



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 08:07 pm BST

PDB ID : 4GKJ  
Title : Structure of the *Thermus thermophilus* 30S ribosomal subunit complexed with a human mitochondrial anticodon stem loop (ASL) of transfer RNA Methionine (TRNAMET) bound to an mRNA with an AUG-codon in the A-site and paromomycin.  
Authors : Cantara, W.A.; Murphy IV, F.V.; Spears, J.L.; Demirci, H.; Agris, P.F.  
Deposited on : 2012-08-11  
Resolution : 3.30 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](mailto: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.

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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 : 2.11  
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) : 2.11

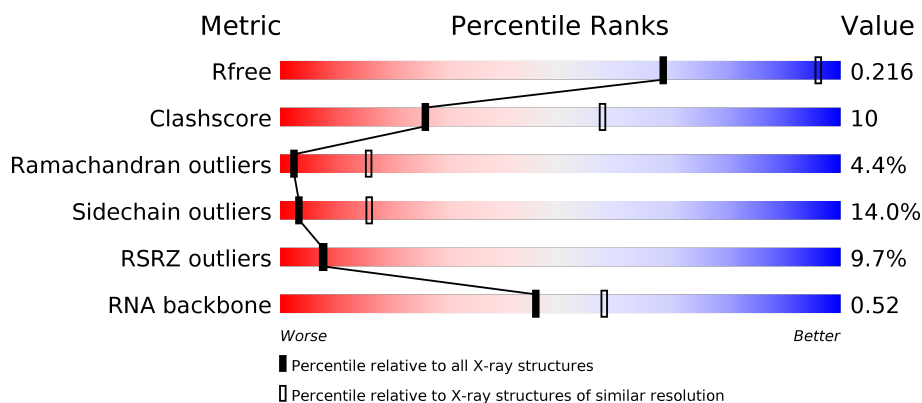
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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.








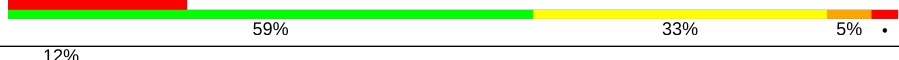

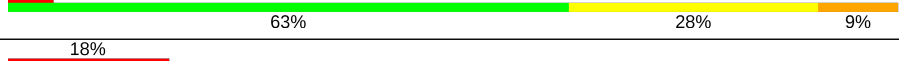

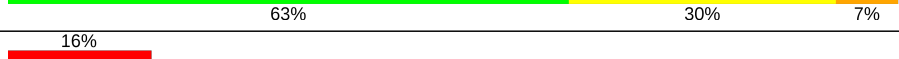
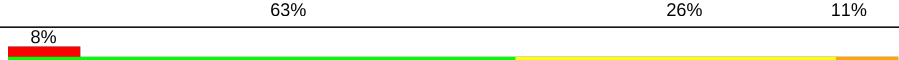
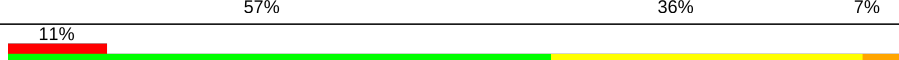
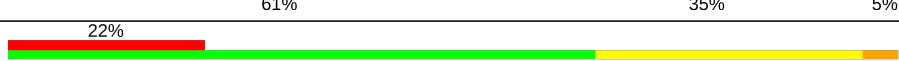
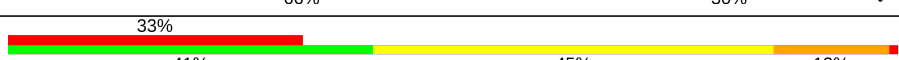
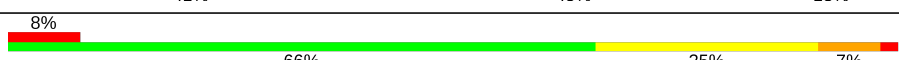


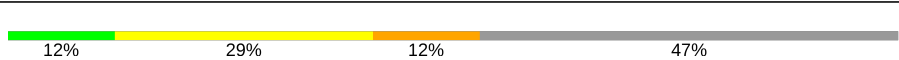

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)
RNA backbone	3102	1117 (3.70-2.90)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1513	<div> <div>7%</div> <div> <div></div> <div>51%</div> <div>35%</div> <div>11%</div> </div> <div></div> </div>
2	B	234	<div> <div>7%</div> <div> <div></div> <div>47%</div> <div>39%</div> <div>12%</div> </div> <div></div> </div>
3	C	206	<div> <div>4%</div> <div> <div></div> <div>63%</div> <div>30%</div> <div>6%</div> </div> <div></div> </div>
4	D	208	<div> <div>15%</div> <div> <div></div> <div>60%</div> <div>32%</div> <div>8%</div> </div> <div></div> </div>

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Mol	Chain	Length	Quality of chain
5	E	150	
6	F	101	
7	G	155	
8	H	138	
9	I	127	
10	J	98	
11	K	119	
12	L	124	
13	M	125	
14	N	60	
15	O	88	
16	P	83	
17	Q	104	
18	R	73	
19	S	80	
20	T	99	
21	V	24	
22	W	6	
23	X	17	

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
24	MG	A	1601	-	-	-	X
24	MG	A	1603	-	-	-	X
24	MG	A	1604	-	-	-	X
24	MG	A	1605	-	-	-	X
24	MG	A	1607	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	MG	A	1609	-	-	-	X
24	MG	A	1619	-	-	-	X
24	MG	A	1621	-	-	-	X
24	MG	A	1627	-	-	-	X
24	MG	A	1629	-	-	-	X
24	MG	A	1636	-	-	-	X
24	MG	A	1638	-	-	-	X
24	MG	A	1639	-	-	-	X
24	MG	A	1642	-	-	-	X
24	MG	A	1645	-	-	-	X
24	MG	A	1646	-	-	-	X
24	MG	A	1650	-	-	-	X
24	MG	A	1654	-	-	-	X
24	MG	A	1657	-	-	-	X
24	MG	A	1665	-	-	-	X
24	MG	A	1670	-	-	-	X
24	MG	A	1672	-	-	-	X
24	MG	A	1676	-	-	-	X
24	MG	A	1681	-	-	-	X
24	MG	A	1682	-	-	-	X
24	MG	A	1687	-	-	-	X
24	MG	A	1689	-	-	-	X
24	MG	A	1690	-	-	-	X
24	MG	A	1695	-	-	-	X
24	MG	A	1696	-	-	-	X
24	MG	A	1697	-	-	-	X
24	MG	A	1698	-	-	-	X
24	MG	A	1703	-	-	-	X
24	MG	A	1709	-	-	-	X
24	MG	A	1713	-	-	-	X
24	MG	A	1716	-	-	-	X
24	MG	A	1717	-	-	-	X
24	MG	A	1718	-	-	-	X
24	MG	A	1721	-	-	-	X
24	MG	A	1724	-	-	-	X
24	MG	A	1728	-	-	-	X
24	MG	A	1733	-	-	-	X
24	MG	A	1739	-	-	-	X
24	MG	A	1741	-	-	-	X
24	MG	A	1742	-	-	-	X
24	MG	A	1751	-	-	-	X
24	MG	A	1753	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	MG	A	1754	-	-	-	X
24	MG	A	1756	-	-	-	X
24	MG	A	1765	-	-	-	X
24	MG	A	1766	-	-	-	X
24	MG	A	1772	-	-	-	X
24	MG	A	1777	-	-	-	X

## 2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 52227 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 16S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1513	Total	C	N	O	P	22	0	0
			32515	14472	6016	10514	1513			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1005	C	-	INSERTION	GB 48256
A	1013	G	-	INSERTION	GB 48256
A	1225	C	-	INSERTION	GB 48256
A	1226	A	-	INSERTION	GB 48256
A	1517	U	C	CONFLICT	GB 48256
A	1519	U	C	CONFLICT	GB 48256

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	234	Total	C	N	O	S	0	0	0
			1900	1213	341	341	5			

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	150	Total	C	N	O	S	0	0	0
			1146	724	217	201	4			

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	I	127	Total	C	N	O	0	0	0
			1011	639	198	174			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	58	ARG	HIS	CONFLICT	UNP P80374

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	98	Total	C	N	O	S	0	0	0
			794	499	156	138	1			

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	124	Total	C	N	O	S	0	0	0
			970	611	195	163	1			

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	125	Total	C	N	O	S	0	0	0
			997	617	207	171	2			

- Molecule 14 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	104	Total	C	N	O	S	0	0	0
			857	547	161	147	2			

There is a discrepancy between the modelled and reference sequences:



Chain	Residue	Modelled	Actual	Comment	Reference
Q	96	GLN	GLU	CONFLICT	UNP Q5SHP7

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	R	73	Total	C	N	O	0	0	0
			597	380	118	99			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	60	GLY	ALA	CONFLICT	UNP Q5SLQ0

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	80	Total	C	N	O	S	0	0	0
			647	414	119	112	2			

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	41	VAL	ILE	CONFLICT	UNP P80380

- Molecule 21 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	V	24	Total	C	N	O	0	0	0
			208	128	50	30			

- Molecule 22 is a RNA chain called mRNA A-site fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	W	3	Total	C	N	O	P	0	0	0
			62	29	12	19	2			

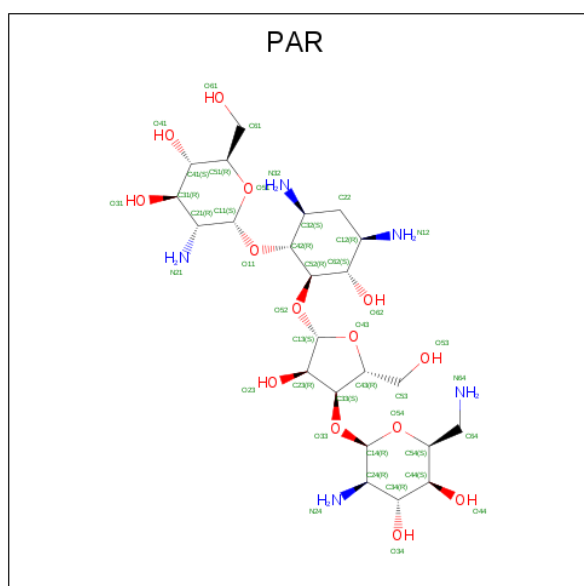
- Molecule 23 is a RNA chain called tRNA ASL human mitochondrial Met.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	X	9	Total	C	N	O	P	0	0	0
			189	85	32	63	9			

- Molecule 24 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	B	1	Total	Mg	0	0
			1	1		
24	A	184	Total	Mg	0	0
			184	184		
24	N	1	Total	Mg	0	0
			1	1		

- Molecule 25 is PAROMOMYCIN (three-letter code: PAR) (formula: C<sub>23</sub>H<sub>45</sub>N<sub>5</sub>O<sub>14</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	N	O	0	0
			42	23	5	14		

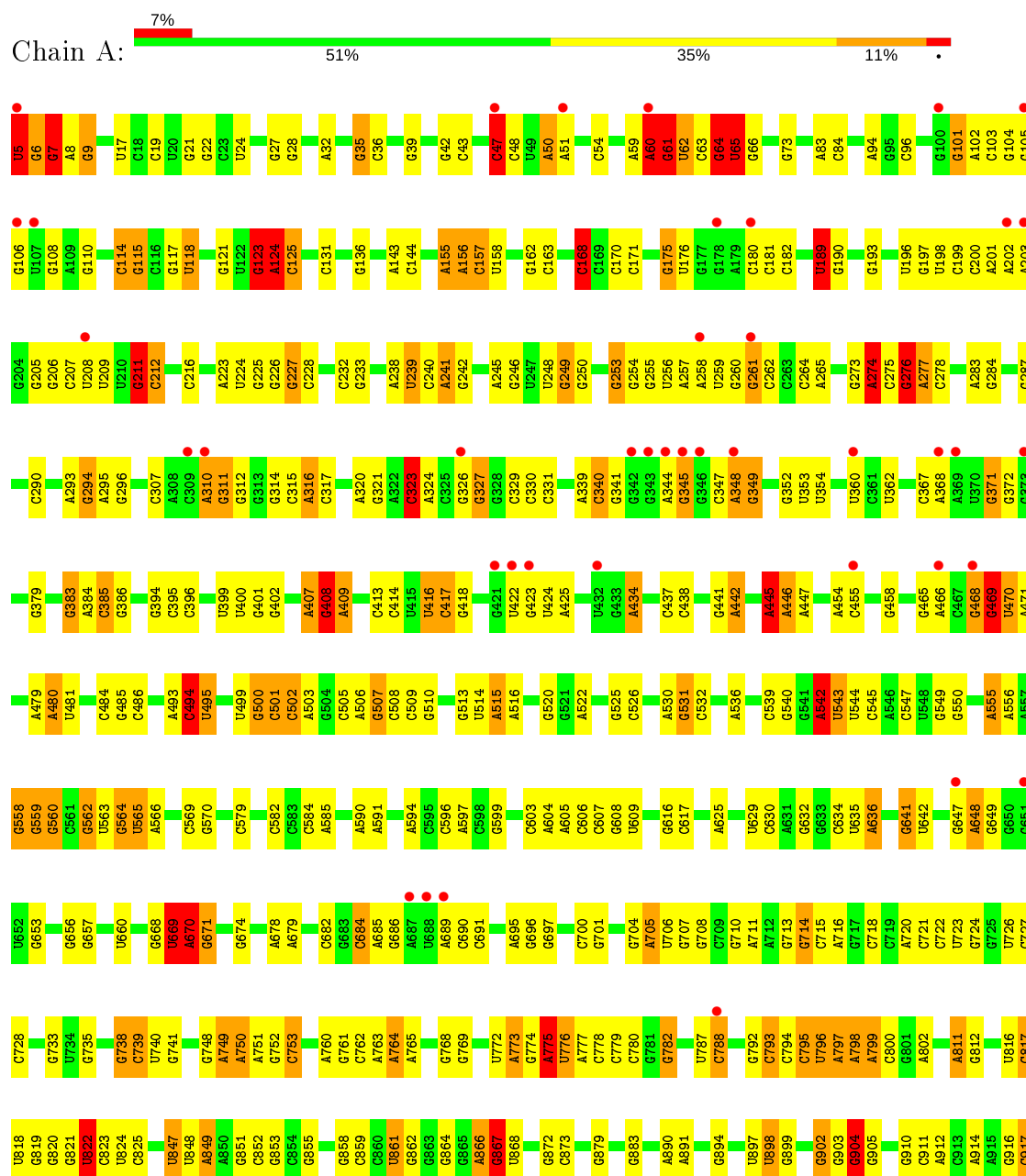
- Molecule 26 is ZINC ION (three-letter code: ZN) (formula: Zn).

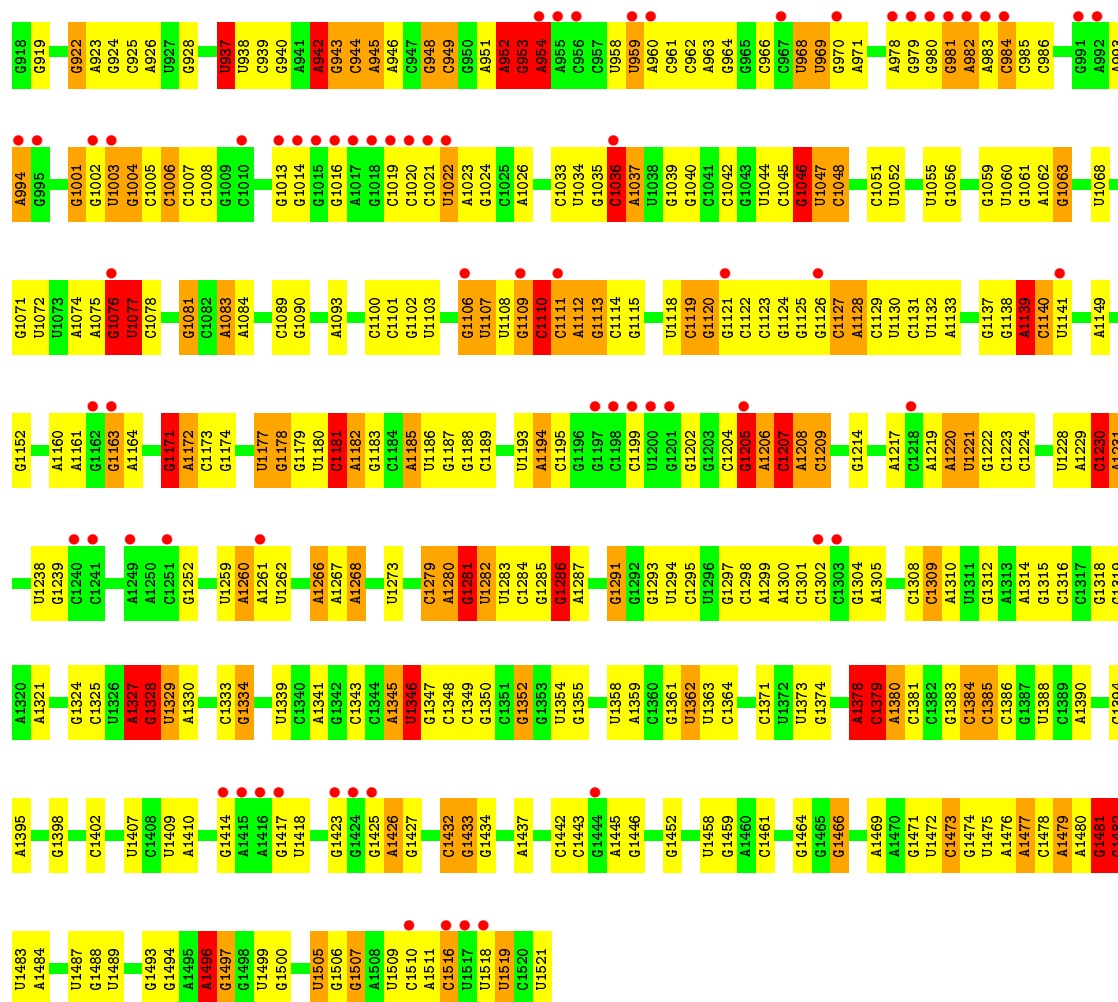
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
26	D	1	Total	Zn	0	0
			1	1		
26	N	1	Total	Zn	0	0
			1	1		

### 3 Residue-property plots

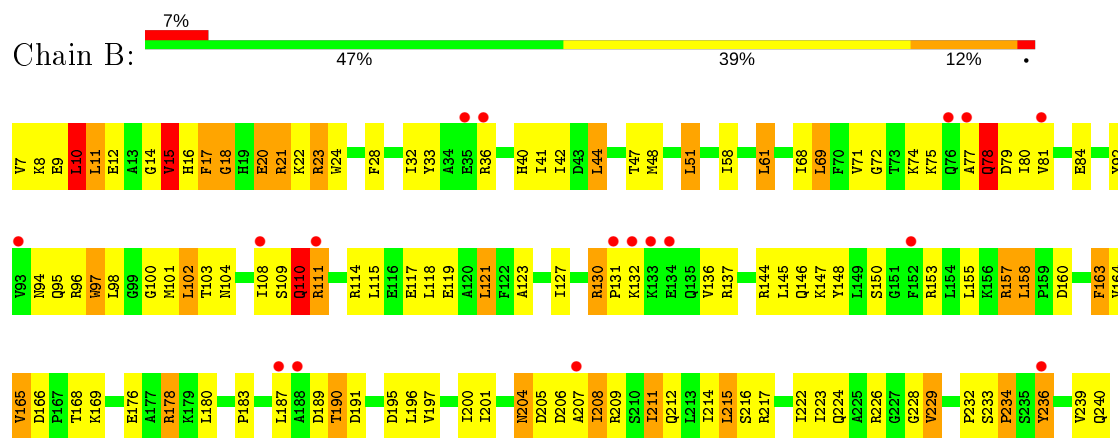
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: 16S rRNA

