



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:01 AM UTC

PDB ID : 4DR4 / pdb_00004dr4
Title : Crystal structure of the *Thermus thermophilus* (HB8) 30S ribosomal subunit with codon, cognate transfer RNA anticodon stem-loop and multiple copies of paromomycin molecules bound
Authors : Demirci, H.; Murphy IV, F.; Murphy, E.; Gregory, S.T.; Dahlberg, A.E.; Jogl, G.
Deposited on : 2012-02-16
Resolution : 3.97 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references](#) ①) were used in the production of this report:

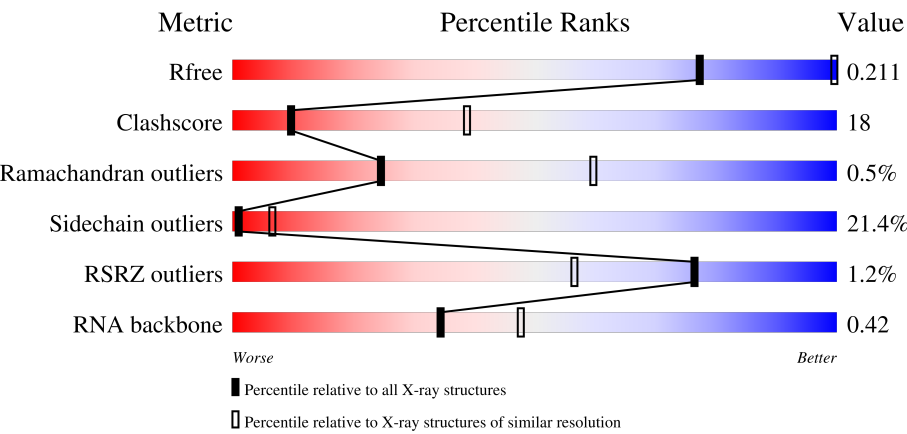
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.97 Å.

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



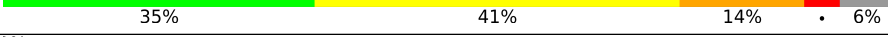
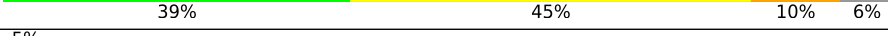
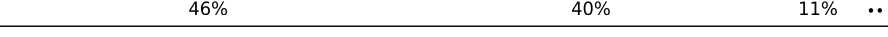
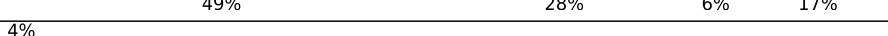
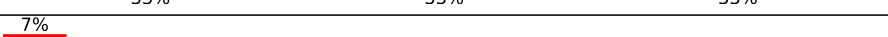
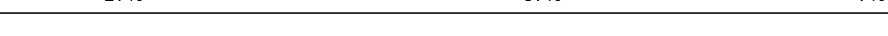
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1046 (4.16-3.76)
Clashscore	190562	1019 (4.14-3.78)
Ramachandran outliers	187476	1031 (4.16-3.76)
Sidechain outliers	187428	1024 (4.16-3.76)
RSRZ outliers	180081	1046 (4.16-3.76)
RNA backbone	3983	1016 (4.80-3.10)

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

Mol	Chain	Length	Quality of chain
1	A	1522	38% 46% 15% .
2	B	256	46% 36% 9% 8%
3	C	239	38% 37% 12% 13%
4	D	209	53% 37% 9% .

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Mol	Chain	Length	Quality of chain
5	E	162	
6	F	101	
7	G	156	
8	H	138	
9	I	128	
10	J	105	
11	K	129	
12	L	135	
13	M	126	
14	N	61	
15	O	89	
16	P	88	
17	Q	105	
18	R	88	
19	S	93	
20	T	106	
21	U	27	
22	V	3	
23	W	15	

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
25	MG	A	1653[B]	-	-	-	X
25	MG	A	1882[A]	-	-	-	X
25	MG	A	1882[B]	-	-	-	X

2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 53651 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	1512	Total	C	N	O	P	0	0	0
			32504	14477	6011	10505	1511			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1534	C	A	conflict	GB M26923.1
A	1535	A	C	conflict	GB M26923.1

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	236	Total	C	N	O	S	0	0	1
			1896	1211	337	343	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	207	Total	C	N	O	S	0	0	1
			1613	1016	315	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	151	Total	C	N	O	S	0	0	1
			1147	724	218	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
			1010	639	197	174			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	99	Total	C	N	O	S	0	0	1
			793	498	157	137	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	125	Total	C	N	O	S	0	0	1
			973	612	196	163	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	118	Total	C	N	O	S	0	0	0
			937	579	193	163	2			

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

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	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	100	Total	C	N	O	S	0	0	0
			834	534	156	142	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
			598	381	118	99				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	81	Total	C	N	O	S	0	0	1
			648	414	120	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
			763	470	162	129	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	U	25	Total	C	N	O	0	0	1
			209	128	51	30			

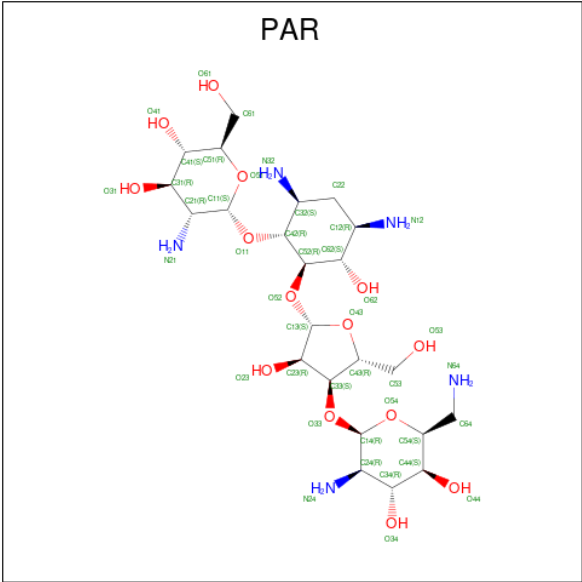
- Molecule 22 is a RNA chain called 5'-R(*UP*UP*U)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	V	3	Total	C	N	O	P	0	0	0
			57	27	6	22	2			

- Molecule 23 is a RNA chain called 5'-R(*GP*GP*GP*AP*UP*UP*GP*AP*AP*AP*AP*UP*CP*CP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	W	15	Total	C	N	O	P	0	0	0
			319	144	60	101	14			

- Molecule 24 is PAROMOMYCIN (CCD ID: PAR) (formula: C₂₃H₄₅N₅O₁₄).



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

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

- Molecule 25 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	A	339	Total	Mg	0	8
			345	345		
25	D	2	Total	Mg	0	0
			2	2		
25	E	4	Total	Mg	0	0
			4	4		
25	H	1	Total	Mg	0	0
			1	1		
25	L	1	Total	Mg	0	0
			1	1		
25	N	1	Total	Mg	0	0
			1	1		
25	O	1	Total	Mg	0	0
			1	1		
25	P	3	Total	Mg	0	0
			3	3		
25	Q	1	Total	Mg	0	0
			1	1		
25	S	2	Total	Mg	0	0
			2	2		
25	T	1	Total	Mg	0	0
			1	1		
25	V	1	Total	Mg	0	0
			1	1		

- Molecule 26 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

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

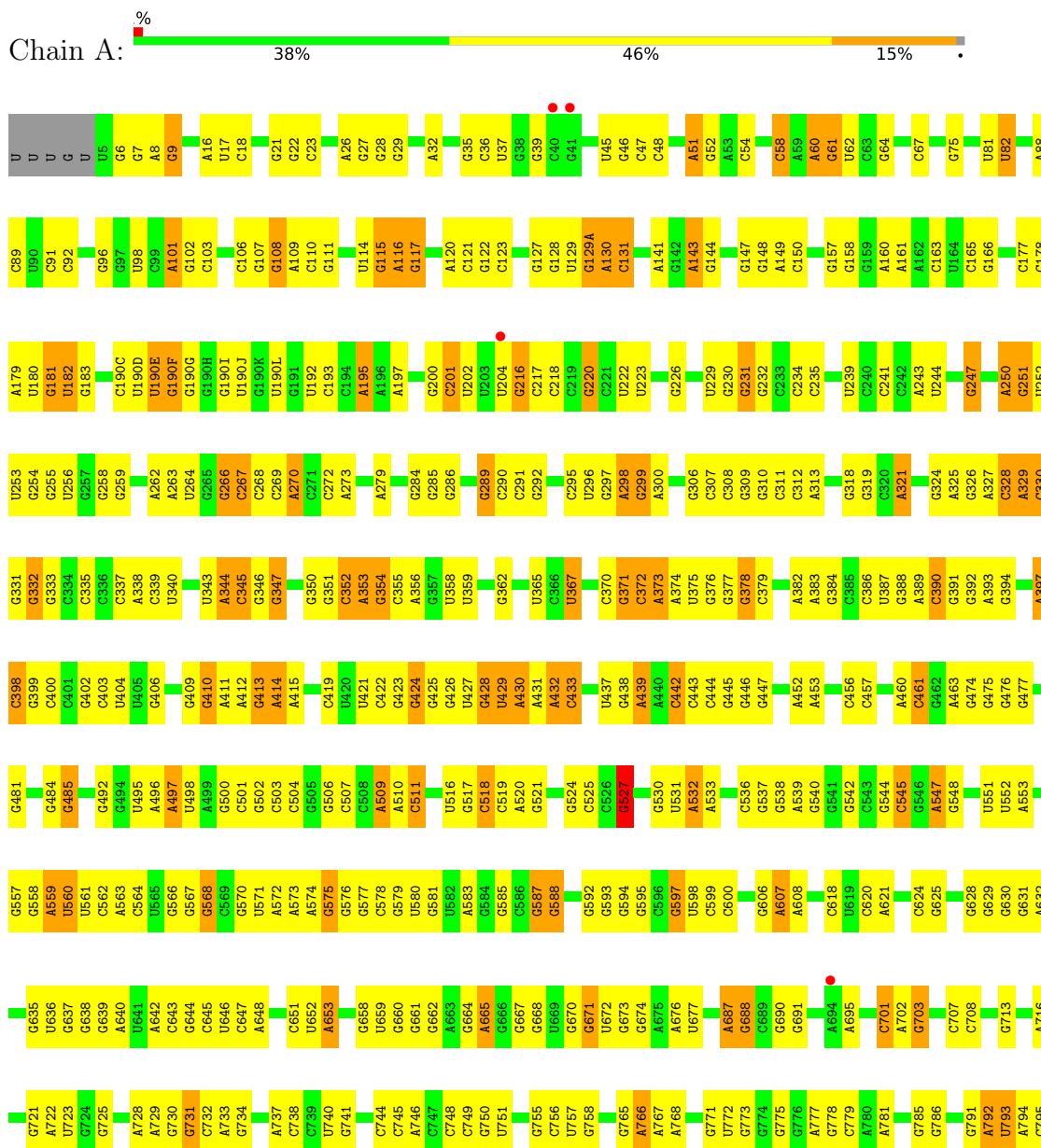
- Molecule 27 is water.

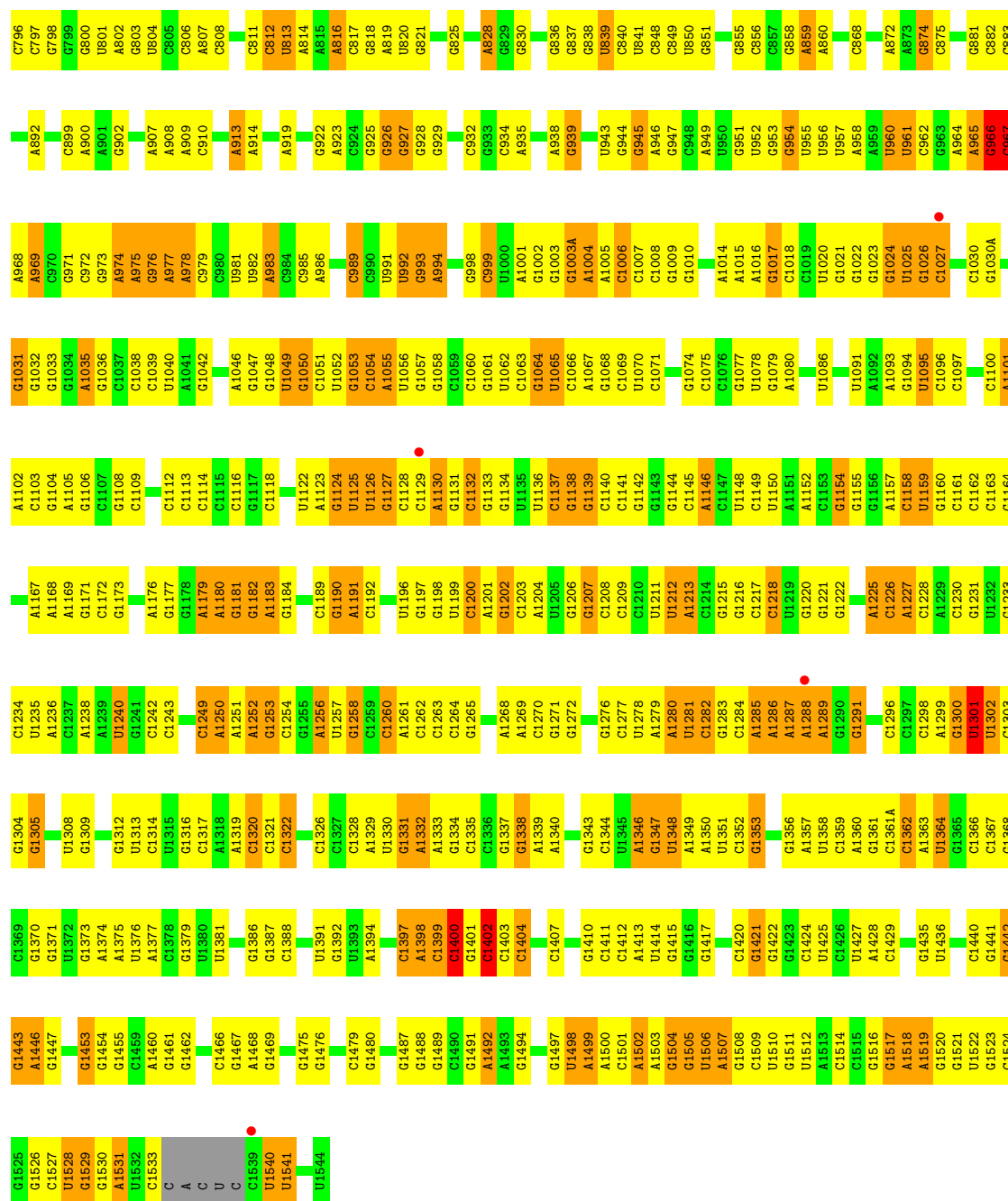
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
27	A	480	Total	O	0	0
			480	480		
27	C	1	Total	O	0	0
			1	1		
27	D	2	Total	O	0	0
			2	2		
27	E	5	Total	O	0	0
			5	5		
27	K	1	Total	O	0	0
			1	1		
27	L	2	Total	O	0	0
			2	2		
27	N	2	Total	O	0	0
			2	2		
27	O	4	Total	O	0	0
			4	4		
27	V	1	Total	O	0	0
			1	1		

3 Residue-property plots

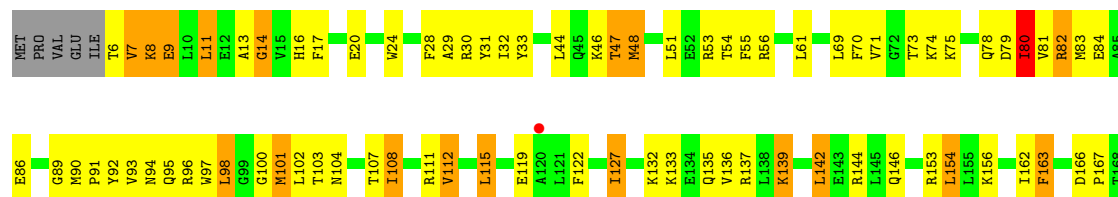
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

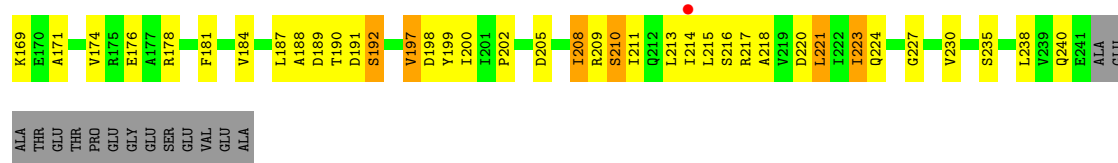
- Molecule 1: 16S rRNA



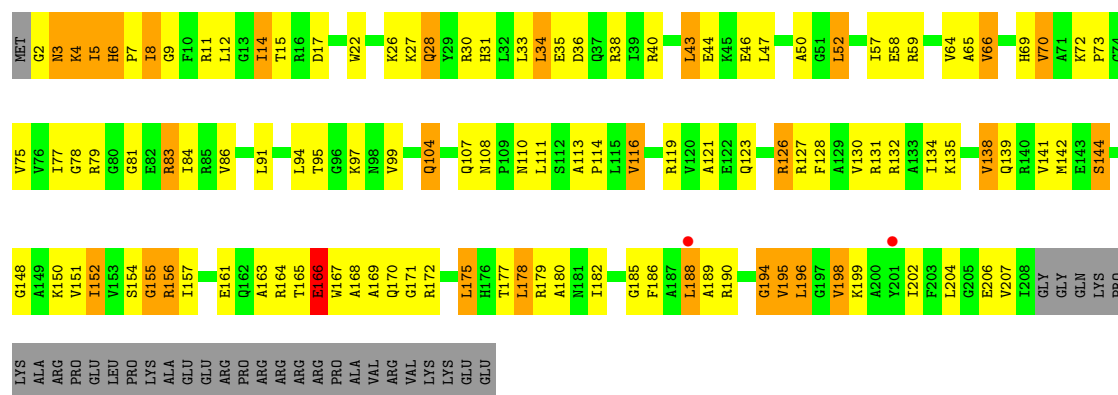


• Molecule 2: 30S ribosomal protein S2

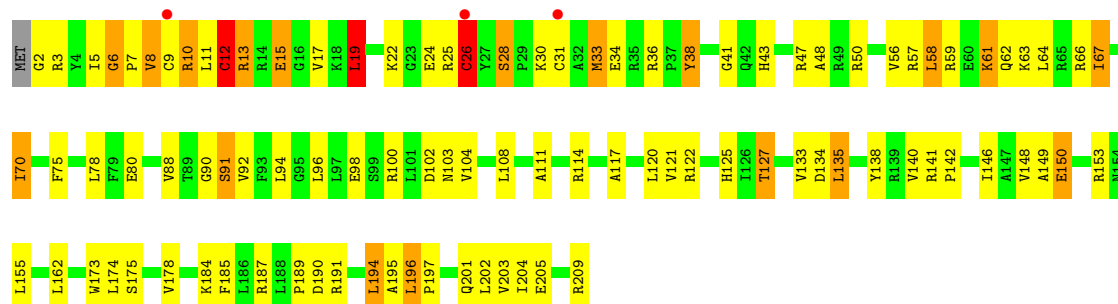




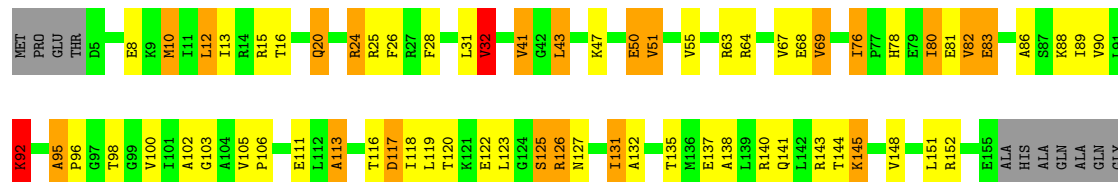
• Molecule 3: 30S ribosomal protein S3



• Molecule 4: 30S ribosomal protein S4

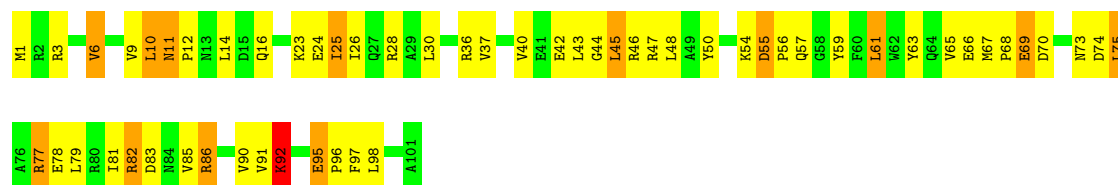


• Molecule 5: 30S ribosomal protein S5

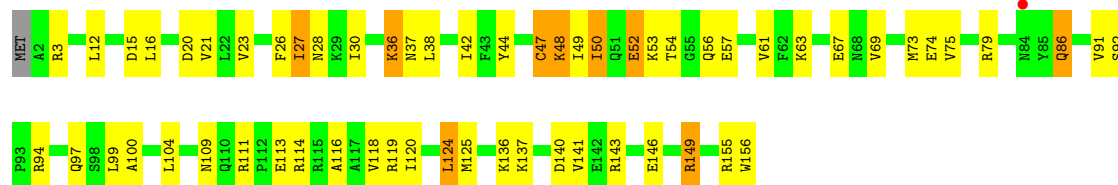


• Molecule 6: 30S ribosomal protein S6

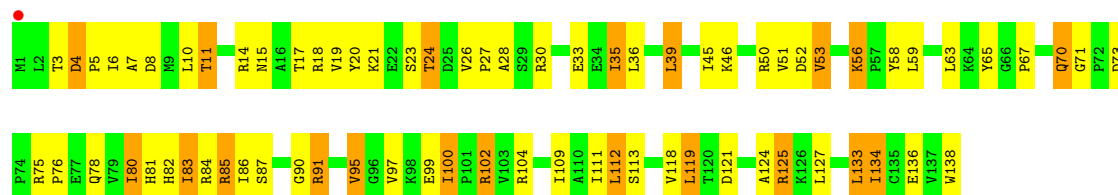




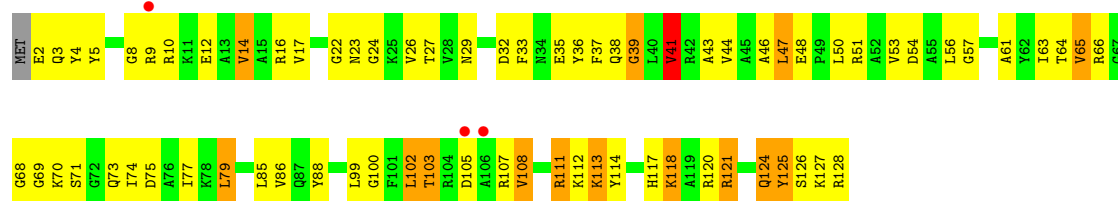
• Molecule 7: 30S ribosomal protein S7



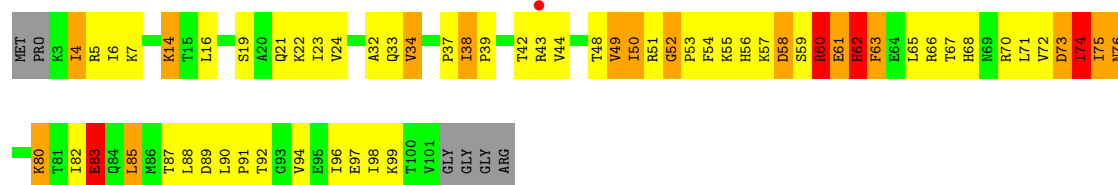
• Molecule 8: 30S ribosomal protein S8



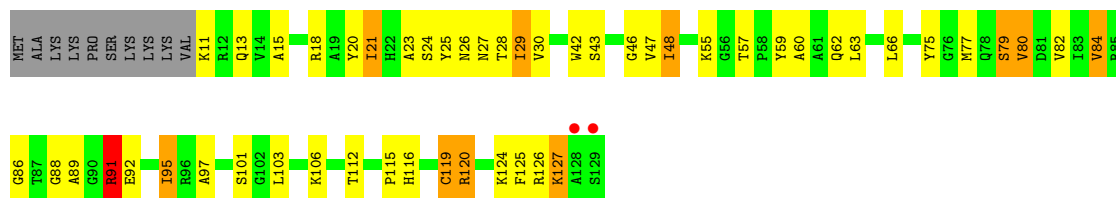
• Molecule 9: 30S ribosomal protein S9



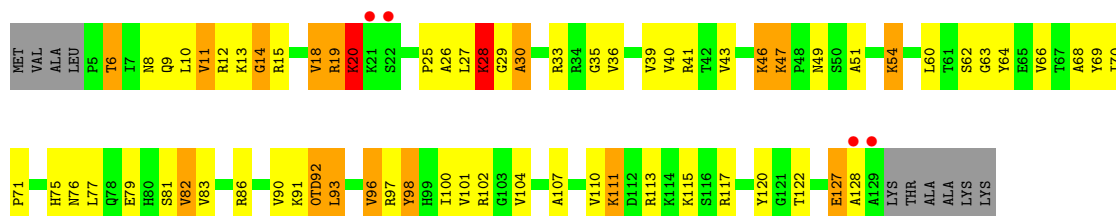
• Molecule 10: 30S ribosomal protein S10



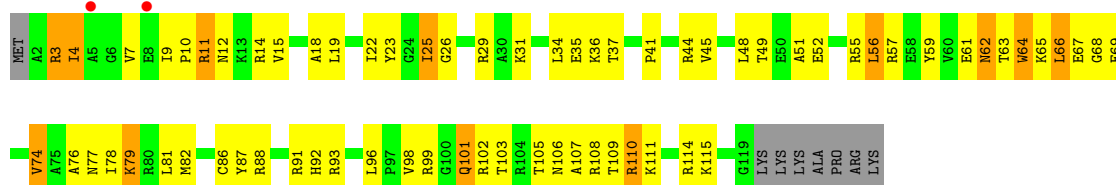
• Molecule 11: 30S ribosomal protein S11



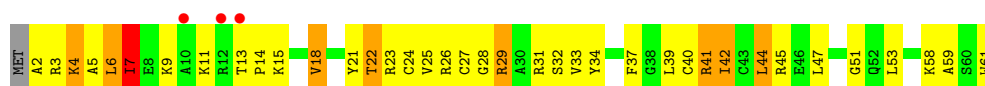
- Molecule 12: 30S ribosomal protein S12



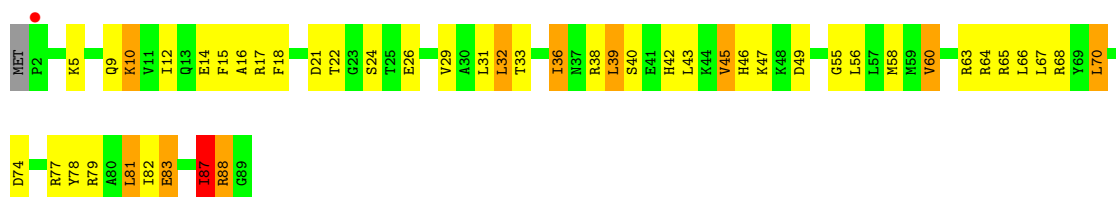
- Molecule 13: 30S ribosomal protein S13



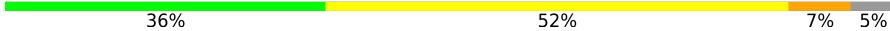
- Molecule 14: 30S ribosomal protein S14



- Molecule 15: 30S ribosomal protein S15



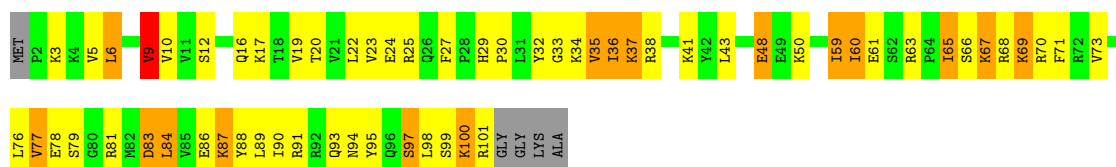
- Molecule 16: 30S ribosomal protein S16

Chain P: 



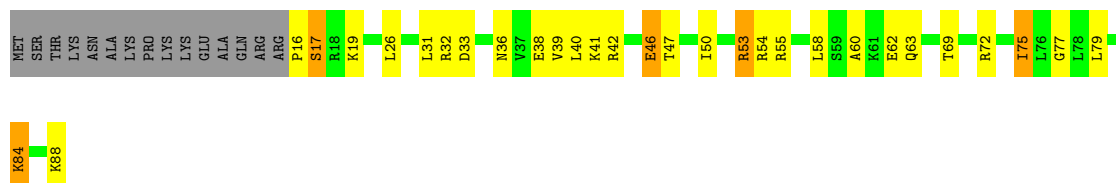
- Molecule 17: 30S ribosomal protein S17

Chain Q: 



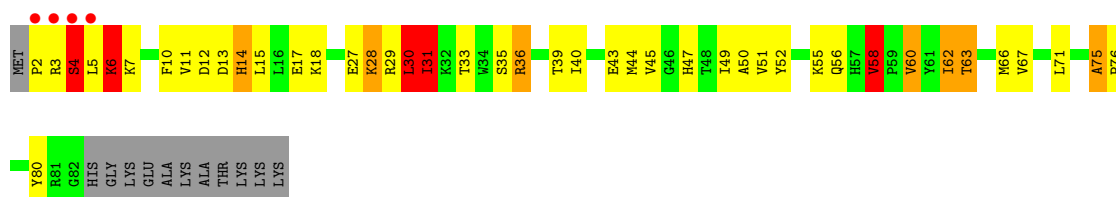
- Molecule 18: 30S ribosomal protein S18

Chain R: 



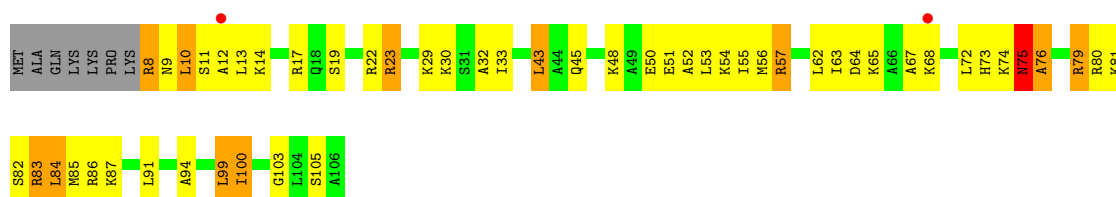
- Molecule 19: 30S ribosomal protein S19

Chain S: 



- Molecule 20: 30S ribosomal protein S20

Chain T: 



- Molecule 21: 30S ribosomal protein THX



● Molecule 22: 5'-R(*UP*UP*U)-3'



● Molecule 23: 5'-R(*GP*GP*GP*AP*UP*UP*GP*AP*AP*AP*AP*UP*CP*CP*C)-3'



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	400.95Å 400.95Å 176.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.73 – 3.97 49.73 – 3.97	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.73-3.97) 99.0 (49.73-3.97)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.94 (at 4.00Å)	Xtriage
Refinement program	PHENIX dev_978	Depositor
R, R_{free}	0.153 , 0.212 0.154 , 0.211	Depositor DCC
R_{free} test set	6190 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	100.0	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 87.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	53651	wwPDB-VP
Average B, all atoms (Å ²)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.58% 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: 4OC, MG, 7MG, 5MC, 2MG, 0TD, PAR, UR3, M2G, MA6, PSU, ZN

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	0.61	1/36037 (0.0%)	0.61	0/56239
2	B	0.85	0/1931	1.25	15/2607 (0.6%)
3	C	0.92	1/1637 (0.1%)	1.25	7/2207 (0.3%)
4	D	0.87	1/1733 (0.1%)	1.32	23/2318 (1.0%)
5	E	1.05	0/1163	1.51	21/1566 (1.3%)
6	F	0.82	0/856	1.21	6/1154 (0.5%)
7	G	0.82	0/1276	1.25	7/1709 (0.4%)
8	H	0.98	1/1136 (0.1%)	1.45	13/1527 (0.9%)
9	I	0.87	1/1029 (0.1%)	1.32	7/1379 (0.5%)
10	J	0.97	3/806 (0.4%)	1.31	8/1084 (0.7%)
11	K	0.90	0/900	1.29	8/1213 (0.7%)
12	L	1.13	4/978 (0.4%)	1.41	10/1308 (0.8%)
13	M	0.90	1/947 (0.1%)	1.18	1/1270 (0.1%)
14	N	0.93	0/501	1.28	3/664 (0.5%)
15	O	0.84	0/745	1.13	0/992
16	P	0.99	1/717 (0.1%)	1.28	2/965 (0.2%)
17	Q	1.08	3/847 (0.4%)	1.42	7/1131 (0.6%)
18	R	0.89	0/604	1.22	2/801 (0.2%)
19	S	0.81	0/662	1.32	8/892 (0.9%)
20	T	0.98	0/765	1.38	6/1007 (0.6%)
21	U	0.82	0/213	1.11	0/279
22	V	0.73	0/62	0.62	0/94
23	W	0.55	0/357	0.51	0/555
All	All	0.73	17/55902 (0.0%)	0.89	154/82961 (0.2%)

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
2	B	0	2
3	C	0	1
4	D	0	1
8	H	0	1
12	L	0	1
13	M	0	1
14	N	0	1
17	Q	0	1
19	S	0	1
All	All	0	10

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	L	26	ALA	CA-CB	8.43	1.68	1.53
13	M	9	ILE	CA-CB	7.78	1.64	1.54
12	L	101	VAL	CA-CB	-7.42	1.45	1.54
17	Q	9	VAL	CA-CB	-6.75	1.46	1.54
17	Q	35	VAL	CA-CB	-6.65	1.46	1.54
16	P	24	ALA	CA-CB	-5.80	1.43	1.53
3	C	206	GLU	CA-C	5.61	1.57	1.52
8	H	134	ILE	CA-CB	-5.58	1.47	1.54
17	Q	23	VAL	CA-CB	-5.52	1.47	1.54
12	L	102	ARG	CA-C	-5.27	1.46	1.52
9	I	41	VAL	CA-CB	-5.24	1.47	1.54
10	J	60	ARG	CA-C	5.23	1.59	1.52
1	A	1301	U	C3'-O3'	5.19	1.50	1.43
10	J	90	LEU	CA-C	5.18	1.59	1.52
4	D	56	VAL	CA-CB	-5.15	1.47	1.54
12	L	18	VAL	CA-CB	5.11	1.59	1.53
10	J	75	ILE	CA-CB	5.09	1.61	1.54

All (154) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	39	GLY	N-CA-C	-13.40	96.76	114.85
17	Q	35	VAL	CB-CA-C	-11.02	97.25	110.91
4	D	26	CYS	N-CA-C	-10.36	100.67	113.20
20	T	75	ASN	N-CA-C	-10.20	100.32	113.17
8	H	73	ASP	CA-C-N	10.15	129.89	119.64
8	H	73	ASP	C-N-CA	10.15	129.89	119.64
12	L	26	ALA	N-CA-C	-10.00	101.10	113.20
3	C	155	GLY	N-CA-C	9.68	122.98	112.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	111	ARG	CA-C-N	9.55	129.21	119.56
7	G	111	ARG	C-N-CA	9.55	129.21	119.56
5	E	145	LYS	N-CA-C	-9.31	101.11	111.07
3	C	6	HIS	CA-C-N	9.23	128.57	118.97
3	C	6	HIS	C-N-CA	9.23	128.57	118.97
20	T	9	ASN	N-CA-C	9.21	120.06	108.45
9	I	117	HIS	N-CA-C	-8.78	98.13	111.56
17	Q	9	VAL	CB-CA-C	-8.68	97.79	110.63
8	H	75	ARG	CA-C-N	8.62	129.14	119.92
8	H	75	ARG	C-N-CA	8.62	129.14	119.92
11	K	101	SER	N-CA-C	-8.48	101.94	113.30
14	N	7	ILE	CB-CA-C	8.23	124.78	111.29
10	J	52	GLY	CA-C-N	8.06	127.73	119.19
10	J	52	GLY	C-N-CA	8.06	127.73	119.19
9	I	22	GLY	N-CA-C	8.04	123.56	111.42
8	H	4	ASP	CA-C-N	8.02	127.69	119.19
8	H	4	ASP	C-N-CA	8.02	127.69	119.19
2	B	8	LYS	N-CA-C	-7.84	102.74	111.28
10	J	60	ARG	N-CA-C	7.82	120.41	110.24
12	L	63	GLY	N-CA-C	-7.82	105.39	114.69
7	G	61	VAL	CB-CA-C	-7.63	101.69	112.22
2	B	7	VAL	CB-CA-C	-7.63	105.23	111.71
19	S	4	SER	N-CA-C	7.62	120.90	108.55
9	I	64	THR	CB-CA-C	-7.30	98.99	110.74
8	H	46	LYS	N-CA-C	-7.25	103.45	111.36
5	E	76	ILE	CA-C-N	7.22	127.22	119.28
5	E	76	ILE	C-N-CA	7.22	127.22	119.28
7	G	36	LYS	N-CA-C	-7.20	103.96	112.89
11	K	25	TYR	N-CA-C	-7.19	104.59	113.15
19	S	58	VAL	N-CA-C	7.14	116.48	108.05
3	C	5	ILE	CB-CA-C	-7.11	103.49	111.45
20	T	76	ALA	N-CA-C	-7.06	103.66	111.36
8	H	71	GLY	CA-C-N	-6.96	113.62	120.52
8	H	71	GLY	C-N-CA	-6.96	113.62	120.52
17	Q	17	LYS	N-CA-C	6.91	120.93	111.54
4	D	6	GLY	CA-C-N	6.83	127.24	119.93
4	D	6	GLY	C-N-CA	6.83	127.24	119.93
4	D	13	ARG	N-CA-C	6.70	118.38	111.14
2	B	7	VAL	N-CA-C	6.69	117.77	111.48
4	D	12	CYS	N-CA-C	-6.62	100.45	111.37
5	E	24	ARG	N-CA-C	-6.54	98.55	109.07
5	E	92	LYS	CA-C-N	6.52	126.87	119.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	92	LYS	C-N-CA	6.52	126.87	119.83
18	R	62	GLU	N-CA-C	-6.50	104.11	111.07
11	K	29	ILE	N-CA-C	6.49	117.65	108.17
5	E	32	VAL	N-CA-C	6.47	118.03	108.45
5	E	41	VAL	CB-CA-C	-6.47	100.36	110.52
2	B	90	MET	N-CA-C	6.47	117.04	109.60
12	L	101	VAL	CB-CA-C	-6.44	102.20	111.34
3	C	198	VAL	CB-CA-C	-6.34	101.86	110.42
12	L	82	VAL	CB-CA-C	-6.30	102.94	111.63
8	H	125	ARG	N-CA-C	-6.27	103.97	111.69
5	E	127	ASN	CA-C-N	6.15	125.64	119.24
5	E	127	ASN	C-N-CA	6.15	125.64	119.24
5	E	95	ALA	CA-C-N	6.14	126.16	119.90
5	E	95	ALA	C-N-CA	6.14	126.16	119.90
6	F	55	ASP	CA-C-N	6.12	126.24	119.87
6	F	55	ASP	C-N-CA	6.12	126.24	119.87
16	P	79	VAL	N-CA-C	-6.11	103.45	111.09
16	P	70	ALA	N-CA-C	-6.06	104.75	111.36
5	E	67	VAL	N-CA-C	6.03	116.31	108.35
4	D	135	LEU	CA-C-N	6.00	125.62	119.56
4	D	135	LEU	C-N-CA	6.00	125.62	119.56
17	Q	99	SER	N-CA-C	5.97	123.51	110.80
7	G	155	ARG	N-CA-C	5.95	119.36	111.75
14	N	37	PHE	N-CA-C	5.95	120.66	113.17
8	H	134	ILE	N-CA-C	5.94	116.58	110.82
20	T	79	ARG	N-CA-C	-5.94	104.72	111.07
6	F	95	GLU	CA-C-N	5.92	126.27	119.93
6	F	95	GLU	C-N-CA	5.92	126.27	119.93
18	R	17	SER	N-CA-C	5.91	119.81	112.24
8	H	67	PRO	CA-C-O	-5.88	114.82	122.12
2	B	188	ALA	N-CA-C	5.86	117.99	108.26
5	E	140	ARG	N-CA-C	-5.80	105.04	111.36
9	I	41	VAL	CB-CA-C	-5.77	104.26	112.22
2	B	80	ILE	N-CA-C	5.77	115.84	110.42
4	D	12	CYS	CA-CB-SG	5.76	127.65	114.40
17	Q	27	PHE	CA-C-N	-5.73	114.06	120.14
17	Q	27	PHE	C-N-CA	-5.73	114.06	120.14
7	G	86	GLN	CA-C-N	-5.69	117.81	123.04
7	G	86	GLN	C-N-CA	-5.69	117.81	123.04
5	E	20	GLN	N-CA-C	-5.68	99.78	108.76
3	C	194	GLY	N-CA-C	5.64	117.79	110.45
11	K	42	TRP	N-CA-C	5.61	116.49	108.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	38	TYR	CA-C-N	5.61	126.16	120.38
4	D	38	TYR	C-N-CA	5.61	126.16	120.38
10	J	62	HIS	N-CA-C	5.60	122.73	110.80
11	K	91	ARG	N-CA-C	-5.60	105.18	111.28
2	B	96	ARG	N-CA-C	5.58	117.55	109.07
10	J	76	ASN	CA-C-N	5.57	126.80	119.84
10	J	76	ASN	C-N-CA	5.57	126.80	119.84
2	B	227	GLY	N-CA-C	5.56	119.20	112.48
9	I	63	ILE	N-CA-C	5.51	116.06	108.12
4	D	19	LEU	CA-C-N	-5.50	115.21	122.85
4	D	19	LEU	C-N-CA	-5.50	115.21	122.85
4	D	33	MET	N-CA-C	-5.48	105.32	112.23
19	S	36	ARG	N-CA-C	-5.48	106.64	113.38
12	L	66	VAL	CB-CA-C	-5.47	102.72	110.82
5	E	111	GLU	N-CA-C	-5.47	105.40	111.36
13	M	25	ILE	N-CA-C	5.45	116.33	108.48
6	F	92	LYS	N-CA-C	-5.45	101.10	109.76
11	K	75	TYR	N-CA-C	-5.44	106.41	113.16
12	L	20	LYS	N-CA-C	5.43	117.69	108.02
19	S	75	ALA	CA-C-N	5.43	125.70	119.83
19	S	75	ALA	C-N-CA	5.43	125.70	119.83
12	L	30	ALA	CA-C-N	5.42	125.04	119.56
12	L	30	ALA	C-N-CA	5.42	125.04	119.56
6	F	11	ASN	N-CA-C	5.42	117.40	109.71
11	K	89	ALA	N-CA-C	-5.41	102.39	110.23
2	B	47	THR	N-CA-CB	5.40	117.79	109.91
2	B	81	VAL	CB-CA-C	-5.39	104.97	112.04
19	S	30	LEU	CB-CA-C	-5.38	109.38	115.79
19	S	60	VAL	N-CA-C	5.37	116.11	107.73
2	B	127	ILE	N-CA-C	5.35	115.98	110.36
17	Q	67	LYS	N-CA-C	-5.33	103.11	110.35
4	D	5	ILE	CB-CA-C	-5.30	104.88	111.08
11	K	82	VAL	N-CA-C	5.30	115.48	107.75
10	J	58	ASP	N-CA-C	5.29	119.42	112.92
2	B	20	GLU	N-CA-C	5.27	116.73	110.19
12	L	79	GLU	N-CA-C	-5.25	105.47	111.14
2	B	192	SER	N-CA-C	5.23	118.22	110.48
4	D	194	LEU	CA-C-N	5.23	127.54	120.38
4	D	194	LEU	C-N-CA	5.23	127.54	120.38
4	D	196	LEU	CA-C-N	5.21	128.94	121.91
4	D	196	LEU	C-N-CA	5.21	128.94	121.91
4	D	10	ARG	N-CA-C	5.18	117.66	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	T	94	ALA	N-CA-C	-5.17	106.95	113.20
10	J	74	ILE	N-CA-C	5.16	115.53	107.99
4	D	204	ILE	CB-CA-C	-5.16	105.37	111.97
5	E	113	ALA	N-CA-C	-5.14	105.85	111.82
12	L	14	GLY	N-CA-C	5.14	118.71	112.48
4	D	196	LEU	N-CA-C	5.13	116.87	109.48
19	S	29	ARG	N-CA-C	5.13	116.77	108.26
9	I	17	VAL	N-CA-C	5.12	115.42	107.28
8	H	35	ILE	CB-CA-C	-5.10	105.25	112.14
5	E	82	VAL	CA-C-N	-5.09	115.69	122.72
5	E	82	VAL	C-N-CA	-5.09	115.69	122.72
4	D	141	ARG	CA-C-N	-5.09	114.74	120.14
4	D	141	ARG	C-N-CA	-5.09	114.74	120.14
2	B	154	LEU	N-CA-C	5.09	117.72	111.82
2	B	71	VAL	CB-CA-C	-5.08	104.68	110.73
20	T	55	ILE	CB-CA-C	-5.05	105.42	112.04
3	C	28	GLN	N-CA-C	5.04	119.50	112.90
14	N	42	ILE	CB-CA-C	-5.02	105.44	112.02
5	E	12	LEU	N-CA-C	5.01	116.81	109.24
5	E	83	GLU	N-CA-C	-5.00	101.09	109.24

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	14	GLY	Peptide
2	B	89	GLY	Peptide
3	C	166	GLU	Peptide
4	D	195	ALA	Peptide
8	H	90	GLY	Peptide
12	L	46	LYS	Peptide
13	M	62	ASN	Peptide
14	N	7	ILE	Peptide
17	Q	79	SER	Peptide
19	S	6	LYS	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	32504	0	16432	806	0
2	B	1896	0	1936	81	0
3	C	1613	0	1677	83	0
4	D	1703	0	1763	82	0
5	E	1147	0	1207	41	0
6	F	843	0	857	33	0
7	G	1257	0	1296	41	0
8	H	1116	0	1177	60	0
9	I	1010	0	1037	50	0
10	J	793	0	835	57	0
11	K	885	0	904	31	0
12	L	973	0	1058	42	0
13	M	937	0	995	46	0
14	N	492	0	529	35	0
15	O	734	0	771	34	0
16	P	701	0	720	40	0
17	Q	834	0	906	46	0
18	R	598	0	670	25	0
19	S	648	0	673	30	0
20	T	763	0	861	29	0
21	U	209	0	221	10	0
22	V	57	0	32	3	0
23	W	319	0	164	9	0
24	A	756	0	810	62	0
25	A	345	0	0	0	0
25	D	2	0	0	0	0
25	E	4	0	0	0	0
25	H	1	0	0	0	0
25	L	1	0	0	0	0
25	N	1	0	0	0	0
25	O	1	0	0	0	0
25	P	3	0	0	0	0
25	Q	1	0	0	0	0
25	S	2	0	0	0	0
25	T	1	0	0	0	0
25	V	1	0	0	0	0
26	D	1	0	0	0	0
26	N	1	0	0	0	0
27	A	480	0	0	6	0
27	C	1	0	0	0	0
27	D	2	0	0	0	0
27	E	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	K	1	0	0	0	0
27	L	2	0	0	0	0
27	N	2	0	0	1	0
27	O	4	0	0	0	0
27	V	1	0	0	0	0
All	All	53651	0	37531	1578	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 18.

