



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 01:05 PM UTC

PDB ID : 4DR2 / pdb_00004dr2
Title : Crystal structure of the *Thermus thermophilus* (HB8) 30S ribosomal subunit with 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 : 3.25 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 ⓘ](#)) 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

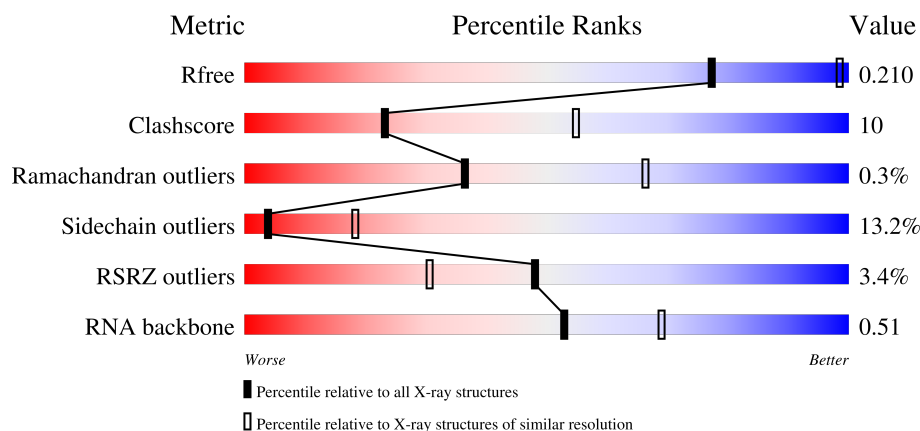
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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.



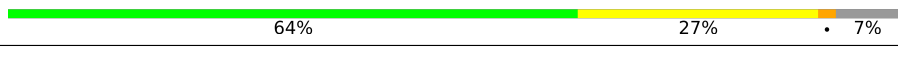
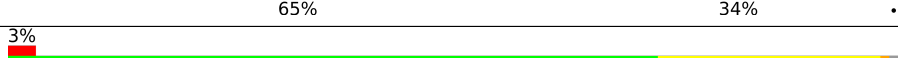
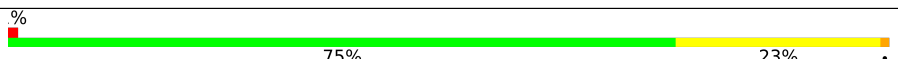
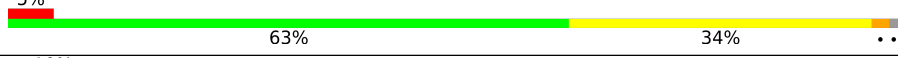
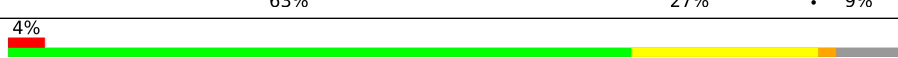
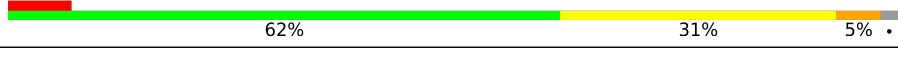
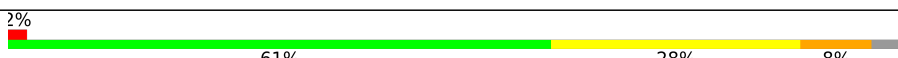
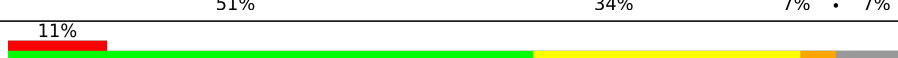
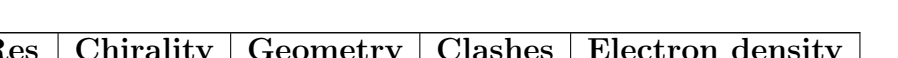
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2153 (3.28-3.20)
Clashscore	190562	2275 (3.28-3.20)
Ramachandran outliers	187476	2233 (3.28-3.20)
Sidechain outliers	187428	2232 (3.28-3.20)
RSRZ outliers	180081	2153 (3.28-3.20)
RNA backbone	3983	1047 (3.52-2.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	3% 57% 33% 9%
2	B	256	% 64% 25% 8%
3	C	239	3% 59% 22% 5% 13%

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Mol	Chain	Length	Quality of chain
4	D	209	
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	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	MG	A	1730	-	-	-	X
23	MG	A	1804	-	-	-	X
23	MG	A	1807	-	-	-	X
23	MG	A	1819	-	-	-	X
23	MG	A	1836	-	-	-	X
23	MG	A	1838	-	-	-	X
23	MG	A	1864	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	MG	A	1880	-	-	-	X
23	MG	A	1882	-	-	-	X
24	ZN	D	301	-	-	-	X

2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 53227 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	117	Total	C	N	O	S	0	0	0
			873	543	166	161	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
			491	311	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	101	Total	C	N	O	S	0	0	0
			838	536	157	143	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			

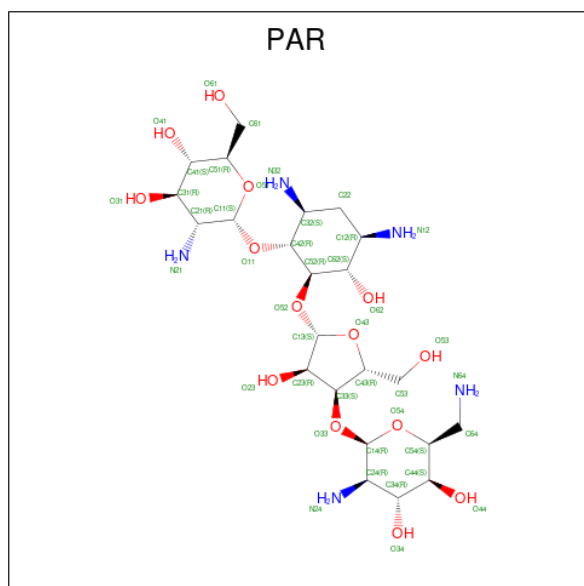
- Molecule 20 is a protein called 30S ribosomal protein S20.

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 PAROMOMYCIN (CCD ID: PAR) (formula: $C_{23}H_{45}N_5O_{14}$).



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

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

- Molecule 23 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	A	305	Total 311	Mg 311	0	6
23	D	2	Total 2	Mg 2	0	0
23	E	2	Total 2	Mg 2	0	0
23	F	1	Total 1	Mg 1	0	0
23	H	2	Total 2	Mg 2	0	0
23	I	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	L	1	Total 1	Mg 1	0	0
23	N	1	Total 1	Mg 1	0	0
23	O	1	Total 1	Mg 1	0	0
23	P	1	Total 1	Mg 1	0	0
23	Q	1	Total 1	Mg 1	0	0
23	S	1	Total 1	Mg 1	0	0
23	T	2	Total 2	Mg 2	0	0

- Molecule 24 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

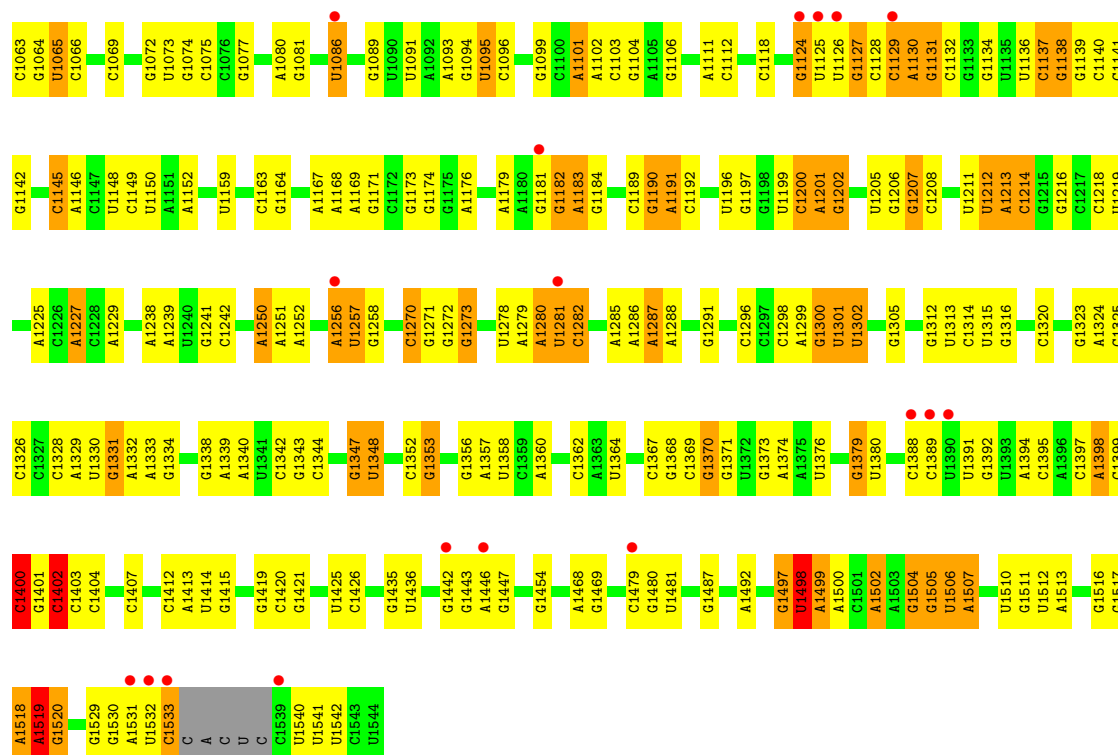
- Molecule 25 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	A	512	Total 512	O 512	0	0
25	C	1	Total 1	O 1	0	0
25	D	7	Total 7	O 7	0	0
25	E	6	Total 6	O 6	0	0
25	H	4	Total 4	O 4	0	0
25	L	2	Total 2	O 2	0	0
25	O	3	Total 3	O 3	0	0
25	T	1	Total 1	O 1	0	0

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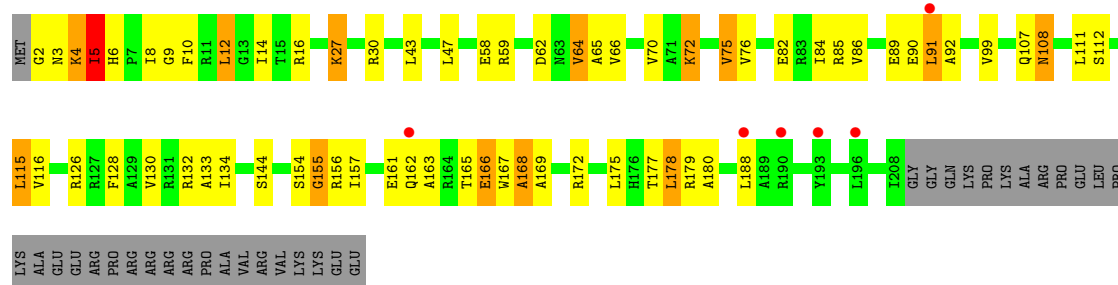
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	U	1	Total	O	0	0
			1	1		



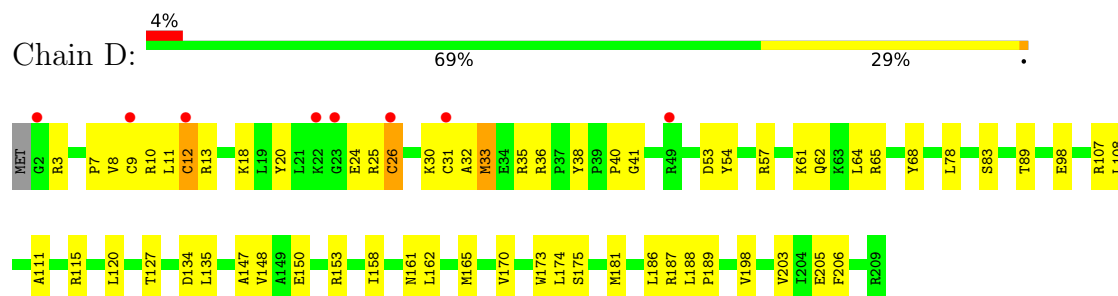
• Molecule 2: 30S ribosomal protein S2



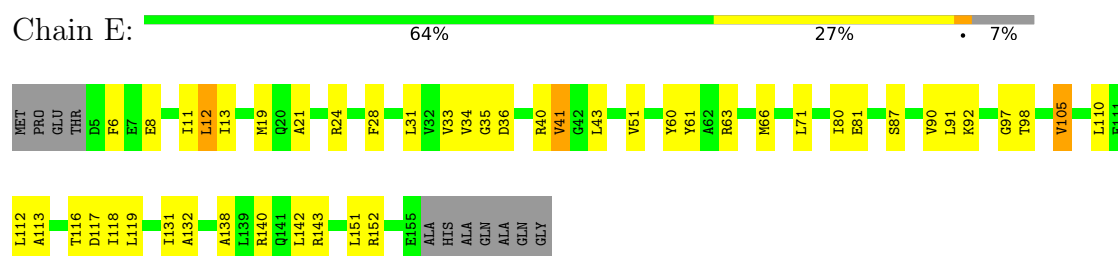
• Molecule 3: 30S ribosomal protein S3



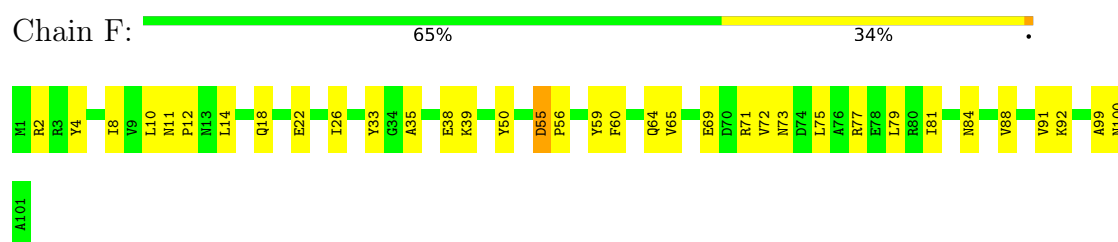
- Molecule 4: 30S ribosomal protein S4



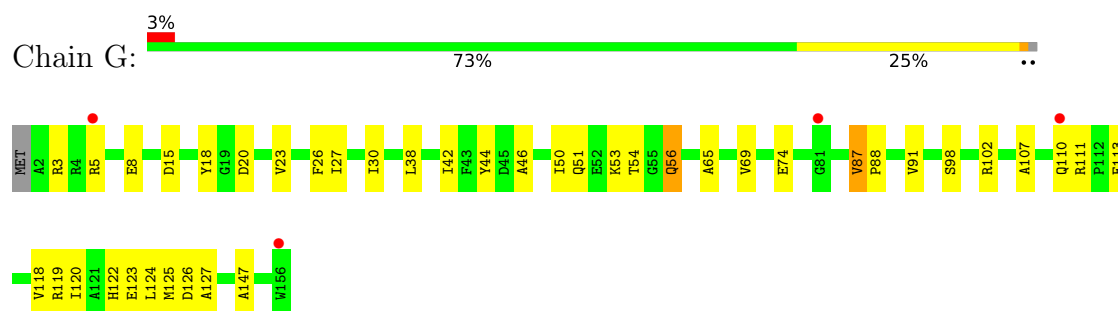
- Molecule 5: 30S ribosomal protein S5



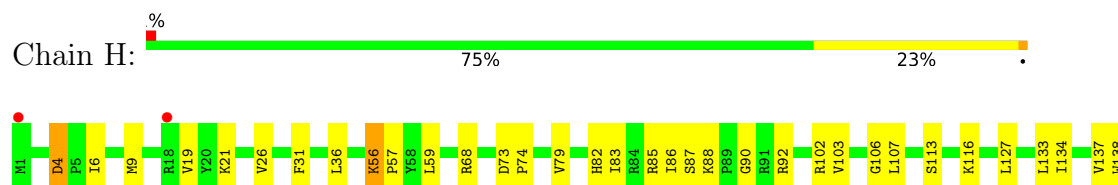
- Molecule 6: 30S ribosomal protein S6



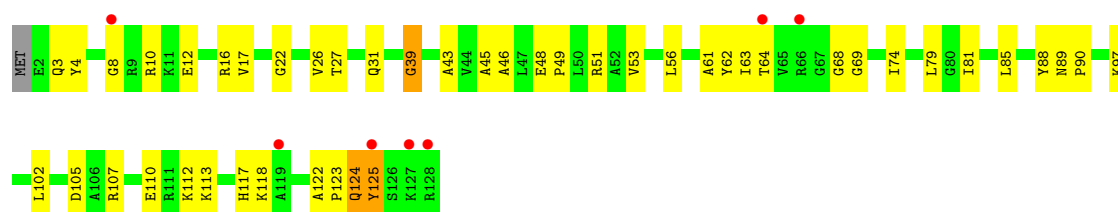
- Molecule 7: 30S ribosomal protein S7



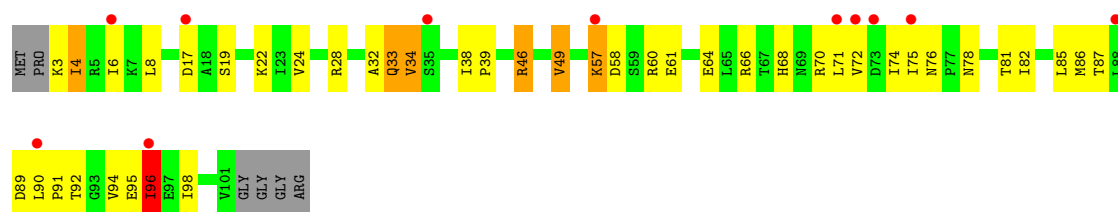
- Molecule 8: 30S ribosomal protein S8



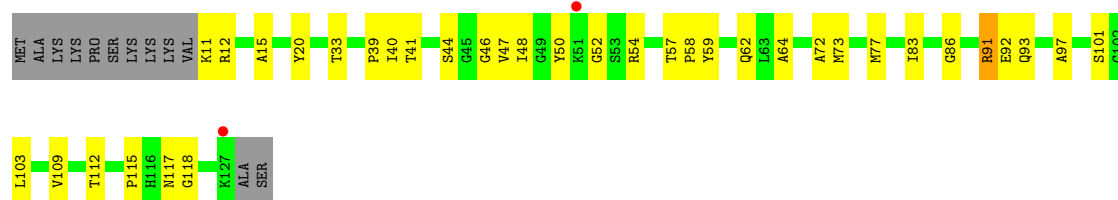
- Molecule 9: 30S ribosomal protein S9



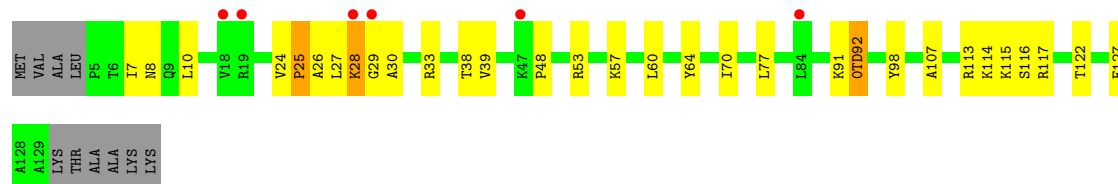
- Molecule 10: 30S ribosomal protein S10



- Molecule 11: 30S ribosomal protein S11

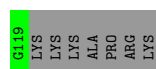


- Molecule 12: 30S ribosomal protein S12

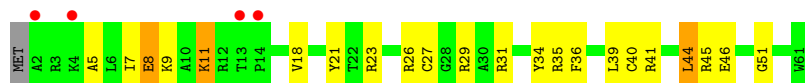


- Molecule 13: 30S ribosomal protein S13

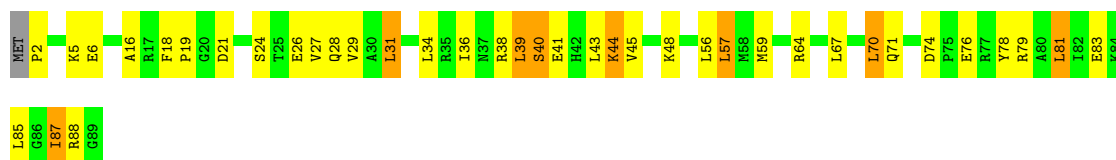




- Molecule 14: 30S ribosomal protein S14



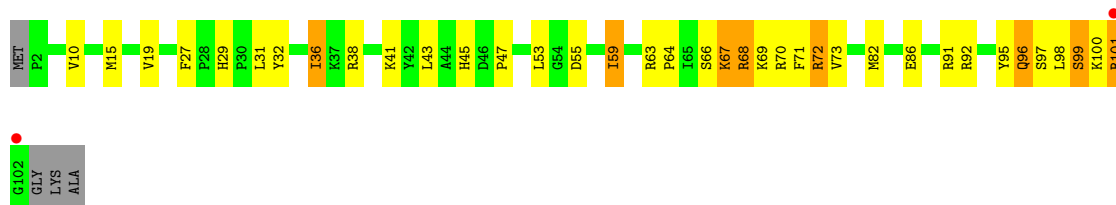
- Molecule 15: 30S ribosomal protein S15



- Molecule 16: 30S ribosomal protein S16



- Molecule 17: 30S ribosomal protein S17

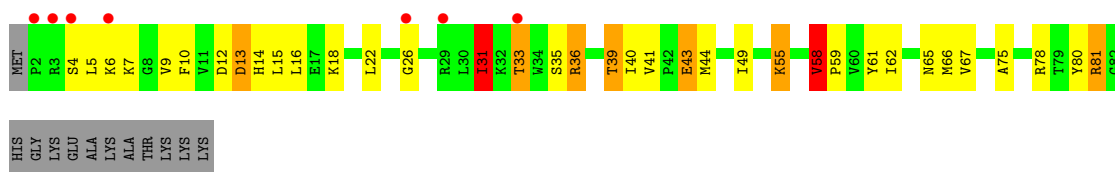


- Molecule 18: 30S ribosomal protein S18

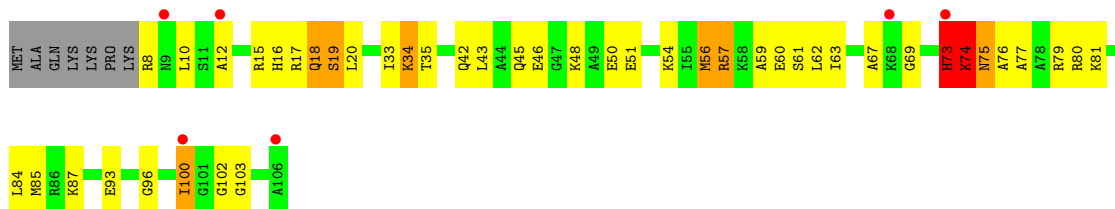


- Molecule 19: 30S ribosomal protein S19





- Molecule 20: 30S ribosomal protein S20



- Molecule 21: 30S ribosomal protein THX



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	402.60Å 402.60Å 177.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.39 – 3.25 44.39 – 3.25	Depositor EDS
% Data completeness (in resolution range)	99.6 (44.39-3.25) 99.3 (44.39-3.25)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 3.25Å)	Xtriage
Refinement program	PHENIX dev_978	Depositor
R, R_{free}	0.171 , 0.211 0.172 , 0.210	Depositor DCC
R_{free} test set	11415 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	88.7	Xtriage
Anisotropy	0.297	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 78.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	53227	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, PSU, 5MC, PAR, M2G, 0TD, UR3, MG, 4OC, 2MG, MA6, 7MG

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	0.37	0/36037	0.45	0/56239
2	B	0.51	0/1931	1.00	5/2607 (0.2%)
3	C	0.57	0/1637	0.99	7/2207 (0.3%)
4	D	0.55	0/1733	0.98	3/2318 (0.1%)
5	E	0.68	0/1163	1.09	4/1566 (0.3%)
6	F	0.49	0/856	0.94	3/1154 (0.3%)
7	G	0.49	0/1276	0.90	3/1709 (0.2%)
8	H	0.62	0/1136	1.10	6/1527 (0.4%)
9	I	0.50	0/1029	1.00	3/1379 (0.2%)
10	J	0.51	0/806	0.99	2/1084 (0.2%)
11	K	0.57	0/888	1.07	2/1198 (0.2%)
12	L	0.61	2/978 (0.2%)	1.07	4/1308 (0.3%)
13	M	0.50	0/947	0.95	1/1270 (0.1%)
14	N	0.50	0/500	1.00	1/663 (0.2%)
15	O	0.53	0/745	0.89	0/992
16	P	0.57	0/717	0.98	2/965 (0.2%)
17	Q	0.66	0/851	1.09	4/1136 (0.4%)
18	R	0.51	0/604	0.88	1/801 (0.1%)
19	S	0.44	0/662	0.96	3/892 (0.3%)
20	T	0.63	0/765	1.03	2/1007 (0.2%)
21	U	0.56	0/213	1.01	0/279
All	All	0.44	2/55474 (0.0%)	0.67	56/82301 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
3	C	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
8	H	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	L	25	PRO	CA-C	5.37	1.57	1.52
12	L	26	ALA	CA-CB	5.14	1.61	1.53

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	73	ASP	CA-C-N	10.10	130.37	119.87
8	H	73	ASP	C-N-CA	10.10	130.37	119.87
12	L	26	ALA	N-CA-C	-9.71	101.60	113.15
9	I	39	GLY	N-CA-C	-9.70	101.06	114.64
4	D	26	CYS	N-CA-C	-8.99	102.01	113.16
2	B	7	VAL	N-CA-C	8.28	118.36	110.42
17	Q	67	LYS	N-CA-C	-8.25	98.27	110.23
11	K	91	ARG	N-CA-C	-7.38	102.62	111.69
2	B	165	VAL	N-CA-C	7.13	118.77	111.00
4	D	12	CYS	N-CA-C	-7.05	102.41	111.02
20	T	96	GLY	N-CA-C	7.03	120.70	111.70
20	T	74	LYS	CB-CA-C	-6.98	107.49	115.79
3	C	180	ALA	N-CA-C	6.95	119.44	111.11
7	G	147	ALA	N-CA-C	-6.88	104.36	112.89
19	S	9	VAL	N-CA-C	6.85	118.27	109.30
12	L	127	GLU	CB-CA-C	-6.72	108.81	116.54
3	C	108	ASN	CA-C-N	6.59	126.28	119.82
3	C	108	ASN	C-N-CA	6.59	126.28	119.82
5	E	12	LEU	N-CA-C	6.45	118.87	109.07
6	F	55	ASP	CA-C-N	6.42	126.54	119.87
6	F	55	ASP	C-N-CA	6.42	126.54	119.87
5	E	41	VAL	CB-CA-C	-6.22	99.80	110.30
19	S	58	VAL	CA-C-N	6.17	127.55	119.84
19	S	58	VAL	C-N-CA	6.17	127.55	119.84
10	J	33	GLN	N-CA-C	6.14	120.24	112.87
11	K	101	SER	N-CA-C	-6.00	105.92	113.72
9	I	53	VAL	N-CA-C	5.99	117.92	112.29
14	N	7	ILE	N-CA-C	-5.98	105.51	112.98
2	B	15	VAL	N-CA-C	5.96	116.13	110.53
8	H	56	LYS	CA-C-N	5.83	126.12	119.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	56	LYS	C-N-CA	5.83	126.12	119.83
17	Q	29	HIS	CA-C-N	5.64	126.01	119.47
17	Q	29	HIS	C-N-CA	5.64	126.01	119.47
17	Q	99	SER	N-CA-C	5.50	122.52	110.80
4	D	33	MET	N-CA-C	-5.44	105.37	112.23
3	C	65	ALA	N-CA-C	5.38	117.96	111.40
7	G	56	GLN	N-CA-C	5.32	117.55	110.53
16	P	79	VAL	N-CA-C	-5.27	104.50	111.09
6	F	60	PHE	N-CA-C	5.26	117.31	108.73
3	C	155	GLY	N-CA-C	5.23	121.13	112.66
3	C	5	ILE	CB-CA-C	-5.22	103.41	111.08
5	E	105	VAL	CA-C-N	-5.20	114.31	119.56
5	E	105	VAL	C-N-CA	-5.20	114.31	119.56
7	G	87	VAL	N-CA-C	5.19	113.65	107.73
8	H	4	ASP	CA-C-N	5.18	125.48	119.47
8	H	4	ASP	C-N-CA	5.18	125.48	119.47
13	M	7	VAL	N-CA-C	5.14	115.76	110.36
2	B	148	TYR	N-CA-C	5.13	118.00	111.69
3	C	4	LYS	N-CA-C	5.13	121.73	110.80
2	B	7	VAL	CB-CA-C	-5.10	105.44	111.97
12	L	115	LYS	CA-C-N	-5.07	115.27	123.23
12	L	115	LYS	C-N-CA	-5.07	115.27	123.23
18	R	50	ILE	CB-CA-C	-5.07	104.53	111.33
10	J	96	ILE	N-CA-C	5.06	115.77	108.48
16	P	9	PHE	N-CA-C	5.02	121.50	110.80
9	I	22	GLY	N-CA-C	5.01	118.99	111.42

