



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 09:07 pm BST

PDB ID : 4GKK
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 AUA-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 : 3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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

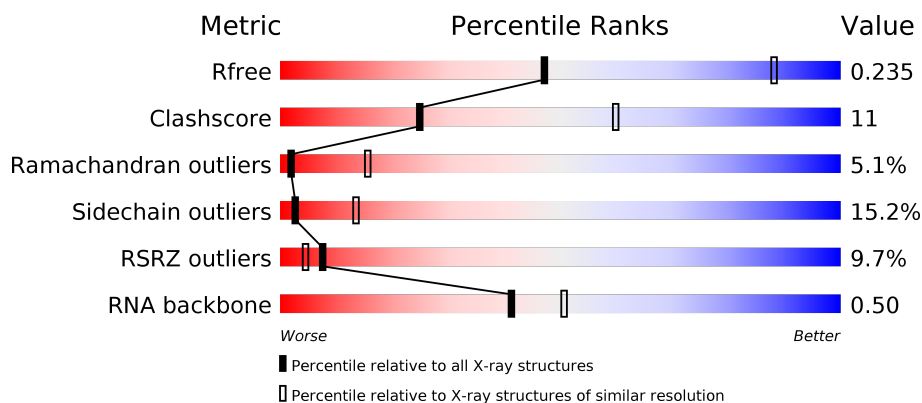
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



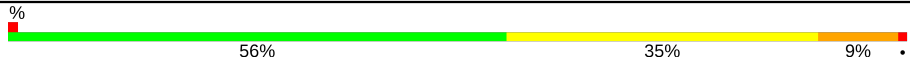




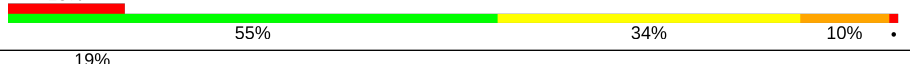
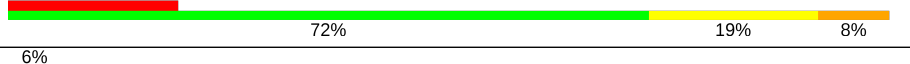

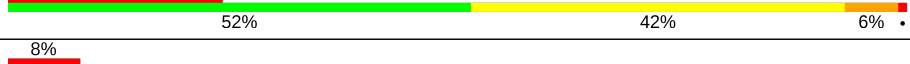








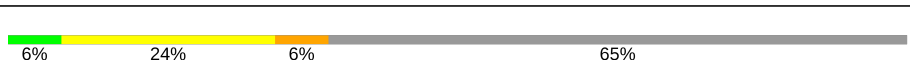

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)
RNA backbone	3102	1010 (3.50-2.90)

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 ≥ 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>4%</div> <div>52%</div> <div>33%</div> <div>11%</div> <div>.</div> </div>
2	B	234	<div> <div>13%</div> <div>50%</div> <div>40%</div> <div>8%</div> <div>.</div> </div>
3	C	206	<div> <div>10%</div> <div>54%</div> <div>39%</div> <div>6%</div> <div>.</div> </div>
4	D	208	<div> <div>22%</div> <div>57%</div> <div>32%</div> <div>11%</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
23	RSQ	X	34	-	-	X	-
24	MG	A	1605	-	-	-	X
24	MG	A	1607	-	-	-	X
24	MG	A	1609	-	-	-	X
24	MG	A	1614	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	MG	A	1615	-	-	-	X
24	MG	A	1622	-	-	-	X
24	MG	A	1626	-	-	-	X
24	MG	A	1628	-	-	-	X
24	MG	A	1633	-	-	-	X
24	MG	A	1639	-	-	-	X
24	MG	A	1640	-	-	-	X
24	MG	A	1652	-	-	-	X
24	MG	A	1666	-	-	-	X
24	MG	A	1668	-	-	-	X
24	MG	A	1671	-	-	-	X
24	MG	A	1673	-	-	-	X
24	MG	A	1677	-	-	-	X
24	MG	A	1690	-	-	-	X
24	MG	A	1697	-	-	-	X
24	MG	A	1699	-	-	-	X
24	MG	A	1701	-	-	-	X
24	MG	A	1702	-	-	-	X
24	MG	A	1705	-	-	-	X
24	MG	A	1713	-	-	-	X
24	MG	A	1716	-	-	-	X
24	MG	A	1721	-	-	-	X
24	MG	A	1722	-	-	-	X
24	MG	A	1724	-	-	-	X
24	MG	A	1742	-	-	-	X
24	MG	A	1747	-	-	-	X
24	MG	A	1755	-	-	-	X
24	MG	A	1756	-	-	-	X
24	MG	A	1759	-	-	-	X
24	MG	A	1764	-	-	-	X
24	MG	A	1768	-	-	-	X
24	MG	A	1777	-	-	-	X
24	MG	A	1778	-	-	-	X
24	MG	A	1784	-	-	-	X

2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 52188 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	-	EXPRESSION TAG	GB 48256
A	1013	G	-	EXPRESSION TAG	GB 48256
A	1225	C	-	EXPRESSION TAG	GB 48256
A	1226	A	-	EXPRESSION TAG	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	4	Total	C	N	O	P	0	0	0
			86	39	17	26	4			

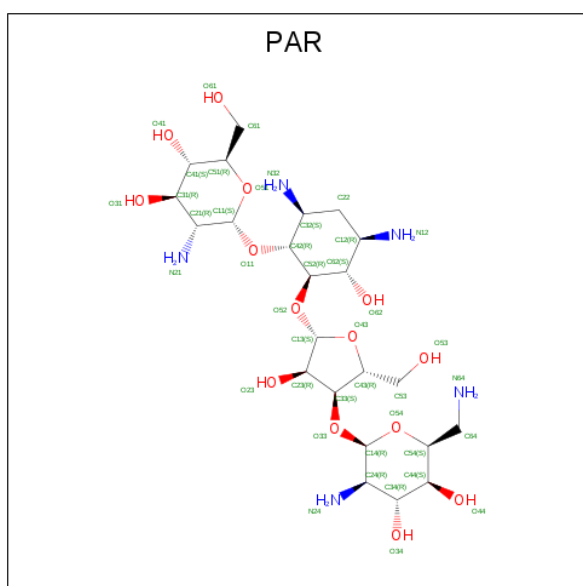
- Molecule 23 is a RNA chain called tRNA ASL human mitochondrial Met.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	X	6	Total	C	N	O	P	0	0	0
			126	57	21	42	6			

- 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	T	1	Total	Mg	0	0
			1	1		

- Molecule 25 is PAROMOMYCIN (three-letter code: PAR) (formula: C₂₃H₄₅N₅O₁₄).



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

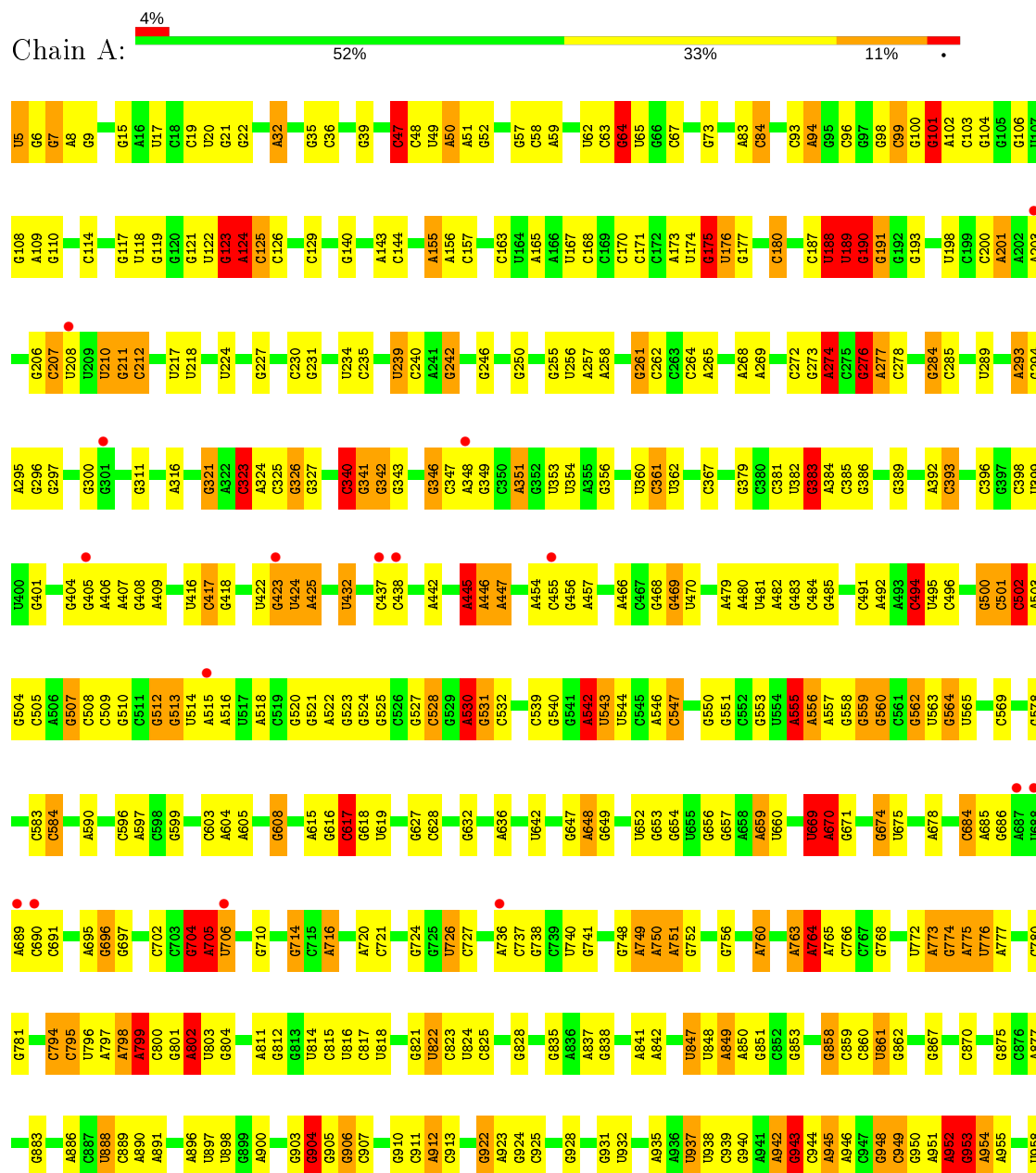
- Molecule 26 is ZINC ION (three-letter code: ZN) (formula: Zn).

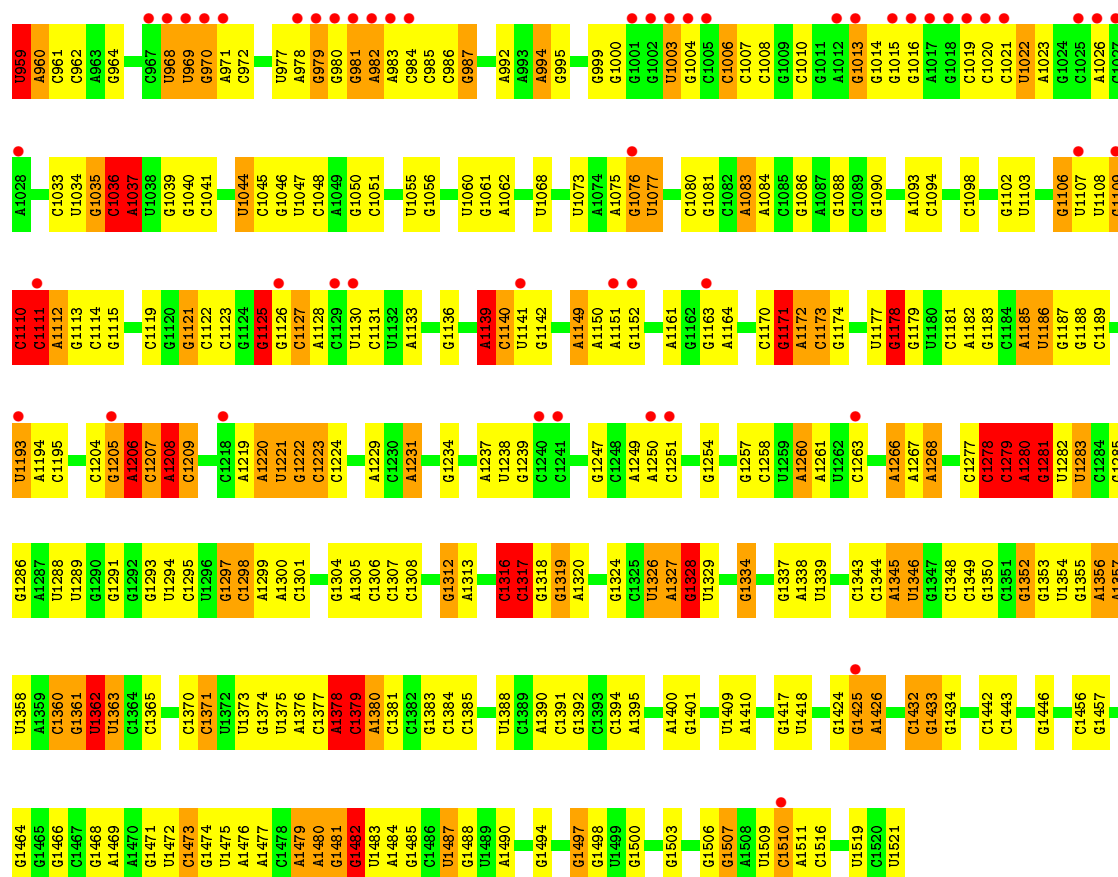
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
26	D	1	Total	Zn	0	0
			1	1		
26	N	1	Total	Zn	0	0
			1	1		

3 Residue-property plots

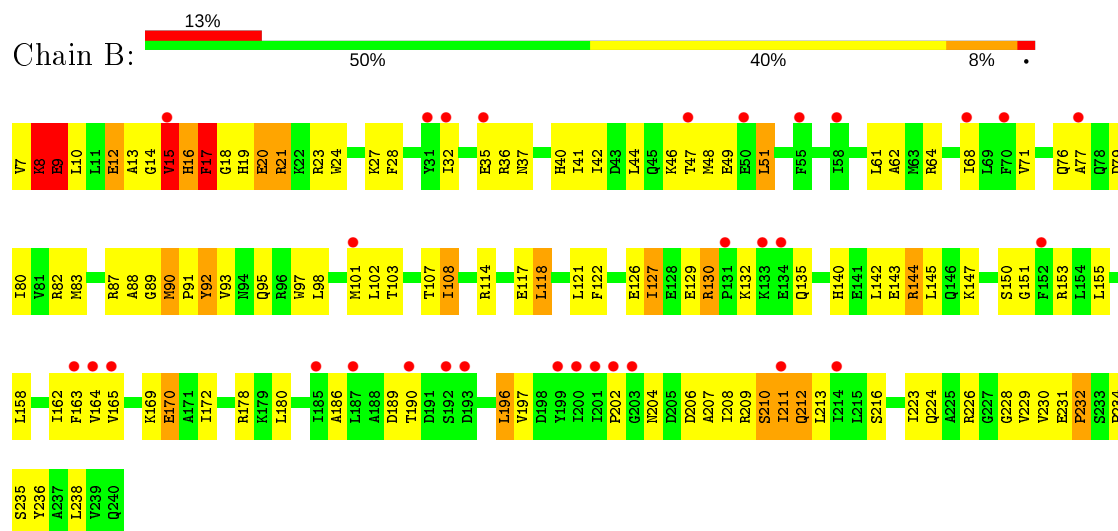
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

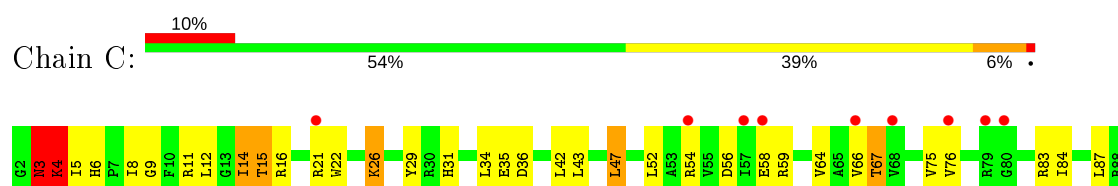


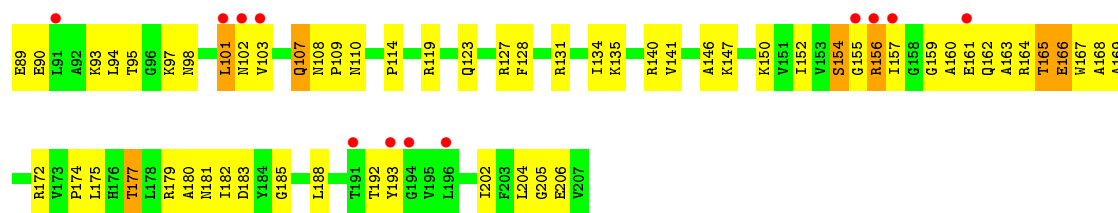


• Molecule 2: 30S ribosomal protein S2

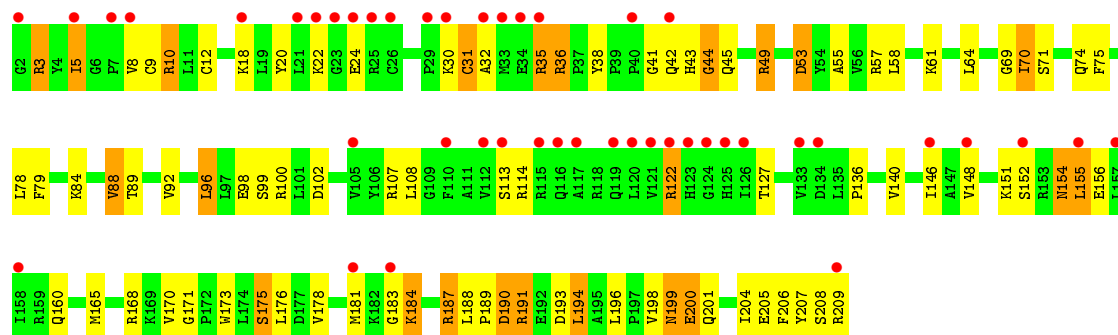


• Molecule 3: 30S ribosomal protein S3

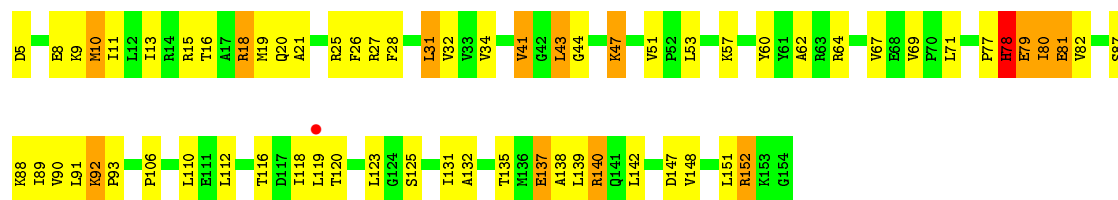




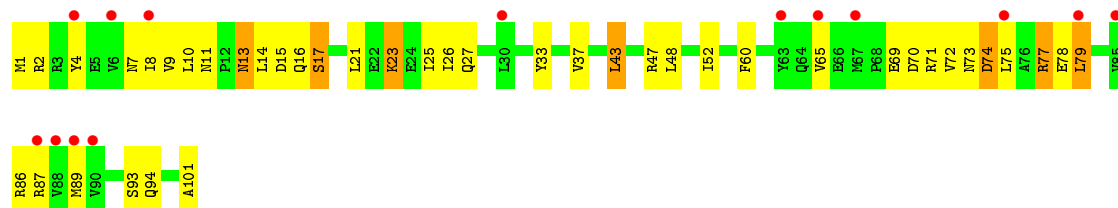
• Molecule 4: 30S ribosomal protein S4



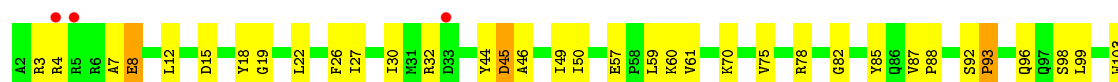
• Molecule 5: 30S ribosomal protein S5



• Molecule 6: 30S ribosomal protein S6

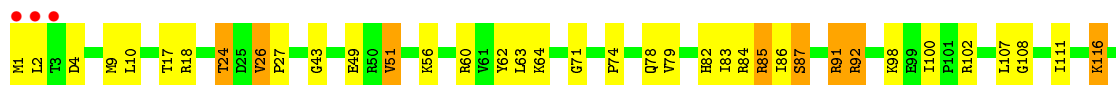


• Molecule 7: 30S ribosomal protein S7





• Molecule 8: 30S ribosomal protein S8



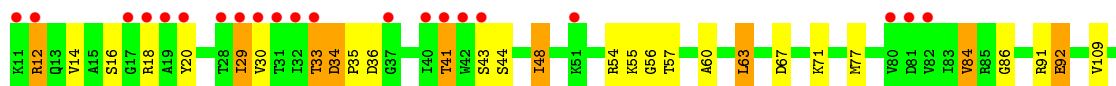
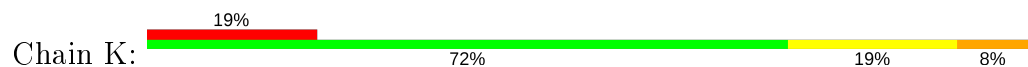
• Molecule 9: 30S ribosomal protein S9



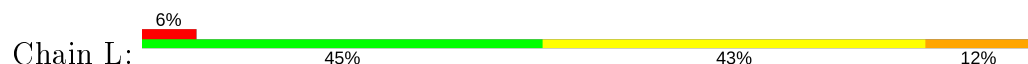
• Molecule 10: 30S ribosomal protein S10

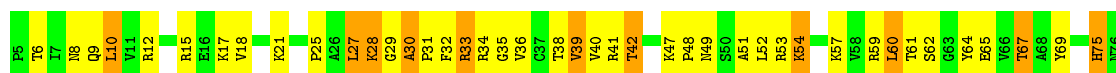


• Molecule 11: 30S ribosomal protein S11

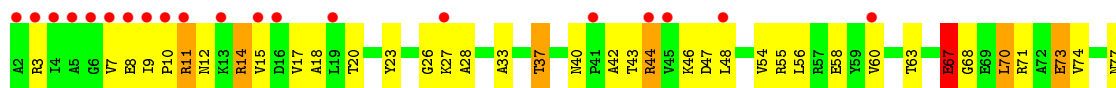


• Molecule 12: 30S ribosomal protein S12

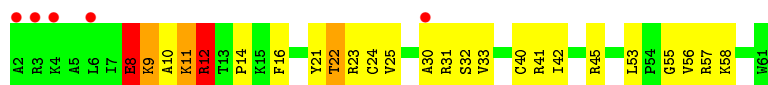




• Molecule 13: 30S ribosomal protein S13



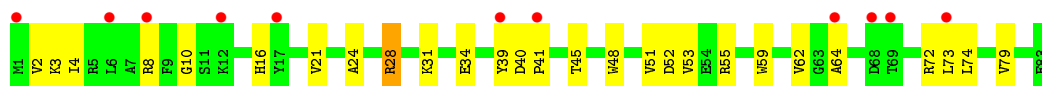
• Molecule 14: 30S ribosomal protein S14 type Z