All (1578) 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)
11:K:15:ALA:HA	11:K:77:MET:HA	1.47	0.97
1:A:1053:G:HO2'	1:A:1199:U:H5	0.97	0.92
1:A:737:A:H1'	6:F:73:ASN:HD21	1.34	0.91
19:S:33:THR:HG22	19:S:35:SER:H	1.38	0.88
1:A:975:A:H4'	1:A:976:G:H5''	1.57	0.87
1:A:983:A:O2'	1:A:1050:G:OP2	1.91	0.86
1:A:1249:C:O2'	9:I:73:GLN:NE2	2.10	0.84
16:P:34:GLU:OE1	16:P:55:ARG:NH1	2.10	0.84
24:A:1608:PAR:N21	24:A:1608:PAR:O43	2.10	0.84
20:T:57:ARG:HH21	20:T:100:ILE:HG23	1.43	0.83
1:A:1271:G:OP1	24:A:1616:PAR:N32	2.11	0.83
10:J:19:SER:HB3	10:J:91:PRO:HG3	1.61	0.83
1:A:537:G:OP1	12:L:113:ARG:NH2	2.11	0.83
5:E:95:ALA:O	5:E:98:THR:OG1	1.96	0.82
1:A:1061:G:OP1	24:A:1608:PAR:O44	1.97	0.82
1:A:664:G:H22	1:A:741:G:H1	1.25	0.81
3:C:58:GLU:HB3	10:J:92:THR:HG21	1.61	0.81
3:C:150:LYS:HG3	3:C:169:ALA:HB2	1.63	0.80
1:A:966:M2G:HM13	1:A:967:5MC:H1'	1.60	0.80
24:A:1605:PAR:N21	24:A:1605:PAR:O53	2.14	0.80
3:C:11:ARG:HD3	3:C:180:ALA:HB3	1.63	0.79
24:A:1608:PAR:H531	24:A:1608:PAR:HN22	1.48	0.79
5:E:83:GLU:HG3	5:E:88:LYS:HE3	1.65	0.79
3:C:180:ALA:HB1	3:C:182:ILE:HG13	1.65	0.78
1:A:108:G:H5''	1:A:109:A:H5''	1.65	0.78
1:A:376:G:H5''	16:P:5:ARG:HD2	1.65	0.78
1:A:946:A:H2'	1:A:947:G:H8	1.47	0.78
17:Q:66:SER:HB3	17:Q:69:LYS:HG3	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1212:U:O2'	1:A:1213:A:O5'	2.02	0.78
1:A:353:A:H5'	1:A:353:A:H8	1.47	0.78
16:P:18:ARG:HD3	16:P:35:LYS:HD2	1.66	0.77
1:A:424:G:N7	24:A:1611:PAR:N21	2.30	0.77
7:G:75:VAL:HG21	7:G:86:GLN:HB3	1.64	0.77
1:A:946:A:H2'	1:A:947:G:C8	2.19	0.77
9:I:43:ALA:HA	9:I:74:ILE:HD13	1.66	0.77
10:J:4:ILE:HD12	10:J:74:ILE:HG13	1.64	0.77
1:A:447:G:H2'	1:A:485:G:H22	1.49	0.77
1:A:1367:C:H5'	10:J:60:ARG:NH1	2.00	0.77
15:O:39:LEU:HD12	15:O:56:LEU:HD13	1.68	0.76
1:A:734:G:H21	18:R:75:ILE:HD11	1.49	0.76
1:A:258:G:H2'	1:A:259:G:H8	1.51	0.76
19:S:55:LYS:HG2	19:S:56:GLN:HG2	1.66	0.75
14:N:27:CYS:SG	14:N:29:ARG:HB2	2.25	0.75
1:A:625:G:O6	24:A:1606:PAR:N24	2.19	0.75
5:E:82:VAL:HG21	5:E:138:ALA:HA	1.68	0.74
4:D:57:ARG:HG3	4:D:57:ARG:HH11	1.52	0.74
1:A:1328:C:H2'	1:A:1329:A:H8	1.52	0.74
1:A:442:C:H42	1:A:492:G:H1	1.35	0.74
1:A:825:G:H21	8:H:11:THR:HG21	1.53	0.74
1:A:951:G:OP2	13:M:102:ARG:NH2	2.21	0.74
2:B:97:TRP:HZ2	2:B:102:LEU:HD13	1.52	0.74
10:J:49:VAL:O	10:J:61:GLU:N	2.20	0.73
1:A:192:U:H1'	20:T:103:GLY:HA2	1.69	0.73
1:A:1127:G:H21	1:A:1146:A:H62	1.36	0.73
1:A:927:G:O2'	1:A:1503:A:N7	2.21	0.73
10:J:48:THR:HA	10:J:62:HIS:HB3	1.71	0.73
1:A:51:A:OP2	24:A:1604:PAR:H24	1.89	0.73
1:A:1399:C:H4'	1:A:1400:5MC:H5''	1.70	0.72
1:A:1387:G:O2'	27:A:2274:HOH:O	2.07	0.72
1:A:47:C:OP1	24:A:1604:PAR:N32	2.23	0.72
8:H:85:ARG:NH1	8:H:87:SER:O	2.21	0.72
16:P:15:PRO:HD2	16:P:42:ARG:HD3	1.70	0.72
1:A:382:A:H2'	1:A:383:A:C8	2.23	0.72
5:E:10:MET:HA	5:E:32:VAL:HG22	1.72	0.72
1:A:1003(A):G:H2'	1:A:1004:A:H4'	1.71	0.72
1:A:235:C:H5'	17:Q:70:ARG:HG2	1.72	0.72
12:L:47:LYS:NZ	22:V:3:U:OP1	2.23	0.72
11:K:24:SER:HB3	11:K:26:ASN:H	1.55	0.72
1:A:1281:U:H5'	1:A:1282:C:H5	1.54	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:737:A:H1'	6:F:73:ASN:ND2	2.05	0.71
7:G:137:LYS:O	7:G:141:VAL:HG23	1.90	0.71
12:L:77:LEU:HD21	12:L:107:ALA:HB2	1.71	0.71
10:J:50:ILE:HA	10:J:60:ARG:HA	1.72	0.71
1:A:1031:G:H2'	1:A:1032:G:H8	1.55	0.71
9:I:53:VAL:HG21	9:I:85:LEU:HD21	1.72	0.71
1:A:1366:C:H2'	1:A:1367:C:C6	2.26	0.71
13:M:49:THR:HG22	13:M:51:ALA:H	1.55	0.71
8:H:17:THR:O	8:H:78:GLN:NE2	2.24	0.71
9:I:51:ARG:HA	9:I:56:LEU:HD22	1.72	0.70
4:D:140:VAL:HG11	4:D:146:ILE:HD11	1.72	0.70
10:J:24:VAL:HG13	10:J:34:VAL:HG11	1.72	0.70
1:A:433:C:H5''	1:A:433:C:H6	1.56	0.70
1:A:795:C:H5''	1:A:796:C:OP2	1.91	0.70
18:R:38:GLU:HA	18:R:41:LYS:HE2	1.72	0.70
1:A:329:A:O2'	1:A:332:G:N7	2.25	0.70
1:A:642:A:N3	8:H:113:SER:OG	2.25	0.70
4:D:13:ARG:HD2	4:D:38:TYR:O	1.91	0.70
1:A:250:A:H4'	1:A:251:G:O5'	1.92	0.70
1:A:114:U:H2'	1:A:115:G:C8	2.27	0.70
1:A:355:C:H5'	1:A:389:A:OP2	1.90	0.70
1:A:1326:C:OP1	21:U:12:LYS:NZ	2.23	0.70
24:A:1613:PAR:O23	24:A:1613:PAR:N21	2.25	0.70
4:D:61:LYS:HB2	4:D:203:VAL:HG13	1.73	0.70
1:A:414:A:P	24:A:1611:PAR:H122	2.15	0.69
1:A:1291:G:H4'	9:I:39:GLY:HA3	1.72	0.69
1:A:1284:C:H3'	1:A:1285:A:H8	1.57	0.69
24:A:1616:PAR:O53	24:A:1616:PAR:N24	2.26	0.69
3:C:78:GLY:HA3	3:C:83:ARG:HB3	1.74	0.69
20:T:64:ASP:OD2	20:T:81:LYS:NZ	2.22	0.69
23:W:36:A:H2'	23:W:37:A:H8	1.55	0.69
24:A:1602:PAR:O44	24:A:1602:PAR:N24	2.24	0.69
1:A:1338:G:H2'	1:A:1339:A:C8	2.28	0.69
1:A:1504:G:OP1	1:A:1507:A:H4'	1.92	0.69
8:H:35:ILE:O	8:H:39:LEU:HD22	1.93	0.69
15:O:10:LYS:HE2	15:O:14:GLU:HB2	1.75	0.69
3:C:131:ARG:HA	3:C:134:ILE:HD12	1.75	0.69
1:A:1360:A:H2'	1:A:1361:G:O4'	1.93	0.69
18:R:17:SER:HB3	18:R:54:ARG:HH11	1.58	0.69
13:M:11:ARG:HG3	13:M:12:ASN:HB2	1.75	0.68
1:A:1328:C:H2'	1:A:1329:A:C8	2.28	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:189:ASP:O	2:B:192:SER:OG	2.09	0.68
9:I:10:ARG:NH1	9:I:75:ASP:OD2	2.27	0.68
3:C:156:ARG:H	3:C:163:ALA:HA	1.58	0.68
3:C:164:ARG:NH1	3:C:166:GLU:OE1	2.26	0.68
10:J:34:VAL:HA	10:J:74:ILE:HG22	1.75	0.68
1:A:1401:G:C2	1:A:1402:4OC:H1'	2.28	0.68
7:G:20:ASP:OD2	7:G:63:LYS:NZ	2.25	0.68
7:G:44:TYR:HA	7:G:47:CYS:HB2	1.75	0.68
24:A:1612:PAR:H42	24:A:1612:PAR:N21	2.09	0.68
1:A:414:A:OP2	24:A:1611:PAR:N12	2.27	0.67
1:A:1023:G:O6	1:A:1024:G:N2	2.24	0.67
5:E:144:THR:O	5:E:148:VAL:HG23	1.94	0.67
11:K:57:THR:HG22	11:K:59:TYR:H	1.59	0.67
12:L:49:ASN:ND2	12:L:92:0TD:SB	2.67	0.67
1:A:37:U:O2'	1:A:500:G:H4'	1.95	0.67
1:A:1356:G:H2'	1:A:1357:A:C8	2.28	0.67
1:A:928:G:O2'	1:A:1533:C:OP1	2.11	0.67
1:A:1154:G:H2'	1:A:1155:G:H8	1.59	0.67
3:C:126:ARG:HG2	3:C:128:PHE:HD1	1.60	0.67
1:A:1124:G:HO2'	1:A:1145:C:N4	1.92	0.67
1:A:972:C:OP1	10:J:57:LYS:NZ	2.22	0.67
1:A:372:C:H4'	1:A:373:A:O5'	1.94	0.67
1:A:1528:U:O2'	1:A:1529:G:OP2	2.12	0.67
20:T:33:ILE:HD13	20:T:63:ILE:HG12	1.77	0.67
10:J:6:ILE:HD13	10:J:72:VAL:HB	1.77	0.66
1:A:1305:G:H5''	21:U:4:GLY:HA3	1.75	0.66
15:O:55:GLY:HA2	15:O:58:MET:HE2	1.75	0.66
1:A:1008:C:N3	1:A:1022:G:N2	2.42	0.66
7:G:74:GLU:HG2	7:G:91:VAL:HG22	1.77	0.66
12:L:62:SER:HB3	12:L:64:TYR:HD1	1.61	0.66
18:R:36:ASN:O	18:R:40:LEU:HD12	1.95	0.66
1:A:475:G:H2'	1:A:476:G:H8	1.59	0.66
1:A:1263:C:H42	1:A:1272:G:H1	1.43	0.66
1:A:1454:G:H2'	1:A:1455:G:H8	1.60	0.66
2:B:197:VAL:HB	2:B:200:ILE:HG12	1.78	0.66
10:J:54:PHE:HD2	10:J:55:LYS:HG2	1.61	0.66
6:F:28:ARG:HH11	6:F:28:ARG:HB2	1.61	0.65
14:N:6:LEU:HD12	14:N:23:ARG:HH21	1.60	0.65
16:P:26:ARG:HD2	16:P:31:LYS:O	1.96	0.65
1:A:1062:U:H2'	1:A:1063:C:C6	2.31	0.65
7:G:15:ASP:HB3	7:G:20:ASP:H	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:61:GLU:OE2	14:N:58:LYS:NZ	2.29	0.65
23:W:36:A:H2'	23:W:37:A:C8	2.32	0.65
1:A:560:U:H5'	1:A:566:G:N2	2.12	0.65
1:A:382:A:H2'	1:A:383:A:H8	1.59	0.65
1:A:975:A:H5''	1:A:975:A:H8	1.62	0.65
1:A:1350:A:OP2	9:I:118:LYS:HE3	1.95	0.65
4:D:31:CYS:C	4:D:33:MET:H	2.04	0.65
13:M:79:LYS:HA	13:M:82:MET:HE2	1.78	0.65
17:Q:67:LYS:HA	17:Q:70:ARG:HH12	1.62	0.65
1:A:542:G:OP1	4:D:10:ARG:NH2	2.30	0.65
1:A:983:A:OP1	14:N:3:ARG:NH2	2.30	0.65
3:C:156:ARG:HH21	3:C:161:GLU:HA	1.62	0.65
1:A:1443:G:H4'	1:A:1446:A:C5'	2.27	0.64
1:A:1488:G:H2'	1:A:1489:G:H8	1.62	0.64
24:A:1610:PAR:O44	24:A:1610:PAR:N24	2.30	0.64
6:F:10:LEU:HD12	6:F:59:TYR:HB3	1.78	0.64
1:A:192:U:C1'	20:T:103:GLY:HA2	2.27	0.64
1:A:1182:G:O2'	1:A:1183:A:OP2	2.13	0.64
1:A:1343:G:H2'	1:A:1344:C:C6	2.32	0.64
16:P:69:THR:HG22	16:P:72:ARG:HD3	1.79	0.64
1:A:204:U:H5'	1:A:216:G:OP1	1.97	0.64
1:A:1060:C:C5	3:C:2:GLY:HA2	2.33	0.64
5:E:81:GLU:HG2	5:E:90:VAL:HG22	1.79	0.64
8:H:86:ILE:HG21	8:H:133:LEU:HD13	1.79	0.64
11:K:24:SER:HB2	11:K:27:ASN:H	1.62	0.64
6:F:25:ILE:HD13	6:F:82:ARG:HD2	1.78	0.64
1:A:665:A:H2'	1:A:732:C:O2	1.96	0.64
1:A:749:C:H2'	1:A:750:G:H8	1.62	0.64
11:K:57:THR:HB	11:K:60:ALA:H	1.63	0.64
3:C:135:LYS:HE3	5:E:50:GLU:HG2	1.80	0.64
17:Q:29:HIS:HB2	17:Q:36:ILE:CD1	2.28	0.64
6:F:91:VAL:HG13	18:R:72:ARG:NH2	2.12	0.64
1:A:976:G:H5'	1:A:1358:U:O2'	1.97	0.64
3:C:116:VAL:HG21	3:C:202:ILE:HD11	1.79	0.64
4:D:111:ALA:HB2	4:D:120:LEU:HD12	1.79	0.64
7:G:23:VAL:O	7:G:27:ILE:HG12	1.98	0.64
19:S:27:GLU:HG2	19:S:28:LYS:H	1.63	0.64
1:A:1498:UR3:O2'	1:A:1499:A:OP2	2.14	0.63
1:A:1031:G:H2'	1:A:1032:G:C8	2.33	0.63
24:A:1603:PAR:H532	24:A:1603:PAR:HN61	1.63	0.63
1:A:217:C:O2'	1:A:461:C:N4	2.30	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:731:G:OP1	1:A:766:A:H1'	1.99	0.63
7:G:26:PHE:CE2	7:G:30:ILE:HD11	2.34	0.63
1:A:1149:C:H2'	1:A:1150:U:H6	1.64	0.63
1:A:390:C:H2'	1:A:391:G:C8	2.33	0.62
24:A:1616:PAR:O44	24:A:1616:PAR:N64	2.30	0.62
2:B:75:LYS:HA	2:B:78:GLN:HB2	1.81	0.62
10:J:49:VAL:HG23	14:N:41:ARG:HD2	1.81	0.62
1:A:447:G:H2'	1:A:485:G:N2	2.12	0.62
1:A:1308:U:OP2	13:M:99:ARG:HG3	1.98	0.62
9:I:46:ALA:HB2	9:I:74:ILE:HG23	1.82	0.62
19:S:31:ILE:HG22	19:S:50:ALA:H	1.64	0.62
3:C:148:GLY:HA3	3:C:172:ARG:O	1.99	0.62
8:H:7:ALA:HA	8:H:85:ARG:HG3	1.81	0.62
1:A:445:G:H2'	1:A:446:G:H8	1.64	0.62
1:A:1060:C:C4	3:C:2:GLY:HA2	2.35	0.62
1:A:1392:G:H21	1:A:1502:A:H8	1.45	0.62
2:B:220:ASP:O	2:B:224:GLN:HB3	1.99	0.62
9:I:4:TYR:CE2	9:I:88:TYR:HD1	2.17	0.62
1:A:353:A:H5'	1:A:353:A:C8	2.31	0.62
1:A:1368:G:H5''	9:I:112:LYS:HD3	1.82	0.62
1:A:1505:G:O2'	1:A:1506:U:OP2	2.12	0.62
14:N:4:LYS:NZ	27:N:202:HOH:O	2.18	0.62
1:A:559:A:OP1	5:E:126:ARG:NH2	2.33	0.61
1:A:981:U:H5'	14:N:21:TYR:CE1	2.35	0.61
1:A:1296:C:H4'	1:A:1302:U:C5	2.34	0.61
5:E:98:THR:HB	5:E:117:ASP:HB3	1.81	0.61
20:T:45:GLN:HA	20:T:91:LEU:HD22	1.81	0.61
1:A:428:G:H4'	1:A:429:U:O5'	2.00	0.61
8:H:5:PRO:HB2	8:H:6:ILE:HD12	1.82	0.61
19:S:31:ILE:HG21	19:S:49:ILE:HG23	1.82	0.61
1:A:978:A:H1'	1:A:1322:C:O2	2.00	0.61
1:A:721:G:H4'	1:A:722:A:O4'	2.01	0.61
1:A:273:A:H1'	17:Q:16:GLN:HE21	1.66	0.61
1:A:592:G:H2'	1:A:593:G:H8	1.65	0.61
1:A:1288:A:H2'	1:A:1289:A:O4'	1.99	0.61
9:I:24:GLY:HA3	9:I:57:GLY:HA2	1.82	0.61
10:J:82:ILE:HA	10:J:85:LEU:HB2	1.81	0.61
1:A:1190:G:HO2'	1:A:1191:A:P	2.23	0.61
13:M:34:LEU:HD12	13:M:41:PRO:HA	1.83	0.61
1:A:1343:G:H2'	1:A:1344:C:H6	1.65	0.61
1:A:344:A:H5'	1:A:345:C:C5	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:598:U:H2'	1:A:599:C:C6	2.36	0.61
1:A:665:A:H3'	1:A:725:G:N2	2.15	0.61
1:A:1494:G:OP1	24:A:1601:PAR:N32	2.34	0.61
1:A:1191:A:OP2	3:C:3:ASN:ND2	2.34	0.61
4:D:8:VAL:O	4:D:11:LEU:N	2.25	0.61
9:I:70:LYS:O	9:I:74:ILE:HG13	2.00	0.61
18:R:33:ASP:O	18:R:40:LEU:HD11	2.01	0.61
12:L:25:PRO:C	12:L:27:LEU:H	2.07	0.60
2:B:80:ILE:HD11	2:B:208:ILE:HG22	1.82	0.60
1:A:109:A:C6	1:A:326:G:C6	2.89	0.60
9:I:29:ASN:ND2	9:I:65:VAL:O	2.26	0.60
1:A:110:C:H2'	1:A:111:G:O4'	2.01	0.60
1:A:595:G:H22	1:A:643:C:N4	1.99	0.60
1:A:81:U:H2'	1:A:82:U:H5''	1.83	0.60
1:A:433:C:H5''	1:A:433:C:C6	2.36	0.60
1:A:1256:A:H5'	1:A:1258:G:H1'	1.83	0.60
1:A:103:C:OP1	20:T:17:ARG:NH1	2.33	0.60
2:B:7:VAL:N	2:B:9:GLU:HG3	2.17	0.60
1:A:179:A:H2'	1:A:180:U:C6	2.37	0.60
3:C:155:GLY:HA2	3:C:164:ARG:H	1.66	0.60
4:D:100:ARG:HB3	4:D:102:ASP:OD1	2.01	0.60
12:L:6:THR:OG1	12:L:9:GLN:HG3	2.02	0.60
1:A:226:G:N7	24:A:1617:PAR:O31	2.34	0.60
1:A:1101:A:H4'	1:A:1102:A:O5'	2.02	0.60
1:A:1127:G:N2	1:A:1145:C:N3	2.50	0.60
2:B:84:GLU:OE1	2:B:216:SER:HA	2.02	0.60
5:E:10:MET:HE1	5:E:13:ILE:HD11	1.83	0.60
8:H:10:LEU:HD22	8:H:83:ILE:HD11	1.83	0.59
11:K:43:SER:HA	11:K:47:VAL:HG21	1.83	0.59
1:A:1256:A:N6	1:A:1278:U:O4'	2.28	0.59
12:L:90:VAL:HB	12:L:93:LEU:HB2	1.84	0.59
1:A:1488:G:H2'	1:A:1489:G:C8	2.37	0.59
2:B:133:LYS:O	2:B:137:ARG:HG3	2.01	0.59
1:A:438:G:O2'	1:A:495:U:O4	2.20	0.59
3:C:11:ARG:HH22	3:C:175:LEU:HD23	1.68	0.59
8:H:6:ILE:O	8:H:10:LEU:HG	2.01	0.59
10:J:39:PRO:HA	10:J:70:ARG:HD3	1.85	0.59
13:M:66:LEU:O	13:M:69:GLU:HB2	2.02	0.59
1:A:362:G:N2	1:A:365:U:OP2	2.36	0.59
1:A:1086:U:O5'	1:A:1086:U:H6	1.85	0.59
24:A:1618:PAR:H322	24:A:1618:PAR:HN21	1.51	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:148:VAL:O	5:E:152:ARG:HG3	2.02	0.59
1:A:1316:G:H4'	14:N:18:VAL:HG11	1.83	0.59
1:A:985:C:C2	1:A:1221:G:N2	2.71	0.59
1:A:1285:A:H4'	1:A:1286:A:O5'	2.03	0.59
1:A:1454:G:H2'	1:A:1455:G:C8	2.38	0.59
18:R:17:SER:OG	18:R:55:ARG:HG2	2.03	0.59
21:U:10:ARG:HD3	21:U:13:ILE:HD11	1.85	0.59
1:A:1065:U:H5''	1:A:1190:G:N2	2.17	0.59
1:A:1112:C:H1'	3:C:179:ARG:HD3	1.83	0.59
3:C:6:HIS:HD2	3:C:8:ILE:H	1.49	0.59
20:T:10:LEU:HG	20:T:12:ALA:H	1.68	0.59
1:A:595:G:H22	1:A:643:C:H42	1.51	0.58
1:A:1212:U:HO2'	1:A:1213:A:P	2.26	0.58
4:D:15:GLU:HG2	4:D:63:LYS:HG3	1.85	0.58
5:E:43:LEU:HD11	5:E:132:ALA:HB1	1.85	0.58
14:N:24:CYS:HB3	14:N:28:GLY:H	1.68	0.58
4:D:173:TRP:O	4:D:174:LEU:HD23	2.03	0.58
7:G:20:ASP:HB3	7:G:23:VAL:HG23	1.84	0.58
1:A:1402:4OC:HM22	1:A:1403:C:H5'	1.85	0.58
4:D:47:ARG:HE	4:D:48:ALA:H	1.51	0.58
4:D:148:VAL:HG12	4:D:149:ALA:H	1.68	0.58
23:W:28:G:H2'	23:W:28:G:N3	2.18	0.58
1:A:370:C:C2'	1:A:371:G:H5'	2.33	0.58
11:K:79:SER:HB2	11:K:106:LYS:HD3	1.85	0.58
15:O:79:ARG:NH1	15:O:83:GLU:HB2	2.18	0.58
1:A:91:C:H2'	1:A:92:C:H6	1.68	0.58
1:A:551:U:H2'	1:A:552:U:C6	2.37	0.58
1:A:1159:U:O4'	1:A:1182:G:N2	2.36	0.58
4:D:13:ARG:HD3	4:D:36:ARG:O	2.04	0.58
13:M:81:LEU:HD22	13:M:88:ARG:HB2	1.86	0.58
1:A:929:G:H1	1:A:1388:C:H42	1.50	0.58
4:D:7:PRO:HB2	4:D:10:ARG:HD2	1.86	0.58
1:A:376:G:H2'	1:A:377:G:H8	1.67	0.58
1:A:558:G:C8	1:A:559:A:H2'	2.38	0.58
1:A:1026:G:H3'	1:A:1027:C:H5''	1.85	0.58
7:G:15:ASP:HB2	7:G:20:ASP:O	2.03	0.58
9:I:48:GLU:HG2	9:I:51:ARG:HH21	1.69	0.58
15:O:56:LEU:O	15:O:60:VAL:HG23	2.03	0.58
16:P:45:THR:HB	16:P:47:ASP:H	1.69	0.58
4:D:100:ARG:O	4:D:104:VAL:HG23	2.04	0.58
15:O:26:GLU:OE1	15:O:77:ARG:HB3	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:677:U:H3	1:A:713:G:H22	1.52	0.57
1:A:975:A:H8	1:A:975:A:C5'	2.17	0.57
4:D:117:ALA:O	4:D:121:VAL:HG23	2.04	0.57
9:I:24:GLY:CA	9:I:57:GLY:HA2	2.33	0.57
7:G:54:THR:HG22	7:G:56:GLN:H	1.68	0.57
12:L:54:LYS:HG2	12:L:75:HIS:CD2	2.39	0.57
16:P:19:ILE:HG22	16:P:36:ILE:HG13	1.86	0.57
1:A:474:G:H2'	1:A:475:G:H8	1.67	0.57
19:S:10:PHE:O	19:S:39:THR:OG1	2.19	0.57
1:A:1517:G:H2'	1:A:1518:MA6:H8	1.87	0.57
8:H:33:GLU:HB2	8:H:59:LEU:HD21	1.85	0.57
17:Q:59:ILE:HD12	17:Q:73:VAL:HA	1.86	0.57
18:R:53:ARG:HG2	18:R:63:GLN:HG2	1.86	0.57
1:A:994:A:N7	1:A:1216:G:H4'	2.19	0.57
1:A:1049:U:H4'	1:A:1050:G:C5'	2.34	0.57
1:A:1179:A:O2'	1:A:1180:A:OP1	2.22	0.57
19:S:33:THR:HG22	19:S:35:SER:N	2.15	0.57
1:A:427:U:H3'	1:A:428:G:H2'	1.86	0.57
1:A:998:G:N2	1:A:999:C:N3	2.53	0.57
1:A:1349:A:OP1	9:I:120:ARG:HB2	2.04	0.57
18:R:53:ARG:HG3	18:R:53:ARG:HH11	1.70	0.57
20:T:82:SER:O	20:T:86:ARG:HG3	2.05	0.57
1:A:376:G:H2'	1:A:377:G:C8	2.40	0.57
1:A:765:G:H5''	1:A:766:A:OP1	2.04	0.57
3:C:155:GLY:HA2	3:C:164:ARG:O	2.05	0.57
7:G:23:VAL:HG12	7:G:27:ILE:HD11	1.87	0.57
11:K:21:ILE:HG23	11:K:30:VAL:HG22	1.86	0.57
1:A:291:C:O2'	1:A:292:G:H5'	2.04	0.57
1:A:1125:U:O2'	1:A:1281:U:O2	2.22	0.57
1:A:432:A:H2'	1:A:433:C:O4'	2.05	0.57
1:A:559:A:H4'	1:A:560:U:O5'	2.03	0.57
5:E:95:ALA:HB1	5:E:96:PRO:HD2	1.87	0.57
1:A:318:G:N2	1:A:335:C:O2	2.36	0.56
1:A:372:C:C4	1:A:387:U:H5	2.23	0.56
4:D:28:SER:O	4:D:30:LYS:N	2.38	0.56
5:E:51:VAL:O	5:E:55:VAL:HG23	2.04	0.56
7:G:50:ILE:HD13	7:G:125:MET:HG3	1.86	0.56
1:A:1048:G:H5''	14:N:3:ARG:HG3	1.86	0.56
24:A:1605:PAR:O44	24:A:1605:PAR:N64	2.36	0.56
17:Q:10:VAL:HG13	17:Q:19:VAL:HB	1.86	0.56
1:A:429:U:H1'	1:A:430:A:H5''	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:C:H2'	1:A:444:C:H6	1.69	0.56
1:A:800:G:O5'	1:A:800:G:H8	1.89	0.56
1:A:872:A:C8	1:A:874:G:C8	2.93	0.56
1:A:958:A:N3	1:A:985:C:O2'	2.35	0.56
6:F:28:ARG:HB2	6:F:28:ARG:NH1	2.19	0.56
6:F:44:GLY:HA2	6:F:59:TYR:CE2	2.40	0.56
17:Q:29:HIS:HB2	17:Q:36:ILE:HD11	1.87	0.56
20:T:81:LYS:O	20:T:85:MET:HG3	2.04	0.56
1:A:413:G:N2	1:A:428:G:H1'	2.20	0.56
1:A:757:U:H2'	1:A:758:G:O4'	2.04	0.56
1:A:1331:G:H4'	1:A:1332:A:H5'	1.88	0.56
11:K:48:ILE:HD13	11:K:48:ILE:H	1.70	0.56
11:K:59:TYR:HE2	11:K:63:LEU:HD11	1.70	0.56
1:A:143:A:H2	1:A:220:G:H22	1.53	0.56
1:A:355:C:OP1	24:A:1604:PAR:N21	2.39	0.56
1:A:807:A:H2'	1:A:808:C:C6	2.41	0.56
1:A:1136:U:H5''	1:A:1137:C:OP2	2.05	0.56
2:B:213:LEU:O	2:B:217:ARG:HG2	2.06	0.56
10:J:61:GLU:HG2	10:J:63:PHE:CE2	2.41	0.56
11:K:23:ALA:HB1	11:K:88:GLY:HA3	1.88	0.56
1:A:372:C:N3	1:A:387:U:H5	2.04	0.56
15:O:70:LEU:HD21	15:O:77:ARG:HB2	1.88	0.56
1:A:502:G:OP1	12:L:117:ARG:N	2.38	0.56
1:A:749:C:H2'	1:A:750:G:C8	2.41	0.56
1:A:954:G:H21	1:A:1227:A:H62	1.53	0.56
1:A:1502:A:H2	1:A:1505:G:H1	1.51	0.56
3:C:43:LEU:O	3:C:47:LEU:HB2	2.06	0.56
9:I:8:GLY:HA2	9:I:79:LEU:HD13	1.88	0.56
9:I:111:ARG:HD2	14:N:61:TRP:OXT	2.05	0.56
10:J:49:VAL:HG23	14:N:41:ARG:HB2	1.87	0.56
17:Q:24:GLU:OE1	17:Q:37:LYS:HD2	2.05	0.56
1:A:1063:C:H2'	1:A:1064:G:C8	2.40	0.56
1:A:258:G:H2'	1:A:259:G:C8	2.39	0.55
4:D:150:GLU:HA	4:D:153:ARG:CZ	2.35	0.55
20:T:65:LYS:O	20:T:68:LYS:HB2	2.06	0.55
1:A:272:C:H2'	1:A:273:A:H8	1.71	0.55
1:A:532:A:N6	1:A:1206:G:O2'	2.39	0.55
1:A:1510:U:H2'	1:A:1511:G:C8	2.41	0.55
2:B:47:THR:HA	2:B:202:PRO:HG2	1.87	0.55
16:P:58:TYR:O	16:P:62:VAL:HG22	2.05	0.55
1:A:1261:A:N6	1:A:1262:C:O2	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:69:VAL:HG21	5:E:113:ALA:HB1	1.87	0.55
7:G:149:ARG:HB3	11:K:59:TYR:CE1	2.42	0.55
12:L:11:VAL:HG22	17:Q:29:HIS:CD2	2.41	0.55
13:M:49:THR:HB	13:M:52:GLU:H	1.71	0.55
3:C:72:LYS:HE3	3:C:75:VAL:HG21	1.88	0.55
13:M:25:ILE:HG23	13:M:29:ARG:HB2	1.88	0.55
20:T:63:ILE:HD13	20:T:80:ARG:HB2	1.87	0.55
1:A:1124:G:O2'	1:A:1145:C:N4	2.40	0.55
2:B:79:ASP:O	2:B:82:ARG:HG3	2.06	0.55
1:A:28:G:O2'	1:A:296:U:OP1	2.24	0.55
1:A:254:G:OP1	17:Q:67:LYS:O	2.25	0.55
1:A:1497:G:C2'	1:A:1498:UR3:H5'	2.37	0.55
13:M:11:ARG:HG3	13:M:12:ASN:N	2.22	0.55
17:Q:3:LYS:HB3	17:Q:61:GLU:HB3	1.89	0.55
1:A:235:C:N4	27:A:2126:HOH:O	2.39	0.55
1:A:437:U:H5''	4:D:155:LEU:HD22	1.88	0.55
2:B:238:LEU:C	2:B:240:GLN:H	2.12	0.55
7:G:50:ILE:HD11	7:G:124:LEU:HB3	1.89	0.55
13:M:34:LEU:CD1	13:M:41:PRO:HA	2.37	0.55
19:S:11:VAL:HG22	19:S:39:THR:HB	1.89	0.55
1:A:600:C:OP1	8:H:97:VAL:HG12	2.07	0.55
1:A:1420:C:H2'	1:A:1421:G:C8	2.42	0.55
2:B:13:ALA:HB1	2:B:209:ARG:HB3	1.89	0.55
4:D:22:LYS:HB2	4:D:26:CYS:SG	2.46	0.55
1:A:756:C:N4	27:A:2114:HOH:O	2.39	0.55
9:I:105:ASP:OD1	9:I:107:ARG:HG3	2.06	0.55
12:L:36:VAL:HG22	12:L:82:VAL:HA	1.88	0.55
18:R:40:LEU:HB3	18:R:79:LEU:HD11	1.89	0.55
20:T:76:ALA:HA	20:T:79:ARG:NH1	2.21	0.55
1:A:1314:C:C5	19:S:6:LYS:HE2	2.42	0.55
1:A:580:U:H2'	1:A:581:G:O4'	2.08	0.54
12:L:70:ILE:HD13	12:L:77:LEU:HD12	1.89	0.54
18:R:32:ARG:HA	18:R:69:THR:HG21	1.88	0.54
1:A:64:G:C2	1:A:67:C:N4	2.75	0.54
1:A:443:C:H2'	1:A:444:C:C6	2.42	0.54
1:A:986:A:C2	1:A:1220:G:C2	2.95	0.54
1:A:1060:C:C5'	10:J:51:ARG:HB3	2.38	0.54
1:A:1420:C:H2'	1:A:1421:G:H8	1.72	0.54
3:C:180:ALA:HB1	3:C:182:ILE:CG1	2.36	0.54
8:H:20:TYR:CE1	8:H:76:PRO:HG2	2.41	0.54
20:T:79:ARG:O	20:T:83:ARG:HG3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:A:H5'	1:A:398:C:OP1	2.07	0.54
1:A:772:U:OP1	24:A:1615:PAR:H222	2.08	0.54
1:A:1435:G:H2'	1:A:1436:U:C6	2.43	0.54
6:F:30:LEU:HD23	6:F:75:LEU:HD11	1.89	0.54
11:K:91:ARG:HD3	11:K:92:GLU:OE1	2.07	0.54
1:A:660:G:OP2	15:O:5:LYS:HE2	2.08	0.54
1:A:1054:C:P	1:A:1197:G:OP2	2.65	0.54
1:A:1347:G:O2'	1:A:1348:U:P	2.65	0.54
2:B:223:ILE:HD12	2:B:224:GLN:H	1.72	0.54
3:C:121:ALA:HB2	3:C:198:VAL:HG21	1.88	0.54
1:A:475:G:H2'	1:A:476:G:C8	2.42	0.54
1:A:855:G:C5	1:A:856:C:C5	2.96	0.54
1:A:976:G:OP1	14:N:32:SER:N	2.33	0.54
1:A:977:A:C2'	1:A:978:A:H5'	2.38	0.54
1:A:1521:G:H2'	1:A:1522:U:C6	2.43	0.54
8:H:36:LEU:HD12	8:H:59:LEU:HD22	1.90	0.54
1:A:263:A:O2'	1:A:264:U:H5'	2.07	0.54
1:A:775:G:N2	1:A:804:U:O4	2.41	0.54
1:A:960:U:H4'	1:A:961:U:C5'	2.38	0.54
1:A:160:A:H2'	1:A:161:A:O4'	2.08	0.54
1:A:1154:G:H2'	1:A:1155:G:C8	2.41	0.54
5:E:86:ALA:HB1	5:E:125:SER:HB3	1.90	0.54
8:H:20:TYR:HA	8:H:65:TYR:CZ	2.43	0.54
1:A:1123:A:H4'	10:J:37:PRO:HD2	1.88	0.54
3:C:33:LEU:HD21	14:N:53:LEU:HD22	1.89	0.54
4:D:25:ARG:HE	4:D:30:LYS:HB2	1.73	0.54
12:L:76:ASN:O	12:L:76:ASN:CG	2.51	0.54
17:Q:5:VAL:C	17:Q:6:LEU:HD23	2.33	0.54
3:C:50:ALA:HB2	3:C:75:VAL:HB	1.88	0.54
8:H:6:ILE:HD12	8:H:6:ILE:N	2.23	0.54
13:M:15:VAL:HB	13:M:34:LEU:HD11	1.90	0.54
17:Q:87:LYS:HA	17:Q:90:ILE:HD12	1.90	0.54
1:A:232:G:H1'	1:A:262:A:N1	2.23	0.53
1:A:390:C:H2'	1:A:391:G:H8	1.73	0.53
1:A:1428:A:H2'	1:A:1429:C:C6	2.42	0.53
1:A:456:C:H2'	1:A:457:C:C6	2.43	0.53
1:A:1006:C:H42	1:A:1024:G:N2	2.06	0.53
3:C:123:GLN:O	3:C:128:PHE:HB2	2.08	0.53
20:T:53:LEU:O	20:T:57:ARG:HD2	2.08	0.53
1:A:413:G:N2	1:A:429:U:OP2	2.23	0.53
1:A:1152:A:OP1	10:J:68:HIS:ND1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:14:ILE:HG23	3:C:15:THR:HG23	1.91	0.53
1:A:778:G:O5'	1:A:778:G:H8	1.92	0.53
1:A:978:A:O2'	1:A:1322:C:N3	2.36	0.53
1:A:1497:G:H2'	1:A:1498:UR3:H5'	1.90	0.53
2:B:181:PHE:CD2	8:H:70:GLN:HB2	2.43	0.53
7:G:120:ILE:O	7:G:124:LEU:HB2	2.08	0.53
8:H:95:VAL:HG12	8:H:99:GLU:HB2	1.89	0.53
9:I:111:ARG:HD3	9:I:113:LYS:HD2	1.90	0.53
4:D:24:GLU:HG2	4:D:25:ARG:N	2.23	0.53
15:O:17:ARG:HD3	15:O:77:ARG:NH1	2.23	0.53
1:A:687:A:H4'	1:A:688:G:O5'	2.09	0.53
5:E:83:GLU:HG2	5:E:88:LYS:HB2	1.91	0.53
1:A:21:G:H2'	1:A:22:G:C8	2.43	0.53
1:A:836:G:C6	1:A:851:G:C6	2.96	0.53
1:A:1527:C:O2'	1:A:1528:U:H5'	2.09	0.53
3:C:134:ILE:HG22	3:C:168:ALA:HB3	1.89	0.53
17:Q:94:ASN:O	17:Q:97:SER:HB3	2.09	0.53
1:A:201:C:H42	1:A:216:G:H1	1.57	0.53
1:A:410:G:N1	1:A:429:U:O2	2.42	0.53
1:A:1240:U:OP2	7:G:116:ALA:N	2.34	0.53
2:B:16:HIS:HB3	2:B:44:LEU:HD11	1.91	0.53
1:A:660:G:C2	1:A:746:A:C2	2.97	0.53
1:A:1347:G:O2'	1:A:1348:U:O5'	2.27	0.53
24:A:1615:PAR:H11	24:A:1615:PAR:O52	2.08	0.53
19:S:50:ALA:HA	19:S:58:VAL:O	2.07	0.53
1:A:60:A:H4'	1:A:61:G:O5'	2.09	0.53
1:A:427:U:OP2	4:D:36:ARG:NH2	2.36	0.53
1:A:1190:G:O5'	1:A:1190:G:H8	1.91	0.53
7:G:109:ASN:OD1	7:G:119:ARG:NH2	2.35	0.53
8:H:24:THR:HG22	8:H:63:LEU:HD21	1.90	0.53
8:H:82:HIS:HE2	8:H:84:ARG:HB2	1.73	0.53
1:A:636:U:O4	24:A:1610:PAR:H54	2.09	0.52
1:A:1202:G:C2	14:N:42:ILE:HG21	2.44	0.52
1:A:1366:C:H2'	1:A:1367:C:H6	1.69	0.52
1:A:414:A:P	24:A:1611:PAR:N12	2.82	0.52
1:A:1128:C:O2'	1:A:1130:A:C8	2.61	0.52
8:H:82:HIS:ND1	8:H:138:TRP:NE1	2.57	0.52
10:J:61:GLU:OE1	14:N:45:ARG:HD2	2.09	0.52
10:J:80:LYS:O	10:J:83:GLU:HB2	2.08	0.52
12:L:20:LYS:H	12:L:20:LYS:HD2	1.74	0.52
1:A:474:G:H5''	16:P:81:ARG:NH2	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1346:A:N1	1:A:1374:A:H5''	2.24	0.52
3:C:5:ILE:HD12	3:C:6:HIS:O	2.09	0.52
14:N:14:PRO:O	14:N:15:LYS:HB3	2.09	0.52
1:A:8:A:N6	4:D:205:GLU:O	2.42	0.52
1:A:644:G:C5	1:A:645:C:C5	2.97	0.52
1:A:1163:C:H2'	1:A:1164:G:C8	2.45	0.52
1:A:1331:G:O2'	1:A:1332:A:P	2.68	0.52
2:B:100:GLY:O	2:B:104:ASN:N	2.41	0.52
3:C:6:HIS:CD2	3:C:8:ILE:H	2.27	0.52
5:E:103:GLY:H	5:E:106:PRO:HG2	1.74	0.52
1:A:1206:G:C6	1:A:1207:2MG:C5	2.98	0.52
2:B:103:THR:HG23	2:B:176:GLU:OE1	2.10	0.52
16:P:15:PRO:HD2	16:P:42:ARG:CD	2.38	0.52
1:A:1015:A:H2'	1:A:1016:A:C8	2.45	0.52
1:A:1097:C:O2'	1:A:1168:A:N3	2.38	0.52
1:A:6:G:O2'	1:A:7:G:H5''	2.10	0.52
1:A:190(E):U:O2	17:Q:63:ARG:NH2	2.43	0.52
1:A:519:C:H2'	1:A:520:A:C8	2.44	0.52
2:B:53:ARG:HA	2:B:56:ARG:NH1	2.25	0.52
3:C:121:ALA:HB1	3:C:189:ALA:HB2	1.92	0.52
5:E:80:ILE:HD12	5:E:138:ALA:HB1	1.92	0.52
6:F:70:ASP:OD1	6:F:70:ASP:N	2.42	0.52
6:F:95:GLU:HG2	6:F:96:PRO:HD2	1.92	0.52
6:F:97:PHE:HB3	18:R:32:ARG:HG3	1.91	0.52
9:I:48:GLU:HG2	9:I:51:ARG:NH2	2.25	0.52
1:A:229:U:H5''	16:P:33:ILE:HD13	1.92	0.52
1:A:665:A:H3'	1:A:725:G:H21	1.75	0.52
8:H:80:ILE:HD12	8:H:80:ILE:H	1.75	0.52
1:A:594:G:H2'	1:A:595:G:H5'	1.91	0.51
1:A:1260:C:O5'	1:A:1284:C:H4'	2.10	0.51
3:C:110:ASN:O	3:C:141:VAL:HG22	2.10	0.51
6:F:12:PRO:HD2	6:F:86:ARG:NH1	2.25	0.51
7:G:37:ASN:OD1	9:I:41:VAL:HG23	2.10	0.51
12:L:69:TYR:HE2	12:L:71:PRO:HA	1.75	0.51
1:A:1312:G:H2'	1:A:1313:U:H6	1.75	0.51
1:A:858:G:O2'	1:A:859:A:H5'	2.10	0.51
1:A:1413:A:C2	1:A:1488:G:C2	2.98	0.51
19:S:31:ILE:HG22	19:S:49:ILE:HA	1.92	0.51
1:A:520:A:OP2	12:L:51:ALA:HB1	2.10	0.51
1:A:254:G:H5''	17:Q:69:LYS:HD2	1.91	0.51
1:A:390:C:O3'	16:P:28:ARG:NH2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1003(A):G:N2	1:A:1038:C:O2	2.43	0.51
1:A:1190:G:O2'	1:A:1191:A:P	2.67	0.51
2:B:97:TRP:CZ2	2:B:102:LEU:HD13	2.39	0.51
2:B:187:LEU:HD12	2:B:214:ILE:HG21	1.92	0.51
7:G:15:ASP:HB3	7:G:20:ASP:N	2.26	0.51
14:N:34:TYR:N	14:N:39:LEU:O	2.41	0.51
1:A:1250:A:H4'	9:I:68:GLY:N	2.25	0.51
24:A:1610:PAR:N24	24:A:1610:PAR:H33	2.23	0.51
15:O:16:ALA:HB1	15:O:21:ASP:HB3	1.92	0.51
1:A:371:G:O2'	1:A:372:C:H5'	2.11	0.51
1:A:539:A:H2'	1:A:540:G:C8	2.46	0.51
1:A:839:U:H2'	1:A:839:U:O2	2.09	0.51
1:A:1242:C:H2'	1:A:1243:C:H6	1.76	0.51
24:A:1610:PAR:O34	24:A:1610:PAR:O54	2.27	0.51
2:B:91:PRO:HB3	2:B:154:LEU:HB2	1.92	0.51
1:A:9:G:OP1	5:E:122:GLU:HG3	2.11	0.51
1:A:262:A:C6	1:A:263:A:C6	2.99	0.51
1:A:324:G:N2	1:A:327:A:C8	2.79	0.51
1:A:1167:A:C6	1:A:1168:A:C6	2.98	0.51
2:B:122:PHE:CE2	2:B:139:LYS:HG2	2.45	0.51
1:A:229:U:H2'	1:A:230:G:H8	1.76	0.51
1:A:974:A:OP2	14:N:29:ARG:NH1	2.38	0.51
1:A:1281:U:H5'	1:A:1282:C:C5	2.39	0.51
2:B:55:PHE:CE2	2:B:218:ALA:HA	2.44	0.51
3:C:6:HIS:HD2	3:C:8:ILE:N	2.09	0.51
3:C:108:ASN:HD21	3:C:144:SER:HB2	1.76	0.51
7:G:140:ASP:OD2	7:G:143:ARG:NH2	2.44	0.51
1:A:552:U:H2'	1:A:553:A:C8	2.46	0.51
1:A:651:C:O2'	1:A:652:U:H5'	2.10	0.51
1:A:665:A:H1'	1:A:733:A:O4'	2.11	0.51
1:A:806:C:H4'	24:A:1613:PAR:H13	1.93	0.51
1:A:892:A:C2	1:A:907:A:C4	2.99	0.51
5:E:144:THR:HG22	5:E:145:LYS:N	2.26	0.51
6:F:91:VAL:HG12	6:F:92:LYS:O	2.11	0.51
9:I:33:PHE:CE2	9:I:47:LEU:HD11	2.46	0.51
11:K:62:GLN:HG3	11:K:97:ALA:HB2	1.93	0.51
17:Q:100:LYS:HG2	17:Q:101:ARG:NH2	2.26	0.51
1:A:803:G:H2'	1:A:804:U:O4'	2.11	0.50
1:A:811:C:H4'	1:A:900:A:N6	2.25	0.50
1:A:1234:C:O2'	1:A:1235:U:H5'	2.11	0.50
12:L:40:VAL:HG21	12:L:77:LEU:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:86:ARG:O	12:L:98:TYR:HB3	2.11	0.50
1:A:370:C:O2'	1:A:371:G:H5'	2.11	0.50
1:A:1010:G:N2	1:A:1020:U:H1'	2.25	0.50
2:B:55:PHE:HE2	2:B:218:ALA:HA	1.76	0.50
9:I:50:LEU:HB3	9:I:56:LEU:H	1.75	0.50
1:A:106:C:O2'	1:A:379:C:OP1	2.29	0.50
1:A:547:A:OP2	4:D:2:GLY:HA3	2.12	0.50
1:A:1208:C:H2'	1:A:1209:C:H6	1.75	0.50
1:A:1213:A:C6	1:A:1215:G:C4	2.99	0.50
5:E:137:GLU:O	5:E:141:GLN:HG3	2.12	0.50
16:P:22:THR:OG1	16:P:23:ASP:N	2.43	0.50
1:A:22:G:H2'	1:A:23:C:C6	2.47	0.50
3:C:38:ARG:HD3	3:C:94:LEU:HD11	1.92	0.50
3:C:52:LEU:HA	3:C:70:VAL:HG13	1.93	0.50
1:A:838:G:N2	1:A:849:C:C2	2.80	0.50
1:A:1314:C:OP2	19:S:6:LYS:HD3	2.12	0.50
2:B:29:ALA:HA	2:B:32:ILE:HD12	1.94	0.50
2:B:189:ASP:HB2	2:B:205:ASP:OD2	2.12	0.50
2:B:211:ILE:O	2:B:215:LEU:HB2	2.11	0.50
3:C:156:ARG:N	3:C:163:ALA:HA	2.25	0.50
10:J:62:HIS:O	14:N:59:ALA:HB3	2.12	0.50
1:A:428:G:H8	1:A:428:G:OP1	1.94	0.50
1:A:932:C:C5	7:G:3:ARG:HD3	2.47	0.50
2:B:174:VAL:O	2:B:178:ARG:HG2	2.12	0.50
3:C:6:HIS:NE2	3:C:8:ILE:HB	2.26	0.50
15:O:45:VAL:HB	15:O:46:HIS:HD2	1.77	0.50
1:A:377:G:N2	1:A:387:U:O2	2.44	0.50
1:A:456:C:H2'	1:A:457:C:H6	1.75	0.50
1:A:1179:A:H2'	1:A:1180:A:O4'	2.12	0.50
1:A:1339:A:H2'	1:A:1340:A:O4'	2.12	0.50
1:A:1403:C:O2'	1:A:1404:5MC:H5'	2.12	0.50
1:A:1475:G:H2'	1:A:1476:G:H8	1.77	0.50
2:B:132:LYS:O	2:B:136:VAL:HG23	2.12	0.50
7:G:54:THR:C	7:G:56:GLN:H	2.20	0.50
19:S:14:HIS:O	19:S:17:GLU:HG2	2.11	0.50
1:A:377:G:OP1	16:P:5:ARG:NH1	2.43	0.50
1:A:431:A:C2'	1:A:432:A:H5'	2.42	0.50
1:A:1252:A:H2'	1:A:1253:G:O4'	2.11	0.50
1:A:1375:A:P	7:G:28:ASN:HD22	2.35	0.50
4:D:6:GLY:O	4:D:8:VAL:HG12	2.11	0.50
6:F:6:VAL:HG13	6:F:90:VAL:HG22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:36:LEU:HA	8:H:39:LEU:HD23	1.94	0.50
8:H:82:HIS:HE1	8:H:136:GLU:OE2	1.94	0.50
1:A:35:G:C6	1:A:36:C:N4	2.80	0.50
1:A:345:C:O2	1:A:346:G:N2	2.44	0.50
1:A:830:G:N2	1:A:856:C:O2	2.39	0.50
1:A:1206:G:O4'	3:C:194:GLY:HA2	2.11	0.50
10:J:51:ARG:HB2	10:J:59:SER:HB2	1.94	0.50
16:P:9:PHE:CD1	16:P:18:ARG:HG3	2.47	0.50
16:P:49:LEU:HD13	16:P:73:LEU:HD22	1.94	0.50
20:T:56:MET:HG3	20:T:84:LEU:HD22	1.94	0.50
9:I:121:ARG:HG2	9:I:121:ARG:HH11	1.77	0.49
13:M:78:ILE:HD13	13:M:92:HIS:CE1	2.47	0.49
19:S:31:ILE:CG2	19:S:49:ILE:HA	2.42	0.49
1:A:658:G:H2'	1:A:659:U:C6	2.47	0.49
1:A:814:A:H2'	1:A:816:A:H5''	1.94	0.49
1:A:1192:C:O2	5:E:25:ARG:NH2	2.32	0.49
1:A:1256:A:H5'	1:A:1258:G:C1'	2.43	0.49
24:A:1603:PAR:HN61	24:A:1603:PAR:C53	2.24	0.49
4:D:57:ARG:HG3	4:D:57:ARG:NH1	2.26	0.49
1:A:1014:A:H4'	19:S:14:HIS:CD2	2.47	0.49
11:K:27:ASN:OD1	11:K:28:THR:N	2.45	0.49
13:M:19:LEU:O	13:M:22:ILE:HG12	2.11	0.49
1:A:673:G:H2'	1:A:674:G:C8	2.46	0.49
1:A:1283:G:H2'	1:A:1284:C:H6	1.76	0.49
2:B:48:MET:HA	2:B:51:LEU:HD12	1.95	0.49
13:M:63:THR:HG23	13:M:64:TRP:H	1.78	0.49
1:A:267:C:O2'	1:A:268:C:H5'	2.12	0.49
1:A:949:A:C2	1:A:1233:G:N3	2.81	0.49
1:A:1002:G:H2'	1:A:1003:G:C8	2.47	0.49
1:A:1038:C:H2'	1:A:1039:C:H6	1.76	0.49
1:A:1056:U:H5'	3:C:163:ALA:HB2	1.93	0.49
3:C:83:ARG:HA	3:C:86:VAL:HG23	1.94	0.49
7:G:48:LYS:HG3	7:G:49:ILE:N	2.26	0.49
10:J:32:ALA:HB3	10:J:75:ILE:O	2.12	0.49
15:O:74:ASP:OD2	15:O:77:ARG:HG3	2.12	0.49
1:A:141:A:H1'	1:A:182:U:O2	2.13	0.49
1:A:812:C:O2'	1:A:813:U:OP2	2.24	0.49
1:A:1060:C:O2'	10:J:56:HIS:ND1	2.43	0.49
1:A:1104:G:OP1	2:B:111:ARG:HD2	2.13	0.49
1:A:1213:A:N6	1:A:1215:G:N3	2.60	0.49
3:C:188:LEU:HD22	3:C:195:VAL:HG22	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:39:LEU:HD12	15:O:56:LEU:HB2	1.94	0.49
21:U:5:ASP:HB3	21:U:8:THR:OG1	2.12	0.49
1:A:325:A:H2'	1:A:326:G:O4'	2.13	0.49
1:A:1511:G:H2'	1:A:1512:U:O4'	2.13	0.49
24:A:1602:PAR:N24	24:A:1602:PAR:H33	2.27	0.49
2:B:53:ARG:HA	2:B:56:ARG:HH12	1.77	0.49
8:H:23:SER:HA	8:H:63:LEU:HD22	1.94	0.49
13:M:36:LYS:HD3	13:M:59:TYR:OH	2.13	0.49
1:A:533:A:C6	1:A:536:C:C2	3.01	0.49
1:A:1004:A:H5'	27:A:2449:HOH:O	2.11	0.49
1:A:1052:U:H2'	1:A:1055:A:OP1	2.13	0.49
1:A:268:C:H2'	1:A:269:C:H6	1.77	0.49
1:A:767:A:H2'	1:A:768:A:O4'	2.12	0.49
9:I:71:SER:O	9:I:74:ILE:HB	2.12	0.49
1:A:637:G:H2'	1:A:638:G:H8	1.76	0.49
1:A:922:G:C6	1:A:923:A:C6	3.01	0.49
1:A:1048:G:O3'	1:A:1049:U:H3'	2.13	0.49
1:A:1220:G:H2'	1:A:1221:G:C8	2.48	0.49
1:A:1347:G:O6	9:I:10:ARG:NH2	2.45	0.49
4:D:121:VAL:O	4:D:134:ASP:HA	2.12	0.49
8:H:100:ILE:HG22	8:H:125:ARG:HH12	1.78	0.49
16:P:28:ARG:HG3	16:P:29:ASP:OD2	2.12	0.49
19:S:45:VAL:HA	19:S:62:ILE:HD13	1.95	0.49
1:A:975:A:H5''	1:A:975:A:C8	2.46	0.48
1:A:1279:A:H5''	1:A:1280:A:OP1	2.13	0.48
1:A:1347:G:H3'	9:I:108:VAL:O	2.13	0.48
1:A:1443:G:H4'	1:A:1446:A:O5'	2.12	0.48
3:C:154:SER:O	3:C:196:LEU:HD11	2.12	0.48
9:I:5:TYR:CE1	9:I:16:ARG:HG2	2.48	0.48
13:M:81:LEU:O	13:M:86:CYS:HB3	2.13	0.48
1:A:518:C:H2'	1:A:530:G:N3	2.28	0.48
1:A:1061:G:C6	1:A:1062:U:N3	2.80	0.48
1:A:1137:C:H4'	1:A:1138:G:C2	2.47	0.48
1:A:1163:C:H2'	1:A:1164:G:H8	1.78	0.48
13:M:23:TYR:HB2	13:M:67:GLU:OE2	2.13	0.48
1:A:511:C:O3'	4:D:43:HIS:NE2	2.45	0.48
1:A:670:G:OP2	24:A:1613:PAR:N24	2.45	0.48
1:A:932:C:H5	7:G:3:ARG:NH1	2.11	0.48
1:A:1264:C:H2'	1:A:1265:G:H8	1.78	0.48
1:A:247:G:OP2	17:Q:100:LYS:HB2	2.12	0.48
1:A:574:A:N3	1:A:883:C:HI'	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:708:C:H6	1:A:708:C:O5'	1.96	0.48
1:A:1288:A:C6	1:A:1289:A:C5	3.02	0.48
4:D:120:LEU:HD23	4:D:125:HIS:CD2	2.48	0.48
10:J:6:ILE:CD1	10:J:72:VAL:HB	2.43	0.48
10:J:54:PHE:CD2	10:J:55:LYS:HG2	2.45	0.48
15:O:29:VAL:HG11	15:O:67:LEU:HD21	1.95	0.48
20:T:29:LYS:O	20:T:32:ALA:HB3	2.13	0.48
1:A:811:C:H4'	1:A:900:A:H62	1.78	0.48
1:A:956:U:C2	1:A:1225:A:C2	3.01	0.48
1:A:1054:C:N3	23:W:34:G:O4'	2.46	0.48
1:A:1128:C:N3	1:A:1144:G:N2	2.61	0.48
3:C:138:VAL:HG23	3:C:151:VAL:HG23	1.95	0.48
4:D:58:LEU:HD22	4:D:62:GLN:HG2	1.96	0.48
12:L:117:ARG:O	12:L:120:TYR:N	2.47	0.48
13:M:57:ARG:HG3	13:M:61:GLU:HG3	1.95	0.48
15:O:32:LEU:HD22	15:O:32:LEU:HA	1.73	0.48
17:Q:9:VAL:HG21	17:Q:84:LEU:HD12	1.95	0.48
19:S:44:MET:O	19:S:47:HIS:HB2	2.12	0.48
1:A:929:G:H1	1:A:1388:C:N4	2.11	0.48
1:A:1158:C:O2	1:A:1181:G:N2	2.34	0.48
18:R:53:ARG:NH1	18:R:60:ALA:HA	2.29	0.48
1:A:989:C:H42	1:A:1216:G:H1	1.62	0.48
1:A:1427:U:H2'	1:A:1428:A:C8	2.48	0.48
6:F:45:LEU:HD12	6:F:47:ARG:HH22	1.79	0.48
8:H:28:ALA:HA	8:H:59:LEU:CD1	2.44	0.48
10:J:42:THR:HG23	10:J:67:THR:O	2.14	0.48
23:W:37:A:H2'	23:W:38:A:O4'	2.14	0.48
1:A:157:G:C2	1:A:158:G:C8	3.02	0.48
1:A:340:U:C2	1:A:350:G:N2	2.82	0.48
1:A:1126:U:C2	1:A:1127:G:C8	3.02	0.48
1:A:1168:A:C6	1:A:1169:A:C6	3.01	0.48
1:A:1401:G:N2	1:A:1402:4OC:H1'	2.28	0.48
1:A:1410:G:H2'	1:A:1411:C:C6	2.49	0.48
1:A:1492:A:OP1	12:L:47:LYS:HA	2.12	0.48
14:N:2:ALA:HB1	14:N:7:ILE:HD11	1.94	0.48
15:O:87:ILE:O	15:O:88:ARG:HB2	2.13	0.48
20:T:43:LEU:HD13	20:T:51:GLU:HB3	1.96	0.48
1:A:592:G:N2	1:A:648:A:C4	2.81	0.48
1:A:966:M2G:HM13	1:A:967:5MC:C1'	2.37	0.48
1:A:1061:G:H2'	1:A:1062:U:O4'	2.13	0.48
2:B:70:PHE:O	2:B:92:TYR:HA	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:12:CYS:HA	4:D:19:LEU:CD2	2.44	0.48
13:M:74:VAL:O	13:M:77:ASN:HB2	2.14	0.48
1:A:269:C:H2'	1:A:270:A:C8	2.49	0.48
1:A:925:G:H1	1:A:1391:U:H3	1.62	0.48
1:A:1007:C:H2'	1:A:1008:C:C6	2.49	0.48
1:A:1287:A:C6	1:A:1288:A:C6	3.01	0.48
1:A:1300:G:C6	1:A:1335:C:C5	3.01	0.48
1:A:1300:G:O2'	1:A:1301:U:P	2.71	0.48
1:A:1351:U:O2'	1:A:1352:C:H5'	2.14	0.48
1:A:1376:U:H2'	1:A:1377:A:C8	2.49	0.48
1:A:1412:C:H2'	1:A:1413:A:C8	2.49	0.48
24:A:1613:PAR:H11	24:A:1613:PAR:H322	1.78	0.48
9:I:118:LYS:O	9:I:120:ARG:N	2.43	0.48
12:L:27:LEU:HD13	12:L:64:TYR:HE1	1.78	0.48
19:S:63:THR:HG23	19:S:66:MET:SD	2.54	0.48
1:A:16:A:C2'	1:A:17:U:H5'	2.44	0.47
1:A:149:A:H2'	1:A:150:C:C6	2.49	0.47
1:A:285:G:O2'	1:A:286:G:H5'	2.14	0.47
1:A:410:G:OP2	4:D:25:ARG:HD2	2.14	0.47
1:A:1095:U:H5''	1:A:1109:C:O2	2.12	0.47
2:B:70:PHE:CE2	2:B:163:PHE:HD1	2.32	0.47
2:B:73:THR:HG23	2:B:95:GLN:O	2.14	0.47
9:I:26:VAL:HG13	9:I:61:ALA:HB3	1.95	0.47
11:K:24:SER:CB	11:K:26:ASN:H	2.26	0.47
17:Q:66:SER:O	17:Q:70:ARG:NH1	2.46	0.47
1:A:179:A:H2'	1:A:180:U:H6	1.76	0.47
1:A:707:C:H5''	11:K:20:TYR:CD2	2.49	0.47
1:A:825:G:N2	8:H:11:THR:HG21	2.26	0.47
1:A:1074:G:C6	1:A:1075:C:C4	3.03	0.47
1:A:1158:C:H5''	1:A:1159:U:OP2	2.15	0.47
4:D:175:SER:HB3	4:D:184:LYS:HB2	1.95	0.47
8:H:102:ARG:H	8:H:102:ARG:HD2	1.79	0.47
1:A:103:C:OP2	20:T:14:LYS:HD2	2.13	0.47