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	14	GLY	Peptide
3	C	166	GLU	Peptide
8	H	90	GLY	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	16434	454	0
2	B	1896	0	1936	36	0
3	C	1613	0	1677	45	0
4	D	1703	0	1763	51	0
5	E	1147	0	1207	36	0
6	F	843	0	857	25	0
7	G	1257	0	1296	30	0
8	H	1116	0	1177	28	0
9	I	1010	0	1037	34	0
10	J	793	0	835	33	0
11	K	873	0	894	22	0
12	L	973	0	1058	26	0
13	M	937	0	995	20	0
14	N	491	0	524	18	0
15	O	734	0	771	26	0
16	P	701	0	720	15	0
17	Q	838	0	909	24	0
18	R	598	0	670	18	0
19	S	648	0	673	22	0
20	T	763	0	861	33	0
21	U	209	0	221	6	0
22	A	714	0	765	34	0
23	A	311	0	0	0	0
23	D	2	0	0	0	0
23	E	2	0	0	0	0
23	F	1	0	0	0	0
23	H	2	0	0	0	0
23	I	1	0	0	0	0
23	L	1	0	0	0	0
23	N	1	0	0	0	0
23	O	1	0	0	0	0
23	P	1	0	0	0	0
23	Q	1	0	0	0	0
23	S	1	0	0	0	0
23	T	2	0	0	0	0
24	D	1	0	0	0	0
24	N	1	0	0	0	0
25	A	512	0	0	8	0
25	C	1	0	0	0	0
25	D	7	0	0	0	0
25	E	6	0	0	0	0
25	H	4	0	0	0	0
25	L	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	O	3	0	0	0	0
25	T	1	0	0	0	0
25	U	1	0	0	0	0
All	All	53227	0	37280	912	0