• Molecule 15: 30S ribosomal protein S15

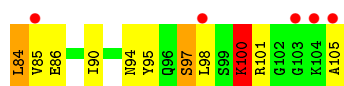


• Molecule 16: 30S ribosomal protein S16

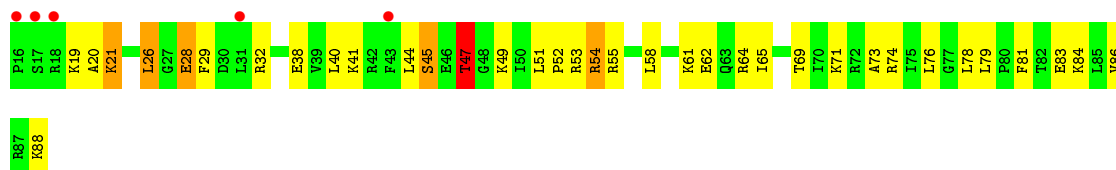


• Molecule 17: 30S ribosomal protein S17

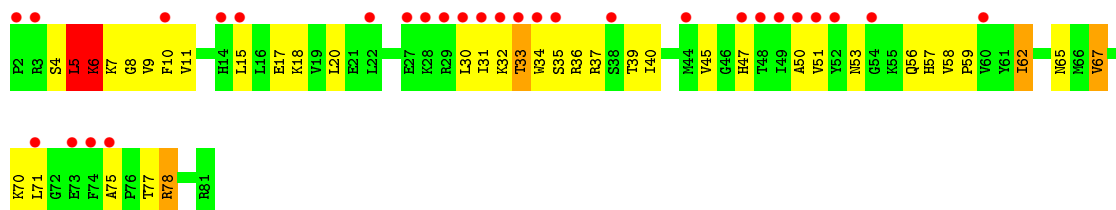




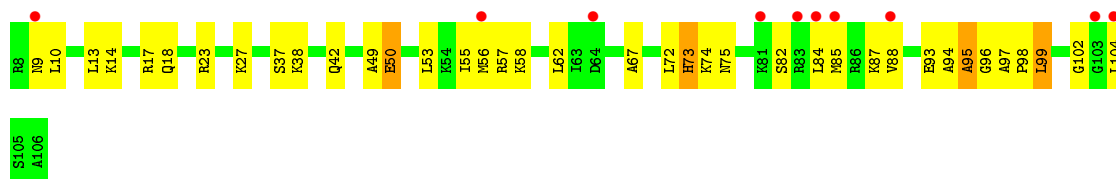
- Molecule 18: 30S ribosomal protein S18



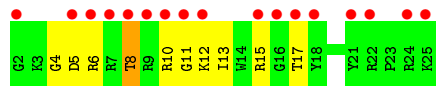
- Molecule 19: 30S ribosomal protein S19



- 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, α , β , γ	402.37Å 402.37Å 175.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	73.47 – 3.20 80.48 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.3 (73.47-3.20) 98.3 (80.48-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.8_1069	Depositor
R, R_{free}	0.195 , 0.236 0.194 , 0.235	Depositor DCC
R_{free} test set	11793 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	99.7	Xtriage
Anisotropy	0.128	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 58.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	52188	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.72% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.80	13/36395 (0.0%)	1.31	291/56801 (0.5%)
2	B	0.40	0/1935	0.61	0/2609
3	C	0.43	0/1636	0.63	0/2205
4	D	0.47	0/1733	0.65	1/2318 (0.0%)
5	E	0.58	0/1162	0.74	1/1564 (0.1%)
6	F	0.39	0/856	0.57	0/1154
7	G	0.42	0/1276	0.60	0/1709
8	H	0.62	0/1136	0.81	1/1527 (0.1%)
9	I	0.42	0/1029	0.62	0/1378
10	J	0.48	0/807	0.67	0/1085
11	K	0.48	0/900	0.65	0/1213
12	L	0.55	0/986	0.78	1/1320 (0.1%)
13	M	0.43	0/1008	0.64	0/1347
14	N	0.41	0/501	0.62	0/664
15	O	0.46	0/745	0.62	0/992
16	P	0.60	0/716	0.75	0/963
17	Q	0.58	0/870	0.81	2/1159 (0.2%)
18	R	0.47	0/603	0.65	0/799
19	S	0.35	0/661	0.63	0/890
20	T	0.54	0/764	0.74	0/1006
21	V	0.42	0/212	0.60	0/277
22	W	0.90	0/96	1.74	5/147 (3.4%)
23	X	0.98	0/115	1.61	4/176 (2.3%)
All	All	0.70	13/56142 (0.0%)	1.15	306/83303 (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
14	N	0	1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	5	U	OP3-P	-10.39	1.48	1.61
1	A	118	U	C4-O4	6.75	1.29	1.23
1	A	274	A	N9-C4	-6.73	1.33	1.37
1	A	261	G	N9-C4	-6.34	1.32	1.38
1	A	799	A	N9-C4	-6.04	1.34	1.37
1	A	1208	A	N9-C4	-5.88	1.34	1.37
1	A	1379	C	N1-C6	5.77	1.40	1.37
1	A	797	A	N7-C5	-5.42	1.36	1.39
1	A	1280	A	N3-C4	-5.22	1.31	1.34
1	A	578	G	N7-C5	-5.18	1.36	1.39
1	A	617	C	N3-C4	-5.12	1.30	1.33
1	A	1377	C	N1-C6	-5.08	1.34	1.37
1	A	794	C	N1-C6	-5.05	1.34	1.37

All (306) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1479	A	N1-C6-N6	10.56	124.94	118.60
1	A	674	G	N1-C6-O6	9.78	125.77	119.90
1	A	101	G	C5-N7-C8	-9.57	99.52	104.30
1	A	1479	A	C2-N3-C4	-9.44	105.88	110.60
1	A	1479	A	C5-N7-C8	-9.24	99.28	103.90
1	A	1479	A	C6-C5-N7	-9.14	125.90	132.30
1	A	1479	A	C4-C5-N7	9.12	115.26	110.70
1	A	804	G	O5'-P-OP1	-9.10	97.51	105.70
1	A	542	A	P-O3'-C3'	9.02	130.53	119.70
1	A	101	G	C4-C5-N7	8.97	114.39	110.80
1	A	261	G	N3-C4-C5	8.71	132.95	128.60
1	A	569	C	C6-N1-C2	8.60	123.74	120.30
1	A	274	A	C5-N7-C8	-8.54	99.63	103.90
1	A	274	A	N1-C6-N6	8.44	123.66	118.60
1	A	1036	C	N3-C2-O2	-8.44	115.99	121.90
1	A	326	G	N1-C6-O6	8.29	124.88	119.90
1	A	795	C	N3-C2-O2	-8.25	116.12	121.90
1	A	118	U	N3-C4-C5	-8.24	109.66	114.60
1	A	1036	C	C4-C5-C6	8.06	121.43	117.40
1	A	1379	C	C5-C6-N1	8.03	125.02	121.00
1	A	1432	C	P-O3'-C3'	7.97	129.26	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	766	C	C6-N1-C2	7.90	123.46	120.30
1	A	323	C	N3-C2-O2	-7.85	116.40	121.90
1	A	323	C	C6-N1-C2	-7.81	117.17	120.30
1	A	189	U	P-O3'-C3'	7.81	129.07	119.70
1	A	7	G	N9-C4-C5	-7.69	102.32	105.40
1	A	274	A	C2-N3-C4	-7.63	106.78	110.60
1	A	1125	G	C8-N9-C4	-7.62	103.35	106.40
1	A	101	G	N7-C8-N9	7.62	116.91	113.10
1	A	1317	C	P-O3'-C3'	7.56	128.78	119.70
1	A	1326	U	P-O3'-C3'	7.45	128.65	119.70
1	A	861	U	P-O3'-C3'	7.44	128.63	119.70
1	A	799	A	C2-N3-C4	-7.35	106.92	110.60
1	A	1179	G	O5'-P-OP1	-7.33	99.10	105.70
1	A	1487	U	C5-C6-N1	-7.33	119.03	122.70
1	A	1281	G	P-O3'-C3'	7.33	128.50	119.70
1	A	117	G	C5-C6-N1	-7.31	107.85	111.50
1	A	858	G	C8-N9-C4	7.31	109.32	106.40
1	A	175	G	N3-C4-C5	-7.30	124.95	128.60
1	A	274	A	C4-C5-N7	7.27	114.33	110.70
1	A	118	U	C5-C4-O4	7.25	130.25	125.90
1	A	1056	G	C5-C6-N1	-7.24	107.88	111.50
1	A	180	C	C6-N1-C2	7.20	123.18	120.30
1	A	123	G	P-O3'-C3'	7.18	128.32	119.70
1	A	1076	G	OP2-P-O3'	7.18	121.00	105.20
1	A	674	G	C6-C5-N7	-7.16	126.10	130.40
1	A	445	A	C8-N9-C4	-7.14	102.94	105.80
1	A	64	G	C8-N9-C1'	-7.11	117.76	127.00
23	X	39	C	C6-N1-C2	-7.06	117.48	120.30
1	A	1479	A	N7-C8-N9	7.06	117.33	113.80
1	A	530	A	P-O3'-C3'	7.03	128.13	119.70
1	A	323	C	P-O3'-C3'	6.99	128.09	119.70
1	A	1111	C	OP2-P-O3'	6.99	120.57	105.20
1	A	539	C	C5-C6-N1	-6.99	117.51	121.00
1	A	361	C	N1-C2-O2	6.97	123.08	118.90
1	A	1497	G	O5'-P-OP2	-6.96	99.43	105.70
1	A	392	A	C8-N9-C4	-6.94	103.03	105.80
1	A	101	G	N1-C6-O6	6.93	124.06	119.90
1	A	1036	C	C5-C6-N1	-6.91	117.55	121.00
1	A	1171	G	P-O3'-C3'	6.89	127.97	119.70
1	A	389	G	C5-C6-O6	6.81	132.69	128.60
1	A	323	C	C2-N1-C1'	6.81	126.29	118.80
1	A	129	C	N1-C2-O2	-6.80	114.82	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1328	G	P-O3'-C3'	6.78	127.84	119.70
1	A	50	A	P-O3'-C3'	6.78	127.84	119.70
1	A	188	U	P-O3'-C3'	6.75	127.80	119.70
1	A	795	C	N1-C2-O2	6.75	122.95	118.90
1	A	261	G	N3-C4-N9	-6.72	121.97	126.00
1	A	274	A	O4'-C1'-N9	-6.68	102.86	108.20
1	A	47	C	C2-N1-C1'	-6.66	111.47	118.80
1	A	530	A	N1-C6-N6	-6.66	114.61	118.60
1	A	766	C	N3-C4-C5	6.65	124.56	121.90
1	A	1035	G	P-O3'-C3'	6.65	127.68	119.70
1	A	1475	U	N1-C2-N3	6.64	118.89	114.90
1	A	670	A	P-O3'-C3'	6.64	127.67	119.70
1	A	7	G	N1-C6-O6	6.62	123.87	119.90
1	A	802	A	N1-C2-N3	6.60	132.60	129.30
1	A	5	U	P-O3'-C3'	6.60	127.62	119.70
1	A	124	A	N1-C6-N6	6.60	122.56	118.60
1	A	562	G	N1-C6-O6	6.56	123.84	119.90
1	A	64	G	C4-N9-C1'	6.55	135.02	126.50
1	A	1036	C	N1-C2-O2	6.55	122.83	118.90
1	A	897	U	C5-C4-O4	6.52	129.81	125.90
1	A	32	A	C8-N9-C4	-6.51	103.20	105.80
1	A	1278	C	P-O3'-C3'	6.50	127.51	119.70
1	A	1125	G	N7-C8-N9	6.50	116.35	113.10
1	A	795	C	C2-N1-C1'	6.47	125.91	118.80
1	A	383	G	P-O3'-C3'	6.46	127.46	119.70
1	A	795	C	P-O3'-C3'	6.46	127.46	119.70
1	A	1477	A	O5'-P-OP2	-6.45	99.90	105.70
1	A	99	C	OP2-P-O3'	6.40	119.27	105.20
8	H	119	LEU	CA-CB-CG	6.38	129.98	115.30
22	W	3	A	C5-N7-C8	-6.38	100.71	103.90
1	A	1479	A	N9-C4-C5	-6.35	103.26	105.80
1	A	539	C	C6-N1-C2	6.33	122.83	120.30
1	A	1173	C	C6-N1-C2	-6.32	117.77	120.30
1	A	7	G	C8-N9-C4	6.30	108.92	106.40
1	A	798	A	OP2-P-O3'	6.29	119.04	105.20
1	A	101	G	O4'-C1'-N9	6.29	113.23	108.20
1	A	351	A	O5'-P-OP2	-6.28	100.05	105.70
1	A	704	G	P-O3'-C3'	6.27	127.23	119.70
1	A	47	C	C6-N1-C2	6.27	122.81	120.30
1	A	512	G	N1-C6-O6	6.25	123.65	119.90
1	A	323	C	N1-C2-O2	6.22	122.63	118.90
1	A	326	G	C6-C5-N7	-6.22	126.67	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	261	G	C5-N7-C8	-6.21	101.19	104.30
1	A	546	A	N1-C6-N6	-6.21	114.88	118.60
23	X	39	C	C5-C6-N1	6.20	124.10	121.00
1	A	578	G	C6-C5-N7	-6.17	126.70	130.40
1	A	239	U	P-O3'-C3'	6.15	127.08	119.70
1	A	716	A	O4'-C1'-N9	6.14	113.12	108.20
1	A	669	U	P-O3'-C3'	6.14	127.07	119.70
1	A	1507	G	N3-C4-C5	6.12	131.66	128.60
1	A	1479	A	N1-C2-N3	6.10	132.35	129.30
1	A	1481	G	P-O3'-C3'	6.08	127.00	119.70
1	A	276	G	P-O3'-C3'	6.07	126.99	119.70
1	A	750	A	N1-C6-N6	-6.07	114.96	118.60
1	A	706	U	C2-N1-C1'	6.07	124.98	117.70
1	A	1280	A	C8-N9-C4	-6.05	103.38	105.80
1	A	494	C	P-O3'-C3'	6.05	126.96	119.70
1	A	569	C	N3-C4-C5	6.05	124.32	121.90
1	A	674	G	C5-C6-O6	-6.03	124.98	128.60
1	A	1179	G	O5'-P-OP2	6.01	117.92	110.70
1	A	1476	A	O5'-P-OP1	-6.01	100.29	105.70
1	A	250	G	N1-C6-O6	6.00	123.50	119.90
1	A	500	G	P-O3'-C3'	6.00	126.91	119.70
1	A	1482	G	OP1-P-OP2	-6.00	110.61	119.60
1	A	1208	A	C5-N7-C8	-5.99	100.90	103.90
1	A	1223	C	C6-N1-C2	5.98	122.69	120.30
22	W	3	A	C4-C5-N7	5.97	113.69	110.70
1	A	445	A	P-O3'-C3'	5.97	126.86	119.70
1	A	117	G	C4-C5-C6	5.97	122.38	118.80
1	A	760	A	N1-C6-N6	5.96	122.17	118.60
1	A	469	G	P-O3'-C3'	5.95	126.84	119.70
1	A	1388	U	N1-C2-N3	5.95	118.47	114.90
1	A	175	G	C4-N9-C1'	5.93	134.22	126.50
1	A	224	U	C5-C6-N1	-5.93	119.74	122.70
1	A	618	G	O5'-P-OP1	-5.93	100.36	105.70
1	A	1378	A	P-O3'-C3'	5.93	126.81	119.70
1	A	7	G	C4-C5-N7	5.92	113.17	110.80
1	A	550	G	OP1-P-OP2	5.91	128.46	119.60
1	A	847	U	P-O3'-C3'	5.90	126.78	119.70
1	A	802	A	C2-N3-C4	-5.90	107.65	110.60
1	A	1379	C	C2-N3-C4	5.89	122.85	119.90
1	A	1500	G	N3-C2-N2	-5.89	115.78	119.90
4	D	12	CYS	CA-CB-SG	5.88	124.58	114.00
22	W	3	A	N7-C8-N9	5.88	116.74	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	274	A	C6-C5-N7	-5.88	128.19	132.30
1	A	417	C	P-O3'-C3'	5.87	126.74	119.70
1	A	748	G	C8-N9-C4	5.87	108.75	106.40
1	A	875	G	O5'-P-OP2	-5.84	100.44	105.70
1	A	250	G	C5-C6-O6	-5.84	125.10	128.60
1	A	1507	G	N1-C6-O6	5.82	123.39	119.90
1	A	64	G	P-O3'-C3'	5.79	126.65	119.70
1	A	1208	A	C2-N3-C4	-5.74	107.73	110.60
1	A	774	G	C6-C5-N7	-5.73	126.96	130.40
1	A	1037	A	O5'-P-OP1	-5.72	100.55	105.70
1	A	1174	G	N1-C6-O6	5.72	123.33	119.90
1	A	1061	G	C8-N9-C1'	-5.71	119.57	127.00
1	A	124	A	N9-C4-C5	-5.71	103.52	105.80
1	A	101	G	C5-C6-O6	-5.71	125.18	128.60
1	A	1379	C	OP2-P-O3'	5.70	117.74	105.20
1	A	1044	U	N3-C2-O2	-5.69	118.21	122.20
1	A	175	G	N3-C4-N9	5.69	129.41	126.00
1	A	798	A	P-O3'-C3'	5.69	126.53	119.70
1	A	190	G	P-O3'-C3'	5.68	126.52	119.70
1	A	540	G	O5'-P-OP1	5.68	117.52	110.70
1	A	250	G	C6-C5-N7	-5.68	126.99	130.40
1	A	1056	G	N1-C6-O6	5.68	123.31	119.90
1	A	106	G	O5'-P-OP1	5.67	117.50	110.70
1	A	261	G	C2-N3-C4	-5.66	109.07	111.90
1	A	804	G	O5'-P-OP2	5.66	117.49	110.70
1	A	726	U	C6-N1-C2	5.65	124.39	121.00
1	A	958	U	N3-C4-O4	5.64	123.35	119.40
1	A	883	G	C4-C5-N7	5.64	113.06	110.80
12	L	10	LEU	CA-CB-CG	-5.63	102.35	115.30
1	A	445	A	N7-C8-N9	5.63	116.61	113.80
1	A	1357	A	C8-N9-C4	-5.62	103.55	105.80
1	A	1111	C	P-O3'-C3'	5.61	126.43	119.70
1	A	560	G	C8-N9-C4	5.61	108.64	106.40
1	A	751	A	N1-C2-N3	5.61	132.10	129.30
1	A	584	C	N1-C2-O2	5.60	122.26	118.90
1	A	649	G	C5-C6-O6	-5.59	125.24	128.60
1	A	276	G	C4-N9-C1'	5.55	133.71	126.50
1	A	1424	G	C4-N9-C1'	5.55	133.71	126.50
1	A	1476	A	O5'-P-OP2	5.55	117.36	110.70
1	A	101	G	C6-C5-N7	-5.53	127.08	130.40
1	A	1370	C	C6-N1-C2	5.51	122.50	120.30
1	A	293	A	N1-C2-N3	5.51	132.06	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	231	G	N1-C6-O6	5.51	123.20	119.90
1	A	1076	G	P-O3'-C3'	5.49	126.29	119.70
1	A	1178	G	O5'-P-OP2	-5.49	100.76	105.70
1	A	323	C	N3-C4-N4	-5.49	114.16	118.00
1	A	705	A	O5'-P-OP1	-5.48	100.77	105.70
1	A	206	G	N1-C6-O6	5.47	123.18	119.90
1	A	669	U	OP1-P-O3'	5.46	117.22	105.20
1	A	1279	C	P-O3'-C3'	5.46	126.25	119.70
1	A	1328	G	OP2-P-O3'	5.46	117.20	105.20
1	A	1056	G	C4-C5-C6	5.46	122.07	118.80
1	A	550	G	C2-N3-C4	-5.45	109.17	111.90
1	A	1485	G	O5'-P-OP2	-5.45	100.80	105.70
1	A	1379	C	N3-C4-N4	5.44	121.81	118.00
1	A	922	G	C4-C5-N7	5.43	112.97	110.80
1	A	952	A	C5-N7-C8	-5.43	101.19	103.90
1	A	1060	U	O5'-P-OP1	-5.43	100.81	105.70
1	A	953	G	O5'-P-OP1	-5.42	100.82	105.70
1	A	684	C	P-O3'-C3'	5.42	126.20	119.70
1	A	1280	A	N7-C8-N9	5.41	116.51	113.80
1	A	799	A	N3-C4-C5	5.40	130.58	126.80
1	A	551	G	C8-N9-C4	-5.40	104.24	106.40
1	A	1050	G	C4-C5-N7	5.39	112.96	110.80
1	A	659	A	C8-N9-C4	5.39	107.96	105.80
1	A	502	C	N1-C2-O2	5.39	122.13	118.90
1	A	389	G	C4-C5-N7	-5.38	108.65	110.80
1	A	1206	A	P-O3'-C3'	5.35	126.12	119.70
1	A	124	A	C5-C6-N6	-5.35	119.42	123.70
1	A	898	U	C5-C6-N1	-5.35	120.03	122.70
1	A	1498	G	N1-C2-N3	5.33	127.10	123.90
1	A	500	G	C4-N9-C1'	5.32	133.42	126.50
1	A	922	G	C6-C5-N7	-5.32	127.21	130.40
17	Q	53	LEU	CA-CB-CG	5.31	127.51	115.30
1	A	943	G	C8-N9-C4	5.30	108.52	106.40
1	A	300	G	N1-C6-O6	5.30	123.08	119.90
1	A	340	C	P-O3'-C3'	5.30	126.06	119.70
1	A	1356	A	C8-N9-C4	-5.30	103.68	105.80
1	A	1125	G	N3-C4-C5	-5.29	125.95	128.60
5	E	41	VAL	CB-CA-C	-5.29	101.35	111.40
1	A	540	G	N3-C4-C5	-5.28	125.96	128.60
1	A	736	A	C6-N1-C2	-5.28	115.43	118.60
1	A	1139	A	P-O3'-C3'	5.28	126.04	119.70
1	A	361	C	C6-N1-C1'	-5.28	114.47	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1208	A	N3-C4-C5	5.28	130.49	126.80
1	A	766	C	C5-C6-N1	-5.28	118.36	121.00
1	A	555	A	C5-C6-N1	5.27	120.34	117.70
1	A	704	G	C8-N9-C4	-5.27	104.29	106.40
22	W	3	A	C5-C6-N6	-5.26	119.49	123.70
1	A	1498	G	N3-C4-N9	5.25	129.15	126.00
1	A	710	G	N9-C4-C5	-5.25	103.30	105.40
1	A	1316	C	C2-N1-C1'	5.25	124.57	118.80
1	A	1473	C	N1-C2-O2	-5.25	115.75	118.90
1	A	500	G	N3-C4-C5	-5.25	125.98	128.60
1	A	888	U	C5-C4-O4	5.24	129.04	125.90
1	A	904	G	N3-C4-C5	5.23	131.22	128.60
1	A	706	U	N1-C2-O2	5.22	126.45	122.80
1	A	360	U	N3-C4-O4	5.21	123.05	119.40
22	W	3	A	N1-C6-N6	5.21	121.72	118.60
1	A	1061	G	C6-C5-N7	-5.19	127.29	130.40
1	A	959	U	P-O3'-C3'	5.19	125.92	119.70
1	A	608	G	C8-N9-C4	5.18	108.47	106.40
1	A	326	G	C5-C6-N1	-5.17	108.91	111.50
1	A	648	A	N1-C6-N6	-5.17	115.50	118.60
1	A	392	A	N7-C8-N9	5.17	116.38	113.80
1	A	84	C	C5-C6-N1	5.17	123.58	121.00
1	A	560	G	C5-C6-O6	-5.17	125.50	128.60
1	A	922	G	N1-C6-O6	5.17	123.00	119.90
1	A	764	A	C8-N9-C4	5.16	107.86	105.80
1	A	774	G	C4-C5-C6	5.16	121.90	118.80
1	A	1479	A	C5-C6-N6	-5.16	119.57	123.70
1	A	52	G	N1-C6-O6	-5.16	116.81	119.90
1	A	1046	G	N3-C2-N2	-5.15	116.29	119.90
1	A	361	C	C2-N1-C1'	5.15	124.46	118.80
1	A	321	G	C5-C6-N1	-5.14	108.93	111.50
23	X	36	U	N3-C2-O2	-5.14	118.60	122.20
1	A	542	A	C8-N9-C4	-5.14	103.75	105.80
1	A	360	U	C5-C4-O4	-5.13	122.82	125.90
1	A	261	G	C4-C5-N7	5.12	112.85	110.80
1	A	737	C	C2-N1-C1'	5.12	124.43	118.80
1	A	231	G	C5-C6-N1	-5.12	108.94	111.50
1	A	509	C	C6-N1-C2	5.12	122.35	120.30
1	A	542	A	N9-C4-C5	5.12	107.85	105.80
1	A	277	A	OP1-P-OP2	-5.11	111.93	119.60
1	A	1263	C	C6-N1-C2	-5.11	118.26	120.30
1	A	578	G	N3-C4-N9	5.11	129.06	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	802	A	OP2-P-O3'	5.11	116.43	105.20
1	A	1312	G	N1-C6-O6	-5.11	116.84	119.90
1	A	1482	G	N3-C4-N9	-5.10	122.94	126.00
1	A	175	G	C8-N9-C4	-5.10	104.36	106.40
1	A	1181	C	N1-C2-O2	5.10	121.96	118.90
1	A	922	G	C5-C6-O6	-5.10	125.54	128.60
1	A	751	A	N1-C6-N6	5.10	121.66	118.60
1	A	250	G	C8-N9-C1'	-5.09	120.38	127.00
1	A	118	U	C2-N3-C4	5.09	130.06	127.00
1	A	140	G	N1-C6-O6	5.08	122.95	119.90
1	A	802	A	O5'-P-OP2	5.07	116.78	110.70
1	A	584	C	N3-C2-O2	-5.06	118.36	121.90
1	A	750	A	C6-N1-C2	-5.06	115.56	118.60
1	A	1371	C	C6-N1-C2	5.06	122.33	120.30
1	A	1446	G	C5-C6-O6	-5.06	125.57	128.60
1	A	1220	A	P-O3'-C3'	5.05	125.76	119.70
1	A	393	C	C6-N1-C2	5.05	122.32	120.30
1	A	704	G	C4-N9-C1'	5.05	133.06	126.50
1	A	1392	G	C8-N9-C4	5.04	108.42	106.40
1	A	559	G	N1-C6-O6	5.04	122.92	119.90
1	A	289	U	C6-N1-C2	5.04	124.02	121.00
1	A	276	G	C8-N9-C1'	-5.04	120.45	127.00
1	A	1110	C	P-O3'-C3'	5.04	125.74	119.70
1	A	1362	U	P-O3'-C3'	5.02	125.73	119.70
23	X	36	U	C2-N1-C1'	5.02	123.72	117.70
1	A	360	U	O4'-C1'-N1	5.02	112.22	108.20
1	A	1377	C	O5'-P-OP2	-5.02	101.19	105.70
1	A	278	C	C5-C6-N1	5.02	123.51	121.00
1	A	381	C	N3-C4-C5	5.01	123.91	121.90
1	A	952	A	C2-N3-C4	-5.01	108.09	110.60
1	A	1280	A	C6-C5-N7	-5.01	128.79	132.30
1	A	797	A	OP1-P-O3'	5.01	116.22	105.20
17	Q	25	ARG	NE-CZ-NH1	5.00	122.80	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
14	N	8	GLU	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32515	0	16411	383	0
2	B	1900	0	1951	77	0
3	C	1612	0	1677	63	0
4	D	1703	0	1764	58	0
5	E	1146	0	1207	42	0
6	F	843	0	857	24	0
7	G	1257	0	1296	35	0
8	H	1116	0	1177	29	0
9	I	1011	0	1043	41	0
10	J	794	0	840	34	0
11	K	885	0	904	22	0
12	L	970	0	1057	44	0
13	M	997	0	1072	34	0
14	N	492	0	529	17	0
15	O	734	0	771	25	0
16	P	700	0	720	11	0
17	Q	857	0	930	39	0
18	R	597	0	668	26	0
19	S	647	0	673	20	0
20	T	762	0	859	16	0
21	V	208	0	221	9	0
22	W	86	0	44	6	0
23	X	126	0	66	8	0
24	A	184	0	0	0	0
24	B	1	0	0	0	0
24	T	1	0	0	0	0
25	A	42	0	45	2	0
26	D	1	0	0	0	0
26	N	1	0	0	0	0
All	All	52188	0	36782	938	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 11.