1:A:177:C:H2'	1:A:178:C:H6	1.79	0.47
1:A:426:G:H2'	1:A:427:U:C6	2.50	0.47
1:A:662:G:O6	24:A:1605:PAR:H62	2.14	0.47
1:A:665:A:N3	1:A:732:C:H2'	2.29	0.47
1:A:668:G:N2	1:A:738:C:O2	2.44	0.47
1:A:728:A:H2'	1:A:729:A:O4'	2.14	0.47
1:A:740:U:H4'	15:O:42:HIS:CD2	2.48	0.47
1:A:803:G:OP1	24:A:1615:PAR:O41	2.31	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1071:C:H42	1:A:1104:G:H1	1.63	0.47
10:J:6:ILE:HB	10:J:72:VAL:CG2	2.44	0.47
10:J:51:ARG:HG2	14:N:45:ARG:NH1	2.28	0.47
1:A:1288:A:N3	1:A:1352:C:O2'	2.36	0.47
1:A:1442:G:C5	1:A:1446:A:N6	2.83	0.47
2:B:238:LEU:C	2:B:240:GLN:N	2.72	0.47
8:H:119:LEU:HD12	8:H:124:ALA:HB2	1.96	0.47
13:M:86:CYS:SG	13:M:87:TYR:N	2.88	0.47
1:A:148:G:H2'	1:A:149:A:H8	1.79	0.47
1:A:558:G:H8	1:A:559:A:H2'	1.79	0.47
1:A:620:C:C2	4:D:135:LEU:HD22	2.50	0.47
1:A:1002:G:C6	1:A:1003:G:C6	3.03	0.47
1:A:1122:U:O4	1:A:1123:A:N6	2.48	0.47
1:A:1391:U:H2'	1:A:1392:G:C8	2.49	0.47
1:A:1466:C:H2'	1:A:1467:G:O4'	2.15	0.47
10:J:5:ARG:HA	10:J:73:ASP:OD1	2.14	0.47
13:M:99:ARG:NH2	19:S:2:PRO:HG2	2.28	0.47
16:P:58:TYR:CD1	16:P:58:TYR:C	2.91	0.47
1:A:781:A:C8	1:A:802:A:C2	3.02	0.47
1:A:955:U:H1'	1:A:1227:A:H61	1.79	0.47
1:A:992:U:H4'	1:A:993:G:O5'	2.14	0.47
1:A:1056:U:C5'	3:C:163:ALA:HB2	2.45	0.47
1:A:1191:A:H5''	3:C:4:LYS:HE2	1.95	0.47
1:A:1392:G:N2	1:A:1502:A:H8	2.11	0.47
2:B:75:LYS:CA	2:B:78:GLN:HB2	2.43	0.47
7:G:54:THR:HG22	7:G:56:GLN:HB3	1.97	0.47
11:K:120:ARG:HH11	11:K:120:ARG:HB3	1.79	0.47
13:M:4:ILE:HD11	13:M:56:LEU:HB3	1.97	0.47
21:U:17:THR:O	21:U:22:ARG:NH1	2.44	0.47
1:A:506:G:C6	1:A:507:C:C4	3.03	0.47
1:A:961:U:H2'	1:A:962:C:H5'	1.95	0.47
1:A:974:A:OP1	1:A:974:A:H8	1.98	0.47
1:A:1057:G:H5''	3:C:154:SER:HB2	1.97	0.47
1:A:1118:C:H1'	1:A:1179:A:C4	2.50	0.47
1:A:1157:A:H4'	1:A:1158:C:O5'	2.15	0.47
24:A:1608:PAR:N21	24:A:1608:PAR:H531	2.24	0.47
4:D:91:SER:HB3	4:D:191:ARG:HB2	1.96	0.47
10:J:19:SER:HA	10:J:22:LYS:HE3	1.97	0.47
14:N:24:CYS:HB3	14:N:28:GLY:N	2.29	0.47
15:O:12:ILE:HG12	15:O:31:LEU:HD11	1.97	0.47
20:T:33:ILE:HD11	20:T:63:ILE:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:G:O2'	1:A:295:C:H4'	2.15	0.47
1:A:393:A:O2'	1:A:394:G:H5'	2.14	0.47
1:A:738:C:H5''	6:F:69:GLU:HB3	1.97	0.47
24:A:1614:PAR:H11	24:A:1614:PAR:H52	1.68	0.47
4:D:25:ARG:HA	4:D:28:SER:HB3	1.97	0.47
6:F:78:GLU:HA	6:F:81:ILE:HG12	1.97	0.47
9:I:32:ASP:HB3	9:I:35:GLU:HB2	1.97	0.47
10:J:91:PRO:HB2	10:J:94:VAL:HB	1.97	0.47
18:R:46:GLU:CD	18:R:46:GLU:H	2.23	0.47
1:A:1091:U:O2	1:A:1093:A:C8	2.67	0.47
1:A:1316:G:N2	1:A:1319:A:OP2	2.41	0.47
1:A:1331:G:HO2'	1:A:1332:A:P	2.37	0.47
24:A:1605:PAR:C51	24:A:1605:PAR:H322	2.27	0.47
2:B:54:THR:HG23	2:B:199:TYR:HB3	1.96	0.47
2:B:235:SER:O	2:B:238:LEU:HB2	2.13	0.47
1:A:123:C:OP1	1:A:311:C:O2'	2.31	0.47
1:A:346:G:H2'	1:A:347:G:O4'	2.15	0.47
1:A:501:C:H2'	1:A:502:G:H8	1.80	0.47
1:A:956:U:H2'	1:A:957:U:O4'	2.14	0.47
1:A:1441:G:O2'	1:A:1460:A:N6	2.46	0.47
8:H:82:HIS:ND1	8:H:138:TRP:CD1	2.83	0.47
16:P:8:ARG:O	16:P:9:PHE:HD2	1.98	0.47
1:A:310:G:OP2	16:P:27:LYS:HE2	2.15	0.46
1:A:432:A:C8	1:A:433:C:C6	3.03	0.46
1:A:737:A:H2'	1:A:738:C:C6	2.50	0.46
1:A:919:A:O2'	1:A:1080:A:N1	2.48	0.46
1:A:943:U:H1'	9:I:124:GLN:HE22	1.80	0.46
1:A:1222:G:OP2	1:A:1322:C:N4	2.48	0.46
1:A:1501:C:N4	1:A:1504:G:C2	2.83	0.46
24:A:1603:PAR:H532	24:A:1603:PAR:N64	2.28	0.46
6:F:10:LEU:CD1	6:F:59:TYR:HB3	2.42	0.46
6:F:50:TYR:CE1	18:R:77:GLY:HA2	2.51	0.46
13:M:45:VAL:HG13	13:M:48:LEU:HD12	1.96	0.46
1:A:101:A:O2'	1:A:102:G:H5'	2.16	0.46
1:A:585:G:H4'	12:L:8:ASN:OD1	2.16	0.46
1:A:661:G:N2	1:A:745:C:C2	2.83	0.46
1:A:745:C:H2'	1:A:746:A:C8	2.50	0.46
1:A:1009:G:N2	1:A:1020:U:O2	2.32	0.46
1:A:1015:A:C6	1:A:1016:A:C6	3.03	0.46
1:A:1182:G:O2'	1:A:1183:A:P	2.74	0.46
3:C:114:PRO:HA	3:C:185:GLY:HA3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:668:G:O4'	15:O:49:ASP:HB2	2.16	0.46
1:A:688:G:H5'	11:K:46:GLY:C	2.40	0.46
1:A:1103:C:H5''	2:B:98:LEU:HD13	1.96	0.46
1:A:1249:C:H2'	9:I:68:GLY:O	2.15	0.46
1:A:1417:G:O5'	1:A:1417:G:H8	1.99	0.46
8:H:17:THR:HB	8:H:78:GLN:HE22	1.80	0.46
19:S:30:LEU:HB3	19:S:31:ILE:H	1.54	0.46
1:A:297:G:N2	1:A:300:A:OP2	2.48	0.46
1:A:620:C:N1	4:D:135:LEU:HD13	2.30	0.46
1:A:625:G:H4'	16:P:16:HIS:CD2	2.50	0.46
1:A:881:G:H2'	1:A:882:C:O4'	2.15	0.46
1:A:1298:C:H4'	1:A:1299:A:O4'	2.16	0.46
1:A:1309:G:C6	1:A:1329:A:C2	3.04	0.46
1:A:716:A:N7	24:A:1613:PAR:O41	2.47	0.46
1:A:965:A:C2	1:A:969:A:C2	3.04	0.46
1:A:1413:A:H2'	1:A:1414:U:O4'	2.16	0.46
13:M:106:ASN:HB3	13:M:107:ALA:H	1.50	0.46
1:A:222:U:H2'	1:A:223:U:C6	2.51	0.46
1:A:266:G:H5''	1:A:267:C:C5	2.51	0.46
1:A:1226:C:H4'	19:S:80:TYR:CZ	2.50	0.46
1:A:1357:A:H61	1:A:1363:A:H2	1.63	0.46
1:A:1386:G:O2'	1:A:1387:G:H5'	2.15	0.46
20:T:75:ASN:OD1	20:T:75:ASN:N	2.49	0.46
1:A:234:C:H2'	1:A:235:C:C6	2.50	0.46
1:A:583:A:N6	1:A:758:G:O2'	2.49	0.46
1:A:730:G:C5	1:A:731:G:H1'	2.51	0.46
1:A:1053:G:N7	1:A:1200:C:H5''	2.30	0.46
1:A:1069:C:O2'	1:A:1192:C:H1'	2.16	0.46
1:A:1230:C:H2'	1:A:1231:G:H8	1.79	0.46
1:A:1358:U:H5''	1:A:1359:C:OP2	2.16	0.46
1:A:1468:A:H2'	1:A:1469:G:O4'	2.15	0.46
1:A:1503:A:H5'	1:A:1531:A:H1'	1.98	0.46
5:E:78:HIS:ND1	8:H:104:ARG:HD2	2.30	0.46
12:L:25:PRO:C	12:L:27:LEU:N	2.73	0.46
17:Q:20:THR:HA	17:Q:43:LEU:HD23	1.98	0.46
17:Q:36:ILE:H	17:Q:36:ILE:HG12	1.49	0.46
20:T:43:LEU:HB2	20:T:52:ALA:HB2	1.98	0.46
1:A:509:A:C8	1:A:509:A:H3'	2.51	0.46
1:A:646:U:H2'	1:A:647:C:C6	2.51	0.46
1:A:875:C:H1'	8:H:15:ASN:HD21	1.81	0.46
1:A:1149:C:H2'	1:A:1150:U:C6	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:31:HIS:O	3:C:34:LEU:HD23	2.16	0.46
4:D:17:VAL:O	4:D:19:LEU:HD23	2.16	0.46
4:D:148:VAL:HG12	4:D:149:ALA:N	2.31	0.46
4:D:191:ARG:HD2	4:D:191:ARG:O	2.16	0.46
7:G:52:GLU:HG2	7:G:53:LYS:HZ2	1.81	0.46
9:I:53:VAL:CG2	9:I:85:LEU:HD21	2.43	0.46
11:K:124:LYS:HE3	11:K:125:PHE:CE2	2.50	0.46
1:A:352:C:O2'	1:A:354:G:OP1	2.32	0.46
1:A:410:G:O6	1:A:429:U:O2'	2.30	0.46
1:A:578:C:O2'	1:A:728:A:N3	2.42	0.46
1:A:922:G:H4'	5:E:20:GLN:HA	1.97	0.46
1:A:1022:G:H2'	1:A:1023:G:C8	2.51	0.46
10:J:14:LYS:HB3	10:J:14:LYS:HE2	1.67	0.46
11:K:24:SER:C	11:K:26:ASN:H	2.23	0.46
11:K:80:VAL:HG11	11:K:103:LEU:HD13	1.97	0.46
1:A:426:G:H2'	1:A:427:U:H6	1.81	0.46
1:A:744:C:H2'	1:A:745:C:C6	2.51	0.46
1:A:792:A:H4'	1:A:793:U:O5'	2.16	0.46
1:A:1051:C:H2'	1:A:1052:U:C6	2.51	0.46
1:A:1055:A:C6	1:A:1206:G:C5	3.04	0.46
24:A:1603:PAR:H11	24:A:1603:PAR:O52	2.16	0.46
2:B:115:LEU:HD11	2:B:146:GLN:HG3	1.97	0.46
4:D:12:CYS:HA	4:D:19:LEU:HD21	1.98	0.46
4:D:47:ARG:NE	4:D:48:ALA:H	2.12	0.46
13:M:67:GLU:HB3	13:M:68:GLY:H	1.51	0.46
13:M:99:ARG:NH1	19:S:2:PRO:HG2	2.31	0.46
21:U:5:ASP:O	21:U:11:GLY:HA3	2.15	0.46
1:A:51:A:H4'	1:A:52:G:C5'	2.47	0.45
1:A:355:C:O2'	1:A:388:G:N3	2.43	0.45
1:A:598:U:H2'	1:A:599:C:H6	1.80	0.45
1:A:1054:C:HO2'	1:A:1055:A:P	2.38	0.45
1:A:1113:C:O2'	1:A:1114:C:H5'	2.16	0.45
1:A:1263:C:N4	1:A:1272:G:H1	2.11	0.45
1:A:1442:G:O6	1:A:1461:G:N2	2.50	0.45
7:G:140:ASP:HA	7:G:143:ARG:NH2	2.31	0.45
8:H:104:ARG:NE	8:H:138:TRP:CZ2	2.84	0.45
11:K:63:LEU:HA	11:K:63:LEU:HD23	1.62	0.45
13:M:37:THR:HG22	13:M:55:ARG:NH1	2.31	0.45
15:O:33:THR:HG23	15:O:63:ARG:HH12	1.81	0.45
1:A:131:C:OP1	1:A:190(F):G:N2	2.46	0.45
1:A:200:G:H2'	1:A:201:C:O4'	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:C:H42	1:A:285:G:H1	1.65	0.45
1:A:786:G:C2	1:A:797:C:C2	3.04	0.45
1:A:820:U:H4'	1:A:821:G:OP2	2.16	0.45
1:A:1057:G:C5	1:A:1204:A:C2	3.04	0.45
1:A:1127:G:H1	1:A:1145:C:H42	1.62	0.45
2:B:101:MET:HA	2:B:108:ILE:HG21	1.98	0.45
3:C:116:VAL:O	3:C:119:ARG:HB3	2.17	0.45
4:D:98:GLU:HG2	4:D:189:PRO:HG3	1.98	0.45
4:D:127:THR:O	4:D:127:THR:OG1	2.29	0.45
9:I:9:ARG:HG3	9:I:14:VAL:HG13	1.98	0.45
9:I:125:TYR:HE1	9:I:127:LYS:HB2	1.81	0.45
12:L:69:TYR:CE2	12:L:71:PRO:HA	2.51	0.45
13:M:64:TRP:HE3	13:M:66:LEU:HD21	1.81	0.45
15:O:39:LEU:O	15:O:43:LEU:HG	2.16	0.45
16:P:15:PRO:CD	16:P:42:ARG:HD3	2.44	0.45
18:R:38:GLU:O	18:R:42:ARG:HG2	2.17	0.45
1:A:231:G:N7	24:A:1612:PAR:H612	2.31	0.45
1:A:778:G:H1'	11:K:119:CYS:HB3	1.98	0.45
1:A:781:A:H2	1:A:1514:C:O4'	1.99	0.45
1:A:1226:C:H2'	13:M:103:THR:OG1	2.16	0.45
2:B:83:MET:HA	2:B:86:GLU:HB2	1.97	0.45
4:D:9:CYS:HA	4:D:12:CYS:HB2	1.98	0.45
17:Q:83:ASP:O	17:Q:86:GLU:HB2	2.16	0.45
1:A:791:G:H2'	1:A:792:A:H5'	1.98	0.45
4:D:92:VAL:O	4:D:96:LEU:HD13	2.16	0.45
6:F:23:LYS:HD2	6:F:42:GLU:OE1	2.16	0.45
7:G:52:GLU:HG2	7:G:53:LYS:NZ	2.32	0.45
13:M:96:LEU:C	13:M:110:ARG:HG2	2.41	0.45
18:R:36:ASN:CG	18:R:39:VAL:HG12	2.41	0.45
1:A:908:A:C2	1:A:909:A:C4	3.04	0.45
1:A:1001:A:H2'	1:A:1002:G:C8	2.52	0.45
1:A:1305:G:H22	1:A:1331:G:H2'	1.81	0.45
2:B:48:MET:HE2	2:B:48:MET:HB3	1.69	0.45
2:B:184:VAL:N	2:B:198:ASP:OD2	2.36	0.45
17:Q:48:GLU:OE1	17:Q:50:LYS:NZ	2.49	0.45
1:A:391:G:C6	1:A:392:G:C5	3.04	0.45
1:A:567:G:H2'	1:A:568:G:O4'	2.16	0.45
1:A:899:C:H2'	1:A:900:A:O4'	2.17	0.45
1:A:1161:C:H2'	1:A:1162:C:H6	1.82	0.45
1:A:1216:G:H5''	14:N:5:ALA:HB2	1.98	0.45
1:A:1330:U:O4	1:A:1331:G:N1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:34:LEU:HB2	14:N:25:VAL:HG21	1.98	0.45
4:D:108:LEU:HD23	4:D:108:LEU:HA	1.79	0.45
16:P:73:LEU:HD23	16:P:73:LEU:HA	1.73	0.45
18:R:53:ARG:HG3	18:R:53:ARG:NH1	2.32	0.45
19:S:58:VAL:HG21	19:S:75:ALA:HB2	1.98	0.45
1:A:27:G:N2	1:A:557:G:H1'	2.32	0.45
1:A:358:U:H2'	1:A:359:U:C6	2.52	0.45
1:A:375:U:H4'	16:P:17:TYR:CE2	2.51	0.45
24:A:1610:PAR:N21	24:A:1610:PAR:O43	2.50	0.45
24:A:1613:PAR:H23	24:A:1613:PAR:H52	1.65	0.45
9:I:24:GLY:O	9:I:26:VAL:HG23	2.17	0.45
20:T:50:GLU:HB2	20:T:99:LEU:HD22	1.99	0.45
1:A:129(A):G:C2	1:A:190(E):U:H5''	2.52	0.45
1:A:148:G:H2'	1:A:149:A:C8	2.52	0.45
1:A:165:C:C2	1:A:166:G:C8	3.05	0.45
1:A:474:G:H5''	16:P:81:ARG:CZ	2.47	0.45
1:A:527:7MG:H5''	1:A:527:7MG:H81	1.98	0.45
1:A:740:U:O3'	15:O:39:LEU:HD23	2.17	0.45
1:A:1148:U:H2'	1:A:1149:C:O4'	2.16	0.45
1:A:1148:U:C5	1:A:1149:C:C4	3.04	0.45
1:A:1254:C:H41	10:J:43:ARG:HH21	1.64	0.45
1:A:1283:G:H2'	1:A:1284:C:C6	2.51	0.45
2:B:28:PHE:CD2	2:B:190:THR:HA	2.52	0.45
2:B:30:ARG:HG3	2:B:31:TYR:CD2	2.52	0.45
5:E:8:GLU:OE1	5:E:63:ARG:NH2	2.49	0.45
5:E:80:ILE:HA	8:H:104:ARG:NH2	2.31	0.45
1:A:355:C:C4	1:A:356:A:N7	2.85	0.45
1:A:1157:A:C2	1:A:1181:G:C4	3.05	0.45
1:A:1172:C:H2'	1:A:1173:G:H8	1.81	0.45
1:A:1189:C:P	10:J:51:ARG:HH22	2.40	0.45
2:B:83:MET:HB3	2:B:83:MET:HE2	1.54	0.45
3:C:188:LEU:HD21	3:C:195:VAL:HG13	1.98	0.45
4:D:57:ARG:HD3	4:D:202:LEU:HD22	1.98	0.45
6:F:95:GLU:CG	6:F:96:PRO:HD2	2.47	0.45
1:A:390:C:O5'	1:A:390:C:H6	1.99	0.45
1:A:500:G:H2'	1:A:501:C:C6	2.52	0.45
1:A:542:G:H5'	4:D:41:GLY:HA3	1.98	0.45
1:A:701:C:H5''	1:A:703:G:O4'	2.17	0.45
1:A:952:U:O2'	1:A:953:G:H5'	2.17	0.45
1:A:1049:U:H4'	1:A:1050:G:O5'	2.16	0.45
1:A:1300:G:O2'	1:A:1301:U:O5'	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1347:G:N2	1:A:1374:A:OP2	2.33	0.45
3:C:50:ALA:O	3:C:70:VAL:HG12	2.15	0.45
4:D:25:ARG:O	4:D:25:ARG:HG2	2.15	0.45
4:D:63:LYS:O	4:D:67:ILE:HD12	2.17	0.45
8:H:36:LEU:HA	8:H:36:LEU:HD23	1.79	0.45
10:J:4:ILE:O	10:J:73:ASP:HA	2.17	0.45
13:M:108:ARG:NH2	13:M:114:ARG:HA	2.32	0.45
14:N:9:LYS:HE3	14:N:21:TYR:O	2.17	0.45
14:N:23:ARG:NH1	14:N:28:GLY:O	2.50	0.45
1:A:373:A:H1'	1:A:481:G:N3	2.32	0.44
1:A:496:A:C2	1:A:497:A:C4	3.05	0.44
1:A:628:G:H2'	1:A:629:G:H8	1.82	0.44
1:A:1251:A:H2'	1:A:1252:A:O4'	2.17	0.44
3:C:186:PHE:HD1	3:C:198:VAL:O	2.00	0.44
4:D:94:LEU:HD23	4:D:94:LEU:HA	1.75	0.44
4:D:150:GLU:HA	4:D:153:ARG:NH2	2.32	0.44
5:E:118:ILE:HG12	5:E:119:LEU:N	2.32	0.44
12:L:27:LEU:O	12:L:29:GLY:N	2.50	0.44
17:Q:59:ILE:HD12	17:Q:59:ILE:HA	1.55	0.44
21:U:10:ARG:O	21:U:13:ILE:HG13	2.17	0.44
1:A:298:A:N6	27:A:2267:HOH:O	2.50	0.44
1:A:837:G:C2	1:A:850:U:O2	2.70	0.44
1:A:1276:G:O5'	1:A:1276:G:H8	2.00	0.44
1:A:1321:C:C5	1:A:1322:C:C2	3.04	0.44
1:A:1333:A:H2'	1:A:1334:G:O4'	2.18	0.44
1:A:1375:A:C2	1:A:1376:U:C2	3.05	0.44
4:D:98:GLU:OE2	4:D:103:ASN:ND2	2.44	0.44
4:D:173:TRP:CD2	4:D:189:PRO:HB3	2.52	0.44
16:P:39:TYR:CD2	16:P:73:LEU:HD11	2.52	0.44
17:Q:100:LYS:HG2	17:Q:101:ARG:HH21	1.80	0.44
18:R:55:ARG:HH11	18:R:55:ARG:HB3	1.82	0.44
1:A:312:C:H2'	1:A:313:A:C8	2.53	0.44
1:A:1030(A):G:N2	1:A:1031:G:O6	2.50	0.44
2:B:154:LEU:HD23	2:B:154:LEU:HA	1.73	0.44
3:C:95:THR:C	3:C:97:LYS:H	2.26	0.44
16:P:9:PHE:HE1	16:P:18:ARG:CZ	2.30	0.44
1:A:284:G:H2'	1:A:285:G:H8	1.82	0.44
1:A:518:C:H2'	1:A:530:G:C2	2.52	0.44
1:A:624:C:H2'	1:A:625:G:C8	2.52	0.44
1:A:945:G:C2	1:A:1337:G:C2	3.06	0.44
1:A:949:A:H1'	1:A:1364:U:N3	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1127:G:N2	1:A:1145:C:C2	2.86	0.44
1:A:1284:C:H3'	1:A:1285:A:C8	2.45	0.44
2:B:97:TRP:HZ3	2:B:176:GLU:OE2	2.01	0.44
4:D:36:ARG:HB3	4:D:38:TYR:CE2	2.52	0.44
1:A:1242:C:H2'	1:A:1243:C:C6	2.52	0.44
5:E:102:ALA:HA	5:E:120:THR:OG1	2.18	0.44
10:J:60:ARG:H	10:J:60:ARG:HG2	1.40	0.44
15:O:26:GLU:HA	15:O:81:LEU:HD13	1.99	0.44
17:Q:76:LEU:HD12	17:Q:77:VAL:N	2.33	0.44
1:A:243:A:H4'	1:A:244:U:O5'	2.18	0.44
1:A:671:G:H2'	1:A:672:U:O4'	2.17	0.44
1:A:1054:C:H42	23:W:34:G:C1'	2.30	0.44
1:A:1357:A:C5	1:A:1358:U:C4	3.06	0.44
1:A:1371:G:O3'	9:I:69:GLY:HA3	2.17	0.44
1:A:1425:U:H3	1:A:1475:G:H1	1.65	0.44
1:A:1503:A:OP1	1:A:1531:A:O2'	2.33	0.44
5:E:15:ARG:HD3	5:E:28:PHE:HE2	1.83	0.44
5:E:135:THR:O	5:E:138:ALA:HB3	2.18	0.44
6:F:56:PRO:HG2	6:F:57:GLN:HG3	1.98	0.44
7:G:56:GLN:HG2	7:G:57:GLU:H	1.81	0.44
8:H:104:ARG:HG3	8:H:138:TRP:CD2	2.53	0.44
1:A:116:A:OP1	27:A:2017:HOH:O	2.21	0.44
1:A:413:G:H21	1:A:428:G:H1'	1.83	0.44
1:A:625:G:H4'	16:P:16:HIS:CG	2.53	0.44
1:A:976:G:N7	1:A:1358:U:C2	2.86	0.44
1:A:1046:A:H3'	1:A:1047:G:H8	1.83	0.44
5:E:78:HIS:HE2	5:E:143:ARG:H	1.65	0.44
6:F:68:PRO:HB2	6:F:70:ASP:OD1	2.18	0.44
7:G:53:LYS:HA	7:G:53:LYS:HD3	1.78	0.44
10:J:66:ARG:HD3	10:J:68:HIS:CE1	2.53	0.44
17:Q:60:ILE:C	17:Q:71:PHE:HD1	2.25	0.44
1:A:530:G:O2'	23:W:35:A:H4'	2.17	0.44
1:A:751:U:H4'	15:O:24:SER:HA	1.99	0.44
1:A:1039:C:H2'	1:A:1040:U:C6	2.53	0.44
1:A:1103:C:H2'	1:A:1104:G:O4'	2.18	0.44
1:A:1236:A:O2'	1:A:1304:G:H4'	2.18	0.44
1:A:1256:A:C2	1:A:1277:C:N4	2.86	0.44
1:A:1440:C:C2	1:A:1462:G:C2	3.06	0.44
2:B:55:PHE:HD2	2:B:221:LEU:HD12	1.81	0.44
3:C:6:HIS:CD2	3:C:9:GLY:H	2.35	0.44
10:J:87:THR:O	10:J:88:LEU:HD23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:10:LEU:HD23	12:L:14:GLY:HA2	2.00	0.44
16:P:10:GLY:H	16:P:16:HIS:H	1.65	0.44
17:Q:68:ARG:NH1	17:Q:68:ARG:HB3	2.32	0.44
20:T:64:ASP:O	20:T:67:ALA:HB3	2.17	0.44
1:A:358:U:O2'	1:A:359:U:H5'	2.18	0.44
1:A:378:G:C2	1:A:386:C:O2	2.71	0.44
1:A:1009:G:H1'	1:A:1021:G:H22	1.83	0.44
1:A:1132:C:H42	1:A:1142:G:H1	1.66	0.44
1:A:1509:C:H2'	1:A:1510:U:O4'	2.17	0.44
24:A:1616:PAR:HN21	24:A:1616:PAR:H42	1.83	0.44
3:C:35:GLU:OE2	3:C:59:ARG:NH2	2.29	0.44
4:D:138:TYR:C	4:D:138:TYR:CD2	2.96	0.44
8:H:6:ILE:HG21	8:H:85:ARG:HH21	1.83	0.44
12:L:111:LYS:HA	12:L:111:LYS:NZ	2.33	0.44
15:O:26:GLU:HA	15:O:81:LEU:CD1	2.48	0.44
16:P:40:ASP:OD1	16:P:44:THR:HG23	2.17	0.44
21:U:10:ARG:HA	21:U:13:ILE:HD11	2.00	0.44
1:A:129:U:O3'	1:A:129(A):G:H3'	2.17	0.43
1:A:321:A:H62	1:A:328:C:H1'	1.83	0.43
1:A:372:C:H1'	1:A:373:A:OP2	2.18	0.43
1:A:439:A:C4	1:A:497:A:C2	3.06	0.43
1:A:1049:U:H4'	1:A:1050:G:H5'	2.00	0.43
5:E:15:ARG:HD2	5:E:26:PHE:CD2	2.53	0.43
7:G:149:ARG:HB3	11:K:59:TYR:HE1	1.83	0.43
8:H:91:ARG:NH1	17:Q:33:GLY:HA3	2.32	0.43
19:S:51:VAL:HG21	19:S:71:LEU:HB3	1.99	0.43
1:A:120:A:OP2	24:A:1603:PAR:O53	2.28	0.43
1:A:558:G:H3'	1:A:559:A:H3'	1.99	0.43
1:A:635:G:N7	24:A:1610:PAR:O34	2.40	0.43
1:A:1361(A):C:H2'	1:A:1362:C:H5''	2.00	0.43
1:A:1507:A:C2	1:A:1508:G:C4	3.05	0.43
1:A:1516:G:H2'	1:A:1518:MA6:OP2	2.18	0.43
4:D:31:CYS:O	4:D:31:CYS:SG	2.77	0.43
6:F:74:ASP:O	6:F:77:ARG:HB3	2.19	0.43
7:G:50:ILE:CD1	7:G:125:MET:HG3	2.48	0.43
10:J:57:LYS:HG2	10:J:58:ASP:OD1	2.18	0.43
1:A:88:A:H2'	1:A:89:C:O4'	2.18	0.43
1:A:157:G:H2'	1:A:158:G:H8	1.83	0.43
1:A:926:G:H3'	1:A:1505:G:H21	1.84	0.43
1:A:938:A:N6	1:A:939:G:C6	2.86	0.43
1:A:1055:A:C8	1:A:1206:G:C2	3.06	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1329:A:H62	21:U:7:ARG:HH21	1.65	0.43
1:A:1421:G:C6	1:A:1480:G:N1	2.86	0.43
24:A:1602:PAR:H51	24:A:1602:PAR:H322	1.82	0.43
2:B:48:MET:O	2:B:51:LEU:HB2	2.19	0.43
2:B:97:TRP:CZ3	2:B:176:GLU:OE2	2.71	0.43
6:F:61:LEU:HB2	6:F:63:TYR:CE2	2.54	0.43
8:H:85:ARG:HD3	8:H:87:SER:O	2.17	0.43
10:J:6:ILE:HG23	10:J:98:ILE:HG12	1.99	0.43
23:W:39:U:H2'	23:W:40:C:C6	2.54	0.43
1:A:266:G:H8	1:A:266:G:H2'	1.58	0.43
1:A:410:G:N1	1:A:429:U:C2	2.86	0.43
3:C:43:LEU:HA	3:C:43:LEU:HD22	1.66	0.43
3:C:81:GLY:O	3:C:84:ILE:HG22	2.18	0.43
4:D:15:GLU:OE1	4:D:66:ARG:NH1	2.52	0.43
4:D:114:ARG:HG3	4:D:114:ARG:HH11	1.83	0.43
1:A:190(C):C:C5	1:A:190(D):U:C5	3.07	0.43
1:A:218:C:H6	1:A:218:C:O5'	2.01	0.43
1:A:345:C:OP2	1:A:345:C:H6	2.02	0.43
1:A:382:A:C2	1:A:383:A:C4	3.06	0.43
1:A:575:G:C5	1:A:881:G:C2	3.06	0.43
1:A:690:G:C6	1:A:691:G:C6	3.07	0.43
1:A:975:A:C5'	1:A:975:A:C8	3.01	0.43
1:A:1376:U:H2'	1:A:1377:A:H8	1.83	0.43
1:A:1399:C:C2	1:A:1401:G:C5	3.07	0.43
1:A:1526:G:O2'	1:A:1527:C:H5'	2.19	0.43
24:A:1614:PAR:O61	24:A:1614:PAR:O41	2.27	0.43
2:B:7:VAL:H	2:B:9:GLU:HG3	1.84	0.43
3:C:77:ILE:O	3:C:81:GLY:HA2	2.19	0.43
4:D:173:TRP:HB2	4:D:187:ARG:O	2.18	0.43
5:E:144:THR:HG22	5:E:145:LYS:H	1.84	0.43
11:K:126:ARG:HB3	11:K:127:LYS:H	1.56	0.43
12:L:28:LYS:C	12:L:30:ALA:N	2.75	0.43
1:A:476:G:C2	1:A:477:G:C4	3.07	0.43
1:A:581:G:H4'	15:O:64:ARG:HH22	1.83	0.43
1:A:1331:G:O2'	1:A:1332:A:O5'	2.37	0.43
2:B:112:VAL:HG21	2:B:153:ARG:HA	2.00	0.43
10:J:49:VAL:HG13	10:J:61:GLU:HB3	2.01	0.43
12:L:110:VAL:HG23	12:L:120:TYR:HB3	2.01	0.43
1:A:35:G:H2'	1:A:36:C:C6	2.54	0.43
1:A:216:G:O2'	1:A:217:C:O5'	2.36	0.43
1:A:329:A:H4'	1:A:330:C:OP2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:892:A:O2'	1:A:1415:G:H4'	2.19	0.43
1:A:1116:C:O2'	9:I:108:VAL:HG21	2.18	0.43
5:E:82:VAL:HG21	5:E:138:ALA:CA	2.41	0.43
1:A:200:G:N2	1:A:218:C:C2	2.87	0.43
1:A:309:G:H1'	1:A:608:A:C2	2.54	0.43
1:A:620:C:H2'	1:A:621:A:O4'	2.18	0.43
1:A:1070:U:O2'	1:A:1071:C:H5'	2.18	0.43
1:A:1134:G:N2	1:A:1140:C:O2	2.49	0.43
8:H:111:ILE:O	8:H:134:ILE:HB	2.18	0.43
8:H:121:ASP:HB2	8:H:125:ARG:NH2	2.34	0.43
12:L:35:GLY:HA3	12:L:60:LEU:HD13	1.99	0.43
16:P:60:LEU:HD23	16:P:60:LEU:HA	1.67	0.43
1:A:255:G:C2	1:A:272:C:C2	3.07	0.43
1:A:255:G:H2'	1:A:256:U:C6	2.53	0.43
1:A:279:A:OP2	17:Q:95:TYR:OH	2.25	0.43
1:A:768:A:H5'	1:A:1524:C:H1'	2.01	0.43
1:A:1018:C:O5'	1:A:1018:C:H6	2.01	0.43
1:A:1404:5MC:O4'	1:A:1499:A:C2	2.71	0.43
1:A:1475:G:H2'	1:A:1476:G:C8	2.53	0.43
3:C:73:PRO:O	3:C:77:ILE:HG12	2.18	0.43
9:I:121:ARG:HG2	9:I:121:ARG:NH1	2.34	0.43
12:L:19:ARG:H	12:L:19:ARG:HG3	1.57	0.43
17:Q:65:ILE:HD12	17:Q:65:ILE:H	1.84	0.43
17:Q:69:LYS:HE2	17:Q:69:LYS:HB3	1.69	0.43
18:R:17:SER:OG	18:R:17:SER:O	2.32	0.43
1:A:9:G:C4	1:A:26:A:N1	2.87	0.43
1:A:75:G:C6	1:A:96:G:C6	3.07	0.43
1:A:181:G:N2	1:A:195:A:C4	2.87	0.43
1:A:399:G:H2'	1:A:400:C:C6	2.53	0.43
1:A:409:G:H1	1:A:433:C:H42	1.65	0.43
1:A:800:G:H2'	1:A:801:U:C6	2.54	0.43
24:A:1601:PAR:H11	24:A:1601:PAR:O52	2.19	0.43
2:B:135:GLN:O	2:B:139:LYS:HB2	2.19	0.43
4:D:15:GLU:OE2	4:D:59:ARG:NE	2.49	0.43
4:D:70:ILE:HD11	4:D:100:ARG:CZ	2.49	0.43
5:E:123:LEU:HA	5:E:123:LEU:HD23	1.67	0.43
10:J:63:PHE:HA	14:N:59:ALA:H	1.84	0.43
15:O:21:ASP:OD2	15:O:24:SER:HB3	2.19	0.43
17:Q:22:LEU:HA	17:Q:22:LEU:HD12	1.56	0.43
1:A:771:G:N2	1:A:808:C:O2	2.44	0.42
1:A:1038:C:H2'	1:A:1039:C:C6	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:24:TRP:HB2	2:B:190:THR:HG22	2.01	0.42
2:B:181:PHE:HD2	8:H:70:GLN:HB2	1.83	0.42
3:C:11:ARG:CD	3:C:180:ALA:HB3	2.43	0.42
12:L:6:THR:HG1	12:L:9:GLN:HG3	1.84	0.42
13:M:91:ARG:HH22	13:M:103:THR:HG21	1.84	0.42
15:O:36:ILE:HD13	15:O:60:VAL:HG22	2.00	0.42
15:O:70:LEU:HD22	15:O:78:TYR:N	2.33	0.42
17:Q:78:GLU:OE1	17:Q:81:ARG:HD2	2.19	0.42
1:A:22:G:O2'	1:A:23:C:H5'	2.18	0.42
1:A:337:C:H2'	1:A:338:A:C8	2.54	0.42
1:A:343:U:O2'	1:A:346:G:O6	2.27	0.42
1:A:965:A:H4'	1:A:966:M2G:OP2	2.19	0.42
1:A:1127:G:H4'	1:A:1148:U:O2	2.18	0.42
1:A:1230:C:H2'	1:A:1231:G:C8	2.54	0.42
1:A:1526:G:C2'	1:A:1527:C:H5'	2.50	0.42
3:C:142:MET:HE3	3:C:142:MET:HB3	1.79	0.42
7:G:99:LEU:HD23	7:G:99:LEU:HA	1.87	0.42
9:I:100:GLY:O	9:I:102:LEU:HD12	2.18	0.42
10:J:6:ILE:HB	10:J:72:VAL:HB	2.02	0.42
12:L:68:ALA:HB1	12:L:100:ILE:HG13	2.01	0.42
15:O:17:ARG:HD3	15:O:77:ARG:HH11	1.83	0.42
1:A:128:G:N7	24:A:1612:PAR:N32	2.63	0.42
1:A:328:C:H2'	1:A:328:C:O2	2.19	0.42
1:A:1304:G:C5	1:A:1305:G:N1	2.88	0.42
1:A:1397:C:H4'	1:A:1398:A:OP2	2.17	0.42
1:A:1505:G:C8	1:A:1505:G:H3'	2.53	0.42
3:C:69:HIS:CE1	3:C:104:GLN:HB3	2.55	0.42
4:D:133:VAL:HG12	4:D:135:LEU:H	1.85	0.42
5:E:89:ILE:HG21	5:E:135:THR:HA	2.01	0.42
7:G:54:THR:HG22	7:G:56:GLN:CB	2.50	0.42
13:M:65:LYS:HB2	13:M:65:LYS:HE3	1.84	0.42
16:P:1:MET:HE2	16:P:1:MET:HB3	1.86	0.42
16:P:6:LEU:HD23	16:P:17:TYR:CB	2.49	0.42
17:Q:90:ILE:O	17:Q:93:GLN:N	2.51	0.42
19:S:75:ALA:HA	19:S:76:PRO:HD2	1.83	0.42
1:A:147:G:C2	1:A:148:G:C8	3.08	0.42
1:A:252:U:C4	1:A:253:U:O4	2.72	0.42
1:A:872:A:H2'	1:A:872:A:N3	2.35	0.42
1:A:913:A:OP1	12:L:91:LYS:HE3	2.19	0.42
1:A:982:U:H4'	1:A:983:A:O5'	2.19	0.42
1:A:1030:C:H42	1:A:1031:G:H1	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1309:G:N2	1:A:1329:A:H1'	2.34	0.42
2:B:167:PRO:O	2:B:171:ALA:HB2	2.18	0.42
4:D:88:VAL:HG12	4:D:90:GLY:H	1.84	0.42
6:F:1:MET:HE3	6:F:66:GLU:HG2	2.00	0.42
16:P:9:PHE:N	16:P:16:HIS:O	2.51	0.42
16:P:74:LEU:HD23	16:P:74:LEU:HA	1.78	0.42
1:A:106:C:H2'	1:A:107:G:H8	1.84	0.42
1:A:239:U:O4	24:A:1603:PAR:H642	2.20	0.42
1:A:285:G:C2	1:A:286:G:C8	3.08	0.42
1:A:344:A:H4'	1:A:345:C:OP2	2.20	0.42
1:A:403:C:O2'	1:A:404:U:H5'	2.19	0.42
1:A:424:G:H2'	1:A:425:G:H8	1.85	0.42
1:A:707:C:H2'	1:A:708:C:C6	2.54	0.42
1:A:1422:G:N2	1:A:1479:C:C2	2.87	0.42
2:B:82:ARG:HB3	2:B:94:ASN:HD21	1.84	0.42
5:E:92:LYS:O	5:E:119:LEU:HB2	2.19	0.42
8:H:91:ARG:NH1	17:Q:32:TYR:O	2.52	0.42
9:I:36:TYR:HD2	9:I:37:PHE:CE2	2.36	0.42
9:I:126:SER:C	9:I:128:ARG:H	2.28	0.42
10:J:7:LYS:HG3	10:J:71:LEU:HD21	2.01	0.42
1:A:130:A:OP2	1:A:190(E):U:O2'	2.36	0.42
1:A:254:G:H2'	1:A:255:G:H8	1.83	0.42
1:A:922:G:O2'	1:A:1398:A:N1	2.46	0.42
1:A:1077:G:N2	1:A:1079:G:H3'	2.34	0.42
1:A:1399:C:C2	1:A:1502:A:N6	2.87	0.42
1:A:1460:A:H2'	1:A:1461:G:O4'	2.20	0.42
2:B:98:LEU:HG	2:B:101:MET:HE3	2.01	0.42
4:D:31:CYS:C	4:D:33:MET:N	2.73	0.42
6:F:23:LYS:HB3	6:F:23:LYS:HE2	1.78	0.42
6:F:61:LEU:HD12	6:F:63:TYR:HE2	1.83	0.42
8:H:81:HIS:HB2	8:H:138:TRP:O	2.20	0.42
8:H:118:VAL:C	8:H:119:LEU:HD23	2.45	0.42
9:I:69:GLY:O	9:I:73:GLN:HG3	2.19	0.42
17:Q:100:LYS:HB3	17:Q:101:ARG:HE	1.84	0.42
1:A:397:A:C6	1:A:548:G:N7	2.88	0.42
1:A:414:A:H2'	1:A:415:A:O4'	2.20	0.42
1:A:430:A:P	4:D:8:VAL:H	2.41	0.42
1:A:653:A:OP1	8:H:56:LYS:HE2	2.19	0.42
1:A:1035:A:H2'	1:A:1036:G:H8	1.83	0.42
1:A:1200:C:H1'	1:A:1204:A:H62	1.85	0.42
2:B:7:VAL:HG13	2:B:48:MET:SD	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:223:ILE:HD12	2:B:224:GLN:N	2.34	0.42
4:D:57:ARG:HH11	4:D:57:ARG:CG	2.29	0.42
8:H:83:ILE:HD13	8:H:83:ILE:HG21	1.73	0.42
16:P:42:ARG:H	16:P:42:ARG:HG2	1.44	0.42
19:S:52:TYR:HA	19:S:56:GLN:O	2.20	0.42
20:T:43:LEU:CD1	20:T:51:GLU:HB3	2.49	0.42
1:A:190(L):U:O2	20:T:105:SER:HB2	2.20	0.42
1:A:503:C:H6	1:A:503:C:O5'	2.03	0.42
1:A:587:G:O2'	1:A:588:G:OP2	2.30	0.42
1:A:593:G:H1	1:A:646:U:H3	1.68	0.42
1:A:778:G:H2'	1:A:779:C:O4'	2.20	0.42
1:A:1402:4OC:O2	1:A:1500:A:N1	2.52	0.42
3:C:6:HIS:HA	3:C:7:PRO:HD2	1.71	0.42
3:C:58:GLU:HB3	10:J:92:THR:CG2	2.42	0.42
3:C:58:GLU:H	3:C:65:ALA:HB3	1.84	0.42
5:E:131:ILE:HD13	5:E:131:ILE:HA	1.78	0.42
8:H:27:PRO:HA	8:H:58:TYR:CD2	2.54	0.42
12:L:127:GLU:HB2	12:L:128:ALA:H	1.63	0.42
14:N:26:ARG:NH1	14:N:47:LEU:HD21	2.34	0.42
14:N:40:CYS:O	14:N:44:LEU:HB3	2.19	0.42
17:Q:66:SER:HB3	17:Q:69:LYS:CG	2.41	0.42
1:A:161:A:N1	1:A:347:G:O2'	2.38	0.42
1:A:691:G:O2'	1:A:797:C:H4'	2.19	0.42
1:A:859:A:H2'	1:A:860:A:O4'	2.20	0.42
1:A:1054:C:OP1	1:A:1197:G:OP2	2.37	0.42
1:A:1161:C:H2'	1:A:1162:C:C6	2.55	0.42
12:L:49:ASN:ND2	12:L:92:0TD:OD2	2.48	0.42
12:L:60:LEU:HB3	12:L:62:SER:H	1.85	0.42
13:M:91:ARG:HD2	13:M:91:ARG:HA	1.75	0.42
16:P:45:THR:HG22	16:P:46:PRO:HD2	2.01	0.42
1:A:117:G:O5'	1:A:117:G:H8	2.03	0.42
1:A:192:U:C2	1:A:193:C:C6	3.08	0.42
1:A:367:U:C6	1:A:394:G:N2	2.88	0.42
1:A:410:G:OP1	4:D:30:LYS:NZ	2.53	0.42
1:A:989:C:O2'	1:A:1017:G:O2'	2.21	0.42
1:A:1375:A:N1	1:A:1376:U:C2	2.88	0.42
2:B:14:GLY:O	2:B:17:PHE:HB2	2.20	0.42
4:D:8:VAL:C	4:D:10:ARG:N	2.77	0.42
10:J:49:VAL:CG2	14:N:41:ARG:HB2	2.50	0.42
13:M:3:ARG:NH2	13:M:7:VAL:HG12	2.35	0.42
14:N:11:LYS:O	14:N:14:PRO:HD3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:G:C2	1:A:123:C:C2	3.08	0.41
1:A:157:G:N3	1:A:158:G:C8	2.88	0.41
1:A:306:G:O2'	1:A:307:C:H5'	2.20	0.41
1:A:431:A:O2'	1:A:432:A:H5'	2.20	0.41
1:A:560:U:H4'	1:A:561:U:H5''	2.01	0.41
1:A:837:G:N2	1:A:850:U:O2	2.53	0.41
1:A:1105:A:H2'	1:A:1106:G:C8	2.54	0.41
1:A:1217:C:H2'	1:A:1218:C:O4'	2.20	0.41
1:A:1334:G:O5'	1:A:1334:G:H8	2.03	0.41
1:A:1348:U:O3'	9:I:120:ARG:HG3	2.19	0.41
2:B:119:GLU:HG3	2:B:142:LEU:HD21	2.02	0.41
2:B:217:ARG:O	2:B:220:ASP:HB2	2.19	0.41
4:D:162:LEU:HD23	4:D:162:LEU:HA	1.74	0.41
10:J:52:GLY:HA2	10:J:53:PRO:HD3	1.68	0.41
1:A:129(A):G:N3	1:A:190(E):U:H5''	2.34	0.41
1:A:268:C:O2'	1:A:269:C:H5'	2.20	0.41
1:A:538:G:OP2	12:L:115:LYS:HG3	2.20	0.41
1:A:828:A:H4'	1:A:828:A:OP1	2.20	0.41
1:A:1176:A:H2'	1:A:1177:G:C8	2.54	0.41
1:A:1281:U:O2'	1:A:1282:C:OP1	2.35	0.41
1:A:1320:C:O2'	1:A:1321:C:H5'	2.19	0.41
1:A:1424:C:H2'	1:A:1425:U:O4'	2.20	0.41
3:C:14:ILE:CG2	3:C:15:THR:HG23	2.51	0.41
3:C:43:LEU:HD13	3:C:47:LEU:HD22	2.01	0.41
7:G:54:THR:C	7:G:56:GLN:N	2.78	0.41
11:K:55:LYS:HB2	11:K:55:LYS:HE3	1.82	0.41
15:O:33:THR:HG23	15:O:63:ARG:NH1	2.34	0.41
1:A:442:C:H6	1:A:442:C:OP2	2.04	0.41
1:A:524:G:H2'	1:A:525:C:C6	2.56	0.41
1:A:955:U:H1'	1:A:1227:A:N6	2.34	0.41
1:A:1453:G:N2	1:A:1454:G:C5	2.89	0.41
24:A:1609:PAR:H24	24:A:1609:PAR:H33	1.74	0.41
3:C:57:ILE:HG12	3:C:66:VAL:HG22	2.02	0.41
3:C:111:LEU:HD23	3:C:111:LEU:HA	1.73	0.41
3:C:113:ALA:HA	3:C:116:VAL:HG23	2.01	0.41
3:C:126:ARG:HG2	3:C:128:PHE:CD1	2.48	0.41
3:C:178:LEU:HD12	3:C:178:LEU:HA	1.59	0.41
4:D:196:LEU:HA	4:D:197:PRO:HD3	1.87	0.41
8:H:53:VAL:HG23	8:H:58:TYR:CD1	2.56	0.41
8:H:91:ARG:HH12	17:Q:33:GLY:HA3	1.86	0.41
8:H:102:ARG:CD	8:H:102:ARG:N	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:83:ASP:OD1	17:Q:83:ASP:N	2.53	0.41
18:R:58:LEU:HA	18:R:58:LEU:HD23	1.73	0.41
1:A:299:G:C6	1:A:300:A:C6	3.09	0.41
2:B:73:THR:O	2:B:75:LYS:N	2.54	0.41
2:B:166:ASP:HB3	2:B:169:LYS:HB3	2.02	0.41
3:C:12:LEU:HA	3:C:12:LEU:HD23	1.80	0.41
4:D:8:VAL:O	4:D:10:ARG:N	2.53	0.41
9:I:100:GLY:O	9:I:103:THR:HB	2.21	0.41
13:M:56:LEU:HD23	13:M:56:LEU:HA	1.71	0.41
1:A:1160:G:O6	1:A:1181:G:O6	2.38	0.41
1:A:1373:G:H5''	7:G:36:LYS:HB2	2.03	0.41
2:B:30:ARG:H	2:B:30:ARG:HG2	1.71	0.41
15:O:17:ARG:HB2	15:O:18:PHE:CD2	2.54	0.41
1:A:321:A:C2	1:A:333:G:C2	3.08	0.41
1:A:325:A:N6	1:A:326:G:C2	2.88	0.41
1:A:504:C:C2	1:A:542:G:C2	3.09	0.41
1:A:1148:U:O3'	9:I:14:VAL:HG11	2.20	0.41
1:A:1447:G:C6	1:A:1460:A:C2	3.08	0.41
24:A:1613:PAR:H11	24:A:1613:PAR:N32	2.35	0.41
2:B:98:LEU:N	2:B:98:LEU:HD23	2.36	0.41
3:C:12:LEU:HD11	14:N:51:GLY:HA2	2.03	0.41
4:D:28:SER:C	4:D:30:LYS:H	2.27	0.41
8:H:6:ILE:N	8:H:6:ILE:CD1	2.84	0.41
8:H:28:ALA:HA	8:H:59:LEU:HD12	2.02	0.41
13:M:31:LYS:HG2	13:M:35:GLU:OE1	2.20	0.41
1:A:190(I):G:C6	1:A:190(J):U:C4	3.09	0.41
1:A:973:G:H3'	1:A:974:A:H5''	2.02	0.41
1:A:1054:C:H3'	1:A:1054:C:O2	2.20	0.41
1:A:1127:G:C2	1:A:1145:C:N3	2.88	0.41
2:B:33:TYR:HD1	2:B:44:LEU:HD22	1.85	0.41
8:H:17:THR:HB	8:H:78:GLN:NE2	2.35	0.41
8:H:112:LEU:N	8:H:112:LEU:HD23	2.36	0.41
11:K:86:GLY:H	11:K:112:THR:HG23	1.86	0.41
15:O:82:ILE:O	15:O:83:GLU:C	2.64	0.41
16:P:43:LYS:HA	16:P:48:TRP:HB3	2.03	0.41
18:R:16:PRO:HB2	18:R:17:SER:H	1.66	0.41
22:V:1:U:N3	23:W:37:A:C2	2.89	0.41
1:A:46:G:O2'	1:A:365:U:H1'	2.19	0.41
1:A:338:A:C2	1:A:339:C:C2	3.08	0.41
2:B:210:SER:O	2:B:214:ILE:HG12	2.20	0.41
4:D:25:ARG:HH21	4:D:30:LYS:HB3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:25:ILE:HG22	13:M:26:GLY:O	2.21	0.41
17:Q:29:HIS:HA	17:Q:30:PRO:HD3	1.88	0.41
18:R:55:ARG:HB3	18:R:55:ARG:NH1	2.35	0.41
20:T:22:ARG:O	20:T:23:ARG:C	2.62	0.41
20:T:43:LEU:HD12	20:T:52:ALA:HA	2.03	0.41
1:A:58:C:H6	1:A:58:C:H3'	1.86	0.41
1:A:127:G:C6	24:A:1612:PAR:H221	2.56	0.41
1:A:177:C:H2'	1:A:178:C:C6	2.55	0.41
1:A:530:G:O6	22:V:3:U:H1'	2.20	0.41
1:A:676:A:H1'	11:K:115:PRO:HB3	2.03	0.41
1:A:964:A:O2'	10:J:55:LYS:HD3	2.21	0.41
1:A:983:A:H1'	1:A:1049:U:O2	2.21	0.41
1:A:1124:G:H2'	1:A:1145:C:H5	1.86	0.41
1:A:1128:C:H1'	1:A:1130:A:N7	2.36	0.41
1:A:1139:G:H4'	1:A:1140:C:OP1	2.21	0.41
1:A:1320:C:N3	19:S:36:ARG:HG3	2.36	0.41
1:A:1348:U:N3	1:A:1374:A:N7	2.69	0.41
1:A:1410:G:N2	1:A:1491:G:C4	2.89	0.41
24:A:1603:PAR:O54	24:A:1603:PAR:H43	2.20	0.41
4:D:64:LEU:HD12	4:D:75:PHE:HZ	1.85	0.41
4:D:142:PRO:HA	4:D:185:PHE:HD2	1.85	0.41
4:D:202:LEU:HA	4:D:202:LEU:HD23	1.66	0.41
5:E:28:PHE:CE1	5:E:51:VAL:HG22	2.55	0.41
8:H:30:ARG:O	8:H:33:GLU:HB3	2.21	0.41
11:K:66:LEU:HD23	11:K:66:LEU:HA	1.84	0.41
12:L:27:LEU:O	12:L:30:ALA:N	2.42	0.41
17:Q:20:THR:HG22	17:Q:41:LYS:HG2	2.02	0.41
17:Q:76:LEU:HD12	17:Q:76:LEU:C	2.45	0.41
17:Q:83:ASP:OD1	17:Q:84:LEU:HD23	2.21	0.41
1:A:98:U:O4	24:A:1618:PAR:H12	2.21	0.41
1:A:181:G:H4'	1:A:182:U:H5'	2.02	0.41
1:A:409:G:N2	1:A:433:C:N3	2.53	0.41
1:A:474:G:OP2	16:P:75:ARG:NH1	2.54	0.41
1:A:557:G:N1	1:A:558:G:C2	2.89	0.41
1:A:855:G:C4	1:A:856:C:C6	3.09	0.41
1:A:1024:G:H5''	1:A:1025:U:OP2	2.21	0.41
1:A:1055:A:N6	1:A:1206:G:C5	2.89	0.41
1:A:1203:C:OP1	14:N:2:ALA:N	2.54	0.41
1:A:1228:C:OP2	13:M:111:LYS:HE3	2.21	0.41
1:A:1522:U:O2'	1:A:1523:G:H5'	2.21	0.41
24:A:1616:PAR:H32	24:A:1616:PAR:H11	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:74:LYS:O	2:B:75:LYS:HB2	2.20	0.41
3:C:22:TRP:NE1	3:C:36:ASP:OD1	2.50	0.41
4:D:64:LEU:HD12	4:D:75:PHE:CZ	2.56	0.41
6:F:67:MET:HB2	6:F:68:PRO:HD2	2.03	0.41
11:K:84:VAL:HG21	11:K:95:ILE:HD11	2.03	0.41
13:M:10:PRO:HB2	13:M:18:ALA:HB1	2.02	0.41
15:O:14:GLU:HG3	15:O:15:PHE:CD1	2.56	0.41
18:R:84:LYS:H	18:R:84:LYS:HG3	1.57	0.41
19:S:40:ILE:O	19:S:67:VAL:HG13	2.21	0.41
20:T:8:ARG:HD2	20:T:8:ARG:N	2.36	0.41
1:A:107:G:C2	1:A:108:G:H1'	2.56	0.40
1:A:289:G:C6	1:A:290:C:N4	2.89	0.40
1:A:386:C:C2'	1:A:387:U:H5'	2.51	0.40
1:A:606:G:H5''	1:A:607:A:H5'	2.03	0.40
1:A:949:A:OP1	13:M:101:GLN:HB3	2.21	0.40
1:A:1060:C:HO2'	10:J:56:HIS:CE1	2.37	0.40
1:A:1256:A:H2	1:A:1277:C:N4	2.19	0.40
1:A:1501:C:C5	1:A:1504:G:C4	3.09	0.40
1:A:1502:A:H2	1:A:1505:G:N1	2.17	0.40
3:C:170:GLN:HG2	3:C:171:GLY:N	2.36	0.40
1:A:45:U:OP1	1:A:307:C:O2'	2.36	0.40
1:A:290:C:O5'	1:A:290:C:H6	2.04	0.40
1:A:961:U:C2'	1:A:962:C:H5'	2.50	0.40
1:A:994:A:N3	1:A:994:A:H2'	2.36	0.40
1:A:1057:G:H2'	1:A:1058:G:O4'	2.21	0.40
2:B:127:ILE:H	2:B:127:ILE:HG13	1.70	0.40
2:B:163:PHE:CE1	2:B:215:LEU:HD23	2.56	0.40
3:C:177:THR:O	3:C:180:ALA:HB2	2.21	0.40
6:F:61:LEU:HD13	6:F:63:TYR:OH	2.21	0.40
8:H:102:ARG:H	8:H:102:ARG:CD	2.34	0.40
9:I:74:ILE:HA	9:I:77:ILE:HD12	2.04	0.40
10:J:32:ALA:HB2	10:J:76:ASN:HB2	2.02	0.40
12:L:15:ARG:HD3	12:L:15:ARG:HA	1.89	0.40
13:M:99:ARG:CZ	19:S:2:PRO:HG2	2.51	0.40
14:N:21:TYR:HD2	14:N:22:THR:O	2.03	0.40
1:A:410:G:C2	1:A:429:U:C2	3.09	0.40
1:A:544:G:C6	1:A:545:C:C4	3.09	0.40
1:A:597:G:C6	1:A:644:G:C6	3.10	0.40
1:A:1313:U:O4	19:S:4:SER:OG	2.26	0.40
1:A:1329:A:H62	21:U:7:ARG:NH2	2.18	0.40
1:A:1442:G:N7	1:A:1446:A:N6	2.70	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:8:LYS:HA	2:B:11:LEU:HD13	2.02	0.40
2:B:82:ARG:HB3	2:B:94:ASN:ND2	2.36	0.40
3:C:40:ARG:O	3:C:44:GLU:HG3	2.21	0.40
3:C:152:ILE:HG22	3:C:199:LYS:HB2	2.02	0.40
4:D:194:LEU:HD13	4:D:194:LEU:HA	1.90	0.40
8:H:4:ASP:OD1	8:H:7:ALA:N	2.41	0.40
10:J:48:THR:OG1	10:J:62:HIS:HB3	2.21	0.40
13:M:59:TYR:CE1	13:M:63:THR:HG21	2.56	0.40
1:A:17:U:H2'	1:A:18:C:C6	2.56	0.40
1:A:415:A:OP1	24:A:1611:PAR:N64	2.55	0.40
1:A:1060:C:H5''	10:J:51:ARG:HB3	2.02	0.40
1:A:1203:C:H6	1:A:1203:C:O5'	2.03	0.40
2:B:162:ILE:HD11	2:B:184:VAL:HG22	2.04	0.40
5:E:83:GLU:HA	5:E:88:LYS:HA	2.02	0.40
6:F:45:LEU:HD12	6:F:47:ARG:NH2	2.36	0.40
6:F:48:LEU:HD22	18:R:77:GLY:HA3	2.03	0.40
7:G:69:VAL:HG12	7:G:100:ALA:HA	2.04	0.40
10:J:38:ILE:CG2	10:J:71:LEU:HB2	2.51	0.40
13:M:76:ALA:HA	13:M:79:LYS:HB3	2.03	0.40
1:A:328:C:H4'	1:A:329:A:C5'	2.51	0.40
1:A:639:G:O2'	1:A:640:A:H5'	2.21	0.40
1:A:909:A:H2'	1:A:910:C:O4'	2.21	0.40
1:A:989:C:N4	1:A:1216:G:H1	2.20	0.40
1:A:1133:G:N2	1:A:1141:C:O2	2.48	0.40
1:A:1190:G:O6	24:A:1608:PAR:N64	2.54	0.40
1:A:1227:A:H3'	1:A:1227:A:C8	2.57	0.40
1:A:1269:A:H2'	1:A:1270:C:O4'	2.21	0.40
1:A:1352:C:H2'	1:A:1353:G:C8	2.57	0.40
24:A:1602:PAR:O54	24:A:1602:PAR:O34	2.35	0.40
2:B:97:TRP:CH2	2:B:176:GLU:CD	3.00	0.40
7:G:104:LEU:HA	7:G:104:LEU:HD23	1.69	0.40
7:G:140:ASP:O	7:G:143:ARG:HB3	2.22	0.40
12:L:93:LEU:HD13	12:L:96:VAL:HG21	2.04	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	234/256 (91%)	204 (87%)	30 (13%)	0	100	100
3	C	205/239 (86%)	184 (90%)	20 (10%)	1 (0%)	24	60
4	D	206/209 (99%)	195 (95%)	11 (5%)	0	100	100
5	E	149/162 (92%)	144 (97%)	5 (3%)	0	100	100
6	F	99/101 (98%)	97 (98%)	2 (2%)	0	100	100
7	G	153/156 (98%)	141 (92%)	12 (8%)	0	100	100
8	H	136/138 (99%)	132 (97%)	4 (3%)	0	100	100
9	I	125/128 (98%)	110 (88%)	14 (11%)	1 (1%)	16	51
10	J	97/105 (92%)	80 (82%)	14 (14%)	3 (3%)	3	25
11	K	117/129 (91%)	105 (90%)	11 (9%)	1 (1%)	14	48
12	L	122/135 (90%)	111 (91%)	10 (8%)	1 (1%)	16	51
13	M	116/126 (92%)	104 (90%)	12 (10%)	0	100	100
14	N	58/61 (95%)	53 (91%)	5 (9%)	0	100	100
15	O	86/89 (97%)	76 (88%)	9 (10%)	1 (1%)	10	42
16	P	82/88 (93%)	77 (94%)	5 (6%)	0	100	100
17	Q	98/105 (93%)	93 (95%)	5 (5%)	0	100	100
18	R	71/88 (81%)	65 (92%)	6 (8%)	0	100	100
19	S	79/93 (85%)	70 (89%)	7 (9%)	2 (2%)	4	29
20	T	97/106 (92%)	82 (84%)	14 (14%)	1 (1%)	12	45
21	U	23/27 (85%)	22 (96%)	1 (4%)	0	100	100
All	All	2353/2541 (93%)	2145 (91%)	197 (8%)	11 (0%)	24	60