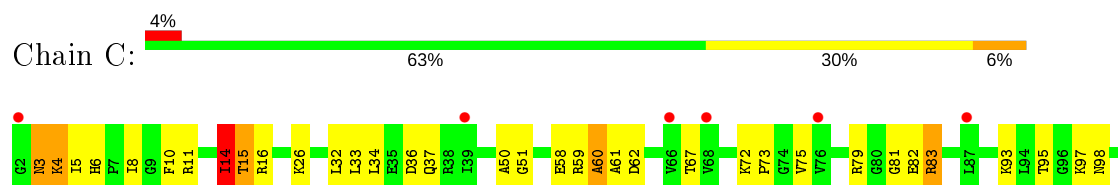


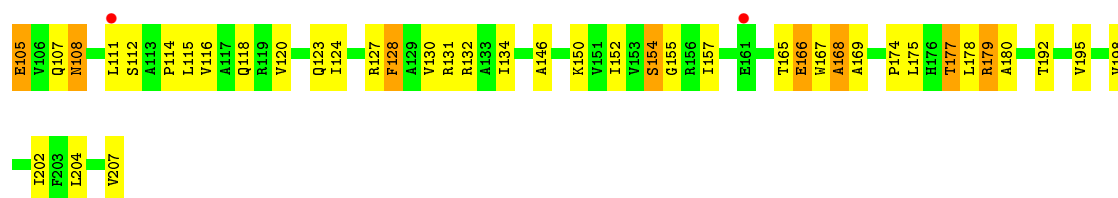


• Molecule 2: 30S ribosomal protein S2

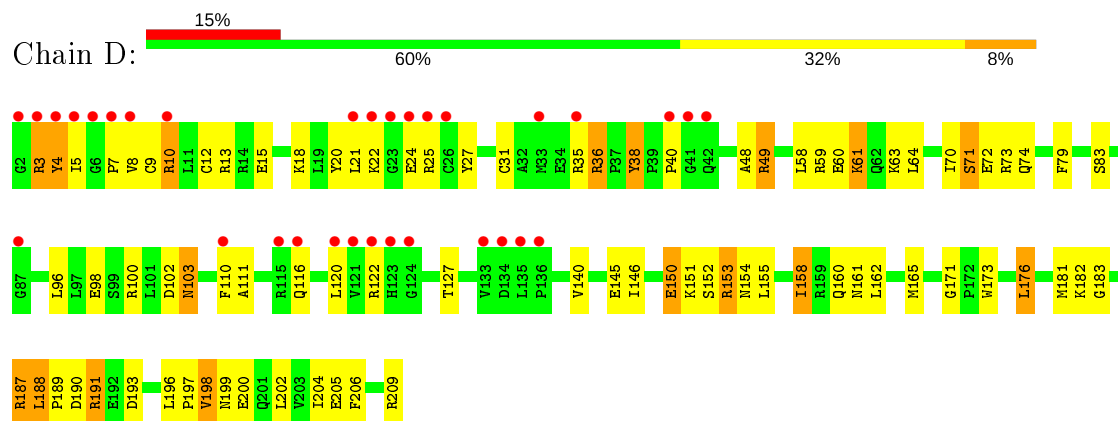


• Molecule 3: 30S ribosomal protein S3

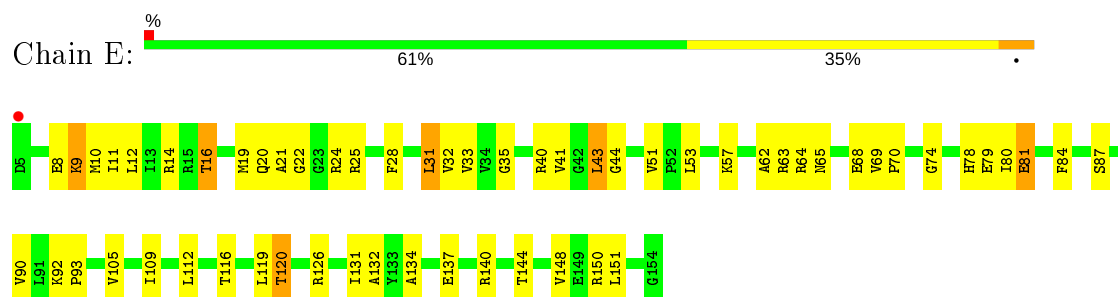




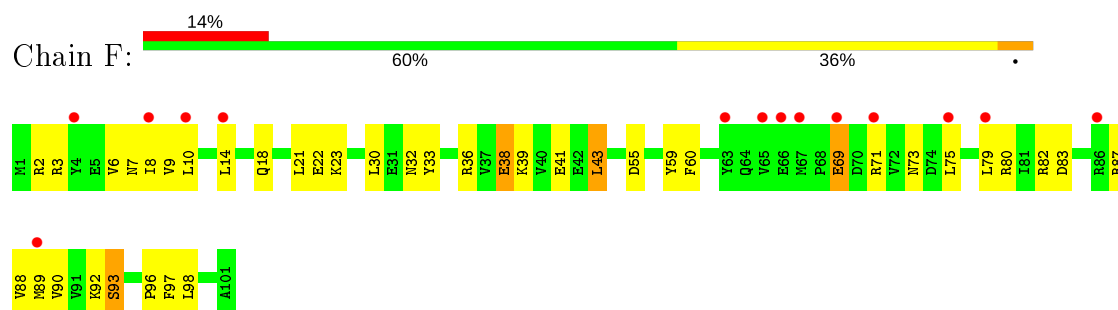
• Molecule 4: 30S ribosomal protein S4



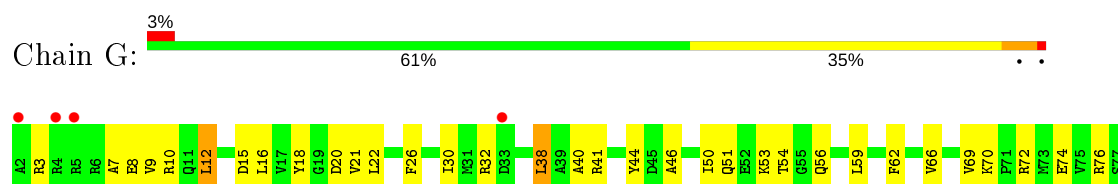
• Molecule 5: 30S ribosomal protein S5

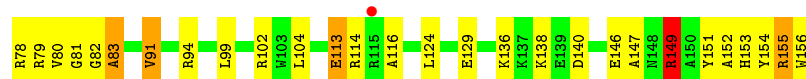


• Molecule 6: 30S ribosomal protein S6

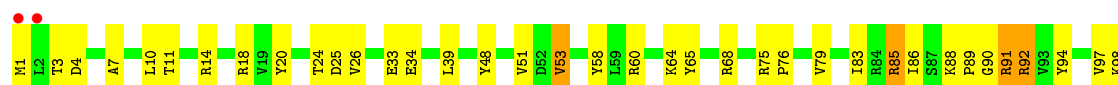


• Molecule 7: 30S ribosomal protein S7





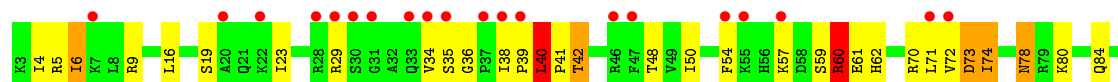
• Molecule 8: 30S ribosomal protein S8



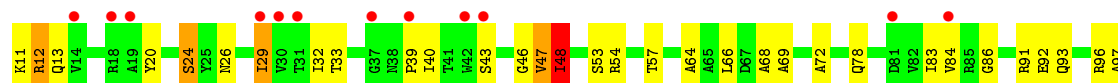
• Molecule 9: 30S ribosomal protein S9



• Molecule 10: 30S ribosomal protein S10



• Molecule 11: 30S ribosomal protein S11

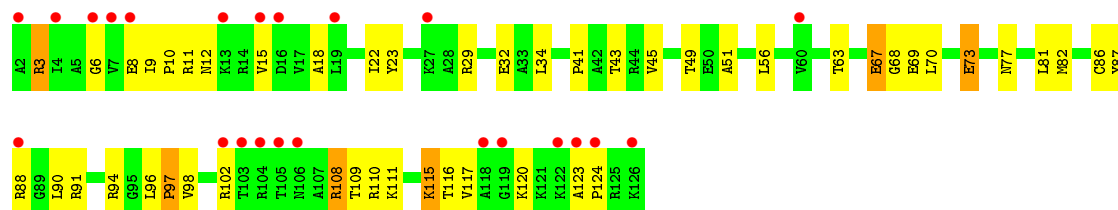


• Molecule 12: 30S ribosomal protein S12

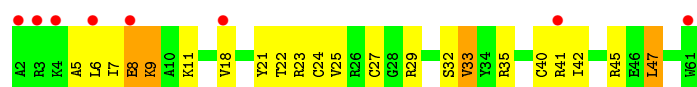




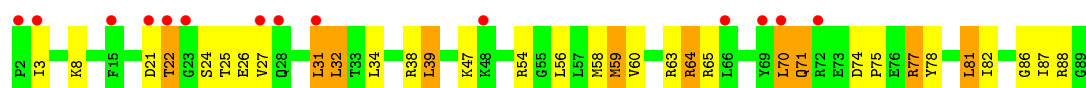
• Molecule 13: 30S ribosomal protein S13



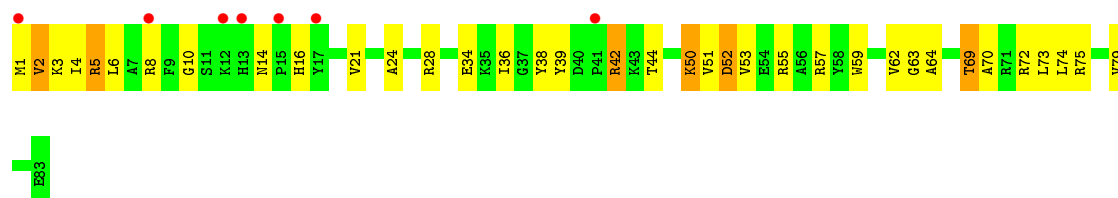
• Molecule 14: 30S ribosomal protein S14 type Z



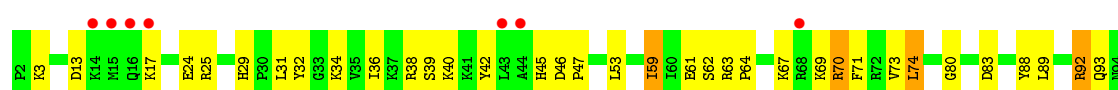
• Molecule 15: 30S ribosomal protein S15

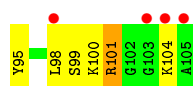


• Molecule 16: 30S ribosomal protein S16

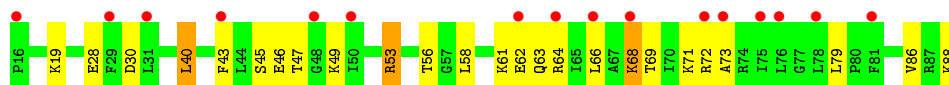


• Molecule 17: 30S ribosomal protein S17

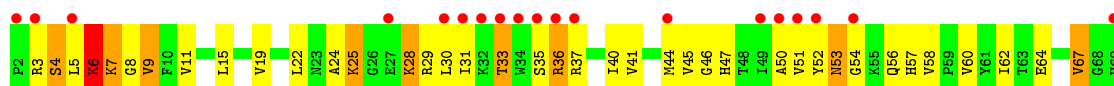




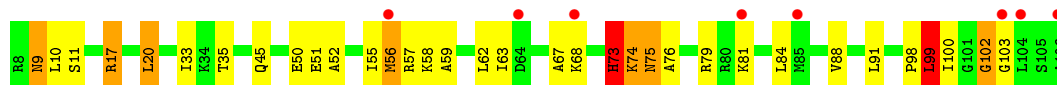
- Molecule 18: 30S ribosomal protein S18



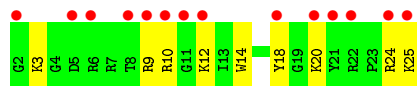
- Molecule 19: 30S ribosomal protein S19



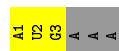
- Molecule 20: 30S ribosomal protein S20



- Molecule 21: 30S ribosomal protein Thx



- Molecule 22: mRNA A-site fragment



- Molecule 23: tRNA ASL human mitochondrial Met





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	400.55Å 400.55Å 176.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	97.15 – 3.30 97.15 – 3.30	Depositor EDS
% Data completeness (in resolution range)	97.3 (97.15-3.30) 97.4 (97.15-3.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.41 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.8_1069	Depositor
R, $R_{free}$	0.188 , 0.222 0.188 , 0.216	Depositor DCC
$R_{free}$ test set	10451 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	100.8	Xtriage
Anisotropy	0.166	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 51.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.84	EDS
Total number of atoms	52227	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.89% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.78	7/36395 (0.0%)	1.33	326/56801 (0.6%)
2	B	0.39	0/1935	0.62	0/2609
3	C	0.45	0/1636	0.64	1/2205 (0.0%)
4	D	0.53	2/1733 (0.1%)	0.68	1/2318 (0.0%)
5	E	0.59	0/1162	0.78	0/1564
6	F	0.41	0/856	0.59	0/1154
7	G	0.42	0/1276	0.61	0/1709
8	H	0.60	0/1136	0.77	1/1527 (0.1%)
9	I	0.43	0/1029	0.61	0/1378
10	J	0.46	0/807	0.63	0/1085
11	K	0.46	0/900	0.64	0/1213
12	L	0.60	0/986	0.80	0/1320
13	M	0.42	0/1008	0.64	0/1347
14	N	0.45	0/501	0.67	0/664
15	O	0.44	0/745	0.62	0/992
16	P	0.55	0/716	0.75	0/963
17	Q	0.54	0/870	0.72	0/1159
18	R	0.46	0/603	0.62	0/799
19	S	0.36	0/661	0.63	0/890
20	T	0.50	0/764	0.76	1/1006 (0.1%)
21	V	0.41	0/212	0.66	0/277
22	W	1.03	0/69	1.53	0/106
23	X	0.78	0/184	1.35	2/281 (0.7%)
All	All	0.69	9/56184 (0.0%)	1.16	332/83367 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
8	H	0	1
20	T	0	1
All	All	0	2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	5	U	OP3-P	-10.37	1.48	1.61
1	A	118	U	C4-O4	7.15	1.29	1.23
1	A	1208	A	N9-C4	-7.01	1.33	1.37
1	A	114	C	N1-C2	6.84	1.47	1.40
1	A	274	A	N9-C4	-6.68	1.33	1.37
1	A	1479	A	C5-C6	-6.30	1.35	1.41
4	D	12	CYS	CB-SG	6.10	1.92	1.82
4	D	9	CYS	CB-SG	5.33	1.91	1.82
1	A	501	C	N1-C2	5.16	1.45	1.40