All (938) 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)
2:B:18:GLY:HA2	2:B:42:ILE:HG12	1.51	0.93
1:A:1479:A:H2	1:A:1482:G:H1	1.14	0.92
1:A:1279:C:OP2	7:G:114:ARG:NH2	2.02	0.92
2:B:12:GLU:HG3	2:B:213:LEU:HD11	1.53	0.88
1:A:647:G:H22	1:A:724:G:H1	1.17	0.88
8:H:24:THR:HG22	8:H:63:LEU:HD21	1.56	0.87
7:G:117:ALA:H	7:G:120:ILE:HD13	1.40	0.85
1:A:1267:A:H2'	1:A:1268:A:H4'	1.59	0.85
12:L:27:LEU:O	12:L:29:GLY:N	2.09	0.84
1:A:1231:A:H4'	9:I:68:GLY:H	1.42	0.83
3:C:36:ASP:OD2	3:C:59:ARG:NH2	2.11	0.83
1:A:432:U:H5'	4:D:155:LEU:HD21	1.61	0.82
1:A:422:U:OP2	4:D:36:ARG:NH2	2.13	0.82
1:A:1171:G:O2'	3:C:3:ASN:HB3	1.79	0.82
3:C:21:ARG:HH22	10:J:93:GLY:H	1.28	0.81
1:A:801:G:O2'	1:A:802:A:H5''	1.81	0.81
1:A:1068:U:H3	1:A:1081:G:H22	1.30	0.80
5:E:106:PRO:HB3	5:E:135:THR:HG21	1.62	0.80
12:L:36:VAL:HG12	12:L:82:VAL:HG23	1.64	0.79
10:J:24:VAL:HG22	10:J:34:VAL:HG11	1.65	0.79
12:L:33:ARG:HD3	12:L:62:SER:HB2	1.65	0.79
1:A:952:A:H4'	1:A:953:G:H5''	1.65	0.78
17:Q:53:LEU:HD13	17:Q:85:VAL:HG11	1.64	0.78
3:C:154:SER:OG	3:C:155:GLY:N	2.16	0.77
19:S:53:ASN:HB2	19:S:56:GLN:H	1.51	0.76
3:C:14:ILE:O	3:C:16:ARG:N	2.19	0.76
4:D:191:ARG:NH1	4:D:200:GLU:OE2	2.17	0.75
1:A:1055:U:OP2	5:E:57:LYS:NZ	2.21	0.74
1:A:1170:C:OP1	10:J:51:ARG:NH2	2.20	0.74
11:K:57:THR:HG23	11:K:60:ALA:H	1.53	0.74
1:A:1417:G:H2'	1:A:1418:U:C6	2.24	0.73
1:A:952:A:H8	1:A:952:A:H5'	1.52	0.73
2:B:132:LYS:HA	2:B:135:GLN:HB2	1.70	0.73
17:Q:6:LEU:HB3	17:Q:23:VAL:HG11	1.71	0.73
13:M:10:PRO:HB2	13:M:18:ALA:HB1	1.70	0.72
5:E:92:LYS:HB3	5:E:119:LEU:HB2	1.70	0.71
19:S:50:ALA:HB1	19:S:57:HIS:HB3	1.71	0.71
1:A:1374:G:H21	1:A:1479:A:H8	1.39	0.71
8:H:4:ASP:OD2	8:H:85:ARG:NH1	2.23	0.71
1:A:818:U:OP1	18:R:64:ARG:NH2	2.24	0.71
2:B:71:VAL:HB	2:B:164:VAL:HG12	1.73	0.71
18:R:32:ARG:HA	18:R:69:THR:HG21	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:154:ASN:OD1	4:D:154:ASN:N	2.23	0.71
12:L:86:ARG:NH1	12:L:87:GLY:O	2.22	0.71
1:A:653:G:H21	6:F:73:ASN:HD21	1.40	0.70
9:I:100:GLY:O	9:I:102:LEU:N	2.23	0.70
5:E:80:ILE:HD13	5:E:138:ALA:HB1	1.74	0.70
2:B:80:ILE:HD12	2:B:80:ILE:H	1.57	0.69
9:I:8:GLY:HA2	9:I:79:LEU:HD13	1.72	0.69
13:M:107:ALA:HB3	13:M:111:LYS:HD2	1.75	0.69
15:O:74:ASP:HB3	15:O:77:ARG:HB3	1.74	0.69
2:B:88:ALA:HA	2:B:226:ARG:HH22	1.58	0.69
1:A:1115:G:N2	1:A:1123:C:O2	2.24	0.68
1:A:942:A:O2'	1:A:943:G:OP2	2.11	0.68
18:R:38:GLU:HA	18:R:41:LYS:HE2	1.76	0.68
5:E:137:GLU:OE2	5:E:140:ARG:NH1	2.27	0.68
1:A:1133:A:H5''	10:J:42:THR:HG23	1.76	0.67
15:O:39:LEU:HD13	15:O:56:LEU:HB2	1.75	0.67
4:D:175:SER:HB3	4:D:184:LYS:HB3	1.77	0.66
8:H:86:ILE:HG21	8:H:133:LEU:HD23	1.77	0.66
2:B:77:ALA:HB2	2:B:211:ILE:HD13	1.76	0.66
17:Q:24:GLU:HG3	17:Q:39:SER:HB3	1.78	0.66
18:R:88:LYS:NZ	18:R:88:LYS:OXT	2.26	0.66
16:P:74:LEU:HD22	16:P:79:VAL:HG21	1.77	0.66
17:Q:100:LYS:HG2	17:Q:101:ARG:HE	1.59	0.66
2:B:18:GLY:HA3	2:B:41:ILE:HA	1.78	0.66
2:B:158:LEU:H	2:B:158:LEU:HD12	1.61	0.65
13:M:11:ARG:HD3	13:M:12:ASN:HB2	1.77	0.65
2:B:89:GLY:H	2:B:226:ARG:HH12	1.44	0.65
4:D:36:ARG:HG3	4:D:38:TYR:CZ	2.30	0.65
7:G:70:LYS:HD3	7:G:96:GLN:HB3	1.78	0.65
15:O:4:THR:OG1	15:O:7:GLU:OE2	2.12	0.65
1:A:180:C:O3'	20:T:82:SER:HB3	1.96	0.65
15:O:4:THR:N	15:O:7:GLU:OE1	2.30	0.65
7:G:15:ASP:OD1	7:G:44:TYR:OH	2.15	0.65
1:A:1390:A:N1	25:A:1785:PAR:O61	2.30	0.64
15:O:38:ARG:HB3	15:O:38:ARG:HH11	1.61	0.64
4:D:199:ASN:O	4:D:201:GLN:N	2.29	0.64
1:A:583:C:H2'	1:A:584:C:H6	1.62	0.64
1:A:660:U:H3	1:A:696:G:H22	1.45	0.64
2:B:20:GLU:OE1	2:B:21:ARG:NH2	2.29	0.64
9:I:9:ARG:HG3	9:I:14:VAL:HG13	1.78	0.64
2:B:7:VAL:O	2:B:8:LYS:NZ	2.19	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:16:ARG:NH1	3:C:183:ASP:OD2	2.31	0.64
1:A:1062:A:O3'	5:E:16:THR:OG1	2.15	0.64
13:M:26:GLY:O	13:M:28:ALA:N	2.31	0.64
1:A:294:G:H2'	1:A:295:A:C8	2.33	0.64
1:A:1209:C:H4'	13:M:116:THR:HA	1.80	0.63
3:C:174:PRO:HB2	3:C:177:THR:HG23	1.80	0.63
10:J:4:ILE:HA	10:J:100:THR:HG22	1.79	0.63
1:A:1207:C:OP2	13:M:91:ARG:NH1	2.30	0.63
7:G:57:GLU:H	7:G:60:LYS:HE2	1.63	0.63
9:I:42:ARG:O	9:I:44:VAL:N	2.31	0.63
1:A:969:U:H3	1:A:1026:A:H62	1.47	0.63
4:D:70:ILE:HD11	4:D:100:ARG:CZ	2.29	0.63
20:T:53:LEU:HD23	20:T:56:MET:HE1	1.80	0.63
2:B:189:ASP:HB3	2:B:204:ASN:HA	1.80	0.62
4:D:190:ASP:N	4:D:190:ASP:OD2	2.29	0.62
1:A:1006:C:N3	1:A:1016:G:N2	2.47	0.62
1:A:1222:G:H2'	1:A:1223:C:C6	2.33	0.62
10:J:4:ILE:HG13	10:J:74:ILE:HG13	1.81	0.62
5:E:89:ILE:HG12	5:E:135:THR:HG22	1.80	0.62
1:A:1295:C:N4	19:S:4:SER:OG	2.32	0.62
1:A:1374:G:N2	1:A:1479:A:H8	1.96	0.62
3:C:58:GLU:HB3	10:J:92:THR:HG21	1.81	0.62
1:A:1279:C:H4'	1:A:1280:A:O4'	1.99	0.62
3:C:109:PRO:HG2	3:C:110:ASN:HD22	1.64	0.62
17:Q:66:SER:OG	17:Q:67:LYS:N	2.33	0.62
1:A:507:G:H2'	1:A:508:C:C6	2.35	0.61
18:R:41:LYS:HA	18:R:44:LEU:HD13	1.82	0.61
1:A:1111:C:H4'	1:A:1112:A:OP2	2.01	0.61
1:A:1204:C:OP2	19:S:78:ARG:NH2	2.33	0.61
12:L:27:LEU:C	12:L:29:GLY:H	2.03	0.61
15:O:26:GLU:OE1	15:O:77:ARG:NH1	2.33	0.61
2:B:62:ALA:HB1	2:B:226:ARG:HG3	1.81	0.61
3:C:156:ARG:H	3:C:163:ALA:HA	1.66	0.61
4:D:108:LEU:HD23	4:D:170:VAL:HG21	1.81	0.61
1:A:953:G:H5'	1:A:1339:U:O2'	2.01	0.61
17:Q:83:ASP:N	17:Q:83:ASP:OD1	2.33	0.61
18:R:38:GLU:OE1	18:R:38:GLU:N	2.33	0.61
12:L:40:VAL:HG21	12:L:77:LEU:O	2.01	0.60
1:A:1307:C:OP2	21:V:6:ARG:NH1	2.34	0.60
1:A:8:A:N6	4:D:205:GLU:O	2.34	0.60
18:R:19:LYS:NZ	18:R:20:ALA:O	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:522:A:H2'	1:A:523:G:C8	2.36	0.60
19:S:32:LYS:HB3	19:S:50:ALA:HB3	1.84	0.60
10:J:50:ILE:HB	14:N:41:ARG:HD2	1.84	0.60
1:A:1229:A:N3	9:I:70:LYS:NZ	2.48	0.60
1:A:775:A:H4'	1:A:776:U:O5'	2.01	0.60
10:J:65:LEU:HD13	14:N:56:VAL:HG22	1.82	0.60
18:R:53:ARG:NH1	18:R:58:LEU:O	2.33	0.60
3:C:11:ARG:HD3	3:C:180:ALA:HB3	1.84	0.60
3:C:95:THR:HG22	3:C:97:LYS:H	1.66	0.60
4:D:196:LEU:HB3	4:D:198:VAL:HG22	1.84	0.59
7:G:103:TRP:CD1	7:G:137:LYS:HD2	2.37	0.59
15:O:26:GLU:HA	15:O:81:LEU:HD11	1.85	0.59
13:M:23:TYR:HB3	13:M:67:GLU:HA	1.85	0.59
1:A:1110:C:N4	1:A:1126:G:O6	2.32	0.59
2:B:18:GLY:O	2:B:19:HIS:ND1	2.35	0.59
3:C:6:HIS:HD2	3:C:8:ILE:H	1.50	0.59
9:I:4:TYR:HB2	9:I:19:LEU:HB2	1.83	0.59
16:P:34:GLU:OE2	16:P:55:ARG:HD3	2.03	0.59
1:A:1278:C:O2'	1:A:1279:C:OP2	2.18	0.59
13:M:125:ARG:O	13:M:125:ARG:NH1	2.34	0.59
1:A:35:G:H2'	1:A:36:C:C6	2.38	0.58
1:A:1487:U:H2'	1:A:1488:G:C8	2.38	0.58
1:A:1222:G:H2'	1:A:1223:C:H6	1.68	0.58
1:A:173:A:H2'	1:A:174:U:C6	2.38	0.58
10:J:49:VAL:HG13	14:N:41:ARG:HG3	1.85	0.58
1:A:1110:C:OP1	9:I:66:ARG:NH2	2.36	0.58
1:A:212:C:O2'	1:A:455:C:N4	2.35	0.58
4:D:98:GLU:OE2	4:D:107:ARG:NE	2.35	0.58
6:F:15:ASP:O	6:F:17:SER:N	2.36	0.58
1:A:501:C:H5''	1:A:502:C:H6	1.67	0.58
1:A:690:C:H2'	1:A:691:C:H6	1.68	0.58
7:G:146:GLU:O	7:G:149:ARG:N	2.35	0.58
12:L:78:GLN:O	12:L:80:HIS:N	2.35	0.58
15:O:74:ASP:O	15:O:77:ARG:N	2.36	0.58
2:B:16:HIS:CD2	2:B:209:ARG:HB3	2.39	0.58
20:T:23:ARG:O	20:T:27:LYS:HB2	2.03	0.58
10:J:6:ILE:HD11	10:J:23:ILE:HD13	1.86	0.58
1:A:406:A:N3	1:A:408:G:O2'	2.27	0.57
2:B:204:ASN:ND2	2:B:206:ASP:O	2.37	0.57
5:E:64:ARG:H	5:E:64:ARG:HD2	1.68	0.57
5:E:8:GLU:HG2	5:E:34:VAL:HG12	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:180:ALA:HB1	3:C:182:ILE:HG13	1.84	0.57
8:H:10:LEU:HD22	8:H:83:ILE:HD11	1.85	0.57
1:A:1204:C:P	19:S:78:ARG:HH21	2.26	0.57
22:W:3:A:H61	23:X:34:RSQ:HN4	1.52	0.57
7:G:111:ARG:NH1	7:G:113:GLU:OE2	2.38	0.57
21:V:10:ARG:HG2	21:V:13:ILE:HD12	1.87	0.57
7:G:18:TYR:CD1	7:G:59:LEU:HB2	2.39	0.57
13:M:37:THR:O	13:M:55:ARG:NH1	2.36	0.57
19:S:50:ALA:HA	19:S:58:VAL:O	2.04	0.57
20:T:14:LYS:O	20:T:18:GLN:HG2	2.04	0.57
1:A:1036:C:O2'	1:A:1037:A:O5'	2.22	0.57
1:A:102:A:H2'	1:A:321:G:N2	2.19	0.57
1:A:501:C:H5''	1:A:502:C:C6	2.39	0.57
17:Q:19:VAL:HG23	17:Q:44:ALA:HB3	1.86	0.57
7:G:78:ARG:NH1	7:G:154:TYR:HB3	2.20	0.57
1:A:925:C:OP1	13:M:109:THR:HG22	2.03	0.57
1:A:1381:C:C2	1:A:1479:A:N6	2.72	0.57
3:C:67:THR:HG23	3:C:102:ASN:HB2	1.85	0.57
22:W:2:U:H2'	22:W:3:A:C8	2.39	0.57
8:H:1:MET:HG2	8:H:2:LEU:H	1.70	0.56
12:L:52:LEU:O	12:L:54:LYS:NZ	2.29	0.56
1:A:1288:U:H2'	1:A:1289:U:C6	2.40	0.56
22:W:2:U:H2'	22:W:3:A:H8	1.70	0.56
8:H:92:ARG:HH11	8:H:92:ARG:CG	2.19	0.56
9:I:25:LYS:N	9:I:60:ASP:OD1	2.38	0.56
13:M:88:ARG:HG2	13:M:98:VAL:HG13	1.87	0.56
16:P:51:VAL:O	16:P:52:ASP:HB3	2.05	0.56
5:E:16:THR:HG23	5:E:27:ARG:HB3	1.88	0.56
1:A:952:A:C8	1:A:952:A:H5'	2.36	0.56
1:A:408:G:O6	4:D:36:ARG:NH1	2.39	0.56
6:F:9:VAL:HG23	6:F:87:ARG:HB2	1.87	0.56
9:I:53:VAL:HG21	9:I:85:LEU:HD21	1.88	0.56
2:B:82:ARG:HA	2:B:92:TYR:CE1	2.40	0.56
12:L:65:GLU:OE1	12:L:65:GLU:N	2.39	0.56
1:A:273:G:OP2	17:Q:41:LYS:NZ	2.35	0.56
17:Q:7:THR:O	17:Q:23:VAL:HG13	2.05	0.56
15:O:82:ILE:O	15:O:86:GLY:N	2.31	0.56
1:A:1328:G:N2	1:A:1355:G:H2'	2.19	0.55
2:B:101:MET:HA	2:B:108:ILE:HD12	1.88	0.55
5:E:80:ILE:HD12	5:E:91:LEU:HB2	1.88	0.55
6:F:13:ASN:N	6:F:13:ASN:OD1	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:985:C:N3	1:A:1000:G:N2	2.50	0.55
2:B:118:LEU:HB3	2:B:142:LEU:HD13	1.88	0.55
11:K:14:VAL:O	11:K:16:SER:N	2.38	0.55
1:A:1109:G:N1	1:A:1126:G:N7	2.50	0.55
2:B:92:TYR:CE2	2:B:151:GLY:HA3	2.41	0.55
1:A:944:C:H2'	1:A:945:A:N7	2.22	0.55
7:G:108:ALA:O	7:G:119:ARG:HD2	2.06	0.55
1:A:937:U:H1'	1:A:1204:C:H5'	1.89	0.55
1:A:1350:G:H5''	9:I:112:LYS:HB3	1.89	0.55
1:A:669:U:H4'	1:A:670:A:OP1	2.07	0.55
1:A:905:G:H5'	1:A:1510:C:OP1	2.07	0.55
2:B:208:ILE:HD12	2:B:209:ARG:N	2.22	0.55
3:C:119:ARG:HG2	3:C:140:ARG:HH12	1.72	0.55
1:A:1206:A:O2'	1:A:1207:C:O5'	2.23	0.55
1:A:35:G:H2'	1:A:36:C:H6	1.72	0.55
7:G:111:ARG:HD2	7:G:123:GLU:HB2	1.88	0.55
17:Q:59:ILE:HD12	17:Q:73:VAL:HA	1.89	0.55
1:A:125:C:H2'	1:A:126:C:C6	2.42	0.55
1:A:1360:C:H5	1:A:1361:G:C4	2.24	0.55
1:A:928:G:OP2	13:M:102:ARG:NH2	2.40	0.55
2:B:9:GLU:HB3	2:B:12:GLU:HB2	1.89	0.55
3:C:22:TRP:HB3	3:C:59:ARG:HB3	1.89	0.55
3:C:22:TRP:NE1	3:C:36:ASP:OD1	2.34	0.55
1:A:978:A:N1	1:A:979:G:N2	2.55	0.54
1:A:188:U:H1'	1:A:189:U:H5''	1.89	0.54
9:I:26:VAL:HB	9:I:33:PHE:HB2	1.89	0.54
13:M:23:TYR:CE2	13:M:71:ARG:HB3	2.41	0.54
1:A:1106:G:HO2'	1:A:1127:C:N4	2.04	0.54
1:A:1204:C:H3'	1:A:1205:G:H5''	1.89	0.54
3:C:6:HIS:CD2	3:C:8:ILE:H	2.25	0.54
1:A:816:U:H2'	1:A:817:C:C6	2.43	0.54
1:A:123:G:N3	1:A:189:U:H3'	2.22	0.54
1:A:656:G:H2'	1:A:657:G:C8	2.42	0.54
1:A:143:A:H2'	1:A:144:C:C6	2.43	0.54
1:A:563:U:H2'	1:A:564:G:O4'	2.08	0.54
1:A:1350:G:OP1	9:I:111:ARG:NH2	2.41	0.54
11:K:18:ARG:HB2	11:K:33:THR:HG22	1.89	0.54
17:Q:15:MET:HG2	17:Q:18:THR:HB	1.90	0.54
7:G:18:TYR:HB3	7:G:59:LEU:HD22	1.89	0.54
13:M:14:ARG:HG3	13:M:44:ARG:NH1	2.22	0.54
1:A:1231:A:H4'	9:I:68:GLY:N	2.18	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:93:LYS:HG3	3:C:94:LEU:HD23	1.90	0.54
6:F:33:TYR:HA	6:F:71:ARG:HH21	1.72	0.54
1:A:858:G:P	12:L:12:ARG:HH22	2.31	0.54
1:A:1221:U:H3'	1:A:1222:G:H5'	1.91	0.53
1:A:525:G:P	4:D:10:ARG:HH22	2.29	0.53
1:A:424:U:H1'	1:A:425:A:H5''	1.90	0.53
2:B:114:ARG:O	2:B:118:LEU:N	2.40	0.53
2:B:140:HIS:HA	2:B:143:GLU:HG3	1.89	0.53
4:D:9:CYS:HB3	4:D:32:ALA:HB2	1.89	0.53
1:A:1121:G:N2	1:A:1126:G:H1	2.07	0.53
1:A:1327:A:N1	1:A:1356:A:H5''	2.23	0.53
17:Q:4:LYS:HE3	17:Q:6:LEU:HD21	1.89	0.53
1:A:1051:C:O2'	1:A:1173:C:H1'	2.08	0.53
1:A:1456:C:H2'	1:A:1457:G:H8	1.73	0.53
1:A:1479:A:H2	1:A:1482:G:N1	1.93	0.53
2:B:97:TRP:HZ2	2:B:102:LEU:HD13	1.73	0.53
1:A:608:G:H4'	16:P:16:HIS:CD2	2.44	0.53
7:G:46:ALA:O	7:G:50:ILE:HG12	2.09	0.53
1:A:1308:C:OP2	21:V:12:LYS:NZ	2.42	0.53
1:A:702:C:H1'	18:R:49:LYS:HG2	1.89	0.53
11:K:48:ILE:HG21	11:K:63:LEU:HD13	1.91	0.53
12:L:54:LYS:HG2	12:L:75:HIS:CD2	2.44	0.53
1:A:1121:G:H22	1:A:1126:G:H22	1.57	0.53
1:A:583:C:H2'	1:A:584:C:C6	2.44	0.53
1:A:923:A:H2'	1:A:924:G:C8	2.43	0.53
2:B:20:GLU:HB2	2:B:190:THR:OG1	2.09	0.53
5:E:10:MET:HA	5:E:32:VAL:HA	1.90	0.53
1:A:1249:A:N3	1:A:1307:C:O2'	2.39	0.53
1:A:922:G:C2	1:A:923:A:C8	2.96	0.53
2:B:223:ILE:HG13	2:B:226:ARG:HH21	1.74	0.53
22:W:3:A:N6	23:X:34:RSQ:HN4	2.07	0.53
2:B:16:HIS:HB3	2:B:210:SER:OG	2.09	0.53
8:H:64:LYS:HG2	8:H:79:VAL:HG21	1.90	0.53
9:I:46:ALA:HB2	9:I:74:ILE:HG23	1.91	0.53
12:L:57:LYS:HD3	12:L:67:THR:HB	1.90	0.53
1:A:1394:C:H2'	1:A:1395:A:C8	2.43	0.52
2:B:178:ARG:NH1	8:H:71:GLY:O	2.42	0.52
1:A:1260:A:H2'	1:A:1260:A:N3	2.24	0.52
1:A:773:A:H5''	1:A:774:G:OP2	2.10	0.52
3:C:11:ARG:NH1	3:C:177:THR:O	2.42	0.52
9:I:66:ARG:HH11	9:I:66:ARG:HB3	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1121:G:H21	1:A:1125:G:N2	2.06	0.52
1:A:1093:A:N1	3:C:177:THR:HB	2.24	0.52
3:C:34:LEU:HD22	14:N:25:VAL:HG21	1.91	0.52
21:V:5:ASP:O	21:V:8:THR:OG1	2.27	0.52
1:A:603:C:H2'	1:A:604:A:O4'	2.09	0.52
4:D:43:HIS:O	4:D:45:GLN:N	2.37	0.52
11:K:84:VAL:HG21	11:K:91:ARG:HD3	1.92	0.52
17:Q:86:GLU:O	17:Q:90:ILE:HG13	2.09	0.52
3:C:147:LYS:HD3	3:C:205:GLY:HA2	1.91	0.52
4:D:18:LYS:HB3	4:D:20:TYR:CE2	2.45	0.52
9:I:38:GLN:OE1	9:I:39:GLY:N	2.43	0.52
11:K:124:LYS:HE2	11:K:125:PHE:CZ	2.45	0.52
12:L:8:ASN:O	12:L:12:ARG:HG3	2.10	0.52
1:A:125:C:H2'	1:A:126:C:H6	1.75	0.52
1:A:274:A:H5''	1:A:276:G:H5'	1.91	0.52
2:B:208:ILE:HD12	2:B:209:ARG:H	1.74	0.52
8:H:111:ILE:HG22	8:H:134:ILE:HD12	1.91	0.52
8:H:116:LYS:HG3	8:H:129:VAL:HG11	1.92	0.52
9:I:3:GLN:HE22	9:I:20:ARG:HH21	1.57	0.52
20:T:67:ALA:HA	20:T:73:HIS:H	1.75	0.52
1:A:1298:C:O2	19:S:37:ARG:NH2	2.40	0.51
1:A:382:U:H5'	1:A:383:G:P	2.50	0.51
2:B:28:PHE:CD2	2:B:190:THR:HA	2.45	0.51
9:I:11:LYS:O	9:I:13:ALA:N	2.43	0.51
1:A:949:C:H4'	10:J:57:LYS:HB3	1.91	0.51
17:Q:81:ARG:NE	17:Q:84:LEU:HD11	2.25	0.51
1:A:987:G:H22	1:A:999:G:H1'	1.76	0.51
13:M:15:VAL:HG21	13:M:48:LEU:HD21	1.92	0.51
19:S:51:VAL:O	19:S:58:VAL:HG22	2.11	0.51
1:A:323:C:O2	1:A:323:C:H2'	2.10	0.51