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	L	28	LYS

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Mol	Chain	Res	Type
19	S	31	ILE
20	T	99	LEU
9	I	38	GLN
19	S	6	LYS
10	J	34	VAL
10	J	83	GLU
10	J	85	LEU
11	K	95	ILE
15	O	87	ILE
3	C	66	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	201/220 (91%)	173 (86%)	28 (14%)	3	17
3	C	160/188 (85%)	117 (73%)	43 (27%)	0	4
4	D	180/181 (99%)	157 (87%)	23 (13%)	4	20
5	E	115/123 (94%)	90 (78%)	25 (22%)	1	6
6	F	90/90 (100%)	60 (67%)	30 (33%)	0	2
7	G	126/127 (99%)	102 (81%)	24 (19%)	1	10
8	H	119/119 (100%)	90 (76%)	29 (24%)	1	5
9	I	98/99 (99%)	73 (74%)	25 (26%)	0	4
10	J	87/92 (95%)	64 (74%)	23 (26%)	0	4
11	K	90/99 (91%)	76 (84%)	14 (16%)	2	15
12	L	103/110 (94%)	78 (76%)	25 (24%)	1	5
13	M	94/101 (93%)	76 (81%)	18 (19%)	1	10
14	N	49/50 (98%)	38 (78%)	11 (22%)	1	6
15	O	79/80 (99%)	60 (76%)	19 (24%)	1	5
16	P	72/74 (97%)	59 (82%)	13 (18%)	2	12
17	Q	95/97 (98%)	71 (75%)	24 (25%)	0	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	R	64/77 (83%)	54 (84%)	10 (16%)	2	15
19	S	71/80 (89%)	54 (76%)	17 (24%)	1	5
20	T	76/82 (93%)	56 (74%)	20 (26%)	0	4
21	U	19/22 (86%)	15 (79%)	4 (21%)	1	7
All	All	1988/2111 (94%)	1563 (79%)	425 (21%)	1	6

All (425) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	6	THR
2	B	9	GLU
2	B	11	LEU
2	B	46	LYS
2	B	48	MET
2	B	61	LEU
2	B	69	LEU
2	B	80	ILE
2	B	82	ARG
2	B	93	VAL
2	B	98	LEU
2	B	101	MET
2	B	107	THR
2	B	108	ILE
2	B	112	VAL
2	B	115	LEU
2	B	139	LYS
2	B	142	LEU
2	B	144	ARG
2	B	156	LYS
2	B	163	PHE
2	B	191	ASP
2	B	197	VAL
2	B	208	ILE
2	B	210	SER
2	B	221	LEU
2	B	223	ILE
2	B	230	VAL
3	C	3	ASN
3	C	4	LYS
3	C	8	ILE
3	C	14	ILE

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Mol	Chain	Res	Type
3	C	17	ASP
3	C	26	LYS
3	C	27	LYS
3	C	28	GLN
3	C	30	ARG
3	C	34	LEU
3	C	43	LEU
3	C	46	GLU
3	C	52	LEU
3	C	64	VAL
3	C	70	VAL
3	C	79	ARG
3	C	83	ARG
3	C	91	LEU
3	C	99	VAL
3	C	104	GLN
3	C	107	GLN
3	C	116	VAL
3	C	126	ARG
3	C	127	ARG
3	C	130	VAL
3	C	132	ARG
3	C	138	VAL
3	C	139	GLN
3	C	144	SER
3	C	152	ILE
3	C	156	ARG
3	C	157	ILE
3	C	165	THR
3	C	166	GLU
3	C	167	TRP
3	C	175	LEU
3	C	178	LEU
3	C	188	LEU
3	C	190	ARG
3	C	195	VAL
3	C	196	LEU
3	C	204	LEU
3	C	207	VAL
4	D	3	ARG
4	D	8	VAL
4	D	12	CYS

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Mol	Chain	Res	Type
4	D	15	GLU
4	D	19	LEU
4	D	26	CYS
4	D	28	SER
4	D	34	GLU
4	D	50	ARG
4	D	58	LEU
4	D	61	LYS
4	D	67	ILE
4	D	70	ILE
4	D	78	LEU
4	D	80	GLU
4	D	91	SER
4	D	122	ARG
4	D	127	THR
4	D	150	GLU
4	D	178	VAL
4	D	190	ASP
4	D	201	GLN
4	D	209	ARG
5	E	10	MET
5	E	12	LEU
5	E	16	THR
5	E	24	ARG
5	E	31	LEU
5	E	32	VAL
5	E	41	VAL
5	E	43	LEU
5	E	47	LYS
5	E	50	GLU
5	E	51	VAL
5	E	64	ARG
5	E	68	GLU
5	E	69	VAL
5	E	76	ILE
5	E	80	ILE
5	E	92	LYS
5	E	100	VAL
5	E	105	VAL
5	E	116	THR
5	E	117	ASP
5	E	125	SER

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Mol	Chain	Res	Type
5	E	126	ARG
5	E	131	ILE
5	E	151	LEU
6	F	3	ARG
6	F	6	VAL
6	F	9	VAL
6	F	10	LEU
6	F	11	ASN
6	F	14	LEU
6	F	16	GLN
6	F	24	GLU
6	F	25	ILE
6	F	26	ILE
6	F	36	ARG
6	F	37	VAL
6	F	40	VAL
6	F	43	LEU
6	F	45	LEU
6	F	46	ARG
6	F	54	LYS
6	F	55	ASP
6	F	61	LEU
6	F	65	VAL
6	F	69	GLU
6	F	75	LEU
6	F	77	ARG
6	F	79	LEU
6	F	82	ARG
6	F	83	ASP
6	F	85	VAL
6	F	86	ARG
6	F	92	LYS
6	F	98	LEU
7	G	12	LEU
7	G	16	LEU
7	G	21	VAL
7	G	27	ILE
7	G	38	LEU
7	G	42	ILE
7	G	47	CYS
7	G	48	LYS
7	G	50	ILE

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Mol	Chain	Res	Type
7	G	52	GLU
7	G	67	GLU
7	G	73	MET
7	G	79	ARG
7	G	92	SER
7	G	94	ARG
7	G	97	GLN
7	G	113	GLU
7	G	114	ARG
7	G	118	VAL
7	G	124	LEU
7	G	136	LYS
7	G	146	GLU
7	G	149	ARG
7	G	156	TRP
8	H	3	THR
8	H	8	ASP
8	H	11	THR
8	H	14	ARG
8	H	18	ARG
8	H	19	VAL
8	H	21	LYS
8	H	24	THR
8	H	26	VAL
8	H	39	LEU
8	H	45	ILE
8	H	50	ARG
8	H	51	VAL
8	H	52	ASP
8	H	53	VAL
8	H	56	LYS
8	H	70	GLN
8	H	80	ILE
8	H	83	ILE
8	H	85	ARG
8	H	91	ARG
8	H	95	VAL
8	H	100	ILE
8	H	102	ARG
8	H	109	ILE
8	H	112	LEU
8	H	119	LEU

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Mol	Chain	Res	Type
8	H	127	LEU
8	H	133	LEU
9	I	2	GLU
9	I	3	GLN
9	I	12	GLU
9	I	14	VAL
9	I	23	ASN
9	I	27	THR
9	I	41	VAL
9	I	44	VAL
9	I	47	LEU
9	I	54	ASP
9	I	65	VAL
9	I	66	ARG
9	I	79	LEU
9	I	86	VAL
9	I	99	LEU
9	I	102	LEU
9	I	103	THR
9	I	108	VAL
9	I	111	ARG
9	I	113	LYS
9	I	114	TYR
9	I	118	LYS
9	I	121	ARG
9	I	124	GLN
9	I	125	TYR
10	J	4	ILE
10	J	14	LYS
10	J	16	LEU
10	J	21	GLN
10	J	23	ILE
10	J	33	GLN
10	J	38	ILE
10	J	44	VAL
10	J	49	VAL
10	J	50	ILE
10	J	60	ARG
10	J	61	GLU
10	J	62	HIS
10	J	63	PHE
10	J	65	LEU