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

All (912) 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	1.51	0.90
1:A:1502:A:H2	1:A:1505:G:H1	1.15	0.89
1:A:1086:U:H3	1:A:1099:G:H22	1.23	0.86
19:S:33:THR:HG22	19:S:35:SER:H	1.41	0.85
1:A:427:U:OP1	4:D:13:ARG:NH2	2.12	0.83
7:G:113:GLU:HG2	7:G:119:ARG:HG3	1.62	0.81
1:A:1532:U:H2'	1:A:1533:C:H3'	1.60	0.81
3:C:58:GLU:HB3	10:J:92:THR:HG21	1.64	0.80
1:A:279:A:OP2	17:Q:95:TYR:OH	1.99	0.79
1:A:230:G:O6	22:A:1611:PAR:N24	2.14	0.79
17:Q:66:SER:O	17:Q:70:ARG:NH1	2.16	0.79
1:A:542:G:OP1	4:D:10:ARG:NH2	2.16	0.78
1:A:835:U:OP1	18:R:64:ARG:NH2	2.16	0.78
1:A:975:A:H4'	1:A:976:G:H5''	1.65	0.78
1:A:821:G:N7	22:A:1602:PAR:H641	1.99	0.77
9:I:8:GLY:HA2	9:I:79:LEU:HD13	1.64	0.77
13:M:14:ARG:HG3	13:M:44:ARG:HH21	1.49	0.77
20:T:43:LEU:HD13	20:T:51:GLU:HG3	1.66	0.77
1:A:774:G:OP2	22:A:1614:PAR:N64	2.18	0.76
20:T:75:ASN:OD1	20:T:75:ASN:N	2.18	0.76
1:A:1182:G:O2'	1:A:1183:A:OP2	2.03	0.75
2:B:84:GLU:HB3	2:B:219:VAL:HG21	1.68	0.74
10:J:19:SER:HB2	10:J:91:PRO:HG3	1.67	0.74
1:A:975:A:H5'	1:A:975:A:H8	1.53	0.74
1:A:972:C:OP1	10:J:57:LYS:NZ	2.13	0.73
1:A:235:C:N4	25:A:2155:HOH:O	2.20	0.73
4:D:7:PRO:HB2	4:D:10:ARG:HD2	1.70	0.72
12:L:39:VAL:HG23	12:L:57:LYS:HB2	1.72	0.71
4:D:98:GLU:OE2	4:D:107:ARG:NH1	2.23	0.71
1:A:664:G:H22	1:A:741:G:H1	1.37	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:927:G:H21	1:A:1532:U:H5''	1.55	0.71
10:J:49:VAL:HG23	14:N:41:ARG:HB2	1.71	0.70
1:A:192:U:H1'	20:T:103:GLY:HA2	1.73	0.70
1:A:1502:A:H2	1:A:1505:G:N1	1.88	0.70
3:C:155:GLY:HA3	3:C:163:ALA:HB1	1.74	0.70
1:A:452:A:HO2'	1:A:453:A:H8	1.39	0.70
1:A:1313:U:O4	19:S:4:SER:OG	2.08	0.70
1:A:946:A:H2'	1:A:947:G:C8	2.27	0.70
5:E:81:GLU:HG2	5:E:90:VAL:HG22	1.72	0.70
11:K:57:THR:HG22	11:K:59:TYR:H	1.56	0.69
13:M:10:PRO:HB3	13:M:18:ALA:HB1	1.72	0.69
1:A:1504:G:OP1	1:A:1507:A:H4'	1.92	0.69
1:A:250:A:H4'	1:A:251:G:O5'	1.91	0.69
3:C:108:ASN:HD21	3:C:144:SER:HB2	1.55	0.69
13:M:49:THR:HG22	13:M:51:ALA:H	1.57	0.69
1:A:390:C:O3'	16:P:28:ARG:NH2	2.26	0.69
1:A:278:G:OP2	17:Q:41:LYS:NZ	2.25	0.69
3:C:5:ILE:HD13	3:C:10:PHE:HB2	1.73	0.69
8:H:102:ARG:H	8:H:102:ARG:NE	1.88	0.69
1:A:1305:G:N2	1:A:1331:G:H1'	2.08	0.68
1:A:503:C:OP2	12:L:116:SER:HB3	1.93	0.68
1:A:261:U:OP2	20:T:79:ARG:NH2	2.26	0.68
1:A:1127:G:N2	1:A:1145:C:N3	2.37	0.68
1:A:1028:C:H42	1:A:1033:G:H1	1.40	0.68
1:A:1028:C:N3	1:A:1033:G:N2	2.43	0.67
10:J:3:LYS:N	10:J:75:ILE:HA	2.10	0.67
22:A:1610:PAR:H33	22:A:1610:PAR:H241	1.58	0.67
1:A:673:G:H2'	1:A:674:G:C8	2.30	0.67
1:A:976:G:H5'	1:A:1358:U:O2'	1.95	0.67
14:N:8:GLU:HG2	14:N:11:LYS:HE2	1.77	0.67
5:E:80:ILE:HG13	5:E:138:ALA:HB1	1.77	0.67
15:O:16:ALA:HB1	15:O:21:ASP:HB3	1.77	0.67
20:T:46:GLU:OE2	20:T:48:LYS:NZ	2.27	0.67
1:A:954:G:H21	1:A:1227:A:H62	1.43	0.66
1:A:1127:G:H1	1:A:1145:C:H42	1.43	0.66
1:A:1218:C:H2'	1:A:1219:U:C6	2.30	0.66
7:G:15:ASP:HB3	7:G:20:ASP:H	1.61	0.66
1:A:69:G:O6	22:A:1613:PAR:H221	1.96	0.66
20:T:60:GLU:HG3	20:T:81:LYS:HD2	1.77	0.66
1:A:344:A:H5''	1:A:345:C:H5	1.60	0.65
2:B:74:LYS:HD2	2:B:166:ASP:HB2	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:36:ARG:NH2	19:S:75:ALA:O	2.28	0.65
22:A:1614:PAR:N64	22:A:1614:PAR:O44	2.30	0.65
6:F:84:ASN:N	6:F:84:ASN:OD1	2.30	0.65
1:A:1291:G:H4'	9:I:39:GLY:HA3	1.78	0.65
1:A:1103:C:OP1	2:B:96:ARG:NH1	2.30	0.64
1:A:1505:G:O2'	1:A:1506:U:OP2	2.10	0.64
5:E:24:ARG:HH11	5:E:24:ARG:HB3	1.62	0.64
5:E:152:ARG:NH2	8:H:107:LEU:O	2.30	0.64
1:A:424:G:N7	22:A:1617:PAR:N21	2.40	0.64
1:A:926:G:H5''	1:A:927:G:OP1	1.98	0.64
2:B:139:LYS:HE2	2:B:143:GLU:HG3	1.78	0.64
1:A:411:A:OP2	4:D:25:ARG:NH2	2.31	0.64
12:L:77:LEU:HD21	12:L:107:ALA:HB2	1.80	0.64
1:A:933:G:O6	7:G:3:ARG:NH2	2.31	0.64
1:A:1131:G:OP1	9:I:3:GLN:NE2	2.31	0.64
7:G:111:ARG:HB2	7:G:119:ARG:HG2	1.79	0.64
1:A:1388:C:H2'	1:A:1389:C:O4'	1.97	0.64
1:A:1326:C:OP1	21:U:12:LYS:NZ	2.29	0.63
9:I:16:ARG:HG3	9:I:64:THR:HB	1.79	0.63
1:A:1281:U:O2'	1:A:1282:C:OP1	2.16	0.63
1:A:353:A:H5'	1:A:353:A:H8	1.63	0.63
1:A:1152:A:OP1	10:J:68:HIS:ND1	2.28	0.63
1:A:939:G:H5''	7:G:102:ARG:NH2	2.13	0.63
1:A:1003(A):G:N2	1:A:1038:C:O2	2.32	0.63
3:C:126:ARG:CZ	3:C:128:PHE:HB2	2.29	0.63
5:E:12:LEU:HD13	5:E:31:LEU:HB2	1.81	0.63
4:D:57:ARG:NH1	4:D:205:GLU:OE2	2.32	0.62
9:I:45:ALA:HA	9:I:48:GLU:HG2	1.81	0.62
1:A:1392:G:H21	1:A:1502:A:H8	1.47	0.62
1:A:537:G:OP1	12:L:113:ARG:NH2	2.32	0.62
1:A:991:U:O2'	1:A:992:U:O5'	2.16	0.62
6:F:100:ASN:HD21	18:R:23:LYS:HG2	1.65	0.62
11:K:33:THR:HG22	11:K:39:PRO:HA	1.80	0.62
12:L:27:LEU:O	12:L:29:GLY:N	2.32	0.62
20:T:54:LYS:HA	20:T:57:ARG:HH11	1.63	0.62
14:N:5:ALA:O	14:N:8:GLU:HB3	2.00	0.62
11:K:73:MET:HG3	11:K:103:LEU:HD21	1.82	0.62
1:A:538:G:H5''	12:L:114:LYS:HB2	1.80	0.62
1:A:1399:C:H4'	1:A:1400:5MC:H5''	1.82	0.62
1:A:235:C:H5'	17:Q:70:ARG:HG2	1.80	0.62
1:A:619:U:N3	4:D:134:ASP:OD2	2.25	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:A:OP2	22:A:1604:PAR:H24	1.99	0.61
1:A:928:G:H2'	1:A:929:G:C8	2.34	0.61
9:I:110:GLU:OE2	9:I:113:LYS:NZ	2.33	0.61
1:A:474:G:H2'	1:A:475:G:H8	1.64	0.61
1:A:1479:C:H2'	1:A:1480:G:H8	1.65	0.61
9:I:46:ALA:HB2	9:I:74:ILE:HG23	1.82	0.61
1:A:359:U:H2'	1:A:360:A:C8	2.36	0.61
1:A:1023:G:O6	1:A:1024:G:N2	2.34	0.61
1:A:1077:G:N2	1:A:1080:A:OP2	2.31	0.61
1:A:1128:C:HO2'	1:A:1130:A:H8	1.47	0.61
1:A:1137:C:H4'	1:A:1138:G:C2	2.36	0.61
1:A:103:C:OP1	20:T:17:ARG:NH1	2.32	0.61
1:A:407:G:H5''	4:D:115:ARG:HB3	1.82	0.61
1:A:1323:G:H2'	1:A:1324:A:C8	2.35	0.61
22:A:1609:PAR:O43	22:A:1609:PAR:N21	2.34	0.61
8:H:19:VAL:HG23	8:H:21:LYS:HD3	1.83	0.61
13:M:52:GLU:HG2	13:M:55:ARG:HH21	1.64	0.61
1:A:1134:G:N2	1:A:1140:C:N3	2.45	0.61
1:A:1189:C:H5''	3:C:5:ILE:HG12	1.81	0.61
18:R:32:ARG:HA	18:R:69:THR:HG21	1.82	0.60
7:G:122:HIS:HA	7:G:125:MET:HE2	1.81	0.60
9:I:51:ARG:HA	9:I:56:LEU:HD11	1.83	0.60
10:J:91:PRO:HB2	10:J:94:VAL:HB	1.83	0.60
15:O:36:ILE:HG13	15:O:59:MET:HE2	1.83	0.60
10:J:24:VAL:HG13	10:J:34:VAL:HG11	1.82	0.60
7:G:111:ARG:NH2	7:G:126:ASP:OD1	2.35	0.60
1:A:1347:G:O2'	1:A:1348:U:OP2	2.19	0.60
16:P:74:LEU:O	16:P:79:VAL:HG23	2.02	0.60
1:A:98:U:O4	22:A:1613:PAR:N12	2.35	0.60
1:A:776:G:O6	22:A:1614:PAR:N24	2.35	0.60
9:I:8:GLY:HA3	9:I:79:LEU:HB3	1.83	0.60
1:A:983:A:O2'	1:A:1050:G:OP2	2.20	0.59
3:C:27:LYS:HD3	3:C:27:LYS:H	1.65	0.59
8:H:85:ARG:NE	8:H:87:SER:O	2.35	0.59
19:S:40:ILE:HG23	19:S:62:ILE:HD11	1.83	0.59
3:C:12:LEU:HD11	14:N:51:GLY:HA2	1.82	0.59
7:G:15:ASP:OD2	7:G:44:TYR:OH	2.15	0.59
1:A:1435:G:H2'	1:A:1436:U:C6	2.36	0.59
7:G:5:ARG:HH12	7:G:8:GLU:HG2	1.67	0.59
7:G:15:ASP:OD1	7:G:18:TYR:N	2.24	0.59
13:M:5:ALA:HB1	13:M:66:LEU:HD12	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1497:G:H2'	1:A:1498:UR3:H5'	1.85	0.59
3:C:156:ARG:H	3:C:163:ALA:HA	1.68	0.59
12:L:25:PRO:C	12:L:27:LEU:H	2.08	0.59
1:A:1376:U:OP1	7:G:98:SER:OG	2.20	0.59
20:T:15:ARG:HA	20:T:18:GLN:HG3	1.85	0.59
6:F:2:ARG:NE	6:F:69:GLU:HG2	2.18	0.59
1:A:670:G:H21	6:F:73:ASN:HD21	1.51	0.58
1:A:975:A:H5'	1:A:975:A:C8	2.37	0.58
1:A:1057:G:H5''	3:C:154:SER:CB	2.33	0.58
1:A:1200:C:O2'	1:A:1205:U:O4	2.20	0.58
1:A:1510:U:H2'	1:A:1511:G:C8	2.38	0.58
1:A:765:G:H5''	1:A:766:A:OP1	2.03	0.58
1:A:1024:G:N1	25:A:2509:HOH:O	2.29	0.58
10:J:64:GLU:OE2	10:J:66:ARG:NH2	2.37	0.58
1:A:328:C:H4'	1:A:329:A:H5'	1.84	0.58
5:E:35:GLY:HA3	5:E:112:LEU:HB3	1.85	0.58
20:T:69:GLY:O	20:T:73:HIS:ND1	2.37	0.58
1:A:580:U:H2'	1:A:581:G:O4'	2.04	0.58
1:A:1148:U:H2'	1:A:1149:C:O4'	2.04	0.58
22:A:1612:PAR:N64	22:A:1612:PAR:O33	2.36	0.58
1:A:1301:U:O2'	1:A:1302:U:O5'	2.21	0.58
1:A:372:C:H4'	1:A:373:A:O5'	2.03	0.58
13:M:11:ARG:HG3	13:M:12:ASN:HB2	1.86	0.58
2:B:215:LEU:O	2:B:219:VAL:HG23	2.03	0.57
5:E:33:VAL:HG12	5:E:112:LEU:HD12	1.85	0.57
1:A:17:U:H2'	1:A:18:C:C6	2.39	0.57
1:A:1065:U:H5''	1:A:1190:G:N2	2.19	0.57
1:A:1513:A:N6	25:A:2425:HOH:O	2.35	0.57
15:O:70:LEU:HD13	15:O:78:TYR:HA	1.87	0.57
11:K:40:ILE:HG22	11:K:41:THR:HG23	1.87	0.57
1:A:1006:C:H42	1:A:1024:G:H21	1.52	0.57
1:A:182:U:OP2	1:A:182:U:H6	1.87	0.57
1:A:974:A:OP1	1:A:974:A:H8	1.88	0.57
1:A:1347:G:O2'	1:A:1348:U:P	2.62	0.57
1:A:974:A:P	14:N:41:ARG:HH12	2.28	0.57
1:A:1168:A:H2'	1:A:1169:A:C8	2.39	0.57
1:A:1305:G:H5''	21:U:4:GLY:HA3	1.86	0.57
11:K:58:PRO:HB3	11:K:93:GLN:HG3	1.86	0.57
1:A:1402:4OC:HM22	1:A:1403:C:H5'	1.86	0.57
3:C:6:HIS:CD2	3:C:8:ILE:HB	2.39	0.57
10:J:46:ARG:HG3	10:J:46:ARG:HH11	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:24:GLU:HG2	4:D:25:ARG:H	1.69	0.57
5:E:80:ILE:HD11	5:E:91:LEU:HD12	1.87	0.57
1:A:1112:C:H1'	3:C:179:ARG:HE	1.70	0.56
3:C:130:VAL:O	3:C:134:ILE:HG13	2.05	0.56
1:A:1392:G:N2	1:A:1502:A:H8	2.03	0.56
5:E:98:THR:HB	5:E:117:ASP:HB3	1.87	0.56
10:J:17:ASP:OD1	10:J:70:ARG:NH1	2.24	0.56
1:A:1300:G:O2'	1:A:1301:U:O5'	2.22	0.56
3:C:128:PHE:HZ	3:C:132:ARG:HD2	1.70	0.56
7:G:113:GLU:HG3	7:G:118:VAL:HG12	1.86	0.56
19:S:13:ASP:HA	19:S:16:LEU:HB3	1.88	0.56
1:A:1207:2MG:HM23	1:A:1208:C:H1'	1.87	0.56
12:L:28:LYS:HB3	12:L:30:ALA:HB2	1.87	0.56
1:A:141:A:H1'	1:A:182:U:O2	2.05	0.56
22:A:1607:PAR:O44	22:A:1607:PAR:N64	2.38	0.56
6:F:39:LYS:HB3	6:F:64:GLN:HB3	1.88	0.56
7:G:46:ALA:O	7:G:50:ILE:HG12	2.05	0.56
1:A:1124:G:H2'	1:A:1145:C:H5	1.71	0.56
1:A:1256:A:H4'	1:A:1257:U:O5'	2.06	0.56
5:E:140:ARG:O	5:E:143:ARG:NH2	2.39	0.56
1:A:581:G:O3'	15:O:64:ARG:NH2	2.38	0.56
19:S:10:PHE:O	19:S:39:THR:OG1	2.19	0.56
1:A:328:C:H2'	1:A:328:C:O2	2.06	0.55
1:A:1343:G:H2'	1:A:1344:C:C6	2.41	0.55
1:A:1497:G:C2'	1:A:1498:UR3:H5'	2.36	0.55
3:C:128:PHE:CZ	3:C:132:ARG:HD2	2.41	0.55
22:A:1617:PAR:O44	22:A:1617:PAR:N64	2.35	0.55
1:A:1057:G:H5''	3:C:154:SER:HB2	1.89	0.55
1:A:1049:U:H4'	1:A:1050:G:O5'	2.06	0.55
8:H:36:LEU:HD12	8:H:59:LEU:HD13	1.87	0.55
1:A:201:C:H42	1:A:216:G:H1	1.54	0.55
1:A:877:C:H5''	8:H:88:LYS:HD3	1.88	0.55
1:A:1129:C:OP1	9:I:62:TYR:OH	2.22	0.55
1:A:1038:C:H2'	1:A:1039:C:H6	1.70	0.55
1:A:1328:C:H2'	1:A:1329:A:C8	2.42	0.55
4:D:31:CYS:C	4:D:33:MET:H	2.14	0.55
15:O:36:ILE:O	15:O:40:SER:OG	2.25	0.55
19:S:18:LYS:HG2	19:S:31:ILE:HD11	1.88	0.55
1:A:646:U:H2'	1:A:647:C:C6	2.42	0.55
1:A:684:A:O3'	11:K:12:ARG:NH2	2.39	0.55
1:A:707:C:H2'	1:A:708:C:H6	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:991:U:HO2'	1:A:992:U:P	2.29	0.55
21:U:5:ASP:O	21:U:11:GLY:HA3	2.07	0.55
8:H:4:ASP:OD1	8:H:85:ARG:NH1	2.41	0.54
12:L:24:VAL:HG13	12:L:98:TYR:CE2	2.43	0.54
2:B:98:LEU:HG	2:B:101:MET:HE3	1.89	0.54
8:H:86:ILE:HD12	8:H:133:LEU:HD22	1.89	0.54
1:A:1241:G:H2'	1:A:1242:C:C6	2.43	0.54
22:A:1610:PAR:H33	22:A:1610:PAR:N24	2.22	0.54
1:A:432:A:HO2'	1:A:433:C:P	2.30	0.54
1:A:939:G:H2'	1:A:940:C:C6	2.42	0.54
10:J:34:VAL:HA	10:J:74:ILE:HG12	1.88	0.54
1:A:7:G:H5'	1:A:298:A:O4'	2.06	0.54
1:A:151:A:H2'	1:A:152:A:O4'	2.07	0.54
1:A:353:A:H5'	1:A:353:A:C8	2.43	0.54
1:A:1328:C:H2'	1:A:1329:A:H8	1.73	0.54
1:A:1532:U:H6	1:A:1532:U:O5'	1.91	0.54
4:D:111:ALA:HB2	4:D:120:LEU:HD12	1.89	0.54
1:A:748:C:H4'	1:A:749:C:O5'	2.06	0.54
4:D:36:ARG:HB3	4:D:38:TYR:CE2	2.43	0.54
13:M:37:THR:HG22	13:M:39:ILE:HG13	1.90	0.54
17:Q:59:ILE:HG23	17:Q:71:PHE:HB3	1.90	0.54
1:A:922:G:N3	1:A:1398:A:H2	2.06	0.54
14:N:27:CYS:SG	14:N:29:ARG:HB2	2.48	0.54
16:P:49:LEU:HD11	16:P:73:LEU:HB3	1.90	0.54
20:T:56:MET:HE1	20:T:85:MET:HA	1.90	0.54
10:J:61:GLU:OE1	14:N:45:ARG:NH1	2.36	0.53
11:K:50:TYR:HD2	11:K:54:ARG:HH11	1.55	0.53
1:A:665:A:H2'	1:A:732:C:O2	2.08	0.53
7:G:38:LEU:O	7:G:42:ILE:HG13	2.08	0.53
9:I:43:ALA:HA	9:I:74:ILE:HD13	1.90	0.53
1:A:877:C:OP1	8:H:88:LYS:NZ	2.34	0.53
4:D:170:VAL:HG13	4:D:174:LEU:HB2	1.89	0.53
7:G:51:GLN:C	7:G:53:LYS:H	2.17	0.53
18:R:47:THR:HG22	18:R:48:GLY:H	1.73	0.53
1:A:371:G:O2'	1:A:372:C:H5'	2.08	0.53
1:A:1250:A:H4'	9:I:68:GLY:N	2.23	0.53
11:K:72:ALA:HB1	11:K:77:MET:HE2	1.89	0.53
1:A:192:U:C1'	20:T:103:GLY:HA2	2.38	0.53
1:A:563:A:H5''	1:A:564:C:OP1	2.07	0.53
1:A:547:A:H4'	1:A:548:G:O5'	2.09	0.53
1:A:563:A:H2'	1:A:567:G:C8	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1057:G:H2'	1:A:1058:G:O4'	2.09	0.53
1:A:1412:C:H2'	1:A:1413:A:C8	2.43	0.53
2:B:91:PRO:HB3	2:B:154:LEU:HB2	1.89	0.53
1:A:180:U:H2'	1:A:181:G:H5'	1.91	0.53
10:J:33:GLN:HB2	10:J:75:ILE:HD11	1.91	0.53
22:A:1610:PAR:O53	22:A:1610:PAR:N21	2.42	0.53
6:F:33:TYR:HA	6:F:71:ARG:HH21	1.74	0.53
8:H:92:ARG:HH11	8:H:92:ARG:CG	2.22	0.53
1:A:421:U:H5'	1:A:422:C:C5	2.44	0.52
1:A:620:C:C2	4:D:135:LEU:HD13	2.44	0.52
1:A:933:G:OP2	7:G:3:ARG:HB3	2.09	0.52
1:A:1064:G:H1'	1:A:1190:G:H21	1.75	0.52
7:G:111:ARG:HD2	7:G:123:GLU:HB2	1.91	0.52
1:A:519:C:H2'	1:A:520:A:C8	2.45	0.52
5:E:97:GLY:N	5:E:117:ASP:OD1	2.43	0.52
15:O:71:GLN:HB2	15:O:78:TYR:CD1	2.45	0.52
1:A:1389:C:H6	1:A:1389:C:O5'	1.92	0.52
8:H:102:ARG:H	8:H:102:ARG:HE	1.57	0.52
1:A:222:U:H2'	1:A:223:U:C6	2.45	0.52
1:A:308:C:H2'	1:A:309:G:C8	2.44	0.52
1:A:390:C:H2'	1:A:391:G:C8	2.45	0.52
1:A:1296:C:H4'	1:A:1302:U:C5	2.44	0.52
1:A:1367:C:H5'	10:J:60:ARG:NH1	2.23	0.52
4:D:61:LYS:HE2	4:D:206:PHE:CE2	2.45	0.52
1:A:1286:A:H2'	1:A:1287:A:H4'	1.91	0.52
3:C:130:VAL:HG12	3:C:134:ILE:HD11	1.91	0.52
10:J:39:PRO:HA	10:J:70:ARG:HD3	1.91	0.52
20:T:50:GLU:HG3	20:T:100:ILE:HG13	1.92	0.52
1:A:116:A:H61	1:A:313:A:H1'	1.75	0.52
1:A:610:G:OP1	22:A:1606:PAR:H641	2.10	0.52
1:A:664:G:OP1	18:R:64:ARG:NH1	2.37	0.52
1:A:972:C:P	10:J:57:LYS:HD2	2.50	0.52
1:A:974:A:OP2	14:N:41:ARG:NH1	2.43	0.52
1:A:1347:G:N7	9:I:10:ARG:NH2	2.57	0.52
13:M:107:ALA:O	13:M:111:LYS:HB2	2.10	0.52
1:A:149:A:H2'	1:A:150:C:C6	2.45	0.52
1:A:1182:G:H4'	1:A:1183:A:O5'	2.10	0.52
2:B:47:THR:HA	2:B:202:PRO:HG2	1.92	0.52
2:B:195:ASP:O	8:H:68:ARG:NH2	2.42	0.52
17:Q:45:HIS:HB3	17:Q:72:ARG:HG3	1.92	0.52
1:A:1069:C:O2'	1:A:1192:C:H1'	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:642:A:N3	8:H:113:SER:OG	2.43	0.51
22:A:1612:PAR:N21	22:A:1612:PAR:O43	2.42	0.51
3:C:134:ILE:HG22	3:C:168:ALA:HB3	1.91	0.51
4:D:20:TYR:HD2	4:D:26:CYS:HB3	1.75	0.51
1:A:308:C:H2'	1:A:309:G:H8	1.75	0.51
1:A:923:A:OP1	5:E:21:ALA:HB2	2.11	0.51
1:A:1128:C:H6	1:A:1128:C:O5'	1.93	0.51
2:B:223:ILE:HD13	2:B:230:VAL:H	1.75	0.51
11:K:20:TYR:CE2	11:K:83:ILE:HD13	2.46	0.51
13:M:16:ASP:OD1	13:M:16:ASP:N	2.43	0.51
1:A:1339:A:H2'	1:A:1340:A:O4'	2.10	0.51
1:A:389:A:C6	1:A:390:C:H1'	2.46	0.51
10:J:89:ASP:HB2	10:J:91:PRO:HD2	1.92	0.51
20:T:10:LEU:HG	20:T:12:ALA:H	1.75	0.51
1:A:559:A:H4'	1:A:560:U:O5'	2.11	0.51
1:A:1516:G:H2'	1:A:1518:MA6:OP2	2.11	0.51
1:A:1300:G:O2'	1:A:1301:U:P	2.68	0.51
1:A:432:A:H2'	1:A:433:C:O4'	2.11	0.51
1:A:820:U:H4'	1:A:821:G:OP2	2.11	0.51
5:E:11:ILE:HG23	5:E:105:VAL:HG22	1.92	0.51
4:D:35:ARG:C	4:D:36:ARG:HG3	2.34	0.50
1:A:1062:U:H2'	1:A:1063:C:C6	2.47	0.50
2:B:82:ARG:O	2:B:86:GLU:HB2	2.11	0.50
11:K:62:GLN:HG3	11:K:97:ALA:HB2	1.92	0.50
15:O:5:LYS:H	15:O:5:LYS:HD2	1.75	0.50
1:A:413:G:N2	1:A:428:G:H1'	2.26	0.50
1:A:1031:G:H2'	1:A:1032:G:C8	2.46	0.50
22:A:1604:PAR:H11	22:A:1604:PAR:O52	2.11	0.50
1:A:509:A:H5'	4:D:54:TYR:HD2	1.76	0.50
12:L:53:ARG:HH12	12:L:92:OTD:CG	2.24	0.50
1:A:299:G:H2'	1:A:300:A:C8	2.47	0.50
1:A:1031:G:H2'	1:A:1032:G:H8	1.75	0.50
4:D:57:ARG:HB2	4:D:206:PHE:HB2	1.94	0.50
9:I:81:ILE:O	9:I:85:LEU:HB2	2.11	0.50
20:T:76:ALA:O	20:T:80:ARG:HG3	2.11	0.50
1:A:1015:A:H2'	1:A:1016:A:C8	2.47	0.50
21:U:6:ARG:HG3	21:U:15:ARG:NH2	2.27	0.50
1:A:129:U:O3'	1:A:129(A):G:H3'	2.11	0.50
1:A:1060:C:C5	3:C:2:GLY:HA3	2.46	0.50
1:A:1216:G:H5''	14:N:5:ALA:HB2	1.93	0.50
1:A:1342:C:O2'	9:I:124:GLN:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:153:ARG:HD3	4:D:181:MET:HG3	1.93	0.50
15:O:41:GLU:O	15:O:44:LYS:HB2	2.11	0.50
1:A:294:U:OP1	1:A:610:G:O2'	2.25	0.49
1:A:1137:C:H4'	1:A:1138:G:N2	2.27	0.49
1:A:254:G:OP1	17:Q:67:LYS:O	2.30	0.49
1:A:457:C:H2'	1:A:458:C:H6	1.78	0.49
22:A:1616:PAR:HN61	22:A:1616:PAR:H33	1.77	0.49
4:D:148:VAL:HG11	4:D:158:ILE:HG21	1.93	0.49
7:G:15:ASP:N	7:G:20:ASP:O	2.43	0.49
1:A:337:C:H2'	1:A:338:A:H8	1.76	0.49
1:A:1128:C:O2'	1:A:1130:A:H8	1.95	0.49
5:E:8:GLU:OE2	5:E:63:ARG:NH2	2.45	0.49
12:L:60:LEU:HB2	12:L:64:TYR:O	2.12	0.49
1:A:194:C:OP1	20:T:61:SER:OG	2.29	0.49
1:A:337:C:H2'	1:A:338:A:C8	2.47	0.49
1:A:382:A:H2'	1:A:383:A:C8	2.48	0.49
1:A:921:U:O2	5:E:19:MET:HB2	2.13	0.49
10:J:6:ILE:HB	10:J:72:VAL:HB	1.94	0.49
13:M:5:ALA:HA	13:M:61:GLU:HG2	1.94	0.49
14:N:21:TYR:HE2	14:N:23:ARG:HE	1.60	0.49
1:A:376:G:OP2	16:P:67:THR:HG21	2.13	0.49
1:A:1285:A:H4'	1:A:1286:A:O5'	2.13	0.49
19:S:61:TYR:HD2	19:S:62:ILE:N	2.10	0.49
8:H:4:ASP:OD2	8:H:85:ARG:HD2	2.13	0.49
10:J:6:ILE:HG12	10:J:98:ILE:HG23	1.93	0.49
10:J:22:LYS:HZ3	10:J:90:LEU:H	1.61	0.49
1:A:1190:G:O2'	1:A:1191:A:P	2.70	0.49
2:B:100:GLY:O	2:B:104:ASN:N	2.46	0.49
4:D:32:ALA:O	4:D:36:ARG:N	2.33	0.49
4:D:173:TRP:CG	4:D:189:PRO:HG3	2.48	0.49
17:Q:63:ARG:HG2	17:Q:64:PRO:HD2	1.95	0.49
20:T:16:HIS:O	20:T:19:SER:HB3	2.13	0.49
1:A:792:A:H4'	1:A:793:U:O5'	2.13	0.49
1:A:920:U:H2'	1:A:921:U:C6	2.47	0.49
1:A:1118:C:H1'	1:A:1179:A:C4	2.48	0.49
1:A:1149:C:H2'	1:A:1150:U:C6	2.48	0.49
13:M:17:VAL:O	13:M:20:THR:HB	2.13	0.49
20:T:50:GLU:HA	20:T:100:ILE:HB	1.94	0.49
1:A:190(F):G:H4'	1:A:190(G):G:OP2	2.13	0.48
1:A:1315:U:H2'	1:A:1316:G:O4'	2.13	0.48
1:A:1519:MA6:H5'	1:A:1520:G:OP2	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:10:LEU:HD22	2:B:15:VAL:HG21	1.94	0.48
1:A:1054:C:H3'	1:A:1054:C:O2	2.13	0.48
8:H:83:ILE:HG13	8:H:137:VAL:HG22	1.94	0.48
1:A:457:C:H2'	1:A:458:C:C6	2.48	0.48
1:A:560:U:H5'	1:A:566:G:C2	2.48	0.48
1:A:1038:C:H2'	1:A:1039:C:C6	2.48	0.48
1:A:1325:C:OP1	21:U:15:ARG:NH1	2.46	0.48
3:C:86:VAL:O	3:C:90:GLU:HG3	2.13	0.48
1:A:45:U:H2'	1:A:46:G:C8	2.48	0.48
1:A:1402:4OC:O2	1:A:1500:A:N1	2.46	0.48
1:A:539:A:H2'	1:A:540:G:C8	2.48	0.48
1:A:1053:G:C3'	1:A:1054:C:H5'	2.44	0.48
20:T:57:ARG:NE	20:T:102:GLY:HA2	2.28	0.48
1:A:1499:A:H1'	1:A:1520:G:H5'	1.94	0.48
6:F:14:LEU:HD22	6:F:18:GLN:HB3	1.94	0.48
20:T:42:GLN:O	20:T:45:GLN:HB2	2.14	0.48
1:A:107:G:N7	20:T:15:ARG:NH2	2.62	0.48
1:A:860:A:H2'	1:A:861:G:O4'	2.13	0.48
10:J:28:ARG:HG2	10:J:34:VAL:HG21	1.96	0.48
19:S:31:ILE:HG22	19:S:49:ILE:HA	1.95	0.48
1:A:266:G:H5''	1:A:267:C:C5	2.48	0.48
1:A:1333:A:H2'	1:A:1334:G:O4'	2.13	0.48
5:E:151:LEU:HD13	8:H:79:VAL:HA	1.96	0.48
12:L:28:LYS:HB2	12:L:33:ARG:HH12	1.78	0.48
15:O:27:VAL:HG12	15:O:31:LEU:HD22	1.96	0.48
1:A:1301:U:HO2'	1:A:1302:U:P	2.37	0.48
6:F:2:ARG:CZ	6:F:69:GLU:HG2	2.44	0.48
1:A:1239:A:C4	1:A:1298:C:N4	2.82	0.47
12:L:27:LEU:HG	12:L:28:LYS:H	1.79	0.47
13:M:15:VAL:HG23	13:M:43:THR:O	2.13	0.47
14:N:26:ARG:NH2	14:N:46:GLU:OE1	2.45	0.47
15:O:18:PHE:HB2	15:O:19:PRO:HD2	1.96	0.47
1:A:1001:A:H2'	1:A:1002:G:C8	2.49	0.47
10:J:82:ILE:HA	10:J:85:LEU:HB2	1.95	0.47
18:R:71:LYS:O	18:R:75:ILE:HG12	2.14	0.47
20:T:16:HIS:CE1	20:T:20:LEU:HD11	2.49	0.47
1:A:994:A:N3	1:A:994:A:H2'	2.29	0.47
3:C:12:LEU:HD23	3:C:12:LEU:HA	1.71	0.47
5:E:92:LYS:HG2	5:E:119:LEU:HB2	1.96	0.47
7:G:113:GLU:OE1	7:G:113:GLU:N	2.46	0.47
1:A:61:G:O2'	25:A:2002:HOH:O	2.20	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:501:C:H2'	1:A:502:G:C8	2.49	0.47
1:A:540:G:H2'	1:A:541:G:O4'	2.15	0.47
1:A:1347:G:N2	1:A:1373:G:H2'	2.29	0.47
6:F:69:GLU:CD	6:F:69:GLU:H	2.22	0.47
10:J:78:ASN:HB2	10:J:81:THR:OG1	2.15	0.47
16:P:8:ARG:HG2	16:P:17:TYR:CE2	2.49	0.47
1:A:397:A:H5'	1:A:398:C:OP1	2.14	0.47
6:F:55:ASP:HA	6:F:56:PRO:HD3	1.71	0.47
1:A:372:C:H1'	1:A:373:A:OP2	2.14	0.47
1:A:501:C:H2'	1:A:502:G:H8	1.79	0.47
1:A:818:G:HO2'	1:A:820:U:H6	1.62	0.47
1:A:1167:A:H8	1:A:1167:A:OP1	1.97	0.47
1:A:1371:G:O3'	9:I:69:GLY:HA3	2.13	0.47
9:I:112:LYS:HD2	9:I:113:LYS:N	2.29	0.47
1:A:247:G:OP2	17:Q:100:LYS:HG3	2.14	0.47
1:A:384:G:H2'	1:A:385:C:C6	2.49	0.47
1:A:474:G:H2'	1:A:475:G:C8	2.47	0.47
1:A:587:G:O2'	1:A:588:G:OP2	2.19	0.47
1:A:695:A:H2'	1:A:696:A:C8	2.48	0.47
1:A:1216:G:H5''	14:N:5:ALA:CB	2.44	0.47
1:A:1352:C:H2'	1:A:1353:G:C8	2.49	0.47
1:A:1511:G:H2'	1:A:1512:U:O4'	2.15	0.47
5:E:24:ARG:HB3	5:E:24:ARG:NH1	2.28	0.47
5:E:80:ILE:HD12	5:E:142:LEU:HD21	1.95	0.47
14:N:34:TYR:N	14:N:39:LEU:O	2.48	0.47
15:O:29:VAL:HG11	15:O:67:LEU:HD21	1.97	0.47
19:S:40:ILE:HG22	19:S:67:VAL:HA	1.96	0.47
1:A:828:A:H4'	1:A:828:A:OP1	2.15	0.47
1:A:1190:G:OP1	3:C:4:LYS:HA	2.15	0.47
1:A:1356:G:H2'	1:A:1357:A:C8	2.49	0.47
1:A:1369:C:H2'	1:A:1370:G:C8	2.50	0.47
1:A:179:A:H2'	1:A:180:U:C6	2.50	0.47
1:A:1419:G:H1	1:A:1481:U:H3	1.63	0.47
6:F:22:GLU:O	6:F:26:ILE:HG12	2.15	0.47
11:K:109:VAL:HG11	18:R:84:LYS:HE2	1.97	0.47
1:A:107:G:C2'	1:A:108:G:H5'	2.45	0.47
1:A:643:C:H4'	8:H:31:PHE:CE2	2.50	0.47
1:A:1057:G:H5''	3:C:154:SER:OG	2.15	0.47
7:G:26:PHE:CE2	7:G:30:ILE:HD11	2.50	0.47
10:J:76:ASN:O	10:J:78:ASN:N	2.48	0.47
1:A:46:G:O2'	1:A:365:U:H1'	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:G:C6	1:A:300:A:C6	3.03	0.46
1:A:452:A:O2'	1:A:453:A:H8	1.95	0.46
1:A:509:A:C8	1:A:509:A:H3'	2.50	0.46
1:A:657:G:H4'	15:O:28:GLN:HG2	1.98	0.46
6:F:8:ILE:HG12	6:F:88:VAL:HG22	1.95	0.46
10:J:90:LEU:N	10:J:91:PRO:HD2	2.30	0.46
17:Q:53:LEU:HD23	17:Q:82:MET:HE1	1.97	0.46
1:A:21:G:H2'	1:A:22:G:C8	2.50	0.46
1:A:35:G:H2'	1:A:36:C:C6	2.50	0.46
1:A:114:U:OP1	22:A:1604:PAR:H32	2.15	0.46
3:C:72:LYS:HB2	3:C:75:VAL:HG23	1.98	0.46
4:D:127:THR:HG23	4:D:147:ALA:HB3	1.96	0.46
4:D:188:LEU:HD23	4:D:188:LEU:HA	1.77	0.46
8:H:31:PHE:HZ	8:H:134:ILE:HD11	1.80	0.46
1:A:266:G:C5'	1:A:268:C:H41	2.28	0.46
1:A:1106:G:H5''	3:C:172:ARG:HG2	1.96	0.46
1:A:1368:G:H5''	9:I:112:LYS:HB3	1.97	0.46
9:I:17:VAL:HG22	9:I:63:ILE:HG12	1.97	0.46
2:B:6:THR:HA	2:B:9:GLU:OE1	2.14	0.46
11:K:115:PRO:C	11:K:117:ASN:H	2.23	0.46
17:Q:100:LYS:HB2	17:Q:101:ARG:CZ	2.45	0.46
1:A:447:G:H2'	1:A:485:G:N2	2.31	0.46
1:A:1016:A:H2'	1:A:1017:G:O4'	2.15	0.46
1:A:1414:U:H2'	1:A:1415:G:H8	1.80	0.46
3:C:112:SER:O	3:C:116:VAL:HG23	2.15	0.46
5:E:43:LEU:HD11	5:E:132:ALA:HB1	1.97	0.46
9:I:4:TYR:CZ	9:I:88:TYR:HD1	2.34	0.46
15:O:26:GLU:HG3	15:O:81:LEU:HG	1.96	0.46
1:A:316:G:OP2	1:A:351:G:O2'	2.33	0.46
1:A:558:G:H3'	1:A:559:A:H3'	1.97	0.46
1:A:1053:G:H3'	1:A:1054:C:H5'	1.97	0.46
1:A:1053:G:O6	1:A:1199:U:H2'	2.15	0.46
4:D:24:GLU:C	4:D:26:CYS:H	2.23	0.46
4:D:173:TRP:CD2	4:D:189:PRO:HG3	2.50	0.46
10:J:8:LEU:HD23	10:J:96:ILE:HG23	1.98	0.46
12:L:10:LEU:HB3	17:Q:32:TYR:CE1	2.51	0.46
4:D:78:LEU:HD23	4:D:78:LEU:HA	1.73	0.46
12:L:38:THR:HG22	12:L:39:VAL:HG22	1.98	0.46
15:O:57:LEU:HD12	15:O:57:LEU:HA	1.67	0.46
1:A:716:A:H1'	11:K:118:GLY:HA2	1.98	0.46
1:A:911:U:H2'	1:A:912:C:C6	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:977:A:H2'	1:A:978:A:H5''	1.98	0.46
1:A:1101:A:H4'	1:A:1102:A:O5'	2.16	0.46
1:A:1212:U:O2'	1:A:1213:A:P	2.74	0.46
1:A:1316:G:H4'	14:N:18:VAL:HG11	1.98	0.46
1:A:1425:U:H2'	1:A:1426:C:H6	1.80	0.46
4:D:62:GLN:OE1	4:D:65:ARG:NH1	2.49	0.46
6:F:10:LEU:HB2	6:F:59:TYR:HB3	1.97	0.46
9:I:56:LEU:HD12	9:I:56:LEU:H	1.81	0.46
7:G:54:THR:HG22	7:G:56:GLN:H	1.81	0.46
8:H:103:VAL:O	8:H:106:GLY:N	2.48	0.46
15:O:70:LEU:HD12	15:O:81:LEU:HD12	1.96	0.46
17:Q:59:ILE:HD13	17:Q:59:ILE:HA	1.57	0.46
3:C:91:LEU:HG	3:C:99:VAL:HG21	1.98	0.46
8:H:116:LYS:NZ	8:H:127:LEU:HD22	2.30	0.46
16:P:3:LYS:HD2	16:P:24:ALA:HB2	1.97	0.46
17:Q:10:VAL:HG13	17:Q:19:VAL:HB	1.97	0.46
1:A:267:C:H2'	1:A:268:C:C6	2.51	0.45
1:A:1504:G:C3'	1:A:1505:G:H5'	2.46	0.45
3:C:157:ILE:HD13	3:C:166:GLU:HG2	1.98	0.45
4:D:83:SER:HA	4:D:89:THR:HG23	1.98	0.45
11:K:86:GLY:H	11:K:112:THR:HG23	1.82	0.45
12:L:70:ILE:HD13	12:L:77:LEU:HD12	1.97	0.45
17:Q:66:SER:OG	17:Q:69:LYS:HB2	2.17	0.45
1:A:316:G:H4'	25:A:2351:HOH:O	2.15	0.45
1:A:991:U:O2'	1:A:992:U:P	2.74	0.45
3:C:128:PHE:HD2	3:C:133:ALA:HB2	1.81	0.45
6:F:4:TYR:CZ	6:F:72:VAL:HG21	2.51	0.45
18:R:18:ARG:HD3	18:R:18:ARG:HA	1.80	0.45
1:A:556:C:H2'	1:A:557:G:O4'	2.17	0.45
1:A:1136:U:H5''	1:A:1137:C:OP2	2.16	0.45
1:A:1256:A:O2'	1:A:1257:U:O5'	2.31	0.45
1:A:1329:A:H5'	13:M:29:ARG:HD2	1.98	0.45
1:A:927:G:H5'	1:A:928:G:OP2	2.17	0.45
1:A:967:5MC:H2'	1:A:968:A:N7	2.32	0.45
3:C:6:HIS:HD2	3:C:9:GLY:H	1.64	0.45
12:L:48:PRO:HD2	12:L:92:0TD:H3	1.99	0.45
1:A:524:G:H2'	1:A:525:C:C6	2.50	0.45
1:A:625:G:H4'	16:P:16:HIS:ND1	2.32	0.45
10:J:57:LYS:HG2	10:J:58:ASP:CG	2.42	0.45
16:P:12:LYS:C	16:P:14:ASN:H	2.24	0.45
1:A:107:G:H2'	1:A:108:G:H5'	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:496:A:H4'	1:A:497:A:OP1	2.15	0.45
1:A:795:C:H5''	1:A:796:C:OP2	2.17	0.45
1:A:1055:A:O2'	3:C:161:GLU:O	2.34	0.45
3:C:59:ARG:HG2	3:C:64:VAL:HG13	1.98	0.45
11:K:91:ARG:HG2	11:K:92:GLU:N	2.30	0.45
1:A:501:C:OP1	12:L:117:ARG:NH2	2.50	0.45
1:A:517:G:N1	1:A:533:A:OP2	2.33	0.45
1:A:1104:G:O5'	2:B:111:ARG:HD2	2.16	0.45
22:A:1616:PAR:H24	25:A:2497:HOH:O	2.16	0.45
10:J:4:ILE:H	10:J:4:ILE:HG13	1.54	0.45
17:Q:96:GLN:H	17:Q:96:GLN:HG2	1.65	0.45
18:R:36:ASN:O	18:R:40:LEU:HG	2.17	0.45
1:A:1103:C:H2'	1:A:1104:G:O4'	2.17	0.45
1:A:1131:G:H2'	1:A:1132:C:C6	2.52	0.45
1:A:142:G:O2'	1:A:196:A:N1	2.48	0.45
2:B:19:HIS:O	2:B:39:ILE:HG12	2.17	0.45
4:D:8:VAL:O	4:D:11:LEU:N	2.43	0.45
18:R:65:ILE:O	18:R:69:THR:HG23	2.17	0.45
1:A:325:A:H2'	1:A:326:G:O4'	2.18	0.44
1:A:1020:U:H2'	1:A:1021:G:C8	2.52	0.44
1:A:1287:A:H2'	1:A:1288:A:C8	2.52	0.44
4:D:53:ASP:O	4:D:57:ARG:HG2	2.17	0.44
4:D:64:LEU:HG	4:D:198:VAL:HG11	1.99	0.44
13:M:14:ARG:HG3	13:M:44:ARG:NH2	2.25	0.44
16:P:31:LYS:O	16:P:31:LYS:HG3	2.17	0.44
17:Q:10:VAL:HG23	17:Q:55:ASP:O	2.17	0.44
1:A:262:A:C6	1:A:263:A:C6	3.05	0.44
1:A:428:G:H4'	1:A:429:U:O5'	2.17	0.44
1:A:670:G:H21	6:F:73:ASN:ND2	2.16	0.44
1:A:688:G:O2'	1:A:704:A:N1	2.44	0.44
1:A:986:A:O2'	19:S:55:LYS:O	2.35	0.44
1:A:1129:C:H4'	1:A:1130:A:OP2	2.17	0.44
2:B:59:GLU:HB2	2:B:221:LEU:HD11	2.00	0.44
2:B:74:LYS:O	2:B:75:LYS:HB2	2.17	0.44
3:C:30:ARG:HB3	14:N:36:PHE:O	2.17	0.44
18:R:40:LEU:HB3	18:R:79:LEU:HD11	1.98	0.44
1:A:130:A:C8	17:Q:63:ARG:HG3	2.53	0.44
1:A:358:U:H2'	1:A:359:U:C6	2.52	0.44
1:A:736:C:H2'	1:A:737:A:C8	2.53	0.44
5:E:80:ILE:N	5:E:80:ILE:HD13	2.32	0.44
6:F:100:ASN:OD1	18:R:23:LYS:HE2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:17:VAL:HG11	9:I:81:ILE:HA	1.99	0.44
17:Q:67:LYS:O	17:Q:68:ARG:HB3	2.16	0.44
1:A:64:G:N1	22:A:1613:PAR:N32	2.66	0.44
1:A:474:G:H5''	16:P:81:ARG:NH1	2.32	0.44
3:C:6:HIS:CD2	3:C:9:GLY:H	2.35	0.44
12:L:113:ARG:NH1	12:L:116:SER:H	2.15	0.44
1:A:109:A:H2'	1:A:326:G:N2	2.33	0.44
1:A:586:C:C2'	1:A:587:G:H5'	2.48	0.44
1:A:802:A:H2'	1:A:803:G:O4'	2.17	0.44
1:A:1347:G:C2'	1:A:1348:U:OP2	2.66	0.44
4:D:120:LEU:HD23	4:D:120:LEU:HA	1.82	0.44
6:F:50:TYR:CE1	18:R:77:GLY:HA2	2.52	0.44
9:I:26:VAL:HG13	9:I:61:ALA:HB3	1.99	0.44
1:A:620:C:N1	4:D:135:LEU:HD13	2.31	0.44
1:A:1270:C:H2'	1:A:1271:G:H8	1.83	0.44
1:A:1279:A:H5''	1:A:1280:A:OP1	2.18	0.44
2:B:183:PRO:HA	2:B:198:ASP:OD2	2.17	0.44
2:B:189:ASP:OD2	2:B:190:THR:N	2.41	0.44
15:O:85:LEU:HB3	15:O:87:ILE:HD11	2.00	0.44
1:A:707:C:H2'	1:A:708:C:C6	2.53	0.44
1:A:1168:A:C6	1:A:1169:A:C6	3.06	0.44
22:A:1616:PAR:H21	22:A:1616:PAR:H42	1.44	0.44
3:C:111:LEU:HD23	3:C:111:LEU:HA	1.73	0.44
9:I:27:THR:HG23	9:I:31:GLN:H	1.83	0.44
1:A:558:G:H2'	1:A:559:A:H2	1.83	0.44
1:A:833:U:H2'	1:A:834:C:C6	2.53	0.44
1:A:1064:G:H1'	1:A:1190:G:N2	2.32	0.44
2:B:124:SER:OG	2:B:126:GLU:HG2	2.18	0.44
20:T:33:ILE:O	20:T:34:LYS:C	2.61	0.44
1:A:109:A:C6	1:A:326:G:C6	3.06	0.44
1:A:633:G:OP2	22:A:1612:PAR:H11	2.18	0.44
1:A:1330:U:H2'	1:A:1331:G:H5'	1.99	0.44
22:A:1601:PAR:H11	22:A:1601:PAR:O52	2.17	0.44
3:C:86:VAL:O	3:C:89:GLU:HB3	2.18	0.44
4:D:53:ASP:OD1	4:D:53:ASP:N	2.50	0.44
5:E:71:LEU:HD11	5:E:113:ALA:O	2.18	0.44
15:O:21:ASP:OD2	15:O:24:SER:HB3	2.18	0.44
19:S:41:VAL:HG23	19:S:43:GLU:HG2	2.00	0.44
1:A:370:C:H2'	1:A:371:G:O4'	2.18	0.43
1:A:775:G:H2'	1:A:776:G:O4'	2.18	0.43
1:A:1074:G:O2'	1:A:1101:A:N1	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1343:G:H4'	9:I:122:ALA:HB3	2.00	0.43
2:B:178:ARG:NH2	8:H:74:PRO:HG3	2.33	0.43
9:I:97:LYS:HA	9:I:102:LEU:HD11	2.00	0.43
20:T:54:LYS:HA	20:T:57:ARG:NH1	2.33	0.43
1:A:945:G:C2	1:A:946:A:C8	3.06	0.43
2:B:74:LYS:C	2:B:76:GLN:H	2.26	0.43
13:M:108:ARG:NH2	13:M:111:LYS:HE2	2.32	0.43
20:T:62:LEU:HA	20:T:62:LEU:HD23	1.74	0.43
20:T:67:ALA:HA	20:T:73:HIS:H	1.83	0.43
3:C:43:LEU:O	3:C:47:LEU:HB2	2.18	0.43
7:G:65:ALA:HB1	7:G:127:ALA:HB3	1.99	0.43
15:O:87:ILE:HG22	15:O:88:ARG:H	1.82	0.43
19:S:44:MET:HB3	19:S:62:ILE:HD13	2.00	0.43
1:A:179:A:H2'	1:A:180:U:H6	1.83	0.43
1:A:1001:A:H2'	1:A:1002:G:H8	1.83	0.43
7:G:23:VAL:O	7:G:27:ILE:HG13	2.19	0.43
7:G:120:ILE:O	7:G:124:LEU:HB2	2.18	0.43
9:I:125:TYR:H	9:I:125:TYR:HD2	1.65	0.43
11:K:46:GLY:HA2	11:K:50:TYR:O	2.17	0.43
1:A:309:G:H1'	1:A:608:A:C2	2.53	0.43
1:A:376:G:P	16:P:67:THR:HG21	2.59	0.43
1:A:421:U:H5'	1:A:422:C:H5	1.84	0.43
1:A:1086:U:O5'	1:A:1086:U:H6	2.00	0.43
2:B:239:VAL:O	2:B:240:GLN:HB3	2.18	0.43
10:J:46:ARG:HH11	10:J:46:ARG:CG	2.30	0.43
1:A:500:G:H2'	1:A:501:C:C6	2.53	0.43
1:A:695:A:H61	1:A:797:C:H1'	1.83	0.43
1:A:1163:C:H2'	1:A:1164:G:H8	1.84	0.43
1:A:1213:A:O2'	1:A:1214:C:H5''	2.17	0.43
1:A:1468:A:H2'	1:A:1469:G:O4'	2.18	0.43
2:B:84:GLU:OE1	2:B:216:SER:HA	2.19	0.43
2:B:240:GLN:O	2:B:240:GLN:HG2	2.19	0.43
5:E:8:GLU:HG2	5:E:34:VAL:HG22	1.99	0.43
11:K:77:MET:HB3	11:K:77:MET:HE3	1.75	0.43
1:A:1206:G:C6	1:A:1207:2MG:C5	3.07	0.43
1:A:1314:C:OP2	19:S:6:LYS:HD3	2.18	0.43
15:O:2:PRO:O	15:O:38:ARG:NH1	2.47	0.43
1:A:162:A:C5	1:A:163:C:H1'	2.54	0.43
1:A:399:G:H2'	1:A:400:C:C6	2.54	0.43
1:A:1141:C:H2'	1:A:1142:G:H8	1.84	0.43
2:B:103:THR:HG23	2:B:176:GLU:OE1	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:18:LYS:HG2	4:D:33:MET:HG2	2.00	0.43
6:F:99:ALA:HB1	18:R:23:LYS:HE3	1.99	0.43
11:K:48:ILE:HD11	11:K:64:ALA:HA	1.99	0.43
12:L:7:ILE:HD13	12:L:7:ILE:HA	1.81	0.43
13:M:40:ASN:HA	13:M:41:PRO:HD3	1.86	0.43
21:U:17:THR:O	21:U:22:ARG:HD3	2.19	0.43
1:A:90:U:H2'	1:A:91:C:C6	2.54	0.43
1:A:117:G:P	25:A:2020:HOH:O	2.77	0.43
1:A:558:G:OP2	1:A:559:A:O2'	2.32	0.43
1:A:1300:G:HO2'	1:A:1301:U:P	2.42	0.43
1:A:1425:U:H2'	1:A:1426:C:C6	2.54	0.43
4:D:13:ARG:NH2	4:D:40:PRO:HA	2.34	0.43
5:E:110:LEU:HD13	5:E:118:ILE:HG21	2.00	0.43
6:F:38:GLU:HB2	6:F:64:GLN:HG2	2.00	0.43
8:H:4:ASP:CG	8:H:85:ARG:HH11	2.27	0.43
15:O:39:LEU:CD1	15:O:56:LEU:HB2	2.48	0.43
19:S:22:LEU:HD22	19:S:26:GLY:O	2.19	0.43
1:A:1298:C:H4'	1:A:1299:A:C4	2.54	0.43
1:A:1498:UR3:OP2	1:A:1542:U:O2'	2.28	0.43
4:D:162:LEU:HD12	4:D:181:MET:SD	2.59	0.43
5:E:131:ILE:HD13	5:E:131:ILE:HA	1.85	0.43
13:M:49:THR:HG22	13:M:51:ALA:N	2.29	0.43
19:S:62:ILE:HA	19:S:66:MET:HE1	2.01	0.43
1:A:390:C:O5'	1:A:390:C:H6	2.01	0.42
1:A:484:G:H5'	1:A:486:U:O4'	2.19	0.42
1:A:689:C:H2'	1:A:690:G:O4'	2.19	0.42
2:B:196:LEU:HD12	2:B:196:LEU:H	1.84	0.42
3:C:5:ILE:HD12	3:C:5:ILE:O	2.19	0.42
5:E:66:MET:HE3	5:E:66:MET:HB3	1.92	0.42
5:E:87:SER:HB3	5:E:131:ILE:HD13	2.01	0.42
11:K:20:TYR:CZ	11:K:83:ILE:HD13	2.53	0.42
15:O:79:ARG:NH1	15:O:83:GLU:HB2	2.34	0.42
1:A:880:C:OP1	12:L:8:ASN:ND2	2.51	0.42
17:Q:31:LEU:HG	17:Q:32:TYR:CE2	2.54	0.42
1:A:62:U:H2'	1:A:63:C:C6	2.54	0.42
1:A:269:C:H2'	1:A:270:A:C8	2.54	0.42
1:A:1518:MA6:O5'	1:A:1518:MA6:H8	2.18	0.42
14:N:40:CYS:O	14:N:44:LEU:HB3	2.19	0.42
1:A:64:G:C6	22:A:1613:PAR:N32	2.88	0.42
1:A:411:A:OP1	4:D:30:LYS:NZ	2.51	0.42
1:A:570:G:H1'	1:A:820:U:C4	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:993:G:H2'	1:A:995:C:H41	1.84	0.42
1:A:1498:UR3:O5'	1:A:1498:UR3:H6	2.19	0.42
22:A:1613:PAR:H52	22:A:1613:PAR:H11	1.82	0.42
12:L:53:ARG:NH1	12:L:92:0TD:OD1	2.52	0.42
12:L:117:ARG:HD2	12:L:122:THR:HG22	2.01	0.42
16:P:1:MET:HB3	16:P:1:MET:HE2	1.72	0.42
17:Q:59:ILE:HD13	17:Q:73:VAL:HA	2.00	0.42
1:A:629:G:N7	22:A:1615:PAR:H221	2.35	0.42
1:A:690:G:H2'	1:A:691:G:O4'	2.19	0.42
1:A:721:G:H4'	1:A:722:A:O4'	2.18	0.42
1:A:791:G:C6	1:A:792:A:N7	2.88	0.42
1:A:955:U:H1'	1:A:1227:A:N6	2.34	0.42
2:B:43:ASP:HB3	2:B:46:LYS:HB2	2.01	0.42
7:G:74:GLU:HG2	7:G:91:VAL:HG22	2.00	0.42
8:H:127:LEU:HA	8:H:127:LEU:HD23	1.87	0.42
20:T:73:HIS:C	20:T:74:LYS:HG2	2.43	0.42
1:A:109:A:C6	1:A:327:A:C6	3.07	0.42
1:A:636:U:O4	22:A:1612:PAR:H54	2.19	0.42
1:A:644:G:C5	1:A:645:C:C5	3.07	0.42
1:A:695:A:OP1	11:K:52:GLY:HA3	2.19	0.42
1:A:1190:G:O2'	1:A:1191:A:O5'	2.36	0.42
8:H:56:LYS:HA	8:H:57:PRO:HD3	1.78	0.42
15:O:74:ASP:OD1	15:O:76:GLU:HB2	2.20	0.42
19:S:62:ILE:HA	19:S:66:MET:CE	2.49	0.42
1:A:1137:C:H5'	1:A:1138:G:C6	2.55	0.42
3:C:16:ARG:HD2	3:C:16:ARG:HA	1.90	0.42
4:D:57:ARG:HG2	4:D:57:ARG:H	1.56	0.42
20:T:77:ALA:O	20:T:81:LYS:HG3	2.19	0.42
1:A:1163:C:H2'	1:A:1164:G:C8	2.54	0.42
2:B:74:LYS:HD2	2:B:166:ASP:CB	2.44	0.42
3:C:167:TRP:HZ3	3:C:169:ALA:HB3	1.84	0.42
10:J:32:ALA:HB3	10:J:75:ILE:O	2.19	0.42
1:A:217:C:O2'	1:A:461:C:N4	2.53	0.42
1:A:224:C:H2'	1:A:225:C:H6	1.84	0.42
1:A:542:G:H5'	4:D:41:GLY:HA3	2.02	0.42
1:A:946:A:H2'	1:A:947:G:H8	1.78	0.42
1:A:954:G:N2	1:A:1227:A:H62	2.13	0.42
2:B:212:GLN:O	2:B:216:SER:OG	2.38	0.42
3:C:115:LEU:HD12	3:C:115:LEU:HA	1.79	0.42
4:D:61:LYS:HA	4:D:203:VAL:HG22	2.01	0.42
6:F:8:ILE:HD11	6:F:79:LEU:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:71:LEU:HD23	10:J:71:LEU:HA	1.88	0.42
18:R:53:ARG:C	18:R:55:ARG:N	2.76	0.42
20:T:59:ALA:O	20:T:63:ILE:HG13	2.20	0.42
1:A:614:A:H2'	1:A:615:C:C6	2.54	0.42
1:A:804:U:H5''	1:A:805:C:OP2	2.20	0.42
1:A:1095:U:H2'	1:A:1096:C:C6	2.54	0.42
1:A:1270:C:H2'	1:A:1271:G:C8	2.54	0.42
1:A:1399:C:C2	1:A:1401:G:C5	3.08	0.42
22:A:1607:PAR:N32	22:A:1607:PAR:O51	2.52	0.42
4:D:173:TRP:HB2	4:D:187:ARG:O	2.20	0.42
5:E:142:LEU:HA	5:E:142:LEU:HD23	1.78	0.42
1:A:857:C:H2'	1:A:858:G:O4'	2.20	0.41
1:A:1074:G:C6	1:A:1075:C:C4	3.08	0.41
1:A:1347:G:H22	1:A:1374:A:P	2.43	0.41
1:A:1379:G:C6	1:A:1380:U:C4	3.08	0.41
2:B:102:LEU:HB3	2:B:180:LEU:HD12	2.01	0.41
20:T:56:MET:HE3	20:T:56:MET:HB2	1.84	0.41
1:A:266:G:H5'	1:A:268:C:H41	1.84	0.41
1:A:757:U:H2'	1:A:758:G:O4'	2.19	0.41
1:A:1201:A:H4'	1:A:1202:G:O5'	2.20	0.41
1:A:1342:C:H2'	1:A:1343:G:C8	2.55	0.41
1:A:1360:A:OP2	14:N:35:ARG:NH2	2.53	0.41
4:D:161:ASN:O	4:D:165:MET:HG2	2.19	0.41
6:F:35:ALA:HB1	6:F:65:VAL:HG21	2.02	0.41
6:F:77:ARG:NH1	6:F:81:ILE:HD11	2.35	0.41
8:H:9:MET:HG3	8:H:26:VAL:HG21	2.02	0.41
16:P:58:TYR:O	16:P:62:VAL:HG22	2.20	0.41
1:A:728:A:O5'	1:A:728:A:H8	2.03	0.41
1:A:1002:G:C6	1:A:1003:G:C6	3.08	0.41
1:A:1272:G:H2'	1:A:1273:G:O4'	2.20	0.41
1:A:1080:A:C8	1:A:1081:G:H1'	2.55	0.41
1:A:1111:A:O5'	1:A:1111:A:H8	2.03	0.41
1:A:1124:G:H2'	1:A:1145:C:C5	2.53	0.41
1:A:1256:A:H4'	1:A:1257:U:C5'	2.51	0.41
1:A:1479:C:H2'	1:A:1480:G:C8	2.49	0.41
1:A:1500:A:OP2	1:A:1505:G:OP1	2.38	0.41
5:E:6:PHE:HE2	5:E:36:ASP:HB3	1.86	0.41
5:E:13:ILE:HD12	5:E:13:ILE:HG23	1.81	0.41
9:I:49:PRO:HB2	9:I:81:ILE:HG22	2.02	0.41
9:I:105:ASP:OD2	9:I:107:ARG:HG3	2.20	0.41
11:K:44:SER:H	11:K:47:VAL:HB	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:74:LYS:HE3	20:T:74:LYS:HB3	1.89	0.41
4:D:98:GLU:HG2	4:D:189:PRO:HG2	2.02	0.41
7:G:124:LEU:HD12	7:G:124:LEU:HA	1.93	0.41
8:H:6:ILE:HD11	8:H:31:PHE:CD2	2.54	0.41
9:I:89:ASN:HA	9:I:90:PRO:HD2	1.92	0.41
14:N:8:GLU:OE1	14:N:9:LYS:HA	2.20	0.41
16:P:66:PRO:HB2	16:P:71:ARG:HB2	2.01	0.41
19:S:43:GLU:CD	19:S:43:GLU:H	2.27	0.41
19:S:80:TYR:CE1	19:S:81:ARG:HD2	2.55	0.41
1:A:6:G:H4'	1:A:298:A:H4'	2.03	0.41
1:A:295:C:H2'	1:A:296:U:O4'	2.20	0.41
1:A:658:G:H2'	1:A:659:U:C6	2.55	0.41
1:A:1003:G:H22	1:A:1039:C:H1'	1.85	0.41
3:C:43:LEU:HD21	3:C:91:LEU:HD13	2.02	0.41
8:H:82:HIS:HD1	8:H:138:TRP:CD1	2.38	0.41
12:L:33:ARG:HD2	12:L:33:ARG:HA	1.64	0.41
12:L:92:OTD:H8	12:L:92:OTD:H4	1.81	0.41
15:O:71:GLN:HB2	15:O:78:TYR:CE1	2.56	0.41
17:Q:15:MET:HE1	17:Q:43:LEU:HD22	2.03	0.41
19:S:22:LEU:HD23	19:S:22:LEU:HA	1.94	0.41
1:A:344:A:H5''	1:A:345:C:C5	2.47	0.41
1:A:687:A:H4'	1:A:688:G:O5'	2.21	0.41
1:A:1091:U:O2	1:A:1093:A:C8	2.73	0.41
1:A:1173:G:H2'	1:A:1174:G:O4'	2.19	0.41
1:A:1229:A:OP2	13:M:114:ARG:HD3	2.21	0.41
1:A:1402:4OC:H2'	1:A:1403:C:O4'	2.20	0.41
2:B:139:LYS:HA	2:B:139:LYS:HD2	1.93	0.41
5:E:28:PHE:CD2	5:E:51:VAL:HG22	2.55	0.41
5:E:41:VAL:HG13	5:E:113:ALA:HA	2.02	0.41
5:E:60:TYR:HD2	5:E:61:TYR:CD1	2.38	0.41
6:F:11:ASN:HA	6:F:12:PRO:HD3	1.89	0.41
6:F:91:VAL:HG12	6:F:92:LYS:O	2.21	0.41
7:G:87:VAL:HA	7:G:88:PRO:HD2	1.93	0.41
17:Q:27:PHE:CE1	17:Q:36:ILE:HD11	2.56	0.41
18:R:47:THR:HG23	18:R:83:GLU:O	2.21	0.41
20:T:57:ARG:HE	20:T:102:GLY:HA2	1.86	0.41
1:A:106:C:O2	1:A:379:C:H4'	2.21	0.41
1:A:232:G:H1'	1:A:262:A:N1	2.36	0.41
1:A:665:A:H1'	1:A:733:A:O4'	2.21	0.41
1:A:1072:G:H2'	1:A:1073:U:C6	2.55	0.41
1:A:526:C:OP2	12:L:91:LYS:HE3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1211:U:H1'	1:A:1213:A:C2	2.56	0.41
1:A:1212:U:O2'	1:A:1213:A:OP2	2.36	0.41
1:A:1251:A:H4'	9:I:12:GLU:OE1	2.20	0.41
1:A:1314:C:C5	19:S:6:LYS:HE2	2.55	0.41
1:A:1329:A:H2'	1:A:1330:U:O4'	2.21	0.41
1:A:1420:C:H2'	1:A:1421:G:H8	1.86	0.41
1:A:1480:G:C6	1:A:1481:U:C4	3.09	0.41
2:B:193:ASP:HB3	2:B:196:LEU:HD11	2.03	0.41
3:C:92:ALA:HB2	3:C:99:VAL:HG22	2.02	0.41
3:C:128:PHE:CD2	3:C:133:ALA:HB2	2.56	0.41
4:D:9:CYS:O	4:D:12:CYS:HB2	2.20	0.41
7:G:65:ALA:O	7:G:69:VAL:HG23	2.21	0.41
8:H:19:VAL:CG2	8:H:21:LYS:HD3	2.49	0.41
15:O:24:SER:OG	15:O:27:VAL:HG23	2.21	0.41
15:O:67:LEU:HA	15:O:67:LEU:HD23	1.79	0.41
1:A:23:C:N4	25:A:2102:HOH:O	2.53	0.41
1:A:328:C:H4'	1:A:329:A:C5'	2.49	0.41
1:A:1391:U:H2'	1:A:1392:G:C8	2.56	0.41
22:A:1613:PAR:H13	22:A:1613:PAR:H42	1.60	0.41
5:E:117:ASP:OD2	5:E:117:ASP:N	2.54	0.41
18:R:53:ARG:C	18:R:55:ARG:H	2.29	0.41
1:A:116:A:OP2	1:A:116:A:C8	2.75	0.40
1:A:243:A:H4'	1:A:244:U:H5''	2.03	0.40
1:A:416:G:H2'	1:A:417:C:C6	2.56	0.40
1:A:1029:C:H2'	1:A:1030:C:C6	2.56	0.40
1:A:1190:G:HO2'	1:A:1191:A:P	2.44	0.40
6:F:75:LEU:HD23	6:F:79:LEU:HG	2.02	0.40
15:O:81:LEU:HD23	15:O:81:LEU:HA	1.88	0.40
1:A:932:C:H5''	7:G:3:ARG:HG2	2.03	0.40
1:A:1251:A:H2'	1:A:1252:A:O4'	2.21	0.40
22:A:1606:PAR:H11	22:A:1606:PAR:O52	2.21	0.40
22:A:1608:PAR:H42	22:A:1608:PAR:H13	1.74	0.40
3:C:178:LEU:HD13	3:C:178:LEU:HA	1.80	0.40
4:D:68:TYR:OH	4:D:98:GLU:OE1	2.30	0.40
4:D:108:LEU:HD23	4:D:108:LEU:HA	1.83	0.40
4:D:175:SER:HB3	4:D:186:LEU:HD11	2.02	0.40
7:G:107:ALA:O	7:G:110:GLN:HB2	2.21	0.40
9:I:4:TYR:CE2	9:I:88:TYR:HD1	2.39	0.40
17:Q:45:HIS:CD2	17:Q:47:PRO:HG3	2.56	0.40
1:A:558:G:C8	1:A:559:A:H2'	2.56	0.40
1:A:811:C:H4'	1:A:900:A:N6	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1020:U:H2'	1:A:1021:G:H8	1.85	0.40
10:J:86:MET:HG3	10:J:87:THR:H	1.86	0.40
16:P:49:LEU:HD13	16:P:73:LEU:HD22	2.03	0.40
19:S:58:VAL:HA	19:S:59:PRO:HD3	1.67	0.40
1:A:912:C:O2'	1:A:913:A:H5'	2.22	0.40
2:B:80:ILE:HG22	2:B:215:LEU:HD12	2.03	0.40
4:D:150:GLU:CD	4:D:150:GLU:N	2.79	0.40
5:E:116:THR:HB	5:E:117:ASP:OD2	2.21	0.40
18:R:31:LEU:O	18:R:69:THR:HG21	2.21	0.40
20:T:67:ALA:HB2	20:T:77:ALA:HB2	2.03	0.40
1:A:148:G:H2'	1:A:149:A:C8	2.56	0.40
1:A:224:C:H2'	1:A:225:C:C6	2.56	0.40
1:A:631:G:H8	1:A:631:G:H5''	1.86	0.40
1:A:918:A:H2'	1:A:919:A:C8	2.56	0.40
1:A:1128:C:C4'	9:I:16:ARG:HH22	2.35	0.40
1:A:1531:A:H8	1:A:1531:A:O5'	2.04	0.40
2:B:48:MET:HE3	2:B:48:MET:HB3	2.00	0.40
5:E:40:ARG:HB2	5:E:66:MET:CE	2.52	0.40
9:I:117:HIS:CD2	9:I:123:PRO:HA	2.56	0.40
13:M:18:ALA:O	13:M:21:TYR:HB2	2.22	0.40
13:M:91:ARG:HA	13:M:91:ARG:HD2	1.91	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%)	218 (93%)	15 (6%)	1 (0%)	30	60
3	C	205/239 (86%)	187 (91%)	16 (8%)	2 (1%)	12	42
4	D	206/209 (99%)	198 (96%)	7 (3%)	1 (0%)	24	56
5	E	149/162 (92%)	143 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	99/101 (98%)	96 (97%)	3 (3%)	0	100	100
7	G	153/156 (98%)	147 (96%)	6 (4%)	0	100	100
8	H	136/138 (99%)	134 (98%)	2 (2%)	0	100	100
9	I	125/128 (98%)	117 (94%)	8 (6%)	0	100	100
10	J	97/105 (92%)	82 (84%)	14 (14%)	1 (1%)	12	42
11	K	115/129 (89%)	109 (95%)	6 (5%)	0	100	100
12	L	122/135 (90%)	111 (91%)	10 (8%)	1 (1%)	16	47
13	M	116/126 (92%)	108 (93%)	8 (7%)	0	100	100
14	N	58/61 (95%)	55 (95%)	3 (5%)	0	100	100
15	O	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
16	P	82/88 (93%)	79 (96%)	3 (4%)	0	100	100
17	Q	99/105 (94%)	94 (95%)	5 (5%)	0	100	100
18	R	71/88 (81%)	64 (90%)	7 (10%)	0	100	100
19	S	79/93 (85%)	70 (89%)	8 (10%)	1 (1%)	9	37
20	T	97/106 (92%)	88 (91%)	8 (8%)	1 (1%)	12	42
21	U	23/27 (85%)	22 (96%)	1 (4%)	0	100	100
All	All	2352/2541 (93%)	2203 (94%)	141 (6%)	8 (0%)	36	66