1:A:720:A:H2'	1:A:721:C:C6	2.46	0.51
2:B:235:SER:O	2:B:238:LEU:HB2	2.10	0.51
17:Q:67:LYS:O	17:Q:69:LYS:N	2.37	0.51
1:A:1080:C:H2'	1:A:1081:G:O4'	2.09	0.51
1:A:67:C:O2'	1:A:165:A:N3	2.34	0.51
1:A:155:A:H61	1:A:342:G:HO2'	1.58	0.51
1:A:689:A:C4'	11:K:29:ILE:HD11	2.41	0.51
2:B:87:ARG:HD2	2:B:234:PRO:HD2	1.91	0.51
1:A:904:G:H4'	1:A:1480:A:N7	2.26	0.51
1:A:931:G:H2'	1:A:932:U:C6	2.45	0.51
11:K:54:ARG:O	11:K:57:THR:HG22	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1139:A:H4'	1:A:1140:C:O5'	2.11	0.51
1:A:268:A:N6	1:A:269:A:C6	2.79	0.51
6:F:60:PHE:CZ	18:R:78:LEU:HD21	2.46	0.51
19:S:15:LEU:HA	19:S:18:LYS:HB3	1.92	0.51
1:A:1039:G:H5''	3:C:154:SER:HB2	1.92	0.51
1:A:1044:U:H2'	1:A:1045:C:C6	2.46	0.51
3:C:35:GLU:OE2	3:C:59:ARG:NH1	2.43	0.51
17:Q:5:VAL:HG22	17:Q:60:ILE:HD12	1.92	0.51
1:A:1088:G:H5''	3:C:172:ARG:HG2	1.93	0.50
1:A:521:G:H2'	1:A:522:A:H8	1.76	0.50
1:A:1172:A:H5''	3:C:4:LYS:HE2	1.93	0.50
6:F:37:VAL:HA	6:F:65:VAL:HG12	1.91	0.50
15:O:71:GLN:HG3	15:O:78:TYR:CD2	2.46	0.50
1:A:484:C:H2'	1:A:485:G:H8	1.76	0.50
1:A:522:A:H2'	1:A:523:G:H8	1.75	0.50
6:F:21:LEU:O	6:F:25:ILE:HG13	2.12	0.50
13:M:54:VAL:O	13:M:58:GLU:HG2	2.11	0.50
1:A:1188:G:H2'	1:A:1189:C:H6	1.75	0.50
1:A:520:G:OP1	12:L:113:ARG:NH2	2.43	0.50
5:E:43:LEU:HD11	5:E:132:ALA:HB1	1.92	0.50
1:A:264:C:H2'	1:A:265:A:C8	2.46	0.50
1:A:814:U:H2'	1:A:815:C:H6	1.76	0.50
18:R:73:ALA:HB3	18:R:79:LEU:HD12	1.92	0.50
2:B:122:PHE:HA	2:B:127:ILE:HD13	1.93	0.50
2:B:178:ARG:HH22	8:H:74:PRO:HG3	1.75	0.50
7:G:145:ALA:O	7:G:147:ALA:N	2.43	0.50
10:J:75:ILE:HG22	10:J:76:ASN:HD22	1.76	0.50
1:A:1409:U:H2'	1:A:1410:A:C8	2.46	0.50
1:A:530:A:H4'	1:A:531:G:O5'	2.11	0.50
1:A:531:G:H2'	1:A:532:C:C6	2.46	0.50
1:A:1019:C:H2'	1:A:1020:C:C6	2.47	0.50
3:C:3:ASN:HB2	3:C:4:LYS:HD2	1.93	0.50
4:D:148:VAL:HB	4:D:181:MET:HB3	1.92	0.50
5:E:87:SER:HB3	5:E:131:ILE:HD13	1.93	0.50
12:L:115:LYS:O	12:L:117:ARG:N	2.42	0.50
17:Q:63:ARG:HG2	17:Q:64:PRO:HD2	1.92	0.50
5:E:135:THR:O	5:E:139:LEU:HG	2.12	0.50
18:R:74:ARG:HB3	18:R:81:PHE:CE2	2.46	0.50
1:A:1014:G:H2'	1:A:1015:G:O4'	2.11	0.50
1:A:21:G:H2'	1:A:22:G:C8	2.47	0.50
1:A:900:A:OP1	5:E:21:ALA:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:69:TYR:CD1	12:L:90:VAL:HG21	2.46	0.50
14:N:57:ARG:HG2	14:N:58:LYS:H	1.77	0.50
2:B:186:ALA:HB3	2:B:197:VAL:HG11	1.94	0.49
15:O:33:THR:HG23	15:O:63:ARG:NH1	2.27	0.49
1:A:695:A:H2'	1:A:696:G:O4'	2.12	0.49
4:D:199:ASN:C	4:D:199:ASN:HD22	2.07	0.49
1:A:1073:U:O2	1:A:1075:A:C8	2.66	0.49
7:G:26:PHE:O	7:G:30:ILE:HG13	2.12	0.49
7:G:8:GLU:CD	7:G:8:GLU:H	2.12	0.49
1:A:1083:A:H4'	1:A:1084:A:O5'	2.13	0.49
1:A:1098:C:O2'	9:I:108:VAL:HG21	2.13	0.49
2:B:143:GLU:O	2:B:147:LYS:HG3	2.12	0.49
7:G:18:TYR:HD1	7:G:59:LEU:HD22	1.77	0.49
3:C:26:LYS:HZ3	10:J:45:ARG:HE	1.60	0.49
12:L:28:LYS:C	12:L:30:ALA:H	2.14	0.49
12:L:34:ARG:O	12:L:61:THR:HG23	2.12	0.49
12:L:54:LYS:HG2	12:L:75:HIS:HD2	1.76	0.49
1:A:1037:A:C6	1:A:1187:G:C5	3.00	0.49
1:A:446:A:HO2'	1:A:447:A:H8	1.61	0.49
4:D:79:PHE:HE1	4:D:204:ILE:HG12	1.78	0.49
6:F:7:ASN:HB2	6:F:89:MET:O	2.12	0.49
9:I:6:GLY:HA3	9:I:83:ARG:HB2	1.94	0.49
12:L:113:ARG:HH12	12:L:116:SER:H	1.61	0.49
1:A:124:A:H1'	1:A:258:A:O2'	2.11	0.49
1:A:994:A:H2'	1:A:995:G:O4'	2.13	0.49
7:G:117:ALA:H	7:G:120:ILE:CD1	2.20	0.49
1:A:242:G:OP2	17:Q:100:LYS:HB3	2.12	0.49
6:F:101:ALA:HA	18:R:28:GLU:HA	1.95	0.49
1:A:311:G:OP2	1:A:346:G:O2'	2.31	0.49
3:C:150:LYS:HG3	3:C:169:ALA:HB2	1.95	0.49
4:D:61:LYS:HD2	4:D:207:TYR:OH	2.13	0.49
4:D:71:SER:OG	4:D:74:GLN:HB2	2.12	0.49
1:A:619:U:H5'	17:Q:2:PRO:HG2	1.95	0.49
1:A:398:C:O2'	4:D:122:ARG:NH1	2.46	0.48
1:A:886:A:OP1	12:L:21:LYS:HE3	2.13	0.48
1:A:951:A:OP2	14:N:41:ARG:NH1	2.33	0.48
1:A:1039:G:H5''	3:C:154:SER:CB	2.43	0.48
7:G:26:PHE:CD2	7:G:30:ILE:HD11	2.48	0.48
11:K:86:GLY:O	11:K:91:ARG:NH1	2.46	0.48
16:P:3:LYS:HG2	16:P:24:ALA:HB2	1.95	0.48
23:X:34:RSQ:H2'	23:X:35:A:H8	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:150:LYS:HE2	3:C:152:ILE:HD11	1.94	0.48
4:D:53:ASP:O	4:D:57:ARG:HG3	2.13	0.48
8:H:92:ARG:HH11	8:H:92:ARG:HG2	1.78	0.48
1:A:385:C:H2'	1:A:386:G:C8	2.48	0.48
1:A:642:U:OP2	15:O:8:LYS:NZ	2.29	0.48
1:A:821:G:H2'	1:A:822:U:H5''	1.93	0.48
1:A:959:U:H4'	1:A:960:A:O5'	2.14	0.48
11:K:54:ARG:O	11:K:56:GLY:N	2.46	0.48
1:A:230:C:H5'	17:Q:70:ARG:HG2	1.95	0.48
3:C:134:ILE:HG22	3:C:168:ALA:HB3	1.94	0.48
3:C:42:LEU:HD21	3:C:90:GLU:HG3	1.94	0.48
4:D:165:MET:SD	4:D:168:ARG:NH1	2.86	0.48
6:F:23:LYS:O	6:F:27:GLN:HG2	2.13	0.48
2:B:92:TYR:HE2	2:B:151:GLY:HA3	1.78	0.48
6:F:69:GLU:CD	6:F:69:GLU:H	2.16	0.48
15:O:36:ILE:HG13	15:O:59:MET:HE3	1.94	0.48
1:A:705:A:H2'	1:A:705:A:N3	2.28	0.48
1:A:726:U:H2'	1:A:727:C:C6	2.49	0.48
1:A:1036:C:HO2'	1:A:1037:A:P	2.37	0.48
1:A:1039:G:H2'	1:A:1040:G:O4'	2.14	0.48
1:A:19:C:H2'	1:A:20:U:H6	1.78	0.48
2:B:126:GLU:HA	2:B:129:GLU:HB2	1.95	0.48
3:C:177:THR:O	3:C:180:ALA:HB2	2.14	0.48
4:D:98:GLU:HG2	4:D:189:PRO:HG3	1.96	0.48
7:G:27:ILE:HA	7:G:30:ILE:HD12	1.96	0.48
8:H:9:MET:HG3	8:H:26:VAL:HG11	1.96	0.48
13:M:15:VAL:HG23	13:M:43:THR:O	2.14	0.48
1:A:1352:G:C2	1:A:1353:G:C8	3.02	0.48
3:C:6:HIS:HE2	3:C:8:ILE:HD12	1.79	0.48
1:A:1383:G:C2	1:A:1384:C:H1'	2.49	0.48
1:A:780:C:H2'	1:A:781:G:H8	1.78	0.48
11:K:34:ASP:O	11:K:36:ASP:N	2.47	0.48
14:N:24:CYS:HB2	14:N:40:CYS:HB3	1.95	0.48
19:S:5:LEU:HA	19:S:6:LYS:NZ	2.28	0.48
14:N:23:ARG:NH1	14:N:30:ALA:HB2	2.29	0.47
1:A:1130:U:H2'	1:A:1131:C:O4'	2.14	0.47
1:A:501:C:H4'	1:A:502:C:O5'	2.13	0.47
1:A:64:G:OP1	1:A:64:G:H3'	2.13	0.47
4:D:75:PHE:HD2	4:D:207:TYR:HH	1.61	0.47
9:I:50:LEU:O	9:I:52:ALA:N	2.43	0.47
10:J:3:LYS:HE3	10:J:3:LYS:HB2	1.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:U:O3'	1:A:123:G:H3'	2.14	0.47
1:A:274:A:OP2	17:Q:95:TYR:OH	2.29	0.47
1:A:968:U:O2	1:A:970:G:H8	1.97	0.47
1:A:985:C:H42	1:A:1000:G:H1	1.61	0.47
9:I:17:VAL:HG11	9:I:81:ILE:HG12	1.95	0.47
1:A:689:A:O4'	11:K:29:ILE:HD11	2.14	0.47
1:A:1409:U:H2'	1:A:1410:A:H8	1.79	0.47
1:A:981:G:C5	1:A:982:A:N7	2.82	0.47
12:L:35:GLY:HA3	12:L:60:LEU:HD13	1.96	0.47
1:A:96:C:OP1	20:T:17:ARG:NH1	2.45	0.47
3:C:83:ARG:HE	3:C:87:LEU:HD11	1.80	0.47
13:M:40:ASN:HD21	13:M:42:ALA:HB3	1.80	0.47
1:A:690:C:H2'	1:A:691:C:C6	2.48	0.47
3:C:159:GLY:HA2	3:C:193:TYR:CE1	2.50	0.47
8:H:10:LEU:HA	8:H:10:LEU:HD23	1.62	0.47
9:I:11:LYS:C	9:I:13:ALA:H	2.17	0.47
9:I:50:LEU:C	9:I:52:ALA:H	2.18	0.47
9:I:19:LEU:HB3	9:I:59:PHE:CE2	2.49	0.47
20:T:93:GLU:O	20:T:95:ALA:N	2.47	0.47
1:A:121:G:O3'	17:Q:3:LYS:NZ	2.47	0.47
1:A:405:G:H2'	1:A:424:U:C5	2.50	0.47
1:A:491:C:H5'	4:D:209:ARG:HH12	1.79	0.47
1:A:119:G:H4'	1:A:617:C:O2	2.15	0.47
1:A:696:G:H2'	1:A:697:G:C8	2.49	0.47
4:D:3:ARG:HD3	4:D:3:ARG:HA	1.54	0.47
12:L:78:GLN:C	12:L:80:HIS:H	2.17	0.47
18:R:61:LYS:O	18:R:65:ILE:HG13	2.15	0.47
1:A:170:C:H2'	1:A:171:C:H6	1.79	0.47
1:A:505:C:OP2	12:L:69:TYR:OH	2.24	0.47
3:C:174:PRO:HB2	3:C:177:THR:CG2	2.45	0.47
13:M:70:LEU:O	13:M:73:GLU:HG3	2.15	0.47
1:A:1305:A:O4'	1:A:1343:C:H4'	2.15	0.47
3:C:156:ARG:HH11	3:C:156:ARG:HG3	1.79	0.47
4:D:88:VAL:O	4:D:92:VAL:HG23	2.14	0.47
9:I:51:ARG:HA	9:I:56:LEU:HD11	1.97	0.47
11:K:41:THR:HG21	11:K:71:LYS:HB3	1.96	0.47
15:O:57:LEU:HA	15:O:57:LEU:HD12	1.59	0.47
19:S:51:VAL:HG21	19:S:71:LEU:HB3	1.97	0.47
1:A:1185:A:H5'	1:A:1186:U:OP2	2.15	0.46
1:A:531:G:H2'	1:A:532:C:H6	1.77	0.46
1:A:555:A:H5'	1:A:556:A:OP2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:85:ARG:NE	8:H:87:SER:O	2.48	0.46
10:J:39:PRO:O	10:J:40:LEU:HB2	2.15	0.46
10:J:50:ILE:H	10:J:50:ILE:HD12	1.79	0.46
15:O:31:LEU:HA	15:O:31:LEU:HD12	1.71	0.46
1:A:1036:C:H5	23:X:34:RSQ:O4'	1.98	0.46
1:A:492:A:H5''	4:D:55:ALA:HB2	1.97	0.46
1:A:93:C:H2'	1:A:94:A:C8	2.50	0.46
2:B:13:ALA:O	2:B:15:VAL:N	2.48	0.46
4:D:30:LYS:C	4:D:32:ALA:N	2.68	0.46
5:E:31:LEU:HD23	5:E:31:LEU:HA	1.65	0.46
12:L:6:THR:OG1	12:L:9:GLN:HG3	2.14	0.46
1:A:1337:G:H2'	1:A:1338:A:C8	2.51	0.46
1:A:399:U:H5'	4:D:122:ARG:HD2	1.97	0.46
1:A:62:U:H2'	1:A:63:C:C6	2.51	0.46
1:A:653:G:H2'	1:A:654:G:O4'	2.15	0.46
14:N:9:LYS:NZ	14:N:22:THR:HA	2.30	0.46
1:A:1036:C:C5	23:X:34:RSQ:O4'	2.69	0.46
1:A:740:U:H2'	1:A:741:G:O4'	2.15	0.46
3:C:3:ASN:H	3:C:3:ASN:ND2	2.14	0.46
5:E:47:LYS:HE3	5:E:47:LYS:HB2	1.74	0.46
7:G:70:LYS:HB2	7:G:96:GLN:HB3	1.98	0.46
12:L:25:PRO:C	12:L:27:LEU:H	2.19	0.46
19:S:15:LEU:HD13	19:S:33:THR:HG21	1.96	0.46
19:S:17:GLU:HA	19:S:20:LEU:HG	1.98	0.46
1:A:1345:A:H4'	1:A:1346:U:H2'	1.96	0.46
1:A:1480:A:H61	1:A:1510:C:H5'	1.80	0.46
1:A:396:C:H1'	1:A:605:A:H1'	1.96	0.46
1:A:690:C:H4'	11:K:20:TYR:CD1	2.50	0.46
2:B:98:LEU:N	2:B:98:LEU:HD23	2.30	0.46
4:D:199:ASN:ND2	4:D:201:GLN:HB3	2.31	0.46
10:J:5:ARG:HB3	10:J:99:LYS:H	1.79	0.46
20:T:85:MET:HG2	20:T:104:LEU:HD21	1.98	0.46
4:D:96:LEU:HD12	4:D:96:LEU:HA	1.77	0.46
1:A:484:C:H2'	1:A:485:G:C8	2.50	0.46
1:A:794:C:H4'	1:A:877:A:N6	2.31	0.46
9:I:70:LYS:HA	9:I:73:GLN:HB2	1.97	0.46
17:Q:60:ILE:HG13	17:Q:61:GLU:N	2.30	0.46
1:A:859:C:O2'	1:A:860:C:H5'	2.16	0.46
2:B:71:VAL:HG12	2:B:170:GLU:HG2	1.98	0.46
10:J:17:ASP:C	10:J:19:SER:H	2.19	0.46
1:A:1041:C:O3'	14:N:45:ARG:NH2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:94:ASN:HA	17:Q:105:ALA:HB1	1.98	0.46
1:A:1286:G:N2	1:A:1312:G:H1'	2.31	0.46
5:E:81:GLU:OE1	5:E:88:LYS:HE2	2.15	0.46
6:F:75:LEU:O	6:F:79:LEU:HB2	2.15	0.46
19:S:11:VAL:HG22	19:S:39:THR:HB	1.98	0.46
1:A:1077:U:P	1:A:1090:G:H1	2.39	0.46
1:A:1425:G:H5''	1:A:1426:A:H3'	1.97	0.46
1:A:1442:C:H2'	1:A:1443:C:O4'	2.16	0.46
1:A:293:A:H2'	1:A:294:G:O4'	2.16	0.46
1:A:596:C:H2'	1:A:597:A:C8	2.51	0.46
3:C:156:ARG:HD3	3:C:156:ARG:HA	1.72	0.46
18:R:21:LYS:HE2	18:R:54:ARG:O	2.15	0.46
18:R:40:LEU:HB3	18:R:79:LEU:HD11	1.98	0.46
1:A:616:G:H2'	1:A:617:C:C6	2.50	0.45
1:A:772:U:O2'	1:A:774:G:N7	2.45	0.45
2:B:46:LYS:HA	2:B:49:GLU:HG2	1.96	0.45
2:B:77:ALA:HA	2:B:80:ILE:HD13	1.97	0.45
3:C:107:GLN:H	3:C:107:GLN:CD	2.20	0.45
10:J:50:ILE:HB	14:N:41:ARG:CD	2.46	0.45
1:A:1224:C:H5''	21:V:8:THR:HG22	1.98	0.45
1:A:110:G:O6	1:A:284:G:H1'	2.16	0.45
1:A:674:G:H2'	1:A:675:U:C6	2.51	0.45
1:A:83:A:H5''	1:A:84:C:OP2	2.16	0.45
1:A:952:A:H4'	1:A:953:G:C5'	2.43	0.45
1:A:982:A:N6	1:A:1019:C:H42	2.14	0.45
2:B:223:ILE:HG21	2:B:230:VAL:HG22	1.98	0.45
3:C:119:ARG:O	3:C:123:GLN:HG3	2.16	0.45
18:R:45:SER:N	18:R:49:LYS:O	2.44	0.45
19:S:8:GLY:O	19:S:10:PHE:N	2.49	0.45
20:T:87:LYS:HE3	20:T:87:LYS:HB2	1.64	0.45
1:A:1013:G:H2'	1:A:1014:G:C8	2.51	0.45
1:A:1472:U:H2'	1:A:1473:C:C6	2.51	0.45
1:A:200:C:H2'	1:A:201:A:H5''	1.97	0.45
3:C:164:ARG:HG2	3:C:165:THR:H	1.81	0.45
10:J:6:ILE:HG23	10:J:72:VAL:HB	1.98	0.45
22:W:3:A:H5''	22:W:4:A:OP2	2.15	0.45
1:A:1187:G:C6	1:A:1188:G:C5	3.04	0.45
1:A:1247:G:N2	1:A:1250:A:OP2	2.40	0.45
1:A:408:G:H2'	1:A:423:G:N2	2.31	0.45
4:D:152:SER:O	4:D:155:LEU:HB2	2.17	0.45
1:A:1020:C:H2'	1:A:1021:C:H5'	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:48:ILE:HD12	11:K:48:ILE:HA	1.68	0.45
1:A:1400:A:H2'	1:A:1401:G:O4'	2.16	0.45
3:C:54:ARG:HD3	3:C:56:ASP:OD2	2.17	0.45
1:A:284:G:C6	1:A:285:C:N4	2.85	0.45
1:A:1094:C:O2	3:C:179:ARG:N	2.43	0.45
1:A:1286:G:C4	1:A:1312:G:N2	2.85	0.45
1:A:1328:G:H3'	9:I:108:VAL:O	2.16	0.45
1:A:799:A:OP1	1:A:1503:G:O2'	2.28	0.45
1:A:912:A:C2	1:A:913:C:C2	3.05	0.45
2:B:231:GLU:HB3	2:B:232:PRO:HD2	1.98	0.45
1:A:1110:C:H4'	9:I:16:ARG:HH22	1.81	0.45
9:I:55:ALA:H	9:I:56:LEU:HD12	1.81	0.45
18:R:26:LEU:HD13	18:R:29:PHE:CE2	2.52	0.45
1:A:801:G:C2'	1:A:802:A:H5''	2.47	0.45
2:B:61:LEU:HD23	2:B:68:ILE:HD11	1.99	0.45
3:C:9:GLY:HA2	3:C:12:LEU:HD13	1.98	0.45
3:C:159:GLY:HA2	3:C:193:TYR:CZ	2.52	0.45
3:C:21:ARG:NH2	10:J:92:THR:HB	2.32	0.45
4:D:36:ARG:HG3	4:D:38:TYR:CE2	2.52	0.45
4:D:78:LEU:HA	4:D:78:LEU:HD23	1.67	0.45
8:H:26:VAL:HG23	8:H:27:PRO:O	2.17	0.45
9:I:16:ARG:N	9:I:64:THR:O	2.49	0.44
13:M:71:ARG:HA	13:M:74:VAL:HG12	1.99	0.44
18:R:47:THR:HA	18:R:83:GLU:HB2	1.98	0.44
20:T:56:MET:HG3	20:T:88:VAL:HG21	2.00	0.44
1:A:198:U:O2'	20:T:57:ARG:HG3	2.17	0.44
1:A:100:G:C2	1:A:101:G:H1'	2.52	0.44
1:A:1417:G:H2'	1:A:1418:U:H6	1.76	0.44
1:A:437:C:H2'	1:A:438:C:C6	2.53	0.44
1:A:437:C:H2'	1:A:438:C:H6	1.82	0.44
1:A:949:C:OP1	10:J:57:LYS:NZ	2.31	0.44
2:B:17:PHE:CD2	2:B:17:PHE:N	2.85	0.44
2:B:210:SER:O	2:B:213:LEU:N	2.50	0.44
2:B:35:GLU:O	2:B:37:ASN:N	2.49	0.44
8:H:108:GLY:HA3	8:H:138:TRP:HB3	1.99	0.44
10:J:81:THR:O	10:J:85:LEU:N	2.45	0.44
13:M:8:GLU:OE2	13:M:67:GLU:HG2	2.16	0.44
18:R:71:LYS:O	18:R:74:ARG:HB2	2.18	0.44
1:A:1285:G:C6	1:A:1286:G:N1	2.85	0.44
1:A:1468:G:C5	25:A:1785:PAR:H21	2.52	0.44
1:A:837:A:H2'	1:A:838:G:O4'	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:935:A:N3	1:A:962:C:O2'	2.43	0.44
2:B:17:PHE:HD2	2:B:17:PHE:H	1.63	0.44
3:C:114:PRO:HA	3:C:185:GLY:HA3	1.97	0.44
3:C:157:ILE:HD12	3:C:164:ARG:HB3	1.98	0.44
5:E:90:VAL:O	5:E:120:THR:HA	2.16	0.44
6:F:11:ASN:HD22	6:F:86:ARG:NH2	2.15	0.44
10:J:49:VAL:HG11	14:N:45:ARG:HB2	1.99	0.44
1:A:1257:G:O5'	1:A:1257:G:H8	2.00	0.44
1:A:1348:C:H2'	1:A:1349:C:C6	2.53	0.44
1:A:340:C:H4'	1:A:341:G:O5'	2.16	0.44
1:A:353:U:H2'	1:A:354:U:H6	1.83	0.44
5:E:10:MET:HB2	5:E:32:VAL:HG23	1.99	0.44
19:S:36:ARG:HH12	19:S:75:ALA:HB3	1.81	0.44
1:A:102:A:C6	1:A:321:G:C6	3.06	0.44
1:A:521:G:H2'	1:A:522:A:C8	2.53	0.44
16:P:39:TYR:CD2	16:P:73:LEU:HD11	2.51	0.44
1:A:750:A:H2'	1:A:751:A:O4'	2.18	0.44
5:E:110:LEU:HD13	5:E:118:ILE:HG21	1.99	0.44
7:G:15:ASP:HB3	7:G:19:GLY:N	2.32	0.44
7:G:26:PHE:CE2	7:G:30:ILE:HD11	2.53	0.44
12:L:87:GLY:H	12:L:98:TYR:HB3	1.83	0.44
13:M:79:LYS:O	13:M:83:ASP:N	2.51	0.44
5:E:69:VAL:HG21	5:E:139:LEU:HD13	2.00	0.44
6:F:4:TYR:CZ	6:F:72:VAL:HG21	2.52	0.44
8:H:49:GLU:HG2	8:H:62:TYR:HE2	1.82	0.44