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Mol	Chain	Res	Type
10	J	73	ASP
10	J	74	ILE
10	J	80	LYS
10	J	83	GLU
10	J	89	ASP
10	J	96	ILE
10	J	97	GLU
10	J	99	LYS
11	K	11	LYS
11	K	13	GLN
11	K	18	ARG
11	K	21	ILE
11	K	29	ILE
11	K	48	ILE
11	K	79	SER
11	K	80	VAL
11	K	84	VAL
11	K	91	ARG
11	K	116	HIS
11	K	119	CYS
11	K	120	ARG
11	K	127	LYS
12	L	6	THR
12	L	11	VAL
12	L	12	ARG
12	L	13	LYS
12	L	18	VAL
12	L	19	ARG
12	L	20	LYS
12	L	28	LYS
12	L	33	ARG
12	L	39	VAL
12	L	41	ARG
12	L	43	VAL
12	L	46	LYS
12	L	47	LYS
12	L	54	LYS
12	L	81	SER
12	L	83	VAL
12	L	93	LEU
12	L	96	VAL
12	L	97	ARG

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Mol	Chain	Res	Type
12	L	98	TYR
12	L	104	VAL
12	L	111	LYS
12	L	122	THR
12	L	127	GLU
13	M	3	ARG
13	M	4	ILE
13	M	11	ARG
13	M	14	ARG
13	M	44	ARG
13	M	56	LEU
13	M	62	ASN
13	M	64	TRP
13	M	66	LEU
13	M	74	VAL
13	M	79	LYS
13	M	93	ARG
13	M	98	VAL
13	M	101	GLN
13	M	105	THR
13	M	109	THR
13	M	110	ARG
13	M	115	LYS
14	N	4	LYS
14	N	6	LEU
14	N	7	ILE
14	N	13	THR
14	N	18	VAL
14	N	22	THR
14	N	29	ARG
14	N	31	ARG
14	N	33	VAL
14	N	41	ARG
14	N	44	LEU
15	O	9	GLN
15	O	10	LYS
15	O	22	THR
15	O	32	LEU
15	O	36	ILE
15	O	38	ARG
15	O	39	LEU
15	O	40	SER

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Mol	Chain	Res	Type
15	O	45	VAL
15	O	47	LYS
15	O	60	VAL
15	O	65	ARG
15	O	66	LEU
15	O	68	ARG
15	O	70	LEU
15	O	81	LEU
15	O	83	GLU
15	O	87	ILE
15	O	88	ARG
16	P	2	VAL
16	P	20	VAL
16	P	27	LYS
16	P	42	ARG
16	P	44	THR
16	P	45	THR
16	P	49	LEU
16	P	53	VAL
16	P	54	GLU
16	P	61	SER
16	P	67	THR
16	P	69	THR
16	P	83	GLU
17	Q	6	LEU
17	Q	9	VAL
17	Q	12	SER
17	Q	25	ARG
17	Q	34	LYS
17	Q	35	VAL
17	Q	36	ILE
17	Q	37	LYS
17	Q	38	ARG
17	Q	48	GLU
17	Q	59	ILE
17	Q	60	ILE
17	Q	65	ILE
17	Q	69	LYS
17	Q	77	VAL
17	Q	83	ASP
17	Q	84	LEU
17	Q	87	LYS

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Mol	Chain	Res	Type
17	Q	88	TYR
17	Q	89	LEU
17	Q	91	ARG
17	Q	97	SER
17	Q	98	LEU
17	Q	100	LYS
18	R	19	LYS
18	R	26	LEU
18	R	31	LEU
18	R	46	GLU
18	R	47	THR
18	R	50	ILE
18	R	53	ARG
18	R	75	ILE
18	R	84	LYS
18	R	88	LYS
19	S	3	ARG
19	S	4	SER
19	S	5	LEU
19	S	7	LYS
19	S	12	ASP
19	S	13	ASP
19	S	14	HIS
19	S	15	LEU
19	S	18	LYS
19	S	28	LYS
19	S	30	LEU
19	S	31	ILE
19	S	43	GLU
19	S	58	VAL
19	S	60	VAL
19	S	62	ILE
19	S	63	THR
20	T	8	ARG
20	T	10	LEU
20	T	11	SER
20	T	13	LEU
20	T	19	SER
20	T	23	ARG
20	T	30	LYS
20	T	43	LEU
20	T	48	LYS

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Mol	Chain	Res	Type
20	T	54	LYS
20	T	57	ARG
20	T	62	LEU
20	T	72	LEU
20	T	73	HIS
20	T	74	LYS
20	T	75	ASN
20	T	83	ARG
20	T	84	LEU
20	T	87	LYS
20	T	100	ILE
21	U	8	THR
21	U	13	ILE
21	U	15	ARG
21	U	17	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	40	HIS
2	B	140	HIS
3	C	6	HIS
3	C	69	HIS
3	C	108	ASN
3	C	118	GLN
4	D	119	GLN
6	F	7	ASN
6	F	32	ASN
6	F	73	ASN
6	F	94	GLN
6	F	100	ASN
7	G	13	GLN
8	H	15	ASN
8	H	78	GLN
8	H	81	HIS
9	I	73	GLN
10	J	33	GLN
10	J	69	ASN
11	K	13	GLN
11	K	62	GLN
16	P	14	ASN
16	P	16	HIS

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Mol	Chain	Res	Type
17	Q	16	GLN
19	S	14	HIS
20	T	18	GLN
20	T	73	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1510/1522 (99%)	321 (21%)	46 (3%)
22	V	2/3 (66%)	1 (50%)	0
23	W	14/15 (93%)	4 (28%)	0
All	All	1526/1540 (99%)	326 (21%)	46 (3%)

All (326) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	9	G
1	A	32	A
1	A	39	G
1	A	48	C
1	A	51	A
1	A	54	C
1	A	58	C
1	A	60	A
1	A	61	G
1	A	62	U
1	A	82	U
1	A	101	A
1	A	108	G
1	A	115	G
1	A	116	A
1	A	117	G
1	A	121	C
1	A	129(A)	G
1	A	130	A
1	A	131	C
1	A	143	A
1	A	144	G
1	A	163	C
1	A	182	U
1	A	183	G

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Mol	Chain	Res	Type
1	A	190(E)	U
1	A	190(F)	G
1	A	190(G)	G
1	A	195	A
1	A	197	A
1	A	201	C
1	A	202	U
1	A	216	G
1	A	220	G
1	A	231	G
1	A	247	G
1	A	251	G
1	A	266	G
1	A	267	C
1	A	270	A
1	A	289	G
1	A	298	A
1	A	299	G
1	A	308	C
1	A	319	G
1	A	321	A
1	A	328	C
1	A	329	A
1	A	330	C
1	A	331	G
1	A	332	G
1	A	344	A
1	A	345	C
1	A	347	G
1	A	351	G
1	A	352	C
1	A	353	A
1	A	354	G
1	A	367	U
1	A	371	G
1	A	372	C
1	A	373	A
1	A	374	A
1	A	378	G
1	A	384	G
1	A	390	C
1	A	397	A

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Mol	Chain	Res	Type
1	A	398	C
1	A	402	G
1	A	406	G
1	A	410	G
1	A	411	A
1	A	412	A
1	A	413	G
1	A	414	A
1	A	419	C
1	A	421	U
1	A	422	C
1	A	423	G
1	A	424	G
1	A	428	G
1	A	429	U
1	A	430	A
1	A	432	A
1	A	433	C
1	A	439	A
1	A	442	C
1	A	452	A
1	A	453	A
1	A	460	A
1	A	461	C
1	A	463	A
1	A	485	G
1	A	497	A
1	A	498	U
1	A	509	A
1	A	510	A
1	A	511	C
1	A	517	G
1	A	518	C
1	A	521	G
1	A	527	7MG
1	A	531	U
1	A	532	A
1	A	545	C
1	A	547	A
1	A	559	A
1	A	560	U
1	A	562	C

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Mol	Chain	Res	Type
1	A	563	A
1	A	564	C
1	A	568	G
1	A	570	G
1	A	571	U
1	A	572	A
1	A	573	A
1	A	575	G
1	A	576	G
1	A	577	G
1	A	579	G
1	A	587	G
1	A	588	G
1	A	597	G
1	A	607	A
1	A	618	C
1	A	630	G
1	A	631	G
1	A	632	A
1	A	653	A
1	A	665	A
1	A	667	G
1	A	671	G
1	A	687	A
1	A	688	G
1	A	695	A
1	A	701	C
1	A	702	A
1	A	703	G
1	A	723	U
1	A	731	G
1	A	748	C
1	A	755	G
1	A	766	A
1	A	773	G
1	A	777	A
1	A	785	G
1	A	792	A
1	A	793	U
1	A	794	A
1	A	798	G
1	A	812	C

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Mol	Chain	Res	Type
1	A	813	U
1	A	816	A
1	A	817	C
1	A	818	G
1	A	819	A
1	A	828	A
1	A	839	U
1	A	840	C
1	A	841	U
1	A	848	C
1	A	859	A
1	A	868	C
1	A	874	G
1	A	902	G
1	A	914	A
1	A	926	G
1	A	927	G
1	A	934	C
1	A	935	A
1	A	939	G
1	A	944	G
1	A	945	G
1	A	954	G
1	A	960	U
1	A	961	U
1	A	966	M2G
1	A	967	5MC
1	A	968	A
1	A	969	A
1	A	971	G
1	A	974	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	978	A
1	A	979	C
1	A	983	A
1	A	989	C
1	A	991	U
1	A	992	U
1	A	993	G
1	A	994	A

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Mol	Chain	Res	Type
1	A	999	C
1	A	1003(A)	G
1	A	1004	A
1	A	1005	A
1	A	1006	C
1	A	1017	G
1	A	1024	G
1	A	1025	U
1	A	1026	G
1	A	1027	C
1	A	1031	G
1	A	1033	G
1	A	1035	A
1	A	1042	G
1	A	1050	G
1	A	1053	G
1	A	1054	C
1	A	1055	A
1	A	1064	G
1	A	1065	U
1	A	1066	C
1	A	1068	G
1	A	1078	U
1	A	1094	G
1	A	1095	U
1	A	1096	C
1	A	1100	C
1	A	1101	A
1	A	1108	G
1	A	1125	U
1	A	1126	U
1	A	1127	G
1	A	1129	C
1	A	1130	A
1	A	1131	G
1	A	1132	C
1	A	1137	C
1	A	1138	G
1	A	1139	G
1	A	1146	A
1	A	1154	G
1	A	1158	C

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Mol	Chain	Res	Type
1	A	1159	U
1	A	1171	G
1	A	1179	A
1	A	1180	A
1	A	1181	G
1	A	1183	A
1	A	1184	G
1	A	1190	G
1	A	1191	A
1	A	1196	U
1	A	1198	G
1	A	1200	C
1	A	1201	A
1	A	1202	G
1	A	1211	U
1	A	1212	U
1	A	1213	A
1	A	1218	C
1	A	1225	A
1	A	1226	C
1	A	1227	A
1	A	1238	A
1	A	1240	U
1	A	1249	C
1	A	1250	A
1	A	1252	A
1	A	1253	G
1	A	1257	U
1	A	1258	G
1	A	1260	C
1	A	1268	A
1	A	1280	A
1	A	1281	U
1	A	1282	C
1	A	1285	A
1	A	1286	A
1	A	1287	A
1	A	1288	A
1	A	1289	A
1	A	1291	G
1	A	1300	G
1	A	1301	U

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Mol	Chain	Res	Type
1	A	1302	U
1	A	1303	C
1	A	1305	G
1	A	1317	C
1	A	1320	C
1	A	1322	C
1	A	1332	A
1	A	1338	G
1	A	1346	A
1	A	1347	G
1	A	1348	U
1	A	1353	G
1	A	1362	C
1	A	1364	U
1	A	1370	G
1	A	1379	G
1	A	1381	U
1	A	1394	A
1	A	1398	A
1	A	1399	C
1	A	1400	5MC
1	A	1402	4OC
1	A	1421	G
1	A	1442	G
1	A	1443	G
1	A	1446	A
1	A	1453	G
1	A	1487	G
1	A	1492	A
1	A	1499	A
1	A	1502	A
1	A	1504	G
1	A	1505	G
1	A	1506	U
1	A	1507	A
1	A	1517	G
1	A	1519	MA6
1	A	1520	G
1	A	1528	U
1	A	1529	G
1	A	1530	G
1	A	1531	A

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Mol	Chain	Res	Type
1	A	1540	PSU
1	A	1541	PSU
22	V	3	U
23	W	30	G
23	W	33	U
23	W	36	A
23	W	42	C

All (46) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	60	A
1	A	115	G
1	A	129(A)	G
1	A	181	G
1	A	250	A
1	A	266	G
1	A	328	C
1	A	329	A
1	A	353	A
1	A	372	C
1	A	428	G
1	A	429	U
1	A	432	A
1	A	484	G
1	A	509	A
1	A	559	A
1	A	560	U
1	A	687	A
1	A	701	C
1	A	793	U
1	A	812	C
1	A	913	A
1	A	960	U
1	A	965	A
1	A	1049	U
1	A	1065	U
1	A	1067	A
1	A	1124	G
1	A	1129	C
1	A	1179	A
1	A	1182	G

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Mol	Chain	Res	Type
1	A	1190	G
1	A	1201	A
1	A	1212	U
1	A	1225	A
1	A	1256	A
1	A	1281	U
1	A	1285	A
1	A	1300	G
1	A	1301	U
1	A	1331	G
1	A	1347	G
1	A	1397	C
1	A	1443	G
1	A	1505	G
1	A	1528	U

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

15 non-standard protein/DNA/RNA residues are 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	$\# Z > 2$
1	5MC	A	967	1	19,22,23	1.41	3 (15%)	26,32,35	0.91	0
1	5MC	A	1407	1	19,22,23	1.68	2 (10%)	26,32,35	1.18	3 (11%)
1	MA6	A	1518	1	23,26,27	0.94	1 (4%)	33,38,41	1.09	1 (3%)
1	MA6	A	1519	1	23,26,27	1.22	5 (21%)	33,38,41	1.08	2 (6%)
1	M2G	A	966	1	24,27,28	0.64	0	33,40,43	1.11	3 (9%)
1	7MG	A	527	25,1	23,26,27	4.27	7 (30%)	27,39,42	2.34	9 (33%)
1	4OC	A	1402	1	20,23,24	0.89	1 (5%)	25,32,35	0.75	0
1	UR3	A	1498	1	19,22,23	0.88	1 (5%)	26,32,35	0.93	0
1	PSU	A	1541	1	18,21,22	1.19	1 (5%)	21,30,33	1.82	4 (19%)
1	2MG	A	1207	1	23,26,27	1.88	4 (17%)	33,38,41	1.36	4 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MC	A	1400	1	19,22,23	1.22	3 (15%)	26,32,35	1.17	3 (11%)
12	0TD	L	92	12	8,9,10	1.33	1 (12%)	6,11,13	2.75	2 (33%)
1	PSU	A	1540	1	18,21,22	1.36	1 (5%)	21,30,33	1.90	6 (28%)
1	PSU	A	516	1	18,21,22	1.39	1 (5%)	21,30,33	1.63	4 (19%)
1	5MC	A	1404	1	19,22,23	1.45	2 (10%)	26,32,35	0.93	1 (3%)

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
1	5MC	A	967	1	-	3/7/25/26	0/2/2/2
1	5MC	A	1407	1	-	0/7/25/26	0/2/2/2
1	MA6	A	1518	1	-	0/11/29/30	0/3/3/3
1	MA6	A	1519	1	-	4/11/29/30	0/3/3/3
1	M2G	A	966	1	-	3/11/29/30	0/3/3/3
1	7MG	A	527	25,1	-	2/7/37/38	0/3/3/3
1	4OC	A	1402	1	-	2/9/29/30	0/2/2/2
1	UR3	A	1498	1	-	2/7/25/26	0/2/2/2
1	PSU	A	1541	1	-	2/7/25/26	0/2/2/2
1	2MG	A	1207	1	-	0/9/27/28	0/3/3/3
1	5MC	A	1400	1	-	2/7/25/26	0/2/2/2
12	0TD	L	92	12	-	3/7/12/14	-
1	PSU	A	1540	1	-	2/7/25/26	0/2/2/2
1	PSU	A	516	1	-	0/7/25/26	0/2/2/2
1	5MC	A	1404	1	-	0/7/25/26	0/2/2/2

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	527	7MG	C8-N9	-18.40	1.33	1.45
1	A	1407	5MC	C5-C4	-5.70	1.39	1.44
1	A	1207	2MG	C2-N1	5.29	1.45	1.36
1	A	1540	PSU	C6-C5	5.07	1.40	1.35
1	A	527	7MG	C2-N2	4.80	1.45	1.34
1	A	516	PSU	C6-C5	4.64	1.40	1.35
1	A	1207	2MG	C6-N1	4.40	1.47	1.38
1	A	1541	PSU	C6-C5	4.31	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	967	5MC	C5-C4	-4.30	1.40	1.44
1	A	1207	2MG	O6-C6	4.23	1.31	1.23
1	A	1404	5MC	C5-C4	-4.22	1.40	1.44
1	A	527	7MG	C5-N7	4.16	1.40	1.35
1	A	527	7MG	C4-N9	-3.37	1.33	1.37
1	A	527	7MG	C4-N3	2.97	1.41	1.34
1	A	1407	5MC	C6-C5	2.89	1.39	1.34
1	A	1404	5MC	C2-N3	2.83	1.42	1.36
1	A	1400	5MC	C2-N3	2.82	1.41	1.36
1	A	967	5MC	C2-N3	2.66	1.41	1.36
1	A	1519	MA6	C2-N1	2.54	1.38	1.33
1	A	1518	MA6	C10-N6	2.45	1.51	1.45
1	A	1519	MA6	C4-N3	2.44	1.39	1.34
12	L	92	0TD	CB-CA	2.39	1.55	1.54
1	A	1519	MA6	C6-N6	2.35	1.43	1.36
1	A	527	7MG	O6-C6	-2.34	1.19	1.23
1	A	1402	4OC	O2-C2	-2.33	1.19	1.23
1	A	967	5MC	C2-N1	2.28	1.44	1.40
1	A	1400	5MC	C4-N3	2.27	1.37	1.34
1	A	1519	MA6	C6-N1	2.25	1.38	1.34
1	A	527	7MG	C8-N7	-2.15	1.31	1.42
1	A	1400	5MC	C2-N1	2.11	1.44	1.40
1	A	1207	2MG	C5-C4	2.09	1.44	1.38
1	A	1519	MA6	C5-C4	2.04	1.42	1.39
1	A	1498	UR3	O2-C2	2.01	1.26	1.22

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	527	7MG	C5-C6-N1	6.11	121.69	110.94
12	L	92	0TD	CSB-SB-CB	-5.71	92.10	102.36
1	A	1541	PSU	C4-N3-C2	-4.54	120.12	126.37
1	A	527	7MG	C2-N3-C4	4.47	119.99	112.30
1	A	1541	PSU	N1-C2-N3	4.38	119.79	115.17
1	A	1540	PSU	N1-C2-N3	4.22	119.62	115.17
1	A	1207	2MG	N2-C2-N3	-4.14	115.23	120.51
1	A	516	PSU	C6-C5-C4	-4.05	115.44	118.17
1	A	1540	PSU	C4-N3-C2	-4.03	120.82	126.37
1	A	527	7MG	N9-C4-N3	3.85	131.09	125.46
1	A	527	7MG	C6-C5-C4	-3.68	115.92	122.40
1	A	527	7MG	C6-C5-N7	3.52	137.38	131.93
1	A	527	7MG	O6-C6-C5	-3.32	119.48	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	527	7MG	C5-C4-N3	-3.29	121.96	128.13
1	A	1407	5MC	C5-C4-N3	3.26	125.10	121.75
1	A	1540	PSU	O2-C2-N1	-3.20	119.49	122.79
1	A	527	7MG	C2-N1-C6	-3.18	119.35	125.11
1	A	1207	2MG	C6-C5-C4	3.10	123.48	118.83
1	A	1540	PSU	C6-N1-C2	-2.99	119.92	122.69
1	A	516	PSU	C4-N3-C2	-2.84	122.46	126.37
1	A	966	M2G	C5-C4-N3	-2.82	123.91	128.39
12	L	92	0TD	CB-CA-N	-2.79	103.44	109.10
1	A	1541	PSU	O4-C4-N3	-2.79	114.87	120.11
1	A	516	PSU	O2-C2-N1	-2.74	119.97	122.79
1	A	1400	5MC	C5-C4-N3	2.70	124.53	121.75
1	A	1400	5MC	C1'-N1-C6	-2.63	116.82	121.15
1	A	527	7MG	N9-C8-N7	2.60	107.05	103.37
1	A	1540	PSU	C6-C5-C4	-2.59	116.42	118.17
1	A	1407	5MC	N4-C4-N3	-2.57	113.86	118.51
1	A	516	PSU	C6-N1-C2	-2.50	120.37	122.69
1	A	1519	MA6	C2-N1-C6	2.50	117.93	111.83
1	A	966	M2G	C6-C5-C4	2.49	122.57	118.83
1	A	1207	2MG	C6-C5-N7	-2.45	125.83	130.29
1	A	1519	MA6	C4-C5-N7	-2.33	107.91	110.58
1	A	966	M2G	O6-C6-C5	2.20	132.33	126.53
1	A	1407	5MC	C5-C6-N1	-2.13	121.00	123.31
1	A	1540	PSU	C3'-C2'-C1'	-2.09	99.22	101.69
1	A	1541	PSU	O2-C2-N1	-2.08	120.65	122.79
1	A	1518	MA6	N1-C6-N6	-2.07	114.33	116.86
1	A	1404	5MC	C1'-N1-C6	-2.07	117.75	121.15
1	A	1207	2MG	C5-C4-N3	-2.05	125.13	128.39
1	A	1400	5MC	N4-C4-N3	-2.04	114.81	118.51

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	967	5MC	O4'-C4'-C5'-O5'
1	A	1400	5MC	O4'-C4'-C5'-O5'
1	A	1519	MA6	O4'-C4'-C5'-O5'
1	A	1541	PSU	C2'-C1'-C5-C4
1	A	1541	PSU	C2'-C1'-C5-C6
12	L	92	0TD	CG-CB-SB-CSB
1	A	966	M2G	C3'-C4'-C5'-O5'
1	A	967	5MC	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	A	1402	4OC	O4'-C4'-C5'-O5'
1	A	1519	MA6	C3'-C4'-C5'-O5'
1	A	1540	PSU	C3'-C4'-C5'-O5'
1	A	1540	PSU	O4'-C4'-C5'-O5'
1	A	527	7MG	O4'-C4'-C5'-O5'
1	A	966	M2G	O4'-C4'-C5'-O5'
1	A	1400	5MC	C3'-C4'-C5'-O5'
1	A	527	7MG	C3'-C4'-C5'-O5'
1	A	1402	4OC	C3'-C4'-C5'-O5'
1	A	1519	MA6	C5-C6-N6-C9
1	A	1519	MA6	C4'-C5'-O5'-P
1	A	966	M2G	C4'-C5'-O5'-P
12	L	92	0TD	SB-CB-CG-OD1
1	A	1498	UR3	O4'-C4'-C5'-O5'
12	L	92	0TD	CA-CB-SB-CSB
1	A	1498	UR3	C3'-C4'-C5'-O5'
1	A	967	5MC	C2'-C1'-N1-C2

There are no ring outliers.

10 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	967	5MC	2	0
1	A	1518	MA6	2	0
1	A	966	M2G	3	0
1	A	527	7MG	1	0
1	A	1402	4OC	4	0
1	A	1498	UR3	3	0
1	A	1207	2MG	1	0
1	A	1400	5MC	1	0
12	L	92	0TD	2	0
1	A	1404	5MC	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 383 ligands modelled in this entry, 365 are monoatomic - leaving 18 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	PAR	A	1606	-	44,45,45	1.46	7 (15%)	63,67,67	1.65	12 (19%)
24	PAR	A	1603	-	44,45,45	1.44	8 (18%)	63,67,67	1.64	12 (19%)
24	PAR	A	1616	-	44,45,45	2.00	11 (25%)	63,67,67	1.68	12 (19%)
24	PAR	A	1608	25	44,45,45	1.31	6 (13%)	63,67,67	1.69	13 (20%)
24	PAR	A	1615	-	44,45,45	2.06	11 (25%)	63,67,67	1.72	14 (22%)
24	PAR	A	1618	-	44,45,45	2.27	16 (36%)	63,67,67	1.67	12 (19%)
24	PAR	A	1607	-	44,45,45	1.68	9 (20%)	63,67,67	1.70	13 (20%)
24	PAR	A	1611	-	44,45,45	1.62	6 (13%)	63,67,67	1.71	13 (20%)
24	PAR	A	1613	-	44,45,45	1.69	10 (22%)	63,67,67	1.68	11 (17%)
24	PAR	A	1614	-	44,45,45	1.71	12 (27%)	63,67,67	1.61	11 (17%)
24	PAR	A	1610	-	44,45,45	1.72	12 (27%)	63,67,67	1.78	13 (20%)
24	PAR	A	1617	25	44,45,45	2.11	15 (34%)	63,67,67	1.71	11 (17%)
24	PAR	A	1604	-	44,45,45	1.32	6 (13%)	63,67,67	1.63	12 (19%)
24	PAR	A	1602	-	44,45,45	1.63	8 (18%)	63,67,67	1.80	10 (15%)
24	PAR	A	1609	-	44,45,45	1.78	15 (34%)	63,67,67	1.73	12 (19%)
24	PAR	A	1605	-	44,45,45	1.26	8 (18%)	63,67,67	1.54	10 (15%)
24	PAR	A	1601	-	44,45,45	1.41	6 (13%)	63,67,67	1.53	11 (17%)
24	PAR	A	1612	-	44,45,45	1.55	8 (18%)	63,67,67	1.66	10 (15%)

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
24	PAR	A	1606	-	-	2/18/94/94	0/4/4/4
24	PAR	A	1603	-	-	5/18/94/94	0/4/4/4
24	PAR	A	1616	-	-	14/18/94/94	1/4/4/4
24	PAR	A	1608	25	-	7/18/94/94	0/4/4/4
24	PAR	A	1615	-	-	8/18/94/94	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	PAR	A	1618	-	-	9/18/94/94	1/4/4/4
24	PAR	A	1607	-	-	9/18/94/94	0/4/4/4
24	PAR	A	1611	-	-	9/18/94/94	0/4/4/4
24	PAR	A	1613	-	-	9/18/94/94	0/4/4/4
24	PAR	A	1614	-	-	11/18/94/94	1/4/4/4
24	PAR	A	1610	-	-	9/18/94/94	1/4/4/4
24	PAR	A	1617	25	-	9/18/94/94	0/4/4/4
24	PAR	A	1604	-	-	8/18/94/94	0/4/4/4
24	PAR	A	1602	-	-	10/18/94/94	1/4/4/4
24	PAR	A	1609	-	-	8/18/94/94	0/4/4/4
24	PAR	A	1605	-	-	3/18/94/94	0/4/4/4
24	PAR	A	1601	-	-	4/18/94/94	0/4/4/4
24	PAR	A	1612	-	-	7/18/94/94	1/4/4/4

All (174) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1615	PAR	C13-C23	6.46	1.61	1.52
24	A	1618	PAR	C34-C24	6.07	1.61	1.53
24	A	1617	PAR	C52-C42	6.00	1.64	1.52
24	A	1618	PAR	C13-C23	5.77	1.60	1.52
24	A	1602	PAR	C14-C24	5.48	1.63	1.52
24	A	1613	PAR	C34-C24	5.35	1.60	1.53
24	A	1616	PAR	C13-C23	5.35	1.59	1.52
24	A	1617	PAR	C13-C23	5.32	1.59	1.52
24	A	1618	PAR	C52-C42	5.24	1.63	1.52
24	A	1611	PAR	C34-C24	5.03	1.59	1.53
24	A	1617	PAR	C34-C24	4.80	1.59	1.53
24	A	1604	PAR	C52-C42	4.75	1.62	1.52
24	A	1615	PAR	O43-C13	4.69	1.50	1.41
24	A	1610	PAR	O43-C13	4.61	1.49	1.41
24	A	1611	PAR	O43-C13	4.57	1.49	1.41
24	A	1603	PAR	C52-C42	4.34	1.61	1.52
24	A	1616	PAR	C34-C24	4.31	1.59	1.53
24	A	1607	PAR	C52-C42	4.30	1.61	1.52
24	A	1615	PAR	C52-C42	4.24	1.61	1.52
24	A	1602	PAR	C31-C21	4.23	1.58	1.53
24	A	1618	PAR	O43-C13	4.22	1.49	1.41
24	A	1612	PAR	C13-C23	4.18	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1615	PAR	O52-C52	4.15	1.54	1.43
24	A	1609	PAR	C14-C24	4.12	1.60	1.52
24	A	1614	PAR	C34-C24	4.01	1.58	1.53
24	A	1616	PAR	C52-C42	3.99	1.60	1.52
24	A	1606	PAR	C34-C24	3.97	1.58	1.53
24	A	1607	PAR	C62-C52	3.86	1.62	1.52
24	A	1609	PAR	C34-C24	3.86	1.58	1.53
24	A	1614	PAR	C14-C24	3.85	1.59	1.52
24	A	1606	PAR	O43-C13	3.84	1.48	1.41
24	A	1610	PAR	C14-C24	3.77	1.59	1.52
24	A	1607	PAR	O43-C13	3.73	1.48	1.41
24	A	1614	PAR	C52-C42	3.72	1.59	1.52
24	A	1616	PAR	C14-C24	3.70	1.59	1.52
24	A	1610	PAR	C11-C21	3.63	1.59	1.52
24	A	1601	PAR	C31-C21	3.63	1.58	1.53
24	A	1606	PAR	C52-C42	3.61	1.59	1.52
24	A	1612	PAR	C14-C24	3.60	1.59	1.52
24	A	1612	PAR	O43-C13	3.58	1.48	1.41
24	A	1615	PAR	O52-C13	3.56	1.51	1.41
24	A	1613	PAR	C14-C24	3.56	1.59	1.52
24	A	1616	PAR	O43-C13	3.55	1.47	1.41
24	A	1618	PAR	C14-C24	3.51	1.59	1.52
24	A	1609	PAR	O43-C13	3.38	1.47	1.41
24	A	1601	PAR	C13-C23	3.34	1.57	1.52
24	A	1618	PAR	O33-C14	3.31	1.51	1.41
24	A	1616	PAR	C31-C21	3.29	1.57	1.53
24	A	1607	PAR	C62-C12	3.26	1.60	1.53
24	A	1603	PAR	C33-C43	3.26	1.61	1.52
24	A	1618	PAR	C31-C21	3.19	1.57	1.53
24	A	1617	PAR	O52-C52	3.18	1.52	1.43
24	A	1611	PAR	C52-C42	3.18	1.58	1.52
24	A	1609	PAR	C13-C23	3.17	1.57	1.52
24	A	1617	PAR	O33-C14	3.11	1.50	1.41
24	A	1601	PAR	C11-C21	3.10	1.58	1.52
24	A	1613	PAR	C62-C52	3.08	1.60	1.52
24	A	1610	PAR	C31-C21	3.08	1.57	1.53
24	A	1613	PAR	C52-C42	3.06	1.58	1.52
24	A	1617	PAR	C62-C52	3.04	1.60	1.52
24	A	1603	PAR	C13-C23	3.02	1.56	1.52
24	A	1613	PAR	C13-C23	3.02	1.56	1.52
24	A	1617	PAR	C14-C24	3.02	1.58	1.52
24	A	1612	PAR	C52-C42	3.02	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1618	PAR	C62-C52	3.01	1.60	1.52
24	A	1601	PAR	C52-C42	2.97	1.58	1.52
24	A	1614	PAR	C31-C21	2.94	1.57	1.53
24	A	1609	PAR	C44-C54	2.93	1.59	1.53
24	A	1607	PAR	C44-C54	2.92	1.59	1.53
24	A	1608	PAR	C62-C12	2.92	1.59	1.53
24	A	1616	PAR	C62-C52	2.87	1.60	1.52
24	A	1602	PAR	C52-C42	2.87	1.58	1.52
24	A	1610	PAR	C41-C51	2.85	1.59	1.53
24	A	1614	PAR	C13-C23	2.80	1.56	1.52
24	A	1611	PAR	C31-C21	2.79	1.57	1.53
24	A	1602	PAR	O43-C13	2.79	1.46	1.41
24	A	1610	PAR	O54-C14	2.78	1.49	1.41
24	A	1618	PAR	O52-C52	2.78	1.51	1.43
24	A	1618	PAR	C42-C32	2.78	1.59	1.53
24	A	1616	PAR	O52-C52	2.77	1.50	1.43
24	A	1603	PAR	C62-C52	2.76	1.59	1.52
24	A	1601	PAR	C33-C43	2.72	1.60	1.52
24	A	1607	PAR	C13-C23	2.72	1.56	1.52
24	A	1609	PAR	C52-C42	2.71	1.57	1.52
24	A	1606	PAR	O52-C52	2.71	1.50	1.43
24	A	1610	PAR	O54-C54	2.70	1.51	1.44
24	A	1606	PAR	C13-C23	2.69	1.56	1.52
24	A	1609	PAR	C62-C52	2.69	1.59	1.52
24	A	1609	PAR	O33-C14	2.63	1.49	1.41
24	A	1615	PAR	C31-C21	2.63	1.56	1.53
24	A	1616	PAR	C11-C21	2.61	1.57	1.52
24	A	1617	PAR	O43-C13	2.61	1.46	1.41
24	A	1615	PAR	C23-C33	2.61	1.58	1.53
24	A	1613	PAR	O33-C14	2.61	1.49	1.41
24	A	1612	PAR	C11-C21	2.60	1.57	1.52
24	A	1605	PAR	C33-C43	2.59	1.59	1.52
24	A	1617	PAR	C42-C32	2.59	1.58	1.53
24	A	1605	PAR	O43-C13	2.59	1.46	1.41
24	A	1609	PAR	C41-C51	2.59	1.58	1.53
24	A	1612	PAR	C41-C51	2.58	1.58	1.53
24	A	1613	PAR	O52-C52	2.56	1.50	1.43
24	A	1615	PAR	C62-C12	2.55	1.58	1.53
24	A	1611	PAR	C14-C24	2.55	1.57	1.52
24	A	1604	PAR	C33-C43	2.55	1.59	1.52
24	A	1608	PAR	C11-C21	2.51	1.57	1.52
24	A	1614	PAR	C62-C52	2.51	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1604	PAR	C42-C32	2.50	1.58	1.53
24	A	1618	PAR	O52-C13	2.49	1.48	1.41
24	A	1614	PAR	C33-C43	2.49	1.59	1.52
24	A	1605	PAR	O54-C14	2.48	1.48	1.41
24	A	1618	PAR	C11-C21	2.47	1.57	1.52
24	A	1602	PAR	O33-C14	2.45	1.48	1.41
24	A	1614	PAR	O52-C52	2.44	1.50	1.43
24	A	1603	PAR	O43-C13	2.44	1.46	1.41
24	A	1605	PAR	C34-C24	2.43	1.56	1.53
24	A	1605	PAR	O33-C14	2.43	1.48	1.41
24	A	1610	PAR	C52-C42	2.42	1.57	1.52
24	A	1608	PAR	O43-C13	2.40	1.45	1.41
24	A	1602	PAR	O54-C14	2.39	1.48	1.41
24	A	1603	PAR	C11-C21	2.38	1.57	1.52
24	A	1616	PAR	O52-C13	2.37	1.48	1.41
24	A	1606	PAR	C33-C43	2.36	1.59	1.52
24	A	1608	PAR	C14-C24	2.36	1.57	1.52
24	A	1617	PAR	O11-C11	2.32	1.48	1.41
24	A	1617	PAR	C44-C54	2.32	1.58	1.53
24	A	1617	PAR	O33-C33	2.31	1.49	1.43
24	A	1608	PAR	C34-C24	2.31	1.56	1.53
24	A	1612	PAR	C34-C24	2.30	1.56	1.53
24	A	1606	PAR	C62-C52	2.28	1.58	1.52
24	A	1618	PAR	C44-C34	2.28	1.58	1.52
24	A	1608	PAR	C62-C52	2.27	1.58	1.52
24	A	1614	PAR	O33-C14	2.27	1.48	1.41
24	A	1601	PAR	C62-C52	2.26	1.58	1.52
24	A	1609	PAR	C31-C21	2.25	1.56	1.53
24	A	1616	PAR	O33-C14	2.21	1.48	1.41
24	A	1604	PAR	C62-C12	-2.21	1.49	1.53
24	A	1604	PAR	O43-C13	2.21	1.45	1.41
24	A	1613	PAR	O52-C13	2.20	1.47	1.41
24	A	1603	PAR	C14-C24	2.20	1.56	1.52
24	A	1610	PAR	C62-C52	2.19	1.58	1.52
24	A	1609	PAR	C24-N24	2.18	1.50	1.47
24	A	1614	PAR	C24-N24	2.18	1.50	1.47
24	A	1609	PAR	C22-C32	-2.17	1.49	1.53
24	A	1613	PAR	C33-C43	2.17	1.58	1.52
24	A	1617	PAR	C33-C43	2.16	1.58	1.52
24	A	1614	PAR	C42-C32	2.15	1.57	1.53
24	A	1605	PAR	C31-C21	2.14	1.56	1.53
24	A	1618	PAR	O11-C11	2.14	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1605	PAR	C13-C23	2.13	1.55	1.52
24	A	1607	PAR	O52-C52	2.12	1.49	1.43
24	A	1611	PAR	O33-C14	2.11	1.47	1.41
24	A	1604	PAR	C13-C23	2.11	1.55	1.52
24	A	1615	PAR	O11-C11	2.11	1.47	1.41
24	A	1610	PAR	O11-C11	2.11	1.47	1.41
24	A	1609	PAR	C33-C43	2.10	1.58	1.52
24	A	1609	PAR	C11-C21	2.10	1.56	1.52
24	A	1609	PAR	O52-C52	2.10	1.49	1.43
24	A	1612	PAR	C62-C52	2.08	1.57	1.52
24	A	1614	PAR	O54-C14	2.08	1.47	1.41
24	A	1607	PAR	C22-C32	-2.08	1.49	1.53
24	A	1610	PAR	C24-N24	2.08	1.50	1.47
24	A	1613	PAR	C62-C12	2.06	1.57	1.53
24	A	1607	PAR	O33-C14	2.06	1.47	1.41
24	A	1617	PAR	C23-C33	2.05	1.57	1.53
24	A	1605	PAR	C23-C33	2.05	1.57	1.53
24	A	1602	PAR	C11-C21	2.05	1.56	1.52
24	A	1602	PAR	C44-C34	-2.05	1.47	1.52
24	A	1618	PAR	O33-C33	2.04	1.49	1.43
24	A	1603	PAR	C41-C51	2.04	1.57	1.53
24	A	1615	PAR	C41-C51	2.04	1.57	1.53
24	A	1617	PAR	O52-C13	2.04	1.47	1.41
24	A	1615	PAR	C42-C32	2.04	1.57	1.53
24	A	1618	PAR	O54-C14	2.02	1.47	1.41
24	A	1610	PAR	C13-C23	2.01	1.55	1.52