All (332) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	114	C	N1-C2-O2	15.99	128.50	118.90
1	A	114	C	N3-C2-O2	-13.45	112.48	121.90
1	A	110	G	N1-C6-O6	11.02	126.51	119.90
1	A	114	C	C2-N1-C1'	10.94	130.83	118.80
1	A	1036	C	C6-N1-C2	-10.65	116.04	120.30
1	A	1479	A	N1-C6-N6	10.41	124.85	118.60
1	A	1479	A	C6-C5-N7	-9.89	125.38	132.30
1	A	323	C	N3-C2-O2	-9.79	115.05	121.90
1	A	674	G	N1-C6-O6	9.62	125.67	119.90
1	A	1479	A	C5-N7-C8	-9.38	99.21	103.90
1	A	323	C	N1-C2-O2	9.29	124.47	118.90
1	A	274	A	C2-N3-C4	-9.16	106.02	110.60
1	A	310	A	P-O3'-C3'	9.12	130.65	119.70
1	A	1398	G	N1-C6-O6	9.06	125.34	119.90
1	A	118	U	N3-C4-C5	-9.01	109.19	114.60
1	A	101	G	N1-C6-O6	9.01	125.31	119.90
1	A	1479	A	C4-C5-N7	8.89	115.14	110.70
1	A	861	U	P-O3'-C3'	8.79	130.25	119.70
1	A	795	C	C6-N1-C2	-8.74	116.81	120.30
1	A	118	U	C5-C4-O4	8.72	131.13	125.90
1	A	101	G	C4-C5-N7	8.66	114.27	110.80
1	A	101	G	C6-C5-N7	-8.46	125.32	130.40
1	A	1479	A	C2-N3-C4	-8.41	106.39	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	114	C	C6-N1-C1'	-8.29	110.85	120.80
1	A	110	G	C5-C6-O6	-8.27	123.64	128.60
1	A	1482	G	OP1-P-OP2	-8.22	107.27	119.60
1	A	317	C	C6-N1-C2	8.13	123.55	120.30
1	A	101	G	C5-N7-C8	-8.13	100.24	104.30
1	A	802	A	N1-C6-N6	8.12	123.47	118.60
1	A	501	C	N3-C2-O2	-8.09	116.23	121.90
1	A	323	C	C6-N1-C2	-8.09	117.06	120.30
1	A	1181	C	N1-C2-O2	8.04	123.73	118.90
1	A	1346	U	P-O3'-C3'	8.04	129.34	119.70
1	A	795	C	P-O3'-C3'	8.02	129.32	119.70
1	A	558	G	C8-N9-C4	7.92	109.57	106.40
1	A	775	A	P-O3'-C3'	7.78	129.04	119.70
1	A	501	C	C2-N1-C1'	7.77	127.35	118.80
4	D	12	CYS	CA-CB-SG	7.74	127.92	114.00
1	A	542	A	P-O3'-C3'	7.68	128.91	119.70
1	A	822	U	C2-N1-C1'	7.66	126.89	117.70
1	A	1521	U	N3-C4-O4	-7.63	114.06	119.40
1	A	501	C	C6-N1-C2	-7.48	117.31	120.30
1	A	1378	A	P-O3'-C3'	7.45	128.64	119.70
1	A	802	A	N1-C2-N3	7.45	133.02	129.30
1	A	948	G	N3-C4-C5	7.45	132.32	128.60
1	A	232	C	N3-C4-C5	7.42	124.87	121.90
1	A	60	A	P-O3'-C3'	7.38	128.56	119.70
1	A	788	C	N3-C4-C5	7.36	124.84	121.90
1	A	569	C	C6-N1-C2	7.33	123.23	120.30
1	A	101	G	O4'-C1'-N9	7.31	114.05	108.20
1	A	1046	G	P-O3'-C3'	7.31	128.47	119.70
1	A	904	G	N3-C4-C5	7.30	132.25	128.60
1	A	17	U	N3-C2-O2	-7.30	117.09	122.20
1	A	1386	C	C4-C5-C6	-7.30	113.75	117.40
1	A	323	C	P-O3'-C3'	7.28	128.44	119.70
1	A	465	G	N1-C6-O6	7.15	124.19	119.90
1	A	1036	C	C5-C6-N1	7.15	124.57	121.00
1	A	1479	A	N7-C8-N9	7.14	117.37	113.80
1	A	1208	A	C2-N3-C4	-7.12	107.04	110.60
1	A	1220	A	P-O3'-C3'	7.12	128.25	119.70
1	A	501	C	N1-C2-O2	7.12	123.17	118.90
1	A	445	A	C8-N9-C4	-7.12	102.95	105.80
1	A	326	G	N1-C6-O6	7.09	124.16	119.90
1	A	110	G	C6-C5-N7	-7.05	126.17	130.40
1	A	500	G	N3-C4-N9	7.05	130.23	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	726	U	C6-N1-C2	7.02	125.21	121.00
1	A	1519	U	N3-C2-O2	-6.99	117.31	122.20
1	A	189	U	P-O3'-C3'	6.99	128.08	119.70
1	A	1364	C	C6-N1-C2	-6.94	117.52	120.30
1	A	494	C	P-O3'-C3'	6.93	128.02	119.70
1	A	250	G	N1-C6-O6	6.90	124.04	119.90
1	A	500	G	N3-C4-C5	-6.88	125.16	128.60
1	A	1286	G	P-O3'-C3'	6.86	127.93	119.70
1	A	1500	G	N3-C2-N2	-6.82	115.12	119.90
1	A	1328	G	P-O3'-C3'	6.76	127.82	119.70
1	A	1036	C	N3-C4-C5	-6.75	119.20	121.90
1	A	101	G	N7-C8-N9	6.74	116.47	113.10
1	A	539	C	C5-C6-N1	-6.73	117.64	121.00
1	A	64	G	C8-N9-C1'	-6.72	118.26	127.00
1	A	852	C	C6-N1-C2	6.71	122.98	120.30
1	A	500	G	P-O3'-C3'	6.69	127.73	119.70
1	A	822	U	N1-C2-O2	6.68	127.47	122.80
1	A	47	C	C6-N1-C2	6.67	122.97	120.30
1	A	124	A	N1-C6-N6	6.66	122.59	118.60
1	A	261	G	N3-C4-C5	6.65	131.92	128.60
1	A	1477	A	O5'-P-OP2	-6.64	99.73	105.70
1	A	1056	G	C5-C6-N1	-6.62	108.19	111.50
1	A	1205	G	P-O3'-C3'	6.58	127.60	119.70
1	A	62	U	C5-C4-O4	6.58	129.85	125.90
1	A	1208	A	N3-C4-C5	6.57	131.40	126.80
1	A	788	C	C6-N1-C2	6.55	122.92	120.30
1	A	21	G	OP2-P-O3'	6.55	119.60	105.20
1	A	1327	A	P-O3'-C3'	6.52	127.53	119.70
1	A	1181	C	C2-N1-C1'	6.47	125.92	118.80
1	A	101	G	C2-N3-C4	-6.47	108.67	111.90
1	A	227	G	N9-C4-C5	-6.45	102.82	105.40
1	A	250	G	C6-C5-N7	-6.45	126.53	130.40
1	A	1207	C	O5'-P-OP2	-6.44	99.90	105.70
1	A	110	G	N9-C4-C5	-6.42	102.83	105.40
1	A	123	G	P-O3'-C3'	6.41	127.39	119.70
1	A	1482	G	O5'-P-OP2	6.40	118.38	110.70
1	A	948	G	N1-C6-O6	6.37	123.72	119.90
1	A	469	G	P-O3'-C3'	6.35	127.33	119.70
1	A	327	G	N1-C6-O6	6.27	123.66	119.90
1	A	669	U	P-O3'-C3'	6.27	127.22	119.70
1	A	802	A	C6-C5-N7	-6.25	127.93	132.30
1	A	904	G	C2-N3-C4	-6.23	108.78	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	323	C	C5-C4-N4	6.23	124.56	120.20
1	A	125	C	N3-C2-O2	-6.23	117.54	121.90
1	A	772	U	N3-C2-O2	-6.21	117.85	122.20
1	A	1507	G	C8-N9-C4	6.21	108.88	106.40
1	A	101	G	C4-N9-C1'	6.20	134.56	126.50
1	A	1505	U	N1-C2-N3	-6.20	111.18	114.90
1	A	1481	G	P-O3'-C3'	6.20	127.14	119.70
1	A	64	G	C4-N9-C1'	6.20	134.56	126.50
1	A	1385	C	C6-N1-C2	-6.20	117.82	120.30
1	A	275	C	C6-N1-C2	6.19	122.78	120.30
1	A	445	A	P-O3'-C3'	6.19	127.12	119.70
1	A	1181	C	C6-N1-C1'	-6.19	113.38	120.80
1	A	19	C	C6-N1-C2	-6.17	117.83	120.30
1	A	445	A	N7-C8-N9	6.17	116.89	113.80
1	A	558	G	N7-C8-N9	-6.17	110.01	113.10
1	A	1496	A	C5-C6-N1	-6.16	114.62	117.70
1	A	64	G	N3-C4-N9	6.16	129.70	126.00
1	A	1398	G	C2-N3-C4	-6.16	108.82	111.90
1	A	772	U	C5-C4-O4	6.15	129.59	125.90
1	A	1379	C	C5-C4-N4	6.14	124.50	120.20
1	A	1432	C	P-O3'-C3'	6.14	127.07	119.70
1	A	233	G	C8-N9-C4	-6.13	103.95	106.40
1	A	569	C	C5-C6-N1	-6.11	117.94	121.00
1	A	847	U	P-O3'-C3'	6.10	127.02	119.70
1	A	64	G	P-O3'-C3'	6.07	126.99	119.70
1	A	65	U	P-O3'-C3'	6.07	126.99	119.70
1	A	684	C	P-O3'-C3'	6.07	126.98	119.70
1	A	1316	C	N1-C2-O2	6.07	122.54	118.90
1	A	1371	C	C6-N1-C2	6.06	122.72	120.30
1	A	910	G	N3-C4-C5	6.06	131.63	128.60
1	A	922	G	N1-C6-O6	6.05	123.53	119.90
1	A	560	G	C8-N9-C4	6.04	108.82	106.40
1	A	239	U	P-O3'-C3'	6.03	126.93	119.70
1	A	1519	U	N1-C2-N3	6.02	118.51	114.90
1	A	954	A	N1-C6-N6	-6.02	114.99	118.60
1	A	118	U	C4-C5-C6	6.02	123.31	119.70
1	A	822	U	C6-N1-C1'	-6.00	112.80	121.20
1	A	84	C	C5-C6-N1	5.98	123.99	121.00
1	A	232	C	C6-N1-C2	5.97	122.69	120.30
1	A	1171	G	P-O3'-C3'	5.96	126.85	119.70
1	A	750	A	N1-C6-N6	-5.96	115.03	118.60
1	A	952	A	O4'-C1'-N9	-5.96	103.44	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1384	C	N3-C4-C5	-5.95	119.52	121.90
1	A	1398	G	C5-C6-O6	-5.94	125.04	128.60
1	A	500	G	C4-N9-C1'	5.93	134.21	126.50
1	A	274	A	O4'-C1'-N9	-5.93	103.45	108.20
1	A	1379	C	N3-C4-N4	-5.93	113.85	118.00
1	A	1464	G	N1-C6-O6	-5.91	116.36	119.90
1	A	1473	C	C6-N1-C2	-5.90	117.94	120.30
1	A	606	C	N1-C2-O2	-5.90	115.36	118.90
1	A	249	G	C8-N9-C4	5.90	108.76	106.40
1	A	7	G	C8-N9-C4	5.88	108.75	106.40
1	A	168	C	C5-C6-N1	5.87	123.93	121.00
1	A	953	G	N1-C6-O6	5.85	123.41	119.90
1	A	1385	C	C5-C6-N1	5.85	123.93	121.00
1	A	959	U	P-O3'-C3'	5.85	126.72	119.70
1	A	948	G	N3-C4-N9	-5.85	122.49	126.00
1	A	417	C	P-O3'-C3'	5.83	126.69	119.70
1	A	782	G	N1-C6-O6	5.82	123.39	119.90
1	A	1177	U	C6-N1-C2	-5.81	117.51	121.00
1	A	175	G	P-O3'-C3'	5.80	126.66	119.70
1	A	867	G	P-O3'-C3'	5.77	126.63	119.70
1	A	223	A	N1-C6-N6	5.77	122.06	118.60
1	A	670	A	P-O3'-C3'	5.75	126.60	119.70
1	A	50	A	P-O3'-C3'	5.74	126.59	119.70
1	A	329	C	C6-N1-C2	-5.74	118.00	120.30
1	A	952	A	C5-N7-C8	-5.74	101.03	103.90
1	A	802	A	C2-N3-C4	-5.73	107.73	110.60
1	A	1072	U	N3-C4-C5	-5.73	111.16	114.60
1	A	952	A	C2-N3-C4	-5.72	107.74	110.60
1	A	797	A	N1-C6-N6	5.72	122.03	118.60
1	A	211	G	O4'-C1'-N9	5.70	112.76	108.20
1	A	326	G	C6-C5-N7	-5.67	127.00	130.40
1	A	1230	C	N1-C2-O2	5.67	122.30	118.90
1	A	1464	G	C4-C5-N7	-5.67	108.53	110.80
1	A	1386	C	C5-C6-N1	5.66	123.83	121.00
1	A	408	G	N1-C6-O6	-5.65	116.51	119.90
1	A	1352	G	N1-C6-O6	5.64	123.29	119.90
1	A	1163	G	P-O3'-C3'	5.63	126.46	119.70
1	A	674	G	C5-C6-N1	-5.63	108.69	111.50
1	A	274	A	N1-C2-N3	5.62	132.11	129.30
1	A	883	G	C4-C5-N7	5.62	113.05	110.80
1	A	1262	U	C5-C6-N1	5.62	125.51	122.70
1	A	261	G	C5-N7-C8	-5.62	101.49	104.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1314	A	C5-C6-N1	5.61	120.50	117.70
1	A	902	G	C8-N9-C4	5.59	108.64	106.40
1	A	641	G	C4-N9-C1'	5.59	133.77	126.50
1	A	817	C	O5'-P-OP2	-5.59	100.67	105.70
1	A	879	G	C8-N9-C4	5.59	108.64	106.40
1	A	708	G	O5'-P-OP1	-5.58	100.67	105.70
1	A	1047	U	P-O3'-C3'	5.58	126.40	119.70
1	A	383	G	C4-N9-C1'	5.58	133.75	126.50
1	A	500	G	C8-N9-C1'	-5.58	119.75	127.00
1	A	274	A	C5-N7-C8	-5.57	101.11	103.90
1	A	501	C	P-O3'-C3'	5.57	126.38	119.70
1	A	952	A	N1-C6-N6	5.56	121.94	118.60
1	A	904	G	N3-C4-N9	-5.55	122.67	126.00
1	A	468	G	P-O3'-C3'	5.54	126.35	119.70
1	A	1521	U	O4'-C1'-N1	5.54	112.63	108.20
1	A	182	C	C6-N1-C2	5.54	122.52	120.30
1	A	1384	C	C4-C5-C6	5.53	120.17	117.40
1	A	948	G	C4-N9-C1'	-5.53	119.31	126.50
1	A	1260	A	C5-N7-C8	-5.53	101.14	103.90
1	A	276	G	P-O3'-C3'	5.53	126.33	119.70
1	A	1081	G	N3-C4-N9	-5.53	122.68	126.00
1	A	864	G	C8-N9-C4	5.53	108.61	106.40
1	A	1362	U	P-O3'-C3'	5.52	126.32	119.70
23	X	31	G	N3-C4-C5	-5.51	125.84	128.60
1	A	1345	A	C8-N9-C4	-5.50	103.60	105.80
1	A	795	C	N3-C2-O2	-5.50	118.05	121.90
1	A	323	C	C2-N1-C1'	5.49	124.84	118.80
1	A	371	G	N1-C6-O6	5.49	123.19	119.90
1	A	594	A	N1-C6-N6	5.49	121.89	118.60
1	A	1208	A	N3-C4-N9	-5.49	123.01	127.40
1	A	668	G	C8-N9-C4	5.48	108.59	106.40
1	A	605	A	O5'-P-OP1	-5.48	100.77	105.70
1	A	674	G	C6-C5-N7	-5.48	127.11	130.40
1	A	669	U	OP1-P-O3'	5.47	117.24	105.20
1	A	115	G	C6-C5-N7	-5.44	127.14	130.40
1	A	1194	A	OP1-P-O3'	5.44	117.17	105.20
1	A	782	G	C5-C6-O6	-5.43	125.34	128.60
1	A	536	A	C2-N3-C4	-5.43	107.88	110.60
1	A	1139	A	P-O3'-C3'	5.43	126.22	119.70
1	A	1194	A	P-O3'-C3'	5.43	126.22	119.70
1	A	739	C	C6-N1-C2	5.43	122.47	120.30
1	A	922	G	C5-C6-O6	-5.43	125.34	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1281	G	P-O3'-C3'	5.41	126.19	119.70
1	A	35	G	N1-C6-O6	5.41	123.15	119.90
1	A	1036	C	C2-N3-C4	5.40	122.60	119.90
1	A	1279	C	P-O3'-C3'	5.40	126.18	119.70
1	A	249	G	O5'-P-OP1	-5.39	100.84	105.70
1	A	1497	G	C2-N3-C4	-5.39	109.20	111.90
1	A	383	G	C8-N9-C1'	-5.39	119.99	127.00
1	A	1519	U	C2-N3-C4	-5.39	123.77	127.00
1	A	682	C	C6-N1-C2	5.38	122.45	120.30
1	A	1077	U	O5'-P-OP2	-5.38	100.86	105.70
20	T	20	LEU	CA-CB-CG	-5.37	102.96	115.30
1	A	227	G	C8-N9-C4	5.36	108.55	106.40
1	A	1379	C	C6-N1-C1'	5.36	127.23	120.80
1	A	794	C	O5'-P-OP1	-5.34	100.89	105.70
1	A	294	G	C5-C6-N1	-5.34	108.83	111.50
1	A	710	G	N3-C4-N9	-5.34	122.80	126.00
1	A	898	U	C5-C6-N1	-5.33	120.03	122.70
1	A	1479	A	N1-C2-N3	5.33	131.97	129.30
1	A	320	A	N9-C4-C5	5.33	107.93	105.80
1	A	793	C	C2-N1-C1'	5.33	124.66	118.80
1	A	949	C	C6-N1-C2	-5.32	118.17	120.30
1	A	383	G	P-O3'-C3'	5.32	126.09	119.70
1	A	283	A	C2-N3-C4	-5.32	107.94	110.60
1	A	323	C	N3-C4-N4	-5.32	114.28	118.00
1	A	1076	G	P-O3'-C3'	5.31	126.08	119.70
1	A	1479	A	C5-C6-N6	-5.31	119.45	123.70
8	H	112	LEU	CA-CB-CG	5.31	127.52	115.30
1	A	83	A	C5-C6-N1	-5.31	115.05	117.70
1	A	802	A	C4-C5-C6	5.31	119.65	117.00
1	A	101	G	C5-C6-N1	-5.30	108.85	111.50
1	A	910	G	C4-N9-C1'	-5.29	119.62	126.50
1	A	110	G	C4-C5-N7	5.29	112.92	110.80
1	A	1388	U	N1-C2-O2	-5.28	119.10	122.80
1	A	1379	C	C2-N1-C1'	-5.26	113.01	118.80
1	A	408	G	P-O3'-C3'	5.26	126.01	119.70
1	A	545	C	C6-N1-C2	5.26	122.40	120.30
1	A	1182	A	P-O3'-C3'	5.26	126.01	119.70
1	A	1178	G	C6-C5-N7	-5.25	127.25	130.40
1	A	594	A	N9-C4-C5	-5.25	103.70	105.80
1	A	83	A	N1-C6-N6	5.24	121.75	118.60
1	A	115	G	N1-C6-O6	5.24	123.05	119.90
1	A	1076	G	OP2-P-O3'	5.24	116.72	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1473	C	C2-N1-C1'	5.23	124.55	118.80
1	A	1398	G	N3-C4-C5	5.23	131.21	128.60
1	A	607	C	C6-N1-C2	5.22	122.39	120.30
1	A	1048	C	C6-N1-C2	-5.21	118.22	120.30
1	A	205	G	N1-C6-O6	5.21	123.03	119.90
1	A	1208	A	C5-C6-N1	-5.21	115.10	117.70
1	A	232	C	C2-N1-C1'	-5.20	113.08	118.80
1	A	937	U	N1-C2-O2	5.20	126.44	122.80
1	A	591	A	OP1-P-O3'	5.20	116.63	105.20
23	X	38	C	N1-C2-O2	5.20	122.02	118.90
1	A	782	G	C6-C5-N7	-5.19	127.29	130.40
1	A	61	G	N1-C6-O6	5.18	123.01	119.90
1	A	566	A	C8-N9-C4	5.16	107.86	105.80
1	A	21	G	O5'-P-OP1	5.15	116.88	110.70
1	A	1042	C	N1-C2-O2	5.15	121.99	118.90
1	A	1475	U	N1-C2-N3	5.15	117.99	114.90
1	A	65	U	OP2-P-O3'	5.15	116.53	105.20
1	A	24	U	C5-C6-N1	-5.15	120.13	122.70
1	A	307	C	C6-N1-C2	5.14	122.36	120.30
1	A	278	C	C5-C6-N1	5.13	123.57	121.00
1	A	555	A	N1-C6-N6	-5.13	115.52	118.60
1	A	1309	C	N1-C2-O2	-5.13	115.82	118.90
1	A	922	G	C8-N9-C1'	-5.12	120.34	127.00
1	A	110	G	C8-N9-C4	5.11	108.44	106.40
1	A	1260	A	N1-C6-N6	5.11	121.67	118.60
1	A	1056	G	N1-C6-O6	5.11	122.96	119.90
1	A	9	G	O5'-P-OP2	-5.10	101.11	105.70
1	A	594	A	C8-N9-C4	5.09	107.84	105.80
1	A	937	U	N3-C2-O2	-5.08	118.64	122.20
1	A	859	C	C6-N1-C2	5.08	122.33	120.30
1	A	649	G	N1-C6-O6	5.08	122.95	119.90
1	A	795	C	N1-C2-N3	5.08	122.76	119.20
1	A	340	C	P-O3'-C3'	5.08	125.79	119.70
1	A	641	G	C8-N9-C1'	-5.08	120.40	127.00
3	C	3	ASN	N-CA-C	5.08	124.70	111.00
1	A	668	G	N3-C4-C5	5.07	131.14	128.60
1	A	101	G	C8-N9-C1'	-5.07	120.42	127.00
1	A	905	G	N1-C6-O6	5.06	122.94	119.90
1	A	290	C	C6-N1-C2	5.06	122.32	120.30
1	A	1521	U	C2-N3-C4	-5.05	123.97	127.00
1	A	550	G	OP2-P-O3'	5.05	116.31	105.20
1	A	1402	C	C6-N1-C2	-5.05	118.28	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	22	G	C8-N9-C4	5.04	108.42	106.40
1	A	952	A	C6-C5-N7	-5.04	128.77	132.30
1	A	35	G	C6-C5-N7	-5.03	127.38	130.40
1	A	1371	C	N3-C2-O2	5.03	125.42	121.90
1	A	408	G	C5-C6-O6	5.03	131.62	128.60
1	A	1475	U	N1-C2-O2	-5.03	119.28	122.80
1	A	1063	G	N1-C6-O6	5.02	122.91	119.90
1	A	276	G	C8-N9-C1'	-5.02	120.47	127.00
1	A	942	A	P-O3'-C3'	5.02	125.72	119.70
1	A	250	G	C8-N9-C1'	-5.01	120.49	127.00
1	A	1466	G	C8-N9-C4	5.01	108.40	106.40
1	A	241	A	O4'-C1'-N9	5.00	112.20	108.20
1	A	1110	C	P-O3'-C3'	5.00	125.70	119.70
1	A	446	A	O5'-P-OP2	5.00	116.70	110.70
1	A	499	U	C5-C6-N1	5.00	125.20	122.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	H	90	GLY	Peptide
20	T	11	SER	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32515	0	16411	405	0
2	B	1900	0	1951	71	0
3	C	1612	0	1677	40	0
4	D	1703	0	1763	52	0
5	E	1146	0	1207	39	0
6	F	843	0	857	21	0
7	G	1257	0	1296	32	0
8	H	1116	0	1177	31	0
9	I	1011	0	1043	37	0
10	J	794	0	840	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	K	885	0	904	22	0
12	L	970	0	1057	28	0
13	M	997	0	1072	29	0
14	N	492	0	529	17	0
15	O	734	0	771	29	0
16	P	700	0	720	21	0
17	Q	857	0	930	24	0
18	R	597	0	668	16	0
19	S	647	0	673	35	0
20	T	762	0	859	30	0
21	V	208	0	221	6	0
22	W	62	0	34	1	0
23	X	189	0	99	5	0
24	A	184	0	0	0	0
24	B	1	0	0	0	0
24	N	1	0	0	0	0
25	A	42	0	45	4	0
26	D	1	0	0	0	0
26	N	1	0	0	0	0
All	All	52227	0	36804	904	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (904) 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)
12:L:27:LEU:O	12:L:29:GLY:N	2.04	0.91
1:A:949:C:OP1	10:J:57:LYS:NZ	2.06	0.86
1:A:1479:A:H2	1:A:1482:G:H1	1.21	0.85
1:A:64:G:H4'	1:A:65:U:H3'	1.57	0.83
3:C:58:GLU:HB3	10:J:92:THR:HG21	1.59	0.82
2:B:15:VAL:HG21	2:B:209:ARG:HB3	1.62	0.82
13:M:10:PRO:HB2	13:M:18:ALA:HB1	1.62	0.81
10:J:40:LEU:HD23	10:J:41:PRO:HD2	1.63	0.80
1:A:952:A:H4'	1:A:953:G:H5''	1.62	0.80
1:A:660:U:H3	1:A:696:G:H22	1.28	0.79
4:D:71:SER:OG	4:D:72:GLU:N	2.13	0.79
1:A:647:G:H22	1:A:724:G:H1	1.29	0.79
1:A:653:G:H21	6:F:73:ASN:HD21	1.28	0.78
12:L:71:PRO:O	12:L:102:ARG:NH1	2.16	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1039:G:H5''	3:C:154:SER:HB2	1.65	0.78
1:A:1077:U:OP1	1:A:1090:G:N1	2.18	0.77
7:G:54:THR:HG22	7:G:56:GLN:H	1.46	0.77
20:T:75:ASN:OD1	20:T:75:ASN:N	2.17	0.77
15:O:74:ASP:HB3	15:O:77:ARG:HG3	1.66	0.77
1:A:980:G:H22	1:A:1021:C:H1'	1.48	0.76
1:A:212:C:O2'	1:A:455:C:N4	2.19	0.75
5:E:81:GLU:HG2	5:E:90:VAL:HG22	1.69	0.74
1:A:1109:G:H22	1:A:1126:G:H22	1.35	0.74
15:O:26:GLU:OE1	15:O:77:ARG:NH1	2.20	0.74
1:A:969:U:H3	1:A:1026:A:H62	1.33	0.73
10:J:90:LEU:H	10:J:91:PRO:HD2	1.53	0.73
3:C:8:ILE:HG23	3:C:16:ARG:HD3	1.71	0.73
4:D:3:ARG:HD3	4:D:4:TYR:H	1.51	0.73
2:B:20:GLU:OE1	2:B:23:ARG:NH1	2.21	0.72
1:A:1273:U:H5'	9:I:38:GLN:HE22	1.53	0.72
1:A:211:G:O2'	1:A:212:C:O5'	2.09	0.71
1:A:818:U:OP1	18:R:64:ARG:NH2	2.23	0.71
1:A:705:A:H2	1:A:716:A:H61	1.35	0.71
5:E:92:LYS:HB3	5:E:119:LEU:HB2	1.73	0.71
1:A:1068:U:H3	1:A:1081:G:H22	1.39	0.71
10:J:61:GLU:OE1	14:N:45:ARG:NH1	2.23	0.70
1:A:96:C:OP1	20:T:17:ARG:NH1	2.24	0.70
1:A:1308:C:OP2	21:V:12:LYS:NZ	2.25	0.70
7:G:15:ASP:OD1	7:G:44:TYR:OH	2.10	0.70
20:T:57:ARG:HE	20:T:102:GLY:HA3	1.55	0.70
1:A:542:A:OP1	5:E:126:ARG:NH2	2.24	0.70
2:B:118:LEU:HA	2:B:121:LEU:HB2	1.72	0.70
8:H:116:LYS:HE3	8:H:127:LEU:HD12	1.73	0.69
19:S:33:THR:HG22	19:S:35:SER:H	1.57	0.69
1:A:981:G:N2	1:A:1020:C:N3	2.39	0.69
1:A:409:A:OP2	1:A:423:G:N2	2.25	0.69
12:L:33:ARG:HD3	12:L:62:SER:HB3	1.74	0.69
1:A:344:A:H2'	1:A:345:G:H5''	1.74	0.69
1:A:1115:G:N2	1:A:1123:C:O2	2.26	0.69
8:H:10:LEU:HD22	8:H:83:ILE:HD11	1.75	0.69
1:A:982:A:OP1	1:A:1003:U:N3	2.26	0.69
7:G:38:LEU:HA	7:G:41:ARG:HB3	1.74	0.68
3:C:154:SER:OG	3:C:155:GLY:N	2.25	0.68
16:P:34:GLU:OE2	16:P:55:ARG:HD3	1.93	0.68
12:L:47:LYS:HB3	12:L:48:PRO:HD3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:86:ILE:HG21	8:H:133:LEU:HD13	1.76	0.68
10:J:57:LYS:O	10:J:60:ARG:NH1	2.27	0.67
1:A:372:G:OP1	16:P:3:LYS:NZ	2.26	0.67
1:A:198:U:H4'	20:T:57:ARG:HD3	1.76	0.67
1:A:1374:G:N2	1:A:1479:A:H8	1.92	0.67
2:B:75:LYS:HA	2:B:78:GLN:HB2	1.75	0.67
6:F:2:ARG:HH21	6:F:69:GLU:HG2	1.59	0.67
1:A:525:G:OP1	4:D:10:ARG:NH2	2.25	0.67
17:Q:67:LYS:HA	17:Q:70:ARG:HH21	1.59	0.67
15:O:63:ARG:O	15:O:65:ARG:N	2.25	0.67
2:B:98:LEU:HB2	2:B:101:MET:HG3	1.77	0.66
1:A:1109:G:H1	1:A:1126:G:H1	1.41	0.66
1:A:953:G:OP2	1:A:1339:U:O2'	2.11	0.66
1:A:596:C:H2'	1:A:597:A:H8	1.61	0.66
16:P:74:LEU:HD22	16:P:79:VAL:HG21	1.77	0.66
8:H:64:LYS:HG2	8:H:79:VAL:HG21	1.78	0.66
4:D:152:SER:O	4:D:154:ASN:N	2.28	0.66
1:A:1109:G:H22	1:A:1126:G:N2	1.94	0.66
1:A:422:U:OP2	4:D:36:ARG:NH2	2.29	0.66
9:I:8:GLY:HA2	9:I:79:LEU:HD13	1.78	0.66
8:H:86:ILE:HG13	8:H:133:LEU:HD22	1.79	0.65
1:A:1516:C:N4	7:G:81:GLY:O	2.27	0.65
1:A:1267:A:H2'	1:A:1268:A:H4'	1.78	0.65
1:A:1390:A:N1	25:A:1785:PAR:O61	2.30	0.65
1:A:952:A:H8	1:A:952:A:H5'	1.62	0.65
15:O:26:GLU:HA	15:O:81:LEU:HD11	1.79	0.65
9:I:9:ARG:HG2	9:I:14:VAL:HG22	1.78	0.65
1:A:348:A:H8	1:A:348:A:H5'	1.62	0.65
12:L:74:GLY:O	12:L:102:ARG:NH2	2.30	0.64
3:C:60:ALA:O	3:C:62:ASP:N	2.30	0.64
1:A:951:A:OP1	14:N:29:ARG:NH2	2.30	0.64
11:K:43:SER:HB3	11:K:68:ALA:HB2	1.78	0.64
1:A:596:C:H2'	1:A:597:A:C8	2.33	0.64
1:A:543:U:H5'	1:A:549:G:N2	2.13	0.63
2:B:10:LEU:O	2:B:12:GLU:N	2.31	0.63
4:D:187:ARG:NH1	4:D:188:LEU:HB2	2.13	0.63
5:E:40:ARG:HH11	5:E:40:ARG:HG2	1.63	0.63
20:T:50:GLU:HG3	20:T:100:ILE:HB	1.79	0.63
1:A:562:G:H5'	1:A:711:A:H1'	1.78	0.63
3:C:11:ARG:NH1	3:C:177:THR:O	2.31	0.63
6:F:22:GLU:OE1	6:F:82:ARG:NH1	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1034:U:O2'	1:A:1037:A:OP2	2.10	0.63
1:A:257:A:H5'	20:T:74:LYS:HD3	1.80	0.63
1:A:565:U:H5''	15:O:64:ARG:HH22	1.64	0.63
23:X:34:RSQ:H6	23:X:34:RSQ:H5'	1.80	0.63
18:R:40:LEU:HD11	18:R:69:THR:HG22	1.80	0.63
1:A:904:G:H4'	1:A:1480:A:N7	2.14	0.62
1:A:1472:U:H2'	1:A:1473:C:H6	1.62	0.62
3:C:6:HIS:HD2	3:C:8:ILE:H	1.46	0.62
2:B:18:GLY:HA3	2:B:41:ILE:HD13	1.79	0.62
2:B:10:LEU:HD23	2:B:11:LEU:HG	1.79	0.62
2:B:109:SER:OG	2:B:110:GLN:N	2.33	0.62
1:A:1409:U:H2'	1:A:1410:A:C8	2.35	0.62
5:E:33:VAL:HG11	5:E:109:ILE:HG12	1.82	0.62
2:B:115:LEU:HD11	2:B:146:GLN:HG3	1.81	0.62
12:L:70:ILE:HD13	12:L:77:LEU:HD12	1.82	0.62
4:D:155:LEU:HD12	4:D:158:ILE:HD11	1.82	0.61
19:S:41:VAL:HG22	19:S:44:MET:HG3	1.83	0.61
1:A:1129:C:O2	9:I:16:ARG:NH1	2.34	0.61
5:E:11:ILE:HD12	5:E:31:LEU:HD13	1.83	0.61
1:A:1339:U:OP1	14:N:35:ARG:HG2	2.01	0.61
1:A:1394:C:H2'	1:A:1395:A:C8	2.36	0.61
4:D:187:ARG:HD2	4:D:188:LEU:H	1.64	0.61
19:S:58:VAL:HG23	19:S:60:VAL:HG23	1.81	0.61
23:X:34:RSQ:C6	23:X:34:RSQ:H5'	2.30	0.61
1:A:775:A:H4'	1:A:776:U:O5'	2.01	0.61
10:J:50:ILE:H	10:J:50:ILE:HD12	1.64	0.61
9:I:10:ARG:NH1	9:I:75:ASP:OD2	2.34	0.60
9:I:43:ALA:HA	9:I:74:ILE:HD13	1.83	0.60
12:L:77:LEU:HD21	12:L:107:ALA:HB2	1.82	0.60
1:A:1109:G:N2	1:A:1126:G:H22	2.00	0.60
1:A:1044:U:H2'	1:A:1045:C:C6	2.36	0.60
1:A:1374:G:H21	1:A:1479:A:H8	1.47	0.60
3:C:50:ALA:HB2	3:C:75:VAL:HG22	1.82	0.60
7:G:74:GLU:HG2	7:G:91:VAL:HG22	1.84	0.60
9:I:18:PHE:HD1	9:I:62:TYR:HD2	1.49	0.60
3:C:95:THR:HG22	3:C:97:LYS:H	1.67	0.60
19:S:50:ALA:HB1	19:S:57:HIS:HB3	1.83	0.60
1:A:982:A:H62	1:A:1019:C:N4	2.00	0.60
3:C:6:HIS:CD2	3:C:8:ILE:HB	2.37	0.60
3:C:134:ILE:HG22	3:C:168:ALA:HB3	1.84	0.60
6:F:10:LEU:HB2	6:F:59:TYR:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:48:THR:OG1	10:J:62:HIS:ND1	2.34	0.60
1:A:1350:G:OP2	9:I:112:LYS:HD2	2.01	0.60
5:E:150:ARG:HB3	5:E:150:ARG:HH11	1.67	0.60
1:A:1110:C:OP1	9:I:66:ARG:NH1	2.33	0.60
1:A:1106:G:H5'	10:J:35:SER:O	2.01	0.60
1:A:256:U:OP2	20:T:79:ARG:NH2	2.34	0.59
1:A:323:C:O2	1:A:323:C:H2'	2.02	0.59
5:E:10:MET:H	5:E:32:VAL:HG23	1.67	0.59
17:Q:24:GLU:HA	17:Q:39:SER:HB3	1.84	0.59
1:A:408:G:N2	1:A:423:G:H1'	2.18	0.59
1:A:547:C:O2'	8:H:91:ARG:NH2	2.36	0.59
13:M:49:THR:HG22	13:M:51:ALA:H	1.66	0.59
1:A:264:C:H2'	1:A:265:A:C8	2.37	0.59
5:E:20:GLN:HG3	5:E:21:ALA:O	2.02	0.59
1:A:954:A:N6	1:A:1205:G:H5''	2.18	0.59
10:J:38:ILE:HB	10:J:71:LEU:HB3	1.85	0.59
16:P:3:LYS:HG2	16:P:24:ALA:HB2	1.85	0.59
23:X:33:C:H2'	23:X:34:RSQ:H5'A	1.84	0.59
19:S:53:ASN:HB3	19:S:56:GLN:H	1.68	0.58
1:A:1076:G:O2'	1:A:1077:U:OP2	2.19	0.58
2:B:103:THR:HA	2:B:180:LEU:HD11	1.85	0.58
1:A:1209:C:H4'	13:M:116:THR:HA	1.83	0.58
15:O:75:PRO:HA	15:O:78:TYR:HB3	1.84	0.58
1:A:951:A:P	14:N:29:ARG:HH22	2.27	0.58
4:D:61:LYS:HE2	4:D:206:PHE:CE2	2.38	0.58
1:A:1328:G:C8	9:I:107:ARG:HG2	2.38	0.58
13:M:98:VAL:HG23	13:M:110:ARG:HH12	1.69	0.58
5:E:79:GLU:HG3	5:E:93:PRO:HD3	1.85	0.58
1:A:1206:A:H3'	1:A:1207:C:C6	2.39	0.58
1:A:1373:U:H2'	1:A:1374:G:C8	2.39	0.58
5:E:11:ILE:HG21	5:E:105:VAL:HG13	1.86	0.57
1:A:1294:U:O4	19:S:4:SER:OG	2.19	0.57
2:B:58:ILE:HG22	2:B:222:ILE:HD11	1.86	0.57
3:C:108:ASN:HB3	3:C:111:LEU:HB2	1.87	0.57
1:A:1409:U:H2'	1:A:1410:A:H8	1.69	0.57
2:B:18:GLY:HA2	2:B:42:ILE:HG12	1.87	0.57
16:P:51:VAL:O	16:P:52:ASP:HB3	2.03	0.57
3:C:174:PRO:HB2	3:C:177:THR:HG23	1.85	0.57
10:J:4:ILE:HD11	10:J:74:ILE:HB	1.86	0.57
1:A:121:G:O3'	17:Q:3:LYS:NZ	2.37	0.57
1:A:1109:G:N2	1:A:1128:A:H62	2.01	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:191:ARG:NH1	4:D:200:GLU:OE1	2.38	0.57
12:L:87:GLY:H	12:L:98:TYR:HB3	1.70	0.57
20:T:59:ALA:O	20:T:63:ILE:HG13	2.05	0.57
1:A:123:G:N3	1:A:189:U:H3'	2.20	0.56
6:F:8:ILE:HG12	6:F:88:VAL:HG22	1.87	0.56
1:A:1348:C:H2'	1:A:1349:C:C6	2.40	0.56
1:A:442:A:OP2	1:A:469:G:N1	2.34	0.56
1:A:563:U:H2'	1:A:564:G:O4'	2.05	0.56
5:E:28:PHE:CD2	5:E:51:VAL:HG22	2.40	0.56
19:S:46:GLY:H	19:S:62:ILE:HG23	1.70	0.56
3:C:14:ILE:O	3:C:16:ARG:N	2.39	0.56
4:D:145:GLU:OE2	4:D:182:LYS:HD2	2.05	0.56
1:A:62:U:H2'	1:A:63:C:C6	2.40	0.56
3:C:150:LYS:HG3	3:C:169:ALA:HB2	1.87	0.56
10:J:4:ILE:HG22	10:J:100:THR:HG22	1.87	0.56
3:C:178:LEU:O	3:C:180:ALA:N	2.38	0.56
8:H:20:TYR:CE1	8:H:76:PRO:HD2	2.40	0.56
13:M:23:TYR:HB3	13:M:67:GLU:HA	1.87	0.56
15:O:63:ARG:C	15:O:65:ARG:H	2.06	0.56
17:Q:59:ILE:HD12	17:Q:73:VAL:HA	1.87	0.56
1:A:1417:G:H2'	1:A:1418:U:C6	2.40	0.56
2:B:189:ASP:O	2:B:191:ASP:N	2.35	0.56
1:A:1076:G:HO2'	1:A:1077:U:P	2.28	0.56
1:A:505:C:OP2	12:L:69:TYR:OH	2.22	0.56
2:B:204:ASN:HD22	2:B:206:ASP:H	1.53	0.56
2:B:32:ILE:HD12	2:B:40:HIS:HB3	1.87	0.56
7:G:15:ASP:HB3	7:G:20:ASP:H	1.71	0.56
17:Q:67:LYS:O	17:Q:69:LYS:N	2.37	0.56
2:B:12:GLU:OE2	2:B:14:GLY:N	2.32	0.55
1:A:1109:G:H1	1:A:1126:G:H22	1.55	0.55
1:A:1221:U:OP1	7:G:116:ALA:HB2	2.07	0.55
1:A:1222:G:H2'	1:A:1223:C:C6	2.40	0.55
1:A:143:A:H2'	1:A:144:C:C6	2.42	0.55
1:A:819:G:OP1	18:R:61:LYS:NZ	2.37	0.55
19:S:40:ILE:HG21	19:S:62:ILE:HD11	1.88	0.55
4:D:7:PRO:HB2	4:D:10:ARG:HG2	1.87	0.55
19:S:51:VAL:HG22	19:S:71:LEU:HD13	1.88	0.55
2:B:97:TRP:HZ3	2:B:176:GLU:OE2	1.90	0.55
18:R:47:THR:HG21	18:R:49:LYS:HE2	1.89	0.55
1:A:922:G:C2	1:A:923:A:C8	2.95	0.55
12:L:47:LYS:CB	12:L:48:PRO:HD3	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:11:ARG:HG2	13:M:12:ASN:N	2.22	0.55
4:D:18:LYS:HE2	4:D:31:CYS:HB3	1.89	0.55
7:G:12:LEU:H	7:G:12:LEU:HD12	1.72	0.55
15:O:71:GLN:HG3	15:O:78:TYR:CE2	2.41	0.55
1:A:952:A:H5'	1:A:952:A:C8	2.41	0.55
3:C:5:ILE:HD13	3:C:10:PHE:HB2	1.89	0.55
5:E:87:SER:HB3	5:E:131:ILE:HD13	1.88	0.55
16:P:50:LYS:HZ2	16:P:51:VAL:H	1.54	0.55
1:A:7:G:H5'	1:A:293:A:O4'	2.07	0.54
1:A:1093:A:N1	3:C:177:THR:HB	2.22	0.54
1:A:1207:C:H5'	13:M:96:LEU:HD13	1.89	0.54
19:S:50:ALA:HA	19:S:58:VAL:O	2.06	0.54
4:D:199:ASN:ND2	4:D:202:LEU:HG	2.23	0.54
1:A:1037:A:C6	1:A:1187:G:C5	2.96	0.54
25:A:1785:PAR:H642	25:A:1785:PAR:H43	1.90	0.54
11:K:126:ARG:O	11:K:128:ALA:N	2.41	0.54
17:Q:101:ARG:H	17:Q:101:ARG:HD2	1.71	0.54
19:S:36:ARG:HH12	19:S:75:ALA:HB3	1.71	0.54
1:A:124:A:H1'	1:A:258:A:O2'	2.08	0.54
1:A:211:G:O2'	1:A:212:C:O4'	2.25	0.54
2:B:197:VAL:HB	2:B:200:ILE:HG12	1.89	0.54
2:B:232:PRO:C	2:B:234:PRO:HD3	2.28	0.54
18:R:46:GLU:OE2	18:R:46:GLU:N	2.38	0.54
1:A:1379:C:H4'	1:A:1380:A:OP2	2.05	0.54
1:A:60:A:H4'	1:A:61:G:O5'	2.07	0.54
7:G:46:ALA:O	7:G:50:ILE:HG12	2.07	0.54
1:A:1005:C:H42	1:A:1016:G:H1	1.53	0.54
1:A:170:C:H2'	1:A:171:C:H6	1.73	0.54
1:A:396:C:O2'	1:A:604:A:N3	2.30	0.54
15:O:82:ILE:HG23	15:O:87:ILE:HB	1.89	0.54
25:A:1785:PAR:H322	25:A:1785:PAR:H51	1.71	0.54
5:E:20:GLN:HG2	5:E:25:ARG:NH2	2.23	0.54
1:A:1472:U:H2'	1:A:1473:C:C6	2.41	0.54
1:A:816:U:H2'	1:A:817:C:C6	2.43	0.54
8:H:60:ARG:HH11	8:H:60:ARG:HG2	1.73	0.54
11:K:93:GLN:HA	11:K:96:ARG:HD2	1.90	0.54
5:E:10:MET:N	5:E:32:VAL:HG23	2.23	0.53
20:T:100:ILE:HG23	20:T:102:GLY:H	1.74	0.53
2:B:72:GLY:HA3	2:B:81:VAL:HG21	1.90	0.53
9:I:17:VAL:HG11	9:I:81:ILE:HA	1.90	0.53
1:A:106:G:H1'	1:A:349:G:H5'	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:953:G:H5'	1:A:1339:U:O2'	2.08	0.53
1:A:1487:U:H2'	1:A:1488:G:C8	2.43	0.53
15:O:56:LEU:HA	15:O:59:MET:HG3	1.90	0.53
1:A:1133:A:H5''	10:J:42:THR:HG22	1.91	0.53
1:A:951:A:OP2	14:N:41:ARG:NH1	2.42	0.53
12:L:27:LEU:C	12:L:29:GLY:H	2.12	0.53
1:A:656:G:H2'	1:A:657:G:C8	2.44	0.53
1:A:923:A:H2'	1:A:924:G:C8	2.43	0.53
1:A:1046:G:H1'	1:A:1171:G:H21	1.73	0.53
1:A:238:A:C2	1:A:241:A:C8	2.97	0.53
1:A:1231:A:H4'	9:I:68:GLY:H	1.74	0.52
20:T:58:LYS:HE3	20:T:62:LEU:HD21	1.91	0.52
8:H:7:ALA:HB2	8:H:85:ARG:HD2	1.91	0.52
16:P:10:GLY:HA3	16:P:14:ASN:O	2.10	0.52
20:T:9:ASN:O	20:T:10:LEU:HD23	2.09	0.52
1:A:1378:A:H4'	1:A:1379:C:O5'	2.08	0.52
1:A:1407:U:H3	1:A:1452:G:H1	1.57	0.52
1:A:1204:C:H3'	1:A:1205:G:H5'	1.91	0.52
1:A:1358:U:H2'	1:A:1359:A:C8	2.44	0.52
1:A:816:U:H2'	1:A:817:C:H6	1.75	0.52
7:G:136:LYS:O	7:G:140:ASP:HB2	2.09	0.52
6:F:30:LEU:HD23	6:F:75:LEU:HD21	1.91	0.52
13:M:8:GLU:HG3	13:M:22:ILE:HG23	1.92	0.52
1:A:294:G:H2'	1:A:295:A:C8	2.45	0.52
1:A:701:G:H5'	11:K:117:ASN:HB2	1.92	0.52
5:E:79:GLU:HG3	5:E:93:PRO:CD	2.41	0.51
8:H:20:TYR:HE2	8:H:75:ARG:HD2	1.75	0.51
1:A:1281:G:O2'	1:A:1282:U:P	2.69	0.51
1:A:855:G:H5'	8:H:89:PRO:HG2	1.92	0.51