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	L	28	LYS
19	S	31	ILE
3	C	168	ALA
4	D	3	ARG
20	T	73	HIS
2	B	229	VAL
3	C	66	VAL
10	J	34	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%)	181 (90%)	20 (10%)	7	28
3	C	137/188 (73%)	114 (83%)	23 (17%)	2	10
9	I	12/99 (12%)	9 (75%)	3 (25%)	0	3
10	J	67/92 (73%)	60 (90%)	7 (10%)	7	26
11	K	3/99 (3%)	2 (67%)	1 (33%)	0	1
12	L	5/110 (4%)	5 (100%)	0	100	100
13	M	64/101 (63%)	57 (89%)	7 (11%)	6	25
14	N	48/50 (96%)	44 (92%)	4 (8%)	10	36
15	O	79/80 (99%)	66 (84%)	13 (16%)	2	10
16	P	72/74 (97%)	66 (92%)	6 (8%)	10	36
17	Q	95/97 (98%)	82 (86%)	13 (14%)	3	17
18	R	64/77 (83%)	59 (92%)	5 (8%)	11	38
19	S	71/80 (89%)	55 (78%)	16 (22%)	1	4
20	T	76/82 (93%)	62 (82%)	14 (18%)	1	8
21	U	19/22 (86%)	17 (90%)	2 (10%)	6	26
All	All	1013/1471 (69%)	879 (87%)	134 (13%)	4	18

All (134) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	9	GLU
2	B	39	ILE
2	B	44	LEU
2	B	46	LYS
2	B	51	LEU
2	B	67	THR
2	B	69	LEU
2	B	86	GLU
2	B	97	TRP
2	B	102	LEU
2	B	121	LEU
2	B	158	LEU
2	B	164	VAL
2	B	169	LYS
2	B	172	ILE
2	B	179	LYS

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Mol	Chain	Res	Type
2	B	187	LEU
2	B	196	LEU
2	B	200	ILE
2	B	208	ILE
3	C	3	ASN
3	C	5	ILE
3	C	12	LEU
3	C	14	ILE
3	C	27	LYS
3	C	62	ASP
3	C	64	VAL
3	C	70	VAL
3	C	72	LYS
3	C	75	VAL
3	C	76	VAL
3	C	82	GLU
3	C	84	ILE
3	C	85	ARG
3	C	91	LEU
3	C	107	GLN
3	C	115	LEU
3	C	162	GLN
3	C	165	THR
3	C	175	LEU
3	C	177	THR
3	C	178	LEU
3	C	188	LEU
9	I	118	LYS
9	I	124	GLN
9	I	125	TYR
10	J	4	ILE
10	J	38	ILE
10	J	46	ARG
10	J	49	VAL
10	J	57	LYS
10	J	95	GLU
10	J	96	ILE
11	K	11	LYS
13	M	44	ARG
13	M	56	LEU
13	M	66	LEU
13	M	70	LEU

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Mol	Chain	Res	Type
13	M	94	ARG
13	M	109	THR
13	M	110	ARG
14	N	8	GLU
14	N	11	LYS
14	N	31	ARG
14	N	44	LEU
15	O	6	GLU
15	O	31	LEU
15	O	34	LEU
15	O	39	LEU
15	O	40	SER
15	O	43	LEU
15	O	44	LYS
15	O	45	VAL
15	O	48	LYS
15	O	57	LEU
15	O	70	LEU
15	O	81	LEU
15	O	87	ILE
16	P	2	VAL
16	P	8	ARG
16	P	27	LYS
16	P	31	LYS
16	P	54	GLU
16	P	62	VAL
17	Q	36	ILE
17	Q	38	ARG
17	Q	59	ILE
17	Q	68	ARG
17	Q	72	ARG
17	Q	86	GLU
17	Q	91	ARG
17	Q	92	ARG
17	Q	96	GLN
17	Q	97	SER
17	Q	98	LEU
17	Q	99	SER
17	Q	101	ARG
18	R	46	GLU
18	R	68	LYS
18	R	76	LEU

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Mol	Chain	Res	Type
18	R	85	LEU
18	R	88	LYS
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	31	ILE
19	S	33	THR
19	S	36	ARG
19	S	39	THR
19	S	43	GLU
19	S	55	LYS
19	S	58	VAL
19	S	65	ASN
19	S	78	ARG
19	S	81	ARG
20	T	8	ARG
20	T	18	GLN
20	T	19	SER
20	T	34	LYS
20	T	35	THR
20	T	56	MET
20	T	57	ARG
20	T	73	HIS
20	T	74	LYS
20	T	75	ASN
20	T	84	LEU
20	T	87	LYS
20	T	93	GLU
20	T	100	ILE
21	U	8	THR
21	U	15	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	76	GLN
3	C	6	HIS
3	C	37	GLN
3	C	63	ASN

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Mol	Chain	Res	Type
3	C	108	ASN
3	C	170	GLN
15	O	53	HIS
16	P	14	ASN
17	Q	96	GLN
19	S	14	HIS
19	S	65	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1510/1522 (99%)	260 (17%)	35 (2%)

All (260) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	9	G
1	A	32	A
1	A	39	G
1	A	44	G
1	A	47	C
1	A	48	C
1	A	50	A
1	A	51	A
1	A	54	C
1	A	81	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	163	C
1	A	169	C
1	A	182	U
1	A	190(I)	G
1	A	195	A
1	A	197	A

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Mol	Chain	Res	Type
1	A	201	C
1	A	202	U
1	A	204	U
1	A	216	G
1	A	220	G
1	A	247	G
1	A	251	G
1	A	266	G
1	A	267	C
1	A	280	C
1	A	289	G
1	A	319	G
1	A	321	A
1	A	328	C
1	A	329	A
1	A	331	G
1	A	332	G
1	A	344	A
1	A	345	C
1	A	347	G
1	A	352	C
1	A	353	A
1	A	354	G
1	A	367	U
1	A	372	C
1	A	373	A
1	A	382	A
1	A	384	G
1	A	390	C
1	A	397	A
1	A	398	C
1	A	406	G
1	A	412	A
1	A	413	G
1	A	421	U
1	A	424	G
1	A	429	U
1	A	432	A
1	A	433	C
1	A	439	A
1	A	442	C
1	A	443	C

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Mol	Chain	Res	Type
1	A	444	C
1	A	452	A
1	A	460	A
1	A	485	G
1	A	496	A
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	519	C
1	A	527	7MG
1	A	532	A
1	A	533	A
1	A	547	A
1	A	559	A
1	A	560	U
1	A	562	C
1	A	563	A
1	A	564	C
1	A	569	C
1	A	572	A
1	A	573	A
1	A	576	G
1	A	577	G
1	A	579	G
1	A	581	G
1	A	588	G
1	A	597	G
1	A	631	G
1	A	632	A
1	A	653	A
1	A	665	A
1	A	687	A
1	A	688	G
1	A	701	C
1	A	702	A
1	A	721	G
1	A	723	U
1	A	749	C

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Mol	Chain	Res	Type
1	A	755	G
1	A	766	A
1	A	777	A
1	A	780	A
1	A	781	A
1	A	782	A
1	A	792	A
1	A	793	U
1	A	794	A
1	A	799	G
1	A	813	U
1	A	816	A
1	A	817	C
1	A	819	A
1	A	820	U
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	876	G
1	A	902	G
1	A	914	A
1	A	926	G
1	A	927	G
1	A	928	G
1	A	934	C
1	A	935	A
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	987	G
1	A	989	C

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Mol	Chain	Res	Type
1	A	991	U
1	A	992	U
1	A	993	G
1	A	1003(A)	G
1	A	1004	A
1	A	1005	A
1	A	1025	U
1	A	1026	G
1	A	1027	C
1	A	1028	C
1	A	1031	G
1	A	1035	A
1	A	1036	G
1	A	1038	C
1	A	1042	G
1	A	1049	U
1	A	1050	G
1	A	1051	C
1	A	1054	C
1	A	1055	A
1	A	1065	U
1	A	1066	C
1	A	1086	U
1	A	1089	G
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1124	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	1137	C
1	A	1138	G
1	A	1139	G
1	A	1145	C
1	A	1146	A
1	A	1159	U
1	A	1171	G
1	A	1176	A

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Mol	Chain	Res	Type
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	1197	G
1	A	1200	C
1	A	1201	A
1	A	1202	G
1	A	1212	U
1	A	1213	A
1	A	1214	C
1	A	1225	A
1	A	1227	A
1	A	1238	A
1	A	1250	A
1	A	1257	U
1	A	1258	G
1	A	1270	C
1	A	1273	G
1	A	1278	U
1	A	1280	A
1	A	1282	C
1	A	1287	A
1	A	1300	G
1	A	1301	U
1	A	1302	U
1	A	1312	G
1	A	1320	C
1	A	1331	G
1	A	1332	A
1	A	1338	G
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	1394	A
1	A	1395	C

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Mol	Chain	Res	Type
1	A	1397	C
1	A	1398	A
1	A	1400	5MC
1	A	1402	4OC
1	A	1442	G
1	A	1443	G
1	A	1446	A
1	A	1447	G
1	A	1454	G
1	A	1487	G
1	A	1492	A
1	A	1497	G
1	A	1498	UR3
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	1529	G
1	A	1530	G
1	A	1533	C

All (35) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	108	G
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	372	C
1	A	428	G
1	A	432	A
1	A	484	G
1	A	496	A
1	A	509	A

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Mol	Chain	Res	Type
1	A	559	A
1	A	575	G
1	A	687	A
1	A	701	C
1	A	748	C
1	A	793	U
1	A	812	C
1	A	913	A
1	A	991	U
1	A	1049	U
1	A	1065	U
1	A	1182	G
1	A	1190	G
1	A	1201	A
1	A	1212	U
1	A	1256	A
1	A	1281	U
1	A	1300	G
1	A	1301	U
1	A	1331	G
1	A	1347	G
1	A	1505	G

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

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	$\# Z > 2$
12	0TD	L	92	12	8,9,10	1.71	1 (12%)	6,11,13	3.11	1 (16%)
1	7MG	A	527	23,1	23,26,27	4.01	4 (17%)	27,39,42	2.21	9 (33%)
1	PSU	A	516	23,1	18,21,22	1.17	1 (5%)	21,30,33	2.02	6 (28%)
1	2MG	A	1207	1	23,26,27	1.38	3 (13%)	33,38,41	1.14	6 (18%)
1	MA6	A	1518	1	23,26,27	1.06	2 (8%)	33,38,41	0.86	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	M2G	A	966	1	24,27,28	0.89	1 (4%)	33,40,43	0.82	0
1	5MC	A	967	1	19,22,23	0.87	1 (5%)	26,32,35	0.87	2 (7%)
1	MA6	A	1519	1	23,26,27	1.13	3 (13%)	33,38,41	1.09	2 (6%)
1	PSU	A	1540	1	18,21,22	1.18	1 (5%)	21,30,33	1.79	4 (19%)
1	5MC	A	1407	1	19,22,23	0.94	0	26,32,35	0.85	1 (3%)
1	UR3	A	1498	1	19,22,23	1.01	1 (5%)	26,32,35	1.04	1 (3%)
1	5MC	A	1404	1	19,22,23	1.22	2 (10%)	26,32,35	0.84	1 (3%)
1	4OC	A	1402	1	20,23,24	1.11	3 (15%)	25,32,35	0.78	1 (4%)
1	5MC	A	1400	1	19,22,23	1.29	2 (10%)	26,32,35	0.98	1 (3%)
1	PSU	A	1541	23,1	18,21,22	1.22	1 (5%)	21,30,33	1.80	4 (19%)

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
12	0TD	L	92	12	-	2/7/12/14	-
1	7MG	A	527	23,1	-	2/7/37/38	0/3/3/3
1	PSU	A	516	23,1	-	0/7/25/26	0/2/2/2
1	2MG	A	1207	1	-	0/9/27/28	0/3/3/3
1	MA6	A	1518	1	-	0/11/29/30	0/3/3/3
1	M2G	A	966	1	-	1/11/29/30	0/3/3/3
1	5MC	A	967	1	-	2/7/25/26	0/2/2/2
1	MA6	A	1519	1	-	1/11/29/30	0/3/3/3
1	PSU	A	1540	1	-	2/7/25/26	0/2/2/2
1	5MC	A	1407	1	-	0/7/25/26	0/2/2/2
1	UR3	A	1498	1	-	0/7/25/26	0/2/2/2
1	5MC	A	1404	1	-	0/7/25/26	0/2/2/2
1	4OC	A	1402	1	-	2/9/29/30	0/2/2/2
1	5MC	A	1400	1	-	2/7/25/26	0/2/2/2
1	PSU	A	1541	23,1	-	1/7/25/26	0/2/2/2

