333	1/1	0.88	0.21	45,45,45,45	0
29	MG	X	3225	1/1	0.88	0.54	56,56,56,56	0
30	MN	X	3199	1/1	0.88	0.46	132,132,132,132	0
30	MN	X	3239	1/1	0.88	0.18	154,154,154,154	0
30	MN	X	3204	1/1	0.88	0.37	141,141,141,141	0
29	MG	X	3021	1/1	0.88	0.27	56,56,56,56	0
30	MN	X	3148	1/1	0.88	0.35	112,112,112,112	0
32	EOH	X	3366	3/3	0.88	0.27	32,32,32,32	0
29	MG	G	201	1/1	0.88	0.29	31,31,31,31	0
30	MN	X	3122	1/1	0.88	0.22	71,71,71,71	0
30	MN	X	3165	1/1	0.88	0.38	83,83,83,83	0
29	MG	X	3323	1/1	0.88	0.13	48,48,48,48	0
29	MG	O	201	1/1	0.88	0.25	0,0,0,0	1
30	MN	X	3140	1/1	0.88	0.28	127,127,127,127	0
28	MPD	X	3008	8/8	0.88	0.34	61,61,61,61	0
28	MPD	X	3004	8/8	0.88	0.26	86,86,86,86	0
29	MG	X	3342	1/1	0.89	0.17	53,53,53,53	0
30	MN	X	3147	1/1	0.89	0.40	89,89,89,89	0
30	MN	X	3131	1/1	0.89	0.56	109,109,109,109	0
30	MN	X	3038	1/1	0.89	0.28	151,151,151,151	0
29	MG	X	3307	1/1	0.89	0.18	49,49,49,49	0
30	MN	X	3073	1/1	0.89	0.24	65,65,65,65	0
30	MN	X	3268	1/1	0.89	0.41	81,81,81,81	0
30	MN	X	3331	1/1	0.89	0.71	119,119,119,119	0
30	MN	X	3085	1/1	0.89	0.35	77,77,77,77	0
29	MG	A	301	1/1	0.89	0.73	45,45,45,45	0
33	EPE	L	201	15/15	0.89	0.13	125,125,125,125	0
29	MG	X	3233	1/1	0.89	0.97	57,57,57,57	0
30	MN	X	3214	1/1	0.89	0.18	78,78,78,78	0
30	MN	X	3142	1/1	0.89	0.17	117,117,117,117	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
29	MG	X	3192	1/1	0.89	0.66	45,45,45,45	0
30	MN	X	3115	1/1	0.89	0.38	65,65,65,65	0
29	MG	X	3344	1/1	0.89	0.09	67,67,67,67	0
30	MN	X	3093	1/1	0.89	0.40	83,83,83,83	0
28	MPD	X	3003	8/8	0.90	0.41	64,64,64,64	0
28	MPD	X	3002	8/8	0.90	0.20	44,44,44,44	0
28	MPD	X	3009	8/8	0.90	0.28	99,99,99,99	0
30	MN	X	3222	1/1	0.90	0.26	101,101,101,101	0
29	MG	X	3372	1/1	0.90	1.47	56,56,56,56	0
29	MG	X	3157	1/1	0.90	0.52	61,61,61,61	0
30	MN	X	3210	1/1	0.90	0.14	128,128,128,128	0
29	MG	X	3352	1/1	0.90	0.39	66,66,66,66	0
27	TEL	X	3001	58/58	0.90	0.39	30,40,52,52	0
30	MN	X	3150	1/1	0.90	0.52	123,123,123,123	0
30	MN	X	3166	1/1	0.90	0.33	72,72,72,72	0
29	MG	X	3023	1/1	0.90	0.28	26,26,26,26	1
29	MG	X	3318	1/1	0.90	0.30	47,47,47,47	0
30	MN	X	3161	1/1	0.90	0.25	93,93,93,93	0