6:F:32:ASN:O	6:F:71:ARG:NH2	2.44	0.51
1:A:1127:C:H4'	1:A:1128:A:O5'	2.10	0.51
15:O:78:TYR:CZ	15:O:82:ILE:HD11	2.44	0.51
1:A:822:U:H2'	1:A:822:U:O2	2.10	0.51
10:J:5:ARG:HA	10:J:73:ASP:OD1	2.11	0.51
1:A:5:U:H4'	1:A:6:G:O5'	2.10	0.51
2:B:80:ILE:HD11	2:B:208:ILE:HG23	1.91	0.51
4:D:111:ALA:HB2	4:D:120:LEU:HD12	1.92	0.51
4:D:48:ALA:HA	4:D:49:ARG:HH21	1.75	0.51
5:E:65:ASN:ND2	5:E:65:ASN:O	2.43	0.51
17:Q:63:ARG:HG2	17:Q:64:PRO:HD2	1.93	0.51
1:A:1111:C:H5'	9:I:62:TYR:OH	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:773:A:H5''	1:A:774:G:OP2	2.10	0.51
1:A:984:C:H2'	1:A:985:C:C6	2.45	0.51
8:H:34:GLU:HB3	8:H:118:VAL:HG21	1.93	0.51
8:H:4:ASP:OD2	8:H:85:ARG:NH1	2.34	0.51
1:A:1324:G:H2'	1:A:1325:C:C6	2.45	0.51
1:A:778:C:H5''	1:A:779:C:OP2	2.11	0.51
3:C:179:ARG:HD3	3:C:207:VAL:HG22	1.93	0.51
1:A:1110:C:H4'	9:I:16:ARG:HH22	1.74	0.51
17:Q:83:ASP:N	17:Q:83:ASP:OD1	2.43	0.51
1:A:635:U:O2'	1:A:636:A:OP2	2.26	0.51
4:D:13:ARG:NH2	4:D:40:PRO:HA	2.26	0.51
7:G:15:ASP:OD1	7:G:16:LEU:N	2.43	0.51
20:T:67:ALA:HA	20:T:73:HIS:H	1.75	0.51
1:A:648:A:N3	1:A:715:C:H2'	2.26	0.51
1:A:1231:A:H4'	9:I:68:GLY:N	2.26	0.51
10:J:40:LEU:HD12	10:J:71:LEU:HB2	1.93	0.51
15:O:39:LEU:HD13	15:O:56:LEU:HB2	1.93	0.51
1:A:952:A:H4'	1:A:953:G:C5'	2.38	0.50
13:M:73:GLU:O	13:M:77:ASN:HB2	2.11	0.50
20:T:45:GLN:HA	20:T:91:LEU:HD22	1.92	0.50
1:A:385:C:H2'	1:A:386:G:C8	2.46	0.50
1:A:937:U:H2'	1:A:937:U:O2	2.10	0.50
6:F:33:TYR:HA	6:F:71:ARG:NH2	2.25	0.50
7:G:69:VAL:O	7:G:138:LYS:HG3	2.10	0.50
13:M:90:LEU:O	13:M:94:ARG:HG2	2.11	0.50
1:A:1061:G:O3'	5:E:14:ARG:NH2	2.44	0.50
1:A:1229:A:H2'	1:A:1230:C:H6	1.76	0.50
1:A:1384:C:H2'	1:A:1385:C:O4'	2.11	0.50
1:A:253:G:H2'	1:A:254:G:H8	1.77	0.50
1:A:255:G:H2'	1:A:256:U:C6	2.46	0.50
1:A:64:G:OP1	1:A:64:G:H3'	2.11	0.50
15:O:54:ARG:O	15:O:58:MET:HG3	2.11	0.50
11:K:110:ASP:HB2	18:R:88:LYS:HG3	1.94	0.50
1:A:584:C:H2'	1:A:585:A:C8	2.47	0.50
1:A:944:C:O3'	9:I:128:ARG:NH2	2.45	0.50
1:A:1107:U:H3	10:J:5:ARG:NH2	2.09	0.50
20:T:57:ARG:HH21	20:T:100:ILE:HG21	1.76	0.50
1:A:1109:G:N3	1:A:1109:G:H2'	2.27	0.50
1:A:1328:G:N2	1:A:1355:G:H2'	2.26	0.50
1:A:155:A:H2'	1:A:156:A:C8	2.46	0.50
2:B:158:LEU:HD21	2:B:180:LEU:HD13	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:51:LEU:HD13	2:B:201:ILE:HG23	1.94	0.50
2:B:207:ALA:O	2:B:209:ARG:N	2.36	0.50
17:Q:24:GLU:HG2	17:Q:39:SER:HB3	1.94	0.50
1:A:1202:G:OP2	19:S:37:ARG:NH2	2.45	0.50
1:A:1333:C:H2'	1:A:1334:G:C8	2.46	0.50
4:D:49:ARG:N	4:D:49:ARG:HE	2.10	0.50
1:A:629:U:H2'	1:A:630:C:C6	2.47	0.49
1:A:522:A:OP2	12:L:115:LYS:HE3	2.12	0.49
7:G:9:VAL:HG21	7:G:94:ARG:HD3	1.95	0.49
1:A:1348:C:H2'	1:A:1349:C:H6	1.77	0.49
1:A:273:G:H21	1:A:274:A:H62	1.59	0.49
1:A:713:G:N2	1:A:748:G:H5''	2.27	0.49
2:B:71:VAL:HG22	2:B:164:VAL:HA	1.94	0.49
8:H:85:ARG:HH21	8:H:134:ILE:HG23	1.78	0.49
11:K:33:THR:HG22	11:K:39:PRO:HA	1.94	0.49
11:K:78:GLN:O	11:K:104:GLN:N	2.43	0.49
1:A:1037:A:N7	1:A:1181:C:N4	2.61	0.49
1:A:1100:C:H1'	1:A:1160:A:C4	2.47	0.49
1:A:8:A:N6	4:D:205:GLU:O	2.45	0.49
2:B:233:SER:N	2:B:234:PRO:HD3	2.28	0.49
1:A:1039:G:C4	1:A:1185:A:C2	3.01	0.49
8:H:25:ASP:OD1	8:H:60:ARG:NE	2.37	0.49
18:R:68:LYS:O	18:R:72:ARG:HG3	2.12	0.49
19:S:53:ASN:HB2	19:S:56:GLN:O	2.13	0.49
1:A:1433:G:N2	1:A:1434:G:N7	2.60	0.49
2:B:71:VAL:HG22	2:B:164:VAL:HG22	1.95	0.49
1:A:315:C:H2'	1:A:316:A:C8	2.47	0.49
1:A:348:A:H5'	1:A:348:A:C8	2.43	0.49
3:C:130:VAL:O	3:C:134:ILE:HG13	2.13	0.49
4:D:140:VAL:HG11	4:D:146:ILE:HD11	1.94	0.49
4:D:196:LEU:HD23	4:D:197:PRO:HD2	1.95	0.49
1:A:168:C:H6	1:A:168:C:H5'	1.78	0.49
2:B:115:LEU:HD13	2:B:145:LEU:HB2	1.95	0.49
2:B:47:THR:O	2:B:51:LEU:HB2	2.12	0.49
6:F:9:VAL:HG22	6:F:60:PHE:CE2	2.47	0.49
12:L:56:ALA:HB2	12:L:70:ILE:HD11	1.93	0.49
15:O:87:ILE:HG22	15:O:88:ARG:H	1.77	0.49
1:A:102:A:H2'	1:A:321:G:N2	2.27	0.49
1:A:642:U:OP2	15:O:8:LYS:NZ	2.41	0.49
9:I:114:TYR:CD2	10:J:60:ARG:HB3	2.48	0.49
1:A:1051:C:O2'	1:A:1173:C:H1'	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:G:O2'	1:A:202:A:N1	2.29	0.48
1:A:733:G:O2'	15:O:21:ASP:OD2	2.31	0.48
2:B:187:LEU:HD12	2:B:201:ILE:O	2.13	0.48
7:G:152:ALA:O	7:G:155:ARG:HG2	2.13	0.48
10:J:19:SER:CB	10:J:91:PRO:HG3	2.43	0.48
13:M:15:VAL:HG23	13:M:43:THR:O	2.13	0.48
2:B:147:LYS:HD2	2:B:148:TYR:CE2	2.48	0.48
7:G:151:TYR:OH	11:K:54:ARG:HD3	2.13	0.48
1:A:1298:C:H2'	1:A:1299:A:O4'	2.13	0.48
1:A:441:G:O6	1:A:469:G:O2'	2.21	0.48
1:A:964:G:H1	1:A:1199:C:H42	1.61	0.48
4:D:187:ARG:HD2	4:D:188:LEU:N	2.27	0.48
5:E:150:ARG:HB3	5:E:150:ARG:NH1	2.27	0.48
8:H:101:PRO:HG3	8:H:133:LEU:HD11	1.94	0.48
8:H:53:VAL:HG23	8:H:58:TYR:CD1	2.48	0.48
12:L:8:ASN:O	12:L:12:ARG:HG3	2.13	0.48
1:A:958:U:H5'	14:N:21:TYR:CE1	2.48	0.48
15:O:60:VAL:O	15:O:64:ARG:HG2	2.12	0.48
1:A:696:G:H2'	1:A:697:G:C8	2.47	0.48
1:A:1022:U:O4	1:A:1023:A:N6	2.47	0.48
1:A:330:C:H2'	1:A:331:C:C6	2.49	0.48
1:A:1106:G:O2'	1:A:1127:C:C4	2.66	0.48
1:A:797:A:H2'	1:A:799:A:H5"	1.96	0.48
1:A:1381:C:C2	1:A:1383:G:C5	3.01	0.48
1:A:897:U:H2'	1:A:898:U:C6	2.48	0.48
3:C:116:VAL:HG21	3:C:202:ILE:HD11	1.95	0.48
4:D:102:ASP:OD2	4:D:103:ASN:N	2.47	0.48
1:A:1204:C:P	19:S:78:ARG:HH21	2.36	0.48
1:A:1458:U:H2'	1:A:1459:G:O4'	2.13	0.48
6:F:7:ASN:HB2	6:F:89:MET:HB3	1.96	0.48
8:H:86:ILE:HG12	8:H:135:CYS:HA	1.95	0.48
1:A:1109:G:H1	1:A:1126:G:N2	2.12	0.48
2:B:204:ASN:HD22	2:B:205:ASP:N	2.11	0.48
2:B:21:ARG:HB2	2:B:22:LYS:H	1.56	0.48
4:D:110:PHE:HD1	4:D:162:LEU:HD11	1.79	0.48
13:M:86:CYS:SG	13:M:87:TYR:N	2.87	0.48
1:A:407:A:H61	4:D:35:ARG:HB3	1.78	0.47
1:A:954:A:H62	1:A:1205:G:H5"	1.79	0.47
1:A:738:G:H1'	8:H:1:MET:HE1	1.95	0.47
1:A:1350:G:OP1	9:I:111:ARG:NH2	2.47	0.47
1:A:506:A:C2	12:L:91:LYS:HB3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:68:LYS:HA	20:T:68:LYS:HD2	1.66	0.47
1:A:1185:A:H5'	1:A:1186:U:OP2	2.14	0.47
1:A:1381:C:C2	1:A:1479:A:N6	2.82	0.47
1:A:797:A:O2'	1:A:798:A:H3'	2.14	0.47
1:A:866:A:H4'	1:A:867:G:OP1	2.14	0.47
4:D:176:LEU:HA	4:D:183:GLY:HA2	1.95	0.47
1:A:1063:G:OP1	5:E:16:THR:OG1	2.32	0.47
5:E:19:MET:SD	5:E:24:ARG:HB3	2.53	0.47
1:A:584:C:H2'	1:A:585:A:H8	1.79	0.47
10:J:5:ARG:HD2	10:J:99:LYS:HB2	1.96	0.47
1:A:394:G:H2'	1:A:395:C:C6	2.49	0.47
1:A:42:G:H2'	1:A:43:C:O4'	2.13	0.47
2:B:217:ARG:NH1	2:B:236:TYR:OH	2.44	0.47
3:C:120:VAL:HB	3:C:198:VAL:HG11	1.96	0.47
6:F:18:GLN:O	6:F:21:LEU:HB3	2.15	0.47
1:A:1139:A:H4'	1:A:1140:C:O5'	2.15	0.47
1:A:1273:U:H5'	9:I:38:GLN:NE2	2.27	0.47
1:A:872:G:H2'	1:A:873:C:C6	2.50	0.47
9:I:4:TYR:CE1	9:I:88:TYR:HD1	2.33	0.47
1:A:1310:A:H5'	13:M:29:ARG:HD2	1.96	0.47
1:A:170:C:H2'	1:A:171:C:C6	2.50	0.47
1:A:180:C:H2'	1:A:181:C:C6	2.50	0.47
2:B:211:ILE:O	2:B:215:LEU:HB2	2.15	0.47
4:D:110:PHE:CD1	4:D:162:LEU:HD11	2.49	0.47
1:A:1445:A:H2'	1:A:1446:G:O4'	2.15	0.47
1:A:582:C:O2'	8:H:129:VAL:HG12	2.15	0.47
15:O:78:TYR:CE1	15:O:82:ILE:HD11	2.49	0.47
16:P:42:ARG:HB3	16:P:44:THR:HG23	1.95	0.47
1:A:197:G:O2'	20:T:102:GLY:O	2.17	0.47
4:D:70:ILE:HD11	4:D:100:ARG:HD2	1.96	0.47
1:A:1131:C:H2'	1:A:1132:U:C6	2.50	0.47
1:A:1373:U:H2'	1:A:1374:G:H8	1.79	0.47
1:A:559:G:H3'	1:A:560:G:H5''	1.97	0.47
7:G:113:GLU:HG2	7:G:113:GLU:H	1.32	0.47
13:M:98:VAL:HG23	13:M:110:ARG:NH1	2.30	0.47
1:A:1305:A:O4'	1:A:1343:C:H4'	2.13	0.47
3:C:112:SER:OG	3:C:112:SER:O	2.32	0.47
9:I:26:VAL:HG13	9:I:61:ALA:HB3	1.97	0.47
1:A:198:U:H1'	20:T:103:GLY:HA2	1.97	0.47
4:D:24:GLU:HG2	4:D:25:ARG:H	1.80	0.47
9:I:18:PHE:HB2	9:I:62:TYR:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:11:LYS:HG3	11:K:12:ARG:NH2	2.30	0.47
1:A:1224:C:OP1	21:V:10:ARG:HG3	2.15	0.47
1:A:1005:C:N4	1:A:1016:G:H22	2.13	0.46
1:A:625:A:N3	8:H:113:SER:OG	2.47	0.46
3:C:73:PRO:HG3	3:C:105:GLU:HG2	1.97	0.46
16:P:53:VAL:O	16:P:57:ARG:HG3	2.14	0.46
20:T:73:HIS:HB3	20:T:74:LYS:HG2	1.97	0.46
1:A:1074:A:C6	1:A:1075:A:C6	3.03	0.46
1:A:603:C:H2'	1:A:604:A:O4'	2.14	0.46
1:A:47:C:C6	1:A:360:U:H2'	2.50	0.46
1:A:634:C:O2'	1:A:635:U:H5'	2.16	0.46
1:A:704:G:H4'	1:A:705:A:O5'	2.16	0.46
4:D:13:ARG:HH21	4:D:40:PRO:HA	1.80	0.46
12:L:34:ARG:O	12:L:61:THR:HG23	2.15	0.46
16:P:50:LYS:HD3	16:P:51:VAL:N	2.30	0.46
1:A:1280:A:C8	1:A:1282:U:H1'	2.51	0.46
1:A:162:G:N1	1:A:163:C:C4	2.83	0.46
1:A:371:G:H5''	16:P:5:ARG:HD2	1.96	0.46
1:A:565:U:H5''	15:O:64:ARG:NH2	2.30	0.46
4:D:35:ARG:O	4:D:36:ARG:HB2	2.16	0.46
12:L:13:LYS:HG2	12:L:13:LYS:H	1.47	0.46
13:M:91:ARG:HH21	13:M:96:LEU:HB3	1.80	0.46
19:S:51:VAL:O	19:S:58:VAL:HG22	2.15	0.46
1:A:1005:C:H42	1:A:1016:G:H22	1.62	0.46
1:A:1006:C:H4'	1:A:1006:C:OP1	2.16	0.46
2:B:18:GLY:HA3	2:B:41:ILE:HA	1.96	0.46
2:B:9:GLU:OE2	2:B:217:ARG:NH2	2.31	0.46
3:C:32:LEU:HD22	3:C:59:ARG:HD3	1.98	0.46
5:E:8:GLU:OE2	5:E:63:ARG:NH2	2.48	0.46
17:Q:45:HIS:NE2	17:Q:47:PRO:HG3	2.30	0.46
1:A:1046:G:H1'	1:A:1171:G:N2	2.31	0.46
1:A:1327:A:O2'	1:A:1328:G:OP2	2.25	0.46
2:B:84:GLU:OE1	2:B:216:SER:HA	2.16	0.46
6:F:8:ILE:HD11	6:F:79:LEU:HD13	1.98	0.46
11:K:32:ILE:HG22	11:K:40:ILE:HD12	1.97	0.46
1:A:442:A:C4	1:A:471:A:C2	3.03	0.46
1:A:727:C:H2'	1:A:728:C:C6	2.50	0.46
2:B:214:ILE:HA	2:B:214:ILE:HD13	1.82	0.46
4:D:173:TRP:HB2	4:D:187:ARG:O	2.16	0.46
4:D:60:GLU:HG2	4:D:202:LEU:HB2	1.98	0.46
8:H:100:ILE:HA	8:H:101:PRO:HD2	1.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:502:C:H2'	1:A:503:A:C8	2.51	0.46
1:A:761:G:H2'	1:A:762:C:O4'	2.15	0.46
2:B:196:LEU:HA	2:B:196:LEU:HD23	1.73	0.46
4:D:36:ARG:HG3	4:D:38:TYR:CZ	2.51	0.46
9:I:70:LYS:O	9:I:74:ILE:HG13	2.15	0.46
11:K:20:TYR:CE2	11:K:83:ILE:HD12	2.51	0.46
17:Q:40:LYS:HD2	17:Q:42:TYR:CZ	2.50	0.46
1:A:198:U:O2'	20:T:57:ARG:HG2	2.16	0.46
1:A:1179:G:H2'	1:A:1180:U:O4'	2.16	0.46
1:A:764:A:O2'	1:A:1499:U:O2	2.34	0.46
4:D:79:PHE:HE1	4:D:204:ILE:HG12	1.81	0.46
5:E:144:THR:O	5:E:148:VAL:HG23	2.15	0.46
5:E:79:GLU:N	5:E:79:GLU:OE2	2.49	0.46
14:N:27:CYS:SG	14:N:29:ARG:HB2	2.56	0.46
20:T:51:GLU:O	20:T:55:ILE:HG12	2.16	0.46
1:A:1229:A:H2'	1:A:1230:C:C6	2.51	0.46
1:A:1442:C:H2'	1:A:1443:C:O4'	2.16	0.46
1:A:942:A:O2'	1:A:943:G:OP2	2.25	0.46
1:A:968:U:O2'	1:A:969:U:H5"	2.16	0.46
9:I:53:VAL:HB	9:I:92:TYR:CE1	2.51	0.46
1:A:971:A:C2	14:N:5:ALA:HA	2.51	0.46
1:A:458:G:OP2	16:P:75:ARG:NH1	2.49	0.46
1:A:1039:G:H2'	1:A:1040:G:O4'	2.16	0.45
1:A:1328:G:O5'	9:I:107:ARG:HG3	2.16	0.45
1:A:713:G:C5	1:A:714:G:H1'	2.51	0.45
1:A:750:A:H2'	1:A:751:A:O4'	2.16	0.45
2:B:233:SER:O	2:B:233:SER:OG	2.30	0.45
2:B:44:LEU:H	2:B:44:LEU:HG	1.34	0.45
5:E:74:GLY:HA3	5:E:116:THR:HG22	1.98	0.45
11:K:47:VAL:HG12	11:K:48:ILE:HD13	1.98	0.45
13:M:12:ASN:H	13:M:45:VAL:HB	1.80	0.45
13:M:34:LEU:HD13	13:M:41:PRO:HA	1.98	0.45
1:A:437:C:H2'	1:A:438:C:H6	1.82	0.45
2:B:61:LEU:HD21	2:B:68:ILE:HD11	1.98	0.45
3:C:157:ILE:CD1	3:C:166:GLU:HB2	2.46	0.45
12:L:41:ARG:HH21	12:L:57:LYS:NZ	2.15	0.45
1:A:1083:A:H4'	1:A:1084:A:O5'	2.16	0.45
1:A:445:A:H8	1:A:445:A:O5'	1.99	0.45
1:A:981:G:H8	1:A:981:G:OP2	1.99	0.45
5:E:90:VAL:O	5:E:120:THR:HA	2.16	0.45
20:T:20:LEU:HA	20:T:20:LEU:HD23	1.67	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:G:H2'	1:A:228:C:O4'	2.17	0.45
6:F:9:VAL:HG22	6:F:60:PHE:HE2	1.81	0.45
7:G:20:ASP:OD2	7:G:21:VAL:N	2.49	0.45
1:A:641:G:O2'	15:O:22:THR:HG21	2.16	0.45
17:Q:67:LYS:HA	17:Q:70:ARG:NH2	2.28	0.45
17:Q:59:ILE:HG23	17:Q:71:PHE:CD1	2.51	0.45
1:A:253:G:H2'	1:A:254:G:C8	2.52	0.45
1:A:849:A:C8	1:A:851:G:C8	3.05	0.45
1:A:928:G:OP2	13:M:102:ARG:NH2	2.50	0.45
4:D:24:GLU:HG2	4:D:25:ARG:N	2.31	0.45
5:E:35:GLY:HA3	5:E:112:LEU:HB3	1.98	0.45
7:G:146:GLU:HA	7:G:149:ARG:HG2	1.98	0.45
21:V:3:LYS:HD3	21:V:14:TRP:CD1	2.52	0.45
7:G:50:ILE:O	7:G:54:THR:HB	2.17	0.45
1:A:1324:G:OP1	9:I:125:TYR:HE2	2.00	0.45
11:K:48:ILE:HD11	11:K:64:ALA:HA	1.99	0.45
1:A:979:G:C2	1:A:980:G:C6	3.05	0.45
2:B:84:GLU:OE2	2:B:234:PRO:HB3	2.17	0.45
23:X:31:G:H2'	23:X:31:G:N3	2.32	0.45
1:A:199:C:H2'	1:A:200:C:C6	2.52	0.45
3:C:114:PRO:O	3:C:118:GLN:HB2	2.17	0.45
1:A:904:G:H4'	1:A:1480:A:C8	2.51	0.45
1:A:714:G:OP1	1:A:749:A:H1'	2.17	0.45
3:C:79:ARG:HB2	3:C:82:GLU:HB3	1.99	0.45
1:A:1208:A:C2	13:M:117:VAL:HG21	2.52	0.45
1:A:1059:G:N2	1:A:1062:A:OP2	2.44	0.45
1:A:922:G:C2	1:A:1318:G:C2	3.05	0.45
1:A:531:G:H2'	1:A:532:C:C6	2.52	0.45
2:B:71:VAL:O	2:B:165:VAL:HG23	2.17	0.45
3:C:174:PRO:HB2	3:C:177:THR:CG2	2.47	0.45
12:L:89:ARG:HH21	12:L:97:ARG:NE	2.15	0.45
1:A:103:C:H2'	1:A:104:G:O4'	2.18	0.44
1:A:198:U:C1'	20:T:103:GLY:HA2	2.46	0.44
7:G:62:PHE:HD1	7:G:124:LEU:HD21	1.81	0.44
7:G:62:PHE:HA	7:G:124:LEU:HD22	2.00	0.44
9:I:10:ARG:HB3	9:I:76:ALA:HB2	1.99	0.44
15:O:25:THR:HG21	15:O:70:LEU:HB2	1.99	0.44
2:B:100:GLY:O	2:B:104:ASN:N	2.43	0.44
2:B:10:LEU:HD12	2:B:48:MET:HE1	1.99	0.44
1:A:917:C:OP1	7:G:102:ARG:NE	2.50	0.44
13:M:3:ARG:HA	13:M:8:GLU:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1106:G:O2'	1:A:1127:C:N4	2.50	0.44
1:A:1309:C:OP1	21:V:20:LYS:NZ	2.50	0.44
1:A:608:G:H4'	16:P:16:HIS:CD2	2.53	0.44
3:C:123:GLN:HB3	3:C:128:PHE:HB2	1.99	0.44
13:M:91:ARG:HD2	13:M:91:ARG:HA	1.69	0.44
1:A:189:U:O2	17:Q:63:ARG:NH2	2.51	0.44
1:A:1008:C:N4	1:A:1014:G:O6	2.50	0.44
2:B:28:PHE:CD2	2:B:190:THR:HA	2.52	0.44
6:F:9:VAL:CG2	6:F:87:ARG:HB2	2.48	0.44
8:H:11:THR:O	8:H:14:ARG:N	2.50	0.44
1:A:1005:C:N4	1:A:1016:G:H1	2.15	0.44
1:A:1112:A:C2	1:A:1128:A:C4	3.06	0.44
1:A:224:U:H2'	1:A:225:G:O4'	2.17	0.44
7:G:18:TYR:CD1	7:G:59:LEU:HB2	2.53	0.44
9:I:89:ASN:HB3	9:I:92:TYR:CD2	2.53	0.44
19:S:52:TYR:CG	19:S:53:ASN:N	2.86	0.44
1:A:293:A:H2'	1:A:294:G:O4'	2.18	0.44
1:A:399:U:H2'	1:A:400:U:C6	2.52	0.44
1:A:402:G:O2'	4:D:116:GLN:HG3	2.18	0.44
1:A:669:U:H4'	1:A:670:A:OP1	2.18	0.44
1:A:671:G:H5'	11:K:46:GLY:C	2.37	0.44
1:A:993:A:H2'	1:A:994:A:C8	2.52	0.44
11:K:24:SER:C	11:K:26:ASN:H	2.20	0.44
1:A:1297:G:H4'	14:N:18:VAL:HG11	1.99	0.44
15:O:32:LEU:HD12	15:O:63:ARG:HB2	1.99	0.44
1:A:1111:C:OP1	1:A:1112:A:C8	2.71	0.44
1:A:259:U:H2'	1:A:260:G:O4'	2.17	0.44
1:A:787:U:H5''	1:A:788:C:OP2	2.17	0.44
1:A:924:G:H2'	1:A:925:C:O4'	2.18	0.44
2:B:69:LEU:O	2:B:163:PHE:N	2.39	0.44
8:H:97:VAL:HG13	8:H:98:LYS:HD2	2.00	0.44
1:A:543:U:H5'	1:A:549:G:C2	2.52	0.44
10:J:90:LEU:H	10:J:91:PRO:CD	2.28	0.44
17:Q:104:LYS:HB3	17:Q:104:LYS:HE2	1.88	0.44
17:Q:59:ILE:HD11	17:Q:73:VAL:HG22	1.99	0.44
19:S:36:ARG:H	19:S:36:ARG:HG2	1.60	0.44
1:A:1302:C:H42	19:S:37:ARG:NH1	2.14	0.44
1:A:609:U:H4'	16:P:38:TYR:CZ	2.53	0.43
1:A:616:G:H2'	1:A:617:C:C6	2.53	0.43
2:B:224:GLN:HA	2:B:229:VAL:HG22	1.99	0.43
3:C:174:PRO:O	3:C:177:THR:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:98:GLU:HG2	4:D:189:PRO:HG3	2.00	0.43
12:L:89:ARG:HH21	12:L:97:ARG:HE	1.66	0.43
1:A:1119:C:O2'	1:A:1120:G:N2	2.51	0.43
1:A:1137:G:H2'	1:A:1138:G:O4'	2.18	0.43
1:A:35:G:H2'	1:A:36:C:C6	2.53	0.43
1:A:493:A:N3	1:A:526:C:H1'	2.33	0.43
1:A:764:A:H5'	1:A:764:A:H8	1.82	0.43
1:A:963:A:H1'	19:S:54:GLY:O	2.18	0.43
3:C:34:LEU:HD22	14:N:25:VAL:HG21	2.00	0.43
18:R:43:PHE:HD2	18:R:56:THR:HG22	1.83	0.43
18:R:40:LEU:HB3	18:R:79:LEU:HD11	2.00	0.43
20:T:52:ALA:O	20:T:56:MET:HB2	2.18	0.43
1:A:1113:G:H2'	1:A:1114:C:C6	2.54	0.43
11:K:86:GLY:O	11:K:91:ARG:NH1	2.51	0.43
19:S:24:ALA:HB3	19:S:25:LYS:HZ3	1.83	0.43
1:A:1130:U:H2'	1:A:1131:C:O4'	2.18	0.43
2:B:204:ASN:ND2	2:B:206:ASP:H	2.14	0.43
4:D:15:GLU:OE1	4:D:59:ARG:NH2	2.51	0.43
8:H:92:ARG:HG2	8:H:94:TYR:OH	2.18	0.43
9:I:10:ARG:HG2	9:I:75:ASP:HB2	2.00	0.43
1:A:926:A:C2	1:A:1214:G:N3	2.87	0.43
1:A:565:U:OP2	1:A:741:G:N1	2.48	0.43
4:D:190:ASP:O	4:D:193:ASP:HB2	2.18	0.43
4:D:196:LEU:HA	4:D:196:LEU:HD23	1.84	0.43
5:E:84:PHE:HB3	5:E:134:ALA:HB2	2.00	0.43
6:F:96:PRO:HB3	18:R:30:ASP:OD2	2.19	0.43
16:P:21:VAL:HG21	16:P:59:TRP:CG	2.54	0.43
16:P:69:THR:HG22	16:P:72:ARG:HD3	2.00	0.43
17:Q:3:LYS:HB3	17:Q:61:GLU:HB3	2.01	0.43
1:A:1107:U:H3	10:J:5:ARG:HH21	1.66	0.43
1:A:748:G:N2	1:A:796:U:OP2	2.51	0.43
3:C:124:ILE:HD13	3:C:130:VAL:HG22	2.00	0.43
4:D:98:GLU:CG	4:D:189:PRO:HG3	2.48	0.43
1:A:858:G:P	12:L:12:ARG:HH22	2.40	0.43
14:N:8:GLU:HG3	14:N:8:GLU:H	1.62	0.43
15:O:24:SER:OG	15:O:27:VAL:HG23	2.19	0.43
19:S:70:LYS:O	19:S:73:GLU:HB2	2.19	0.43
1:A:27:G:H2'	1:A:28:G:O4'	2.17	0.43
1:A:413:C:H2'	1:A:414:C:H6	1.84	0.43
1:A:507:G:H2'	1:A:508:C:C6	2.54	0.43
1:A:939:C:H2'	1:A:940:G:O4'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:87:SER:HB3	5:E:131:ILE:CD1	2.49	0.43
7:G:51:GLN:C	7:G:53:LYS:H	2.22	0.43
15:O:71:GLN:HG3	15:O:78:TYR:CZ	2.53	0.43
16:P:4:ILE:HG22	16:P:70:ALA:HB1	2.01	0.43
18:R:53:ARG:HD2	18:R:58:LEU:O	2.19	0.43
20:T:74:LYS:HB3	20:T:74:LYS:HE3	1.74	0.43
20:T:99:LEU:HA	20:T:99:LEU:HD22	1.82	0.43
1:A:954:A:C2	1:A:1205:G:C6	3.07	0.43
1:A:1281:G:HO2'	1:A:1282:U:P	2.41	0.43
1:A:961:C:H2'	1:A:962:C:H6	1.84	0.43
9:I:118:LYS:HB3	9:I:121:ARG:HB2	2.01	0.43
1:A:1204:C:OP2	19:S:78:ARG:NH2	2.52	0.43
1:A:276:G:O2'	1:A:277:A:OP2	2.29	0.43
1:A:353:U:H2'	1:A:354:U:C6	2.54	0.43
1:A:689:A:H1'	11:K:29:ILE:HD11	2.01	0.43
1:A:695:A:H2'	1:A:696:G:O4'	2.18	0.43
12:L:28:LYS:C	12:L:30:ALA:H	2.22	0.43
14:N:24:CYS:HB2	14:N:40:CYS:HB3	2.00	0.43
19:S:15:LEU:O	19:S:19:VAL:HG12	2.19	0.43
1:A:323:C:O2	1:A:323:C:C2'	2.67	0.43
14:N:47:LEU:HA	14:N:47:LEU:HD13	1.64	0.43
19:S:11:VAL:HG21	19:S:41:VAL:CG1	2.49	0.43
20:T:56:MET:HG3	20:T:88:VAL:HG21	2.01	0.43
1:A:515:A:H2	1:A:1187:G:H21	1.67	0.42
1:A:1228:U:O2'	1:A:1229:A:H5'	2.19	0.42
1:A:206:G:H2'	1:A:207:C:O4'	2.19	0.42
2:B:166:ASP:OD2	2:B:169:LYS:HB2	2.19	0.42
3:C:112:SER:OG	3:C:115:LEU:HD12	2.19	0.42
1:A:949:C:H4'	10:J:57:LYS:HB3	2.00	0.42
17:Q:31:LEU:HD23	17:Q:32:TYR:CZ	2.54	0.42
18:R:28:GLU:OE1	18:R:28:GLU:N	2.51	0.42
19:S:5:LEU:HD13	19:S:9:VAL:HG13	2.00	0.42
20:T:74:LYS:HB2	20:T:76:ALA:H	1.83	0.42
1:A:1124:G:H2'	1:A:1125:G:O4'	2.19	0.42
1:A:1188:G:H2'	1:A:1189:C:C6	2.54	0.42
1:A:1378:A:H2	5:E:19:MET:HG3	1.84	0.42
1:A:274:A:H5''	1:A:276:G:H5'	2.01	0.42
1:A:352:G:C2	1:A:353:U:C5	3.06	0.42
12:L:57:LYS:HE2	12:L:57:LYS:HB2	1.86	0.42
14:N:6:LEU:HD23	14:N:6:LEU:HA	1.76	0.42
1:A:311:G:C2	1:A:312:G:C8	3.07	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:G:C5'	1:A:345:G:H8	2.32	0.42
1:A:485:G:C2	1:A:486:C:C2	3.07	0.42
1:A:752:G:C2'	1:A:753:C:H5'	2.50	0.42
4:D:15:GLU:HB3	4:D:63:LYS:HG3	2.01	0.42
5:E:43:LEU:HD23	5:E:43:LEU:HA	1.76	0.42
7:G:78:ARG:HH11	7:G:154:TYR:HB3	1.84	0.42
7:G:79:ARG:NH1	7:G:83:ALA:HA	2.34	0.42
1:A:1414:G:O2'	1:A:1445:A:N6	2.52	0.42
1:A:811:A:OP1	1:A:811:A:H4'	2.19	0.42
1:A:820:G:H2'	1:A:821:G:C8	2.54	0.42
5:E:44:GLY:HA3	5:E:62:ALA:HB2	2.00	0.42
6:F:6:VAL:HG22	6:F:90:VAL:HG22	2.01	0.42
11:K:84:VAL:HG11	11:K:91:ARG:HD3	2.00	0.42
12:L:89:ARG:HE	12:L:97:ARG:HG2	1.84	0.42
18:R:53:ARG:HG2	18:R:63:GLN:OE1	2.20	0.42
22:W:1:A:O2'	22:W:2:U:H5'	2.20	0.42
2:B:109:SER:C	2:B:111:ARG:H	2.22	0.42
1:A:525:G:P	4:D:10:ARG:HH22	2.38	0.42
19:S:7:LYS:HG3	19:S:7:LYS:H	1.67	0.42
1:A:1493:G:N1	1:A:1496:A:OP2	2.53	0.42
1:A:469:G:H1'	1:A:470:U:OP2	2.20	0.42
2:B:71:VAL:CG2	2:B:164:VAL:HG22	2.50	0.42
2:B:77:ALA:HB2	2:B:211:ILE:HG21	2.01	0.42
6:F:3:ARG:O	6:F:93:SER:HB2	2.18	0.42
8:H:20:TYR:HA	8:H:65:TYR:CZ	2.54	0.42
9:I:51:ARG:HB2	9:I:51:ARG:NH1	2.35	0.42
14:N:33:VAL:HA	14:N:40:CYS:HA	2.02	0.42
17:Q:36:ILE:HG12	17:Q:36:ILE:H	1.72	0.42
1:A:117:G:C6	1:A:118:U:C4	3.08	0.42
1:A:1350:G:H5''	9:I:112:LYS:HB3	2.00	0.42
1:A:1476:A:C2	1:A:1477:A:C8	3.07	0.42
2:B:130:ARG:HA	2:B:130:ARG:HD3	1.85	0.42
2:B:132:LYS:O	2:B:136:VAL:HG23	2.20	0.42
5:E:43:LEU:HD11	5:E:132:ALA:HB1	2.00	0.42
13:M:8:GLU:OE1	13:M:22:ILE:HA	2.19	0.42
15:O:31:LEU:HA	15:O:31:LEU:HD12	1.88	0.42
21:V:25:LYS:HD2	21:V:25:LYS:HA	1.90	0.42
10:J:78:ASN:ND2	10:J:80:LYS:H	2.18	0.42
1:A:1291:G:OP2	13:M:88:ARG:NH2	2.50	0.42
1:A:722:C:C4	1:A:723:U:C5	3.08	0.42
2:B:144:ARG:O	2:B:147:LYS:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:196:LEU:HB3	4:D:198:VAL:CG1	2.50	0.42
10:J:84:GLN:O	10:J:88:LEU:HD12	2.19	0.42
1:A:1033:C:H2'	1:A:1034:U:C6	2.55	0.42
1:A:1284:C:N4	1:A:1285:G:C6	2.88	0.42
1:A:323:C:OP1	1:A:323:C:H4'	2.20	0.42
1:A:562:G:H2'	1:A:563:U:C6	2.55	0.42
1:A:769:G:C2	1:A:780:C:C2	3.08	0.42
3:C:175:LEU:HA	3:C:175:LEU:HD23	1.75	0.42
5:E:137:GLU:OE2	5:E:140:ARG:HD2	2.20	0.42
7:G:66:VAL:O	7:G:70:LYS:HG3	2.20	0.42
8:H:106:GLY:C	8:H:108:GLY:H	2.22	0.42
8:H:111:ILE:O	8:H:134:ILE:HB	2.20	0.42
16:P:39:TYR:CD2	16:P:73:LEU:HD11	2.55	0.42
17:Q:29:HIS:HB2	17:Q:36:ILE:HD13	2.01	0.42
1:A:1037:A:N6	1:A:1187:G:C5	2.88	0.41
2:B:110:GLN:H	2:B:110:GLN:HG3	1.60	0.41
4:D:20:TYR:HE2	4:D:27:TYR:CE2	2.38	0.41
12:L:44:THR:HA	12:L:45:PRO:HD3	1.76	0.41
17:Q:17:LYS:HA	17:Q:46:ASP:O	2.20	0.41
17:Q:89:LEU:HD23	17:Q:89:LEU:HA	1.84	0.41
19:S:22:LEU:HD13	19:S:28:LYS:HB2	2.02	0.41
1:A:1102:G:H2'	1:A:1103:U:C6	2.55	0.41
1:A:1119:C:H5'	1:A:1120:G:OP1	2.20	0.41
1:A:1160:A:H2'	1:A:1161:A:O4'	2.21	0.41
1:A:520:G:H4'	12:L:73:GLU:OE1	2.19	0.41
1:A:727:C:H2'	1:A:728:C:H6	1.85	0.41
1:A:914:A:O5'	1:A:914:A:H8	2.03	0.41
4:D:191:ARG:HD3	4:D:200:GLU:OE2	2.20	0.41
9:I:116:LYS:HD2	9:I:122:ALA:HA	2.01	0.41
11:K:66:LEU:HG	11:K:97:ALA:HB1	2.02	0.41
12:L:78:GLN:O	12:L:80:HIS:N	2.53	0.41
19:S:3:ARG:HB3	19:S:4:SER:H	1.61	0.41
1:A:1202:G:O3'	19:S:77:THR:HG21	2.20	0.41
1:A:1036:C:C6	23:X:34:RSQ:H4'	2.55	0.41
1:A:1139:A:C6	1:A:1161:A:C6	3.08	0.41
2:B:102:LEU:HD12	2:B:102:LEU:HA	1.79	0.41
7:G:26:PHE:CE2	7:G:30:ILE:HD11	2.56	0.41
7:G:40:ALA:HB3	9:I:41:VAL:HG21	2.02	0.41
9:I:97:LYS:N	9:I:98:PRO:HD2	2.35	0.41
14:N:9:LYS:NZ	14:N:21:TYR:O	2.39	0.41
21:V:18:TYR:CD2	21:V:24:ARG:HA	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1055:U:OP2	5:E:57:LYS:NZ	2.40	0.41
1:A:248:U:H2'	1:A:249:G:C8	2.54	0.41
2:B:101:MET:HG2	2:B:108:ILE:HG21	2.03	0.41
2:B:121:LEU:O	2:B:127:ILE:HG21	2.20	0.41
2:B:22:LYS:HA	2:B:22:LYS:HD3	1.87	0.41
1:A:416:U:O4	3:C:127:ARG:NE	2.53	0.41
4:D:162:LEU:HD22	4:D:181:MET:HG2	2.01	0.41
6:F:23:LYS:HB3	6:F:23:LYS:NZ	2.35	0.41
13:M:120:LYS:HD3	13:M:123:ALA:HB3	2.02	0.41
1:A:105:G:H21	1:A:349:G:C4'	2.33	0.41
1:A:944:C:H2'	1:A:945:A:N7	2.35	0.41
5:E:131:ILE:HD13	5:E:131:ILE:HA	1.94	0.41
11:K:69:ALA:O	11:K:72:ALA:N	2.53	0.41
13:M:108:ARG:NE	13:M:108:ARG:HA	2.34	0.41
15:O:71:GLN:HG3	15:O:78:TYR:CD2	2.56	0.41
1:A:131:C:O4'	16:P:63:GLY:HA3	2.20	0.41
1:A:1001:G:O6	1:A:1002:G:N2	2.45	0.41
1:A:1111:C:O5'	1:A:1112:A:H5'	2.21	0.41
1:A:1346:U:O5'	1:A:1346:U:H6	2.03	0.41
1:A:102:A:C6	1:A:321:G:C6	3.09	0.41
1:A:344:A:C2'	1:A:345:G:H5''	2.44	0.41
1:A:434:A:C4	1:A:480:A:C2	3.08	0.41
1:A:720:A:H2'	1:A:721:C:C6	2.55	0.41
2:B:115:LEU:O	2:B:119:GLU:N	2.54	0.41
5:E:69:VAL:HA	5:E:70:PRO:HD3	1.93	0.41
10:J:6:ILE:HG22	10:J:98:ILE:HG22	2.03	0.41
15:O:87:ILE:HG22	15:O:88:ARG:N	2.34	0.41
19:S:24:ALA:HB3	19:S:25:LYS:NZ	2.35	0.41
19:S:6:LYS:HE2	19:S:6:LYS:H	1.85	0.41
20:T:58:LYS:HA	20:T:58:LYS:HD2	1.88	0.41
20:T:67:ALA:HA	20:T:73:HIS:N	2.36	0.41
1:A:1004:G:N3	1:A:1004:G:H2'	2.35	0.41
2:B:155:LEU:HD22	2:B:157:ARG:O	2.21	0.41
7:G:104:LEU:HD23	7:G:104:LEU:HA	1.84	0.41
1:A:780:C:OP1	11:K:124:LYS:HD3	2.21	0.41
16:P:21:VAL:HG21	16:P:59:TRP:CD1	2.56	0.41
16:P:2:VAL:O	16:P:64:ALA:HA	2.21	0.41
1:A:1208:A:O3'	13:M:115:LYS:NZ	2.54	0.41
2:B:195:ASP:O	8:H:68:ARG:NH2	2.50	0.41
6:F:80:ARG:NH1	6:F:88:VAL:O	2.53	0.41
15:O:3:ILE:O	15:O:3:ILE:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1089:C:C4	1:A:1090:G:C8	3.09	0.41
1:A:547:C:OP1	12:L:15:ARG:NE	2.43	0.41
1:A:690:C:H2'	1:A:691:C:H6	1.86	0.41
1:A:902:G:C2	1:A:904:G:C8	3.08	0.41
15:O:38:ARG:HA	15:O:38:ARG:HD3	1.79	0.41
1:A:1478:C:N4	1:A:1481:G:C2	2.89	0.41
1:A:157:C:H2'	1:A:158:U:O4'	2.21	0.41
25:A:1785:PAR:H642	25:A:1785:PAR:C43	2.51	0.41
2:B:109:SER:O	2:B:111:ARG:N	2.54	0.41
2:B:160:ASP:O	2:B:183:PRO:HD2	2.20	0.41
8:H:103:VAL:HG21	8:H:110:ALA:HB2	2.03	0.41
14:N:41:ARG:HG3	14:N:42:ILE:N	2.35	0.41
17:Q:88:TYR:OH	17:Q:92:ARG:NH1	2.53	0.41
1:A:1206:A:O2'	19:S:78:ARG:HD3	2.20	0.41
1:A:1217:A:O2'	1:A:1285:G:H4'	2.21	0.41
1:A:1425:G:H4'	1:A:1426:A:H5''	2.03	0.41
1:A:27:G:C5	1:A:540:G:C2	3.08	0.41
1:A:437:C:H2'	1:A:438:C:C6	2.55	0.41
1:A:494:C:H4'	1:A:495:U:OP1	2.21	0.41
1:A:484:C:H1'	1:A:532:C:H1'	2.03	0.41
3:C:157:ILE:HD13	3:C:166:GLU:HB2	2.01	0.41
5:E:9:LYS:O	5:E:10:MET:HB3	2.20	0.41
6:F:43:LEU:HA	6:F:43:LEU:HD22	1.88	0.41
1:A:1062:A:N7	1:A:1063:G:H1'	2.36	0.40
1:A:1101:C:H2'	1:A:1102:G:H8	1.86	0.40
1:A:1171:G:O2'	1:A:1172:A:P	2.79	0.40
1:A:1488:G:H2'	1:A:1489:U:O4'	2.21	0.40
1:A:64:G:H8	1:A:64:G:H2'	1.64	0.40
5:E:78:HIS:HB2	5:E:79:GLU:H	1.65	0.40
18:R:58:LEU:HB3	18:R:62:GLU:HB2	2.02	0.40
19:S:71:LEU:HD23	19:S:71:LEU:HA	1.81	0.40
1:A:1423:G:H21	1:A:1437:A:H62	1.69	0.40
1:A:227:G:H1'	1:A:257:A:N1	2.37	0.40
1:A:718:C:H5'	18:R:71:LYS:HD3	2.03	0.40
2:B:92:TYR:CD1	2:B:94:ASN:HB2	2.56	0.40
4:D:152:SER:C	4:D:154:ASN:H	2.24	0.40
6:F:36:ARG:NH2	6:F:38:GLU:HG2	2.36	0.40
7:G:26:PHE:CD2	7:G:30:ILE:HD11	2.56	0.40
7:G:99:LEU:HD23	7:G:99:LEU:HA	1.95	0.40
13:M:94:ARG:HH21	19:S:80:TYR:HD2	1.68	0.40
19:S:40:ILE:HB	19:S:67:VAL:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1286:G:N2	1:A:1312:G:H1'	2.37	0.40
1:A:199:C:H2'	1:A:200:C:H6	1.84	0.40
1:A:59:A:H1'	1:A:349:G:N2	2.36	0.40
1:A:678:A:C6	1:A:679:A:C6	3.08	0.40
1:A:792:G:C6	1:A:793:C:C5	3.10	0.40
3:C:81:GLY:O	3:C:83:ARG:N	2.47	0.40
4:D:150:GLU:HA	4:D:153:ARG:HG3	2.04	0.40
4:D:154:ASN:N	4:D:154:ASN:OD1	2.53	0.40
4:D:18:LYS:HB3	4:D:20:TYR:CE1	2.56	0.40
8:H:33:GLU:HG3	8:H:48:TYR:CE1	2.57	0.40
11:K:124:LYS:HB3	11:K:124:LYS:HE2	1.69	0.40
18:R:73:ALA:HB3	18:R:79:LEU:HD12	2.03	0.40
1:A:1266:A:H4'	1:A:1267:A:O5'	2.22	0.40
1:A:1252:G:H5'	1:A:1295:C:H5''	2.04	0.40
1:A:1354:U:H5''	9:I:71:SER:HB3	2.04	0.40
1:A:274:A:OP2	17:Q:95:TYR:OH	2.32	0.40
1:A:345:G:H8	1:A:345:G:H5'	1.86	0.40
1:A:739:C:H2'	1:A:740:U:O4'	2.22	0.40
9:I:5:TYR:H	9:I:87:GLN:HE21	1.69	0.40
13:M:67:GLU:HB3	13:M:68:GLY:H	1.64	0.40
1:A:1329:U:H2'	1:A:1330:A:H8	1.87	0.40
1:A:409:A:P	1:A:423:G:H22	2.44	0.40
1:A:690:C:H2'	1:A:691:C:C6	2.56	0.40
2:B:117:GLU:O	2:B:121:LEU:HB2	2.21	0.40
3:C:120:VAL:O	3:C:124:ILE:HG12	2.21	0.40
3:C:33:LEU:O	3:C:37:GLN:HG2	2.21	0.40
10:J:16:LEU:HD13	10:J:70:ARG:HG2	2.04	0.40
13:M:97:PRO:HD3	13:M:110:ARG:HB3	2.03	0.40
20:T:33:ILE:HD13	20:T:63:ILE:HG12	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	232/234 (99%)	184 (79%)	26 (11%)	22 (10%)	0	4
3	C	204/206 (99%)	162 (79%)	28 (14%)	14 (7%)	1	8
4	D	206/208 (99%)	180 (87%)	19 (9%)	7 (3%)	3	22
5	E	148/150 (99%)	132 (89%)	15 (10%)	1 (1%)	22	54
6	F	99/101 (98%)	90 (91%)	7 (7%)	2 (2%)	7	32
7	G	153/155 (99%)	133 (87%)	13 (8%)	7 (5%)	2	15
8	H	136/138 (99%)	116 (85%)	19 (14%)	1 (1%)	22	54
9	I	125/127 (98%)	103 (82%)	20 (16%)	2 (2%)	9	36
10	J	96/98 (98%)	68 (71%)	18 (19%)	10 (10%)	0	3
11	K	117/119 (98%)	94 (80%)	18 (15%)	5 (4%)	2	16
12	L	122/124 (98%)	99 (81%)	15 (12%)	8 (7%)	1	8
13	M	123/125 (98%)	103 (84%)	16 (13%)	4 (3%)	4	22
14	N	58/60 (97%)	47 (81%)	8 (14%)	3 (5%)	2	13
15	O	86/88 (98%)	75 (87%)	9 (10%)	2 (2%)	6	29
16	P	81/83 (98%)	76 (94%)	4 (5%)	1 (1%)	13	42
17	Q	102/104 (98%)	90 (88%)	9 (9%)	3 (3%)	4	24
18	R	71/73 (97%)	58 (82%)	12 (17%)	1 (1%)	11	38
19	S	78/80 (98%)	60 (77%)	12 (15%)	6 (8%)	1	6
20	T	97/99 (98%)	79 (81%)	13 (13%)	5 (5%)	2	13
21	V	22/24 (92%)	18 (82%)	4 (18%)	0	100	100
All	All	2356/2396 (98%)	1967 (84%)	285 (12%)	104 (4%)	2	16