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	527	7MG	C8-N9	-17.70	1.34	1.45
1	A	1541	PSU	C6-C5	4.20	1.39	1.35
1	A	527	7MG	C2-N2	4.04	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1540	PSU	C6-C5	4.04	1.39	1.35
1	A	527	7MG	C4-N3	3.98	1.43	1.34
1	A	527	7MG	C5-N7	3.97	1.40	1.35
1	A	516	PSU	C6-C5	3.92	1.39	1.35
1	A	1404	5MC	C2-N3	3.82	1.43	1.36
12	L	92	0TD	CB-CA	3.70	1.56	1.54
1	A	1207	2MG	C2-N2	3.60	1.40	1.33
1	A	1207	2MG	C2-N1	3.49	1.42	1.36
1	A	1400	5MC	C2-N3	2.85	1.42	1.36
1	A	1400	5MC	C2-N1	2.71	1.45	1.40
1	A	1519	MA6	C5-C4	2.61	1.43	1.39
1	A	1498	UR3	C2-N1	2.61	1.42	1.38
1	A	1519	MA6	C8-N9	2.59	1.42	1.37
1	A	966	M2G	C2-N2	2.48	1.39	1.35
1	A	1518	MA6	C5-C4	2.43	1.43	1.39
1	A	1402	4OC	C2-N3	2.43	1.41	1.36
1	A	1519	MA6	C8-N7	2.31	1.36	1.31
1	A	1402	4OC	O2-C2	-2.29	1.19	1.23
1	A	1402	4OC	C4-N4	2.27	1.40	1.36
1	A	1518	MA6	C8-N9	2.06	1.41	1.37
1	A	1404	5MC	C4-N4	2.05	1.39	1.34
1	A	967	5MC	C4-N4	2.01	1.39	1.34
1	A	1207	2MG	C6-N1	2.00	1.42	1.38

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	92	0TD	CSB-SB-CB	-7.34	89.17	102.36
1	A	516	PSU	N1-C2-N3	5.38	120.85	115.17
1	A	527	7MG	C5-C6-N1	5.36	120.38	110.94
1	A	527	7MG	N9-C4-N3	4.79	132.48	125.46
1	A	1540	PSU	C4-N3-C2	-4.65	119.96	126.37
1	A	1541	PSU	C4-N3-C2	-4.58	120.06	126.37
1	A	516	PSU	C4-N3-C2	-4.55	120.10	126.37
1	A	1541	PSU	N1-C2-N3	4.45	119.86	115.17
1	A	1540	PSU	N1-C2-N3	4.35	119.76	115.17
1	A	527	7MG	C2-N3-C4	4.12	119.39	112.30
1	A	527	7MG	C5-C4-N3	-3.80	120.99	128.13
1	A	516	PSU	C6-N1-C2	-3.32	119.61	122.69
1	A	527	7MG	C6-C5-C4	-3.05	117.03	122.40
1	A	527	7MG	N9-C8-N7	2.99	107.61	103.37
1	A	527	7MG	O6-C6-C5	-2.90	120.49	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1540	PSU	O2-C2-N1	-2.77	119.93	122.79
1	A	527	7MG	C2-N1-C6	-2.74	120.15	125.11
1	A	527	7MG	C6-C5-N7	2.69	136.09	131.93
1	A	1541	PSU	O2-C2-N1	-2.62	120.09	122.79
1	A	516	PSU	C6-C5-C4	2.61	119.93	118.17
1	A	1207	2MG	C2-N1-C6	-2.47	121.57	124.55
1	A	1207	2MG	C5-C4-N3	-2.46	124.47	128.39
1	A	1540	PSU	C6-N1-C2	-2.44	120.43	122.69
1	A	1541	PSU	C6-N1-C2	-2.40	120.46	122.69
1	A	1518	MA6	C2-N1-C6	2.37	117.62	111.83
1	A	1207	2MG	N9-C4-N3	2.32	130.59	125.95
1	A	1404	5MC	C4-N3-C2	-2.32	117.59	120.81
1	A	1498	UR3	C6-N1-C2	-2.29	119.93	121.80
1	A	1519	MA6	C2-N1-C6	2.29	117.41	111.83
1	A	967	5MC	N4-C4-N3	-2.26	114.41	118.51
1	A	1407	5MC	C5-C4-N3	2.23	124.04	121.75
1	A	516	PSU	O2-C2-N3	-2.19	117.97	121.86
1	A	1519	MA6	C5-C4-N9	2.14	108.15	105.81
1	A	1207	2MG	C6-C5-N7	-2.12	126.44	130.29
1	A	1400	5MC	C4-N3-C2	-2.10	117.89	120.81
1	A	967	5MC	C5-C4-N3	2.07	123.88	121.75
1	A	1207	2MG	C6-C5-C4	2.07	121.94	118.83
1	A	516	PSU	O4'-C1'-C2'	2.05	107.99	105.15
1	A	1207	2MG	O6-C6-N1	-2.02	116.31	120.11
1	A	1402	4OC	C5-C4-N4	-2.00	118.00	122.40

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	527	7MG	O4'-C4'-C5'-O5'
1	A	1400	5MC	O4'-C4'-C5'-O5'
12	L	92	0TD	SB-CB-CG-OD2
1	A	527	7MG	C3'-C4'-C5'-O5'
1	A	967	5MC	O4'-C4'-C5'-O5'
1	A	1402	4OC	O4'-C4'-C5'-O5'
1	A	1400	5MC	C3'-C4'-C5'-O5'
1	A	1402	4OC	C3'-C4'-C5'-O5'
1	A	967	5MC	C3'-C4'-C5'-O5'
12	L	92	0TD	CG-CB-SB-CSB
1	A	1519	MA6	C4'-C5'-O5'-P
1	A	1540	PSU	O4'-C1'-C5-C4

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Mol	Chain	Res	Type	Atoms
1	A	966	M2G	C4'-C5'-O5'-P
1	A	1540	PSU	O4'-C1'-C5-C6
1	A	1541	PSU	O4'-C1'-C5-C6

There are no ring outliers.

8 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	L	92	0TD	4	0
1	A	1207	2MG	2	0
1	A	1518	MA6	2	0
1	A	967	5MC	1	0
1	A	1519	MA6	1	0
1	A	1498	UR3	4	0
1	A	1402	4OC	3	0
1	A	1400	5MC	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 346 ligands modelled in this entry, 329 are monoatomic - leaving 17 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	$\# Z > 2$
22	PAR	A	1606	-	44,45,45	1.24	5 (11%)	63,67,67	1.58	16 (25%)
22	PAR	A	1611	-	44,45,45	1.91	11 (25%)	63,67,67	1.62	9 (14%)
22	PAR	A	1616	-	44,45,45	1.36	5 (11%)	63,67,67	1.64	11 (17%)
22	PAR	A	1601	-	44,45,45	1.02	4 (9%)	63,67,67	1.51	11 (17%)
22	PAR	A	1607	-	44,45,45	1.26	4 (9%)	63,67,67	1.64	12 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	PAR	A	1610	-	44,45,45	1.58	7 (15%)	63,67,67	1.71	11 (17%)
22	PAR	A	1612	-	44,45,45	1.55	7 (15%)	63,67,67	1.74	11 (17%)
22	PAR	A	1605	-	44,45,45	1.17	3 (6%)	63,67,67	1.69	12 (19%)
22	PAR	A	1615	-	44,45,45	1.51	7 (15%)	63,67,67	1.63	13 (20%)
22	PAR	A	1617	-	44,45,45	1.33	5 (11%)	63,67,67	1.65	12 (19%)
22	PAR	A	1614	-	44,45,45	1.50	10 (22%)	63,67,67	1.66	12 (19%)
22	PAR	A	1613	-	44,45,45	1.67	10 (22%)	63,67,67	1.68	12 (19%)
22	PAR	A	1603	-	44,45,45	1.32	3 (6%)	63,67,67	1.55	9 (14%)
22	PAR	A	1609	-	44,45,45	1.16	5 (11%)	63,67,67	1.56	13 (20%)
22	PAR	A	1608	-	44,45,45	1.15	3 (6%)	63,67,67	1.68	12 (19%)
22	PAR	A	1604	-	44,45,45	1.18	2 (4%)	63,67,67	1.62	12 (19%)
22	PAR	A	1602	-	44,45,45	1.04	3 (6%)	63,67,67	1.76	12 (19%)

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
22	PAR	A	1606	-	-	7/18/94/94	0/4/4/4
22	PAR	A	1611	-	-	7/18/94/94	0/4/4/4
22	PAR	A	1616	-	-	9/18/94/94	1/4/4/4
22	PAR	A	1601	-	-	4/18/94/94	0/4/4/4
22	PAR	A	1607	-	-	4/18/94/94	0/4/4/4
22	PAR	A	1610	-	-	7/18/94/94	0/4/4/4
22	PAR	A	1612	-	-	8/18/94/94	0/4/4/4
22	PAR	A	1605	-	-	3/18/94/94	0/4/4/4
22	PAR	A	1615	-	-	11/18/94/94	1/4/4/4
22	PAR	A	1617	-	-	3/18/94/94	1/4/4/4
22	PAR	A	1614	-	-	5/18/94/94	0/4/4/4
22	PAR	A	1613	-	-	11/18/94/94	0/4/4/4
22	PAR	A	1603	-	-	3/18/94/94	0/4/4/4
22	PAR	A	1609	-	-	2/18/94/94	0/4/4/4
22	PAR	A	1608	-	-	8/18/94/94	0/4/4/4
22	PAR	A	1604	-	-	6/18/94/94	0/4/4/4
22	PAR	A	1602	-	-	7/18/94/94	0/4/4/4

All (94) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	1611	PAR	C13-C23	5.17	1.59	1.52
22	A	1611	PAR	C52-C42	4.90	1.62	1.52
22	A	1603	PAR	C31-C21	4.79	1.59	1.53
22	A	1615	PAR	C34-C24	4.57	1.59	1.53
22	A	1612	PAR	C14-C24	4.36	1.60	1.52
22	A	1612	PAR	O43-C13	4.30	1.49	1.41
22	A	1614	PAR	C13-C23	4.26	1.58	1.52
22	A	1604	PAR	C52-C42	4.21	1.60	1.52
22	A	1610	PAR	C34-C24	4.16	1.58	1.53
22	A	1617	PAR	O43-C13	4.14	1.49	1.41
22	A	1613	PAR	C13-C23	4.13	1.58	1.52
22	A	1613	PAR	C31-C21	3.74	1.58	1.53
22	A	1613	PAR	C52-C42	3.63	1.59	1.52
22	A	1607	PAR	O43-C13	3.62	1.48	1.41
22	A	1610	PAR	C52-C42	3.55	1.59	1.52
22	A	1610	PAR	C13-C23	3.53	1.57	1.52
22	A	1611	PAR	C31-C21	3.53	1.58	1.53
22	A	1612	PAR	C34-C24	3.50	1.57	1.53
22	A	1611	PAR	C14-C24	3.43	1.59	1.52
22	A	1613	PAR	C34-C24	3.38	1.57	1.53
22	A	1615	PAR	C52-C42	3.36	1.59	1.52
22	A	1607	PAR	C13-C23	3.36	1.57	1.52
22	A	1616	PAR	O43-C13	3.34	1.47	1.41
22	A	1610	PAR	C14-C24	3.32	1.58	1.52
22	A	1603	PAR	C52-C42	3.28	1.59	1.52
22	A	1612	PAR	C52-C42	3.25	1.58	1.52
22	A	1617	PAR	C52-C42	3.21	1.58	1.52
22	A	1610	PAR	O43-C13	3.21	1.47	1.41
22	A	1614	PAR	C14-C24	3.20	1.58	1.52
22	A	1614	PAR	C52-C42	3.20	1.58	1.52
22	A	1612	PAR	C13-C23	3.15	1.56	1.52
22	A	1606	PAR	C52-C42	3.13	1.58	1.52
22	A	1617	PAR	C34-C24	3.07	1.57	1.53
22	A	1616	PAR	C52-C42	3.06	1.58	1.52
22	A	1611	PAR	C34-C24	3.05	1.57	1.53
22	A	1611	PAR	C62-C52	3.03	1.60	1.52
22	A	1616	PAR	C31-C21	3.01	1.57	1.53
22	A	1611	PAR	O33-C14	2.99	1.50	1.41
22	A	1615	PAR	C13-C23	2.97	1.56	1.52
22	A	1613	PAR	C62-C52	2.95	1.60	1.52
22	A	1605	PAR	C13-C23	2.94	1.56	1.52
22	A	1615	PAR	C14-C24	2.93	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	1606	PAR	C31-C21	2.85	1.57	1.53
22	A	1613	PAR	C14-C24	2.84	1.57	1.52
22	A	1608	PAR	O43-C13	2.83	1.46	1.41
22	A	1608	PAR	C34-C24	2.78	1.57	1.53
22	A	1611	PAR	O52-C52	2.73	1.50	1.43
22	A	1601	PAR	C31-C21	2.71	1.56	1.53
22	A	1607	PAR	C34-C24	2.71	1.56	1.53
22	A	1606	PAR	O43-C13	2.70	1.46	1.41
22	A	1609	PAR	C52-C42	2.69	1.57	1.52
22	A	1610	PAR	O33-C14	2.65	1.49	1.41
22	A	1617	PAR	C13-C23	2.65	1.56	1.52
22	A	1606	PAR	C13-C23	2.60	1.56	1.52
22	A	1605	PAR	C52-C42	2.60	1.57	1.52
22	A	1609	PAR	C33-C43	2.56	1.59	1.52
22	A	1614	PAR	C33-C43	2.54	1.59	1.52
22	A	1616	PAR	C13-C23	2.54	1.56	1.52
22	A	1601	PAR	C52-C42	2.52	1.57	1.52
22	A	1602	PAR	C11-C21	2.44	1.57	1.52
22	A	1607	PAR	C52-C42	2.44	1.57	1.52
22	A	1609	PAR	C31-C21	2.43	1.56	1.53
22	A	1606	PAR	C33-C43	2.42	1.59	1.52
22	A	1613	PAR	O43-C13	2.41	1.45	1.41
22	A	1615	PAR	C33-C43	2.40	1.59	1.52
22	A	1612	PAR	O33-C14	2.39	1.48	1.41
22	A	1604	PAR	C33-C43	2.38	1.59	1.52
22	A	1616	PAR	O33-C14	2.34	1.48	1.41
22	A	1602	PAR	O43-C13	2.31	1.45	1.41
22	A	1601	PAR	C33-C43	2.31	1.58	1.52
22	A	1611	PAR	C22-C12	-2.31	1.48	1.53
22	A	1602	PAR	C33-C43	2.29	1.58	1.52
22	A	1614	PAR	C31-C21	2.27	1.56	1.53
22	A	1614	PAR	C62-C52	2.26	1.58	1.52
22	A	1611	PAR	O33-C33	2.22	1.49	1.43
22	A	1617	PAR	C31-C21	2.20	1.56	1.53
22	A	1609	PAR	C34-C24	2.20	1.56	1.53
22	A	1608	PAR	C13-C23	2.17	1.55	1.52
22	A	1615	PAR	O52-C52	2.17	1.49	1.43
22	A	1610	PAR	C44-C54	2.17	1.57	1.53
22	A	1614	PAR	O52-C52	2.17	1.49	1.43
22	A	1603	PAR	O43-C13	2.14	1.45	1.41
22	A	1605	PAR	O43-C13	2.12	1.45	1.41
22	A	1613	PAR	O11-C42	2.11	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	1609	PAR	C13-C23	2.09	1.55	1.52
22	A	1613	PAR	C11-C21	2.08	1.56	1.52
22	A	1612	PAR	C41-C51	2.06	1.57	1.53
22	A	1615	PAR	O43-C13	2.05	1.45	1.41
22	A	1614	PAR	C34-C24	2.04	1.56	1.53
22	A	1601	PAR	C14-C24	2.02	1.56	1.52
22	A	1613	PAR	O52-C52	2.02	1.49	1.43
22	A	1611	PAR	O43-C13	2.02	1.45	1.41
22	A	1614	PAR	O43-C13	2.01	1.45	1.41
22	A	1614	PAR	C11-C21	2.00	1.56	1.52

All (200) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1612	PAR	O33-C14-C24	7.86	120.94	108.08
22	A	1610	PAR	O33-C14-C24	7.53	120.40	108.08
22	A	1602	PAR	O33-C14-C24	7.26	119.96	108.08
22	A	1611	PAR	O33-C14-C24	6.96	119.46	108.08
22	A	1605	PAR	O33-C14-C24	6.92	119.40	108.08
22	A	1616	PAR	O33-C14-C24	6.90	119.38	108.08
22	A	1617	PAR	O33-C14-C24	6.85	119.29	108.08
22	A	1608	PAR	O33-C14-C24	6.84	119.28	108.08
22	A	1613	PAR	O33-C14-C24	6.59	118.86	108.08
22	A	1614	PAR	O33-C14-C24	6.51	118.73	108.08
22	A	1607	PAR	O33-C14-C24	6.46	118.64	108.08
22	A	1615	PAR	O33-C14-C24	6.35	118.47	108.08
22	A	1604	PAR	O33-C14-C24	6.00	117.89	108.08
22	A	1606	PAR	O33-C14-C24	5.73	117.46	108.08
22	A	1601	PAR	O33-C14-C24	5.60	117.25	108.08
22	A	1603	PAR	O33-C14-C24	5.52	117.11	108.08
22	A	1609	PAR	O33-C14-C24	5.39	116.90	108.08
22	A	1602	PAR	O52-C13-O43	-3.99	107.29	111.37
22	A	1602	PAR	O43-C13-C23	-3.96	99.94	104.98
22	A	1613	PAR	C13-C23-C33	3.82	106.69	102.10
22	A	1605	PAR	C13-C23-C33	3.61	106.45	102.10
22	A	1614	PAR	C13-C23-C33	3.60	106.43	102.10
22	A	1611	PAR	C13-C23-C33	3.57	106.39	102.10
22	A	1617	PAR	C14-O33-C33	-3.50	109.69	117.98
22	A	1605	PAR	C14-O33-C33	-3.42	109.87	117.98
22	A	1602	PAR	O34-C34-C44	-3.36	102.46	110.38
22	A	1614	PAR	C34-C24-N24	-3.24	104.41	111.05
22	A	1605	PAR	C34-C24-N24	-3.24	104.42	111.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1606	PAR	C34-C24-N24	-3.23	104.43	111.05
22	A	1609	PAR	C34-C24-N24	-3.20	104.49	111.05
22	A	1610	PAR	C34-C24-N24	-3.19	104.52	111.05
22	A	1613	PAR	O52-C13-O43	-3.17	108.13	111.37
22	A	1612	PAR	O34-C34-C44	-3.16	102.93	110.38
22	A	1614	PAR	O11-C11-O51	3.16	119.01	110.69
22	A	1616	PAR	C14-O33-C33	-3.16	110.49	117.98
22	A	1613	PAR	C14-O33-C33	-3.14	110.54	117.98
22	A	1611	PAR	C34-C24-N24	-3.13	104.65	111.05
22	A	1607	PAR	C14-O33-C33	-3.12	110.59	117.98
22	A	1606	PAR	O11-C11-O51	3.11	118.88	110.69
22	A	1615	PAR	O11-C11-O51	3.06	118.75	110.69
22	A	1609	PAR	O34-C34-C44	-3.05	103.18	110.38
22	A	1603	PAR	O34-C34-C44	-3.02	103.25	110.38
22	A	1612	PAR	O52-C13-O43	-3.02	108.28	111.37
22	A	1603	PAR	C34-C24-N24	-3.02	104.87	111.05
22	A	1608	PAR	C34-C24-N24	-3.01	104.88	111.05
22	A	1601	PAR	O34-C34-C44	-3.01	103.27	110.38
22	A	1611	PAR	O11-C11-O51	3.01	118.61	110.69
22	A	1601	PAR	C34-C24-N24	-3.01	104.89	111.05
22	A	1616	PAR	O11-C11-O51	3.00	118.58	110.69
22	A	1604	PAR	C34-C24-N24	-3.00	104.91	111.05
22	A	1610	PAR	O52-C13-O43	-2.99	108.31	111.37
22	A	1607	PAR	C34-C24-N24	-2.98	104.95	111.05
22	A	1603	PAR	C13-O52-C52	-2.97	110.93	117.98
22	A	1613	PAR	C34-C24-N24	-2.97	104.96	111.05
22	A	1612	PAR	C34-C24-N24	-2.97	104.97	111.05
22	A	1613	PAR	O11-C11-O51	2.96	118.47	110.69
22	A	1607	PAR	O34-C34-C44	-2.95	103.41	110.38
22	A	1617	PAR	C34-C24-N24	-2.95	105.00	111.05
22	A	1608	PAR	O52-C13-O43	-2.95	108.36	111.37
22	A	1602	PAR	C14-O33-C33	-2.93	111.02	117.98
22	A	1605	PAR	O54-C54-C44	2.92	114.96	109.70
22	A	1608	PAR	O34-C34-C44	-2.92	103.50	110.38
22	A	1616	PAR	C34-C24-N24	-2.91	105.09	111.05
22	A	1617	PAR	O34-C34-C44	-2.89	103.56	110.38
22	A	1605	PAR	O34-C34-C44	-2.89	103.57	110.38
22	A	1609	PAR	C13-O52-C52	-2.87	111.17	117.98
22	A	1604	PAR	O11-C11-O51	2.87	118.24	110.69
22	A	1617	PAR	O11-C11-O51	2.86	118.22	110.69
22	A	1612	PAR	O54-C54-C44	2.86	114.85	109.70
22	A	1612	PAR	O11-C11-O51	2.86	118.22	110.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1603	PAR	O11-C11-O51	2.85	118.20	110.69
22	A	1609	PAR	O11-C11-O51	2.83	118.15	110.69
22	A	1604	PAR	O34-C34-C44	-2.81	103.74	110.38
22	A	1615	PAR	C34-C24-N24	-2.81	105.30	111.05
22	A	1610	PAR	O11-C11-O51	2.78	118.00	110.69
22	A	1615	PAR	C13-C23-C33	2.77	105.44	102.10
22	A	1611	PAR	O34-C34-C44	-2.77	103.84	110.38
22	A	1612	PAR	C14-O33-C33	-2.76	111.42	117.98
22	A	1607	PAR	O11-C11-O51	2.76	117.96	110.69
22	A	1616	PAR	O34-C34-C44	-2.76	103.88	110.38
22	A	1608	PAR	C14-O33-C33	-2.76	111.45	117.98
22	A	1613	PAR	O34-C34-C44	-2.75	103.90	110.38
22	A	1607	PAR	O51-C51-C61	2.73	113.21	106.44
22	A	1601	PAR	O11-C11-O51	2.73	117.87	110.69
22	A	1615	PAR	C14-O33-C33	-2.72	111.52	117.98
22	A	1611	PAR	C14-O33-C33	-2.72	111.54	117.98
22	A	1614	PAR	O34-C34-C44	-2.71	103.98	110.38
22	A	1616	PAR	O54-C54-C44	2.71	114.58	109.70
22	A	1605	PAR	O11-C11-O51	2.71	117.82	110.69
22	A	1604	PAR	C13-C23-C33	2.71	105.36	102.10
22	A	1613	PAR	O11-C42-C52	2.69	114.25	107.42
22	A	1604	PAR	C13-O52-C52	-2.68	111.62	117.98
22	A	1615	PAR	O34-C34-C44	-2.66	104.09	110.38
22	A	1607	PAR	O52-C13-O43	-2.66	108.65	111.37
22	A	1616	PAR	O52-C13-O43	-2.66	108.65	111.37
22	A	1606	PAR	C13-O52-C52	-2.66	111.67	117.98
22	A	1602	PAR	C34-C24-N24	-2.66	105.61	111.05
22	A	1608	PAR	C22-C12-C62	2.65	114.04	110.08
22	A	1614	PAR	C14-O33-C33	-2.64	111.72	117.98
22	A	1615	PAR	C13-O52-C52	-2.63	111.74	117.98
22	A	1604	PAR	O54-C54-C44	2.62	114.42	109.70
22	A	1604	PAR	O52-C13-O43	-2.61	108.70	111.37
22	A	1610	PAR	C14-O33-C33	-2.61	111.80	117.98
22	A	1602	PAR	O11-C11-O51	2.61	117.55	110.69
22	A	1608	PAR	O11-C11-O51	2.60	117.55	110.69
22	A	1604	PAR	O11-C11-C21	-2.59	103.83	108.08
22	A	1610	PAR	O34-C34-C44	-2.58	104.30	110.38
22	A	1605	PAR	C13-O52-C52	-2.57	111.88	117.98
22	A	1606	PAR	O34-C34-C44	-2.57	104.31	110.38
22	A	1601	PAR	C13-O52-C52	-2.57	111.89	117.98
22	A	1606	PAR	O43-C13-C23	-2.56	101.72	104.98
22	A	1610	PAR	O51-C51-C61	2.56	112.78	106.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1608	PAR	C13-C23-C33	2.55	105.17	102.10
22	A	1603	PAR	O52-C13-O43	-2.54	108.77	111.37
22	A	1609	PAR	C14-O33-C33	-2.53	111.98	117.98
22	A	1616	PAR	O51-C51-C61	2.53	112.70	106.44
22	A	1605	PAR	O52-C13-O43	-2.51	108.81	111.37
22	A	1614	PAR	C11-O51-C51	2.50	118.60	113.72
22	A	1607	PAR	C22-C12-C62	2.49	113.81	110.08
22	A	1614	PAR	C22-C12-C62	2.49	113.80	110.08
22	A	1608	PAR	C13-O52-C52	-2.48	112.09	117.98
22	A	1610	PAR	O54-C54-C44	2.48	114.16	109.70
22	A	1616	PAR	C13-O52-C52	-2.48	112.11	117.98
22	A	1614	PAR	C13-O52-C52	-2.48	112.11	117.98
22	A	1609	PAR	O43-C13-C23	-2.47	101.83	104.98
22	A	1604	PAR	C14-O33-C33	-2.47	112.12	117.98
22	A	1610	PAR	C13-O52-C52	-2.47	112.13	117.98
22	A	1610	PAR	C11-O51-C51	2.47	118.54	113.72
22	A	1606	PAR	C31-C41-C51	2.46	114.69	110.23
22	A	1613	PAR	O52-C52-C42	2.45	113.65	107.42
22	A	1612	PAR	C23-C33-C43	-2.45	98.96	103.24
22	A	1602	PAR	O34-C34-C24	-2.44	105.84	110.22
22	A	1613	PAR	C22-C12-C62	2.41	113.69	110.08
22	A	1608	PAR	O51-C51-C61	2.40	112.40	106.44
22	A	1611	PAR	C11-O51-C51	2.39	118.39	113.72
22	A	1617	PAR	C13-O52-C52	-2.39	112.31	117.98
22	A	1601	PAR	C23-C33-C43	-2.38	99.07	103.24
22	A	1607	PAR	C13-C23-C33	2.38	104.96	102.10
22	A	1605	PAR	O51-C51-C61	2.38	112.33	106.44
22	A	1617	PAR	O52-C13-O43	-2.36	108.96	111.37
22	A	1613	PAR	O51-C51-C61	2.36	112.28	106.44
22	A	1601	PAR	O43-C13-C23	-2.35	101.99	104.98
22	A	1615	PAR	O51-C51-C61	2.34	112.23	106.44
22	A	1617	PAR	C22-C12-C62	2.33	113.57	110.08
22	A	1606	PAR	C23-C33-C43	-2.33	99.17	103.24
22	A	1601	PAR	O34-C34-C24	-2.31	106.06	110.22
22	A	1603	PAR	O34-C34-C24	-2.31	106.08	110.22
22	A	1601	PAR	C14-O33-C33	-2.30	112.53	117.98
22	A	1611	PAR	O51-C51-C61	2.30	112.14	106.44
22	A	1606	PAR	O11-C11-C21	-2.30	104.31	108.08
22	A	1603	PAR	C14-O33-C33	-2.28	112.56	117.98
22	A	1617	PAR	O54-C54-C44	2.27	113.79	109.70
22	A	1602	PAR	C23-C33-C43	-2.27	99.27	103.24
22	A	1617	PAR	O51-C51-C61	2.26	112.05	106.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1601	PAR	O51-C51-C61	2.26	112.05	106.44
22	A	1612	PAR	C11-O51-C51	2.26	118.14	113.72
22	A	1607	PAR	C13-O52-C52	-2.26	112.62	117.98
22	A	1610	PAR	C13-C23-C33	2.26	104.82	102.10
22	A	1601	PAR	O33-C14-O54	-2.25	104.76	110.69
22	A	1609	PAR	C22-C12-C62	2.25	113.45	110.08
22	A	1614	PAR	O51-C51-C61	2.25	112.02	106.44
22	A	1603	PAR	O51-C51-C61	2.24	112.00	106.44
22	A	1609	PAR	O33-C14-O54	-2.23	104.82	110.69
22	A	1604	PAR	O51-C51-C61	2.22	111.95	106.44
22	A	1617	PAR	C11-O51-C51	2.22	118.06	113.72
22	A	1606	PAR	O51-C51-C41	2.22	113.69	109.70
22	A	1607	PAR	O54-C54-C44	2.21	113.68	109.70
22	A	1608	PAR	O54-C54-C44	2.21	113.67	109.70
22	A	1606	PAR	O54-C54-C44	2.20	113.66	109.70
22	A	1612	PAR	C13-O52-C52	-2.19	112.79	117.98
22	A	1609	PAR	O51-C51-C61	2.16	111.80	106.44
22	A	1606	PAR	O52-C13-O43	-2.15	109.17	111.37
22	A	1602	PAR	C11-O51-C51	2.15	117.92	113.72
22	A	1614	PAR	O52-C13-O43	-2.15	109.17	111.37
22	A	1602	PAR	O51-C51-C61	2.15	111.76	106.44
22	A	1612	PAR	O51-C51-C61	2.15	111.76	106.44
22	A	1613	PAR	C13-O52-C52	-2.14	112.89	117.98
22	A	1616	PAR	C22-C12-C62	2.14	113.28	110.08
22	A	1615	PAR	C22-C12-C62	2.14	113.28	110.08
22	A	1615	PAR	O52-C13-O43	-2.13	109.19	111.37
22	A	1606	PAR	C22-C32-C42	2.13	114.72	109.50
22	A	1616	PAR	C13-C23-C33	2.12	104.66	102.10
22	A	1606	PAR	O51-C51-C61	2.12	111.69	106.44
22	A	1609	PAR	O43-C43-C53	2.12	113.69	109.22
22	A	1615	PAR	O54-C54-C44	2.12	113.51	109.70
22	A	1606	PAR	C14-O33-C33	-2.11	112.97	117.98
22	A	1602	PAR	O54-C54-C44	2.10	113.48	109.70
22	A	1607	PAR	C11-O51-C51	2.10	117.82	113.72
22	A	1606	PAR	C11-O51-C51	2.08	117.78	113.72
22	A	1608	PAR	C11-O51-C51	2.07	117.76	113.72
22	A	1609	PAR	C11-O51-C51	2.07	117.76	113.72
22	A	1617	PAR	O33-C14-O54	-2.07	105.26	110.69
22	A	1614	PAR	O54-C54-C44	2.05	113.39	109.70
22	A	1609	PAR	O52-C13-O43	-2.05	109.28	111.37
22	A	1605	PAR	C22-C12-C62	2.05	113.14	110.08
22	A	1615	PAR	O52-C52-C42	2.04	112.61	107.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1604	PAR	C11-O51-C51	2.04	117.70	113.72
22	A	1611	PAR	O54-C54-C44	2.02	113.34	109.70
22	A	1615	PAR	O43-C13-C23	-2.02	102.42	104.98
22	A	1605	PAR	O33-C14-O54	-2.00	105.43	110.69

There are no chirality outliers.