30	MN	X	3120	1/1	0.90	0.20	98,98,98,98	0
29	MG	X	3295	1/1	0.90	0.47	57,57,57,57	0
29	MG	X	3306	1/1	0.90	0.64	66,66,66,66	0
30	MN	X	3207	1/1	0.90	0.34	130,130,130,130	0
30	MN	X	3159	1/1	0.91	0.20	81,81,81,81	0
29	MG	X	3319	1/1	0.91	0.63	53,53,53,53	0
29	MG	X	3287	1/1	0.91	0.55	36,36,36,36	0
30	MN	X	3248	1/1	0.91	0.12	115,115,115,115	0
30	MN	X	3076	1/1	0.91	0.18	85,85,85,85	0
30	MN	X	3055	1/1	0.91	0.63	121,121,121,121	0
29	MG	X	3299	1/1	0.91	1.21	52,52,52,52	0
30	MN	X	3244	1/1	0.91	0.18	96,96,96,96	0
30	MN	Y	210	1/1	0.91	1.02	176,176,176,176	0
29	MG	X	3322	1/1	0.91	0.10	67,67,67,67	0
30	MN	X	3212	1/1	0.91	0.19	94,94,94,94	0
29	MG	X	3314	1/1	0.91	0.44	55,55,55,55	0
29	MG	X	3359	1/1	0.91	0.46	60,60,60,60	0
29	MG	X	3232	1/1	0.91	0.21	42,42,42,42	0
29	MG	R	201	1/1	0.91	0.20	24,24,24,24	0
30	MN	X	3056	1/1	0.92	0.21	135,135,135,135	0
28	MPD	X	3007	8/8	0.92	0.46	70,70,70,70	0
29	MG	X	3290	1/1	0.92	0.56	45,45,45,45	0
29	MG	X	3281	1/1	0.92	0.43	21,21,21,21	0
30	MN	X	3178	1/1	0.92	0.25	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
30	MN	I	202	1/1	0.92	0.33	100,100,100,100	0
29	MG	X	3012	1/1	0.92	0.47	16,16,16,16	1
29	MG	X	3341	1/1	0.92	0.14	92,92,92,92	0
28	MPD	X	3006	8/8	0.92	0.25	74,74,74,74	0
29	MG	X	3304	1/1	0.92	0.66	40,40,40,40	0
29	MG	X	3234	1/1	0.92	0.20	34,34,34,34	0
29	MG	X	3298	1/1	0.92	0.47	41,41,41,41	0
29	MG	X	3293	1/1	0.92	0.36	32,32,32,32	0
29	MG	X	3351	1/1	0.92	0.07	57,57,57,57	0
30	MN	X	3269	1/1	0.92	0.37	134,134,134,134	0
29	MG	X	3334	1/1	0.92	0.18	64,64,64,64	0
29	MG	X	3017	1/1	0.92	0.92	46,46,46,46	0
29	MG	X	3350	1/1	0.93	0.30	71,71,71,71	0
30	MN	X	3080	1/1	0.93	0.24	55,55,55,55	0
29	MG	X	3027	1/1	0.93	0.32	38,38,38,38	0
29	MG	X	3313	1/1	0.93	0.28	67,67,67,67	0
30	MN	X	3107	1/1	0.93	0.42	62,62,62,62	0
30	MN	X	3176	1/1	0.93	0.29	78,78,78,78	0
29	MG	X	3251	1/1	0.93	0.24	59,59,59,59	0
30	MN	X	3202	1/1	0.93	0.16	124,124,124,124	0
29	MG	X	3288	1/1	0.93	1.05	39,39,39,39	0
29	MG	X	3312	1/1	0.93	0.49	36,36,36,36	0
30	MN	X	3039	1/1	0.93	0.41	107,107,107,107	0
29	MG	X	3337	1/1	0.93	0.28	69,69,69,69	0