9:I:9:ARG:HB3	9:I:104:ARG:NH2	2.32	0.44
23:X:34:RSQ:H2'	23:X:35:A:C8	2.52	0.44
1:A:1384:C:H2'	1:A:1385:C:O4'	2.17	0.44
1:A:510:G:O2'	1:A:518:A:N1	2.41	0.44
1:A:523:G:H2'	1:A:524:G:O4'	2.18	0.44
4:D:30:LYS:O	4:D:32:ALA:N	2.51	0.44
1:A:234:U:H5''	1:A:235:C:OP1	2.18	0.44
5:E:152:ARG:HB3	8:H:43:GLY:O	2.18	0.44
7:G:18:TYR:HD1	7:G:59:LEU:HB2	1.82	0.44
1:A:858:G:P	12:L:12:ARG:NH2	2.90	0.44
17:Q:65:ILE:N	17:Q:65:ILE:HD12	2.32	0.44
1:A:1371:C:H6	1:A:1371:C:O5'	2.00	0.43
2:B:32:ILE:HG21	2:B:40:HIS:CD2	2.54	0.43
4:D:31:CYS:SG	4:D:31:CYS:O	2.76	0.43
10:J:12:ASP:OD1	10:J:15:THR:HB	2.18	0.43
15:O:14:GLU:HG3	15:O:15:PHE:CD1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:49:ALA:O	20:T:53:LEU:HD12	2.17	0.43
1:A:1297:G:N2	1:A:1299:A:H3'	2.33	0.43
1:A:1231:A:H2	1:A:1334:G:H21	1.63	0.43
1:A:1357:A:H2'	1:A:1358:U:O4'	2.18	0.43
2:B:103:THR:HA	2:B:180:LEU:HD11	2.00	0.43
4:D:187:ARG:NE	4:D:188:LEU:H	2.16	0.43
4:D:173:TRP:CD1	4:D:189:PRO:HD3	2.53	0.43
1:A:951:A:P	14:N:41:ARG:HH22	2.41	0.43
15:O:3:ILE:HG21	15:O:34:LEU:HD11	1.99	0.43
20:T:55:ILE:O	20:T:58:LYS:N	2.51	0.43
1:A:255:G:H2'	1:A:256:U:C6	2.53	0.43
3:C:131:ARG:HD2	3:C:135:LYS:HE3	1.99	0.43
5:E:82:VAL:HG21	5:E:138:ALA:HA	2.00	0.43
17:Q:67:LYS:C	17:Q:69:LYS:H	2.21	0.43
1:A:1008:C:H42	1:A:1013:G:H1	1.65	0.43
1:A:721:C:H5''	6:F:69:GLU:HB3	2.01	0.43
2:B:196:LEU:HA	2:B:196:LEU:HD23	1.71	0.43
4:D:9:CYS:HB3	4:D:32:ALA:CB	2.48	0.43
7:G:92:SER:HA	7:G:93:PRO:HD2	1.65	0.43
9:I:50:LEU:HB3	9:I:56:LEU:H	1.84	0.43
1:A:1208:A:C2	13:M:117:VAL:HG21	2.53	0.43
19:S:58:VAL:HA	19:S:59:PRO:HD3	1.91	0.43
1:A:968:U:C5	1:A:1193:U:H1'	2.54	0.43
1:A:445:A:H8	1:A:445:A:O5'	2.02	0.43
1:A:659:A:H1'	11:K:115:PRO:HB3	2.00	0.43
1:A:982:A:H5''	1:A:1003:U:C4	2.53	0.43
2:B:47:THR:O	2:B:51:LEU:HB2	2.18	0.43
6:F:48:LEU:HD13	6:F:52:ILE:HG13	2.01	0.43
12:L:48:PRO:C	12:L:49:ASN:HD22	2.22	0.43
15:O:69:TYR:CZ	15:O:73:GLU:HG3	2.53	0.43
20:T:50:GLU:HB2	20:T:99:LEU:HD13	1.99	0.43
1:A:888:U:H2'	1:A:889:C:C6	2.54	0.43
10:J:3:LYS:C	10:J:4:ILE:HD13	2.38	0.43
1:A:227:G:H1'	1:A:257:A:N1	2.33	0.43
1:A:599:G:H1'	1:A:608:G:N2	2.34	0.43
2:B:17:PHE:HD2	2:B:17:PHE:N	2.17	0.43
1:A:385:C:H4'	16:P:28:ARG:NH2	2.33	0.43
1:A:1291:G:OP1	13:M:80:ARG:NH2	2.52	0.43
1:A:143:A:H2'	1:A:144:C:H6	1.83	0.43
1:A:49:U:C2	1:A:356:G:N2	2.87	0.43
1:A:424:U:O2	1:A:425:A:C8	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:484:C:OP1	12:L:117:ARG:NH2	2.45	0.43
3:C:21:ARG:HH12	10:J:93:GLY:HA3	1.83	0.43
7:G:45:ASP:O	7:G:49:ILE:HG13	2.18	0.43
11:K:124:LYS:HE2	11:K:125:PHE:CE1	2.53	0.43
1:A:714:G:OP1	1:A:749:A:H1'	2.19	0.43
2:B:47:THR:HA	2:B:202:PRO:HG2	2.01	0.43
5:E:118:ILE:HG12	5:E:119:LEU:N	2.34	0.43
7:G:57:GLU:O	7:G:61:VAL:HG23	2.18	0.43
12:L:27:LEU:C	12:L:29:GLY:N	2.67	0.43
17:Q:43:LEU:HD12	17:Q:68:ARG:HB3	1.99	0.43
1:A:1354:U:H2'	1:A:1355:G:O4'	2.18	0.43
1:A:353:U:H2'	1:A:354:U:C6	2.54	0.43
1:A:910:G:OP2	7:G:3:ARG:HB2	2.18	0.43
4:D:61:LYS:HD3	4:D:206:PHE:CE2	2.54	0.43
1:A:1173:C:O2	5:E:25:ARG:NH2	2.52	0.43
5:E:67:VAL:HG22	5:E:140:ARG:HE	1.83	0.43
6:F:26:ILE:HG23	6:F:79:LEU:HD11	2.01	0.43
1:A:1328:G:H22	1:A:1355:G:H2'	1.84	0.42
1:A:627:G:C5	1:A:628:C:C5	3.07	0.42
2:B:10:LEU:C	2:B:12:GLU:H	2.21	0.42
2:B:91:PRO:HG2	2:B:155:LEU:HG	2.00	0.42
6:F:7:ASN:HB2	6:F:89:MET:HB3	2.01	0.42
12:L:59:ARG:HG3	12:L:65:GLU:HG3	2.00	0.42
1:A:1288:U:H5'	13:M:109:THR:HG21	2.00	0.42
13:M:67:GLU:HB3	13:M:68:GLY:H	1.55	0.42
16:P:4:ILE:HG13	16:P:64:ALA:HB1	2.01	0.42
1:A:1149:A:C6	1:A:1150:A:C6	3.07	0.42
1:A:422:U:OP2	1:A:423:G:O2'	2.33	0.42
1:A:954:A:H2'	1:A:955:A:H5''	2.01	0.42
5:E:92:LYS:HA	5:E:93:PRO:HD3	1.86	0.42
6:F:74:ASP:HA	6:F:77:ARG:HD2	2.00	0.42
8:H:84:ARG:HB3	8:H:84:ARG:HE	1.46	0.42
15:O:74:ASP:O	15:O:76:GLU:N	2.52	0.42
16:P:21:VAL:HG21	16:P:59:TRP:CD1	2.54	0.42
17:Q:10:VAL:HB	17:Q:53:LEU:HA	2.01	0.42
1:A:108:G:H1'	1:A:109:A:N7	2.34	0.42
1:A:1102:G:H2'	1:A:1103:U:C6	2.54	0.42
1:A:1348:C:H2'	1:A:1349:C:H6	1.85	0.42
1:A:170:C:H2'	1:A:171:C:C6	2.53	0.42
1:A:207:C:H42	1:A:211:G:H1	1.67	0.42
1:A:849:A:O2'	1:A:850:A:H3'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:82:HIS:ND1	8:H:138:TRP:CE2	2.88	0.42
1:A:888:U:OP1	12:L:95:GLY:HA2	2.19	0.42
17:Q:60:ILE:HG22	17:Q:72:ARG:O	2.19	0.42
18:R:58:LEU:HD13	18:R:62:GLU:HB3	2.02	0.42
1:A:1306:C:H4'	21:V:17:THR:HG21	2.01	0.42
1:A:1319:G:C6	1:A:1320:A:C6	3.08	0.42
1:A:1381:C:C2	1:A:1383:G:C5	3.07	0.42
1:A:542:A:H4'	1:A:543:U:O5'	2.19	0.42
1:A:704:G:H4'	1:A:705:A:O5'	2.19	0.42
1:A:841:A:H2'	1:A:842:A:C8	2.54	0.42
1:A:889:C:O2'	1:A:890:A:H5'	2.19	0.42
2:B:10:LEU:H	2:B:10:LEU:HD23	1.84	0.42
9:I:43:ALA:C	9:I:45:ALA:H	2.22	0.42
11:K:12:ARG:HA	11:K:12:ARG:CZ	2.49	0.42
22:W:3:A:N1	23:X:34:RSQ:N3	2.68	0.42
1:A:1480:A:N6	1:A:1510:C:H5'	2.34	0.42
1:A:780:C:H2'	1:A:781:G:C8	2.54	0.42
2:B:212:GLN:O	2:B:216:SER:OG	2.20	0.42
6:F:8:ILE:HD13	6:F:26:ILE:HD13	2.00	0.42
10:J:24:VAL:O	10:J:26:ALA:N	2.50	0.42
3:C:26:LYS:NZ	10:J:45:ARG:HE	2.17	0.42
19:S:45:VAL:HA	19:S:62:ILE:HD13	2.00	0.42
1:A:1019:C:H2'	1:A:1020:C:H6	1.84	0.42
1:A:1033:C:H2'	1:A:1034:U:H6	1.85	0.42
2:B:178:ARG:HH22	8:H:74:PRO:CG	2.32	0.42
2:B:83:MET:SD	2:B:234:PRO:HB2	2.59	0.42
6:F:2:ARG:NH1	6:F:69:GLU:HG2	2.35	0.42
8:H:91:ARG:NH1	17:Q:32:TYR:O	2.53	0.42
9:I:37:PHE:CE2	9:I:74:ILE:HG13	2.55	0.42
13:M:91:ARG:HD2	13:M:91:ARG:HA	1.82	0.42
17:Q:59:ILE:HG23	17:Q:71:PHE:CD1	2.55	0.42
1:A:1266:A:H4'	1:A:1267:A:O5'	2.20	0.42
2:B:32:ILE:HD13	2:B:40:HIS:CG	2.55	0.42
4:D:156:GLU:O	4:D:160:GLN:HG2	2.19	0.42
6:F:77:ARG:HG2	6:F:78:GLU:N	2.34	0.42
9:I:17:VAL:HG11	9:I:81:ILE:HA	2.02	0.42
10:J:5:ARG:O	10:J:98:ILE:HA	2.19	0.42
15:O:17:ARG:HH11	15:O:17:ARG:HG3	1.85	0.42
1:A:1433:G:H2'	1:A:1434:G:O4'	2.20	0.42
1:A:190:G:H4'	1:A:191:G:OP2	2.20	0.42
1:A:816:U:H2'	1:A:817:C:H6	1.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:9:VAL:CG2	6:F:87:ARG:HB2	2.50	0.42
9:I:36:TYR:OH	9:I:73:GLN:NE2	2.47	0.42
17:Q:3:LYS:HD3	17:Q:61:GLU:O	2.20	0.42
1:A:906:G:C6	1:A:907:C:C4	3.08	0.42
2:B:118:LEU:HA	2:B:118:LEU:HD23	1.93	0.42
13:M:17:VAL:O	13:M:20:THR:HB	2.20	0.42
1:A:1286:G:H5''	21:V:4:GLY:HA3	2.01	0.42
1:A:1083:A:H8	2:B:172:ILE:HD13	1.84	0.42
1:A:1277:C:H5''	13:M:14:ARG:HD2	2.01	0.42
1:A:849:A:C8	1:A:851:G:C8	3.08	0.42
3:C:76:VAL:HG11	3:C:103:VAL:HG21	2.02	0.42
5:E:78:HIS:HB2	5:E:79:GLU:H	1.71	0.42
8:H:86:ILE:HG12	8:H:135:CYS:HA	2.01	0.42
15:O:3:ILE:HG21	15:O:34:LEU:CD1	2.50	0.42
17:Q:29:HIS:CE1	17:Q:30:PRO:HG2	2.55	0.42
17:Q:43:LEU:HD23	17:Q:43:LEU:HA	1.91	0.42
1:A:1036:C:OP1	1:A:1178:G:OP2	2.37	0.41
1:A:272:C:H5'	17:Q:68:ARG:HH12	1.84	0.41
1:A:501:C:OP2	1:A:513:G:H4'	2.20	0.41
1:A:557:A:N3	1:A:860:C:H1'	2.35	0.41
17:Q:29:HIS:HA	17:Q:30:PRO:HD2	1.85	0.41
19:S:33:THR:OG1	19:S:34:TRP:N	2.51	0.41
1:A:217:U:H2'	1:A:218:U:C6	2.55	0.41
1:A:47:C:OP2	1:A:361:C:N4	2.39	0.41
2:B:71:VAL:O	2:B:164:VAL:HA	2.20	0.41
2:B:90:MET:HA	2:B:91:PRO:HD3	1.82	0.41
4:D:108:LEU:HD13	4:D:183:GLY:HA3	2.01	0.41
7:G:87:VAL:HA	7:G:88:PRO:HD3	1.92	0.41
10:J:50:ILE:N	10:J:50:ILE:HD12	2.34	0.41
10:J:34:VAL:HG22	10:J:74:ILE:HG22	2.01	0.41
11:K:43:SER:OG	11:K:44:SER:N	2.52	0.41
14:N:10:ALA:O	14:N:12:ARG:N	2.53	0.41
1:A:1306:C:P	21:V:6:ARG:HH22	2.44	0.41
1:A:652:U:H2'	1:A:653:G:C8	2.54	0.41
2:B:144:ARG:HG3	2:B:145:LEU:N	2.35	0.41
3:C:3:ASN:N	3:C:3:ASN:ND2	2.67	0.41
4:D:113:SER:OG	4:D:114:ARG:N	2.52	0.41
5:E:148:VAL:O	5:E:152:ARG:HG3	2.20	0.41
5:E:15:ARG:HD3	5:E:26:PHE:CD1	2.56	0.41
9:I:118:LYS:HB2	9:I:121:ARG:HB3	2.01	0.41
11:K:92:GLU:OE2	18:R:88:LYS:NZ	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:503:A:OP2	12:L:51:ALA:HB1	2.19	0.41
13:M:23:TYR:CB	13:M:67:GLU:HA	2.48	0.41
2:B:8:LYS:HB3	2:B:9:GLU:H	1.48	0.41
4:D:194:LEU:HD22	4:D:194:LEU:H	1.85	0.41
1:A:689:A:H4'	11:K:29:ILE:HD11	2.02	0.41
12:L:41:ARG:HH22	12:L:57:LYS:HE3	1.86	0.41
15:O:60:VAL:O	15:O:64:ARG:HG2	2.21	0.41
16:P:40:ASP:HA	16:P:41:PRO:HD3	1.87	0.41
1:A:1374:G:O2'	1:A:1375:U:H5'	2.20	0.41
1:A:17:U:H1'	1:A:1062:A:N3	2.34	0.41
1:A:341:G:H2'	1:A:342:G:O4'	2.20	0.41
1:A:512:G:H22	12:L:51:ALA:HB2	1.85	0.41
4:D:102:ASP:HB3	4:D:136:PRO:HB3	2.02	0.41
8:H:121:ASP:N	8:H:121:ASP:OD1	2.52	0.41
14:N:9:LYS:HG3	14:N:21:TYR:O	2.19	0.41
16:P:39:TYR:HA	16:P:48:TRP:O	2.21	0.41
1:A:752:G:H4'	1:A:1490:A:H4'	2.02	0.41
1:A:904:G:N2	1:A:1373:U:H1'	2.36	0.41
1:A:939:C:H2'	1:A:940:G:O4'	2.20	0.41
2:B:97:TRP:CZ2	2:B:102:LEU:HD13	2.53	0.41
3:C:15:THR:OG1	3:C:16:ARG:N	2.53	0.41
10:J:65:LEU:HD12	14:N:55:GLY:O	2.21	0.41
17:Q:97:SER:OG	17:Q:98:LEU:HD12	2.20	0.41
20:T:37:SER:O	20:T:38:LYS:C	2.59	0.41
1:A:1390:A:H2'	1:A:1391:C:C6	2.54	0.41
1:A:64:G:H2'	1:A:64:G:H8	1.51	0.41
1:A:763:A:O2'	1:A:764:A:H5''	2.21	0.41
2:B:230:VAL:HB	2:B:231:GLU:H	1.53	0.41
3:C:154:SER:O	3:C:165:THR:HA	2.21	0.41
5:E:88:LYS:HB3	5:E:123:LEU:HB2	2.03	0.41
12:L:92:ASP:O	12:L:94:PRO:HD3	2.21	0.41
13:M:46:LYS:H	13:M:46:LYS:HG3	1.56	0.41
1:A:1362:U:H4'	1:A:1363:U:O5'	2.21	0.41
1:A:187:C:C4	1:A:188:U:C4	3.09	0.41
1:A:155:A:N6	1:A:342:G:HO2'	2.18	0.41
1:A:424:U:O3'	4:D:22:LYS:NZ	2.53	0.41
2:B:32:ILE:HD13	2:B:40:HIS:CD2	2.56	0.41
3:C:141:VAL:HG11	3:C:202:ILE:HG12	2.03	0.41
7:G:85:TYR:HA	7:G:85:TYR:HD2	1.75	0.41
18:R:51:LEU:HA	18:R:52:PRO:HD3	1.82	0.41
18:R:76:LEU:HA	18:R:76:LEU:HD23	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:G:H4'	1:A:176:U:H5'	2.03	0.41
1:A:520:G:H2'	1:A:521:G:H8	1.85	0.41
1:A:617:C:O2	1:A:617:C:H2'	2.20	0.41
3:C:164:ARG:HD2	3:C:166:GLU:OE2	2.21	0.41
4:D:30:LYS:C	4:D:32:ALA:H	2.23	0.41
1:A:525:G:H5'	4:D:41:GLY:HA3	2.02	0.41
4:D:38:TYR:HB2	4:D:44:GLY:O	2.21	0.41
5:E:78:HIS:HE1	5:E:142:LEU:HA	1.85	0.41
5:E:80:ILE:H	5:E:80:ILE:HD12	1.85	0.41
8:H:51:VAL:HG11	8:H:60:ARG:CZ	2.50	0.41
1:A:1324:G:H1'	9:I:121:ARG:NH2	2.36	0.41
1:A:210:U:H4'	1:A:211:G:O5'	2.20	0.41
1:A:527:G:C6	1:A:528:C:C4	3.09	0.41
1:A:948:G:H4'	1:A:949:C:C5'	2.51	0.41
2:B:82:ARG:HA	2:B:92:TYR:CD1	2.56	0.41
5:E:28:PHE:CD2	5:E:51:VAL:HG22	2.56	0.41
5:E:9:LYS:HD2	5:E:9:LYS:HA	1.83	0.41
12:L:10:LEU:HA	12:L:10:LEU:HD23	1.69	0.41
13:M:33:ALA:O	13:M:37:THR:HB	2.21	0.41
15:O:29:VAL:HG11	15:O:67:LEU:HD21	2.01	0.41
15:O:33:THR:HA	15:O:36:ILE:HD12	2.03	0.41
15:O:3:ILE:HG23	15:O:38:ARG:NH2	2.36	0.41
17:Q:67:LYS:HA	17:Q:70:ARG:NH2	2.35	0.41
20:T:104:LEU:HD23	20:T:104:LEU:HA	1.90	0.41
1:A:57:G:H2'	1:A:58:C:C6	2.56	0.41
4:D:79:PHE:CE1	4:D:204:ILE:HG12	2.56	0.41
11:K:48:ILE:HD11	11:K:67:ASP:HB2	2.02	0.41
12:L:38:THR:O	12:L:39:VAL:HB	2.21	0.41
13:M:3:ARG:HH12	13:M:7:VAL:HA	1.86	0.41
1:A:1277:C:H4'	1:A:1283:U:C5	2.55	0.40
1:A:950:G:O3'	14:N:41:ARG:NH2	2.52	0.40
4:D:49:ARG:NE	4:D:49:ARG:H	2.19	0.40
1:A:1008:C:N4	1:A:1013:G:H1	2.19	0.40
1:A:1036:C:H41	23:X:34:RSQ:C1'	2.33	0.40
1:A:103:C:H2'	1:A:104:G:O4'	2.21	0.40
1:A:1139:A:C5	1:A:1161:A:C6	3.09	0.40
1:A:406:A:H62	1:A:408:G:N2	2.20	0.40
1:A:494:C:H2'	1:A:494:C:H6	1.67	0.40
1:A:547:C:OP1	12:L:15:ARG:NE	2.50	0.40
1:A:615:A:H2'	1:A:616:G:O4'	2.21	0.40
2:B:44:LEU:H	2:B:44:LEU:HG	1.70	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:140:VAL:HG11	4:D:146:ILE:HD11	2.03	0.40
5:E:131:ILE:HD13	5:E:131:ILE:HA	1.93	0.40
7:G:137:LYS:HB2	7:G:137:LYS:HE3	1.86	0.40
7:G:99:LEU:HD23	7:G:99:LEU:HA	1.87	0.40
8:H:1:MET:HG2	8:H:2:LEU:N	2.35	0.40
9:I:4:TYR:CE2	9:I:88:TYR:HA	2.56	0.40
12:L:31:PRO:HB2	12:L:32:PHE:CE2	2.55	0.40
12:L:41:ARG:HG2	12:L:42:THR:N	2.35	0.40
13:M:124:PRO:C	13:M:126:LYS:H	2.25	0.40
17:Q:53:LEU:O	17:Q:53:LEU:HD12	2.21	0.40
21:V:5:ASP:O	21:V:11:GLY:HA3	2.21	0.40
1:A:1378:A:H2	5:E:19:MET:HG3	1.85	0.40
1:A:398:C:OP1	4:D:136:PRO:HD2	2.20	0.40
1:A:98:G:H2'	1:A:99:C:C6	2.56	0.40
5:E:151:LEU:HA	5:E:151:LEU:HD23	1.93	0.40
7:G:8:GLU:N	7:G:8:GLU:OE2	2.46	0.40
8:H:17:THR:HB	8:H:78:GLN:OE1	2.21	0.40
8:H:4:ASP:CG	8:H:85:ARG:HH11	2.22	0.40
1:A:1317:C:O5'	1:A:1317:C:H6	2.03	0.40
1:A:297:G:H5''	12:L:17:LYS:HE3	2.04	0.40
1:A:423:G:H4'	1:A:424:U:O5'	2.21	0.40
2:B:93:VAL:HG11	2:B:97:TRP:CD1	2.56	0.40
1:A:15:G:H21	5:E:18:ARG:HA	1.86	0.40
5:E:44:GLY:HA3	5:E:62:ALA:HB2	2.03	0.40
7:G:120:ILE:N	7:G:120:ILE:HD12	2.36	0.40
12:L:93:LEU:HB2	12:L:96:VAL:CG2	2.51	0.40
1:A:704:G:OP2	18:R:53:ARG:HG3	2.22	0.40
1:A:1022:U:C2	1:A:1023:A:C8	3.10	0.40
1:A:1281:G:C6	1:A:1316:C:C5	3.09	0.40
1:A:1379:C:H4'	1:A:1380:A:OP2	2.20	0.40
1:A:675:U:H1'	1:A:678:A:N7	2.37	0.40
1:A:948:G:H3'	1:A:948:G:P	2.62	0.40
1:A:982:A:C8	1:A:1020:C:N3	2.89	0.40
3:C:155:GLY:O	3:C:156:ARG:HB2	2.21	0.40
18:R:83:GLU:HB3	18:R:84:LYS:H	1.62	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%)	33 (14%)	15 (6%)	1	10
3	C	204/206 (99%)	147 (72%)	40 (20%)	17 (8%)	1	5
4	D	206/208 (99%)	172 (84%)	24 (12%)	10 (5%)	2	17
5	E	148/150 (99%)	126 (85%)	19 (13%)	3 (2%)	7	38
6	F	99/101 (98%)	88 (89%)	9 (9%)	2 (2%)	7	38
7	G	153/155 (99%)	130 (85%)	18 (12%)	5 (3%)	4	25
8	H	136/138 (99%)	117 (86%)	18 (13%)	1 (1%)	22	61
9	I	125/127 (98%)	96 (77%)	20 (16%)	9 (7%)	1	7
10	J	96/98 (98%)	67 (70%)	18 (19%)	11 (12%)	0	2
11	K	117/119 (98%)	99 (85%)	16 (14%)	2 (2%)	9	42
12	L	122/124 (98%)	96 (79%)	18 (15%)	8 (7%)	1	9
13	M	123/125 (98%)	98 (80%)	19 (15%)	6 (5%)	2	17
14	N	58/60 (97%)	49 (84%)	5 (9%)	4 (7%)	1	8
15	O	86/88 (98%)	75 (87%)	9 (10%)	2 (2%)	6	34
16	P	81/83 (98%)	72 (89%)	8 (10%)	1 (1%)	13	49
17	Q	102/104 (98%)	85 (83%)	11 (11%)	6 (6%)	1	12
18	R	71/73 (97%)	63 (89%)	6 (8%)	2 (3%)	5	29
19	S	78/80 (98%)	60 (77%)	10 (13%)	8 (10%)	0	3
20	T	97/99 (98%)	75 (77%)	13 (13%)	9 (9%)	0	3
21	V	22/24 (92%)	20 (91%)	2 (9%)	0	100	100
All	All	2356/2396 (98%)	1919 (82%)	316 (13%)	121 (5%)	2	15