All (105) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
22	A	1617	PAR	C44-C54-C64-N64
22	A	1612	PAR	O54-C14-O33-C33
22	A	1616	PAR	O51-C11-O11-C42
22	A	1608	PAR	O54-C14-O33-C33
22	A	1613	PAR	O54-C14-O33-C33
22	A	1614	PAR	O54-C14-O33-C33
22	A	1616	PAR	O54-C14-O33-C33
22	A	1613	PAR	C52-C42-O11-C11
22	A	1608	PAR	O51-C11-O11-C42
22	A	1615	PAR	O43-C43-C53-O53
22	A	1602	PAR	C33-C43-C53-O53
22	A	1602	PAR	O43-C43-C53-O53
22	A	1606	PAR	O43-C43-C53-O53
22	A	1605	PAR	O54-C14-O33-C33
22	A	1615	PAR	O51-C11-O11-C42
22	A	1613	PAR	C33-C43-C53-O53
22	A	1613	PAR	O43-C43-C53-O53
22	A	1614	PAR	O51-C51-C61-O61
22	A	1616	PAR	C33-C43-C53-O53
22	A	1616	PAR	O51-C51-C61-O61
22	A	1606	PAR	O54-C14-O33-C33
22	A	1608	PAR	C42-C52-O52-C13
22	A	1616	PAR	O43-C43-C53-O53
22	A	1608	PAR	C41-C51-C61-O61
22	A	1615	PAR	C33-C43-C53-O53
22	A	1615	PAR	O51-C51-C61-O61
22	A	1610	PAR	O51-C51-C61-O61
22	A	1604	PAR	C52-C42-O11-C11
22	A	1608	PAR	O51-C51-C61-O61
22	A	1603	PAR	O51-C11-O11-C42
22	A	1614	PAR	C41-C51-C61-O61
22	A	1615	PAR	C41-C51-C61-O61
22	A	1604	PAR	O54-C14-O33-C33
22	A	1612	PAR	O51-C51-C61-O61
22	A	1611	PAR	C62-C52-O52-C13
22	A	1616	PAR	C41-C51-C61-O61
22	A	1601	PAR	O43-C43-C53-O53
22	A	1612	PAR	O43-C13-O52-C52
22	A	1613	PAR	O43-C13-O52-C52
22	A	1615	PAR	O43-C13-O52-C52
22	A	1611	PAR	C42-C52-O52-C13
22	A	1601	PAR	O54-C14-O33-C33

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Mol	Chain	Res	Type	Atoms
22	A	1610	PAR	O54-C14-O33-C33
22	A	1605	PAR	C41-C51-C61-O61
22	A	1608	PAR	C62-C52-O52-C13
22	A	1617	PAR	O54-C14-O33-C33
22	A	1606	PAR	C52-C42-O11-C11
22	A	1603	PAR	O43-C43-C53-O53
22	A	1611	PAR	C23-C13-O52-C52
22	A	1601	PAR	C52-C42-O11-C11
22	A	1604	PAR	C32-C42-O11-C11
22	A	1610	PAR	C41-C51-C61-O61
22	A	1612	PAR	O54-C54-C64-N64
22	A	1601	PAR	C33-C43-C53-O53
22	A	1602	PAR	O54-C14-O33-C33
22	A	1609	PAR	C24-C14-O33-C33
22	A	1614	PAR	C44-C54-C64-N64
22	A	1607	PAR	O51-C11-O11-C42
22	A	1608	PAR	O43-C13-O52-C52
22	A	1612	PAR	C23-C33-O33-C14
22	A	1606	PAR	O51-C51-C61-O61
22	A	1603	PAR	O54-C14-O33-C33
22	A	1608	PAR	C23-C13-O52-C52
22	A	1609	PAR	C21-C11-O11-C42
22	A	1613	PAR	C21-C11-O11-C42
22	A	1604	PAR	C62-C52-O52-C13
22	A	1610	PAR	C43-C33-O33-C14
22	A	1611	PAR	C43-C33-O33-C14
22	A	1612	PAR	C43-C33-O33-C14
22	A	1613	PAR	C23-C33-O33-C14
22	A	1615	PAR	C43-C33-O33-C14
22	A	1617	PAR	C43-C33-O33-C14

All (3) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A	1616	PAR	C12-C22-C32-C42-C52-C62
22	A	1615	PAR	C12-C22-C32-C42-C52-C62
22	A	1617	PAR	C12-C22-C32-C42-C52-C62

15 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	1606	PAR	2	0

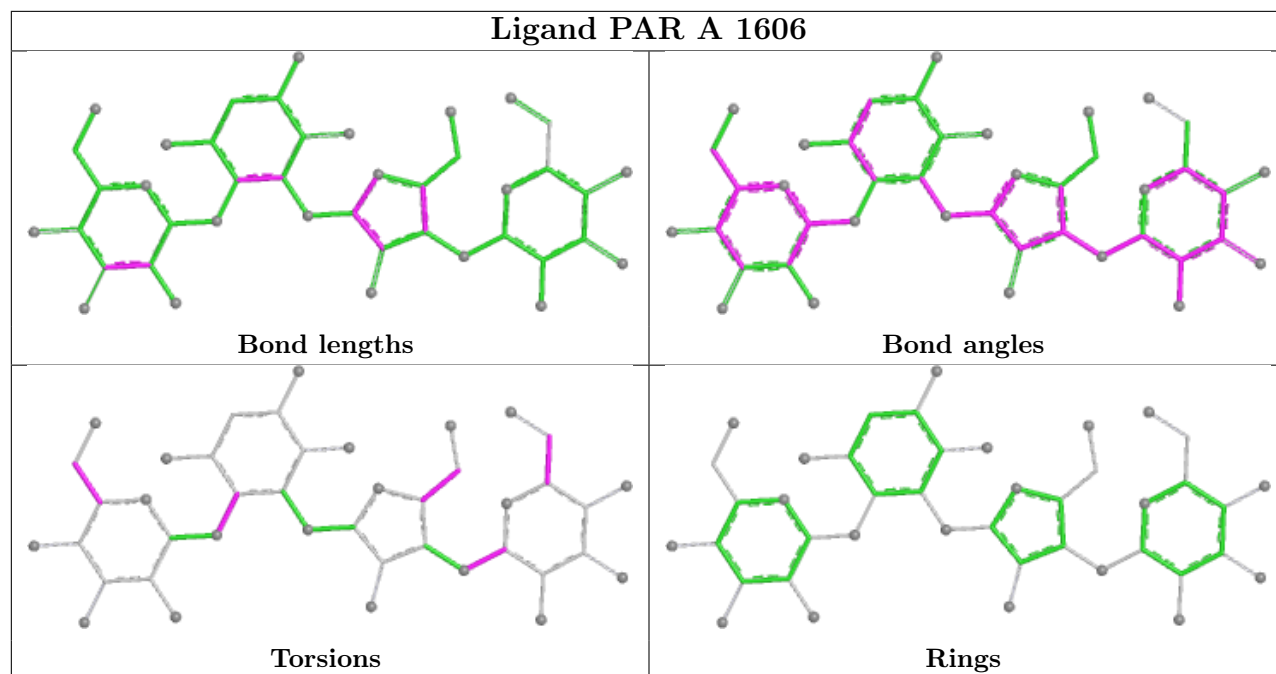
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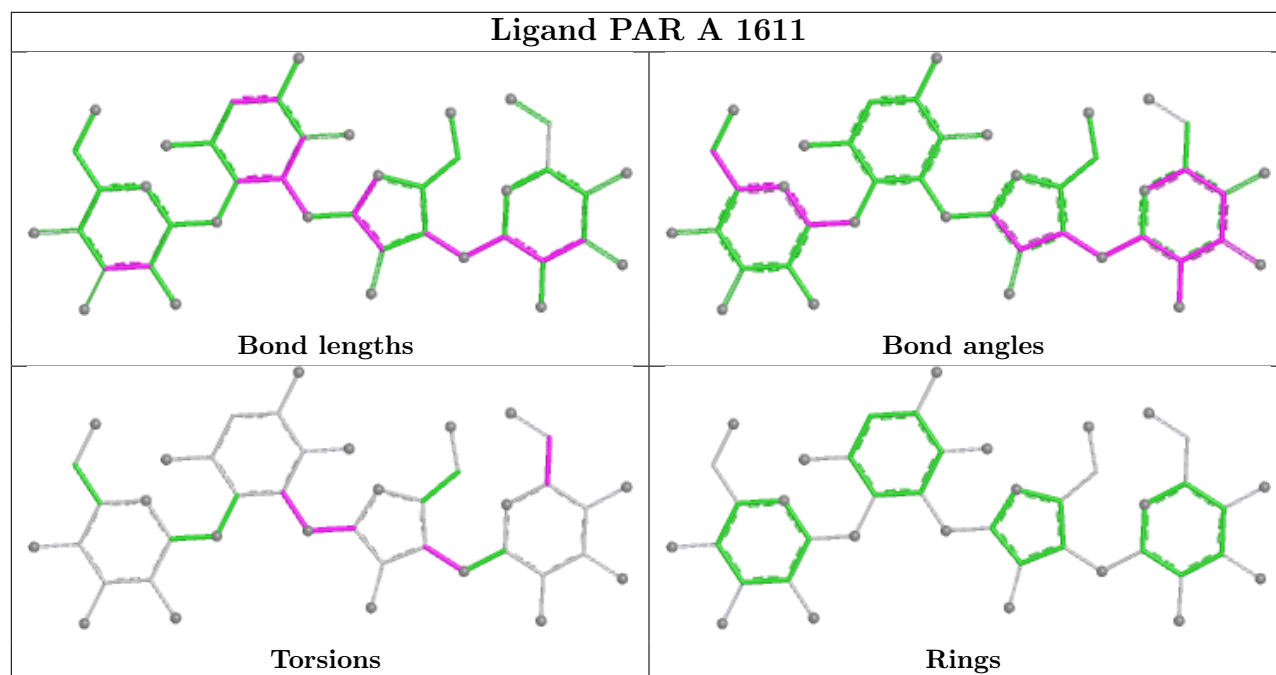
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	1611	PAR	1	0
22	A	1616	PAR	3	0
22	A	1601	PAR	1	0
22	A	1607	PAR	2	0
22	A	1610	PAR	3	0
22	A	1612	PAR	4	0
22	A	1615	PAR	1	0
22	A	1617	PAR	2	0
22	A	1614	PAR	3	0
22	A	1613	PAR	6	0
22	A	1609	PAR	1	0
22	A	1608	PAR	1	0
22	A	1604	PAR	3	0
22	A	1602	PAR	1	0

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.