29	MG	X	3195	1/1	0.93	0.79	28,28,28,28	0
30	MN	X	3075	1/1	0.93	0.20	33,33,33,33	0
30	MN	X	3139	1/1	0.93	0.29	121,121,121,121	0
30	MN	X	3245	1/1	0.93	0.48	98,98,98,98	0
30	MN	X	3217	1/1	0.93	0.28	116,116,116,116	0
31	SPD	X	3362	10/10	0.93	0.24	16,16,16,16	0
30	MN	X	3047	1/1	0.93	0.31	94,94,94,94	0
30	MN	X	3263	1/1	0.93	0.21	114,114,114,114	0
29	MG	X	3302	1/1	0.93	0.11	61,61,61,61	0
29	MG	X	3305	1/1	0.93	0.47	60,60,60,60	0
30	MN	X	3068	1/1	0.93	0.25	102,102,102,102	0
30	MN	X	3261	1/1	0.94	0.21	89,89,89,89	0
29	MG	X	3155	1/1	0.94	0.67	21,21,21,21	0
28	MPD	X	3005	8/8	0.94	0.28	20,20,20,20	0
30	MN	X	3162	1/1	0.94	0.22	114,114,114,114	0
30	MN	X	3132	1/1	0.94	0.70	116,116,116,116	0
30	MN	X	3243	1/1	0.94	0.58	107,107,107,107	0
29	MG	X	3286	1/1	0.94	0.12	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
30	MN	X	3172	1/1	0.94	0.58	113,113,113,113	0
30	MN	X	3236	1/1	0.94	0.31	105,105,105,105	0
30	MN	X	3219	1/1	0.94	0.22	90,90,90,90	0
30	MN	X	3262	1/1	0.94	0.09	130,130,130,130	0
30	MN	X	3098	1/1	0.94	0.26	94,94,94,94	0
31	SPD	X	3365	10/10	0.94	0.20	54,54,54,54	0
29	MG	X	3019	1/1	0.94	0.23	32,32,32,32	0
30	MN	X	3201	1/1	0.94	0.38	106,106,106,106	0
29	MG	X	3336	1/1	0.94	0.61	40,40,40,40	0
29	MG	X	3321	1/1	0.94	0.49	74,74,74,74	0
30	MN	X	3100	1/1	0.94	0.23	57,57,57,57	0
29	MG	X	3300	1/1	0.94	0.66	59,59,59,59	0
30	MN	X	3045	1/1	0.94	0.08	82,82,82,82	0
29	MG	X	3277	1/1	0.94	0.29	51,51,51,51	0
30	MN	X	3254	1/1	0.94	0.27	105,105,105,105	0
30	MN	X	3105	1/1	0.94	0.49	48,48,48,48	0
30	MN	X	3043	1/1	0.94	0.28	67,67,67,67	0
29	MG	X	3278	1/1	0.94	0.56	63,63,63,63	0
30	MN	X	3082	1/1	0.94	0.33	71,71,71,71	0
30	MN	I	201	1/1	0.95	0.27	71,71,71,71	0
29	MG	X	3326	1/1	0.95	0.56	71,71,71,71	0
29	MG	X	3196	1/1	0.95	1.06	41,41,41,41	0
30	MN	X	3109	1/1	0.95	0.22	62,62,62,62	0
29	MG	C	302	1/1	0.95	0.44	44,44,44,44	0
29	MG	X	3197	1/1	0.95	0.15	58,58,58,58	0
30	MN	X	3163	1/1	0.95	0.35	118,118,118,118	0
30	MN	X	3126	1/1	0.95	0.24	62,62,62,62	0
29	MG	Y	209	1/1	0.95	0.35	59,59,59,59	0
30	MN	X	3071	1/1	0.95	0.36	77,77,77,77	0
29	MG	X	3294	1/1	0.95	0.43	32,32,32,32	0