All (212) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1602	PAR	O33-C14-C24	8.58	122.12	108.08
24	A	1610	PAR	O33-C14-C24	7.92	121.04	108.08
24	A	1609	PAR	O33-C14-C24	7.26	119.96	108.08
24	A	1607	PAR	O33-C14-C24	7.22	119.90	108.08
24	A	1618	PAR	O33-C14-C24	7.11	119.72	108.08
24	A	1612	PAR	O33-C14-C24	7.04	119.60	108.08
24	A	1616	PAR	O33-C14-C24	6.91	119.39	108.08
24	A	1611	PAR	O33-C14-C24	6.89	119.36	108.08
24	A	1613	PAR	O33-C14-C24	6.86	119.31	108.08
24	A	1617	PAR	O33-C14-C24	6.77	119.16	108.08
24	A	1606	PAR	O33-C14-C24	6.73	119.09	108.08
24	A	1608	PAR	O33-C14-C24	6.64	118.94	108.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1614	PAR	O33-C14-C24	6.41	118.56	108.08
24	A	1615	PAR	O33-C14-C24	6.30	118.39	108.08
24	A	1605	PAR	O33-C14-C24	6.21	118.24	108.08
24	A	1604	PAR	O33-C14-C24	5.89	117.72	108.08
24	A	1603	PAR	O33-C14-C24	5.85	117.65	108.08
24	A	1601	PAR	O33-C14-C24	5.71	117.42	108.08
24	A	1617	PAR	C13-C23-C33	4.13	107.07	102.10
24	A	1616	PAR	C13-C23-C33	3.88	106.76	102.10
24	A	1602	PAR	C34-C24-N24	-3.80	103.27	111.05
24	A	1615	PAR	C13-C23-C33	3.78	106.65	102.10
24	A	1612	PAR	O11-C11-O51	3.72	120.49	110.69
24	A	1615	PAR	O11-C11-O51	3.65	120.30	110.69
24	A	1608	PAR	C14-O33-C33	-3.65	109.33	117.98
24	A	1609	PAR	C11-O51-C51	3.58	120.71	113.72
24	A	1618	PAR	O11-C11-O51	3.57	120.10	110.69
24	A	1607	PAR	C14-O33-C33	-3.53	109.60	117.98
24	A	1617	PAR	O11-C11-O51	3.52	119.95	110.69
24	A	1602	PAR	O52-C13-O43	-3.48	107.81	111.37
24	A	1608	PAR	C22-C12-C62	3.46	115.26	110.08
24	A	1613	PAR	C13-C23-C33	3.44	106.25	102.10
24	A	1603	PAR	C34-C24-N24	-3.44	104.00	111.05
24	A	1610	PAR	C34-C24-N24	-3.44	104.01	111.05
24	A	1604	PAR	C13-C23-C33	3.41	106.20	102.10
24	A	1611	PAR	C14-O33-C33	-3.41	109.91	117.98
24	A	1618	PAR	C14-O33-C33	-3.36	110.00	117.98
24	A	1615	PAR	C14-O33-C33	-3.31	110.14	117.98
24	A	1605	PAR	C13-C23-C33	3.27	106.03	102.10
24	A	1612	PAR	C34-C24-N24	-3.25	104.39	111.05
24	A	1611	PAR	O52-C13-O43	-3.25	108.05	111.37
24	A	1607	PAR	O34-C34-C44	-3.23	102.76	110.38
24	A	1606	PAR	O11-C11-O51	3.21	119.13	110.69
24	A	1612	PAR	C14-O33-C33	-3.20	110.40	117.98
24	A	1602	PAR	O34-C34-C44	-3.19	102.86	110.38
24	A	1613	PAR	O34-C34-C44	-3.18	102.88	110.38
24	A	1605	PAR	C34-C24-N24	-3.15	104.60	111.05
24	A	1614	PAR	O11-C11-O51	3.15	118.97	110.69
24	A	1606	PAR	C14-O33-C33	-3.15	110.52	117.98
24	A	1615	PAR	C22-C12-C62	3.14	114.79	110.08
24	A	1606	PAR	C34-C24-N24	-3.14	104.62	111.05
24	A	1610	PAR	O52-C13-O43	-3.13	108.17	111.37
24	A	1610	PAR	O34-C34-C44	-3.13	103.00	110.38
24	A	1612	PAR	C13-C23-C33	3.12	105.86	102.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1608	PAR	C13-C23-C33	3.11	105.85	102.10
24	A	1603	PAR	O11-C11-O51	3.11	118.87	110.69
24	A	1608	PAR	C34-C24-N24	-3.11	104.69	111.05
24	A	1601	PAR	C34-C24-N24	-3.10	104.69	111.05
24	A	1609	PAR	C34-C24-N24	-3.10	104.70	111.05
24	A	1604	PAR	O11-C11-O51	3.09	118.83	110.69
24	A	1609	PAR	O52-C13-O43	-3.08	108.22	111.37
24	A	1604	PAR	C13-O52-C52	-3.01	110.84	117.98
24	A	1603	PAR	C13-O52-C52	-3.00	110.88	117.98
24	A	1611	PAR	O11-C11-O51	2.99	118.56	110.69
24	A	1609	PAR	C22-C12-C62	2.95	114.50	110.08
24	A	1616	PAR	C14-O33-C33	-2.93	111.04	117.98
24	A	1604	PAR	C14-O33-C33	-2.92	111.05	117.98
24	A	1610	PAR	O11-C11-O51	2.92	118.37	110.69
24	A	1615	PAR	C34-C24-N24	-2.91	105.09	111.05
24	A	1601	PAR	C13-O52-C52	-2.91	111.09	117.98
24	A	1617	PAR	C34-C24-N24	-2.90	105.12	111.05
24	A	1613	PAR	O52-C13-O43	-2.89	108.42	111.37
24	A	1608	PAR	O11-C11-O51	2.89	118.29	110.69
24	A	1614	PAR	O34-C34-C44	-2.88	103.59	110.38
24	A	1609	PAR	C14-O33-C33	-2.87	111.18	117.98
24	A	1604	PAR	C22-C32-C42	2.86	116.52	109.50
24	A	1616	PAR	O11-C11-O51	2.86	118.22	110.69
24	A	1603	PAR	C22-C12-C62	2.82	114.30	110.08
24	A	1616	PAR	C34-C24-N24	-2.80	105.31	111.05
24	A	1611	PAR	C11-O51-C51	2.80	119.19	113.72
24	A	1615	PAR	O52-C52-C42	2.79	114.52	107.42
24	A	1617	PAR	O54-C54-C44	2.78	114.71	109.70
24	A	1615	PAR	O34-C34-C44	-2.78	103.83	110.38
24	A	1611	PAR	C34-C24-N24	-2.77	105.38	111.05
24	A	1614	PAR	C13-C23-C33	2.76	105.42	102.10
24	A	1607	PAR	O11-C11-O51	2.76	117.96	110.69
24	A	1614	PAR	C34-C24-N24	-2.75	105.42	111.05
24	A	1607	PAR	C52-C62-C12	2.74	116.54	109.93
24	A	1613	PAR	C14-O33-C33	-2.73	111.52	117.98
24	A	1607	PAR	C22-C12-C62	2.72	114.15	110.08
24	A	1604	PAR	C34-C24-N24	-2.72	105.49	111.05
24	A	1617	PAR	C14-O33-C33	-2.70	111.57	117.98
24	A	1616	PAR	O34-C34-C44	-2.70	104.01	110.38
24	A	1603	PAR	O34-C34-C44	-2.70	104.02	110.38
24	A	1612	PAR	O52-C13-O43	-2.70	108.61	111.37
24	A	1605	PAR	O34-C34-C44	-2.69	104.03	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1607	PAR	C34-C24-N24	-2.68	105.55	111.05
24	A	1617	PAR	O34-C34-C44	-2.68	104.05	110.38
24	A	1614	PAR	O43-C13-C23	-2.68	101.57	104.98
24	A	1601	PAR	O43-C13-C23	-2.67	101.58	104.98
24	A	1601	PAR	O34-C34-C44	-2.66	104.10	110.38
24	A	1613	PAR	O11-C11-O51	2.66	117.68	110.69
24	A	1605	PAR	C14-O33-C33	-2.62	111.77	117.98
24	A	1608	PAR	O34-C34-C44	-2.61	104.22	110.38
24	A	1618	PAR	C34-C24-N24	-2.61	105.70	111.05
24	A	1605	PAR	C13-O52-C52	-2.60	111.82	117.98
24	A	1606	PAR	C22-C12-C62	2.59	113.95	110.08
24	A	1610	PAR	C14-O33-C33	-2.58	111.86	117.98
24	A	1609	PAR	O11-C11-O51	2.58	117.48	110.69
24	A	1601	PAR	C14-O33-C33	-2.57	111.88	117.98
24	A	1618	PAR	O51-C51-C61	2.57	112.81	106.44
24	A	1602	PAR	O54-C54-C44	2.57	114.33	109.70
24	A	1609	PAR	O51-C51-C61	2.57	112.80	106.44
24	A	1612	PAR	C13-O52-C52	-2.56	111.91	117.98
24	A	1611	PAR	O34-C34-C44	-2.56	104.34	110.38
24	A	1604	PAR	O34-C34-C44	-2.55	104.37	110.38
24	A	1602	PAR	O51-C51-C61	2.54	112.73	106.44
24	A	1618	PAR	O34-C34-C44	-2.54	104.40	110.38
24	A	1618	PAR	C44-C34-C24	2.53	115.20	110.99
24	A	1608	PAR	C13-O52-C52	-2.52	112.00	117.98
24	A	1613	PAR	C22-C12-C62	2.52	113.84	110.08
24	A	1606	PAR	O34-C34-C44	-2.51	104.45	110.38
24	A	1605	PAR	O11-C11-O51	2.51	117.30	110.69
24	A	1613	PAR	C34-C24-N24	-2.51	105.91	111.05
24	A	1614	PAR	C14-O33-C33	-2.51	112.04	117.98
24	A	1601	PAR	O11-C11-O51	2.50	117.28	110.69
24	A	1604	PAR	C11-O51-C51	2.50	118.59	113.72
24	A	1614	PAR	C22-C12-C62	2.49	113.81	110.08
24	A	1609	PAR	O51-C51-C41	2.48	114.17	109.70
24	A	1607	PAR	C13-O52-C52	-2.46	112.15	117.98
24	A	1606	PAR	C11-O51-C51	2.46	118.52	113.72
24	A	1615	PAR	O11-C42-C52	2.45	113.65	107.42
24	A	1612	PAR	O34-C34-C44	-2.45	104.59	110.38
24	A	1610	PAR	C22-C12-C62	2.44	113.73	110.08
24	A	1603	PAR	O51-C51-C61	2.44	112.49	106.44
24	A	1602	PAR	O11-C11-O51	2.43	117.09	110.69
24	A	1616	PAR	C13-O52-C52	-2.42	112.23	117.98
24	A	1615	PAR	O54-C54-C44	2.42	114.05	109.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1617	PAR	C13-O52-C52	-2.42	112.25	117.98
24	A	1615	PAR	C32-C22-C12	2.41	115.16	111.02
24	A	1602	PAR	C22-C12-C62	2.41	113.69	110.08
24	A	1608	PAR	O52-C13-O43	-2.41	108.91	111.37
24	A	1616	PAR	C22-C12-C62	2.40	113.67	110.08
24	A	1609	PAR	O34-C34-C44	-2.40	104.73	110.38
24	A	1616	PAR	O52-C52-C42	2.39	113.48	107.42
24	A	1607	PAR	O52-C13-O43	-2.39	108.93	111.37
24	A	1603	PAR	C14-O33-C33	-2.37	112.36	117.98
24	A	1603	PAR	C11-O51-C51	2.37	118.34	113.72
24	A	1611	PAR	C22-C32-C42	2.36	115.28	109.50
24	A	1610	PAR	O54-C54-C44	2.35	113.94	109.70
24	A	1601	PAR	O51-C51-C61	2.35	112.27	106.44
24	A	1604	PAR	O51-C51-C61	2.33	112.22	106.44
24	A	1616	PAR	O51-C51-C61	2.33	112.20	106.44
24	A	1602	PAR	C14-O33-C33	-2.32	112.47	117.98
24	A	1615	PAR	O52-C13-O43	-2.32	109.00	111.37
24	A	1612	PAR	O51-C51-C61	2.32	112.18	106.44
24	A	1614	PAR	O51-C51-C61	2.32	112.18	106.44
24	A	1618	PAR	O52-C52-C42	2.31	113.29	107.42
24	A	1607	PAR	C13-C23-C33	2.31	104.88	102.10
24	A	1610	PAR	O34-C34-C24	-2.30	106.09	110.22
24	A	1607	PAR	O34-C34-C24	-2.29	106.10	110.22
24	A	1609	PAR	O54-C54-C44	2.29	113.83	109.70
24	A	1607	PAR	O54-C54-C44	2.26	113.78	109.70
24	A	1610	PAR	C13-O52-C52	-2.26	112.63	117.98
24	A	1608	PAR	C11-O51-C51	2.26	118.12	113.72
24	A	1610	PAR	C31-C41-C51	2.25	114.32	110.23
24	A	1608	PAR	O51-C51-C61	2.24	112.00	106.44
24	A	1605	PAR	O51-C51-C61	2.24	111.98	106.44
24	A	1611	PAR	O51-C51-C61	2.24	111.98	106.44
24	A	1618	PAR	O52-C13-O43	-2.23	109.09	111.37
24	A	1615	PAR	O51-C51-C61	2.22	111.94	106.44
24	A	1606	PAR	C13-O52-C52	-2.22	112.72	117.98
24	A	1617	PAR	C44-C34-C24	2.22	114.67	110.99
24	A	1618	PAR	C22-C12-C62	2.20	113.38	110.08
24	A	1611	PAR	O54-C54-C44	2.19	113.65	109.70
24	A	1601	PAR	O33-C14-O54	-2.19	104.93	110.69
24	A	1605	PAR	O54-C54-C44	2.19	113.65	109.70
24	A	1606	PAR	O54-C54-C44	2.19	113.64	109.70
24	A	1613	PAR	C13-O52-C52	-2.18	112.82	117.98
24	A	1609	PAR	C13-O52-C52	-2.18	112.82	117.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1608	PAR	O33-C14-O54	-2.16	105.01	110.69
24	A	1614	PAR	O43-C43-C53	2.16	113.79	109.22
24	A	1601	PAR	O52-C13-O43	-2.16	109.16	111.37
24	A	1617	PAR	O52-C52-C42	2.15	112.88	107.42
24	A	1606	PAR	O43-C13-C23	-2.15	102.25	104.98
24	A	1607	PAR	O51-C51-C61	2.14	111.75	106.44
24	A	1618	PAR	O54-C54-C44	2.14	113.56	109.70
24	A	1604	PAR	O52-C13-O43	-2.12	109.20	111.37
24	A	1603	PAR	O43-C13-C23	-2.12	102.28	104.98
24	A	1617	PAR	O51-C51-C61	2.12	111.68	106.44
24	A	1612	PAR	O33-C14-O54	-2.11	105.14	110.69
24	A	1616	PAR	C11-O51-C51	2.10	117.83	113.72
24	A	1606	PAR	O51-C51-C61	2.10	111.65	106.44
24	A	1606	PAR	O33-C14-O54	-2.10	105.17	110.69
24	A	1613	PAR	O52-C52-C42	2.09	112.74	107.42
24	A	1603	PAR	O34-C34-C24	-2.09	106.46	110.22
24	A	1616	PAR	O54-C54-C44	2.09	113.47	109.70
24	A	1618	PAR	C23-C33-C43	-2.09	99.58	103.24
24	A	1605	PAR	O52-C13-O43	-2.09	109.24	111.37
24	A	1613	PAR	O51-C51-C61	2.08	111.59	106.44
24	A	1611	PAR	C23-C33-C43	-2.07	99.61	103.24
24	A	1610	PAR	O51-C51-C61	2.07	111.57	106.44
24	A	1601	PAR	O34-C34-C24	-2.07	106.50	110.22
24	A	1603	PAR	O51-C51-C41	2.05	113.40	109.70
24	A	1615	PAR	O34-C34-C24	-2.05	106.54	110.22
24	A	1604	PAR	O33-C14-O54	-2.04	105.32	110.69
24	A	1614	PAR	O54-C54-C44	2.04	113.37	109.70
24	A	1610	PAR	O51-C51-C41	2.03	113.36	109.70
24	A	1611	PAR	C44-C34-C24	2.03	114.36	110.99
24	A	1602	PAR	C13-O52-C52	-2.03	113.17	117.98
24	A	1608	PAR	C32-C22-C12	2.01	114.47	111.02
24	A	1611	PAR	C32-C22-C12	2.01	114.46	111.02

There are no chirality outliers.

All (141) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	1601	PAR	C44-C54-C64-N64
24	A	1601	PAR	O54-C54-C64-N64
24	A	1602	PAR	C23-C13-O52-C52
24	A	1602	PAR	O43-C13-O52-C52
24	A	1602	PAR	C24-C14-O33-C33

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Mol	Chain	Res	Type	Atoms
24	A	1604	PAR	C23-C13-O52-C52
24	A	1604	PAR	C44-C54-C64-N64
24	A	1604	PAR	O54-C54-C64-N64
24	A	1605	PAR	C44-C54-C64-N64
24	A	1606	PAR	O54-C54-C64-N64
24	A	1607	PAR	C24-C14-O33-C33
24	A	1607	PAR	O43-C43-C53-O53
24	A	1607	PAR	C44-C54-C64-N64
24	A	1607	PAR	O54-C54-C64-N64
24	A	1608	PAR	C24-C14-O33-C33
24	A	1609	PAR	C21-C11-O11-C42
24	A	1609	PAR	C23-C13-O52-C52
24	A	1609	PAR	O43-C13-O52-C52
24	A	1609	PAR	C24-C14-O33-C33
24	A	1610	PAR	C23-C13-O52-C52
24	A	1610	PAR	O43-C13-O52-C52
24	A	1610	PAR	C24-C14-O33-C33
24	A	1611	PAR	C44-C54-C64-N64
24	A	1611	PAR	O54-C54-C64-N64
24	A	1612	PAR	C21-C11-O11-C42
24	A	1612	PAR	C23-C13-O52-C52
24	A	1613	PAR	C21-C11-O11-C42
24	A	1613	PAR	C23-C13-O52-C52
24	A	1613	PAR	C24-C14-O33-C33
24	A	1614	PAR	C44-C54-C64-N64
24	A	1614	PAR	O54-C54-C64-N64
24	A	1615	PAR	C23-C13-O52-C52
24	A	1615	PAR	O43-C13-O52-C52
24	A	1615	PAR	C24-C14-O33-C33
24	A	1615	PAR	O54-C54-C64-N64
24	A	1616	PAR	C21-C11-O11-C42
24	A	1616	PAR	C32-C42-O11-C11
24	A	1616	PAR	C23-C13-O52-C52
24	A	1616	PAR	O43-C13-O52-C52
24	A	1616	PAR	C24-C14-O33-C33
24	A	1617	PAR	O51-C11-O11-C42
24	A	1617	PAR	C23-C13-O52-C52
24	A	1617	PAR	O43-C13-O52-C52
24	A	1617	PAR	C24-C14-O33-C33
24	A	1618	PAR	C21-C11-O11-C42
24	A	1618	PAR	C24-C14-O33-C33
24	A	1602	PAR	O54-C14-O33-C33

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Mol	Chain	Res	Type	Atoms
24	A	1605	PAR	O54-C14-O33-C33
24	A	1610	PAR	O54-C14-O33-C33
24	A	1613	PAR	O54-C14-O33-C33
24	A	1615	PAR	O54-C14-O33-C33
24	A	1604	PAR	O51-C11-O11-C42
24	A	1616	PAR	O54-C14-O33-C33
24	A	1618	PAR	O51-C11-O11-C42
24	A	1612	PAR	O54-C14-O33-C33
24	A	1613	PAR	O51-C11-O11-C42
24	A	1618	PAR	O54-C14-O33-C33
24	A	1608	PAR	O43-C43-C53-O53
24	A	1607	PAR	C33-C43-C53-O53
24	A	1608	PAR	C33-C43-C53-O53
24	A	1614	PAR	C52-C42-O11-C11
24	A	1616	PAR	C41-C51-C61-O61
24	A	1603	PAR	C33-C43-C53-O53
24	A	1610	PAR	O51-C51-C61-O61
24	A	1603	PAR	O43-C43-C53-O53
24	A	1611	PAR	O43-C43-C53-O53
24	A	1611	PAR	C33-C43-C53-O53
24	A	1607	PAR	O51-C51-C61-O61
24	A	1613	PAR	O43-C43-C53-O53
24	A	1618	PAR	O43-C43-C53-O53
24	A	1616	PAR	O51-C51-C61-O61
24	A	1602	PAR	O43-C43-C53-O53
24	A	1614	PAR	O51-C11-O11-C42
24	A	1614	PAR	O51-C51-C61-O61
24	A	1602	PAR	C33-C43-C53-O53
24	A	1613	PAR	C33-C43-C53-O53
24	A	1618	PAR	C33-C43-C53-O53
24	A	1604	PAR	C33-C43-C53-O53
24	A	1607	PAR	O54-C14-O33-C33
24	A	1609	PAR	C42-C52-O52-C13
24	A	1609	PAR	C62-C52-O52-C13
24	A	1609	PAR	O54-C14-O33-C33
24	A	1604	PAR	O43-C13-O52-C52
24	A	1612	PAR	O43-C13-O52-C52
24	A	1615	PAR	C52-C42-O11-C11
24	A	1618	PAR	O51-C51-C61-O61
24	A	1612	PAR	O51-C51-C61-O61
24	A	1603	PAR	C52-C42-O11-C11
24	A	1604	PAR	C52-C42-O11-C11

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Mol	Chain	Res	Type	Atoms
24	A	1617	PAR	C21-C11-O11-C42
24	A	1616	PAR	O43-C43-C53-O53
24	A	1617	PAR	C41-C51-C61-O61
24	A	1610	PAR	C41-C51-C61-O61
24	A	1611	PAR	O43-C13-O52-C52
24	A	1601	PAR	C52-C42-O11-C11
24	A	1614	PAR	C62-C52-O52-C13
24	A	1614	PAR	C32-C42-O11-C11
24	A	1616	PAR	C52-C42-O11-C11
24	A	1617	PAR	C62-C52-O52-C13
24	A	1602	PAR	O54-C54-C64-N64
24	A	1608	PAR	O54-C54-C64-N64
24	A	1610	PAR	O54-C54-C64-N64
24	A	1612	PAR	O54-C54-C64-N64
24	A	1613	PAR	O54-C54-C64-N64
24	A	1618	PAR	O54-C54-C64-N64
24	A	1611	PAR	O54-C14-O33-C33
24	A	1614	PAR	C41-C51-C61-O61
24	A	1616	PAR	O51-C11-O11-C42
24	A	1610	PAR	C21-C11-O11-C42
24	A	1616	PAR	C44-C54-C64-N64
24	A	1601	PAR	O43-C13-O52-C52
24	A	1608	PAR	O43-C13-O52-C52
24	A	1615	PAR	O51-C11-O11-C42
24	A	1602	PAR	C23-C33-O33-C14
24	A	1615	PAR	C43-C33-O33-C14
24	A	1616	PAR	C23-C33-O33-C14
24	A	1618	PAR	C43-C33-O33-C14
24	A	1602	PAR	C62-C52-O52-C13
24	A	1611	PAR	O51-C11-O11-C42
24	A	1614	PAR	C42-C52-O52-C13
24	A	1607	PAR	C41-C51-C61-O61
24	A	1606	PAR	C52-C42-O11-C11
24	A	1614	PAR	O43-C13-O52-C52
24	A	1608	PAR	C23-C13-O52-C52
24	A	1611	PAR	C23-C13-O52-C52
24	A	1602	PAR	C42-C52-O52-C13
24	A	1603	PAR	O54-C14-O33-C33
24	A	1617	PAR	C42-C52-O52-C13
24	A	1603	PAR	C62-C52-O52-C13
24	A	1616	PAR	C33-C43-C53-O53
24	A	1604	PAR	C23-C33-O33-C14

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Mol	Chain	Res	Type	Atoms
24	A	1605	PAR	C43-C33-O33-C14
24	A	1607	PAR	C23-C33-O33-C14
24	A	1608	PAR	C43-C33-O33-C14
24	A	1609	PAR	C23-C33-O33-C14
24	A	1610	PAR	C23-C33-O33-C14
24	A	1611	PAR	C43-C33-O33-C14
24	A	1612	PAR	C23-C33-O33-C14
24	A	1613	PAR	C23-C33-O33-C14
24	A	1614	PAR	C23-C33-O33-C14
24	A	1617	PAR	O54-C14-O33-C33

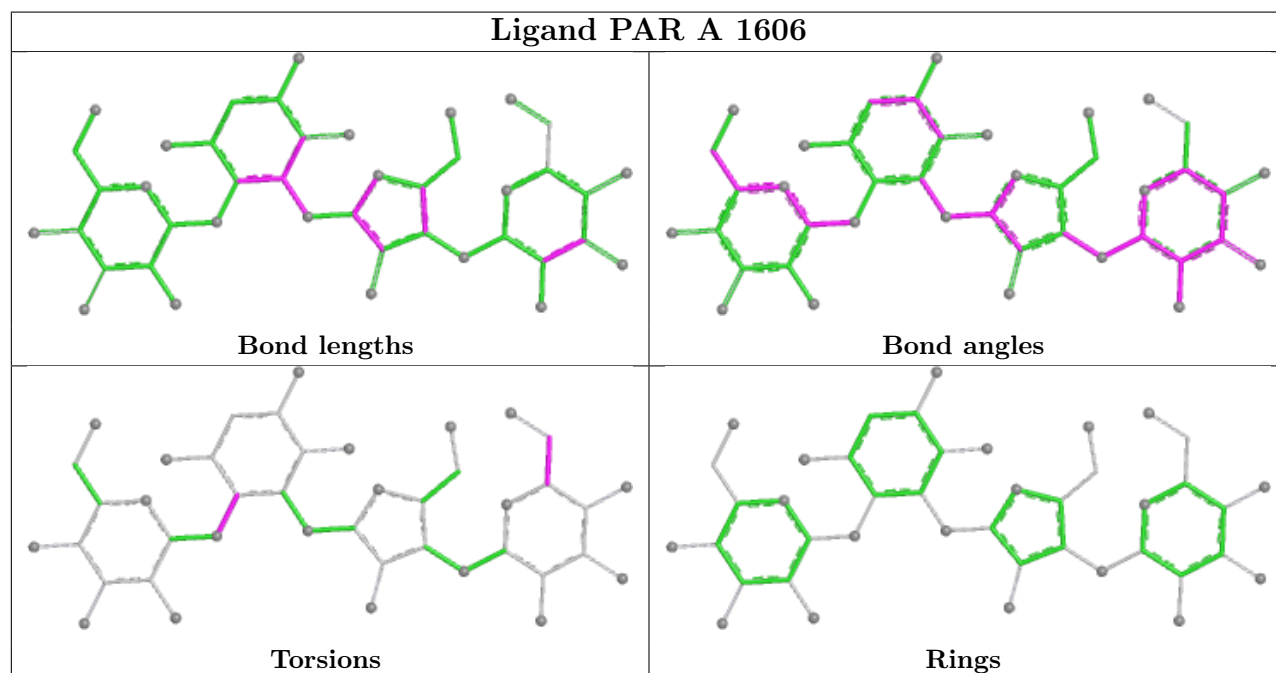
All (6) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	1616	PAR	C12-C22-C32-C42-C52-C62
24	A	1602	PAR	C14-C24-C34-C44-C54-O54
24	A	1618	PAR	C12-C22-C32-C42-C52-C62
24	A	1614	PAR	C12-C22-C32-C42-C52-C62
24	A	1610	PAR	C14-C24-C34-C44-C54-O54
24	A	1612	PAR	C12-C22-C32-C42-C52-C62

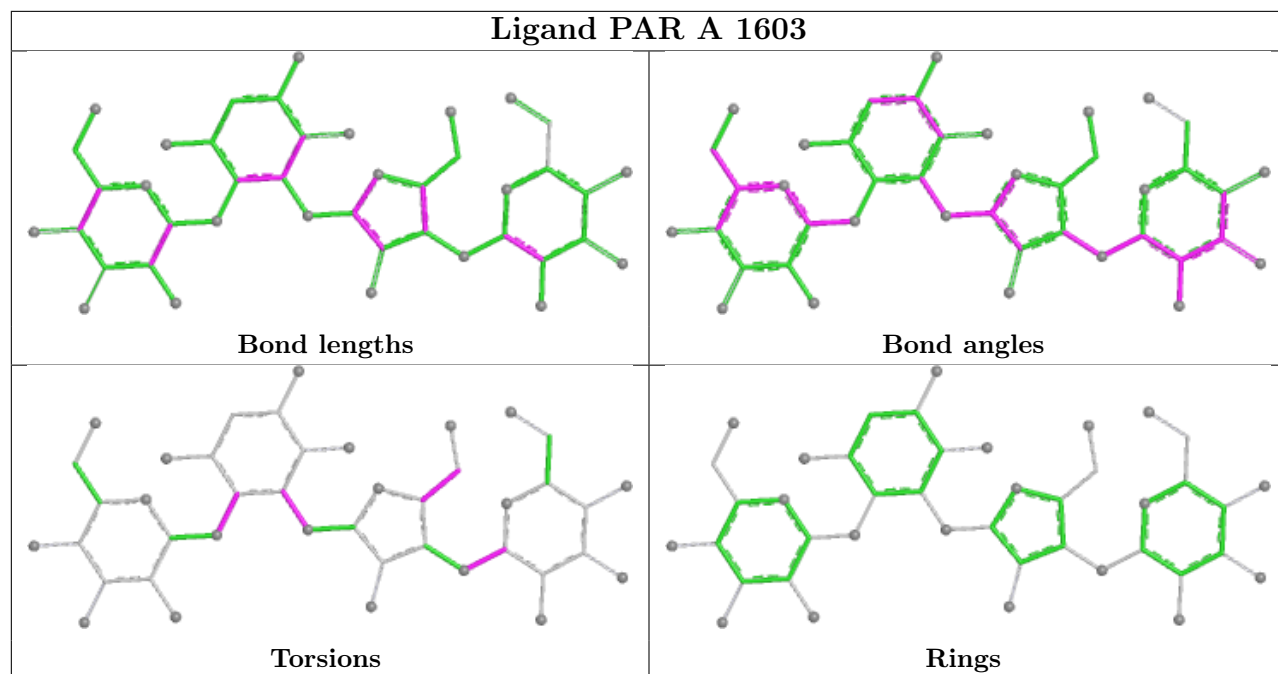
17 monomers are involved in 62 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A	1606	PAR	1	0
24	A	1603	PAR	7	0
24	A	1616	PAR	5	0
24	A	1608	PAR	5	0
24	A	1615	PAR	3	0
24	A	1618	PAR	2	0
24	A	1611	PAR	5	0
24	A	1613	PAR	7	0
24	A	1614	PAR	2	0
24	A	1610	PAR	6	0
24	A	1617	PAR	1	0
24	A	1604	PAR	3	0
24	A	1602	PAR	4	0
24	A	1609	PAR	1	0
24	A	1605	PAR	4	0
24	A	1601	PAR	2	0
24	A	1612	PAR	4	0

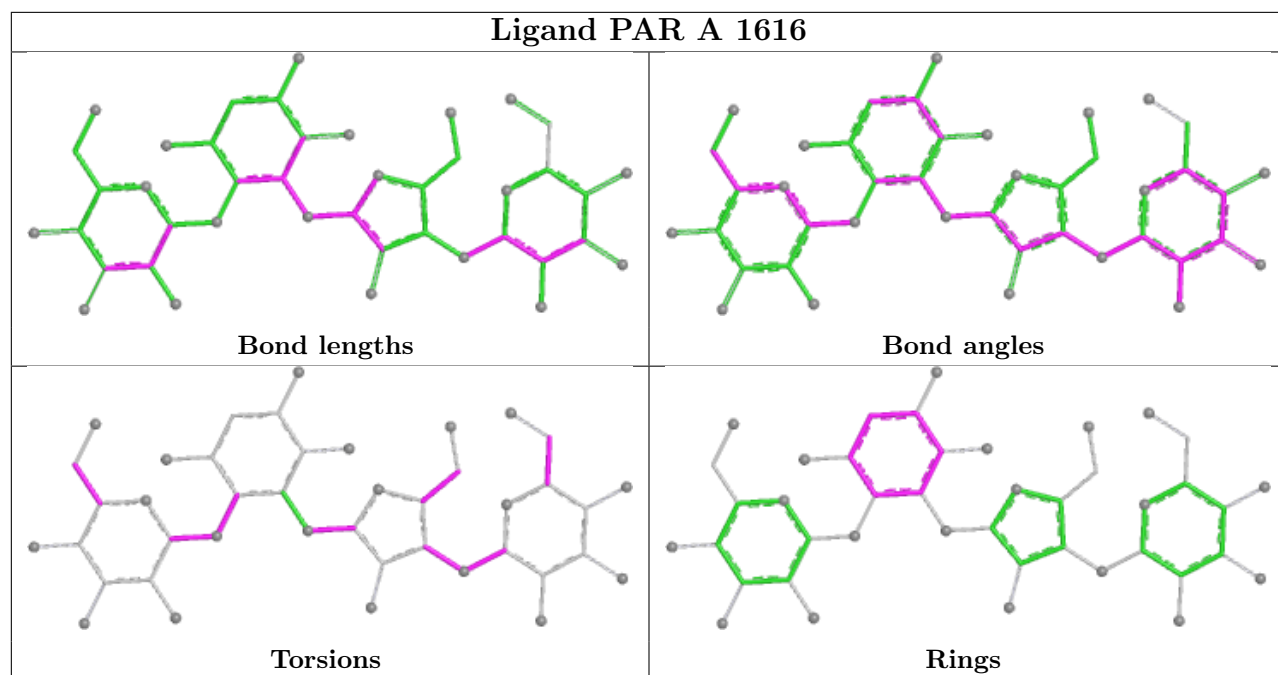
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