All (104) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	10	LEU
2	B	36	ARG
2	B	95	GLN
2	B	190	THR
2	B	234	PRO
3	C	3	ASN
3	C	15	THR
3	C	61	ALA
3	C	154	SER
3	C	179	ARG
4	D	71	SER

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Mol	Chain	Res	Type
4	D	153	ARG
4	D	171	GLY
9	I	118	LYS
10	J	54	PHE
11	K	117	ASN
11	K	127	LYS
12	L	27	LEU
12	L	28	LYS
12	L	30	ALA
12	L	47	LYS
13	M	124	PRO
14	N	32	SER
19	S	9	VAL
20	T	73	HIS
2	B	11	LEU
2	B	15	VAL
2	B	131	PRO
2	B	228	GLY
3	C	14	ILE
10	J	73	ASP
10	J	90	LEU
12	L	48	PRO
15	O	64	ARG
17	Q	80	GLY
19	S	6	LYS
19	S	53	ASN
20	T	9	ASN
20	T	102	GLY
2	B	17	PHE
2	B	20	GLU
2	B	123	ALA
4	D	4	TYR
4	D	22	LYS
4	D	36	ARG
5	E	22	GLY
6	F	38	GLU
7	G	7	ALA
7	G	82	GLY
7	G	147	ALA
7	G	149	ARG
9	I	127	LYS
10	J	36	GLY