30	MN	X	3227	1/1	0.95	0.47	116,116,116,116	0
29	MG	X	3029	1/1	0.95	0.13	51,51,51,51	0
29	MG	X	3015	1/1	0.95	0.42	48,48,48,48	0
30	MN	X	3077	1/1	0.95	0.21	62,62,62,62	0
30	MN	X	3177	1/1	0.95	0.32	89,89,89,89	0
30	MN	X	3215	1/1	0.95	0.24	95,95,95,95	0
29	MG	X	3026	1/1	0.95	0.30	41,41,41,41	0
30	MN	X	3138	1/1	0.95	0.12	91,91,91,91	0
30	MN	X	3121	1/1	0.95	0.33	71,71,71,71	0
29	MG	X	3292	1/1	0.95	0.32	30,30,30,30	0
30	MN	X	3369	1/1	0.95	0.41	70,70,70,70	0
30	MN	X	3137	1/1	0.95	0.29	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
29	MG	X	3279	1/1	0.95	0.29	66,66,66,66	0
29	MG	X	3311	1/1	0.95	0.15	39,39,39,39	0
30	MN	X	3095	1/1	0.95	0.51	87,87,87,87	0
30	MN	X	3086	1/1	0.95	0.22	74,74,74,74	0
29	MG	X	3345	1/1	0.95	0.13	56,56,56,56	0
30	MN	X	3124	1/1	0.95	0.21	67,67,67,67	0
29	MG	X	3257	1/1	0.95	0.08	48,48,48,48	0
29	MG	X	3280	1/1	0.95	0.27	51,51,51,51	0
30	MN	X	3373	1/1	0.95	0.27	44,44,44,44	0
30	MN	X	3167	1/1	0.95	0.59	110,110,110,110	0
30	MN	X	3145	1/1	0.95	0.39	122,122,122,122	0
30	MN	X	3128	1/1	0.95	0.19	55,55,55,55	0
29	MG	X	3250	1/1	0.96	0.59	25,25,25,25	0
30	MN	X	3069	1/1	0.96	0.54	76,76,76,76	0
30	MN	X	3208	1/1	0.96	0.40	109,109,109,109	0
30	MN	X	3059	1/1	0.96	0.41	111,111,111,111	0
30	MN	X	3053	1/1	0.96	0.22	63,63,63,63	0
30	MN	X	3153	1/1	0.96	0.37	41,41,41,41	0
30	MN	X	3099	1/1	0.96	0.57	88,88,88,88	0
30	MN	X	3328	1/1	0.96	0.39	88,88,88,88	0
30	MN	X	3108	1/1	0.96	0.29	70,70,70,70	0
30	MN	X	3072	1/1	0.96	0.25	74,74,74,74	0
30	MN	X	3064	1/1	0.96	0.35	94,94,94,94	0
29	MG	X	3228	1/1	0.96	0.41	62,62,62,62	0
30	MN	X	3070	1/1	0.96	0.44	74,74,74,74	0
29	MG	X	3317	1/1	0.96	0.17	49,49,49,49	0
29	MG	C	303	1/1	0.96	0.15	38,38,38,38	0
30	MN	X	3160	1/1	0.96	0.23	101,101,101,101	0
30	MN	Y	204	1/1	0.96	0.40	146,146,146,146	0
30	MN	X	3110	1/1	0.96	0.30	51,51,51,51	0
29	MG	X	3346	1/1	0.96	0.24	31,31,31,31	0
29	MG	X	3310	1/1	0.96	0.44	36,36,36,36	0
30	MN	X	3169	1/1	0.96	0.13	85,85,85,85	0
29	MG	X	3193	1/1	0.96	0.23	27,27,27,27	0
30	MN	X	3114	1/1	0.96	0.17	59,59,59,59	0
29	MG	X	3338	1/1	0.96	0.33	64,64,64,64	0
30	MN	X	3104	1/1	0.96	0.47	53,53,53,53	0