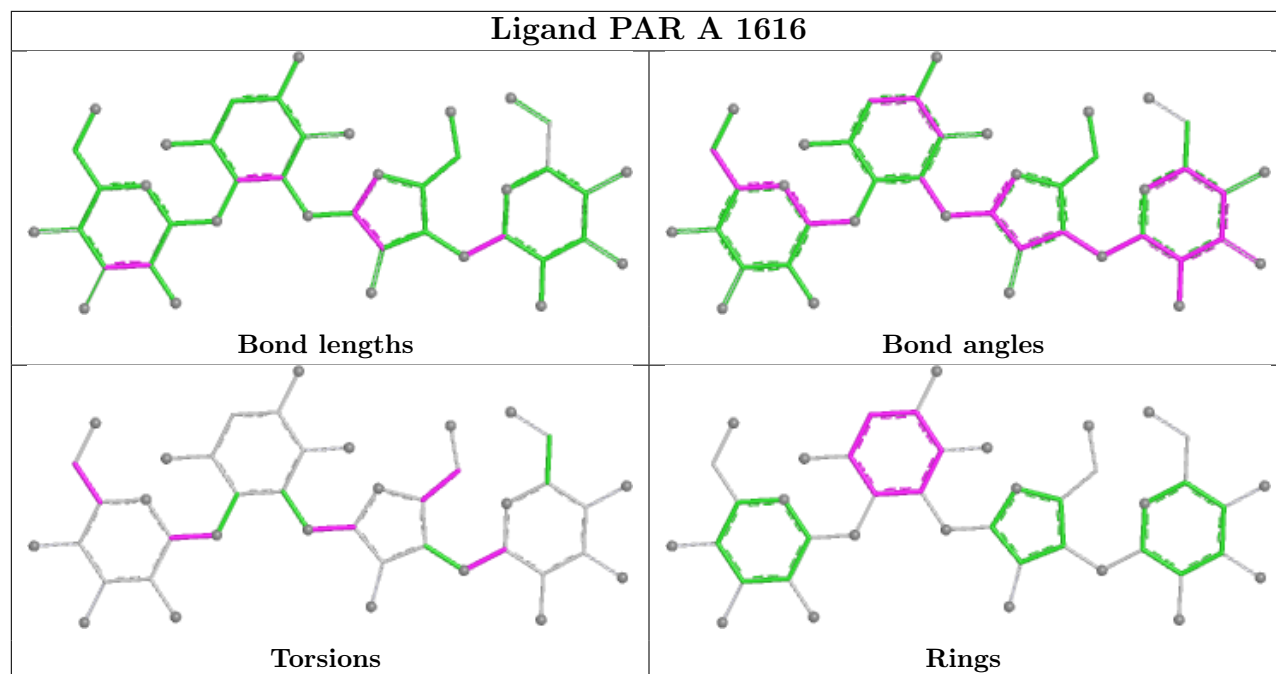
Ligand PAR A 1606



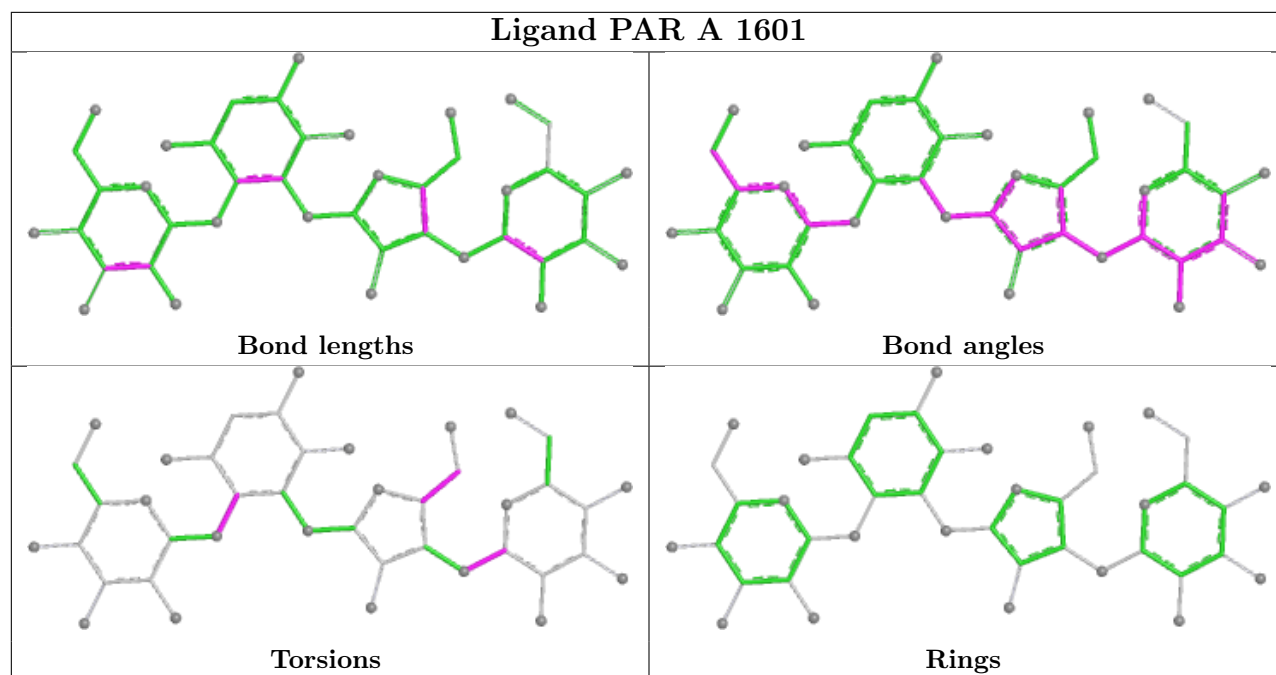
Ligand PAR A 1611



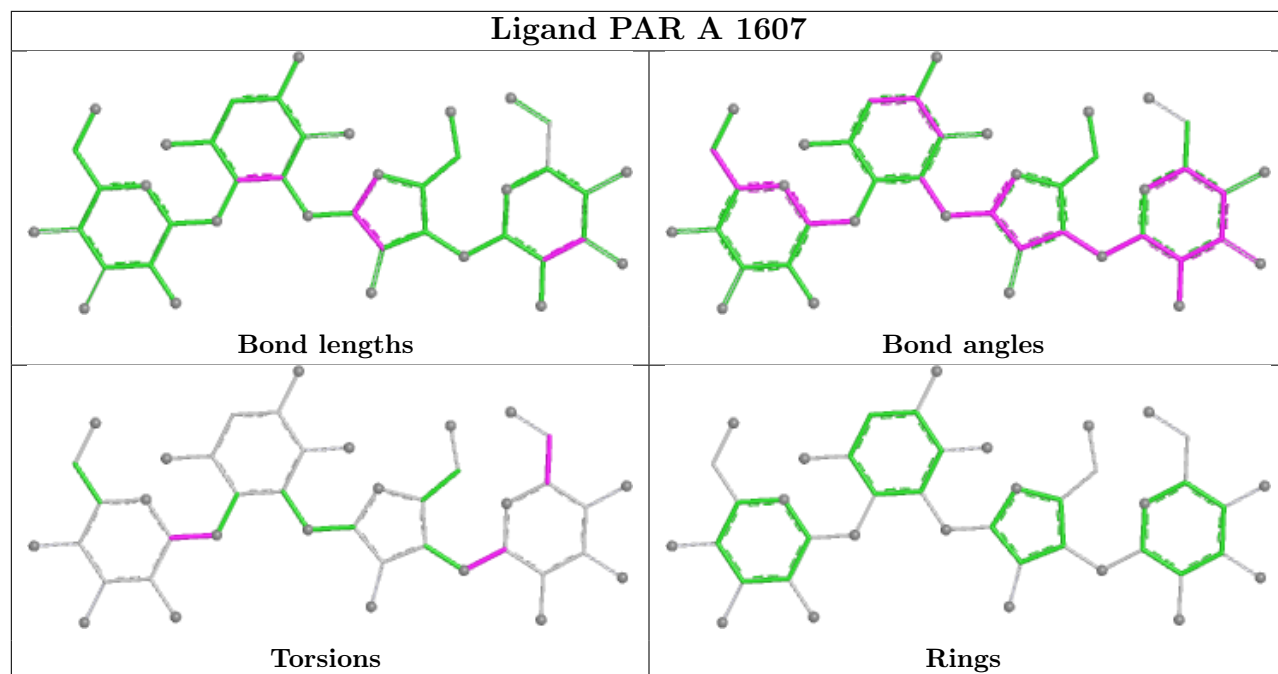
Ligand PAR A 1616



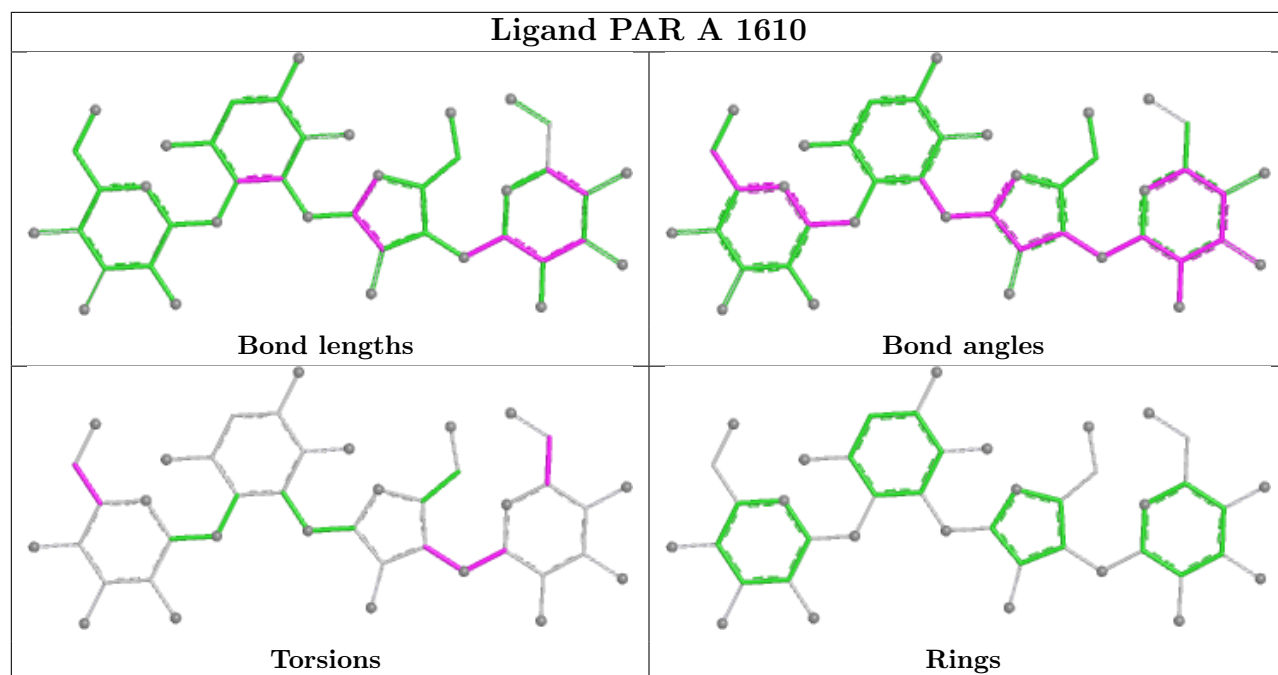
Ligand PAR A 1601



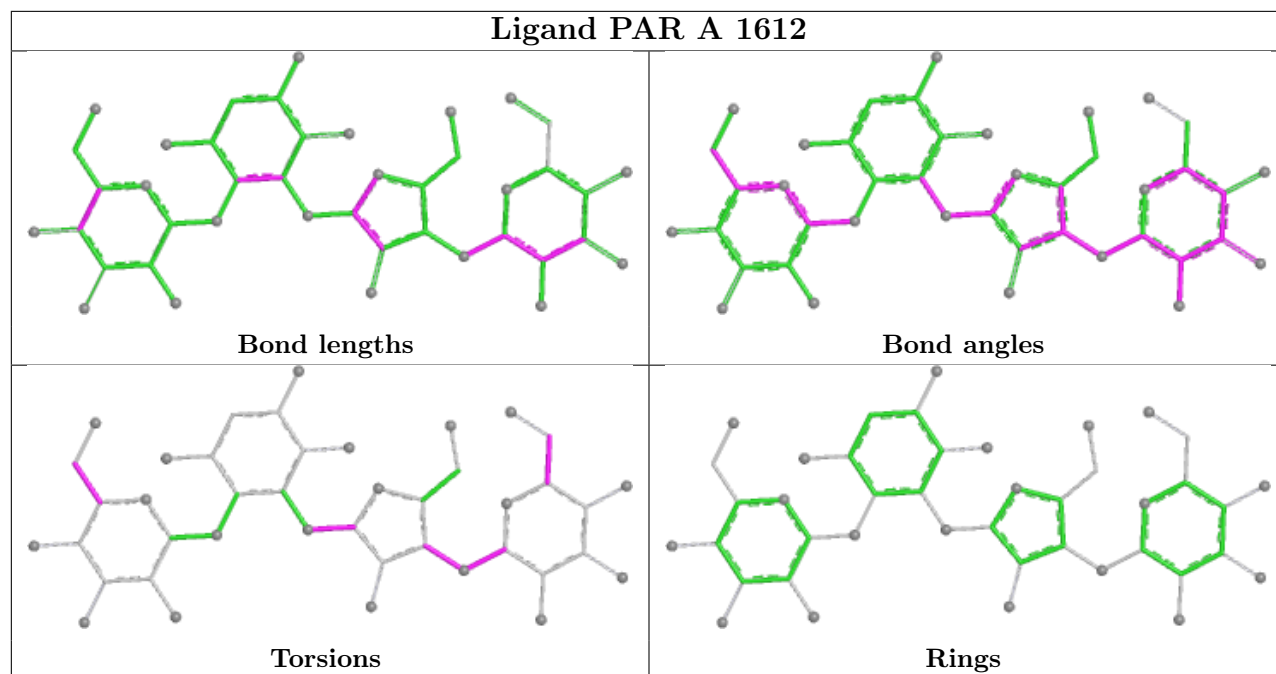
Ligand PAR A 1607



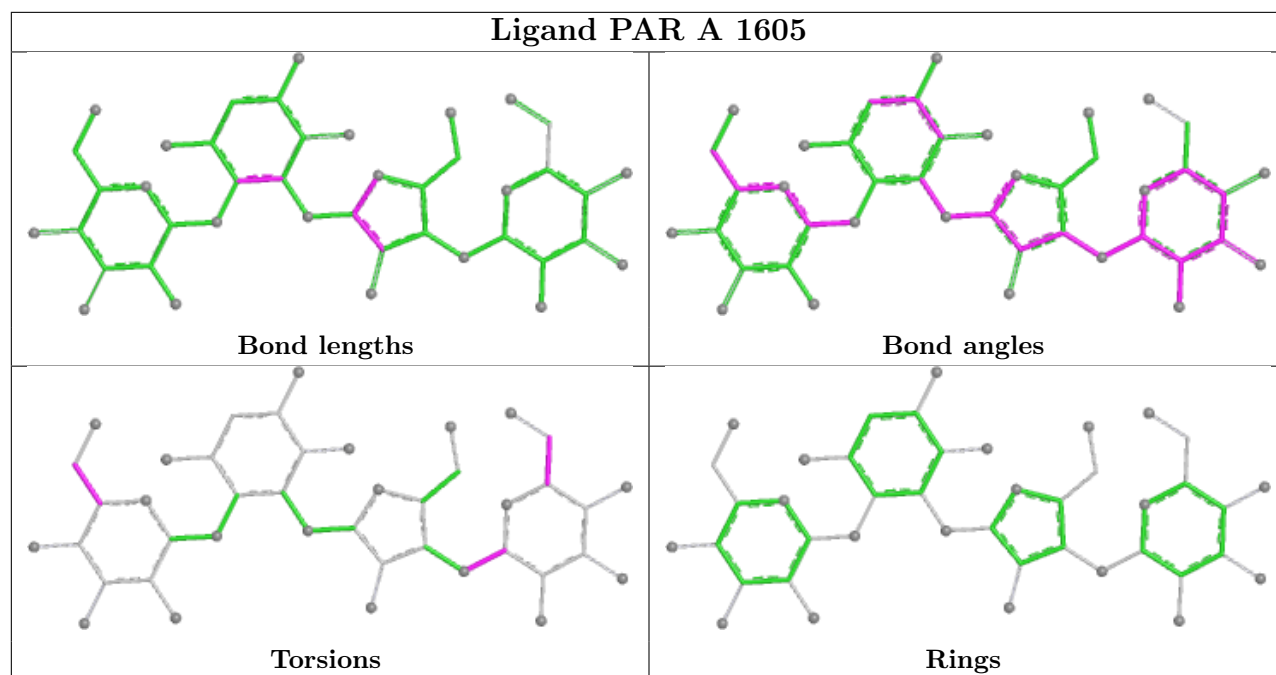
Ligand PAR A 1610



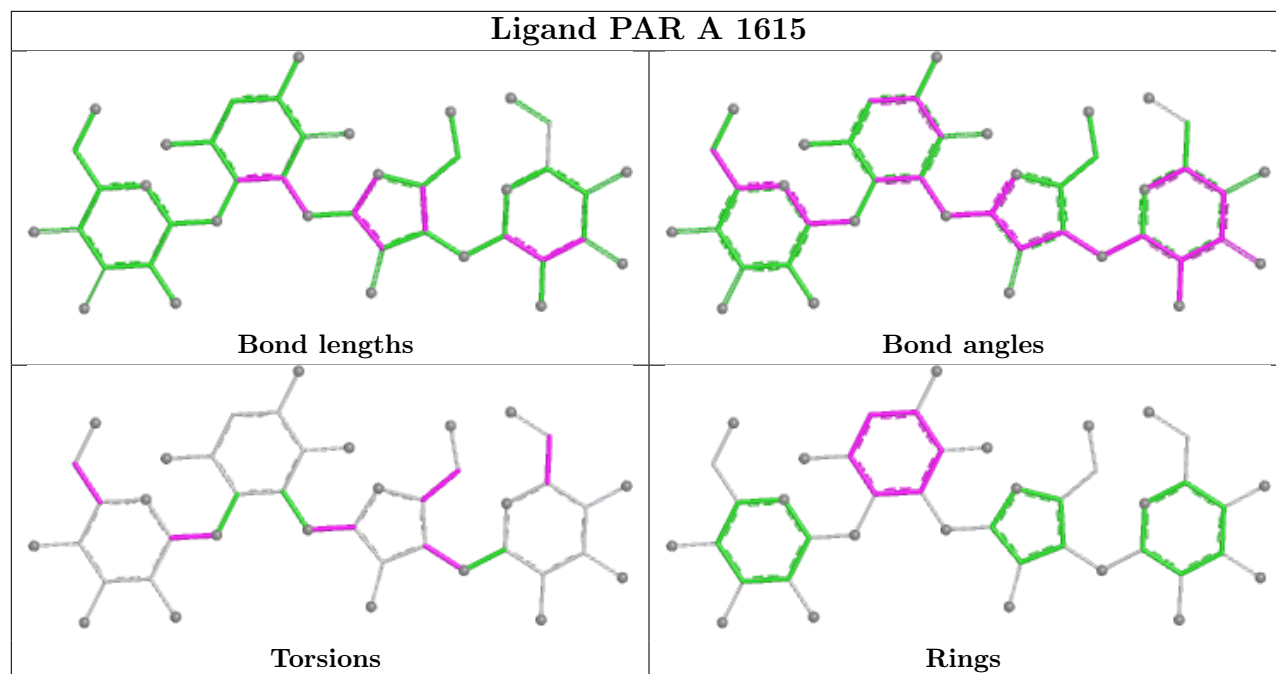
Ligand PAR A 1612



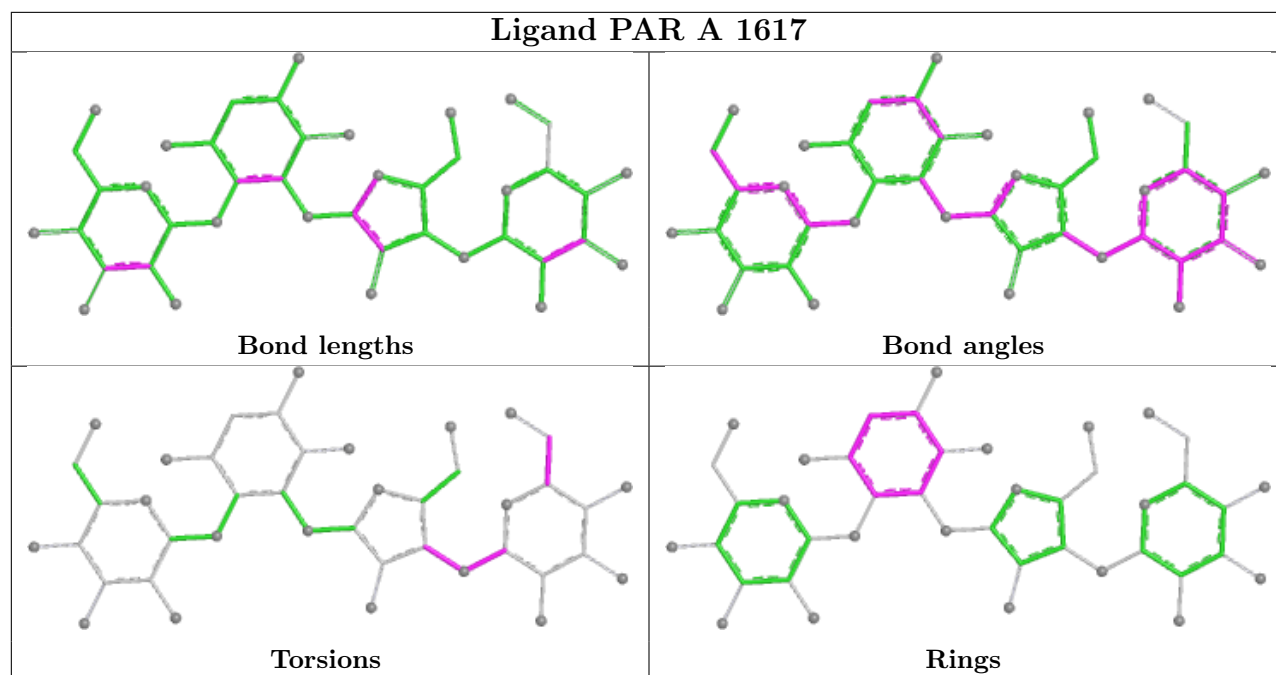
Ligand PAR A 1605



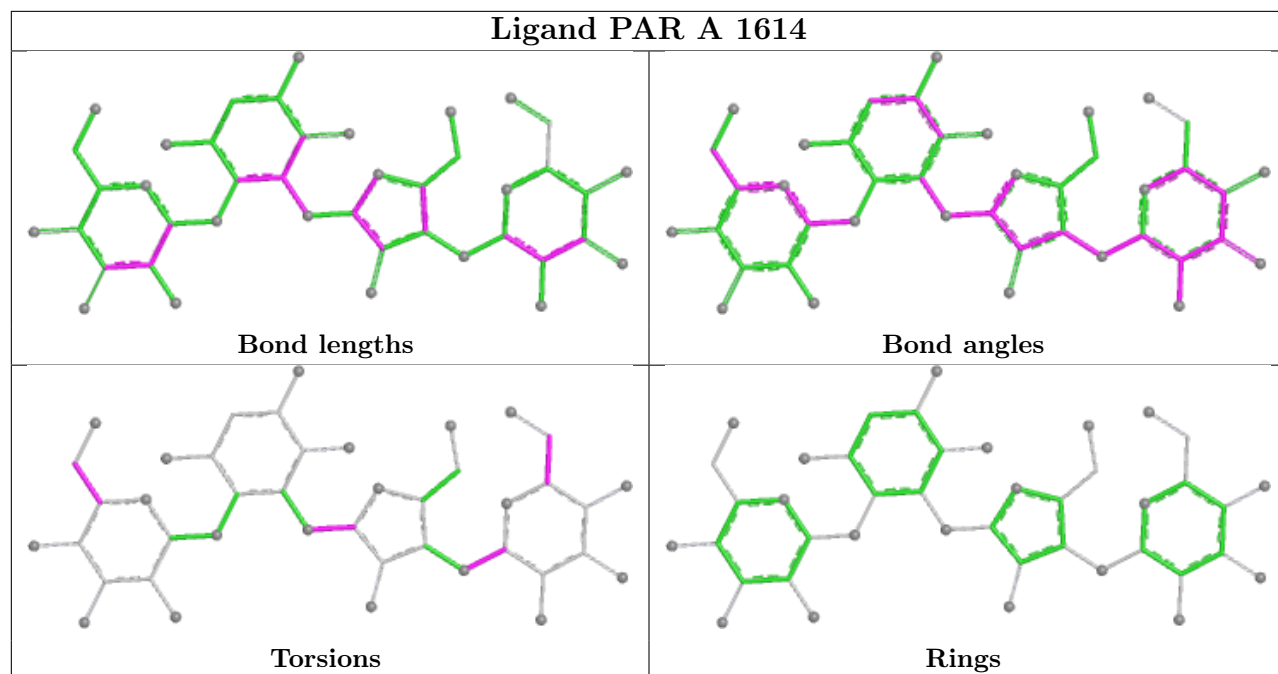
Ligand PAR A 1615



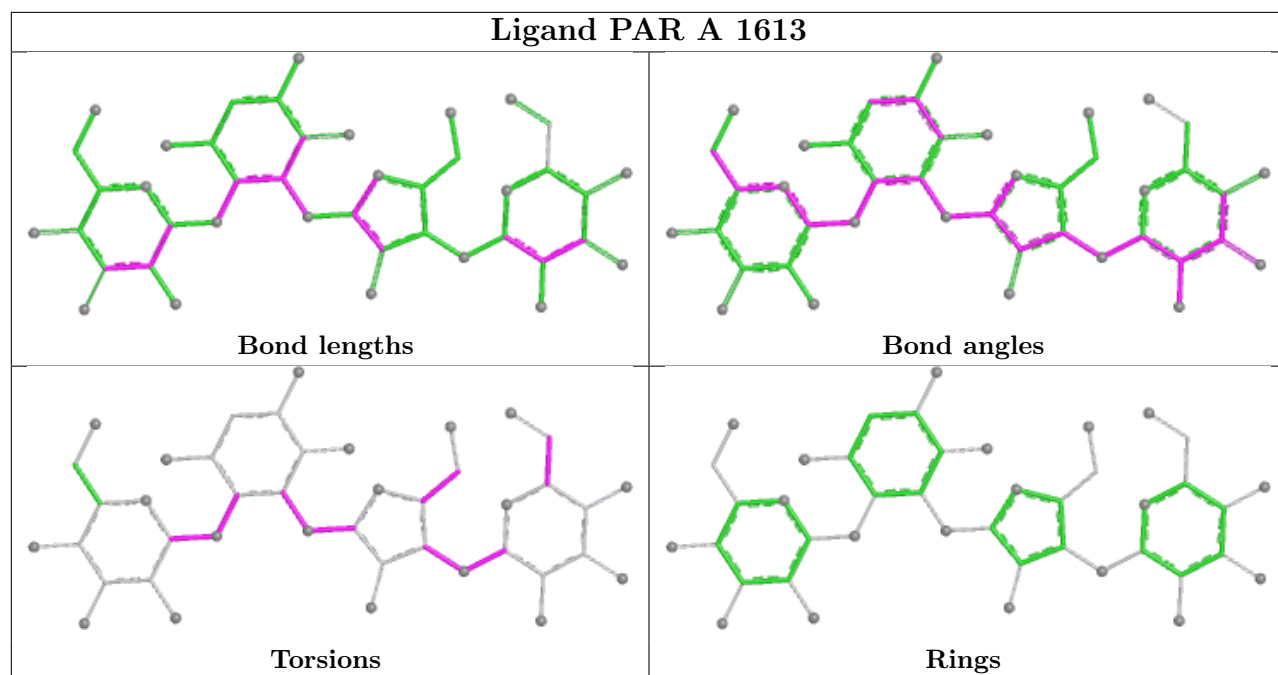
Ligand PAR A 1617



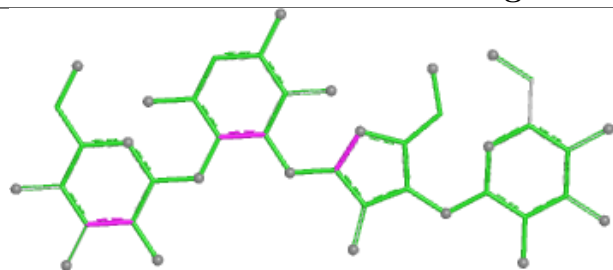
Ligand PAR A 1614



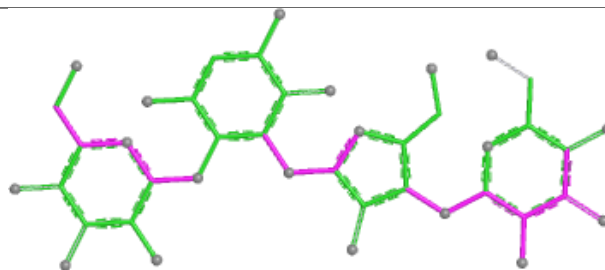
Ligand PAR A 1613



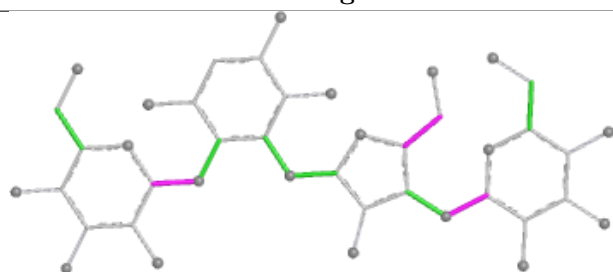
Ligand PAR A 1603



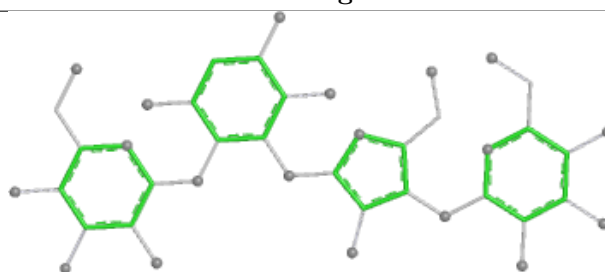
Bond lengths



Bond angles

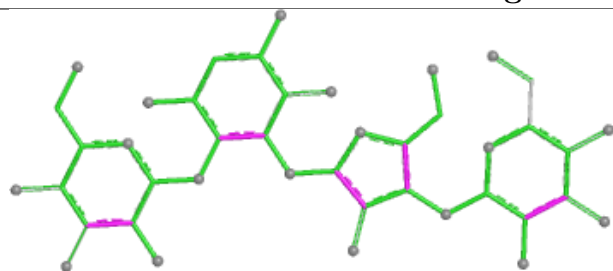


Torsions

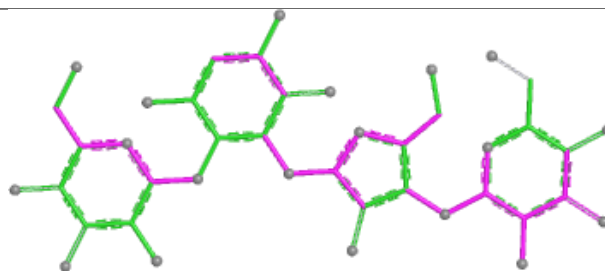


Rings

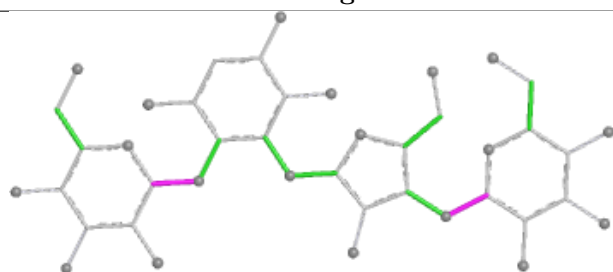
Ligand PAR A 1609



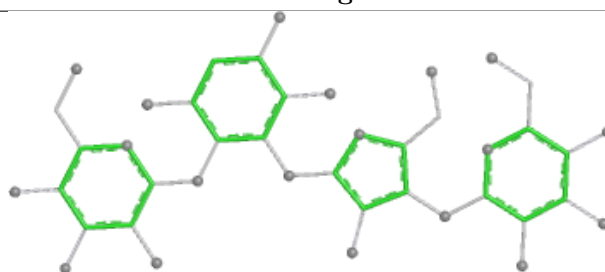
Bond lengths



Bond angles

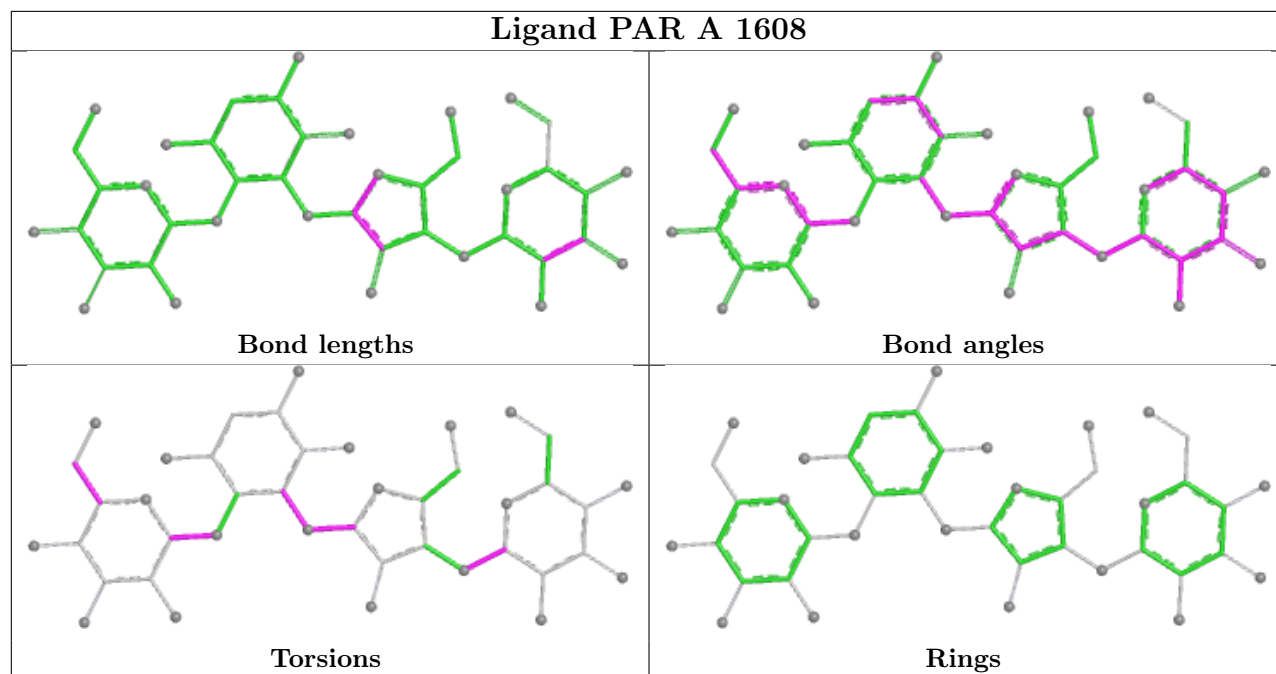


Torsions

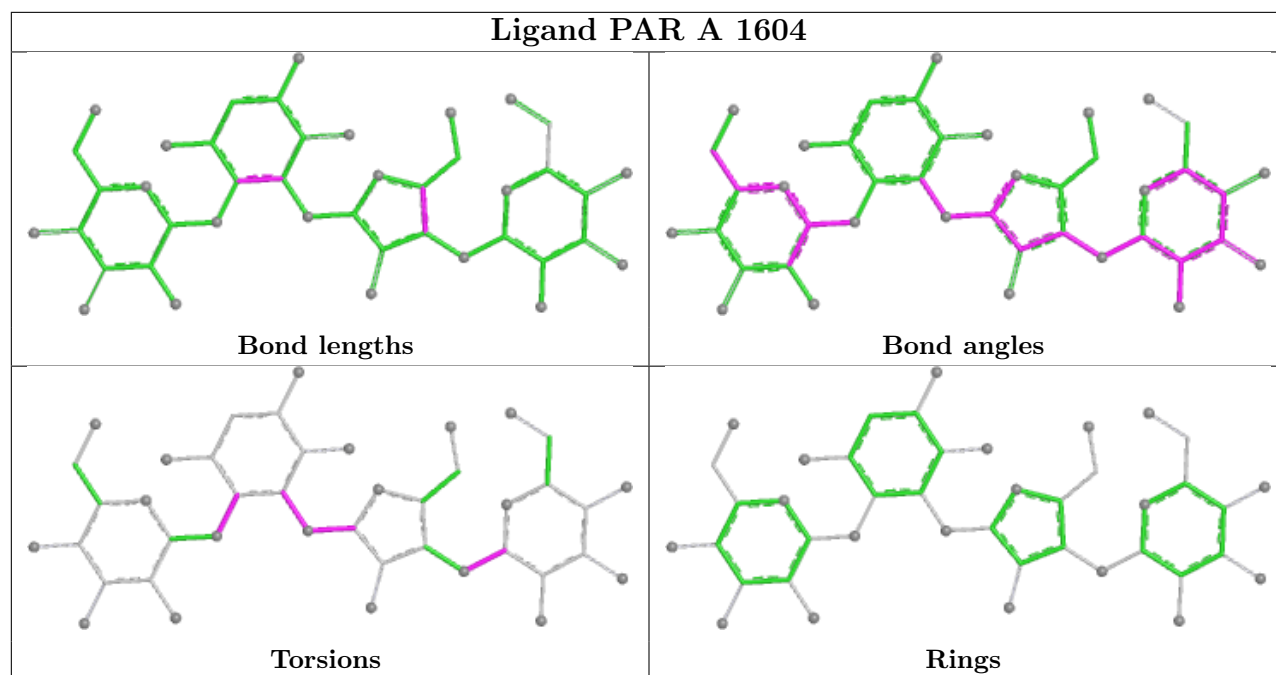


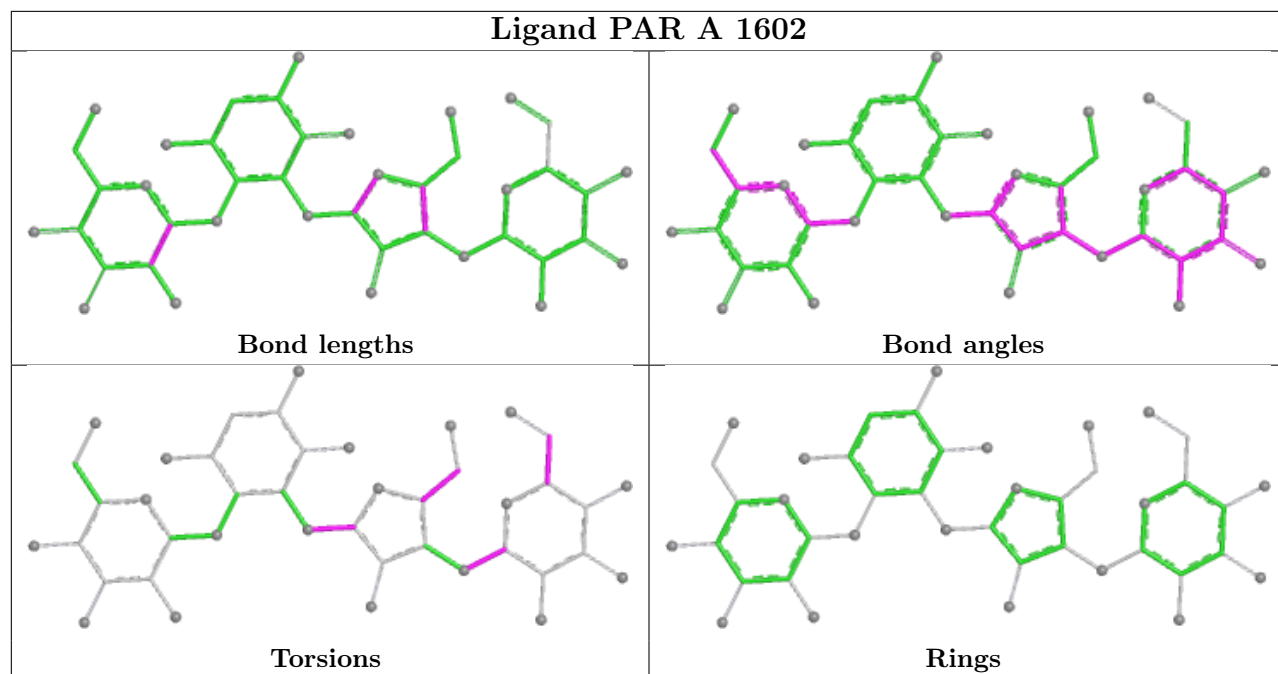
Rings

Ligand PAR A 1608



Ligand PAR A 1604





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%)	-0.34	53 (3%) 47 30	48, 80, 183, 551	0
2	B	236/256 (92%)	-0.00	3 (1%) 75 56	60, 104, 154, 168	0
3	C	207/239 (86%)	0.14	6 (2%) 53 35	69, 106, 153, 184	0
4	D	208/209 (99%)	0.02	8 (3%) 44 28	53, 86, 123, 147	0
5	E	151/162 (93%)	-0.43	0 100 100	50, 70, 105, 144	0
6	F	101/101 (100%)	0.07	0 100 100	73, 111, 136, 155	0
7	G	155/156 (99%)	0.00	4 (2%) 57 38	66, 100, 155, 187	0
8	H	138/138 (100%)	-0.49	2 (1%) 73 54	45, 68, 95, 127	0
9	I	127/128 (99%)	0.37	7 (5%) 30 20	67, 110, 140, 169	0
10	J	99/105 (94%)	0.85	11 (11%) 10 7	69, 133, 194, 209	0
11	K	117/129 (90%)	-0.12	2 (1%) 69 49	57, 85, 120, 137	0
12	L	124/135 (91%)	0.18	6 (4%) 35 23	46, 87, 123, 166	0
13	M	118/126 (93%)	0.22	7 (5%) 28 18	72, 106, 131, 151	0
14	N	60/61 (98%)	0.37	4 (6%) 24 16	76, 97, 143, 194	0
15	O	88/89 (98%)	-0.16	0 100 100	67, 87, 119, 163	0
16	P	84/88 (95%)	-0.13	0 100 100	61, 77, 109, 166	0
17	Q	101/105 (96%)	-0.18	2 (1%) 65 45	54, 74, 108, 154	0
18	R	73/88 (82%)	-0.26	1 (1%) 73 54	65, 87, 190, 221	0
19	S	81/93 (87%)	0.59	7 (8%) 16 11	93, 124, 165, 187	0
20	T	99/106 (93%)	0.16	6 (6%) 27 18	61, 85, 130, 156	0
21	U	25/27 (92%)	0.61	3 (12%) 9 7	77, 95, 129, 151	0
All	All	3890/4063 (95%)	-0.10	132 (3%) 48 30	45, 89, 156, 551	0

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1033	G	9.8
19	S	3	ARG	8.9
1	A	1129	C	8.0
1	A	1034	G	7.8
4	D	31	CYS	7.4
1	A	1002	G	7.0
1	A	1003	G	6.4
1	A	930	C	6.4
19	S	4	SER	6.0
1	A	81	U	5.9
1	A	1032	G	5.6
13	M	5	ALA	5.4
19	S	2	PRO	5.2
12	L	19	ARG	5.2
13	M	8	GLU	4.9
13	M	7	VAL	4.8
1	A	1027	C	4.6
1	A	1532	U	4.5
9	I	127	LYS	4.5
4	D	2	GLY	4.4
4	D	26	CYS	4.4
4	D	9	CYS	4.4
1	A	1389	C	4.3
1	A	1028	C	4.2
1	A	1531	A	4.2
1	A	1181	G	4.1
17	Q	101	ARG	4.0
12	L	47	LYS	4.0
4	D	23	GLY	4.0
1	A	1030(C)	G	3.9
20	T	100	ILE	3.9
1	A	1030(B)	C	3.9
1	A	1388	C	3.8
1	A	202	U	3.7
17	Q	102	GLY	3.7
10	J	73	ASP	3.7
1	A	1031	G	3.6
1	A	1036	G	3.6
9	I	66	ARG	3.6
1	A	1029	C	3.5
1	A	1124	G	3.5
3	C	188	LEU	3.4
21	U	25	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	1281	U	3.4
7	G	5	ARG	3.3
14	N	14	PRO	3.2
14	N	2	ALA	3.2
1	A	1003(A)	G	3.2
10	J	6	ILE	3.2
1	A	1037	C	3.2
9	I	125	TYR	3.2
2	B	240	GLN	3.2
1	A	1030(A)	G	3.1
4	D	12	CYS	3.1
20	T	68	LYS	3.1
1	A	929	G	3.1
1	A	1030(D)	A	3.1
1	A	1539	C	3.0
21	U	26	LYS	3.0
9	I	8	GLY	3.0
10	J	35	SER	2.9
1	A	1005	A	2.9
10	J	88	LEU	2.8
1	A	1001	A	2.8
10	J	17	ASP	2.8
1	A	204	U	2.7
1	A	1125	U	2.7
10	J	96	ILE	2.7
1	A	1021	G	2.7
11	K	51	LYS	2.7
1	A	1006	C	2.7
19	S	29	ARG	2.7
10	J	90	LEU	2.7
19	S	6	LYS	2.6
8	H	1	MET	2.6
1	A	1390	U	2.6
12	L	28	LYS	2.6
1	A	1030	C	2.6
2	B	137	ARG	2.6
1	A	1533	C	2.6
1	A	1022	G	2.5
4	D	49	ARG	2.5
13	M	11	ARG	2.5
1	A	1479	C	2.5
20	T	73	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	1126	U	2.5
12	L	18	VAL	2.5
12	L	84	LEU	2.5
1	A	1023	G	2.5
1	A	1024	G	2.5
1	A	931	C	2.5
7	G	156	TRP	2.5
14	N	4	LYS	2.4
10	J	71	LEU	2.4
2	B	44	LEU	2.4
7	G	81	GLY	2.4
1	A	1004	A	2.4
4	D	22	LYS	2.4
21	U	6	ARG	2.4
18	R	16	PRO	2.4
10	J	57	LYS	2.3
20	T	12	ALA	2.3
3	C	196	LEU	2.3
13	M	100	GLY	2.3
14	N	13	THR	2.3
3	C	91	LEU	2.3
1	A	1256	A	2.3
10	J	72	VAL	2.3
1	A	1086	U	2.3
7	G	110	GLN	2.2
9	I	119	ALA	2.2
9	I	64	THR	2.2
20	T	9	ASN	2.2
1	A	461	C	2.2
3	C	162	GLN	2.2
20	T	106	ALA	2.2
3	C	190	ARG	2.2
19	S	33	THR	2.2
9	I	128	ARG	2.2
3	C	193	TYR	2.1
11	K	127	LYS	2.1
1	A	928	G	2.1
19	S	26	GLY	2.1
1	A	1020	U	2.1
8	H	18	ARG	2.1
1	A	1035	A	2.1
1	A	1442	G	2.1