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Mol	Chain	Res	Type
10	J	39	PRO
10	J	72	VAL
11	K	13	GLN
14	N	23	ARG
15	O	86	GLY
20	T	99	LEU
2	B	78	GLN
2	B	130	ARG
2	B	178	ARG
3	C	83	ARG
3	C	98	ASN
3	C	146	ALA
3	C	168	ALA
6	F	97	PHE
7	G	83	ALA
10	J	29	ARG
10	J	34	VAL
10	J	40	LEU
10	J	60	ARG
12	L	79	GLU
12	L	105	TYR
13	M	97	PRO
14	N	11	LYS
17	Q	74	LEU
20	T	98	PRO
2	B	110	GLN
2	B	165	VAL
2	B	229	VAL
3	C	4	LYS
3	C	60	ALA
4	D	5	ILE
7	G	80	VAL
7	G	155	ARG
8	H	51	VAL
11	K	107	SER
12	L	115	LYS
13	M	67	GLU
16	P	52	ASP
17	Q	99	SER
19	S	30	LEU
2	B	21	ARG
2	B	239	VAL

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Mol	Chain	Res	Type
13	M	6	GLY
18	R	45	SER
2	B	18	GLY
2	B	208	ILE
3	C	108	ASN
11	K	48	ILE
3	C	51	GLY
19	S	8	GLY
19	S	45	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	
2	B	202/202 (100%)	163 (81%)	39 (19%)	1	6
3	C	160/160 (100%)	139 (87%)	21 (13%)	4	17
4	D	180/180 (100%)	152 (84%)	28 (16%)	2	12
5	E	115/115 (100%)	102 (89%)	13 (11%)	6	22
6	F	90/90 (100%)	80 (89%)	10 (11%)	6	23
7	G	126/126 (100%)	110 (87%)	16 (13%)	4	19
8	H	119/119 (100%)	103 (87%)	16 (13%)	4	16
9	I	98/98 (100%)	84 (86%)	14 (14%)	3	15
10	J	88/88 (100%)	77 (88%)	11 (12%)	4	19
11	K	90/90 (100%)	79 (88%)	11 (12%)	5	20
12	L	104/104 (100%)	90 (86%)	14 (14%)	4	16
13	M	100/100 (100%)	86 (86%)	14 (14%)	3	16
14	N	49/49 (100%)	43 (88%)	6 (12%)	5	20
15	O	79/79 (100%)	68 (86%)	11 (14%)	3	16
16	P	72/72 (100%)	61 (85%)	11 (15%)	2	12
17	Q	96/96 (100%)	82 (85%)	14 (15%)	3	14
18	R	64/64 (100%)	58 (91%)	6 (9%)	8	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	S	71/71 (100%)	57 (80%)	14 (20%)	1	5
20	T	76/76 (100%)	67 (88%)	9 (12%)	5	21
21	V	19/19 (100%)	18 (95%)	1 (5%)	22	53
All	All	1998/1998 (100%)	1719 (86%)	279 (14%)	3	16

All (279) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	7	VAL
2	B	8	LYS
2	B	10	LEU
2	B	15	VAL
2	B	16	HIS
2	B	17	PHE
2	B	23	ARG
2	B	24	TRP
2	B	33	TYR
2	B	44	LEU
2	B	51	LEU
2	B	61	LEU
2	B	69	LEU
2	B	74	LYS
2	B	78	GLN
2	B	79	ASP
2	B	96	ARG
2	B	97	TRP
2	B	102	LEU
2	B	110	GLN
2	B	111	ARG
2	B	114	ARG
2	B	121	LEU
2	B	137	ARG
2	B	150	SER
2	B	153	ARG
2	B	157	ARG
2	B	158	LEU
2	B	163	PHE
2	B	168	THR
2	B	178	ARG
2	B	204	ASN
2	B	211	ILE

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Mol	Chain	Res	Type
2	B	212	GLN
2	B	215	LEU
2	B	223	ILE
2	B	226	ARG
2	B	236	TYR
2	B	240	GLN
3	C	4	LYS
3	C	14	ILE
3	C	15	THR
3	C	26	LYS
3	C	36	ASP
3	C	67	THR
3	C	72	LYS
3	C	93	LYS
3	C	105	GLU
3	C	107	GLN
3	C	128	PHE
3	C	131	ARG
3	C	132	ARG
3	C	152	ILE
3	C	165	THR
3	C	166	GLU
3	C	167	TRP
3	C	177	THR
3	C	192	THR
3	C	195	VAL
3	C	204	LEU
4	D	3	ARG
4	D	8	VAL
4	D	10	ARG
4	D	21	LEU
4	D	38	TYR
4	D	49	ARG
4	D	58	LEU
4	D	61	LYS
4	D	64	LEU
4	D	73	ARG
4	D	74	GLN
4	D	83	SER
4	D	96	LEU
4	D	103	ASN
4	D	122	ARG

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Mol	Chain	Res	Type
4	D	127	THR
4	D	150	GLU
4	D	151	LYS
4	D	158	ILE
4	D	160	GLN
4	D	161	ASN
4	D	165	MET
4	D	176	LEU
4	D	187	ARG
4	D	188	LEU
4	D	191	ARG
4	D	198	VAL
4	D	209	ARG
5	E	9	LYS
5	E	12	LEU
5	E	16	THR
5	E	31	LEU
5	E	41	VAL
5	E	43	LEU
5	E	53	LEU
5	E	64	ARG
5	E	68	GLU
5	E	80	ILE
5	E	81	GLU
5	E	120	THR
5	E	151	LEU
6	F	14	LEU
6	F	39	LYS
6	F	41	GLU
6	F	43	LEU
6	F	55	ASP
6	F	69	GLU
6	F	83	ASP
6	F	92	LYS
6	F	93	SER
6	F	98	LEU
7	G	3	ARG
7	G	8	GLU
7	G	10	ARG
7	G	12	LEU
7	G	22	LEU
7	G	32	ARG

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Mol	Chain	Res	Type
7	G	38	LEU
7	G	72	ARG
7	G	76	ARG
7	G	91	VAL
7	G	113	GLU
7	G	114	ARG
7	G	129	GLU
7	G	149	ARG
7	G	153	HIS
7	G	156	TRP
8	H	3	THR
8	H	18	ARG
8	H	24	THR
8	H	26	VAL
8	H	39	LEU
8	H	53	VAL
8	H	85	ARG
8	H	88	LYS
8	H	91	ARG
8	H	92	ARG
8	H	99	GLU
8	H	104	ARG
8	H	112	LEU
8	H	115	SER
8	H	129	VAL
8	H	133	LEU
9	I	2	GLU
9	I	3	GLN
9	I	38	GLN
9	I	64	THR
9	I	66	ARG
9	I	79	LEU
9	I	85	LEU
9	I	104	ARG
9	I	108	VAL
9	I	111	ARG
9	I	113	LYS
9	I	114	TYR
9	I	121	ARG
9	I	127	LYS
10	J	6	ILE
10	J	9	ARG

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Mol	Chain	Res	Type
10	J	23	ILE
10	J	40	LEU
10	J	42	THR
10	J	59	SER
10	J	60	ARG
10	J	74	ILE
10	J	78	ASN
10	J	90	LEU
10	J	96	ILE
11	K	12	ARG
11	K	24	SER
11	K	29	ILE
11	K	47	VAL
11	K	48	ILE
11	K	53	SER
11	K	57	THR
11	K	92	GLU
11	K	98	LEU
11	K	114	VAL
11	K	117	ASN
12	L	13	LYS
12	L	33	ARG
12	L	38	THR
12	L	42	THR
12	L	44	THR
12	L	52	LEU
12	L	54	LYS
12	L	60	LEU
12	L	67	THR
12	L	70	ILE
12	L	89	ARG
12	L	118	SER
12	L	122	THR
12	L	127	GLU
13	M	3	ARG
13	M	9	ILE
13	M	32	GLU
13	M	56	LEU
13	M	63	THR
13	M	69	GLU
13	M	70	LEU
13	M	73	GLU

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Mol	Chain	Res	Type
13	M	81	LEU
13	M	82	MET
13	M	108	ARG
13	M	109	THR
13	M	111	LYS
13	M	115	LYS
14	N	7	ILE
14	N	8	GLU
14	N	9	LYS
14	N	22	THR
14	N	33	VAL
14	N	47	LEU
15	O	22	THR
15	O	31	LEU
15	O	32	LEU
15	O	34	LEU
15	O	39	LEU
15	O	47	LYS
15	O	59	MET
15	O	70	LEU
15	O	71	GLN
15	O	77	ARG
15	O	81	LEU
16	P	1	MET
16	P	2	VAL
16	P	5	ARG
16	P	6	LEU
16	P	8	ARG
16	P	28	ARG
16	P	36	ILE
16	P	42	ARG
16	P	50	LYS
16	P	62	VAL
16	P	69	THR
17	Q	13	ASP
17	Q	25	ARG
17	Q	34	LYS
17	Q	38	ARG
17	Q	53	LEU
17	Q	59	ILE
17	Q	62	SER
17	Q	70	ARG