All (121) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	36	ARG

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Mol	Chain	Res	Type
2	B	211	ILE
2	B	229	VAL
3	C	15	THR
3	C	160	ALA
4	D	31	CYS
4	D	36	ARG
4	D	171	GLY
5	E	77	PRO
7	G	134	ALA
9	I	12	GLU
9	I	101	PHE
11	K	55	LYS
12	L	27	LEU
12	L	28	LYS
12	L	47	LYS
13	M	27	LYS
13	M	86	CYS
14	N	11	LYS
17	Q	49	GLU
17	Q	100	LYS
19	S	9	VAL
20	T	73	HIS
20	T	99	LEU
2	B	8	LYS
2	B	14	GLY
2	B	17	PHE
2	B	210	SER
3	C	4	LYS
3	C	47	LEU
3	C	64	VAL
3	C	98	ASN
3	C	101	LEU
3	C	154	SER
4	D	69	GLY
4	D	208	SER
7	G	4	ARG
7	G	93	PRO
9	I	42	ARG
9	I	43	ALA
9	I	93	ARG
10	J	4	ILE
10	J	34	VAL

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Mol	Chain	Res	Type
10	J	54	PHE
10	J	90	LEU
12	L	39	VAL
12	L	79	GLU
19	S	5	LEU
19	S	6	LYS
20	T	9	ASN
20	T	94	ALA
2	B	20	GLU
2	B	207	ALA
3	C	43	LEU
3	C	66	VAL
3	C	127	ARG
3	C	146	ALA
3	C	181	ASN
4	D	5	ILE
5	E	71	LEU
6	F	16	GLN
9	I	51	ARG
9	I	54	ASP
9	I	88	TYR
10	J	73	ASP
12	L	105	TYR
13	M	113	PRO
15	O	10	LYS
17	Q	97	SER
18	R	47	THR
19	S	47	HIS
19	S	77	THR
20	T	95	ALA
2	B	9	GLU
2	B	95	GLN
2	B	228	GLY
2	B	232	PRO
3	C	29	TYR
3	C	206	GLU
4	D	35	ARG
6	F	43	LEU
7	G	7	ALA
10	J	39	PRO
10	J	40	LEU
10	J	72	VAL

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Mol	Chain	Res	Type
12	L	123	LYS
14	N	8	GLU
14	N	14	PRO
15	O	72	ARG
17	Q	30	PRO
18	R	45	SER
19	S	30	LEU
19	S	78	ARG
20	T	96	GLY
20	T	98	PRO
2	B	15	VAL
2	B	130	ARG
3	C	3	ASN
3	C	108	ASN
9	I	105	ASP
10	J	26	ALA
11	K	35	PRO
14	N	12	ARG
20	T	102	GLY
4	D	184	LYS
5	E	78	HIS
10	J	25	GLU
13	M	67	GLU
13	M	84	ILE
20	T	97	ALA
8	H	51	VAL
7	G	82	GLY
13	M	97	PRO
16	P	10	GLY
17	Q	77	VAL
4	D	44	GLY
4	D	88	VAL
10	J	77	PRO
12	L	30	ALA
17	Q	80	GLY
19	S	67	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%)	166 (82%)	36 (18%)	2	9
3	C	160/160 (100%)	134 (84%)	26 (16%)	2	11
4	D	180/180 (100%)	149 (83%)	31 (17%)	2	10
5	E	115/115 (100%)	91 (79%)	24 (21%)	1	6
6	F	90/90 (100%)	76 (84%)	14 (16%)	2	12
7	G	126/126 (100%)	115 (91%)	11 (9%)	10	37
8	H	119/119 (100%)	106 (89%)	13 (11%)	6	26
9	I	98/98 (100%)	83 (85%)	15 (15%)	2	13
10	J	88/88 (100%)	75 (85%)	13 (15%)	3	14
11	K	90/90 (100%)	76 (84%)	14 (16%)	2	12
12	L	104/104 (100%)	85 (82%)	19 (18%)	1	8
13	M	100/100 (100%)	83 (83%)	17 (17%)	2	10
14	N	49/49 (100%)	38 (78%)	11 (22%)	1	4
15	O	79/79 (100%)	66 (84%)	13 (16%)	2	10
16	P	72/72 (100%)	64 (89%)	8 (11%)	6	25
17	Q	96/96 (100%)	86 (90%)	10 (10%)	7	28
18	R	64/64 (100%)	57 (89%)	7 (11%)	6	26
19	S	71/71 (100%)	60 (84%)	11 (16%)	2	12
20	T	76/76 (100%)	67 (88%)	9 (12%)	5	23
21	V	19/19 (100%)	17 (90%)	2 (10%)	7	28
All	All	1998/1998 (100%)	1694 (85%)	304 (15%)	3	13

All (304) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	8	LYS
2	B	9	GLU
2	B	12	GLU
2	B	15	VAL
2	B	16	HIS
2	B	17	PHE
2	B	21	ARG
2	B	23	ARG

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Mol	Chain	Res	Type
2	B	24	TRP
2	B	27	LYS
2	B	48	MET
2	B	51	LEU
2	B	64	ARG
2	B	76	GLN
2	B	79	ASP
2	B	90	MET
2	B	92	TYR
2	B	107	THR
2	B	108	ILE
2	B	117	GLU
2	B	118	LEU
2	B	121	LEU
2	B	127	ILE
2	B	130	ARG
2	B	144	ARG
2	B	150	SER
2	B	153	ARG
2	B	162	ILE
2	B	163	PHE
2	B	165	VAL
2	B	169	LYS
2	B	170	GLU
2	B	196	LEU
2	B	212	GLN
2	B	224	GLN
2	B	236	TYR
3	C	3	ASN
3	C	4	LYS
3	C	5	ILE
3	C	14	ILE
3	C	26	LYS
3	C	31	HIS
3	C	47	LEU
3	C	52	LEU
3	C	67	THR
3	C	75	VAL
3	C	84	ILE
3	C	89	GLU
3	C	101	LEU
3	C	107	GLN

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Mol	Chain	Res	Type
3	C	128	PHE
3	C	156	ARG
3	C	161	GLU
3	C	162	GLN
3	C	165	THR
3	C	166	GLU
3	C	167	TRP
3	C	175	LEU
3	C	177	THR
3	C	188	LEU
3	C	192	THR
3	C	204	LEU
4	D	3	ARG
4	D	5	ILE
4	D	8	VAL
4	D	10	ARG
4	D	24	GLU
4	D	35	ARG
4	D	42	GLN
4	D	49	ARG
4	D	53	ASP
4	D	58	LEU
4	D	64	LEU
4	D	70	ILE
4	D	84	LYS
4	D	89	THR
4	D	96	LEU
4	D	99	SER
4	D	122	ARG
4	D	127	THR
4	D	151	LYS
4	D	154	ASN
4	D	155	LEU
4	D	175	SER
4	D	176	LEU
4	D	178	VAL
4	D	187	ARG
4	D	190	ASP
4	D	191	ARG
4	D	193	ASP
4	D	194	LEU
4	D	199	ASN

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Mol	Chain	Res	Type
4	D	200	GLU
5	E	5	ASP
5	E	10	MET
5	E	11	ILE
5	E	13	ILE
5	E	18	ARG
5	E	20	GLN
5	E	31	LEU
5	E	41	VAL
5	E	43	LEU
5	E	47	LYS
5	E	53	LEU
5	E	60	TYR
5	E	78	HIS
5	E	79	GLU
5	E	80	ILE
5	E	81	GLU
5	E	92	LYS
5	E	112	LEU
5	E	116	THR
5	E	125	SER
5	E	137	GLU
5	E	140	ARG
5	E	147	ASP
5	E	152	ARG
6	F	1	MET
6	F	10	LEU
6	F	13	ASN
6	F	14	LEU
6	F	17	SER
6	F	23	LYS
6	F	43	LEU
6	F	47	ARG
6	F	70	ASP
6	F	74	ASP
6	F	77	ARG
6	F	79	LEU
6	F	93	SER
6	F	94	GLN
7	G	8	GLU
7	G	12	LEU
7	G	22	LEU

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Mol	Chain	Res	Type
7	G	32	ARG
7	G	45	ASP
7	G	75	VAL
7	G	98	SER
7	G	104	LEU
7	G	114	ARG
7	G	129	GLU
7	G	136	LYS
8	H	18	ARG
8	H	24	THR
8	H	26	VAL
8	H	56	LYS
8	H	85	ARG
8	H	87	SER
8	H	91	ARG
8	H	92	ARG
8	H	98	LYS
8	H	100	ILE
8	H	102	ARG
8	H	107	LEU
8	H	116	LYS
9	I	2	GLU
9	I	12	GLU
9	I	25	LYS
9	I	27	THR
9	I	38	GLN
9	I	51	ARG
9	I	58	ARG
9	I	59	PHE
9	I	62	TYR
9	I	66	ARG
9	I	79	LEU
9	I	88	TYR
9	I	105	ASP
9	I	114	TYR
9	I	124	GLN
10	J	4	ILE
10	J	6	ILE
10	J	15	THR
10	J	16	LEU
10	J	23	ILE
10	J	35	SER

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Mol	Chain	Res	Type
10	J	38	ILE
10	J	45	ARG
10	J	71	LEU
10	J	83	GLU
10	J	86	MET
10	J	90	LEU
10	J	96	ILE
11	K	12	ARG
11	K	29	ILE
11	K	30	VAL
11	K	33	THR
11	K	34	ASP
11	K	41	THR
11	K	48	ILE
11	K	63	LEU
11	K	77	MET
11	K	84	VAL
11	K	92	GLU
11	K	109	VAL
11	K	114	VAL
11	K	124	LYS
12	L	18	VAL
12	L	33	ARG
12	L	42	THR
12	L	53	ARG
12	L	54	LYS
12	L	60	LEU
12	L	64	TYR
12	L	67	THR
12	L	75	HIS
12	L	79	GLU
12	L	80	HIS
12	L	81	SER
12	L	82	VAL
12	L	83	VAL
12	L	85	ILE
12	L	89	ARG
12	L	93	LEU
12	L	111	LYS
12	L	127	GLU
13	M	9	ILE
13	M	11	ARG

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Mol	Chain	Res	Type
13	M	14	ARG
13	M	37	THR
13	M	44	ARG
13	M	47	ASP
13	M	56	LEU
13	M	60	VAL
13	M	63	THR
13	M	67	GLU
13	M	70	LEU
13	M	73	GLU
13	M	77	ASN
13	M	92	HIS
13	M	105	THR
13	M	108	ARG
13	M	125	ARG
14	N	8	GLU
14	N	9	LYS
14	N	11	LYS
14	N	12	ARG
14	N	16	PHE
14	N	22	THR
14	N	31	ARG
14	N	32	SER
14	N	33	VAL
14	N	42	ILE
14	N	53	LEU
15	O	7	GLU
15	O	13	GLN
15	O	21	ASP
15	O	22	THR
15	O	31	LEU
15	O	34	LEU
15	O	38	ARG
15	O	39	LEU
15	O	57	LEU
15	O	70	LEU
15	O	76	GLU
15	O	81	LEU
15	O	83	GLU
16	P	2	VAL
16	P	8	ARG
16	P	28	ARG