30	MN	X	3329	1/1	0.96	0.06	95,95,95,95	0
30	MN	Y	201	1/1	0.96	0.13	84,84,84,84	0
30	MN	Y	202	1/1	0.96	0.17	126,126,126,126	0
30	MN	X	3241	1/1	0.96	0.24	66,66,66,66	0
30	MN	X	3221	1/1	0.97	0.47	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
30	MN	X	3060	1/1	0.97	0.12	67,67,67,67	0
29	MG	X	3283	1/1	0.97	0.28	36,36,36,36	0
29	MG	X	3285	1/1	0.97	0.28	56,56,56,56	0
30	MN	X	3061	1/1	0.97	0.34	69,69,69,69	0
30	MN	X	3149	1/1	0.97	0.33	112,112,112,112	0
30	MN	X	3179	1/1	0.97	0.18	69,69,69,69	0
30	MN	X	3054	1/1	0.97	0.19	76,76,76,76	0
30	MN	X	3356	1/1	0.97	0.41	41,41,41,41	0
29	MG	X	3320	1/1	0.97	0.22	53,53,53,53	0
30	MN	X	3044	1/1	0.97	0.35	34,34,34,34	0
30	MN	X	3136	1/1	0.97	0.25	59,59,59,59	0
30	MN	X	3123	1/1	0.97	0.22	38,38,38,38	0
30	MN	X	3270	1/1	0.97	0.41	120,120,120,120	0
29	MG	X	3296	1/1	0.97	0.38	56,56,56,56	0
30	MN	X	3074	1/1	0.97	0.44	68,68,68,68	0
30	MN	X	3184	1/1	0.97	0.17	99,99,99,99	0
30	MN	X	3203	1/1	0.97	0.31	78,78,78,78	0
29	MG	X	3013	1/1	0.97	0.96	41,41,41,41	0
30	MN	X	3154	1/1	0.97	0.47	47,47,47,47	0
30	MN	X	3066	1/1	0.97	0.38	49,49,49,49	0
30	MN	X	3143	1/1	0.97	0.12	85,85,85,85	0
30	MN	X	3134	1/1	0.97	0.28	90,90,90,90	0
30	MN	X	3186	1/1	0.97	0.13	142,142,142,142	0
30	MN	X	3050	1/1	0.97	0.22	87,87,87,87	0
30	MN	X	3174	1/1	0.97	0.21	77,77,77,77	0
30	MN	X	3119	1/1	0.97	0.33	87,87,87,87	0
30	MN	X	3062	1/1	0.97	0.32	72,72,72,72	0
30	MN	X	3216	1/1	0.98	0.24	78,78,78,78	0
29	MG	Y	203	1/1	0.98	0.39	19,19,19,19	0
30	MN	X	3096	1/1	0.98	0.22	46,46,46,46	0
30	MN	X	3088	1/1	0.98	0.24	97,97,97,97	0
30	MN	X	3371	1/1	0.98	0.25	34,34,34,34	0
30	MN	X	3238	1/1	0.98	0.36	126,126,126,126	0
30	MN	X	3097	1/1	0.98	0.23	64,64,64,64	0
30	MN	X	3189	1/1	0.98	0.25	43,43,43,43	0
30	MN	X	3158	1/1	0.98	0.37	91,91,91,91	0
30	MN	X	3089	1/1	0.98	0.14	89,89,89,89	0
30	MN	X	3106	1/1	0.98	0.36	42,42,42,42	0
30	MN	X	3067	1/1	0.98	0.47	83,83,83,83	0
30	MN	X	3133	1/1	0.98	0.17	81,81,81,81	0
30	MN	X	3035	1/1	0.98	0.55	149,149,149,149	0
30	MN	X	3034	1/1	0.98	0.18	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
30	MN	X	3240	1/1	0.98	0.58	52,52,52,52	0