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Mol	Chain	Res	Type
17	Q	74	LEU
17	Q	92	ARG
17	Q	93	GLN
17	Q	98	LEU
17	Q	100	LYS
17	Q	101	ARG
18	R	19	LYS
18	R	40	LEU
18	R	53	ARG
18	R	66	LEU
18	R	68	LYS
18	R	86	VAL
19	S	4	SER
19	S	6	LYS
19	S	7	LYS
19	S	25	LYS
19	S	28	LYS
19	S	29	ARG
19	S	31	ILE
19	S	33	THR
19	S	36	ARG
19	S	47	HIS
19	S	64	GLU
19	S	67	VAL
19	S	70	LYS
19	S	79	THR
20	T	17	ARG
20	T	35	THR
20	T	56	MET
20	T	73	HIS
20	T	74	LYS
20	T	75	ASN
20	T	81	LYS
20	T	84	LEU
20	T	99	LEU
21	V	9	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	204	ASN
3	C	6	HIS

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Mol	Chain	Res	Type
9	I	38	GLN
16	P	82	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1513/1513 (100%)	315 (20%)	73 (4%)
22	W	2/6 (33%)	1 (50%)	0
23	X	7/17 (41%)	4 (57%)	0
All	All	1522/1536 (99%)	320 (21%)	73 (4%)

All (320) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	7	G
1	A	9	G
1	A	32	A
1	A	39	G
1	A	47	C
1	A	48	C
1	A	50	A
1	A	51	A
1	A	54	C
1	A	60	A
1	A	61	G
1	A	64	G
1	A	65	U
1	A	66	G
1	A	73	G
1	A	94	A
1	A	108	G
1	A	114	C
1	A	115	G
1	A	123	G
1	A	124	A
1	A	125	C
1	A	156	A
1	A	157	C
1	A	168	C
1	A	176	U

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Mol	Chain	Res	Type
1	A	189	U
1	A	190	G
1	A	193	G
1	A	196	U
1	A	201	A
1	A	203	A
1	A	208	U
1	A	209	U
1	A	211	G
1	A	212	C
1	A	216	C
1	A	226	G
1	A	239	U
1	A	240	C
1	A	242	G
1	A	245	A
1	A	246	G
1	A	253	G
1	A	261	G
1	A	262	C
1	A	274	A
1	A	276	G
1	A	277	A
1	A	284	G
1	A	287	G
1	A	296	G
1	A	311	G
1	A	314	G
1	A	316	A
1	A	323	C
1	A	324	A
1	A	327	G
1	A	339	A
1	A	340	C
1	A	341	G
1	A	345	G
1	A	347	C
1	A	348	A
1	A	349	G
1	A	362	U
1	A	367	C
1	A	368	A

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Mol	Chain	Res	Type
1	A	379	G
1	A	384	A
1	A	385	C
1	A	401	G
1	A	407	A
1	A	408	G
1	A	409	A
1	A	416	U
1	A	417	C
1	A	418	G
1	A	424	U
1	A	425	A
1	A	434	A
1	A	442	A
1	A	445	A
1	A	446	A
1	A	447	A
1	A	454	A
1	A	466	A
1	A	468	G
1	A	469	G
1	A	470	U
1	A	479	A
1	A	480	A
1	A	481	U
1	A	494	C
1	A	495	U
1	A	501	C
1	A	502	C
1	A	507	G
1	A	509	C
1	A	510	G
1	A	513	G
1	A	514	U
1	A	515	A
1	A	516	A
1	A	530	A
1	A	531	G
1	A	542	A
1	A	543	U
1	A	544	U
1	A	555	A

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Mol	Chain	Res	Type
1	A	556	A
1	A	559	G
1	A	562	G
1	A	564	G
1	A	565	U
1	A	570	G
1	A	579	C
1	A	590	A
1	A	599	G
1	A	632	G
1	A	636	A
1	A	648	A
1	A	670	A
1	A	671	G
1	A	684	C
1	A	685	A
1	A	686	G
1	A	700	C
1	A	705	A
1	A	706	U
1	A	707	G
1	A	714	G
1	A	735	G
1	A	738	G
1	A	749	A
1	A	753	C
1	A	760	A
1	A	763	A
1	A	764	A
1	A	765	A
1	A	768	G
1	A	773	A
1	A	775	A
1	A	776	U
1	A	777	A
1	A	782	G
1	A	796	U
1	A	798	A
1	A	799	A
1	A	800	C
1	A	811	A
1	A	812	G

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Mol	Chain	Res	Type
1	A	822	U
1	A	823	C
1	A	824	U
1	A	825	C
1	A	847	U
1	A	848	U
1	A	849	A
1	A	853	G
1	A	861	U
1	A	862	G
1	A	867	G
1	A	868	U
1	A	890	A
1	A	891	A
1	A	894	G
1	A	899	G
1	A	903	G
1	A	904	G
1	A	911	C
1	A	912	A
1	A	916	G
1	A	917	C
1	A	919	G
1	A	937	U
1	A	938	U
1	A	943	G
1	A	944	C
1	A	945	A
1	A	946	A
1	A	948	G
1	A	952	A
1	A	953	G
1	A	954	A
1	A	960	A
1	A	966	C
1	A	968	U
1	A	969	U
1	A	970	G
1	A	978	A
1	A	981	G
1	A	982	A
1	A	983	A

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Mol	Chain	Res	Type
1	A	984	C
1	A	986	C
1	A	994	A
1	A	1001	G
1	A	1003	U
1	A	1004	G
1	A	1006	C
1	A	1007	C
1	A	1013	G
1	A	1022	U
1	A	1024	G
1	A	1035	G
1	A	1036	C
1	A	1037	A
1	A	1047	U
1	A	1048	C
1	A	1052	U
1	A	1060	U
1	A	1071	G
1	A	1076	G
1	A	1077	U
1	A	1078	C
1	A	1083	A
1	A	1106	G
1	A	1107	U
1	A	1108	U
1	A	1109	G
1	A	1111	C
1	A	1112	A
1	A	1113	G
1	A	1119	C
1	A	1120	G
1	A	1121	G
1	A	1122	C
1	A	1128	A
1	A	1139	A
1	A	1140	C
1	A	1141	U
1	A	1149	A
1	A	1152	G
1	A	1163	G
1	A	1164	A

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Mol	Chain	Res	Type
1	A	1172	A
1	A	1174	G
1	A	1177	U
1	A	1178	G
1	A	1181	C
1	A	1182	A
1	A	1183	G
1	A	1185	A
1	A	1193	U
1	A	1194	A
1	A	1195	C
1	A	1205	G
1	A	1206	A
1	A	1207	C
1	A	1209	C
1	A	1219	A
1	A	1220	A
1	A	1221	U
1	A	1230	C
1	A	1231	A
1	A	1238	U
1	A	1239	G
1	A	1259	U
1	A	1260	A
1	A	1261	A
1	A	1266	A
1	A	1268	A
1	A	1279	C
1	A	1280	A
1	A	1281	G
1	A	1282	U
1	A	1283	U
1	A	1287	A
1	A	1291	G
1	A	1293	G
1	A	1300	A
1	A	1301	C
1	A	1304	G
1	A	1315	G
1	A	1319	G
1	A	1321	A
1	A	1327	A

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Mol	Chain	Res	Type
1	A	1328	G
1	A	1329	U
1	A	1334	G
1	A	1341	A
1	A	1345	A
1	A	1346	U
1	A	1347	G
1	A	1352	G
1	A	1361	G
1	A	1363	U
1	A	1379	C
1	A	1380	A
1	A	1426	A
1	A	1427	G
1	A	1432	C
1	A	1433	G
1	A	1461	C
1	A	1466	G
1	A	1469	A
1	A	1471	G
1	A	1474	G
1	A	1481	G
1	A	1482	G
1	A	1483	U
1	A	1484	A
1	A	1494	G
1	A	1496	A
1	A	1497	G
1	A	1506	G
1	A	1507	G
1	A	1509	U
1	A	1510	C
1	A	1511	A
1	A	1516	C
1	A	1518	U
1	A	1519	U
22	W	3	G
23	X	32	C
23	X	33	C
23	X	36	U
23	X	39	C

All (73) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	5	U
1	A	50	A
1	A	60	A
1	A	64	G
1	A	65	U
1	A	101	G
1	A	123	G
1	A	155	A
1	A	175	G
1	A	189	U
1	A	239	U
1	A	276	G
1	A	310	A
1	A	323	C
1	A	340	C
1	A	348	A
1	A	383	G
1	A	407	A
1	A	408	G
1	A	417	C
1	A	424	U
1	A	445	A
1	A	468	G
1	A	469	G
1	A	494	C
1	A	500	G
1	A	501	C
1	A	542	A
1	A	543	U
1	A	558	G
1	A	669	U
1	A	670	A
1	A	684	C
1	A	775	A
1	A	776	U
1	A	795	C
1	A	798	A
1	A	847	U
1	A	861	U
1	A	866	A
1	A	867	G
1	A	937	U
1	A	942	A

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Mol	Chain	Res	Type
1	A	959	U
1	A	969	U
1	A	1035	G
1	A	1046	G
1	A	1047	U
1	A	1076	G
1	A	1110	C
1	A	1118	U
1	A	1127	C
1	A	1139	A
1	A	1163	G
1	A	1171	G
1	A	1182	A
1	A	1194	A
1	A	1205	G
1	A	1206	A
1	A	1220	A
1	A	1279	C
1	A	1281	G
1	A	1286	G
1	A	1300	A
1	A	1328	G
1	A	1345	A
1	A	1346	U
1	A	1362	U
1	A	1378	A
1	A	1379	C
1	A	1432	C
1	A	1481	G
1	A	1505	U

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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
23	RSQ	X	34	23	16,23,24	1.92	3 (18%)	20,33,36	1.70	2 (10%)

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
23	RSQ	X	34	23	-	5/7/27/28	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	X	34	RSQ	O30-C10	5.19	1.39	1.21
23	X	34	RSQ	C5-C4	3.50	1.45	1.41
23	X	34	RSQ	C5-C10	2.75	1.53	1.47

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	X	34	RSQ	O30-C10-C5	-4.56	112.29	124.36
23	X	34	RSQ	C2-N3-C4	4.45	121.39	116.02

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	X	34	RSQ	C2'-C1'-N1-C6
23	X	34	RSQ	O30-C10-C5-C4
23	X	34	RSQ	O30-C10-C5-C6
23	X	34	RSQ	C3'-C4'-C5'-O5'
23	X	34	RSQ	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	X	34	RSQ	4	0



## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 189 ligands modelled in this entry, 188 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
25	PAR	A	1785	-	45,45,45	1.41	6 (13%)	64,67,67	1.71	15 (23%)

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
25	PAR	A	1785	-	-	4/18/94/94	0/4/4/4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	1785	PAR	C52-C42	4.23	1.61	1.52
25	A	1785	PAR	C64-C54	3.26	1.56	1.52
25	A	1785	PAR	C31-C21	2.78	1.57	1.53
25	A	1785	PAR	C13-C23	2.56	1.56	1.52
25	A	1785	PAR	C33-C43	2.27	1.59	1.52
25	A	1785	PAR	C22-C12	-2.19	1.49	1.53

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	1785	PAR	O33-C14-C24	6.14	118.80	108.22
25	A	1785	PAR	O54-C54-C44	4.02	116.99	109.69
25	A	1785	PAR	O52-C13-C23	3.77	115.78	107.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	1785	PAR	C34-C24-N24	-3.50	103.89	111.05
25	A	1785	PAR	O34-C34-C44	-2.98	103.47	110.35
25	A	1785	PAR	O11-C11-O51	2.81	118.53	110.67
25	A	1785	PAR	C14-O33-C33	-2.75	111.15	117.96
25	A	1785	PAR	O43-C13-C23	-2.67	101.53	104.98
25	A	1785	PAR	C13-O52-C52	-2.49	111.81	117.96
25	A	1785	PAR	C11-O51-C51	2.31	118.22	113.69
25	A	1785	PAR	O51-C51-C61	2.18	111.87	106.44
25	A	1785	PAR	O34-C34-C24	-2.13	106.39	110.22
25	A	1785	PAR	O52-C13-O43	-2.12	109.14	111.43
25	A	1785	PAR	O11-C11-C21	-2.09	104.62	108.22
25	A	1785	PAR	C22-C32-C42	2.03	114.67	109.53

There are no chirality outliers.

All (4) torsion outliers are listed below:

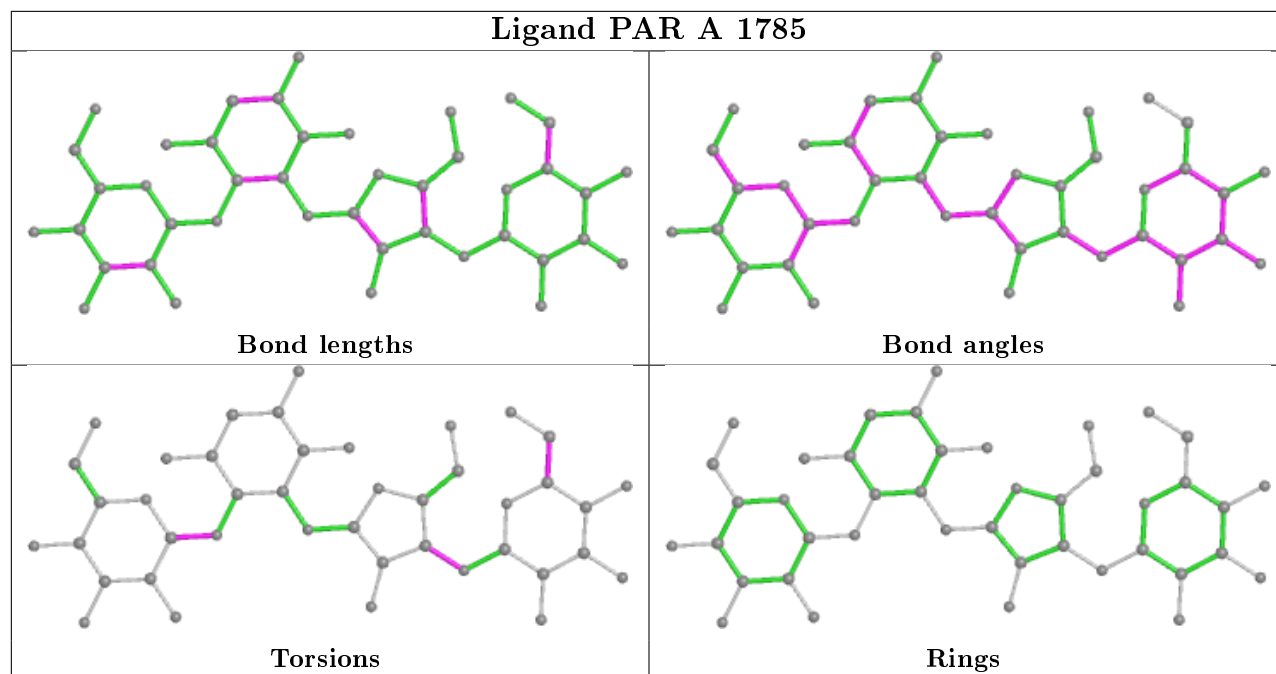
Mol	Chain	Res	Type	Atoms
25	A	1785	PAR	C44-C54-C64-N64
25	A	1785	PAR	O54-C54-C64-N64
25	A	1785	PAR	O51-C11-O11-C42
25	A	1785	PAR	C43-C33-O33-C14

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	A	1785	PAR	4	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 than 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1512/1513 (99%)	0.83	108 (7%)	16 16	37, 67, 149, 244	0
2	B	234/234 (100%)	0.44	17 (7%)	15 15	55, 100, 170, 244	0
3	C	206/206 (100%)	0.30	8 (3%)	39 37	58, 96, 152, 177	0
4	D	208/208 (100%)	0.80	32 (15%)	2 2	49, 70, 118, 161	0
5	E	150/150 (100%)	0.48	1 (0%)	87 88	41, 54, 86, 133	0
6	F	101/101 (100%)	0.68	14 (13%)	2 2	57, 93, 131, 152	0
7	G	155/155 (100%)	0.26	5 (3%)	47 46	62, 84, 135, 224	0
8	H	138/138 (100%)	0.41	3 (2%)	62 60	40, 54, 85, 121	0
9	I	127/127 (100%)	0.96	24 (18%)	1 1	58, 94, 134, 169	0
10	J	98/98 (100%)	1.06	20 (20%)	1 1	60, 114, 197, 259	0
11	K	119/119 (100%)	0.67	14 (11%)	4 4	42, 72, 130, 152	0
12	L	124/124 (100%)	0.47	6 (4%)	30 28	37, 58, 111, 186	0
13	M	125/125 (100%)	0.99	23 (18%)	1 1	63, 98, 158, 233	0
14	N	60/60 (100%)	0.70	8 (13%)	3 3	67, 81, 129, 185	0
15	O	88/88 (100%)	0.80	14 (15%)	1 2	44, 69, 130, 168	0
16	P	83/83 (100%)	0.69	7 (8%)	11 10	47, 56, 94, 135	0
17	Q	104/104 (100%)	0.86	11 (10%)	6 6	39, 65, 120, 239	0
18	R	73/73 (100%)	0.98	16 (21%)	0 1	51, 74, 152, 184	0
19	S	80/80 (100%)	1.83	26 (32%)	0 0	75, 113, 164, 228	0
20	T	99/99 (100%)	0.71	8 (8%)	12 11	51, 70, 119, 159	0
21	V	24/24 (100%)	2.32	14 (58%)	0 0	74, 88, 108, 138	0
22	W	3/6 (50%)	0.82	0	100 100	45, 45, 56, 58	0
23	X	8/17 (47%)	0.46	0	100 100	60, 73, 131, 140	0
All	All	3919/3932 (99%)	0.74	379 (9%)	7 8	37, 75, 148, 259	0

All (379) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
10	J	30	SER	16.3
17	Q	105	ALA	13.6
17	Q	103	GLY	12.7
1	A	1517	U	12.6
1	A	1516	C	12.1
19	S	3	ARG	12.0
17	Q	104	LYS	11.7
4	D	2	GLY	11.7
19	S	2	PRO	11.2
10	J	29	ARG	9.3
8	H	1	MET	8.6
19	S	5	LEU	8.4
10	J	31	GLY	7.7
19	S	34	TRP	7.6
1	A	1016	G	7.1
19	S	37	ARG	6.6
9	I	66	ARG	6.2
4	D	23	GLY	6.0
1	A	1111	C	5.7
1	A	1021	C	5.6
21	V	24	ARG	5.5
14	N	6	LEU	5.5
1	A	981	G	5.5
1	A	1020	C	5.3
2	B	133	LYS	5.2
9	I	14	VAL	5.1
19	S	32	LYS	5.1
13	M	102	ARG	5.1
11	K	42	TRP	4.9
1	A	1036	C	4.8
9	I	9	ARG	4.7
1	A	970	G	4.7
1	A	1424	G	4.7
13	M	123	ALA	4.7
13	M	27	LYS	4.7
9	I	15	ALA	4.6
1	A	208	U	4.5
13	M	2	ALA	4.4
4	D	3	ARG	4.3
15	O	22	THR	4.3
1	A	1510	C	4.3
4	D	7	PRO	4.3

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Mol	Chain	Res	Type	RSRZ
14	N	3	ARG	4.3
4	D	42	GLN	4.3
1	A	348	A	4.2
20	T	103	GLY	4.2
1	A	1425	G	4.2
19	S	51	VAL	4.2
20	T	68	LYS	4.2
1	A	455	C	4.1
21	V	5	ASP	4.1
19	S	36	ARG	4.1
1	A	995	G	4.1
19	S	70	LYS	4.1
4	D	5	ILE	4.1
4	D	4	TYR	4.1
1	A	1205	G	4.0
21	V	6	ARG	4.0
21	V	18	TYR	4.0
19	S	73	GLU	4.0
4	D	41	GLY	4.0
19	S	71	LEU	4.0
4	D	115	ARG	3.9
2	B	132	LYS	3.9
1	A	1015	G	3.9
4	D	134	ASP	3.9
19	S	35	SER	3.9
5	E	5	ASP	3.9
17	Q	68	ARG	3.8
6	F	67	MET	3.8
13	M	8	GLU	3.8
9	I	128	ARG	3.8
11	K	31	THR	3.8
13	M	16	ASP	3.7
19	S	69	HIS	3.7
1	A	1109	G	3.7
8	H	2	LEU	3.7
17	Q	16	GLN	3.7
21	V	25	LYS	3.6
1	A	346	G	3.6
1	A	978	A	3.6
1	A	980	G	3.6
1	A	687	A	3.6
18	R	76	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
10	J	33	GLN	3.6
4	D	35	ARG	3.6
10	J	37	PRO	3.6
2	B	236	TYR	3.5
19	S	52	TYR	3.5
2	B	207	ALA	3.5
9	I	110	GLU	3.5
13	M	103	THR	3.4
15	O	21	ASP	3.4
2	B	131	PRO	3.4
4	D	8	VAL	3.4
10	J	72	VAL	3.4
9	I	102	LEU	3.4
16	P	12	LYS	3.4
1	A	967	C	3.4
13	M	124	PRO	3.3
16	P	8	ARG	3.3
19	S	33	THR	3.3
4	D	21	LEU	3.3
6	F	4	TYR	3.3
13	M	106	ASN	3.3
17	Q	15	MET	3.3
15	O	3	ILE	3.3
18	R	62	GLU	3.3
1	A	983	A	3.3
10	J	71	LEU	3.3
17	Q	43	LEU	3.3
3	C	161	GLU	3.3
17	Q	98	LEU	3.3
21	V	2	GLY	3.3
1	A	423	G	3.3
15	O	2	PRO	3.3
13	M	105	THR	3.3
4	D	33	MET	3.2
7	G	5	ARG	3.2
13	M	15	VAL	3.2
20	T	64	ASP	3.2
2	B	76	GLN	3.2
15	O	48	LYS	3.2
9	I	8	GLY	3.2
1	A	1303	C	3.2
21	V	22	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
4	D	123	HIS	3.2
1	A	688	U	3.1
1	A	1199	C	3.1
1	A	1163	G	3.1
4	D	6	GLY	3.1
9	I	70	LYS	3.1
3	C	76	VAL	3.1
15	O	27	VAL	3.1
1	A	107	U	3.1
13	M	7	VAL	3.1
20	T	104	LEU	3.1
1	A	1014	G	3.0
2	B	111	ARG	3.0
14	N	41	ARG	3.0
7	G	33	ASP	3.0
19	S	49	ILE	3.0
1	A	422	U	3.0
10	J	28	ARG	3.0
1	A	1200	U	3.0
13	M	4	ILE	3.0
21	V	9	ARG	3.0
1	A	1518	U	2.9
14	N	2	ALA	2.9
1	A	1444	G	2.9
1	A	984	C	2.9
1	A	992	A	2.9
2	B	77	ALA	2.9
19	S	74	PHE	2.9
2	B	35	GLU	2.9
20	T	106	ALA	2.9
1	A	1201	G	2.9
19	S	30	LEU	2.9
1	A	1017	A	2.9
11	K	19	ALA	2.9
9	I	7	THR	2.9
6	F	65	VAL	2.9
13	M	88	ARG	2.9
12	L	115	LYS	2.9
10	J	38	ILE	2.9
15	O	70	LEU	2.9
4	D	24	GLU	2.9
1	A	1241	C	2.8