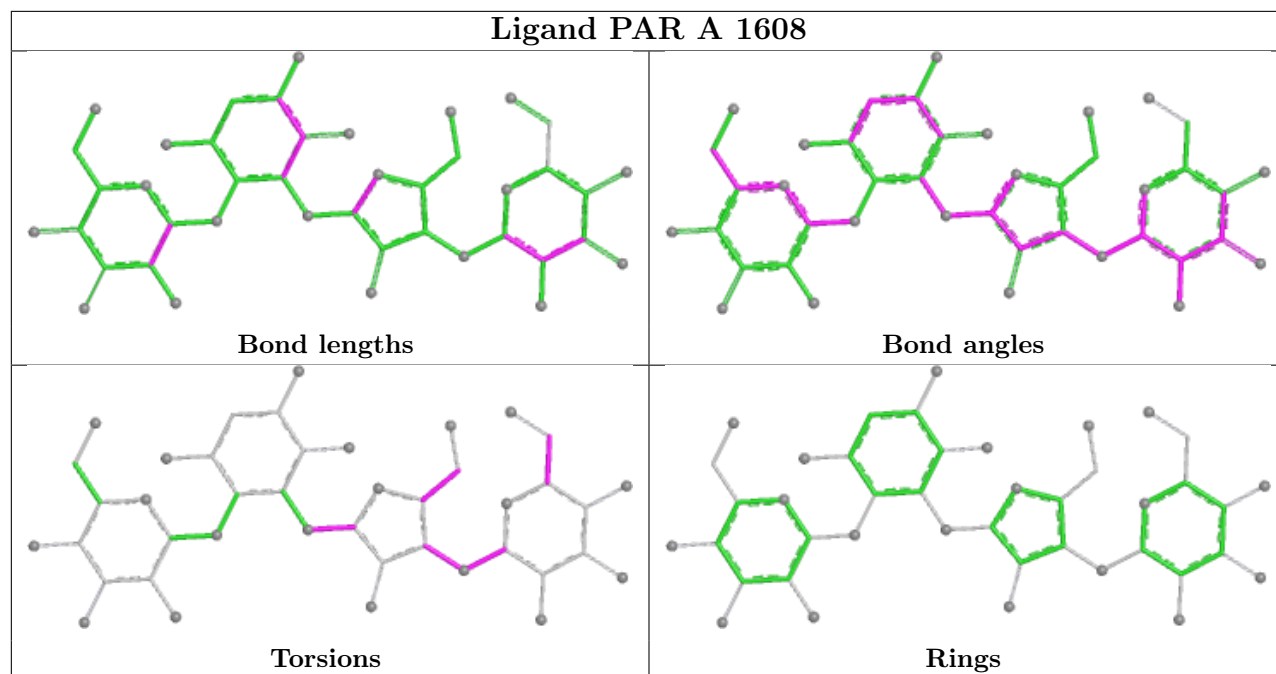
Ligand PAR A 1603



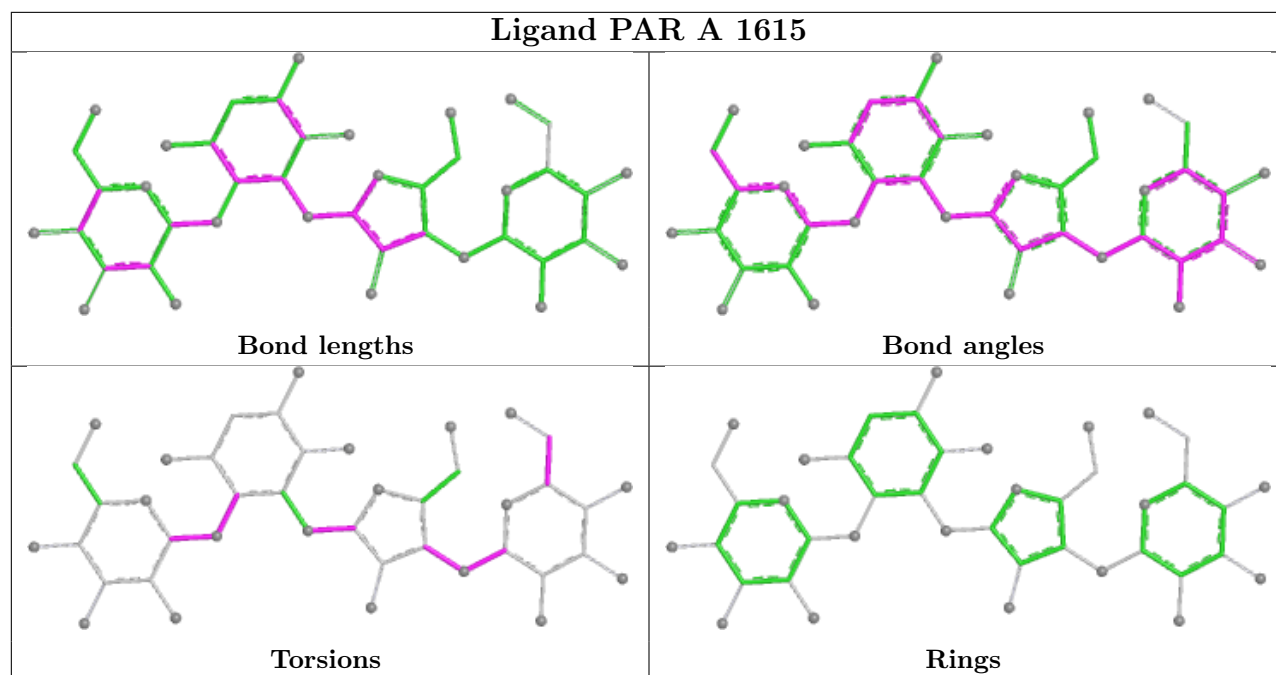
Ligand PAR A 1616



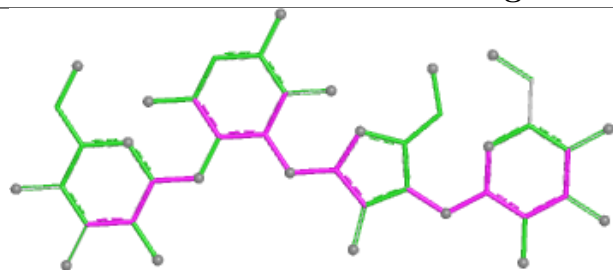
Ligand PAR A 1608



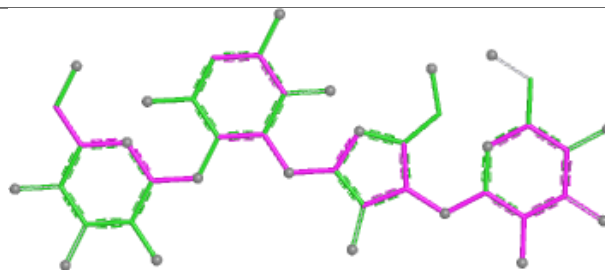
Ligand PAR A 1615



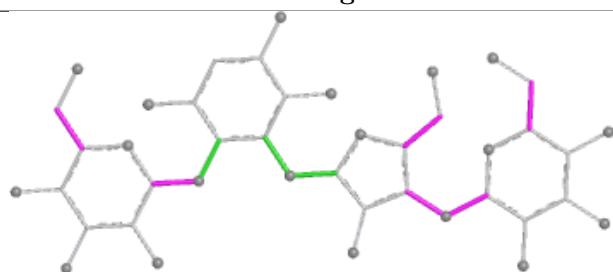
Ligand PAR A 1618



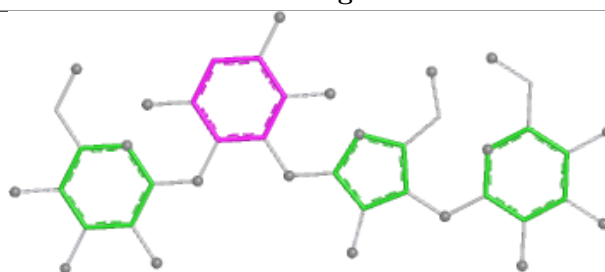
Bond lengths



Bond angles

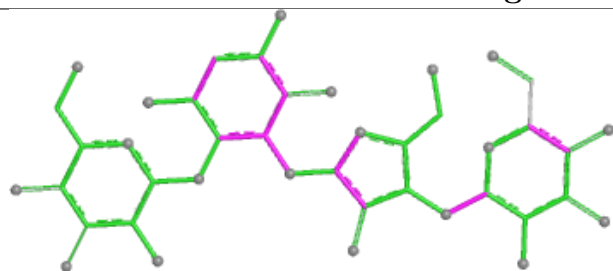


Torsions

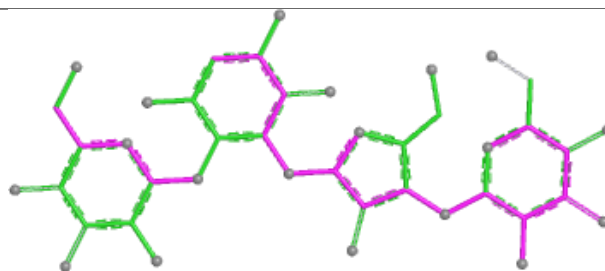


Rings

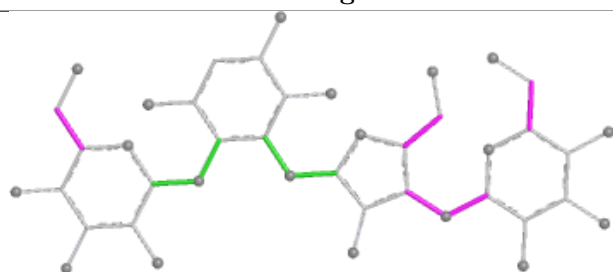
Ligand PAR A 1607



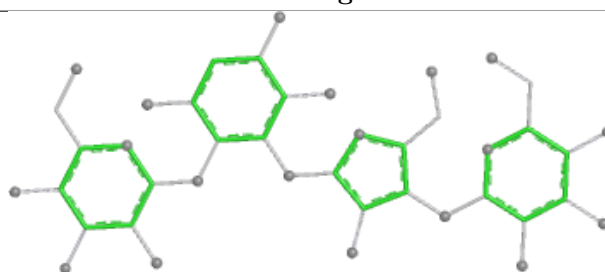
Bond lengths



Bond angles

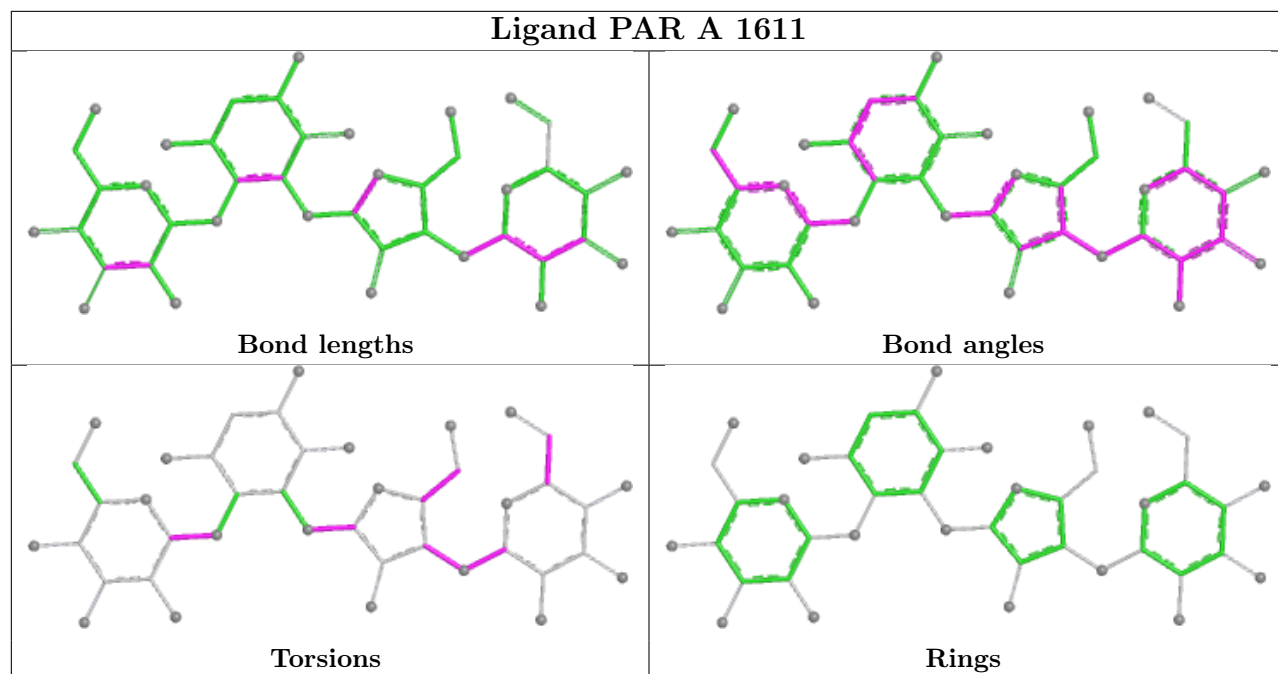


Torsions

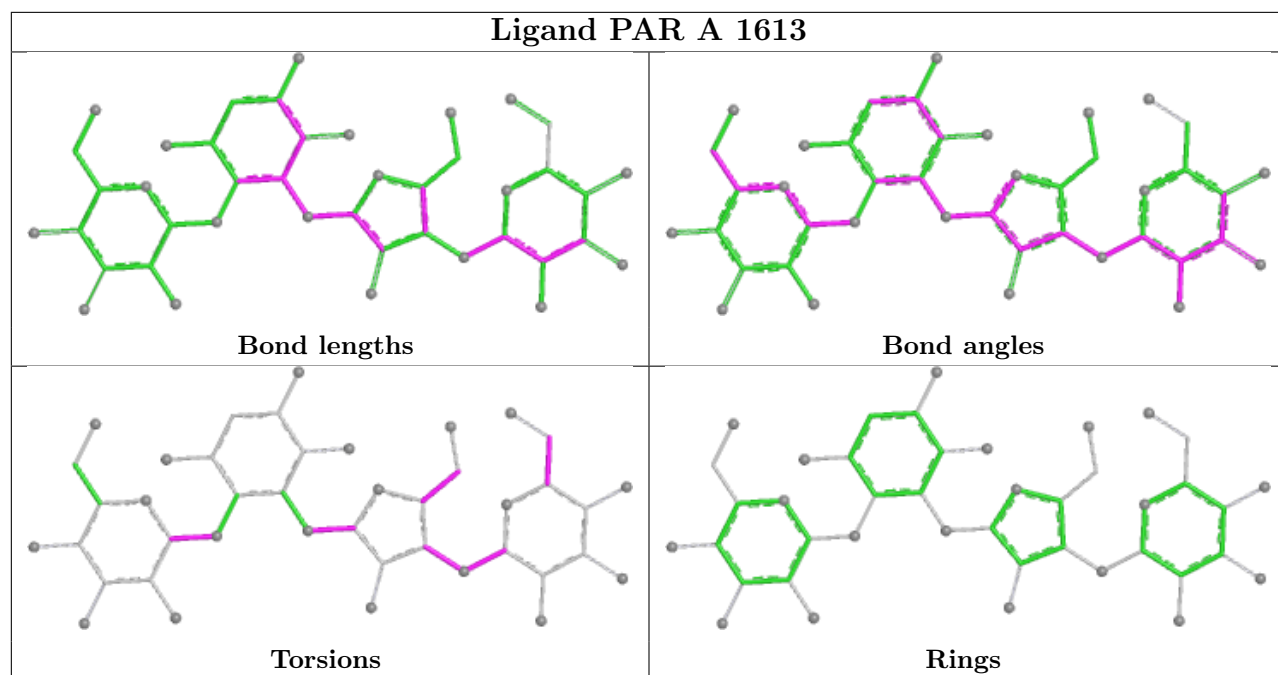


Rings

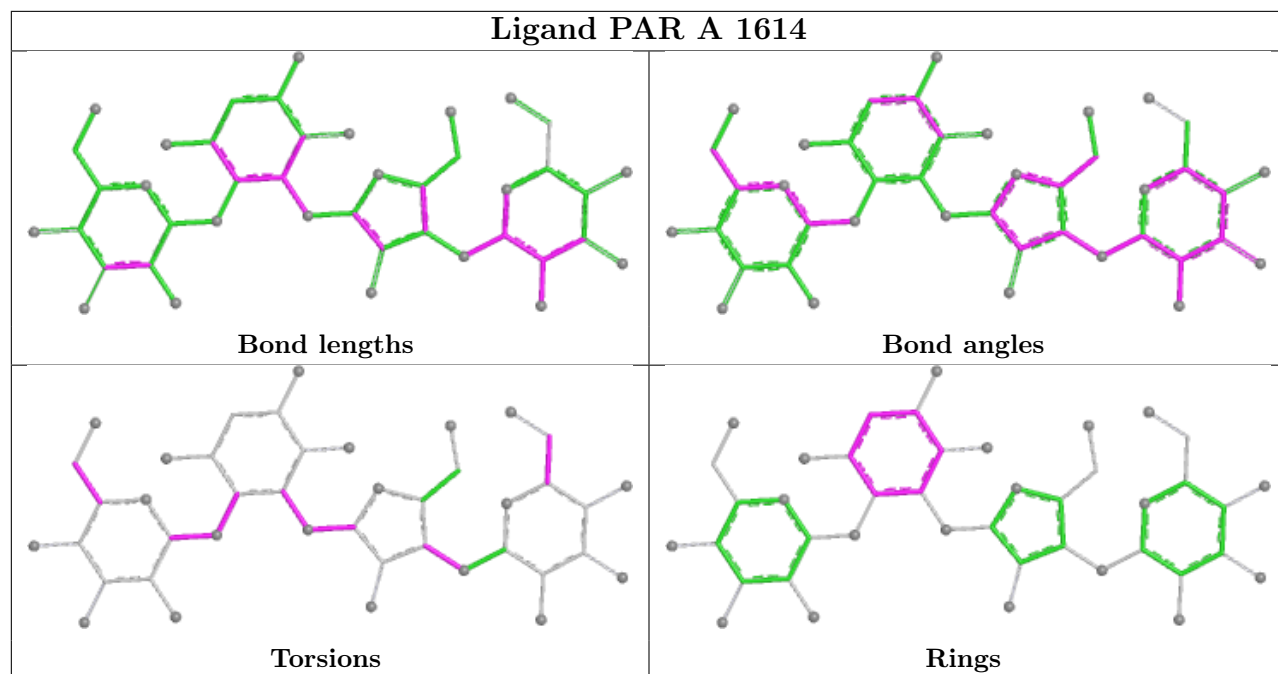
Ligand PAR A 1611



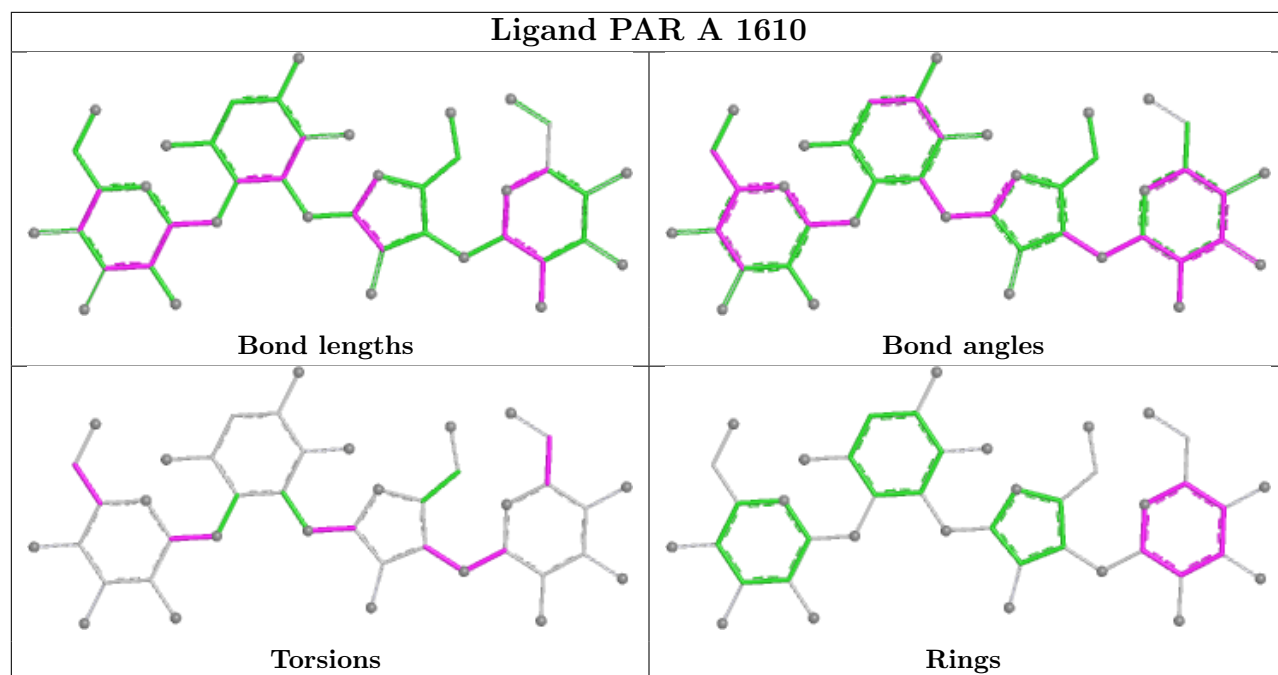
Ligand PAR A 1613



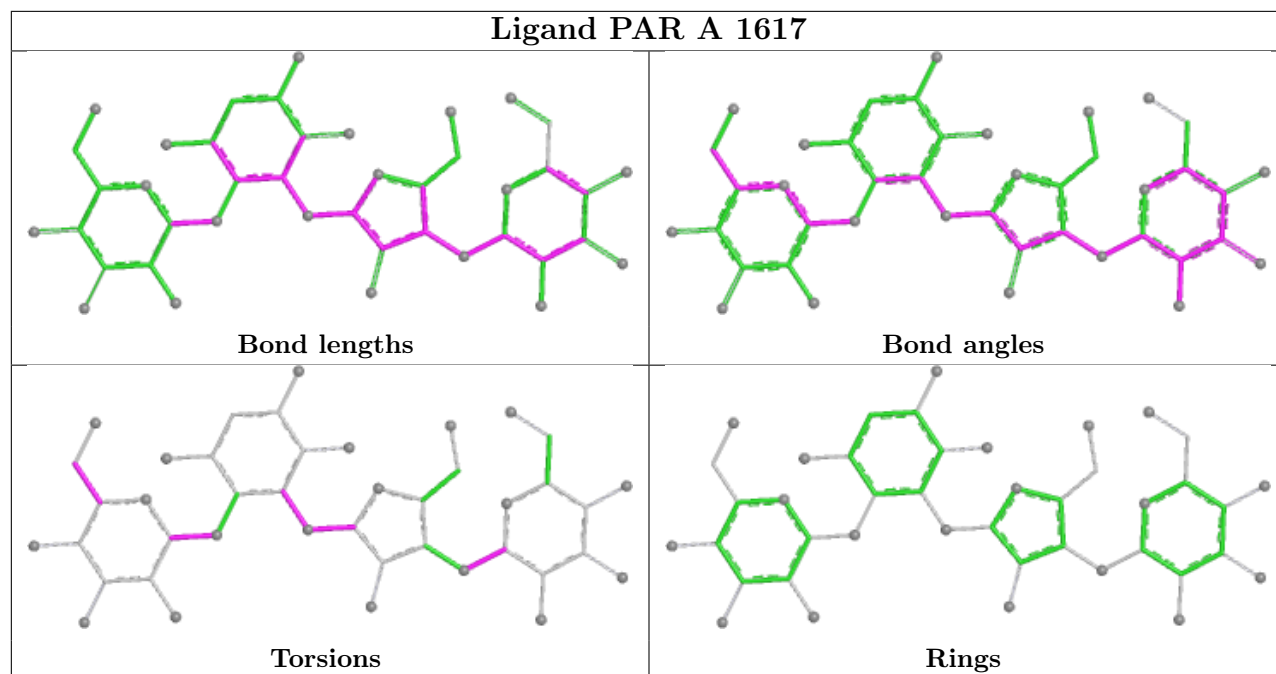
Ligand PAR A 1614



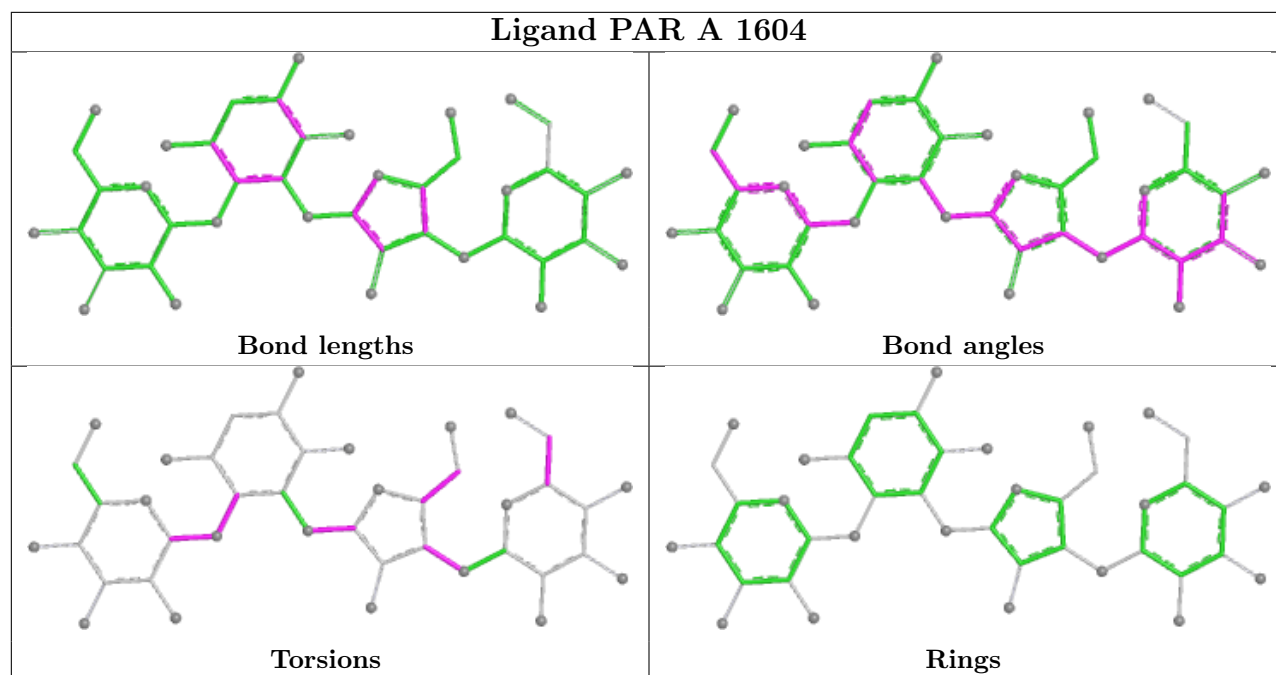
Ligand PAR A 1610



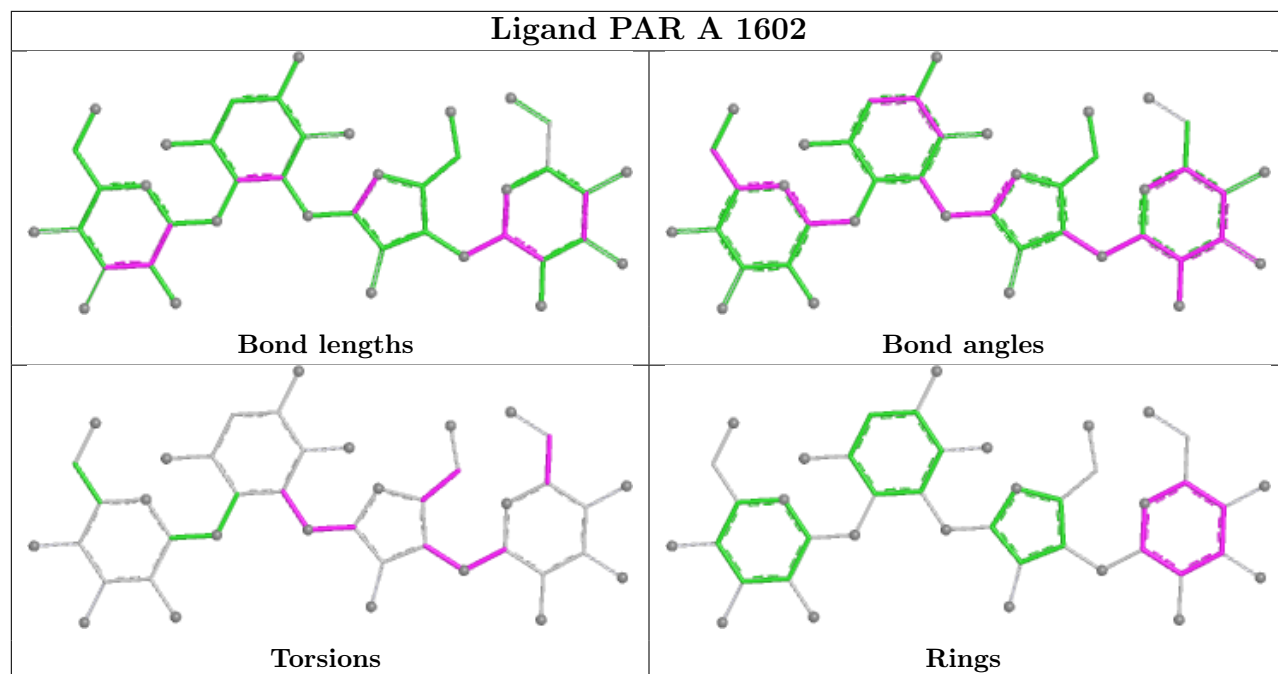
Ligand PAR A 1617



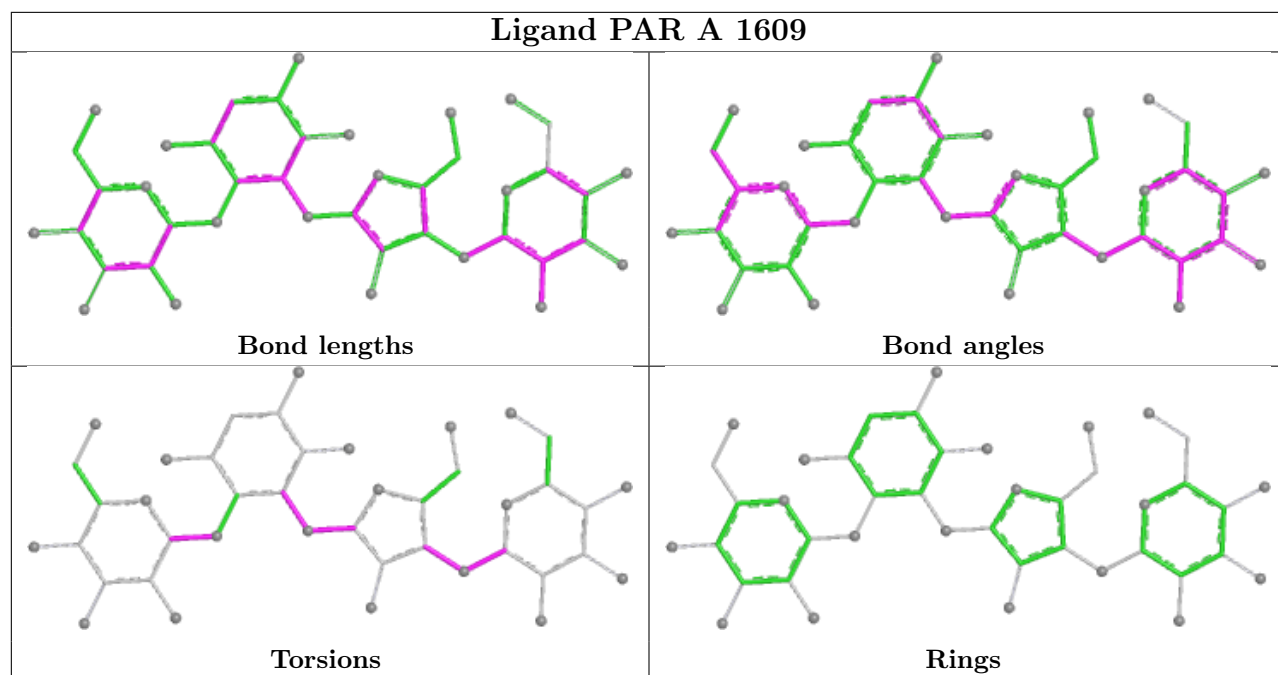
Ligand PAR A 1604



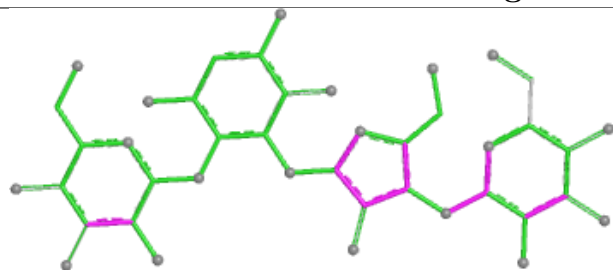
Ligand PAR A 1602



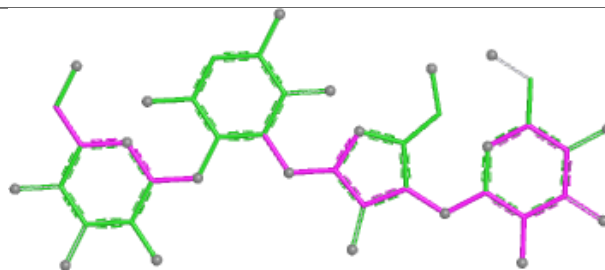
Ligand PAR A 1609



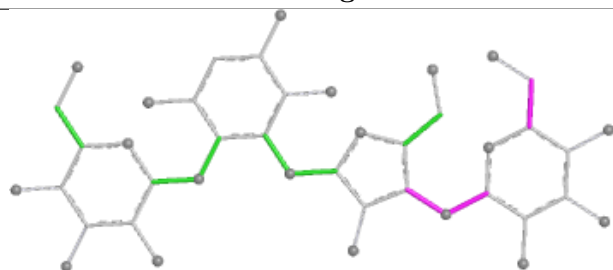
Ligand PAR A 1605



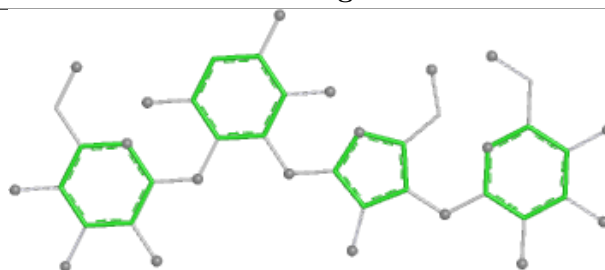
Bond lengths



Bond angles

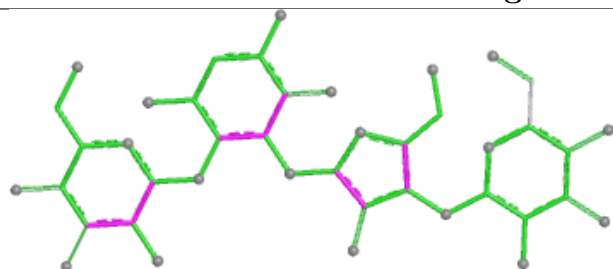


Torsions

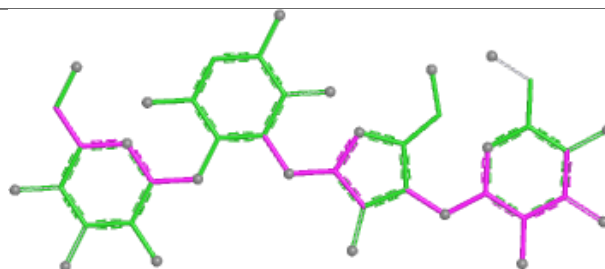


Rings

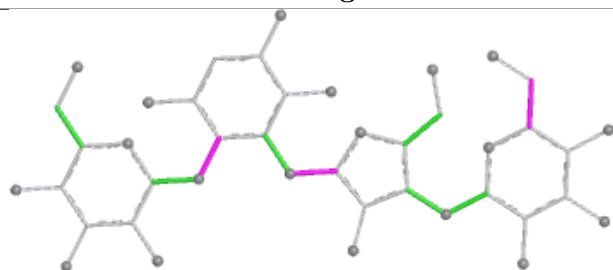
Ligand PAR A 1601



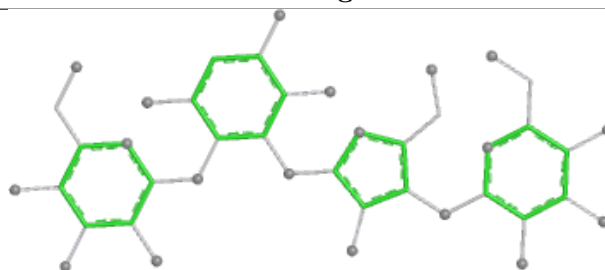
Bond lengths



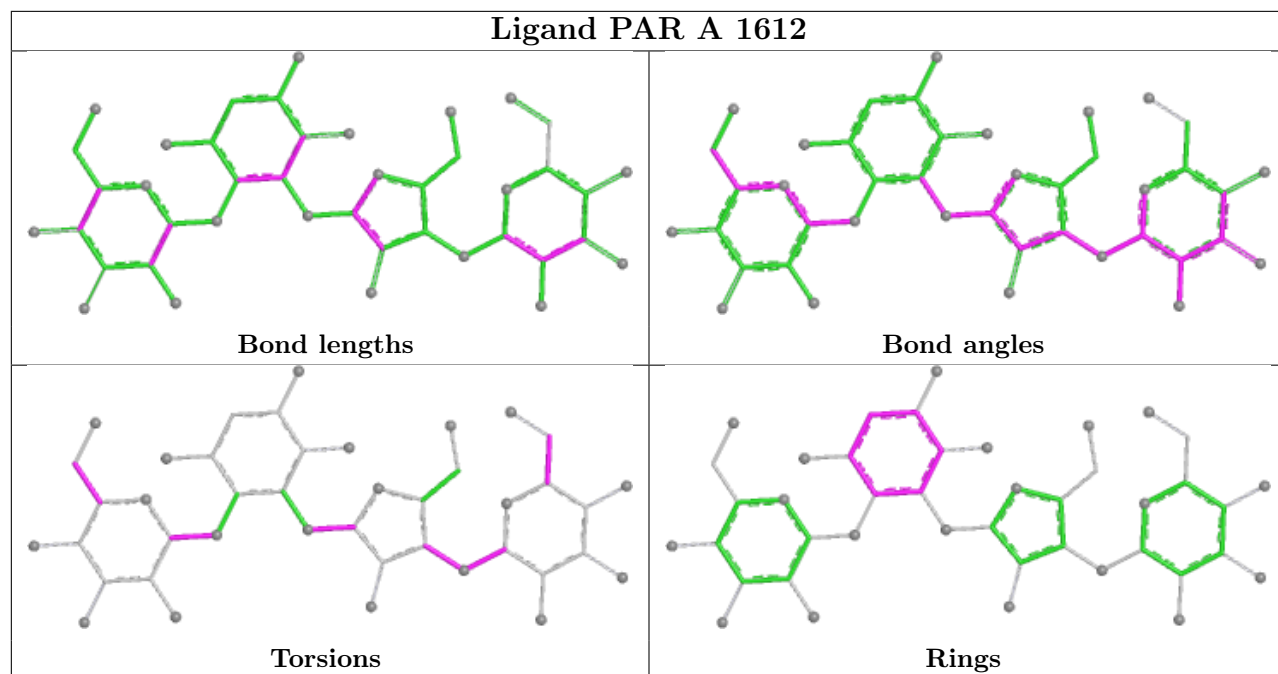
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1498/1522 (98%)	-0.40	8 (0%) 87 72	49, 88, 175, 339	0
2	B	236/256 (92%)	-0.06	2 (0%) 82 64	70, 114, 159, 187	0
3	C	207/239 (86%)	-0.18	2 (0%) 79 59	80, 108, 146, 160	0
4	D	208/209 (99%)	-0.19	3 (1%) 73 53	56, 92, 128, 166	0
5	E	151/162 (93%)	-0.52	0 100 100	47, 73, 107, 151	0
6	F	101/101 (100%)	-0.46	0 100 100	68, 108, 134, 160	0
7	G	155/156 (99%)	-0.24	1 (0%) 85 70	66, 106, 162, 193	0
8	H	138/138 (100%)	-0.46	1 (0%) 84 67	47, 74, 104, 132	0
9	I	127/128 (99%)	-0.05	3 (2%) 59 43	69, 112, 142, 158	0
10	J	99/105 (94%)	0.17	1 (1%) 79 59	75, 127, 185, 199	0
11	K	119/129 (92%)	-0.27	2 (1%) 69 49	54, 94, 132, 210	0
12	L	124/135 (91%)	-0.01	4 (3%) 50 36	55, 80, 124, 185	0
13	M	118/126 (93%)	-0.17	2 (1%) 69 49	78, 108, 137, 149	0
14	N	60/61 (98%)	0.13	3 (5%) 34 27	75, 99, 139, 181	0
15	O	88/89 (98%)	-0.17	1 (1%) 78 58	56, 90, 123, 172	0
16	P	84/88 (95%)	-0.21	0 100 100	58, 77, 107, 151	0
17	Q	100/105 (95%)	-0.30	0 100 100	63, 81, 120, 155	0
18	R	73/88 (82%)	-0.35	0 100 100	68, 100, 153, 221	0
19	S	81/93 (87%)	-0.01	4 (4%) 35 28	89, 124, 151, 179	0
20	T	99/106 (93%)	0.01	2 (2%) 65 46	65, 85, 130, 168	0
21	U	25/27 (92%)	0.69	5 (20%) 3 5	87, 113, 132, 139	0
22	V	3/3 (100%)	-0.55	0 100 100	98, 98, 103, 105	0
23	W	15/15 (100%)	0.63	1 (6%) 24 21	127, 144, 218, 227	0
All	All	3909/4081 (95%)	-0.26	45 (1%) 76 56	47, 96, 156, 339	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	K	129	SER	8.8
12	L	129	ALA	6.6
11	K	128	ALA	6.1
1	A	1539	C	5.6
19	S	3	ARG	5.0
14	N	12	ARG	4.9
12	L	21	LYS	4.7
12	L	128	ALA	4.3
19	S	2	PRO	3.9
1	A	1129	C	3.8
7	G	84	ASN	3.7
15	O	2	PRO	3.6
9	I	105	ASP	3.6
14	N	13	THR	3.5
3	C	188	LEU	3.3
4	D	31	CYS	3.2
21	U	25	LYS	3.2
1	A	40	C	3.0
4	D	9	CYS	2.9
13	M	5	ALA	2.9
21	U	16	GLY	2.9
23	W	28	G	2.9
9	I	106	ALA	2.8
1	A	41	G	2.7
1	A	1288	A	2.7
8	H	1	MET	2.7
13	M	8	GLU	2.7
10	J	43	ARG	2.6
21	U	6	ARG	2.6
21	U	9	ARG	2.6
21	U	26	LYS	2.6
19	S	5	LEU	2.6
9	I	9	ARG	2.5
20	T	12	ALA	2.5
4	D	26	CYS	2.5
14	N	10	ALA	2.4
20	T	68	LYS	2.3
3	C	201	TYR	2.3
12	L	22	SER	2.3
1	A	694	A	2.2
1	A	1027	C	2.2
2	B	120	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	214	ILE	2.0
19	S	4	SER	2.0
1	A	204	U	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
1	PSU	A	1540	20/21	0.88	0.32	210,258,270,270	0
1	PSU	A	1541	20/21	0.92	0.26	228,249,272,273	0
1	2MG	A	1207	24/25	0.95	0.07	91,106,114,118	0
1	PSU	A	516	20/21	0.96	0.11	83,94,105,108	0
1	MA6	A	1518	24/25	0.97	0.08	58,69,75,78	0
1	MA6	A	1519	24/25	0.97	0.11	55,57,64,67	0
1	5MC	A	967	21/22	0.97	0.11	59,75,118,121	0
1	M2G	A	966	25/26	0.97	0.11	66,100,115,127	0
12	0TD	L	92	10/11	0.97	0.15	55,83,98,428	0
1	7MG	A	527	24/25	0.98	0.09	63,69,82,84	0
1	5MC	A	1400	21/22	0.98	0.09	44,73,95,101	0
1	4OC	A	1402	22/23	0.98	0.07	57,63,67,91	0
1	5MC	A	1404	21/22	0.98	0.07	55,64,71,72	0
1	UR3	A	1498	21/22	0.98	0.09	63,71,81,88	0
1	5MC	A	1407	21/22	0.99	0.05	61,67,72,74	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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
25	MG	A	1882[A]	1/1	0.38	0.50	0,0,0,0	1
25	MG	A	1882[B]	1/1	0.38	0.50	0,0,0,0	1
25	MG	A	1869	1/1	0.58	0.20	59,59,59,59	0
25	MG	A	1949	1/1	0.58	0.17	228,228,228,228	0
25	MG	A	1803	1/1	0.63	0.24	71,71,71,71	0
25	MG	A	1919[B]	1/1	0.64	0.13	9,9,9,9	1
25	MG	A	1919[A]	1/1	0.64	0.13	9,9,9,9	1
25	MG	A	1836	1/1	0.66	0.11	75,75,75,75	0
25	MG	S	102	1/1	0.66	0.20	73,73,73,73	0
25	MG	A	1841	1/1	0.68	0.31	64,64,64,64	0
25	MG	A	1652[A]	1/1	0.68	0.36	11,11,11,11	1
25	MG	A	1653[B]	1/1	0.69	0.47	11,11,11,11	1
25	MG	A	1810	1/1	0.70	0.25	71,71,71,71	0
25	MG	A	1813	1/1	0.71	0.16	53,53,53,53	0
25	MG	A	1806	1/1	0.71	0.30	91,91,91,91	0
25	MG	A	1807	1/1	0.72	0.24	83,83,83,83	0
25	MG	A	1889	1/1	0.72	0.23	66,66,66,66	0
25	MG	A	1887	1/1	0.73	0.19	64,64,64,64	0
25	MG	A	1903	1/1	0.73	0.13	74,74,74,74	0
25	MG	A	1876	1/1	0.74	0.10	69,69,69,69	0
25	MG	A	1930	1/1	0.74	0.21	79,79,79,79	0
25	MG	A	1837	1/1	0.75	0.22	54,54,54,54	0
25	MG	A	1798	1/1	0.76	0.30	70,70,70,70	0
24	PAR	A	1616	42/42	0.77	0.19	216,216,216,216	0
25	MG	A	1719	1/1	0.77	0.20	72,72,72,72	0
25	MG	A	1787	1/1	0.77	0.11	66,66,66,66	0
25	MG	A	1726	1/1	0.78	0.10	93,93,93,93	0
25	MG	A	1932	1/1	0.78	0.22	71,71,71,71	0
25	MG	A	1827	1/1	0.78	0.23	78,78,78,78	0
25	MG	A	1833	1/1	0.78	0.23	59,59,59,59	0
25	MG	A	1891	1/1	0.79	0.23	50,50,50,50	0
25	MG	E	201	1/1	0.79	0.12	92,92,92,92	0
25	MG	A	1811	1/1	0.79	0.09	56,56,56,56	0
24	PAR	A	1614	42/42	0.80	0.12	174,174,174,174	0
25	MG	A	1790	1/1	0.80	0.12	162,162,162,162	0
25	MG	L	201	1/1	0.80	0.10	57,57,57,57	0
25	MG	O	101	1/1	0.80	0.14	112,112,112,112	0
25	MG	A	1936	1/1	0.80	0.15	68,68,68,68	0
25	MG	V	101	1/1	0.80	0.14	75,75,75,75	0
25	MG	A	1916	1/1	0.81	0.13	51,51,51,51	0
24	PAR	A	1615	42/42	0.81	0.14	149,149,149,149	0
25	MG	A	1871	1/1	0.81	0.08	63,63,63,63	0
25	MG	A	1638	1/1	0.81	0.15	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	MG	A	1908	1/1	0.82	0.09	66,66,66,66	0
25	MG	A	1927	1/1	0.82	0.13	62,62,62,62	0
25	MG	A	1898	1/1	0.82	0.15	61,61,61,61	0
25	MG	A	1931	1/1	0.82	0.25	58,58,58,58	0
25	MG	A	1917	1/1	0.82	0.24	61,61,61,61	0
25	MG	A	1784	1/1	0.82	0.09	89,89,89,89	0
25	MG	A	1800[B]	1/1	0.83	0.59	7,7,7,7	1
25	MG	A	1812	1/1	0.83	0.37	65,65,65,65	0
25	MG	A	1717	1/1	0.83	0.11	110,110,110,110	0
25	MG	A	1817	1/1	0.83	0.17	54,54,54,54	0
25	MG	A	1728	1/1	0.83	0.10	103,103,103,103	0
25	MG	A	1623	1/1	0.83	0.14	64,64,64,64	0
25	MG	A	1800[A]	1/1	0.83	0.59	7,7,7,7	1
25	MG	A	1830	1/1	0.84	0.06	70,70,70,70	0
25	MG	A	1945	1/1	0.84	0.12	156,156,156,156	0
25	MG	A	1736	1/1	0.84	0.10	88,88,88,88	0
25	MG	A	1786	1/1	0.84	0.14	97,97,97,97	0
25	MG	A	1839	1/1	0.85	0.16	56,56,56,56	0
25	MG	A	1789	1/1	0.85	0.10	127,127,127,127	0
25	MG	A	1639	1/1	0.85	0.20	55,55,55,55	0
25	MG	A	1956	1/1	0.85	0.07	193,193,193,193	0
25	MG	A	1771	1/1	0.85	0.23	89,89,89,89	0
25	MG	A	1929	1/1	0.85	0.34	44,44,44,44	0
25	MG	A	1725	1/1	0.85	0.11	67,67,67,67	0
25	MG	A	1662	1/1	0.85	0.12	77,77,77,77	0
24	PAR	A	1618	42/42	0.85	0.19	166,166,166,166	0
25	MG	A	1650	1/1	0.86	0.13	86,86,86,86	0
25	MG	A	1939	1/1	0.86	0.08	57,57,57,57	0
25	MG	A	1890	1/1	0.86	0.46	59,59,59,59	0
24	PAR	A	1611	42/42	0.86	0.11	131,131,131,131	0
25	MG	A	1926	1/1	0.86	0.08	58,58,58,58	0
25	MG	A	1892	1/1	0.86	0.10	46,46,46,46	0
25	MG	A	1847	1/1	0.86	0.35	85,85,85,85	0
25	MG	A	1868	1/1	0.86	0.08	68,68,68,68	0
25	MG	A	1885	1/1	0.86	0.09	45,45,45,45	0
25	MG	A	1816	1/1	0.86	0.25	53,53,53,53	0
25	MG	A	1734	1/1	0.87	0.10	63,63,63,63	0
25	MG	A	1902	1/1	0.87	0.16	64,64,64,64	0
25	MG	A	1880	1/1	0.87	0.06	60,60,60,60	0
24	PAR	A	1610	42/42	0.87	0.15	144,144,144,144	0
25	MG	A	1713	1/1	0.87	0.11	63,63,63,63	0
25	MG	A	1772	1/1	0.87	0.10	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	MG	A	1724	1/1	0.87	0.09	82,82,82,82	0
25	MG	A	1888	1/1	0.87	0.23	71,71,71,71	0
25	MG	A	1856	1/1	0.87	0.13	59,59,59,59	0
25	MG	A	1832	1/1	0.87	0.10	77,77,77,77	0
25	MG	P	102	1/1	0.87	0.07	51,51,51,51	0
25	MG	A	1732	1/1	0.87	0.17	84,84,84,84	0
25	MG	T	201	1/1	0.87	0.34	88,88,88,88	0
25	MG	A	1835	1/1	0.87	0.21	71,71,71,71	0
25	MG	A	1940	1/1	0.88	0.18	82,82,82,82	0
25	MG	A	1682	1/1	0.88	0.10	104,104,104,104	0
25	MG	A	1925	1/1	0.88	0.08	42,42,42,42	0
25	MG	A	1761	1/1	0.88	0.10	155,155,155,155	0
25	MG	D	302	1/1	0.88	0.20	71,71,71,71	0
25	MG	A	1707	1/1	0.88	0.17	80,80,80,80	0
25	MG	H	201	1/1	0.88	0.14	53,53,53,53	0
25	MG	A	1712	1/1	0.88	0.10	34,34,34,34	0
25	MG	A	1911	1/1	0.88	0.06	49,49,49,49	0
25	MG	A	1883	1/1	0.88	0.10	62,62,62,62	0
25	MG	A	1669	1/1	0.88	0.16	76,76,76,76	0
25	MG	A	1918	1/1	0.88	0.15	39,39,39,39	0
25	MG	A	1893	1/1	0.88	0.31	53,53,53,53	0
25	MG	A	1905	1/1	0.89	0.33	83,83,83,83	0
25	MG	A	1906	1/1	0.89	0.18	73,73,73,73	0
25	MG	A	1954	1/1	0.89	0.13	150,150,150,150	0
25	MG	A	1862	1/1	0.89	0.17	38,38,38,38	0
25	MG	A	1909	1/1	0.89	0.26	68,68,68,68	0
25	MG	D	303	1/1	0.89	0.15	73,73,73,73	0
25	MG	A	1866	1/1	0.89	0.37	53,53,53,53	0
25	MG	E	203	1/1	0.89	0.07	80,80,80,80	0
25	MG	A	1695	1/1	0.89	0.07	94,94,94,94	0
25	MG	A	1701	1/1	0.89	0.12	85,85,85,85	0
25	MG	A	1933	1/1	0.89	0.10	82,82,82,82	0
25	MG	A	1935	1/1	0.89	0.13	57,57,57,57	0
25	MG	A	1690	1/1	0.89	0.13	100,100,100,100	0
25	MG	A	1710	1/1	0.89	0.08	82,82,82,82	0
25	MG	A	1769	1/1	0.89	0.05	114,114,114,114	0
25	MG	A	1922	1/1	0.90	0.25	76,76,76,76	0
25	MG	A	1721	1/1	0.90	0.21	43,43,43,43	0
25	MG	A	1651	1/1	0.90	0.11	48,48,48,48	0
25	MG	A	1770	1/1	0.90	0.13	90,90,90,90	0
25	MG	A	1861	1/1	0.90	0.12	57,57,57,57	0
25	MG	A	1907	1/1	0.90	0.05	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
25	MG	A	1809	1/1	0.90	0.24	76,76,76,76	0
25	MG	A	1645	1/1	0.90	0.12	53,53,53,53	0
25	MG	A	1834	1/1	0.90	0.11	57,57,57,57	0
25	MG	A	1796	1/1	0.90	0.23	58,58,58,58	0
24	PAR	A	1617	42/42	0.90	0.27	189,189,189,189	0
25	MG	A	1780	1/1	0.90	0.31	72,72,72,72	0
25	MG	A	1877	1/1	0.90	0.11	59,59,59,59	0
25	MG	A	1750	1/1	0.90	0.30	67,67,67,67	0
25	MG	A	1714	1/1	0.91	0.07	66,66,66,66	0
25	MG	A	1765	1/1	0.91	0.14	113,113,113,113	0
25	MG	A	1702	1/1	0.91	0.06	104,104,104,104	0
25	MG	A	1636	1/1	0.91	0.11	68,68,68,68	0
25	MG	A	1870	1/1	0.91	0.13	35,35,35,35	0
25	MG	A	1693	1/1	0.91	0.05	96,96,96,96	0
25	MG	A	1894	1/1	0.91	0.17	66,66,66,66	0
25	MG	A	1677	1/1	0.91	0.12	118,118,118,118	0
25	MG	A	1777	1/1	0.91	0.11	60,60,60,60	0
25	MG	A	1928	1/1	0.91	0.26	93,93,93,93	0
25	MG	A	1843	1/1	0.91	0.11	35,35,35,35	0
25	MG	A	1881	1/1	0.91	0.15	63,63,63,63	0
25	MG	A	1742	1/1	0.91	0.12	72,72,72,72	0
25	MG	A	1851	1/1	0.91	0.21	57,57,57,57	0
25	MG	A	1853	1/1	0.91	0.22	44,44,44,44	0
25	MG	A	1747	1/1	0.91	0.09	108,108,108,108	0
25	MG	A	1665	1/1	0.91	0.17	57,57,57,57	0
25	MG	A	1884	1/1	0.92	0.20	55,55,55,55	0
25	MG	A	1924	1/1	0.92	0.26	54,54,54,54	0
25	MG	A	1952	1/1	0.92	0.08	148,148,148,148	0
25	MG	A	1801	1/1	0.92	0.28	57,57,57,57	0
25	MG	A	1955	1/1	0.92	0.10	179,179,179,179	0
25	MG	A	1753	1/1	0.92	0.08	94,94,94,94	0
25	MG	A	1852	1/1	0.92	0.11	47,47,47,47	0
25	MG	A	1657	1/1	0.92	0.14	101,101,101,101	0
24	PAR	A	1605	42/42	0.92	0.21	94,94,94,94	42
25	MG	E	202	1/1	0.92	0.13	45,45,45,45	0
25	MG	A	1860	1/1	0.92	0.15	55,55,55,55	0
25	MG	A	1825	1/1	0.92	0.09	59,59,59,59	0
25	MG	A	1912	1/1	0.92	0.19	51,51,51,51	0
25	MG	A	1706	1/1	0.92	0.06	52,52,52,52	0
25	MG	A	1731	1/1	0.92	0.09	121,121,121,121	0
25	MG	A	1895	1/1	0.92	0.20	44,44,44,44	0
24	PAR	A	1612	42/42	0.92	0.14	131,131,131,131	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
25	MG	A	1899	1/1	0.92	0.12	18,18,18,18	0
25	MG	A	1946	1/1	0.93	0.05	146,146,146,146	0
25	MG	A	1901[B]	1/1	0.93	0.13	16,16,16,16	1
25	MG	A	1635	1/1	0.93	0.17	45,45,45,45	0
25	MG	A	1820	1/1	0.93	0.13	70,70,70,70	0
25	MG	A	1715	1/1	0.93	0.09	82,82,82,82	0
25	MG	A	1844	1/1	0.93	0.12	35,35,35,35	0
25	MG	A	1957	1/1	0.93	0.08	103,103,103,103	0
25	MG	A	1688	1/1	0.93	0.09	60,60,60,60	0
25	MG	A	1874	1/1	0.93	0.15	13,13,13,13	0
25	MG	A	1768	1/1	0.93	0.10	103,103,103,103	0
25	MG	A	1671	1/1	0.93	0.10	66,66,66,66	0
25	MG	A	1692	1/1	0.93	0.09	74,74,74,74	0
25	MG	A	1914	1/1	0.93	0.12	44,44,44,44	0
25	MG	A	1934	1/1	0.93	0.07	69,69,69,69	0
25	MG	A	1675	1/1	0.93	0.15	74,74,74,74	0
24	PAR	A	1609	42/42	0.93	0.21	121,121,121,121	42
25	MG	A	1773	1/1	0.93	0.09	74,74,74,74	0
25	MG	A	1699	1/1	0.93	0.06	79,79,79,79	0
25	MG	A	1901[A]	1/1	0.93	0.13	16,16,16,16	1
25	MG	A	1720	1/1	0.94	0.11	89,89,89,89	0
25	MG	A	1904	1/1	0.94	0.09	49,49,49,49	0
25	MG	A	1808	1/1	0.94	0.15	31,31,31,31	0
25	MG	A	1838	1/1	0.94	0.30	50,50,50,50	0
25	MG	A	1739	1/1	0.94	0.13	85,85,85,85	0
25	MG	A	1630	1/1	0.94	0.08	83,83,83,83	0
25	MG	A	1723	1/1	0.94	0.06	94,94,94,94	0
24	PAR	A	1606	42/42	0.94	0.14	113,113,113,113	0
25	MG	A	1751	1/1	0.94	0.10	95,95,95,95	0
25	MG	A	1950	1/1	0.94	0.05	177,177,177,177	0
25	MG	A	1621	1/1	0.94	0.09	69,69,69,69	0
25	MG	A	1953	1/1	0.94	0.08	179,179,179,179	0
25	MG	A	1759	1/1	0.94	0.10	121,121,121,121	0
25	MG	A	1795	1/1	0.94	0.09	57,57,57,57	0
25	MG	A	1824	1/1	0.94	0.34	64,64,64,64	0
25	MG	A	1857	1/1	0.94	0.12	54,54,54,54	0
25	MG	A	1696	1/1	0.94	0.10	136,136,136,136	0
25	MG	A	1920	1/1	0.94	0.29	50,50,50,50	0
25	MG	A	1622	1/1	0.94	0.09	106,106,106,106	0
25	MG	A	1828	1/1	0.94	0.15	107,107,107,107	0
25	MG	A	1864[A]	1/1	0.94	0.67	11,11,11,11	1
25	MG	A	1864[B]	1/1	0.94	0.67	11,11,11,11	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
25	MG	A	1730	1/1	0.94	0.09	118,118,118,118	0
24	PAR	A	1608	42/42	0.94	0.18	81,81,81,81	42
25	MG	P	101	1/1	0.94	0.12	13,13,13,13	0
25	MG	A	1628	1/1	0.94	0.07	48,48,48,48	0
25	MG	A	1733	1/1	0.94	0.10	61,61,61,61	0
25	MG	A	1649	1/1	0.94	0.15	47,47,47,47	0
25	MG	A	1873	1/1	0.94	0.27	29,29,29,29	0
25	MG	A	1703	1/1	0.95	0.11	57,57,57,57	0
25	MG	A	1670	1/1	0.95	0.12	64,64,64,64	0
25	MG	A	1947	1/1	0.95	0.06	133,133,133,133	0
25	MG	A	1727	1/1	0.95	0.06	101,101,101,101	0
25	MG	A	1792	1/1	0.95	0.10	32,32,32,32	0
25	MG	A	1951	1/1	0.95	0.14	110,110,110,110	0
25	MG	A	1718	1/1	0.95	0.30	80,80,80,80	0
25	MG	A	1840	1/1	0.95	0.14	22,22,22,22	0
25	MG	A	1897[A]	1/1	0.95	0.46	0,0,0,0	1
25	MG	A	1897[B]	1/1	0.95	0.46	0,0,0,0	1
25	MG	A	1815	1/1	0.95	0.16	45,45,45,45	0
25	MG	A	1685	1/1	0.95	0.17	57,57,57,57	0
25	MG	A	1797	1/1	0.95	0.12	47,47,47,47	0
24	PAR	A	1613	42/42	0.95	0.12	120,120,120,120	0
25	MG	A	1752	1/1	0.95	0.07	147,147,147,147	0
25	MG	A	1643	1/1	0.95	0.09	40,40,40,40	0
25	MG	A	1826	1/1	0.95	0.11	44,44,44,44	0
25	MG	A	1778	1/1	0.95	0.30	59,59,59,59	0
25	MG	A	1755	1/1	0.95	0.19	74,74,74,74	0
25	MG	A	1859	1/1	0.95	0.06	73,73,73,73	0
25	MG	A	1805	1/1	0.95	0.10	34,34,34,34	0
25	MG	A	1783	1/1	0.95	0.10	41,41,41,41	0
25	MG	P	103	1/1	0.95	0.14	44,44,44,44	0
25	MG	A	1691	1/1	0.95	0.06	111,111,111,111	0
24	PAR	A	1603	42/42	0.95	0.13	103,103,103,103	3
25	MG	A	1913	1/1	0.95	0.08	49,49,49,49	0
25	MG	A	1943	1/1	0.96	0.05	178,178,178,178	0
25	MG	A	1823	1/1	0.96	0.12	57,57,57,57	0
25	MG	A	1842	1/1	0.96	0.21	43,43,43,43	0
25	MG	A	1697	1/1	0.96	0.12	77,77,77,77	0
25	MG	A	1791	1/1	0.96	0.18	30,30,30,30	0
25	MG	A	1845	1/1	0.96	0.33	64,64,64,64	0
24	PAR	A	1601	42/42	0.96	0.08	64,64,64,64	0
25	MG	A	1850	1/1	0.96	0.26	71,71,71,71	0
25	MG	A	1776	1/1	0.96	0.07	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	MG	A	1900	1/1	0.96	0.10	27,27,27,27	0
25	MG	A	1757	1/1	0.96	0.11	133,133,133,133	0
24	PAR	A	1607	42/42	0.96	0.15	99,99,99,99	42
25	MG	A	1746	1/1	0.96	0.07	146,146,146,146	0
25	MG	A	1679	1/1	0.96	0.07	47,47,47,47	0
25	MG	A	1748	1/1	0.96	0.11	87,87,87,87	0
25	MG	A	1625	1/1	0.96	0.07	30,30,30,30	0
25	MG	A	1664	1/1	0.96	0.12	74,74,74,74	0
25	MG	A	1886	1/1	0.96	0.12	50,50,50,50	0
25	MG	A	1819	1/1	0.96	0.13	64,64,64,64	0
25	MG	A	1672	1/1	0.96	0.12	56,56,56,56	0
25	MG	A	1910	1/1	0.96	0.05	45,45,45,45	0
25	MG	A	1821	1/1	0.96	0.11	33,33,33,33	0
25	MG	A	1937	1/1	0.96	0.29	61,61,61,61	0
25	MG	A	1822	1/1	0.96	0.07	63,63,63,63	0
25	MG	Q	201	1/1	0.96	0.09	60,60,60,60	0
25	MG	S	101	1/1	0.96	0.07	22,22,22,22	0
25	MG	A	1867	1/1	0.96	0.08	29,29,29,29	0
25	MG	A	1941	1/1	0.96	0.05	145,145,145,145	0
25	MG	A	1942	1/1	0.96	0.05	143,143,143,143	0
26	ZN	D	301	1/1	0.96	0.24	141,141,141,141	0
25	MG	A	1938	1/1	0.97	0.07	43,43,43,43	0
25	MG	A	1872	1/1	0.97	0.17	30,30,30,30	0
25	MG	A	1641	1/1	0.97	0.10	56,56,56,56	0
25	MG	A	1700	1/1	0.97	0.09	26,26,26,26	0
25	MG	A	1683	1/1	0.97	0.08	102,102,102,102	0
25	MG	A	1668	1/1	0.97	0.10	66,66,66,66	0
25	MG	A	1878	1/1	0.97	0.12	13,13,13,13	0
25	MG	A	1788	1/1	0.97	0.09	95,95,95,95	0
25	MG	A	1686	1/1	0.97	0.12	91,91,91,91	0
25	MG	A	1818	1/1	0.97	0.08	36,36,36,36	0
25	MG	A	1705	1/1	0.97	0.07	57,57,57,57	0
25	MG	A	1848	1/1	0.97	0.06	42,42,42,42	0
25	MG	A	1915	1/1	0.97	0.20	59,59,59,59	0
25	MG	A	1849	1/1	0.97	0.17	40,40,40,40	0
25	MG	A	1642	1/1	0.97	0.10	70,70,70,70	0
25	MG	A	1689	1/1	0.97	0.05	75,75,75,75	0
24	PAR	A	1602	42/42	0.97	0.09	71,71,71,71	0
24	PAR	A	1604	42/42	0.97	0.08	64,64,64,64	0
25	MG	A	1855	1/1	0.97	0.05	24,24,24,24	0
25	MG	A	1921	1/1	0.97	0.12	48,48,48,48	0
25	MG	A	1659	1/1	0.97	0.05	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	MG	A	1673	1/1	0.97	0.08	73,73,73,73	0
25	MG	A	1799	1/1	0.97	0.12	59,59,59,59	0
25	MG	A	1694	1/1	0.97	0.12	108,108,108,108	0
25	MG	A	1735	1/1	0.97	0.07	67,67,67,67	0
25	MG	N	102	1/1	0.97	0.34	82,82,82,82	0
25	MG	A	1829	1/1	0.97	0.09	37,37,37,37	0
25	MG	A	1863	1/1	0.97	0.10	53,53,53,53	0
25	MG	A	1716	1/1	0.97	0.24	92,92,92,92	0
25	MG	A	1738	1/1	0.97	0.14	59,59,59,59	0
25	MG	A	1660	1/1	0.97	0.08	84,84,84,84	0
25	MG	A	1626	1/1	0.97	0.12	100,100,100,100	0
25	MG	A	1743	1/1	0.97	0.04	71,71,71,71	0
25	MG	A	1745	1/1	0.97	0.03	64,64,64,64	0
25	MG	A	1779	1/1	0.97	0.10	55,55,55,55	0
25	MG	A	1640	1/1	0.97	0.06	59,59,59,59	0
25	MG	A	1767	1/1	0.98	0.10	72,72,72,72	0
25	MG	A	1637	1/1	0.98	0.06	29,29,29,29	0
25	MG	A	1654	1/1	0.98	0.05	75,75,75,75	0
25	MG	A	1804	1/1	0.98	0.06	62,62,62,62	0
25	MG	A	1655	1/1	0.98	0.04	78,78,78,78	0
25	MG	A	1740	1/1	0.98	0.09	113,113,113,113	0
25	MG	A	1741	1/1	0.98	0.16	52,52,52,52	0
25	MG	A	1687	1/1	0.98	0.04	53,53,53,53	0
25	MG	A	1875	1/1	0.98	0.04	14,14,14,14	0
25	MG	A	1629	1/1	0.98	0.09	60,60,60,60	0
25	MG	A	1948	1/1	0.98	0.07	122,122,122,122	0
25	MG	A	1744	1/1	0.98	0.04	62,62,62,62	0
25	MG	A	1704	1/1	0.98	0.07	83,83,83,83	0
25	MG	A	1648	1/1	0.98	0.06	64,64,64,64	0
25	MG	A	1624	1/1	0.98	0.07	58,58,58,58	0
25	MG	A	1846	1/1	0.98	0.08	49,49,49,49	0
25	MG	A	1781	1/1	0.98	0.16	67,67,67,67	0
25	MG	A	1632	1/1	0.98	0.07	65,65,65,65	0
25	MG	A	1708	1/1	0.98	0.07	55,55,55,55	0
25	MG	A	1709	1/1	0.98	0.05	94,94,94,94	0
25	MG	A	1729	1/1	0.98	0.06	73,73,73,73	0
25	MG	A	1676	1/1	0.98	0.11	75,75,75,75	0
25	MG	A	1627	1/1	0.98	0.07	30,30,30,30	0
25	MG	A	1678	1/1	0.98	0.09	48,48,48,48	0
25	MG	A	1923	1/1	0.98	0.05	29,29,29,29	0
25	MG	E	204	1/1	0.98	0.12	70,70,70,70	0
25	MG	A	1758	1/1	0.98	0.09	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	MG	A	1619	1/1	0.98	0.18	69,69,69,69	0
25	MG	A	1858	1/1	0.98	0.04	37,37,37,37	0
25	MG	A	1794	1/1	0.98	0.20	61,61,61,61	0
25	MG	A	1681	1/1	0.98	0.06	30,30,30,30	0
25	MG	A	1762	1/1	0.98	0.05	63,63,63,63	0
25	MG	A	1896	1/1	0.98	0.20	57,57,57,57	0
25	MG	A	1763	1/1	0.98	0.06	65,65,65,65	0
25	MG	A	1764	1/1	0.98	0.09	65,65,65,65	0
25	MG	A	1667	1/1	0.98	0.06	56,56,56,56	0
25	MG	A	1831	1/1	0.98	0.11	40,40,40,40	0
25	MG	A	1865	1/1	0.98	0.22	58,58,58,58	0
25	MG	A	1766	1/1	0.98	0.05	97,97,97,97	0
25	MG	A	1647	1/1	0.99	0.08	72,72,72,72	0
25	MG	A	1663	1/1	0.99	0.06	36,36,36,36	0
25	MG	A	1633	1/1	0.99	0.04	54,54,54,54	0
25	MG	A	1793	1/1	0.99	0.04	22,22,22,22	0
25	MG	A	1749	1/1	0.99	0.07	72,72,72,72	0
25	MG	A	1634	1/1	0.99	0.03	42,42,42,42	0
25	MG	A	1666	1/1	0.99	0.04	91,91,91,91	0
25	MG	A	1656	1/1	0.99	0.07	67,67,67,67	0
25	MG	A	1680	1/1	0.99	0.07	67,67,67,67	0
25	MG	A	1774	1/1	0.99	0.03	71,71,71,71	0
25	MG	A	1754	1/1	0.99	0.06	67,67,67,67	0
25	MG	A	1737	1/1	0.99	0.05	63,63,63,63	0
25	MG	A	1879	1/1	0.99	0.02	56,56,56,56	0
25	MG	A	1756	1/1	0.99	0.09	93,93,93,93	0
25	MG	A	1854	1/1	0.99	0.12	40,40,40,40	0
25	MG	A	1802	1/1	0.99	0.11	46,46,46,46	0
25	MG	A	1722	1/1	0.99	0.05	43,43,43,43	0
25	MG	A	1631	1/1	0.99	0.03	75,75,75,75	0
25	MG	A	1658	1/1	0.99	0.05	57,57,57,57	0
25	MG	A	1782	1/1	0.99	0.06	68,68,68,68	0
25	MG	A	1760	1/1	0.99	0.03	44,44,44,44	0
25	MG	A	1620	1/1	0.99	0.03	70,70,70,70	0
25	MG	A	1785	1/1	0.99	0.04	51,51,51,51	0
25	MG	A	1711	1/1	0.99	0.04	64,64,64,64	0
25	MG	A	1684	1/1	0.99	0.04	25,25,25,25	0
25	MG	A	1944	1/1	0.99	0.03	74,74,74,74	0
25	MG	A	1646	1/1	0.99	0.04	69,69,69,69	0
25	MG	A	1661	1/1	0.99	0.03	90,90,90,90	0
25	MG	A	1814	1/1	0.99	0.12	26,26,26,26	0
25	MG	A	1775	1/1	1.00	0.03	75,75,75,75	0