30	MN	X	3173	1/1	0.98	0.39	72,72,72,72	0
30	MN	X	3141	1/1	0.98	0.24	99,99,99,99	0
30	MN	X	3264	1/1	0.98	0.32	103,103,103,103	0
30	MN	X	3355	1/1	0.98	0.35	68,68,68,68	0
29	MG	X	3291	1/1	0.98	0.27	26,26,26,26	0
30	MN	X	3081	1/1	0.98	0.32	49,49,49,49	0
30	MN	X	3102	1/1	0.98	0.47	100,100,100,100	0
30	MN	X	3187	1/1	0.98	0.21	45,45,45,45	0
29	MG	X	3289	1/1	0.98	0.15	61,61,61,61	0
29	MG	X	3223	1/1	0.98	0.10	42,42,42,42	0
30	MN	X	3129	1/1	0.98	0.24	61,61,61,61	0
30	MN	X	3116	1/1	0.98	0.48	70,70,70,70	0
30	MN	X	3113	1/1	0.98	0.35	62,62,62,62	0
30	MN	X	3079	1/1	0.98	0.20	52,52,52,52	0
29	MG	X	3156	1/1	0.98	0.44	14,14,14,14	0
30	MN	X	3370	1/1	0.99	0.31	98,98,98,98	0
30	MN	X	3087	1/1	0.99	0.30	85,85,85,85	0
30	MN	X	3103	1/1	0.99	0.48	41,41,41,41	0
30	MN	X	3190	1/1	0.99	0.20	77,77,77,77	0
30	MN	X	3048	1/1	0.99	0.27	90,90,90,90	0
29	MG	X	3194	1/1	0.99	0.46	34,34,34,34	0
30	MN	X	3049	1/1	0.99	0.17	81,81,81,81	0
30	MN	X	3090	1/1	0.99	0.27	54,54,54,54	0
30	MN	X	3130	1/1	0.99	0.19	63,63,63,63	0
30	MN	X	3078	1/1	0.99	0.28	54,54,54,54	0
30	MN	X	3127	1/1	0.99	0.23	48,48,48,48	0
30	MN	X	3125	1/1	0.99	0.20	60,60,60,60	0
30	MN	X	3242	1/1	0.99	0.19	68,68,68,68	0
29	MG	X	3284	1/1	0.99	0.22	12,12,12,12	0
30	MN	X	3057	1/1	0.99	0.35	28,28,28,28	0
30	MN	X	3330	1/1	0.99	0.25	83,83,83,83	0
30	MN	X	3188	1/1	0.99	0.26	54,54,54,54	0
29	MG	X	3309	1/1	0.99	0.19	30,30,30,30	0
30	MN	X	3063	1/1	0.99	0.27	42,42,42,42	0
30	MN	X	3111	1/1	0.99	0.56	71,71,71,71	0
30	MN	X	3256	1/1	0.99	0.08	79,79,79,79	0
30	MN	X	3118	1/1	0.99	0.20	32,32,32,32	0
30	MN	X	3211	1/1	0.99	0.13	64,64,64,64	0
30	MN	X	3052	1/1	0.99	0.23	57,57,57,57	0
30	MN	X	3168	1/1	0.99	0.21	40,40,40,40	0
30	MN	X	3213	1/1	0.99	0.24	63,63,63,63	0

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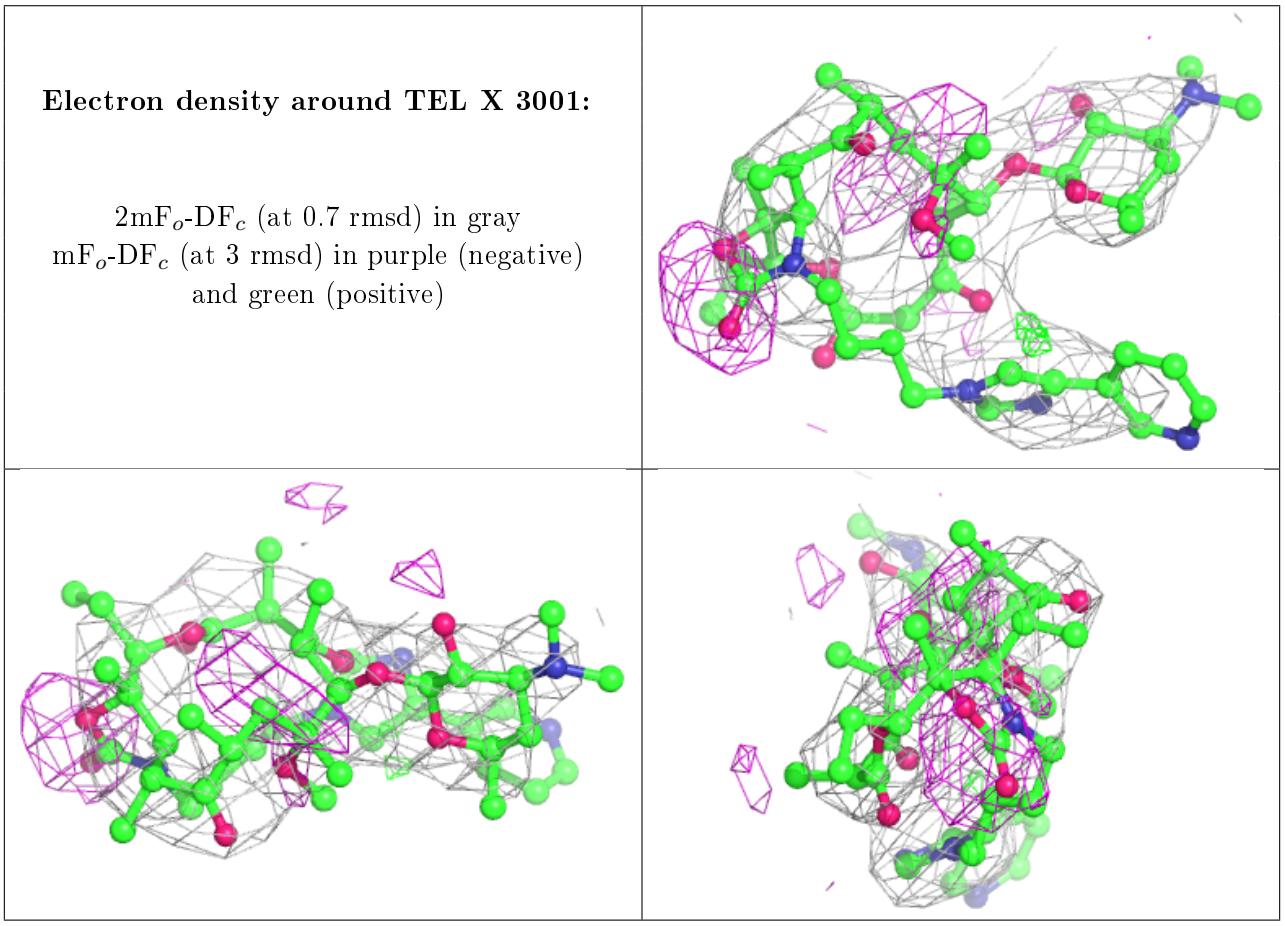
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
30	MN	X	3083	1/1	0.99	0.19	59,59,59,59	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around TEL X 3001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers

There are no such residues in this entry.