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Mol	Chain	Res	Type	RSRZ
10	J	46	ARG	2.8
1	A	100	G	2.8
1	A	689	A	2.8
18	R	48	GLY	2.8
1	A	979	G	2.8
9	I	64	THR	2.8
19	S	54	GLY	2.8
13	M	104	ARG	2.8
1	A	1121	G	2.8
21	V	21	TYR	2.8
14	N	18	VAL	2.8
11	K	29	ILE	2.8
13	M	6	GLY	2.8
1	A	60	A	2.8
17	Q	14	LYS	2.8
10	J	7	LYS	2.7
21	V	20	LYS	2.7
6	F	75	LEU	2.7
1	A	203	A	2.7
1	A	1126	G	2.7
18	R	43	PHE	2.7
1	A	982	A	2.7
9	I	63	ILE	2.7
9	I	13	ALA	2.7
4	D	120	LEU	2.6
1	A	994	A	2.6
1	A	202	A	2.6
2	B	188	ALA	2.6
4	D	121	VAL	2.6
7	G	4	ARG	2.6
3	C	39	ILE	2.6
11	K	18	ARG	2.6
4	D	122	ARG	2.6
19	S	78	ARG	2.6
1	A	991	G	2.6
10	J	39	PRO	2.6
15	O	28	GLN	2.6
16	P	41	PRO	2.6
18	R	72	ARG	2.6
1	A	360	U	2.6
3	C	87	LEU	2.6
1	A	647	G	2.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	1415	A	2.6
16	P	15	PRO	2.5
1	A	51	A	2.5
11	K	81	ASP	2.5
10	J	47	PHE	2.5
17	Q	44	ALA	2.5
16	P	17	TYR	2.5
14	N	4	LYS	2.5
1	A	954	A	2.5
1	A	960	A	2.5
1	A	1249	A	2.5
3	C	66	VAL	2.5
1	A	1018	G	2.5
19	S	27	GLU	2.5
3	C	2	GLY	2.5
6	F	86	ARG	2.5
18	R	66	LEU	2.5
19	S	31	ILE	2.5
1	A	955	A	2.5
9	I	16	ARG	2.5
11	K	84	VAL	2.5
6	F	79	LEU	2.5
9	I	61	ALA	2.5
9	I	37	PHE	2.5
2	B	36	ARG	2.5
1	A	651	G	2.5
18	R	31	LEU	2.5
1	A	310	A	2.5
20	T	56	MET	2.5
10	J	54	PHE	2.5
11	K	30	VAL	2.4
4	D	22	LYS	2.4
20	T	81	LYS	2.4
1	A	106	G	2.4
1	A	1002	G	2.4
4	D	40	PRO	2.4
17	Q	17	LYS	2.4
18	R	75	ILE	2.4
14	N	8	GLU	2.4
2	B	187	LEU	2.4
1	A	1013	G	2.4
6	F	10	LEU	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
4	D	26	CYS	2.4
11	K	43	SER	2.4
19	S	77	THR	2.4
19	S	50	ALA	2.4
1	A	432	U	2.4
7	G	115	ARG	2.4
1	A	421	G	2.4
18	R	50	ILE	2.4
13	M	13	LYS	2.4
1	A	1022	U	2.4
1	A	1076	G	2.4
6	F	89	MET	2.4
1	A	1198	C	2.4
4	D	116	GLN	2.3
6	F	63	TYR	2.3
10	J	20	ALA	2.3
15	O	31	LEU	2.3
1	A	342	G	2.3
1	A	1417	G	2.3
16	P	13	HIS	2.3
2	B	134	GLU	2.3
18	R	78	LEU	2.3
4	D	133	VAL	2.3
10	J	55	LYS	2.3
1	A	345	G	2.3
1	A	1414	G	2.3
12	L	101	VAL	2.3
15	O	23	GLY	2.3
1	A	788	C	2.3
1	A	343	G	2.3
1	A	959	U	2.3
11	K	39	PRO	2.3
1	A	180	C	2.3
1	A	1019	C	2.3
9	I	79	LEU	2.3
3	C	68	VAL	2.3
15	O	72	ARG	2.3
21	V	10	ARG	2.3
1	A	1197	G	2.3
16	P	1	MET	2.3
10	J	57	LYS	2.3
21	V	12	LYS	2.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	369	A	2.3
1	A	1010	C	2.3
9	I	82	ALA	2.3
4	D	87	GLY	2.2
13	M	126	LYS	2.2
4	D	10	ARG	2.2
3	C	111	LEU	2.2
10	J	34	VAL	2.2
1	A	261	G	2.2
1	A	1423	G	2.2
18	R	73	ALA	2.2
9	I	83	ARG	2.2
1	A	1106	G	2.2
1	A	1302	C	2.2
4	D	110	PHE	2.2
9	I	18	PHE	2.2
13	M	122	LYS	2.2
6	F	14	LEU	2.2
15	O	15	PHE	2.2
1	A	1162	G	2.2
7	G	2	ALA	2.2
12	L	120	TYR	2.2
6	F	8	ILE	2.2
1	A	373	G	2.2
9	I	85	LEU	2.2
2	B	152	PHE	2.2
1	A	105	G	2.2
1	A	5	U	2.2
6	F	66	GLU	2.2
20	T	85	MET	2.2
13	M	119	GLY	2.2
4	D	25	ARG	2.2
18	R	81	PHE	2.2
2	B	108	ILE	2.2
18	R	29	PHE	2.1
13	M	60	VAL	2.1
1	A	1416	A	2.1
1	A	1218	C	2.1
11	K	129	SER	2.1
18	R	16	PRO	2.1
14	N	61	TRP	2.1
1	A	468	G	2.1

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Mol	Chain	Res	Type	RSRZ
9	I	67	GLY	2.1
13	M	19	LEU	2.1
21	V	8	THR	2.1
4	D	135	LEU	2.1
11	K	37	GLY	2.1
19	S	44	MET	2.1
15	O	69	TYR	2.1
6	F	69	GLU	2.1
9	I	109	VAL	2.1
15	O	66	LEU	2.1
21	V	11	GLY	2.1
12	L	28	LYS	2.1
1	A	368	A	2.1
1	A	47	C	2.1
1	A	326	G	2.1
11	K	14	VAL	2.1
6	F	71	ARG	2.1
1	A	258	A	2.1
1	A	956	C	2.1
1	A	1240	C	2.1
19	S	72	GLY	2.1
1	A	1003	U	2.1
1	A	1261	A	2.1
4	D	136	PRO	2.1
10	J	22	LYS	2.1
18	R	68	LYS	2.1
1	A	309	C	2.1
1	A	1141	U	2.0
2	B	93	VAL	2.0
13	M	118	ALA	2.0
1	A	344	A	2.0
1	A	178	G	2.0
12	L	119	LYS	2.0
8	H	102	ARG	2.0
10	J	35	SER	2.0
1	A	466	A	2.0
12	L	104	VAL	2.0
1	A	1251	C	2.0
11	K	98	LEU	2.0
4	D	124	GLY	2.0
18	R	64	ARG	2.0
9	I	19	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	81	VAL	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
23	RSQ	X	34	22/23	0.94	0.23	65,67,69,70	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
24	MG	A	1713	1/1	0.04	0.95	92,92,92,92	0
24	MG	A	1639	1/1	0.23	0.95	85,85,85,85	0
24	MG	A	1670	1/1	0.24	0.91	72,72,72,72	0
24	MG	A	1741	1/1	0.25	0.69	91,91,91,91	0
24	MG	A	1772	1/1	0.29	0.53	92,92,92,92	0
24	MG	A	1643	1/1	0.37	0.20	74,74,74,74	0
24	MG	A	1609	1/1	0.40	0.81	67,67,67,67	0
24	MG	A	1603	1/1	0.42	0.44	65,65,65,65	0
24	MG	A	1742	1/1	0.44	1.13	96,96,96,96	0
24	MG	A	1778	1/1	0.45	0.30	94,94,94,94	0
24	MG	A	1697	1/1	0.48	0.50	58,58,58,58	0
24	MG	A	1676	1/1	0.50	0.62	73,73,73,73	0
24	MG	A	1753	1/1	0.50	0.44	71,71,71,71	0
24	MG	A	1645	1/1	0.53	0.65	108,108,108,108	0
24	MG	A	1695	1/1	0.53	0.94	86,86,86,86	0
24	MG	A	1690	1/1	0.55	1.45	135,135,135,135	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
24	MG	A	1621	1/1	0.58	0.43	50,50,50,50	0
24	MG	A	1703	1/1	0.58	2.54	106,106,106,106	1
24	MG	A	1764	1/1	0.59	0.37	51,51,51,51	0
24	MG	A	1605	1/1	0.59	0.46	59,59,59,59	0
24	MG	A	1698	1/1	0.60	0.66	77,77,77,77	0
24	MG	A	1681	1/1	0.60	0.51	58,58,58,58	0
24	MG	A	1721	1/1	0.61	0.47	88,88,88,88	0
24	MG	A	1749	1/1	0.62	0.36	67,67,67,67	0
24	MG	A	1724	1/1	0.63	0.50	53,53,53,53	0
24	MG	A	1733	1/1	0.63	0.57	82,82,82,82	0
24	MG	A	1691	1/1	0.64	0.18	109,109,109,109	0
24	MG	A	1665	1/1	0.65	0.50	53,53,53,53	0
24	MG	A	1638	1/1	0.65	0.49	50,50,50,50	0
24	MG	A	1601	1/1	0.66	0.68	59,59,59,59	0
24	MG	A	1682	1/1	0.67	1.67	84,84,84,84	0
24	MG	A	1604	1/1	0.68	0.85	93,93,93,93	0
24	MG	A	1654	1/1	0.68	0.51	46,46,46,46	0
24	MG	A	1718	1/1	0.69	0.45	66,66,66,66	0
24	MG	A	1709	1/1	0.69	0.51	76,76,76,76	0
24	MG	A	1777	1/1	0.71	0.79	89,89,89,89	0
24	MG	A	1751	1/1	0.72	0.48	67,67,67,67	0
24	MG	A	1739	1/1	0.72	0.75	69,69,69,69	0
24	MG	A	1619	1/1	0.73	0.61	67,67,67,67	0
24	MG	A	1636	1/1	0.74	0.54	41,41,41,41	0
24	MG	A	1766	1/1	0.74	0.57	70,70,70,70	0
24	MG	A	1627	1/1	0.74	0.48	68,68,68,68	0
24	MG	A	1762	1/1	0.74	0.25	66,66,66,66	0
24	MG	A	1616	1/1	0.74	0.19	70,70,70,70	0
24	MG	A	1602	1/1	0.74	0.17	74,74,74,74	0
24	MG	A	1754	1/1	0.74	1.95	97,97,97,97	0
24	MG	A	1687	1/1	0.75	0.43	86,86,86,86	0
24	MG	A	1731	1/1	0.75	0.35	98,98,98,98	0
24	MG	A	1728	1/1	0.75	0.47	76,76,76,76	0
24	MG	A	1716	1/1	0.75	0.90	87,87,87,87	0
24	MG	A	1692	1/1	0.75	0.20	112,112,112,112	0
24	MG	A	1702	1/1	0.75	0.36	81,81,81,81	0
24	MG	A	1683	1/1	0.76	0.23	64,64,64,64	0
24	MG	A	1696	1/1	0.76	0.73	78,78,78,78	0
24	MG	A	1756	1/1	0.76	0.47	66,66,66,66	0
24	MG	A	1707	1/1	0.76	0.24	50,50,50,50	0
24	MG	A	1607	1/1	0.76	0.75	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
24	MG	A	1642	1/1	0.77	1.11	64,64,64,64	0
24	MG	A	1657	1/1	0.77	0.55	70,70,70,70	0
24	MG	A	1629	1/1	0.77	0.67	42,42,42,42	0
24	MG	A	1759	1/1	0.77	0.38	49,49,49,49	0
24	MG	A	1771	1/1	0.77	0.34	63,63,63,63	0
24	MG	A	1699	1/1	0.78	0.38	60,60,60,60	0
24	MG	A	1689	1/1	0.78	0.65	80,80,80,80	0
24	MG	A	1650	1/1	0.78	0.92	75,75,75,75	0
24	MG	A	1767	1/1	0.78	0.40	49,49,49,49	0
24	MG	A	1765	1/1	0.78	1.52	82,82,82,82	0
24	MG	A	1701	1/1	0.78	0.38	84,84,84,84	0
24	MG	A	1781	1/1	0.79	0.16	74,74,74,74	0
24	MG	A	1646	1/1	0.79	0.46	69,69,69,69	0
24	MG	A	1746	1/1	0.79	0.23	63,63,63,63	0
24	MG	A	1717	1/1	0.79	0.75	88,88,88,88	0
24	MG	A	1704	1/1	0.79	0.18	58,58,58,58	0
24	MG	A	1672	1/1	0.79	0.86	60,60,60,60	0
24	MG	A	1729	1/1	0.80	0.55	38,38,38,38	0
24	MG	A	1631	1/1	0.80	0.47	48,48,48,48	0
24	MG	A	1712	1/1	0.80	0.28	53,53,53,53	0
24	MG	A	1664	1/1	0.81	0.12	82,82,82,82	0
24	MG	A	1780	1/1	0.81	0.51	68,68,68,68	0
24	MG	A	1738	1/1	0.81	0.17	44,44,44,44	0
24	MG	A	1625	1/1	0.82	0.20	57,57,57,57	0
24	MG	A	1655	1/1	0.82	0.20	47,47,47,47	0
24	MG	A	1633	1/1	0.82	1.61	67,67,67,67	0
24	MG	A	1750	1/1	0.82	0.55	66,66,66,66	0
24	MG	N	101	1/1	0.82	0.37	70,70,70,70	0
24	MG	A	1671	1/1	0.82	0.49	37,37,37,37	0
24	MG	A	1734	1/1	0.83	0.87	46,46,46,46	0
24	MG	A	1618	1/1	0.84	0.43	62,62,62,62	0
24	MG	A	1632	1/1	0.84	1.03	77,77,77,77	0
24	MG	A	1673	1/1	0.84	0.54	53,53,53,53	0
24	MG	A	1774	1/1	0.85	0.55	72,72,72,72	0
24	MG	A	1669	1/1	0.85	0.41	51,51,51,51	0
24	MG	A	1620	1/1	0.85	0.36	55,55,55,55	0
24	MG	A	1637	1/1	0.85	0.26	76,76,76,76	0
24	MG	A	1722	1/1	0.86	0.86	73,73,73,73	0
24	MG	A	1678	1/1	0.86	0.68	60,60,60,60	0
24	MG	A	1660	1/1	0.86	0.57	41,41,41,41	0
24	MG	A	1651	1/1	0.86	0.18	92,92,92,92	0
24	MG	A	1610	1/1	0.87	0.11	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
24	MG	B	301	1/1	0.87	0.37	87,87,87,87	0
24	MG	A	1714	1/1	0.87	0.32	54,54,54,54	0
24	MG	A	1736	1/1	0.87	0.30	56,56,56,56	0
24	MG	A	1680	1/1	0.87	0.57	54,54,54,54	0
24	MG	A	1779	1/1	0.88	0.40	95,95,95,95	0
24	MG	A	1693	1/1	0.88	0.42	80,80,80,80	0
24	MG	A	1613	1/1	0.88	0.49	53,53,53,53	0
24	MG	A	1752	1/1	0.89	0.42	61,61,61,61	0
24	MG	A	1783	1/1	0.89	0.42	77,77,77,77	0
24	MG	A	1737	1/1	0.89	0.44	66,66,66,66	0
24	MG	A	1666	1/1	0.89	0.35	46,46,46,46	0
24	MG	A	1740	1/1	0.89	0.80	39,39,39,39	0
24	MG	A	1732	1/1	0.90	0.51	89,89,89,89	0
24	MG	A	1622	1/1	0.90	0.33	98,98,98,98	0
24	MG	A	1745	1/1	0.90	0.20	50,50,50,50	0
24	MG	A	1667	1/1	0.90	0.30	39,39,39,39	0
24	MG	A	1744	1/1	0.90	0.37	61,61,61,61	0
24	MG	A	1755	1/1	0.90	1.13	64,64,64,64	0
24	MG	A	1623	1/1	0.90	1.06	115,115,115,115	0
24	MG	A	1735	1/1	0.90	0.52	56,56,56,56	0
24	MG	A	1782	1/1	0.90	0.53	55,55,55,55	0
24	MG	A	1674	1/1	0.91	0.34	57,57,57,57	0
24	MG	A	1694	1/1	0.91	0.13	79,79,79,79	0
24	MG	A	1719	1/1	0.91	0.58	66,66,66,66	0
24	MG	A	1700	1/1	0.91	0.49	39,39,39,39	0
24	MG	A	1747	1/1	0.91	0.42	99,99,99,99	0
24	MG	A	1776	1/1	0.91	0.29	75,75,75,75	0
24	MG	A	1612	1/1	0.91	0.68	39,39,39,39	0
24	MG	A	1663	1/1	0.91	0.23	50,50,50,50	0
24	MG	A	1630	1/1	0.91	0.33	44,44,44,44	0
24	MG	A	1685	1/1	0.91	0.38	54,54,54,54	0
24	MG	A	1615	1/1	0.91	0.37	40,40,40,40	0
24	MG	A	1675	1/1	0.91	0.43	60,60,60,60	0
24	MG	A	1641	1/1	0.92	0.49	53,53,53,53	0
24	MG	A	1608	1/1	0.92	0.17	86,86,86,86	0
24	MG	A	1773	1/1	0.92	0.29	57,57,57,57	0
24	MG	A	1679	1/1	0.92	0.87	47,47,47,47	0
24	MG	A	1784	1/1	0.92	0.90	42,42,42,42	0
24	MG	A	1614	1/1	0.92	0.60	79,79,79,79	1
24	MG	A	1688	1/1	0.92	0.13	76,76,76,76	0
24	MG	A	1677	1/1	0.92	0.51	68,68,68,68	0
24	MG	A	1635	1/1	0.92	0.47	36,36,36,36	0

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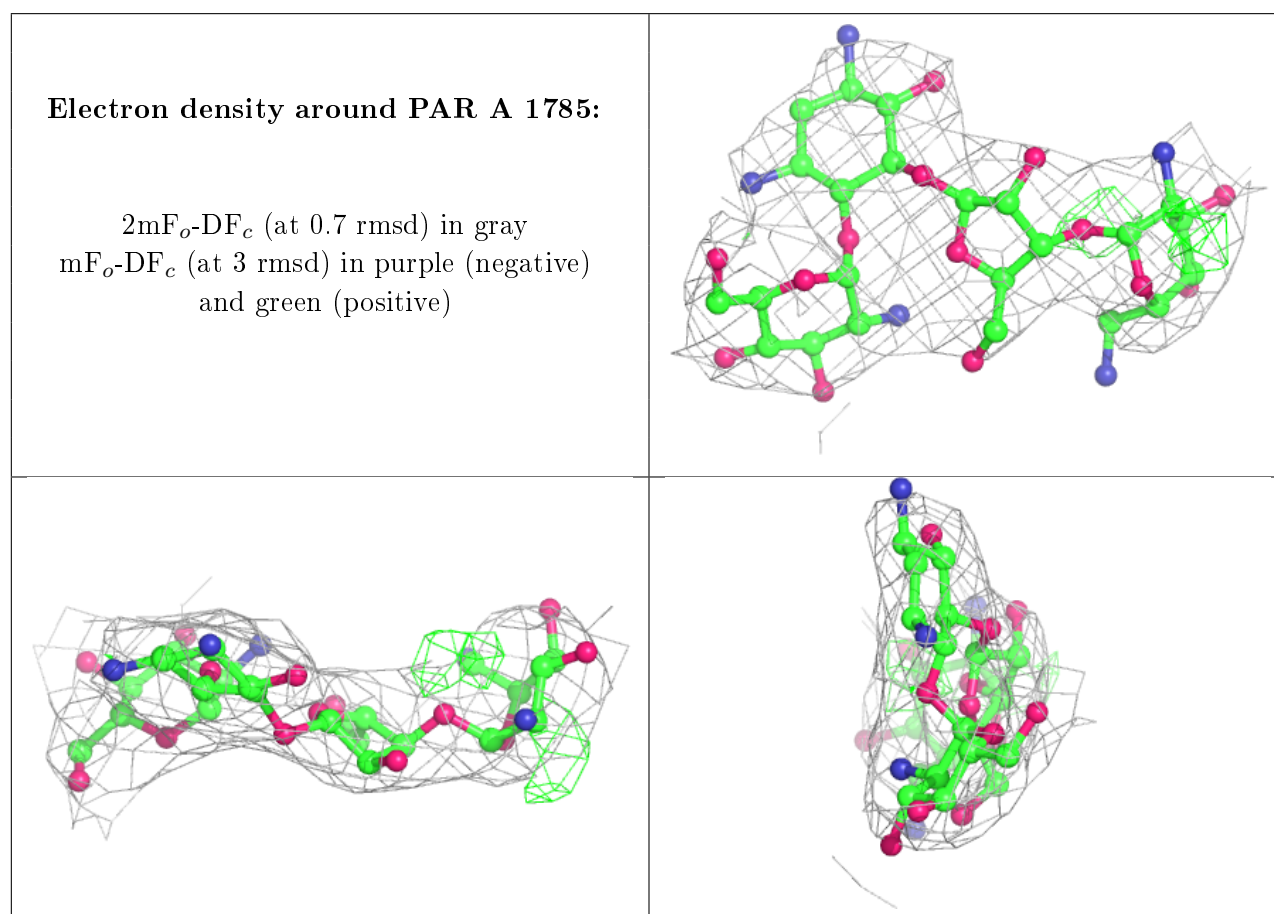
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
24	MG	A	1708	1/1	0.92	0.61	69,69,69,69	0
24	MG	A	1748	1/1	0.92	0.29	59,59,59,59	0
24	MG	A	1606	1/1	0.92	0.51	53,53,53,53	0
24	MG	A	1686	1/1	0.93	0.41	60,60,60,60	0
24	MG	A	1628	1/1	0.93	0.15	80,80,80,80	0
24	MG	A	1617	1/1	0.93	0.71	59,59,59,59	0
24	MG	A	1652	1/1	0.93	0.33	44,44,44,44	0
24	MG	A	1640	1/1	0.93	0.17	78,78,78,78	0
24	MG	A	1725	1/1	0.93	0.21	43,43,43,43	0
24	MG	A	1626	1/1	0.94	0.38	39,39,39,39	0
24	MG	A	1706	1/1	0.94	0.41	65,65,65,65	0
25	PAR	A	1785	42/42	0.94	0.27	45,48,55,57	0
24	MG	A	1656	1/1	0.94	0.34	57,57,57,57	0
24	MG	A	1684	1/1	0.94	0.39	44,44,44,44	0
24	MG	A	1761	1/1	0.94	0.12	53,53,53,53	0
24	MG	A	1705	1/1	0.94	0.78	39,39,39,39	0
24	MG	A	1644	1/1	0.94	0.18	54,54,54,54	0
24	MG	A	1770	1/1	0.94	0.65	52,52,52,52	0
24	MG	A	1647	1/1	0.95	0.46	39,39,39,39	0
24	MG	A	1768	1/1	0.95	0.33	44,44,44,44	0
24	MG	A	1624	1/1	0.95	0.46	82,82,82,82	0
24	MG	A	1775	1/1	0.95	0.56	82,82,82,82	0
24	MG	A	1760	1/1	0.95	0.23	49,49,49,49	0
24	MG	A	1720	1/1	0.96	0.21	46,46,46,46	0
24	MG	A	1758	1/1	0.96	0.29	40,40,40,40	0
24	MG	A	1727	1/1	0.96	0.17	58,58,58,58	0
24	MG	A	1715	1/1	0.96	0.26	50,50,50,50	0
24	MG	A	1730	1/1	0.96	0.47	66,66,66,66	0
24	MG	A	1662	1/1	0.96	0.14	43,43,43,43	0
24	MG	A	1769	1/1	0.97	0.33	40,40,40,40	0
24	MG	A	1711	1/1	0.97	0.33	36,36,36,36	0
24	MG	A	1634	1/1	0.97	0.63	57,57,57,57	0
24	MG	A	1658	1/1	0.97	0.39	49,49,49,49	0
24	MG	A	1763	1/1	0.97	0.26	65,65,65,65	0
24	MG	A	1611	1/1	0.97	0.44	42,42,42,42	0
24	MG	A	1661	1/1	0.97	0.63	37,37,37,37	0
24	MG	A	1757	1/1	0.97	0.39	47,47,47,47	0
24	MG	A	1653	1/1	0.97	0.50	38,38,38,38	0
24	MG	A	1743	1/1	0.97	0.32	40,40,40,40	0
24	MG	A	1648	1/1	0.98	0.39	40,40,40,40	0
24	MG	A	1710	1/1	0.98	0.19	54,54,54,54	0
24	MG	A	1649	1/1	0.98	0.47	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
24	MG	A	1668	1/1	0.98	0.82	40,40,40,40	0
24	MG	A	1726	1/1	0.98	0.35	51,51,51,51	0
24	MG	A	1723	1/1	0.98	0.60	62,62,62,62	0
24	MG	A	1659	1/1	0.98	0.58	38,38,38,38	0
26	ZN	D	301	1/1	1.00	0.41	64,64,64,64	0
26	ZN	N	102	1/1	1.00	0.21	73,73,73,73	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.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.