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Mol	Chain	Res	Type
16	P	31	LYS
16	P	45	THR
16	P	53	VAL
16	P	62	VAL
16	P	72	ARG
17	Q	38	ARG
17	Q	59	ILE
17	Q	69	LYS
17	Q	70	ARG
17	Q	74	LEU
17	Q	78	GLU
17	Q	79	SER
17	Q	83	ASP
17	Q	84	LEU
17	Q	100	LYS
18	R	21	LYS
18	R	26	LEU
18	R	28	GLU
18	R	47	THR
18	R	54	ARG
18	R	55	ARG
18	R	86	VAL
19	S	5	LEU
19	S	6	LYS
19	S	7	LYS
19	S	31	ILE
19	S	33	THR
19	S	35	SER
19	S	40	ILE
19	S	62	ILE
19	S	65	ASN
19	S	67	VAL
19	S	70	LYS
20	T	10	LEU
20	T	13	LEU
20	T	42	GLN
20	T	50	GLU
20	T	62	LEU
20	T	72	LEU
20	T	74	LYS
20	T	75	ASN
20	T	84	LEU

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Mol	Chain	Res	Type
21	V	8	THR
21	V	15	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	16	HIS
2	B	40	HIS
3	C	110	ASN
4	D	42	GLN
5	E	78	HIS
6	F	73	ASN
10	J	76	ASN
11	K	93	GLN
16	P	16	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1513/1513 (100%)	327 (21%)	73 (4%)
22	W	3/6 (50%)	1 (33%)	0
23	X	4/17 (23%)	2 (50%)	0
All	All	1520/1536 (98%)	330 (21%)	73 (4%)

All (330) 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	59	A
1	A	65	U
1	A	73	G
1	A	94	A

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Mol	Chain	Res	Type
1	A	114	C
1	A	123	G
1	A	124	A
1	A	125	C
1	A	156	A
1	A	157	C
1	A	163	C
1	A	167	U
1	A	168	C
1	A	176	U
1	A	177	G
1	A	189	U
1	A	190	G
1	A	191	G
1	A	193	G
1	A	201	A
1	A	203	A
1	A	207	C
1	A	208	U
1	A	211	G
1	A	212	C
1	A	239	U
1	A	240	C
1	A	242	G
1	A	246	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	296	G
1	A	316	A
1	A	323	C
1	A	324	A
1	A	325	C
1	A	326	G
1	A	327	G
1	A	340	C
1	A	341	G
1	A	342	G
1	A	343	G

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Mol	Chain	Res	Type
1	A	346	G
1	A	347	C
1	A	348	A
1	A	349	G
1	A	351	A
1	A	362	U
1	A	367	C
1	A	379	G
1	A	383	G
1	A	384	A
1	A	393	C
1	A	401	G
1	A	404	G
1	A	407	A
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	432	U
1	A	442	A
1	A	445	A
1	A	446	A
1	A	447	A
1	A	454	A
1	A	456	G
1	A	457	A
1	A	466	A
1	A	469	G
1	A	470	U
1	A	479	A
1	A	480	A
1	A	481	U
1	A	483	G
1	A	494	C
1	A	495	U
1	A	496	C
1	A	501	C
1	A	502	C
1	A	504	G
1	A	507	G

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Mol	Chain	Res	Type
1	A	513	G
1	A	514	U
1	A	515	A
1	A	516	A
1	A	528	C
1	A	530	A
1	A	531	G
1	A	542	A
1	A	543	U
1	A	544	U
1	A	547	C
1	A	553	G
1	A	555	A
1	A	556	A
1	A	559	G
1	A	560	G
1	A	562	G
1	A	564	G
1	A	565	U
1	A	590	A
1	A	617	C
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	696	G
1	A	705	A
1	A	706	U
1	A	714	G
1	A	716	A
1	A	738	G
1	A	749	A
1	A	756	G
1	A	760	A
1	A	763	A
1	A	764	A
1	A	765	A
1	A	768	G

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Mol	Chain	Res	Type
1	A	773	A
1	A	775	A
1	A	776	U
1	A	777	A
1	A	795	C
1	A	796	U
1	A	798	A
1	A	799	A
1	A	800	C
1	A	802	A
1	A	803	U
1	A	811	A
1	A	812	G
1	A	822	U
1	A	823	C
1	A	824	U
1	A	825	C
1	A	828	G
1	A	835	G
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	870	C
1	A	891	A
1	A	896	A
1	A	903	G
1	A	904	G
1	A	906	G
1	A	911	C
1	A	912	A
1	A	937	U
1	A	938	U
1	A	943	G
1	A	945	A
1	A	946	A
1	A	948	G
1	A	949	C
1	A	952	A

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Mol	Chain	Res	Type
1	A	953	G
1	A	954	A
1	A	960	A
1	A	961	C
1	A	964	G
1	A	968	U
1	A	969	U
1	A	970	G
1	A	971	A
1	A	972	C
1	A	977	U
1	A	979	G
1	A	980	G
1	A	981	G
1	A	982	A
1	A	983	A
1	A	984	C
1	A	986	C
1	A	987	G
1	A	992	A
1	A	994	A
1	A	1003	U
1	A	1004	G
1	A	1006	C
1	A	1007	C
1	A	1010	C
1	A	1013	G
1	A	1022	U
1	A	1035	G
1	A	1036	C
1	A	1037	A
1	A	1047	U
1	A	1048	C
1	A	1076	G
1	A	1077	U
1	A	1083	A
1	A	1086	G
1	A	1106	G
1	A	1107	U
1	A	1108	U
1	A	1109	G
1	A	1111	C

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Mol	Chain	Res	Type
1	A	1112	A
1	A	1113	G
1	A	1114	C
1	A	1119	C
1	A	1121	G
1	A	1122	C
1	A	1125	G
1	A	1127	C
1	A	1128	A
1	A	1136	G
1	A	1139	A
1	A	1140	C
1	A	1141	U
1	A	1142	G
1	A	1149	A
1	A	1151	A
1	A	1152	G
1	A	1163	G
1	A	1164	A
1	A	1172	A
1	A	1177	U
1	A	1178	G
1	A	1182	A
1	A	1183	G
1	A	1185	A
1	A	1186	U
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	1208	A
1	A	1209	C
1	A	1219	A
1	A	1221	U
1	A	1222	G
1	A	1231	A
1	A	1234	G
1	A	1237	A
1	A	1238	U
1	A	1239	G

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Mol	Chain	Res	Type
1	A	1251	C
1	A	1254	G
1	A	1258	C
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	1293	G
1	A	1294	U
1	A	1297	G
1	A	1298	C
1	A	1300	A
1	A	1301	C
1	A	1304	G
1	A	1313	A
1	A	1316	C
1	A	1317	C
1	A	1318	G
1	A	1319	G
1	A	1326	U
1	A	1327	A
1	A	1329	U
1	A	1334	G
1	A	1344	C
1	A	1345	A
1	A	1346	U
1	A	1352	G
1	A	1360	C
1	A	1361	G
1	A	1363	U
1	A	1365	C
1	A	1376	A
1	A	1379	C
1	A	1380	A
1	A	1425	G
1	A	1426	A
1	A	1433	G

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Mol	Chain	Res	Type
1	A	1464	G
1	A	1466	G
1	A	1469	A
1	A	1471	G
1	A	1474	G
1	A	1480	A
1	A	1481	G
1	A	1482	G
1	A	1483	U
1	A	1484	A
1	A	1494	G
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	1519	U
1	A	1521	U
22	W	3	A
23	X	38	C
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	64	G
1	A	101	G
1	A	123	G
1	A	155	A
1	A	175	G
1	A	188	U
1	A	189	U
1	A	190	G
1	A	210	U
1	A	239	U
1	A	276	G
1	A	323	C
1	A	340	C

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Mol	Chain	Res	Type
1	A	347	C
1	A	383	G
1	A	417	C
1	A	423	G
1	A	424	U
1	A	445	A
1	A	468	G
1	A	469	G
1	A	479	A
1	A	482	A
1	A	494	C
1	A	500	G
1	A	501	C
1	A	530	A
1	A	542	A
1	A	558	G
1	A	669	U
1	A	670	A
1	A	684	C
1	A	704	G
1	A	705	A
1	A	776	U
1	A	795	C
1	A	798	A
1	A	802	A
1	A	847	U
1	A	861	U
1	A	937	U
1	A	942	A
1	A	948	G
1	A	959	U
1	A	969	U
1	A	1035	G
1	A	1036	C
1	A	1076	G
1	A	1110	C
1	A	1111	C
1	A	1139	A
1	A	1163	G
1	A	1171	G
1	A	1182	A
1	A	1194	A

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Mol	Chain	Res	Type
1	A	1206	A
1	A	1220	A
1	A	1278	C
1	A	1279	C
1	A	1281	G
1	A	1316	C
1	A	1317	C
1	A	1326	U
1	A	1328	G
1	A	1345	A
1	A	1362	U
1	A	1378	A
1	A	1379	C
1	A	1432	C
1	A	1481	G
1	A	1510	C

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	-	16,23,24	2.09	3 (18%)	20,33,36	1.62	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	-	-	2/7/27/28	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	6.17	1.42	1.21
23	X	34	RSQ	C5-C10	4.00	1.56	1.47
23	X	34	RSQ	C5-C4	3.43	1.45	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	X	34	RSQ	C2-N3-C4	4.79	121.80	116.02
23	X	34	RSQ	O30-C10-C5	-3.81	114.29	124.36

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	X	34	RSQ	O30-C10-C5-C4
23	X	34	RSQ	O30-C10-C5-C6

There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	X	34	RSQ	8	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	1.14	3 (6%)	64,67,67	1.70	13 (20%)

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	-	-	6/18/94/94	0/4/4/4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	1785	PAR	C52-C42	3.64	1.59	1.52
25	A	1785	PAR	C64-C54	3.01	1.56	1.52
25	A	1785	PAR	C22-C12	-2.31	1.48	1.53

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	1785	PAR	O33-C14-C24	6.55	119.50	108.22
25	A	1785	PAR	O52-C13-C23	3.83	115.90	107.96
25	A	1785	PAR	C34-C24-N24	-3.46	103.96	111.05
25	A	1785	PAR	O34-C34-C44	-3.05	103.31	110.35
25	A	1785	PAR	C14-O33-C33	-3.02	110.49	117.96
25	A	1785	PAR	O54-C54-C44	2.91	114.98	109.69
25	A	1785	PAR	C13-O52-C52	-2.84	110.94	117.96
25	A	1785	PAR	O11-C11-O51	2.80	118.50	110.67
25	A	1785	PAR	O43-C13-C23	-2.77	101.41	104.98
25	A	1785	PAR	C11-O51-C51	2.54	118.68	113.69
25	A	1785	PAR	O34-C34-C24	-2.18	106.30	110.22
25	A	1785	PAR	O51-C51-C61	2.12	111.71	106.44
25	A	1785	PAR	O52-C13-O43	-2.09	109.17	111.43

There are no chirality outliers.

All (6) torsion outliers are listed below:

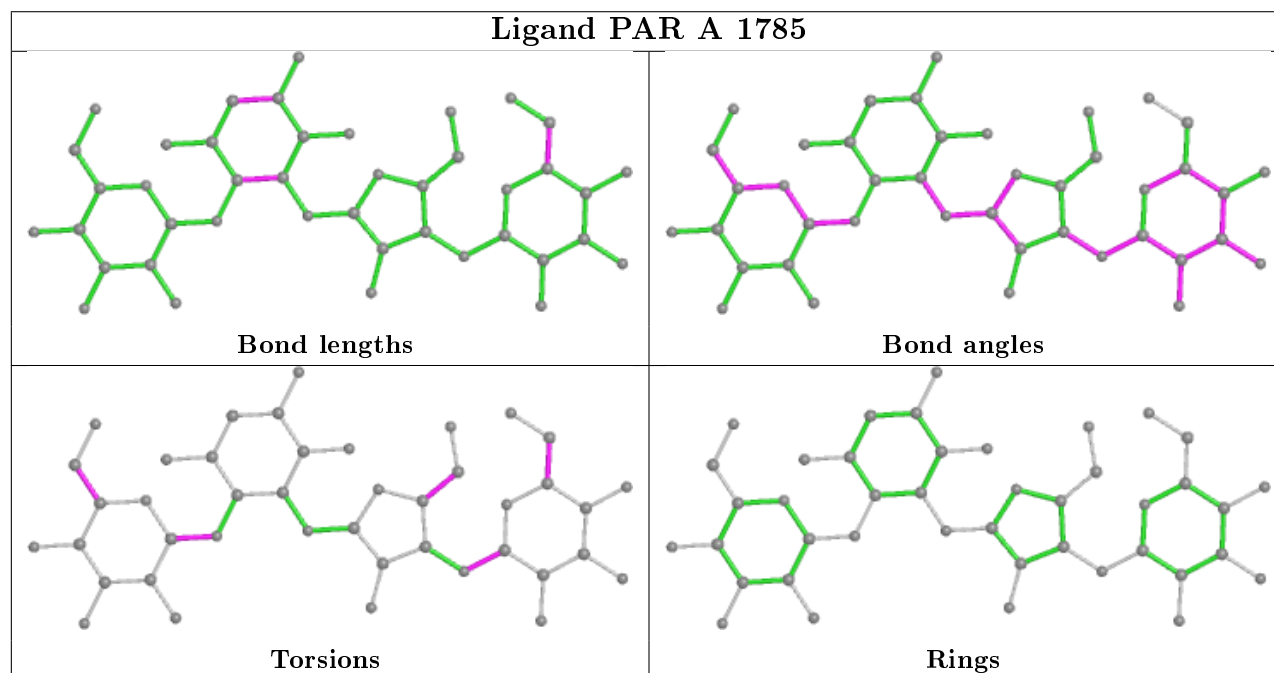
Mol	Chain	Res	Type	Atoms
25	A	1785	PAR	C44-C54-C64-N64
25	A	1785	PAR	O54-C54-C64-N64
25	A	1785	PAR	O51-C11-O11-C42
25	A	1785	PAR	C33-C43-C53-O53
25	A	1785	PAR	O54-C14-O33-C33
25	A	1785	PAR	O51-C51-C61-O61

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	A	1785	PAR	2	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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1512/1513 (99%)	0.46	67 (4%) 34 21	40, 73, 157, 278	0
2	B	234/234 (100%)	0.68	31 (13%) 3 2	60, 107, 182, 222	0
3	C	206/206 (100%)	0.26	21 (10%) 6 4	64, 103, 161, 188	0
4	D	208/208 (100%)	0.94	45 (21%) 0 1	55, 83, 134, 205	0
5	E	150/150 (100%)	0.17	1 (0%) 87 81	44, 63, 103, 123	0
6	F	101/101 (100%)	0.60	14 (13%) 2 1	66, 100, 135, 195	0
7	G	155/155 (100%)	-0.12	3 (1%) 66 53	62, 94, 149, 222	0
8	H	138/138 (100%)	0.18	3 (2%) 62 48	43, 61, 98, 138	0
9	I	127/127 (100%)	1.26	31 (24%) 0 0	65, 110, 155, 202	0
10	J	98/98 (100%)	0.54	13 (13%) 3 2	69, 129, 214, 238	0
11	K	119/119 (100%)	0.83	23 (19%) 1 1	45, 73, 122, 179	0
12	L	124/124 (100%)	0.38	7 (5%) 24 13	40, 70, 122, 195	0
13	M	125/125 (100%)	1.05	30 (24%) 0 0	70, 104, 151, 281	0
14	N	60/60 (100%)	0.43	5 (8%) 11 6	75, 91, 148, 195	0
15	O	88/88 (100%)	0.46	5 (5%) 23 13	48, 77, 130, 176	0
16	P	83/83 (100%)	0.57	11 (13%) 3 2	50, 59, 91, 147	0
17	Q	104/104 (100%)	0.69	8 (7%) 13 7	42, 68, 138, 202	0
18	R	73/73 (100%)	0.40	5 (6%) 17 10	55, 81, 157, 194	0
19	S	80/80 (100%)	1.65	29 (36%) 0 0	81, 127, 179, 205	0
20	T	99/99 (100%)	0.53	10 (10%) 7 4	55, 71, 131, 163	0
21	V	24/24 (100%)	3.02	17 (70%) 0 0	79, 96, 120, 141	0
22	W	4/6 (66%)	-0.02	0 100 100	69, 78, 80, 83	0
23	X	5/17 (29%)	-0.07	0 100 100	82, 85, 96, 112	0
All	All	3917/3932 (99%)	0.55	379 (9%) 7 4	40, 82, 157, 281	0

All (379) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	M	119	GLY	9.9
9	I	15	ALA	9.2
19	S	3	ARG	8.9
9	I	7	THR	8.9
4	D	2	GLY	8.7
8	H	1	MET	8.1
9	I	8	GLY	7.2
21	V	18	TYR	7.1
4	D	35	ARG	7.0
9	I	14	VAL	7.0
1	A	970	G	7.0
9	I	64	THR	6.8
1	A	983	A	6.8
9	I	9	ARG	6.6
19	S	28	LYS	6.6
21	V	24	ARG	6.4
9	I	66	ARG	6.4
13	M	7	VAL	6.4
17	Q	105	ALA	6.3
11	K	31	THR	6.2
4	D	23	GLY	6.0
1	A	971	A	5.8
13	M	4	ILE	5.8
19	S	31	ILE	5.6
19	S	34	TRP	5.4
19	S	49	ILE	5.3
13	M	2	ALA	5.3
12	L	115	LYS	5.3
3	C	193	TYR	5.3
1	A	1510	C	5.3
11	K	42	TRP	5.2
13	M	120	LYS	5.1
1	A	984	C	5.1
1	A	1020	C	5.1
13	M	8	GLU	5.0
2	B	31	TYR	5.0
1	A	981	G	5.0
20	T	103	GLY	4.9
1	A	982	A	4.9
17	Q	104	LYS	4.9
4	D	123	HIS	4.9
2	B	163	PHE	4.9

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Mol	Chain	Res	Type	RSRZ
4	D	125	HIS	4.9
1	A	1002	G	4.9
4	D	120	LEU	4.8
13	M	44	ARG	4.8
19	S	32	LYS	4.8
1	A	1003	U	4.8
9	I	65	VAL	4.8
1	A	208	U	4.8
17	Q	103	GLY	4.7
19	S	2	PRO	4.6
9	I	102	LEU	4.6
2	B	200	ILE	4.6
13	M	13	LYS	4.5
6	F	89	MET	4.5
1	A	1152	G	4.5
9	I	105	ASP	4.5
4	D	25	ARG	4.4
13	M	16	ASP	4.4
12	L	120	TYR	4.4
1	A	1193	U	4.4
10	J	99	LYS	4.4
14	N	3	ARG	4.4
4	D	21	LEU	4.4
2	B	187	LEU	4.3
1	A	1018	G	4.3
4	D	24	GLU	4.3
1	A	1019	C	4.3
1	A	1241	C	4.2
21	V	6	ARG	4.2
15	O	22	THR	4.2
11	K	18	ARG	4.1
4	D	115	ARG	4.1
1	A	968	U	4.1
2	B	165	VAL	4.1
4	D	157	LEU	4.1
14	N	6	LEU	4.0
1	A	1004	G	4.0
21	V	17	THR	4.0
4	D	116	GLN	4.0
21	V	22	ARG	4.0
11	K	129	SER	4.0
16	P	1	MET	4.0

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Mol	Chain	Res	Type	RSRZ
21	V	25	LYS	4.0
19	S	15	LEU	3.9
9	I	17	VAL	3.9
11	K	32	ILE	3.9
2	B	134	GLU	3.9
10	J	73	ASP	3.8
9	I	6	GLY	3.8
2	B	185	ILE	3.8
21	V	9	ARG	3.8
3	C	76	VAL	3.8
3	C	161	GLU	3.7
4	D	22	LYS	3.7
9	I	83	ARG	3.7
10	J	5	ARG	3.7
20	T	64	ASP	3.7
9	I	5	TYR	3.6
1	A	1027	C	3.6
2	B	68	ILE	3.6
8	H	2	LEU	3.6
4	D	7	PRO	3.6
9	I	103	THR	3.6
1	A	1111	C	3.6
3	C	68	VAL	3.6
20	T	104	LEU	3.6
11	K	81	ASP	3.6
11	K	11	LYS	3.5
4	D	126	ILE	3.5
19	S	30	LEU	3.5
2	B	201	ILE	3.5
19	S	47	HIS	3.5
6	F	88	VAL	3.5
4	D	110	PHE	3.5
4	D	32	ALA	3.5
4	D	33	MET	3.5
1	A	969	U	3.5
11	K	128	ALA	3.5
18	R	18	ARG	3.4
3	C	156	ARG	3.4
2	B	211	ILE	3.4
19	S	60	VAL	3.4
9	I	16	ARG	3.4
21	V	5	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
2	B	192	SER	3.4
11	K	20	TYR	3.3
12	L	116	SER	3.3
21	V	12	LYS	3.3
4	D	119	GLN	3.3
19	S	14	HIS	3.3
13	M	6	GLY	3.3
9	I	19	LEU	3.3
6	F	63	TYR	3.3
1	A	967	C	3.3
1	A	1163	G	3.3
6	F	30	LEU	3.3
1	A	1021	C	3.3
11	K	28	THR	3.3
21	V	11	GLY	3.2
1	A	1109	G	3.2
20	T	84	LEU	3.2
9	I	101	PHE	3.2
4	D	181	MET	3.2
1	A	1130	U	3.2
15	O	23	GLY	3.2
13	M	88	ARG	3.2
12	L	113	ARG	3.1
1	A	1250	A	3.1
13	M	87	TYR	3.1
21	V	2	GLY	3.1
1	A	405	G	3.1
20	T	85	MET	3.1
16	P	41	PRO	3.1
4	D	146	ILE	3.1
4	D	8	VAL	3.1
10	J	43	ARG	3.1
12	L	114	LYS	3.1
6	F	87	ARG	3.0
1	A	1425	G	3.0
6	F	8	ILE	3.0
6	F	6	VAL	3.0
12	L	112	ASP	3.0
21	V	21	TYR	3.0
1	A	1141	U	3.0
2	B	35	GLU	3.0
20	T	88	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	55	PHE	2.9
2	B	70	PHE	2.9
9	I	18	PHE	2.9
19	S	29	ARG	2.9
10	J	38	ILE	2.9
9	I	13	ALA	2.9
21	V	15	ARG	2.9
11	K	41	THR	2.9
17	Q	2	PRO	2.9
19	S	38	SER	2.9
3	C	58	GLU	2.9
13	M	19	LEU	2.9
11	K	29	ILE	2.8
1	A	1129	C	2.8
3	C	191	THR	2.8
5	E	119	LEU	2.8
3	C	91	LEU	2.8
9	I	92	TYR	2.8
12	L	128	ALA	2.8
20	T	56	MET	2.8
6	F	79	LEU	2.8
1	A	1028	A	2.8
3	C	54	ARG	2.8
9	I	10	ARG	2.8
15	O	21	ASP	2.8
17	Q	85	VAL	2.8
19	S	33	THR	2.8
10	J	7	LYS	2.8
19	S	35	SER	2.8
19	S	44	MET	2.8
6	F	75	LEU	2.8
19	S	73	GLU	2.8
1	A	978	A	2.7
1	A	1025	C	2.7
1	A	1013	G	2.7
2	B	15	VAL	2.7
1	A	1151	A	2.7
1	A	688	U	2.7
17	Q	68	ARG	2.7
4	D	148	VAL	2.7
18	R	31	LEU	2.7
1	A	690	C	2.7