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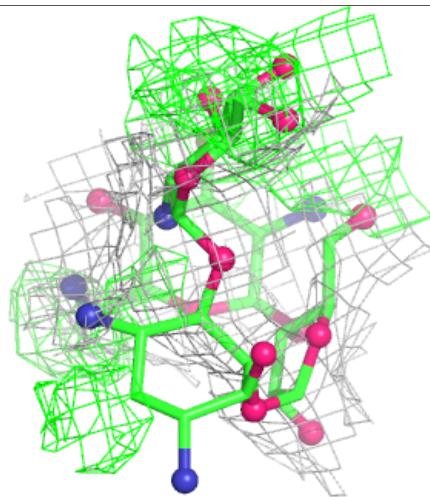
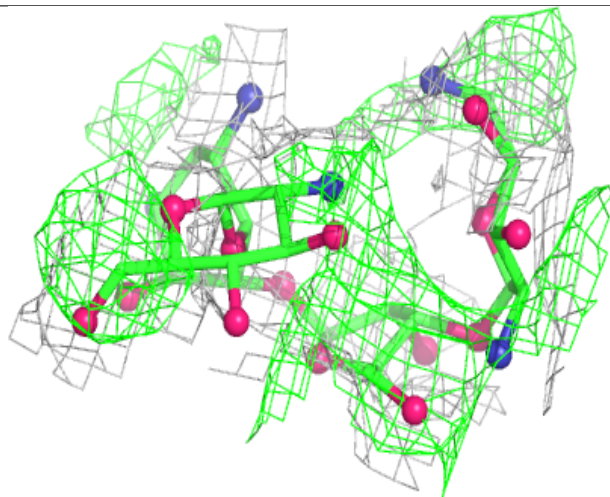
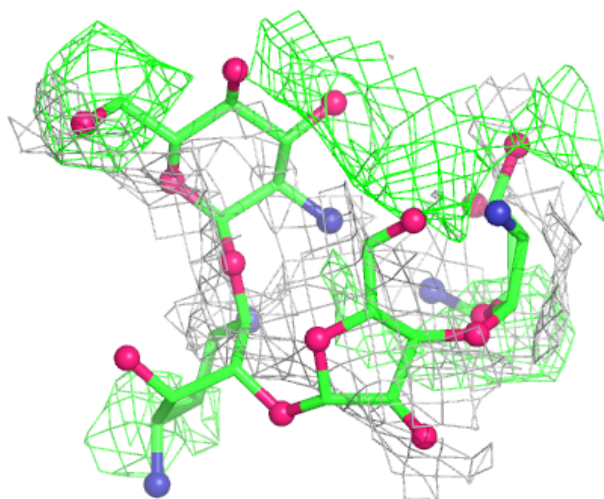
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	MG	A	1644	1/1	1.00	0.02	40,40,40,40	0
25	MG	A	1698	1/1	1.00	0.02	56,56,56,56	0
25	MG	A	1674	1/1	1.00	0.27	18,18,18,18	0
26	ZN	N	101	1/1	1.00	0.05	88,88,88,88	0

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

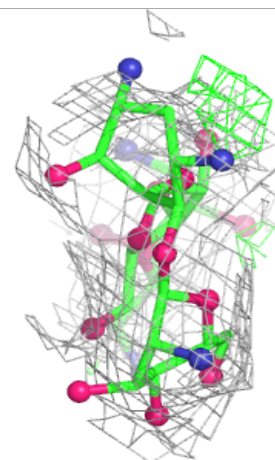
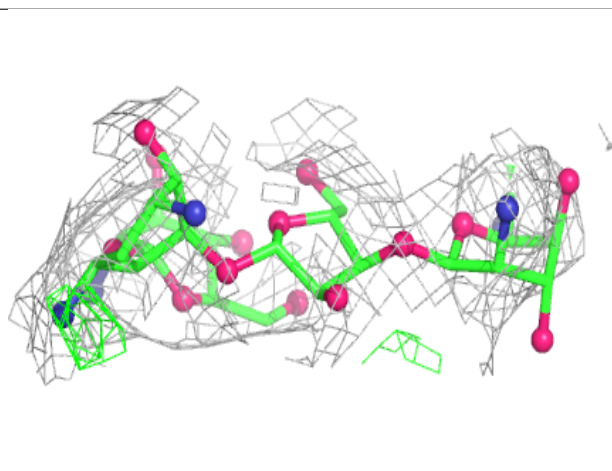
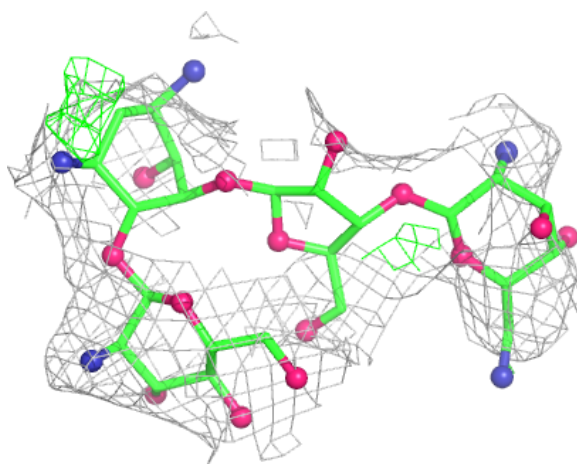
Electron density around PAR A 1616:

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



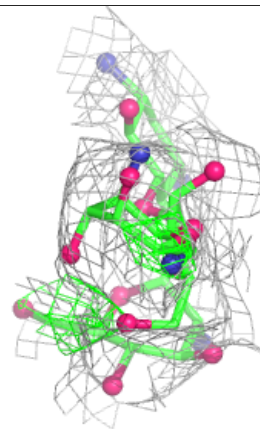
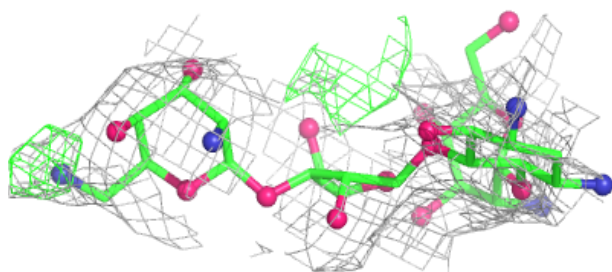
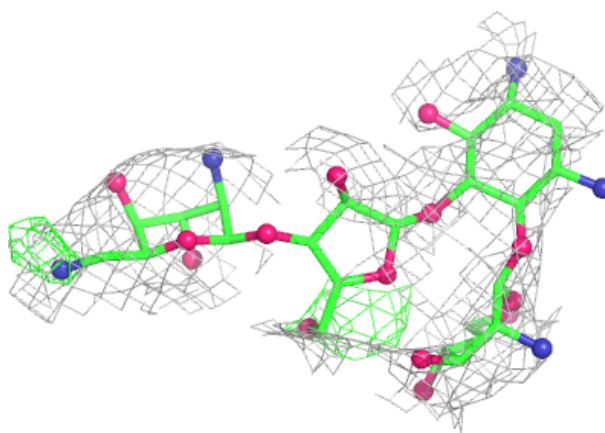
Electron density around PAR A 1614:

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



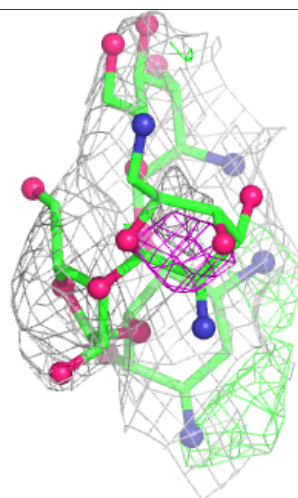
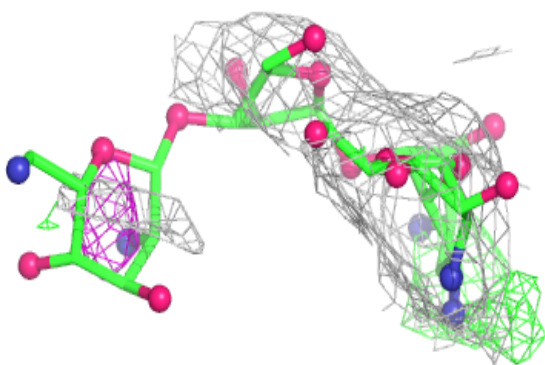
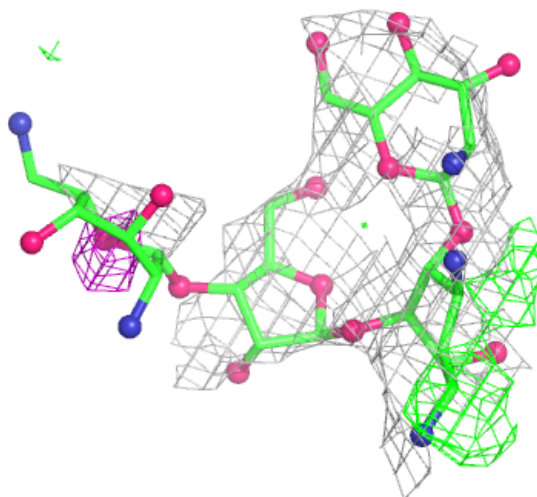
Electron density around PAR A 1615:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



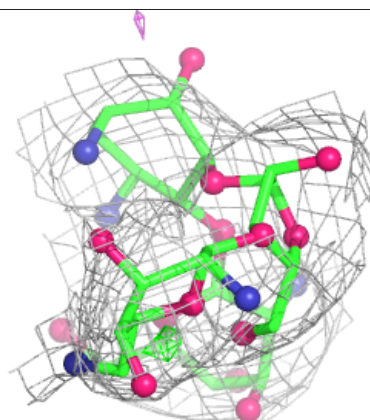
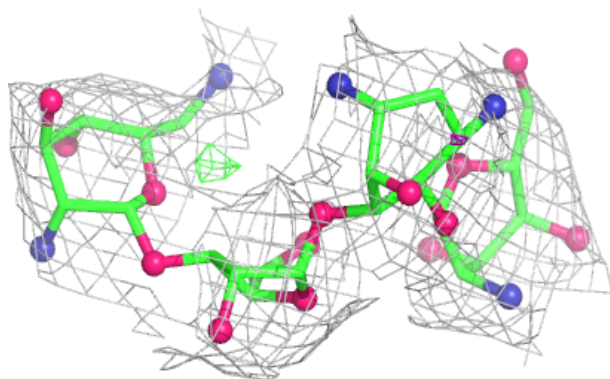
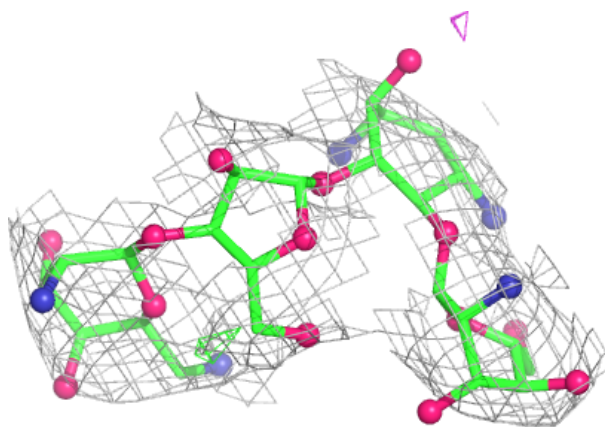
Electron density around PAR A 1618:

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

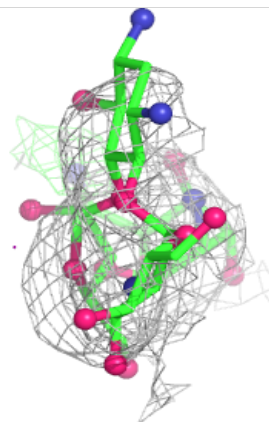
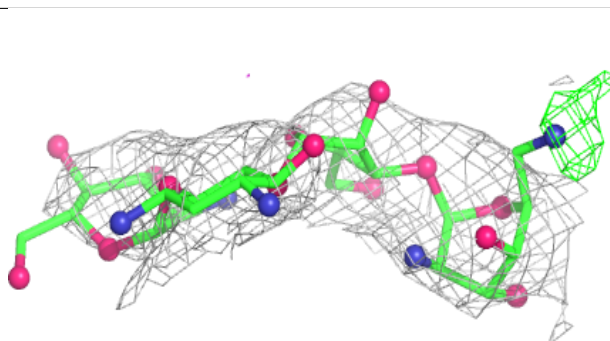
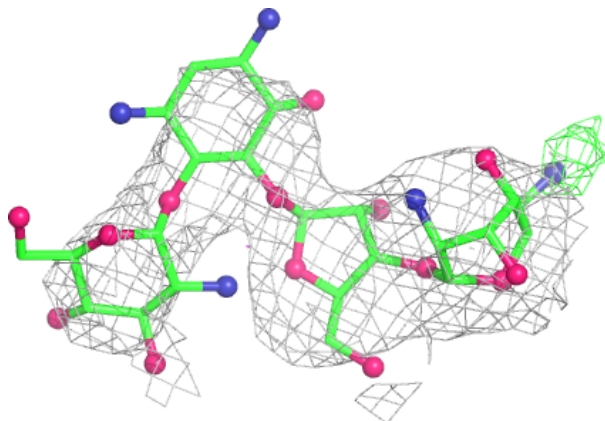


Electron density around PAR A 1611:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

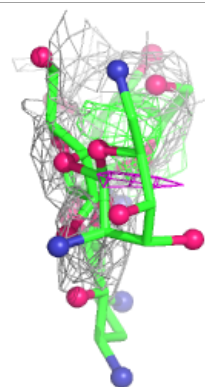
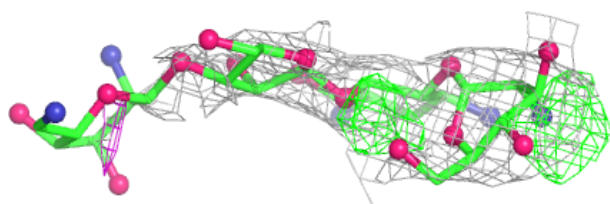
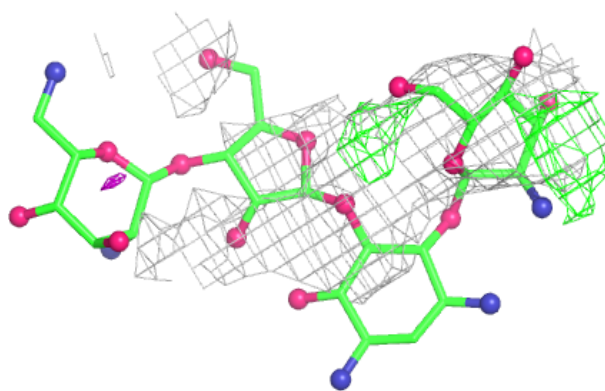
**Electron density around PAR A 1610:**

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



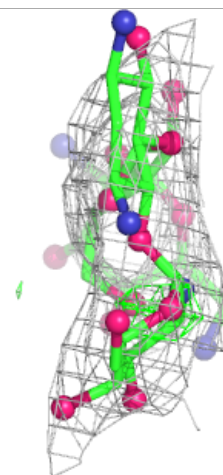
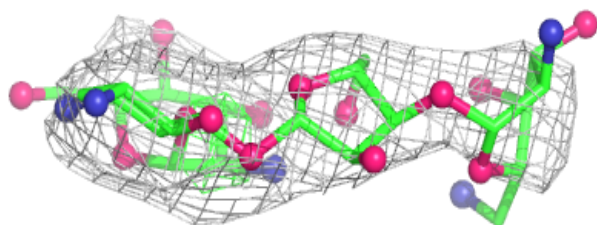
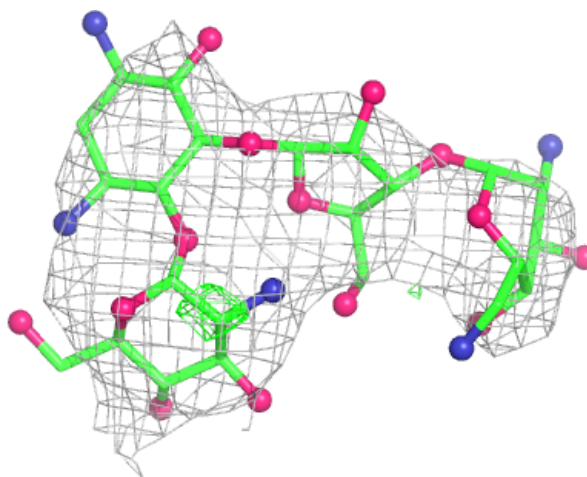
Electron density around PAR A 1617:

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



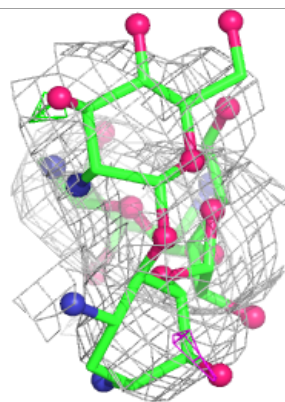
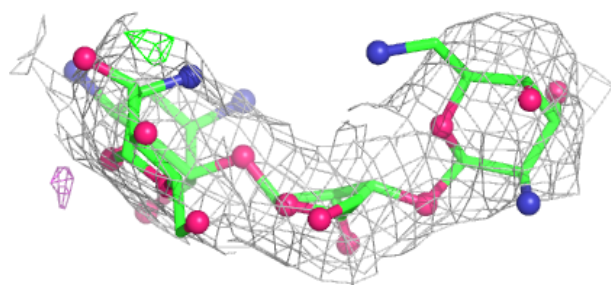
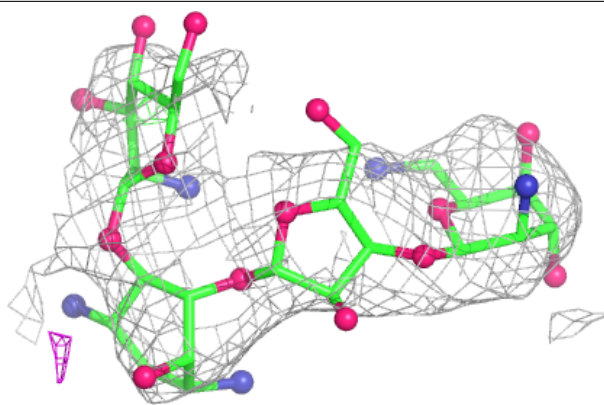
Electron density around PAR A 1605:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

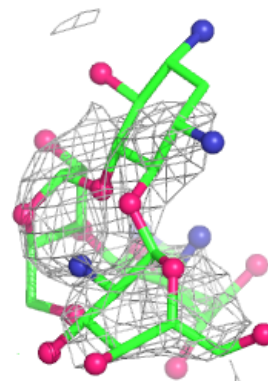
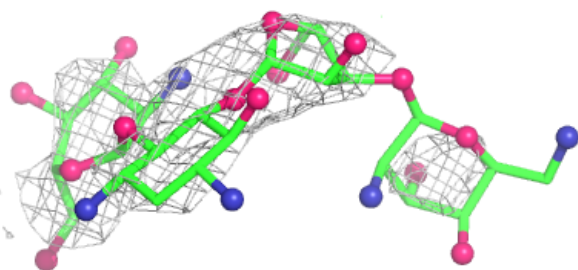
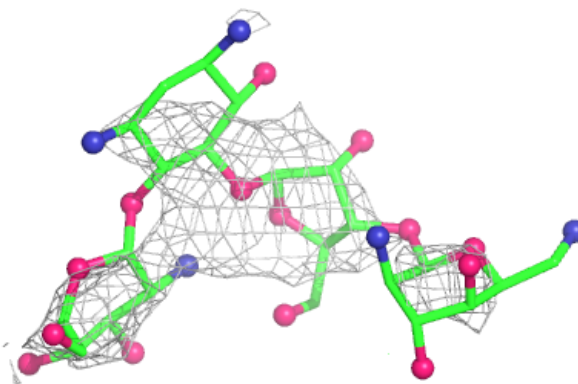


Electron density around PAR A 1612:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

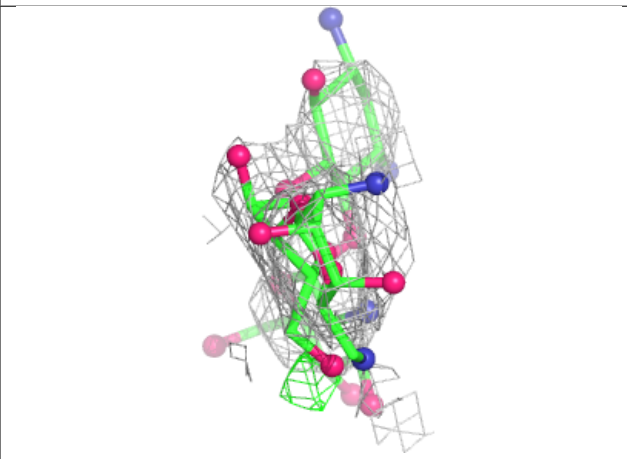
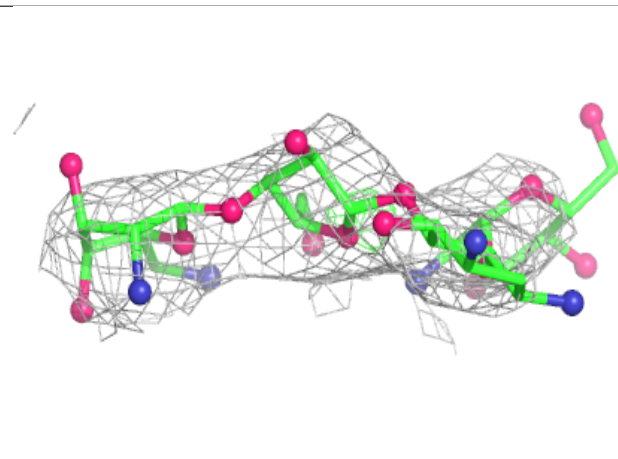
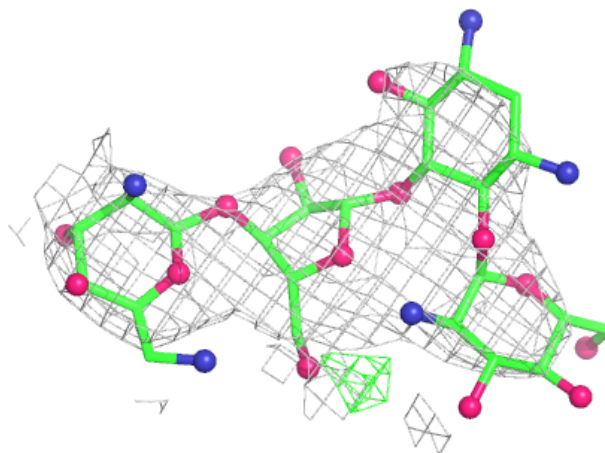
**Electron density around PAR A 1609:**

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



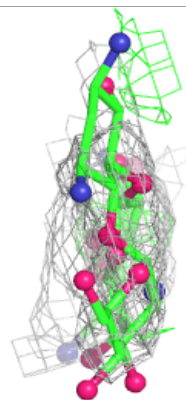
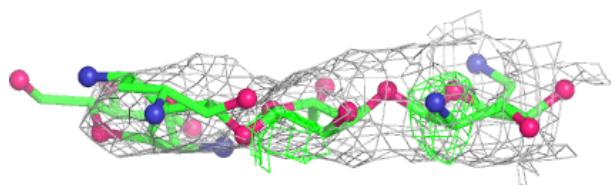
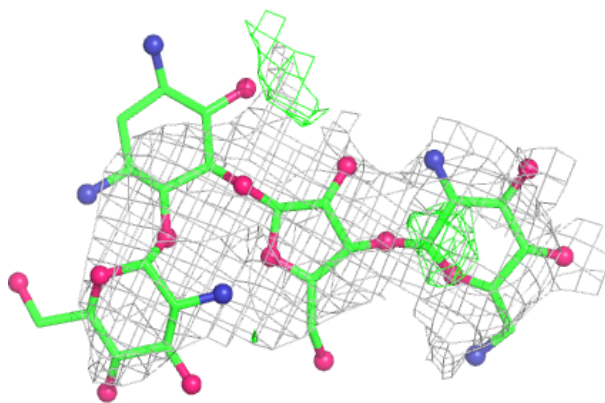
Electron density around PAR A 1606:

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



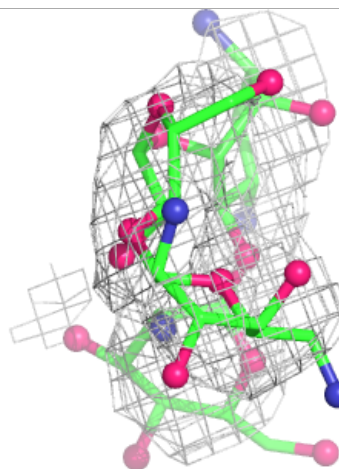
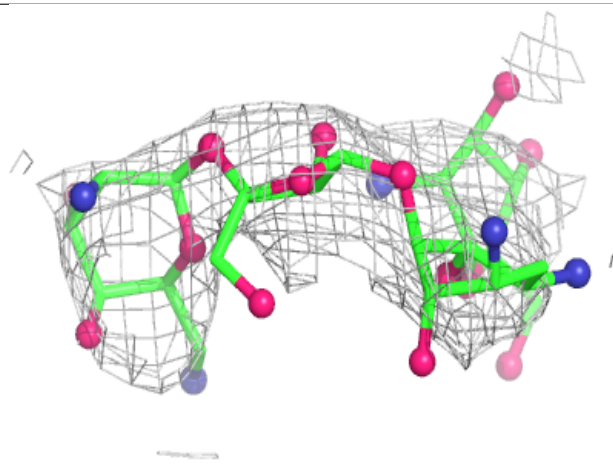
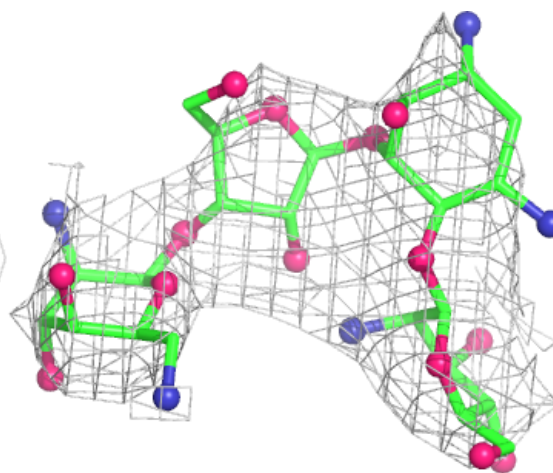
Electron density around PAR A 1608:

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



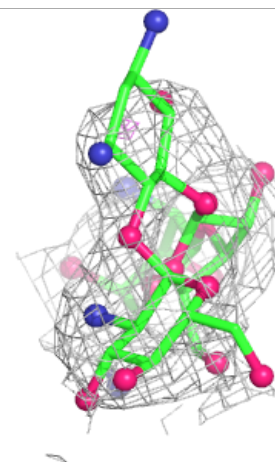
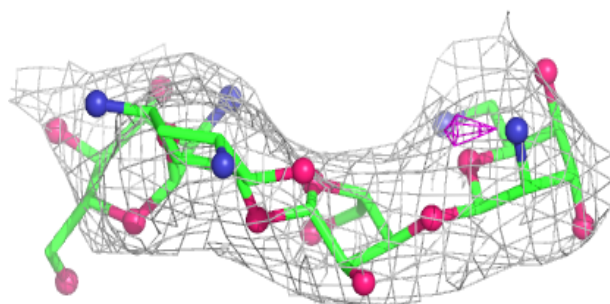
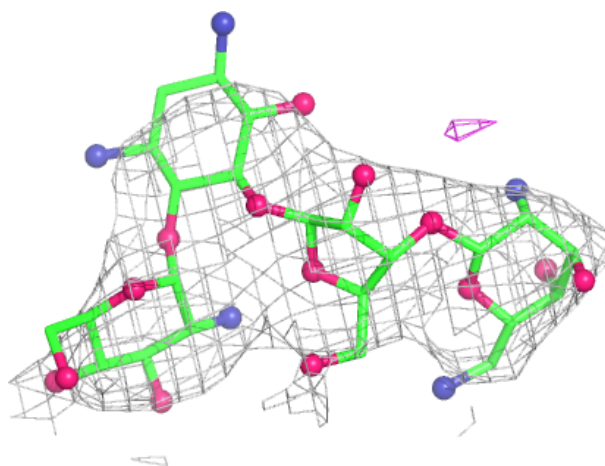
Electron density around PAR A 1613:

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



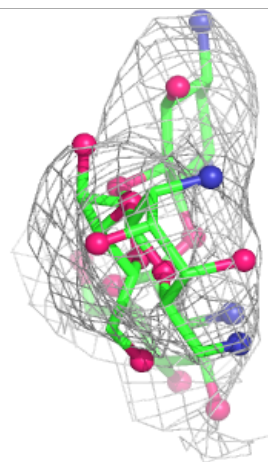
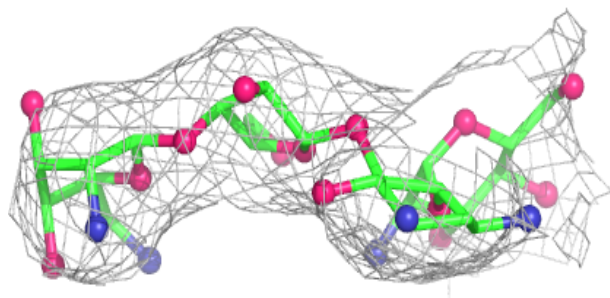
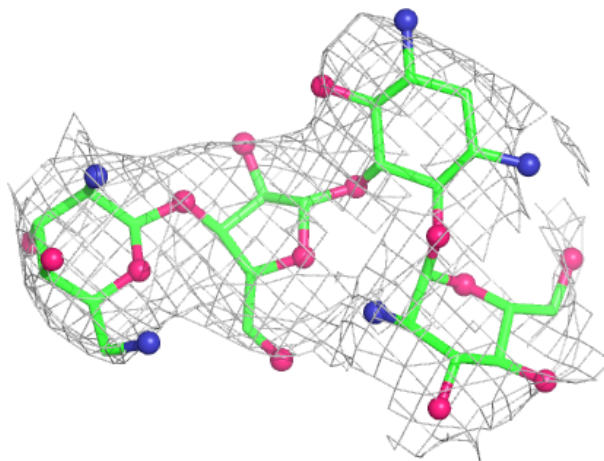
Electron density around PAR A 1603:

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



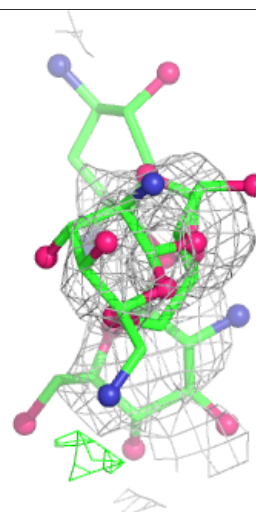
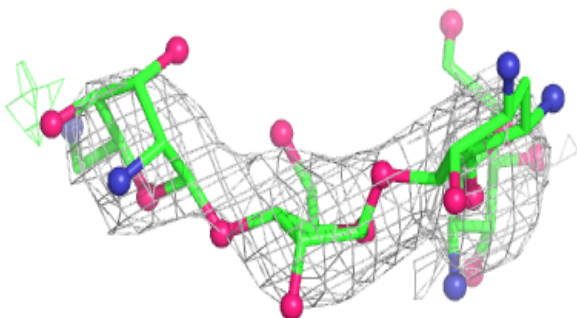
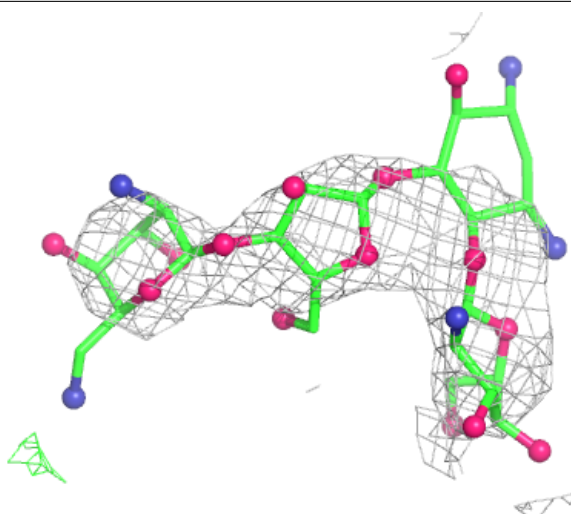
Electron density around PAR A 1601:

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



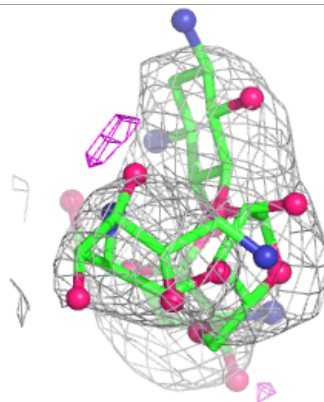
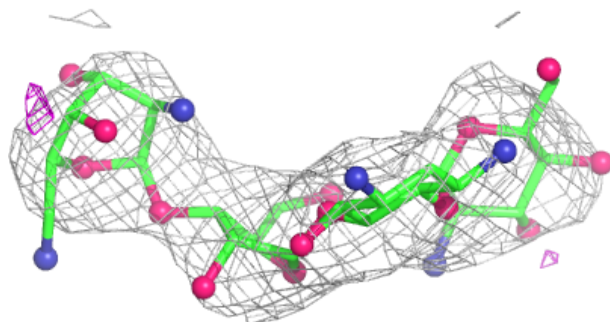
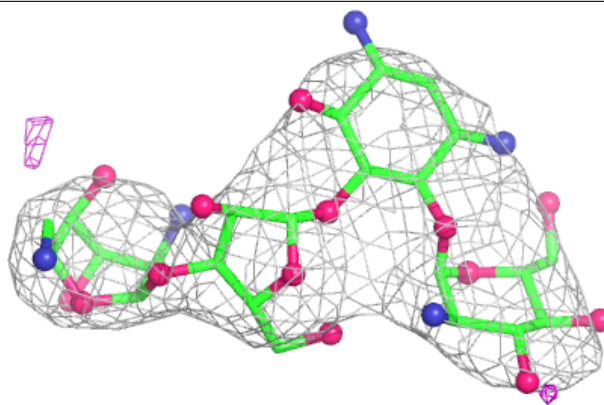
Electron density around PAR A 1607:

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



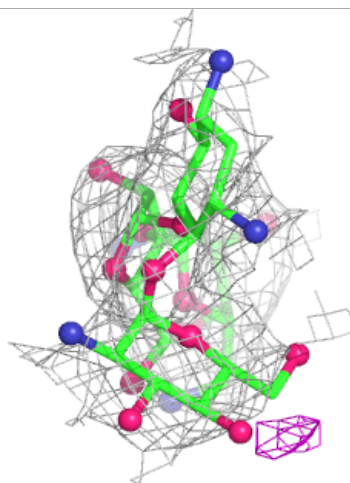
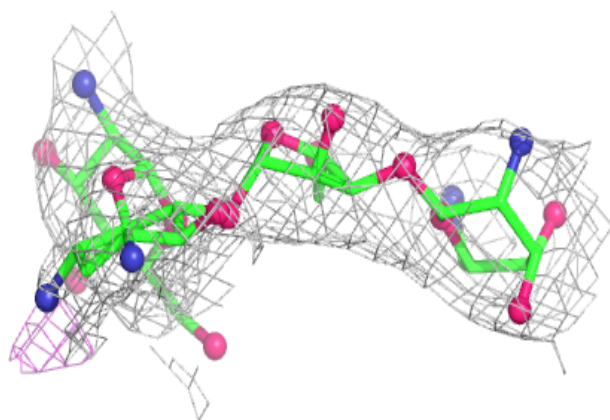
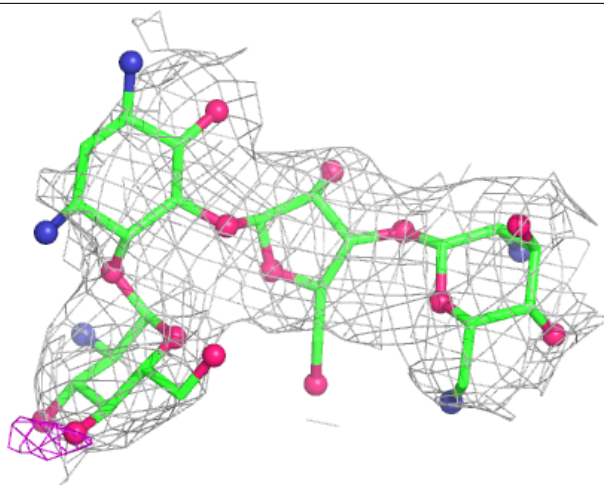
Electron density around PAR A 1602:

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



Electron density around PAR A 1604:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.