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Mol	Chain	Res	Type	RSRZ
13	M	11	ARG	2.7
21	V	10	ARG	2.7
2	B	199	TYR	2.7
4	D	122	ARG	2.7
7	G	5	ARG	2.7
3	C	21	ARG	2.7
4	D	158	ILE	2.7
13	M	9	ILE	2.7
4	D	29	PRO	2.7
20	T	83	ARG	2.6
4	D	183	GLY	2.6
21	V	7	ARG	2.6
1	A	1005	C	2.6
3	C	102	ASN	2.6
4	D	112	VAL	2.6
11	K	12	ARG	2.6
3	C	57	ILE	2.6
9	I	104	ARG	2.6
9	I	106	ALA	2.6
19	S	48	THR	2.6
1	A	437	C	2.6
3	C	155	GLY	2.6
11	K	40	ILE	2.6
3	C	101	LEU	2.6
4	D	30	LYS	2.6
2	B	47	THR	2.6
16	P	64	ALA	2.5
13	M	60	VAL	2.5
1	A	301	G	2.5
19	S	74	PHE	2.5
16	P	12	LYS	2.5
10	J	74	ILE	2.5
4	D	34	GLU	2.5
1	A	980	G	2.5
20	T	9	ASN	2.5
10	J	71	LEU	2.5
19	S	71	LEU	2.5
4	D	133	VAL	2.5
4	D	42	GLN	2.5
4	D	26	CYS	2.5
10	J	72	VAL	2.5
4	D	152	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	423	G	2.5
9	I	79	LEU	2.5
4	D	124	GLY	2.5
16	P	8	ARG	2.5
1	A	1107	U	2.5
1	A	515	A	2.4
11	K	30	VAL	2.4
15	O	69	TYR	2.4
19	S	54	GLY	2.4
19	S	75	ALA	2.4
18	R	16	PRO	2.4
13	M	45	VAL	2.4
21	V	16	GLY	2.4
1	A	438	C	2.4
6	F	4	TYR	2.4
3	C	157	ILE	2.4
14	N	4	LYS	2.4
1	A	689	A	2.4
1	A	1001	G	2.4
2	B	58	ILE	2.4
11	K	80	VAL	2.4
1	A	1263	C	2.4
3	C	66	VAL	2.4
13	M	124	PRO	2.4
16	P	39	TYR	2.4
2	B	193	ASP	2.4
1	A	1251	C	2.4
11	K	51	LYS	2.4
13	M	15	VAL	2.4
14	N	2	ALA	2.4
4	D	5	ILE	2.4
16	P	68	ASP	2.4
3	C	103	VAL	2.4
21	V	8	THR	2.4
18	R	17	SER	2.4
10	J	54	PHE	2.3
20	T	81	LYS	2.3
10	J	34	VAL	2.3
2	B	50	GLU	2.3
2	B	214	ILE	2.3
1	A	203	A	2.3
1	A	706	U	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	203	GLY	2.3
1	A	1026	A	2.3
13	M	102	ARG	2.3
3	C	196	LEU	2.3
17	Q	14	LYS	2.3
1	A	1076	G	2.3
19	S	27	GLU	2.3
4	D	134	ASP	2.3
6	F	65	VAL	2.3
3	C	194	GLY	2.3
13	M	118	ALA	2.3
1	A	1017	A	2.3
9	I	124	GLN	2.3
3	C	79	ARG	2.3
4	D	121	VAL	2.3
13	M	41	PRO	2.3
6	F	85	VAL	2.3
10	J	29	ARG	2.2
2	B	32	ILE	2.2
18	R	43	PHE	2.2
2	B	131	PRO	2.2
13	M	3	ARG	2.2
2	B	133	LYS	2.2
13	M	5	ALA	2.2
1	A	1016	G	2.2
13	M	126	LYS	2.2
19	S	50	ALA	2.2
1	A	455	C	2.2
4	D	18	LYS	2.2
11	K	43	SER	2.2
2	B	77	ALA	2.2
7	G	4	ARG	2.2
10	J	40	LEU	2.2
1	A	1012	A	2.2
2	B	152	PHE	2.2
9	I	37	PHE	2.1
9	I	63	ILE	2.1
13	M	10	PRO	2.1
3	C	80	GLY	2.1
8	H	3	THR	2.1
4	D	117	ALA	2.1
19	S	10	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
11	K	37	GLY	2.1
9	I	82	ALA	2.1
9	I	110	GLU	2.1
19	S	51	VAL	2.1
2	B	101	MET	2.1
4	D	155	LEU	2.1
16	P	73	LEU	2.1
2	B	202	PRO	2.1
1	A	1015	G	2.1
2	B	164	VAL	2.1
4	D	40	PRO	2.1
13	M	27	LYS	2.1
16	P	6	LEU	2.1
1	A	979	G	2.1
1	A	1240	C	2.1
14	N	30	ALA	2.1
4	D	113	SER	2.1
11	K	33	THR	2.1
1	A	348	A	2.1
1	A	1205	G	2.1
2	B	190	THR	2.1
6	F	90	VAL	2.1
11	K	19	ALA	2.1
1	A	1218	C	2.1
6	F	67	MET	2.1
4	D	209	ARG	2.0
1	A	1126	G	2.0
16	P	69	THR	2.0
17	Q	98	LEU	2.0
19	S	22	LEU	2.0
4	D	105	VAL	2.0
13	M	86	CYS	2.0
16	P	17	TYR	2.0
7	G	33	ASP	2.0
13	M	48	LEU	2.0
19	S	52	TYR	2.0
11	K	82	VAL	2.0
13	M	125	ARG	2.0
15	O	24	SER	2.0
11	K	17	GLY	2.0
1	A	687	A	2.0
1	A	736	A	2.0

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Mol	Chain	Res	Type	RSRZ
9	I	12	GLU	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
23	RSQ	X	34	22/23	0.92	0.26	94,96,98,100	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
24	MG	A	1691	1/1	-0.09	0.17	156,156,156,156	0
24	MG	A	1756	1/1	0.18	0.41	81,81,81,81	0
24	MG	A	1633	1/1	0.20	2.70	90,90,90,90	0
24	MG	A	1742	1/1	0.22	0.48	90,90,90,90	0
24	MG	A	1628	1/1	0.24	0.77	78,78,78,78	0
24	MG	A	1666	1/1	0.28	1.02	61,61,61,61	0
24	MG	A	1607	1/1	0.40	0.83	76,76,76,76	0
24	MG	A	1700	1/1	0.44	0.27	81,81,81,81	0
24	MG	A	1717	1/1	0.47	0.37	109,109,109,109	0
24	MG	A	1677	1/1	0.47	1.52	99,99,99,99	0
24	MG	A	1739	1/1	0.51	0.39	53,53,53,53	1
24	MG	A	1724	1/1	0.53	0.41	84,84,84,84	0
24	MG	A	1609	1/1	0.54	0.43	66,66,66,66	0
24	MG	A	1644	1/1	0.55	0.18	87,87,87,87	0
24	MG	A	1621	1/1	0.57	0.28	70,70,70,70	0
24	MG	A	1698	1/1	0.57	0.37	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
24	MG	A	1613	1/1	0.57	0.37	64,64,64,64	0
24	MG	A	1768	1/1	0.58	0.54	62,62,62,62	0
24	MG	A	1716	1/1	0.58	1.05	106,106,106,106	0
24	MG	A	1671	1/1	0.60	0.43	84,84,84,84	0
24	MG	A	1608	1/1	0.60	0.32	96,96,96,96	0
24	MG	A	1626	1/1	0.60	0.62	81,81,81,81	0
24	MG	A	1728	1/1	0.61	0.28	99,99,99,99	0
24	MG	A	1682	1/1	0.62	0.28	46,46,46,46	0
24	MG	A	1651	1/1	0.63	0.23	65,65,65,65	0
24	MG	A	1713	1/1	0.63	0.46	81,81,81,81	0
24	MG	A	1775	1/1	0.64	0.30	80,80,80,80	0
24	MG	A	1652	1/1	0.64	0.51	93,93,93,93	0
24	MG	A	1699	1/1	0.65	1.06	82,82,82,82	0
24	MG	A	1601	1/1	0.65	0.27	59,59,59,59	0
24	MG	A	1616	1/1	0.66	0.32	83,83,83,83	0
24	MG	A	1665	1/1	0.66	0.18	82,82,82,82	0
24	MG	A	1749	1/1	0.66	0.19	59,59,59,59	0
24	MG	A	1719	1/1	0.67	0.28	69,69,69,69	0
24	MG	A	1605	1/1	0.68	1.05	77,77,77,77	0
24	MG	A	1622	1/1	0.68	1.84	85,85,85,85	0
24	MG	A	1767	1/1	0.69	0.26	65,65,65,65	0
24	MG	A	1712	1/1	0.69	0.22	59,59,59,59	0
24	MG	A	1764	1/1	0.70	0.76	78,78,78,78	0
24	MG	A	1693	1/1	0.71	0.14	122,122,122,122	0
24	MG	A	1615	1/1	0.71	0.41	43,43,43,43	0
24	MG	A	1602	1/1	0.72	0.25	90,90,90,90	0
24	MG	A	1690	1/1	0.72	0.93	90,90,90,90	0
24	MG	A	1766	1/1	0.72	0.36	77,77,77,77	0
24	MG	A	1705	1/1	0.72	1.26	58,58,58,58	0
24	MG	A	1697	1/1	0.73	0.53	81,81,81,81	0
24	MG	A	1759	1/1	0.73	0.45	52,52,52,52	0
24	MG	A	1755	1/1	0.73	0.41	86,86,86,86	0
24	MG	T	201	1/1	0.74	0.35	99,99,99,99	0
24	MG	A	1614	1/1	0.74	0.87	76,76,76,76	0
24	MG	A	1778	1/1	0.74	0.73	77,77,77,77	0
24	MG	A	1772	1/1	0.75	0.37	96,96,96,96	0
24	MG	A	1704	1/1	0.75	0.27	61,61,61,61	0
24	MG	A	1721	1/1	0.75	0.76	64,64,64,64	0
24	MG	A	1784	1/1	0.76	1.24	68,68,68,68	0
24	MG	A	1668	1/1	0.76	0.46	58,58,58,58	0
24	MG	A	1625	1/1	0.77	0.23	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
24	MG	A	1777	1/1	0.77	0.54	83,83,83,83	0
24	MG	A	1673	1/1	0.77	0.79	74,74,74,74	0
24	MG	A	1701	1/1	0.77	0.58	63,63,63,63	0
24	MG	A	1718	1/1	0.78	0.28	65,65,65,65	0
24	MG	A	1670	1/1	0.78	0.39	56,56,56,56	0
24	MG	A	1684	1/1	0.78	0.24	63,63,63,63	0
24	MG	A	1722	1/1	0.78	0.57	76,76,76,76	0
24	MG	A	1783	1/1	0.78	0.38	65,65,65,65	0
24	MG	A	1640	1/1	0.79	0.65	105,105,105,105	0
24	MG	A	1771	1/1	0.79	0.32	60,60,60,60	0
24	MG	A	1747	1/1	0.79	0.44	84,84,84,84	0
24	MG	A	1695	1/1	0.79	0.18	101,101,101,101	0
24	MG	A	1702	1/1	0.79	1.39	90,90,90,90	0
24	MG	A	1780	1/1	0.80	0.30	81,81,81,81	0
24	MG	A	1639	1/1	0.80	0.59	56,56,56,56	0
24	MG	A	1638	1/1	0.80	0.18	72,72,72,72	0
24	MG	A	1758	1/1	0.81	0.17	43,43,43,43	0
24	MG	A	1629	1/1	0.82	0.25	65,65,65,65	0
24	MG	A	1753	1/1	0.82	0.24	87,87,87,87	0
24	MG	A	1692	1/1	0.82	0.28	122,122,122,122	0
24	MG	A	1737	1/1	0.82	0.89	76,76,76,76	0
24	MG	A	1643	1/1	0.82	1.02	61,61,61,61	0
24	MG	A	1617	1/1	0.83	1.79	66,66,66,66	0
24	MG	A	1708	1/1	0.83	0.62	74,74,74,74	0
24	MG	A	1714	1/1	0.83	0.37	53,53,53,53	0
24	MG	A	1750	1/1	0.83	0.39	72,72,72,72	0
24	MG	A	1703	1/1	0.83	1.27	100,100,100,100	0
24	MG	A	1779	1/1	0.84	0.49	97,97,97,97	0
24	MG	A	1731	1/1	0.84	0.38	108,108,108,108	0
24	MG	A	1781	1/1	0.84	0.78	92,92,92,92	0
24	MG	A	1672	1/1	0.85	1.00	50,50,50,50	0
24	MG	A	1645	1/1	0.85	0.25	58,58,58,58	0
24	MG	A	1637	1/1	0.85	0.60	48,48,48,48	0
24	MG	A	1606	1/1	0.85	0.87	50,50,50,50	0
24	MG	A	1741	1/1	0.85	0.57	85,85,85,85	0
24	MG	A	1694	1/1	0.85	0.33	89,89,89,89	0
24	MG	A	1686	1/1	0.85	0.28	58,58,58,58	0
24	MG	A	1658	1/1	0.85	0.22	101,101,101,101	0
24	MG	A	1751	1/1	0.86	0.39	70,70,70,70	0
24	MG	A	1688	1/1	0.86	0.29	71,71,71,71	0
24	MG	A	1603	1/1	0.86	0.12	61,61,61,61	0
24	MG	A	1630	1/1	0.86	0.66	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
24	MG	A	1729	1/1	0.87	1.12	58,58,58,58	0
24	MG	A	1679	1/1	0.87	0.58	63,63,63,63	0
24	MG	A	1675	1/1	0.88	0.34	74,74,74,74	0
24	MG	A	1735	1/1	0.88	0.61	62,62,62,62	0
24	MG	A	1774	1/1	0.88	0.22	67,67,67,67	0
24	MG	A	1619	1/1	0.88	0.36	73,73,73,73	0
24	MG	A	1632	1/1	0.88	0.70	51,51,51,51	0
24	MG	A	1624	1/1	0.88	0.54	120,120,120,120	0
24	MG	A	1744	1/1	0.88	0.52	63,63,63,63	0
24	MG	A	1657	1/1	0.88	0.44	66,66,66,66	0
24	MG	A	1636	1/1	0.88	0.38	59,59,59,59	0
24	MG	A	1681	1/1	0.88	0.66	59,59,59,59	0
24	MG	A	1620	1/1	0.88	0.66	68,68,68,68	0
24	MG	A	1773	1/1	0.88	0.40	64,64,64,64	0
24	MG	A	1623	1/1	0.88	0.51	79,79,79,79	0
24	MG	A	1761	1/1	0.89	0.13	57,57,57,57	0
24	MG	A	1754	1/1	0.89	0.24	67,67,67,67	0
24	MG	A	1647	1/1	0.89	0.46	67,67,67,67	0
24	MG	A	1664	1/1	0.89	0.14	47,47,47,47	0
24	MG	A	1656	1/1	0.89	0.54	52,52,52,52	0
24	MG	A	1740	1/1	0.89	0.66	41,41,41,41	0
24	MG	A	1752	1/1	0.89	0.27	62,62,62,62	0
24	MG	A	1646	1/1	0.90	0.25	89,89,89,89	0
24	MG	A	1746	1/1	0.90	0.61	76,76,76,76	0
24	MG	A	1674	1/1	0.90	0.81	57,57,57,57	0
24	MG	A	1678	1/1	0.90	0.84	75,75,75,75	0
24	MG	A	1733	1/1	0.90	0.62	77,77,77,77	0
24	MG	A	1707	1/1	0.90	0.56	52,52,52,52	0
24	MG	A	1696	1/1	0.91	0.08	75,75,75,75	0
24	MG	A	1732	1/1	0.91	0.34	91,91,91,91	0
24	MG	A	1762	1/1	0.91	0.24	75,75,75,75	0
24	MG	A	1709	1/1	0.91	0.24	82,82,82,82	0
24	MG	A	1641	1/1	0.91	0.47	87,87,87,87	0
24	MG	A	1765	1/1	0.91	0.58	73,73,73,73	0
24	MG	A	1610	1/1	0.91	0.10	89,89,89,89	0
24	MG	A	1627	1/1	0.91	0.46	44,44,44,44	0
24	MG	A	1604	1/1	0.91	0.85	105,105,105,105	0
24	MG	A	1770	1/1	0.92	0.35	65,65,65,65	0
24	MG	A	1734	1/1	0.92	1.39	58,58,58,58	0
24	MG	A	1736	1/1	0.92	0.46	62,62,62,62	0
24	MG	A	1782	1/1	0.92	0.51	62,62,62,62	0
24	MG	A	1745	1/1	0.92	0.41	55,55,55,55	0

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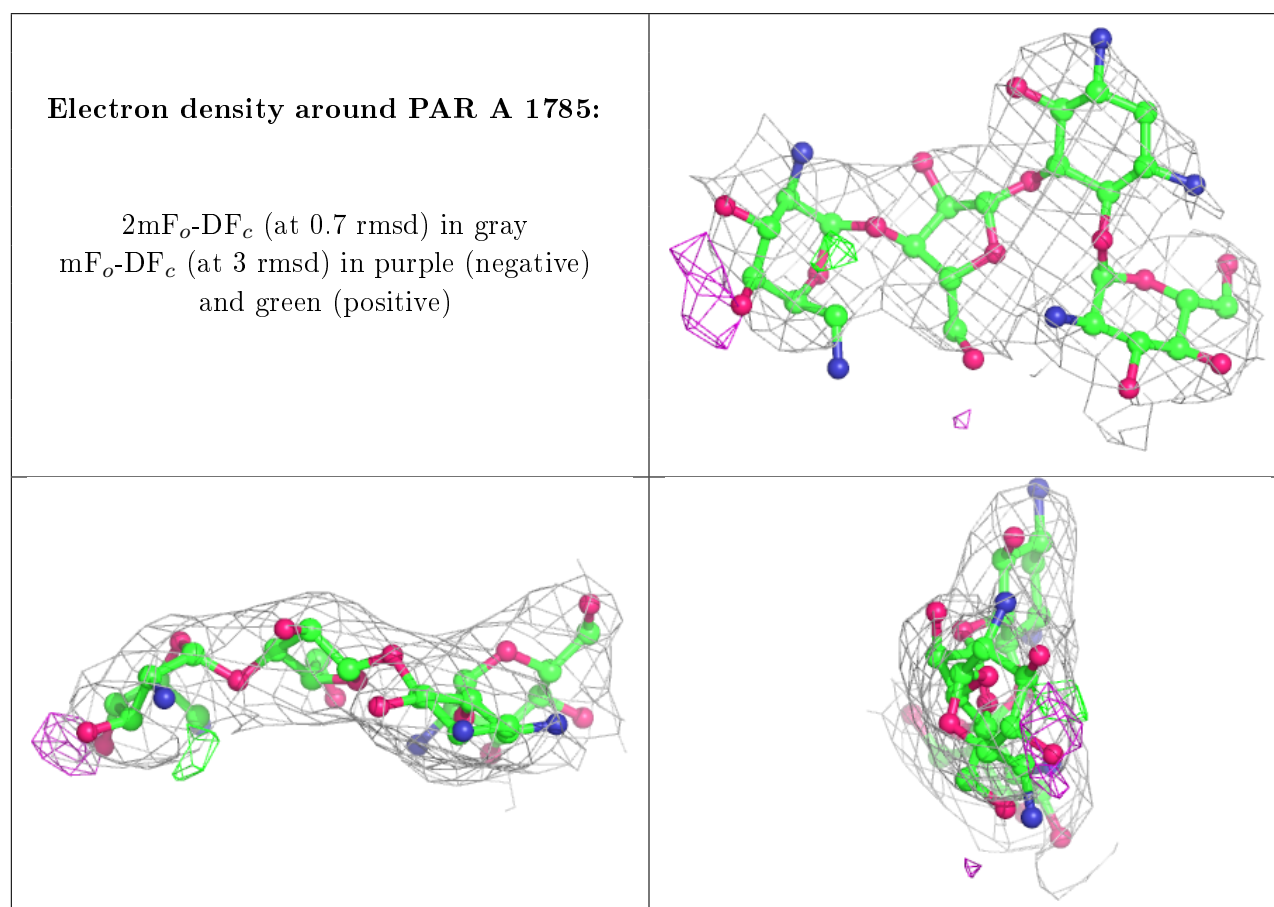
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
24	MG	A	1689	1/1	0.93	0.10	89,89,89,89	0
24	MG	A	1720	1/1	0.93	0.29	58,58,58,58	0
24	MG	A	1631	1/1	0.93	0.58	50,50,50,50	1
24	MG	A	1642	1/1	0.93	0.76	57,57,57,57	0
24	MG	A	1662	1/1	0.93	0.67	41,41,41,41	0
24	MG	A	1727	1/1	0.93	0.26	64,64,64,64	0
24	MG	A	1655	1/1	0.93	0.38	49,49,49,49	0
24	MG	B	301	1/1	0.93	0.17	115,115,115,115	0
24	MG	A	1676	1/1	0.94	0.48	68,68,68,68	0
24	MG	A	1683	1/1	0.94	0.72	66,66,66,66	0
24	MG	A	1757	1/1	0.94	0.34	53,53,53,53	0
24	MG	A	1763	1/1	0.94	0.20	52,52,52,52	0
24	MG	A	1723	1/1	0.94	0.71	68,68,68,68	0
24	MG	A	1635	1/1	0.94	0.51	60,60,60,60	0
24	MG	A	1687	1/1	0.95	0.55	66,66,66,66	0
24	MG	A	1711	1/1	0.95	0.36	39,39,39,39	0
25	PAR	A	1785	42/42	0.95	0.26	48,51,58,59	0
24	MG	A	1659	1/1	0.95	0.50	55,55,55,55	0
24	MG	A	1611	1/1	0.95	0.59	44,44,44,44	0
24	MG	A	1618	1/1	0.95	0.41	72,72,72,72	0
24	MG	A	1660	1/1	0.95	0.57	41,41,41,41	0
24	MG	A	1738	1/1	0.95	0.24	48,48,48,48	0
24	MG	A	1760	1/1	0.95	0.37	52,52,52,52	0
24	MG	A	1715	1/1	0.95	0.38	53,53,53,53	0
24	MG	A	1706	1/1	0.95	0.44	56,56,56,56	0
24	MG	A	1649	1/1	0.95	0.41	43,43,43,43	0
24	MG	A	1748	1/1	0.95	0.21	77,77,77,77	0
24	MG	A	1612	1/1	0.96	0.63	43,43,43,43	0
24	MG	A	1726	1/1	0.96	0.42	56,56,56,56	0
24	MG	A	1776	1/1	0.96	0.38	82,82,82,82	0
24	MG	A	1667	1/1	0.96	0.51	47,47,47,47	0
24	MG	A	1685	1/1	0.96	0.15	48,48,48,48	0
24	MG	A	1769	1/1	0.96	0.27	43,43,43,43	0
24	MG	A	1725	1/1	0.96	0.20	58,58,58,58	0
24	MG	A	1634	1/1	0.96	1.12	56,56,56,56	0
24	MG	A	1710	1/1	0.97	0.14	64,64,64,64	0
24	MG	A	1648	1/1	0.97	0.48	41,41,41,41	0
24	MG	A	1680	1/1	0.97	0.81	53,53,53,53	0
24	MG	A	1650	1/1	0.97	0.33	45,45,45,45	0
24	MG	A	1730	1/1	0.97	0.61	73,73,73,73	0
24	MG	A	1653	1/1	0.97	0.27	46,46,46,46	0
24	MG	A	1663	1/1	0.97	0.24	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
24	MG	A	1669	1/1	0.97	0.90	44,44,44,44	0
24	MG	A	1743	1/1	0.98	0.31	43,43,43,43	0
24	MG	A	1654	1/1	0.98	0.60	40,40,40,40	0
24	MG	A	1661	1/1	0.98	0.67	40,40,40,40	0
26	ZN	N	101	1/1	0.99	0.25	90,90,90,90	0
26	ZN	D	301	1/1	0.99	0.35	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 ⓘ

There are no such residues in this entry.