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Mol	Chain	Res	Type	RSRZ
10	J	75	ILE	2.1
12	L	29	GLY	2.1
13	M	9	ILE	2.0
13	M	2	ALA	2.0
1	A	1446	A	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	0.82	0.24	197,257,265,266	0
1	PSU	A	1541	20/21	0.90	0.17	205,208,212,214	0
1	PSU	A	516	20/21	0.95	0.08	91,99,107,112	0
1	5MC	A	967	21/22	0.97	0.09	53,66,76,80	0
1	2MG	A	1207	24/25	0.97	0.07	84,91,99,100	0
1	5MC	A	1400	21/22	0.97	0.09	56,78,91,92	0
1	5MC	A	1407	21/22	0.97	0.09	58,69,78,82	0
1	7MG	A	527	24/25	0.97	0.09	60,65,76,80	0
1	M2G	A	966	25/26	0.97	0.07	65,74,83,93	0
12	0TD	L	92	10/11	0.97	0.11	47,89,101,397	0
1	MA6	A	1518	24/25	0.98	0.07	57,62,73,74	0
1	MA6	A	1519	24/25	0.98	0.10	50,57,68,73	0
1	5MC	A	1404	21/22	0.98	0.08	52,62,70,73	0
1	4OC	A	1402	22/23	0.98	0.07	56,67,76,80	0
1	UR3	A	1498	21/22	0.98	0.10	57,68,78,81	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($\text{\AA}^2$)	Q<0.9
23	MG	A	1882	1/1	0.51	0.41	94,94,94,94	0
23	MG	A	1768	1/1	0.52	0.34	122,122,122,122	0
23	MG	A	1758	1/1	0.55	0.12	149,149,149,149	0
23	MG	A	1807	1/1	0.56	0.41	96,96,96,96	0
23	MG	A	1902	1/1	0.57	0.36	93,93,93,93	0
23	MG	A	1804	1/1	0.58	0.57	103,103,103,103	0
23	MG	A	1824	1/1	0.58	0.16	92,92,92,92	0
24	ZN	D	301	1/1	0.60	0.51	194,194,194,194	0
23	MG	A	1756	1/1	0.63	0.23	158,158,158,158	0
23	MG	A	1637	1/1	0.65	0.27	90,90,90,90	0
23	MG	A	1852	1/1	0.68	0.15	65,65,65,65	0
23	MG	A	1730	1/1	0.68	0.47	98,98,98,98	0
23	MG	A	1828	1/1	0.69	0.22	100,100,100,100	0
23	MG	A	1693	1/1	0.70	0.12	129,129,129,129	0
23	MG	A	1915	1/1	0.70	0.26	101,101,101,101	0
23	MG	O	101	1/1	0.70	0.12	104,104,104,104	0
23	MG	A	1889	1/1	0.70	0.37	92,92,92,92	0
23	MG	A	1909	1/1	0.71	0.23	91,91,91,91	0
23	MG	A	1864	1/1	0.71	0.56	96,96,96,96	0
23	MG	A	1748	1/1	0.72	0.24	115,115,115,115	0
23	MG	A	1819	1/1	0.73	0.48	96,96,96,96	0
23	MG	A	1880	1/1	0.73	0.44	96,96,96,96	0
23	MG	A	1714	1/1	0.73	0.15	115,115,115,115	0
23	MG	A	1874	1/1	0.74	0.32	90,90,90,90	0
23	MG	A	1795	1/1	0.74	0.36	101,101,101,101	0
23	MG	A	1767	1/1	0.74	0.11	113,113,113,113	0
22	PAR	A	1614	42/42	0.75	0.21	147,147,147,147	0
23	MG	A	1836	1/1	0.76	0.50	86,86,86,86	0
23	MG	A	1783	1/1	0.76	0.31	132,132,132,132	0
23	MG	A	1830	1/1	0.77	0.35	92,92,92,92	0
23	MG	A	1808	1/1	0.77	0.28	93,93,93,93	0
23	MG	A	1786	1/1	0.77	0.15	154,154,154,154	0
23	MG	A	1881	1/1	0.77	0.38	102,102,102,102	0
23	MG	N	102	1/1	0.77	0.28	76,76,76,76	0
23	MG	A	1863	1/1	0.77	0.26	90,90,90,90	0
23	MG	A	1883	1/1	0.77	0.15	68,68,68,68	0
22	PAR	A	1611	42/42	0.78	0.24	130,130,130,130	0
23	MG	A	1798	1/1	0.78	0.25	75,75,75,75	0
23	MG	A	1838	1/1	0.78	0.49	80,80,80,80	0
23	MG	A	1823	1/1	0.78	0.38	82,82,82,82	0
23	MG	A	1747	1/1	0.78	0.32	166,166,166,166	0
23	MG	A	1718	1/1	0.78	0.33	89,89,89,89	0
23	MG	A	1785	1/1	0.79	0.16	142,142,142,142	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
23	MG	A	1856	1/1	0.79	0.31	90,90,90,90	0
23	MG	A	1723	1/1	0.79	0.12	103,103,103,103	0
23	MG	A	1851	1/1	0.79	0.32	89,89,89,89	0
23	MG	D	302	1/1	0.80	0.12	112,112,112,112	0
23	MG	A	1629	1/1	0.80	0.15	96,96,96,96	0
23	MG	A	1759	1/1	0.80	0.30	79,79,79,79	0
23	MG	A	1817	1/1	0.80	0.58	99,99,99,99	0
23	MG	A	1899[B]	1/1	0.81	0.96	45,45,45,45	1
23	MG	A	1749	1/1	0.81	0.09	138,138,138,138	0
23	MG	A	1799	1/1	0.81	0.21	74,74,74,74	0
23	MG	A	1829	1/1	0.81	0.19	90,90,90,90	0
23	MG	A	1789	1/1	0.81	0.30	100,100,100,100	0
23	MG	A	1706	1/1	0.81	0.26	123,123,123,123	0
23	MG	A	1837	1/1	0.81	0.40	84,84,84,84	0
23	MG	A	1899[A]	1/1	0.81	0.96	45,45,45,45	1
23	MG	A	1827	1/1	0.82	0.36	91,91,91,91	0
23	MG	A	1877	1/1	0.82	0.31	105,105,105,105	0
23	MG	A	1731	1/1	0.82	0.13	140,140,140,140	0
23	MG	A	1910	1/1	0.82	0.21	80,80,80,80	0
23	MG	A	1736	1/1	0.82	0.12	138,138,138,138	0
23	MG	A	1737	1/1	0.82	0.19	105,105,105,105	0
23	MG	A	1787	1/1	0.82	0.07	165,165,165,165	0
23	MG	A	1744	1/1	0.82	0.12	99,99,99,99	0
23	MG	Q	201	1/1	0.82	0.17	86,86,86,86	0
23	MG	A	1872	1/1	0.82	0.16	59,59,59,59	0
23	MG	A	1622	1/1	0.83	0.18	111,111,111,111	0
23	MG	A	1811	1/1	0.83	0.37	87,87,87,87	0
23	MG	A	1826	1/1	0.83	0.32	82,82,82,82	0
22	PAR	A	1613	42/42	0.83	0.34	152,152,152,152	0
23	MG	A	1703	1/1	0.83	0.16	85,85,85,85	0
23	MG	A	1849	1/1	0.83	0.31	63,63,63,63	0
23	MG	A	1792	1/1	0.84	0.23	100,100,100,100	0
23	MG	A	1866	1/1	0.84	0.50	83,83,83,83	0
23	MG	A	1870	1/1	0.84	0.54	75,75,75,75	0
22	PAR	A	1615	42/42	0.84	0.24	169,169,169,169	0
23	MG	A	1800	1/1	0.84	0.32	83,83,83,83	0
23	MG	S	101	1/1	0.84	0.18	83,83,83,83	0
23	MG	A	1885	1/1	0.84	0.31	96,96,96,96	0
23	MG	A	1641	1/1	0.85	0.10	92,92,92,92	0
23	MG	A	1844	1/1	0.85	0.26	71,71,71,71	0
23	MG	A	1722	1/1	0.85	0.09	100,100,100,100	0
23	MG	A	1896	1/1	0.85	0.22	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
23	MG	A	1762	1/1	0.85	0.14	127,127,127,127	0
23	MG	T	201	1/1	0.85	0.23	100,100,100,100	0
23	MG	A	1922	1/1	0.85	0.21	77,77,77,77	0
23	MG	A	1802	1/1	0.86	0.18	71,71,71,71	0
23	MG	A	1742	1/1	0.86	0.13	146,146,146,146	0
23	MG	A	1698	1/1	0.86	0.18	91,91,91,91	0
23	MG	A	1784	1/1	0.86	0.11	127,127,127,127	0
23	MG	A	1679	1/1	0.86	0.14	73,73,73,73	0
23	MG	A	1715	1/1	0.86	0.09	107,107,107,107	0
23	MG	A	1728	1/1	0.86	0.11	144,144,144,144	0
23	MG	A	1918	1/1	0.86	0.29	90,90,90,90	0
23	MG	A	1831	1/1	0.87	0.27	85,85,85,85	0
23	MG	A	1905	1/1	0.87	0.34	100,100,100,100	0
23	MG	A	1835	1/1	0.87	0.38	72,72,72,72	0
23	MG	A	1814	1/1	0.87	0.29	85,85,85,85	0
23	MG	A	1913	1/1	0.87	0.24	69,69,69,69	0
23	MG	A	1859[A]	1/1	0.87	1.12	59,59,59,59	1
23	MG	A	1859[B]	1/1	0.87	1.12	59,59,59,59	1
23	MG	A	1919	1/1	0.87	0.25	85,85,85,85	0
23	MG	A	1861	1/1	0.87	0.38	75,75,75,75	0
23	MG	A	1862	1/1	0.87	0.40	70,70,70,70	0
23	MG	E	201	1/1	0.87	0.11	110,110,110,110	0
23	MG	A	1805	1/1	0.87	0.24	83,83,83,83	0
23	MG	A	1770	1/1	0.87	0.08	101,101,101,101	0
23	MG	A	1893	1/1	0.87	0.31	71,71,71,71	0
23	MG	A	1777	1/1	0.87	0.17	84,84,84,84	0
23	MG	A	1867	1/1	0.87	0.50	75,75,75,75	0
23	MG	A	1628	1/1	0.87	0.15	44,44,44,44	0
23	MG	A	1791	1/1	0.88	0.28	84,84,84,84	0
23	MG	A	1750	1/1	0.88	0.16	100,100,100,100	0
23	MG	A	1907	1/1	0.88	0.19	81,81,81,81	0
23	MG	A	1842	1/1	0.88	0.25	70,70,70,70	0
23	MG	A	1860	1/1	0.88	0.50	102,102,102,102	0
23	MG	A	1621	1/1	0.88	0.12	131,131,131,131	0
23	MG	A	1825	1/1	0.88	0.12	88,88,88,88	0
23	MG	A	1796	1/1	0.88	0.45	94,94,94,94	0
23	MG	A	1630	1/1	0.88	0.14	87,87,87,87	0
22	PAR	A	1616	42/42	0.89	0.23	126,126,126,126	42
23	MG	A	1733	1/1	0.89	0.07	142,142,142,142	0
23	MG	A	1735	1/1	0.89	0.15	92,92,92,92	0
23	MG	A	1854	1/1	0.89	0.20	76,76,76,76	0
23	MG	A	1879	1/1	0.89	0.31	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
23	MG	A	1694	1/1	0.89	0.10	97,97,97,97	0
23	MG	A	1717	1/1	0.89	0.21	110,110,110,110	0
23	MG	A	1652	1/1	0.89	0.32	86,86,86,86	0
23	MG	A	1921[A]	1/1	0.89	0.30	28,28,28,28	1
23	MG	A	1921[B]	1/1	0.89	0.30	28,28,28,28	1
23	MG	A	1809	1/1	0.89	0.21	58,58,58,58	0
23	MG	A	1699	1/1	0.89	0.05	112,112,112,112	0
23	MG	A	1886	1/1	0.89	0.31	86,86,86,86	0
22	PAR	A	1617	42/42	0.89	0.23	137,137,137,137	0
23	MG	A	1775	1/1	0.89	0.12	83,83,83,83	0
23	MG	A	1797	1/1	0.89	0.36	85,85,85,85	0
23	MG	A	1865	1/1	0.89	0.15	66,66,66,66	0
23	MG	A	1692	1/1	0.89	0.08	98,98,98,98	0
23	MG	A	1710	1/1	0.89	0.18	92,92,92,92	0
23	MG	A	1726	1/1	0.90	0.11	91,91,91,91	0
23	MG	A	1920	1/1	0.90	0.14	72,72,72,72	0
23	MG	A	1709	1/1	0.90	0.29	87,87,87,87	0
22	PAR	A	1610	42/42	0.90	0.18	111,111,111,111	0
23	MG	A	1740	1/1	0.90	0.14	96,96,96,96	0
23	MG	A	1846	1/1	0.90	0.45	81,81,81,81	0
23	MG	A	1816	1/1	0.90	0.24	75,75,75,75	0
23	MG	E	202	1/1	0.90	0.27	74,74,74,74	0
23	MG	F	201	1/1	0.90	0.33	80,80,80,80	0
23	MG	A	1753	1/1	0.90	0.10	109,109,109,109	0
23	MG	A	1691	1/1	0.90	0.26	118,118,118,118	0
23	MG	A	1743	1/1	0.90	0.09	145,145,145,145	0
23	MG	A	1670	1/1	0.90	0.20	84,84,84,84	0
23	MG	A	1888	1/1	0.90	0.28	71,71,71,71	0
23	MG	A	1857	1/1	0.90	0.31	59,59,59,59	0
22	PAR	A	1605	42/42	0.91	0.16	93,93,93,93	0
23	MG	A	1916[A]	1/1	0.91	0.42	50,50,50,50	1
23	MG	A	1916[B]	1/1	0.91	0.42	50,50,50,50	1
23	MG	A	1704	1/1	0.91	0.10	87,87,87,87	0
23	MG	A	1887	1/1	0.91	0.42	93,93,93,93	0
23	MG	A	1821	1/1	0.91	0.26	82,82,82,82	0
23	MG	A	1832	1/1	0.91	0.26	68,68,68,68	0
23	MG	A	1834	1/1	0.91	0.26	77,77,77,77	0
23	MG	A	1620	1/1	0.91	0.18	91,91,91,91	0
23	MG	A	1725	1/1	0.91	0.07	94,94,94,94	0
23	MG	A	1788	1/1	0.91	0.42	75,75,75,75	0
23	MG	A	1900	1/1	0.91	0.19	77,77,77,77	0
23	MG	A	1683	1/1	0.91	0.14	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	MG	A	1841	1/1	0.91	0.14	74,74,74,74	0
23	MG	A	1790	1/1	0.91	0.26	89,89,89,89	0
23	MG	A	1843	1/1	0.91	0.12	62,62,62,62	0
23	MG	A	1766	1/1	0.91	0.08	118,118,118,118	0
23	MG	A	1884	1/1	0.91	0.32	85,85,85,85	0
23	MG	A	1914	1/1	0.91	0.50	81,81,81,81	0
23	MG	A	1801	1/1	0.92	0.49	87,87,87,87	0
23	MG	A	1822	1/1	0.92	0.28	69,69,69,69	0
23	MG	A	1640	1/1	0.92	0.18	78,78,78,78	0
23	MG	A	1917	1/1	0.92	0.46	68,68,68,68	0
23	MG	A	1840	1/1	0.92	0.19	79,79,79,79	0
23	MG	A	1678	1/1	0.92	0.11	101,101,101,101	0
22	PAR	A	1607	42/42	0.92	0.16	92,92,92,92	42
23	MG	A	1806	1/1	0.92	0.22	81,81,81,81	0
23	MG	A	1774	1/1	0.92	0.13	95,95,95,95	0
23	MG	A	1845	1/1	0.92	0.15	63,63,63,63	0
23	MG	A	1713	1/1	0.92	0.10	95,95,95,95	0
23	MG	A	1741	1/1	0.92	0.14	76,76,76,76	0
23	MG	A	1850	1/1	0.92	0.19	60,60,60,60	0
23	MG	A	1904	1/1	0.92	0.14	80,80,80,80	0
23	MG	I	201	1/1	0.92	0.18	92,92,92,92	0
23	MG	L	201	1/1	0.92	0.17	81,81,81,81	0
23	MG	A	1649	1/1	0.92	0.09	90,90,90,90	0
23	MG	A	1700	1/1	0.92	0.27	90,90,90,90	0
23	MG	A	1761	1/1	0.92	0.11	103,103,103,103	0
23	MG	A	1833	1/1	0.92	0.24	58,58,58,58	0
22	PAR	A	1612	42/42	0.92	0.16	69,69,69,69	42
23	MG	T	202	1/1	0.92	0.33	56,56,56,56	0
23	MG	A	1653	1/1	0.92	0.09	96,96,96,96	0
23	MG	A	1732	1/1	0.93	0.18	86,86,86,86	0
23	MG	A	1793	1/1	0.93	0.51	84,84,84,84	0
23	MG	A	1643	1/1	0.93	0.33	74,74,74,74	0
23	MG	A	1684	1/1	0.93	0.12	81,81,81,81	0
23	MG	A	1687	1/1	0.93	0.10	92,92,92,92	0
23	MG	A	1763	1/1	0.93	0.15	102,102,102,102	0
23	MG	A	1912	1/1	0.93	0.12	70,70,70,70	0
23	MG	A	1632	1/1	0.93	0.07	68,68,68,68	0
23	MG	A	1739	1/1	0.93	0.30	84,84,84,84	0
23	MG	A	1635	1/1	0.93	0.18	65,65,65,65	0
22	PAR	A	1608	42/42	0.93	0.17	97,97,97,97	0
23	MG	A	1773	1/1	0.93	0.16	91,91,91,91	0
23	MG	A	1656	1/1	0.93	0.16	124,124,124,124	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	MG	A	1720	1/1	0.93	0.08	94,94,94,94	0
23	MG	A	1664	1/1	0.93	0.15	94,94,94,94	0
23	MG	A	1878	1/1	0.93	0.19	49,49,49,49	0
23	MG	A	1778	1/1	0.93	0.13	107,107,107,107	0
23	MG	A	1781	1/1	0.93	0.09	104,104,104,104	0
23	MG	A	1745	1/1	0.93	0.11	79,79,79,79	0
23	MG	A	1812	1/1	0.93	0.33	77,77,77,77	0
23	MG	A	1813	1/1	0.93	0.10	55,55,55,55	0
23	MG	A	1638	1/1	0.93	0.20	93,93,93,93	0
23	MG	A	1671	1/1	0.93	0.16	68,68,68,68	0
23	MG	H	201	1/1	0.93	0.06	85,85,85,85	0
22	PAR	A	1603	42/42	0.93	0.13	83,83,83,83	3
23	MG	A	1624	1/1	0.93	0.09	95,95,95,95	0
23	MG	A	1820	1/1	0.93	0.29	88,88,88,88	0
23	MG	A	1680	1/1	0.93	0.08	85,85,85,85	0
23	MG	A	1853	1/1	0.93	0.19	55,55,55,55	0
23	MG	A	1754	1/1	0.93	0.09	111,111,111,111	0
23	MG	A	1855	1/1	0.93	0.25	74,74,74,74	0
23	MG	A	1755	1/1	0.93	0.14	96,96,96,96	0
23	MG	A	1707	1/1	0.93	0.10	112,112,112,112	0
23	MG	A	1636	1/1	0.94	0.10	72,72,72,72	0
23	MG	A	1727	1/1	0.94	0.08	117,117,117,117	0
23	MG	A	1839	1/1	0.94	0.24	84,84,84,84	0
23	MG	A	1868	1/1	0.94	0.31	73,73,73,73	0
23	MG	A	1701	1/1	0.94	0.16	83,83,83,83	0
22	PAR	A	1609	42/42	0.94	0.13	77,77,77,77	42
23	MG	A	1682	1/1	0.94	0.10	33,33,33,33	0
23	MG	A	1655	1/1	0.94	0.08	87,87,87,87	0
23	MG	A	1818	1/1	0.94	0.24	79,79,79,79	0
23	MG	A	1642	1/1	0.94	0.08	77,77,77,77	0
23	MG	A	1760	1/1	0.94	0.15	77,77,77,77	0
23	MG	A	1847	1/1	0.94	0.30	70,70,70,70	0
23	MG	A	1848	1/1	0.94	0.38	71,71,71,71	0
23	MG	A	1685	1/1	0.94	0.27	90,90,90,90	0
23	MG	A	1686	1/1	0.94	0.08	73,73,73,73	0
23	MG	A	1712	1/1	0.94	0.07	112,112,112,112	0
23	MG	A	1738	1/1	0.94	0.21	116,116,116,116	0
22	PAR	A	1606	42/42	0.94	0.11	64,64,64,64	42
23	MG	A	1689	1/1	0.94	0.11	87,87,87,87	0
23	MG	A	1639	1/1	0.94	0.20	72,72,72,72	0
23	MG	H	202	1/1	0.94	0.10	72,72,72,72	0
23	MG	A	1650	1/1	0.94	0.09	106,106,106,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
23	MG	A	1674	1/1	0.94	0.12	96,96,96,96	0
23	MG	A	1803	1/1	0.94	0.24	62,62,62,62	0
23	MG	A	1676	1/1	0.94	0.10	82,82,82,82	0
23	MG	A	1721	1/1	0.94	0.10	93,93,93,93	0
23	MG	A	1746	1/1	0.94	0.12	88,88,88,88	0
23	MG	A	1697	1/1	0.94	0.39	66,66,66,66	0
23	MG	A	1677	1/1	0.94	0.08	70,70,70,70	0
23	MG	A	1651	1/1	0.94	0.42	61,61,61,61	0
23	MG	A	1892	1/1	0.95	0.11	58,58,58,58	0
23	MG	A	1810	1/1	0.95	0.18	63,63,63,63	0
23	MG	A	1895[A]	1/1	0.95	0.36	30,30,30,30	1
23	MG	A	1895[B]	1/1	0.95	0.36	30,30,30,30	1
23	MG	A	1876	1/1	0.95	0.14	60,60,60,60	0
23	MG	A	1708	1/1	0.95	0.09	77,77,77,77	0
23	MG	A	1663	1/1	0.95	0.17	92,92,92,92	0
23	MG	A	1645	1/1	0.95	0.17	64,64,64,64	0
23	MG	A	1901	1/1	0.95	0.27	81,81,81,81	0
23	MG	A	1667	1/1	0.95	0.09	78,78,78,78	0
23	MG	A	1688	1/1	0.95	0.18	115,115,115,115	0
22	PAR	A	1602	42/42	0.95	0.10	58,58,58,58	0
23	MG	A	1906	1/1	0.95	0.13	75,75,75,75	0
23	MG	A	1681	1/1	0.95	0.07	89,89,89,89	0
23	MG	A	1908	1/1	0.95	0.19	69,69,69,69	0
23	MG	A	1654	1/1	0.95	0.10	104,104,104,104	0
22	PAR	A	1601	42/42	0.95	0.11	70,70,70,70	0
23	MG	A	1911	1/1	0.95	0.19	62,62,62,62	0
23	MG	P	101	1/1	0.95	0.21	63,63,63,63	0
23	MG	A	1869	1/1	0.95	0.33	71,71,71,71	0
22	PAR	A	1604	42/42	0.95	0.12	70,70,70,70	0
23	MG	A	1871	1/1	0.95	0.36	85,85,85,85	0
23	MG	A	1769	1/1	0.95	0.05	108,108,108,108	0
23	MG	A	1890	1/1	0.95	0.20	86,86,86,86	0
23	MG	A	1711	1/1	0.96	0.15	102,102,102,102	0
23	MG	A	1646	1/1	0.96	0.12	85,85,85,85	0
23	MG	A	1875	1/1	0.96	0.11	55,55,55,55	0
23	MG	A	1765	1/1	0.96	0.09	107,107,107,107	0
23	MG	A	1724	1/1	0.96	0.05	97,97,97,97	0
23	MG	A	1858[A]	1/1	0.96	0.68	32,32,32,32	1
23	MG	A	1858[B]	1/1	0.96	0.68	32,32,32,32	1
23	MG	A	1668	1/1	0.96	0.07	92,92,92,92	0
23	MG	A	1751	1/1	0.96	0.13	81,81,81,81	0
23	MG	A	1669	1/1	0.96	0.08	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
23	MG	A	1661	1/1	0.96	0.16	112,112,112,112	0
23	MG	A	1716	1/1	0.96	0.06	74,74,74,74	0
23	MG	A	1729	1/1	0.96	0.09	93,93,93,93	0
23	MG	A	1647	1/1	0.96	0.14	101,101,101,101	0
23	MG	A	1794	1/1	0.96	0.22	80,80,80,80	0
23	MG	A	1627	1/1	0.96	0.08	70,70,70,70	0
23	MG	A	1675	1/1	0.96	0.08	101,101,101,101	0
23	MG	A	1779	1/1	0.96	0.11	70,70,70,70	0
23	MG	A	1815	1/1	0.96	0.07	71,71,71,71	0
23	MG	A	1780	1/1	0.96	0.07	66,66,66,66	0
23	MG	A	1894	1/1	0.96	0.22	64,64,64,64	0
23	MG	A	1690	1/1	0.96	0.08	108,108,108,108	0
23	MG	A	1618	1/1	0.97	0.12	79,79,79,79	0
23	MG	A	1634	1/1	0.97	0.06	44,44,44,44	0
23	MG	A	1658	1/1	0.97	0.07	103,103,103,103	0
23	MG	A	1719	1/1	0.97	0.10	71,71,71,71	0
23	MG	A	1897	1/1	0.97	0.10	47,47,47,47	0
23	MG	A	1660	1/1	0.97	0.05	66,66,66,66	0
23	MG	A	1752	1/1	0.97	0.09	105,105,105,105	0
23	MG	A	1644	1/1	0.97	0.05	50,50,50,50	0
23	MG	A	1702	1/1	0.97	0.08	68,68,68,68	0
23	MG	A	1873	1/1	0.97	0.33	59,59,59,59	0
23	MG	A	1903	1/1	0.97	0.06	46,46,46,46	0
23	MG	A	1619	1/1	0.97	0.06	79,79,79,79	0
23	MG	A	1673	1/1	0.97	0.06	70,70,70,70	0
23	MG	A	1757	1/1	0.97	0.16	61,61,61,61	0
23	MG	A	1771	1/1	0.97	0.04	67,67,67,67	0
23	MG	A	1696	1/1	0.97	0.05	84,84,84,84	0
23	MG	A	1764	1/1	0.98	0.11	107,107,107,107	0
23	MG	A	1633	1/1	0.98	0.06	64,64,64,64	0
23	MG	A	1705	1/1	0.98	0.07	76,76,76,76	0
23	MG	A	1734	1/1	0.98	0.08	96,96,96,96	0
23	MG	A	1657	1/1	0.98	0.06	54,54,54,54	0
23	MG	A	1898	1/1	0.98	0.14	55,55,55,55	0
23	MG	A	1625	1/1	0.98	0.08	90,90,90,90	0
23	MG	A	1659	1/1	0.98	0.05	84,84,84,84	0
23	MG	A	1782	1/1	0.98	0.10	62,62,62,62	0
23	MG	A	1891	1/1	0.98	0.49	70,70,70,70	0
23	MG	D	303	1/1	0.98	0.08	63,63,63,63	0
23	MG	A	1665	1/1	0.98	0.04	90,90,90,90	0
23	MG	A	1672	1/1	0.98	0.05	58,58,58,58	0
23	MG	A	1666	1/1	0.99	0.05	54,54,54,54	0

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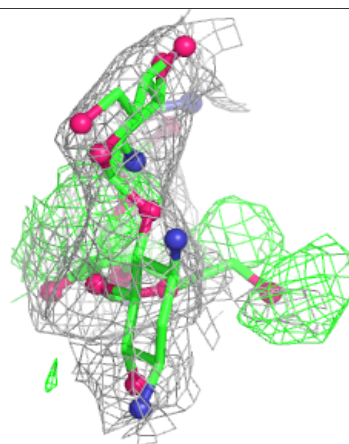
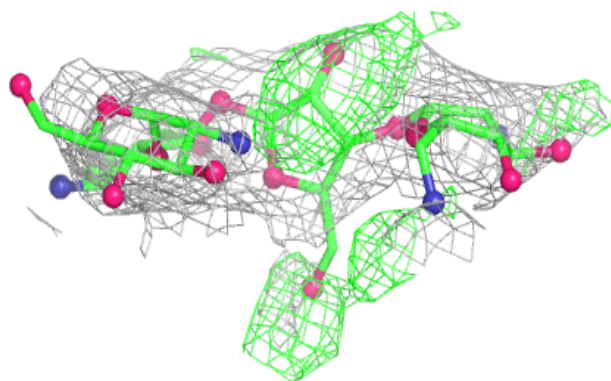
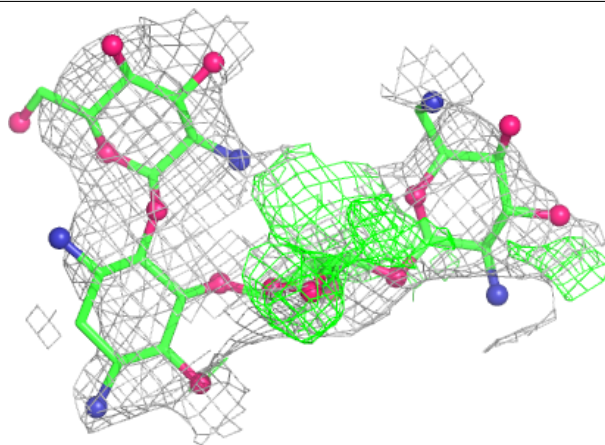
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	MG	A	1776	1/1	0.99	0.10	86,86,86,86	0
23	MG	A	1626	1/1	0.99	0.09	53,53,53,53	0
23	MG	A	1662	1/1	0.99	0.16	59,59,59,59	0
23	MG	A	1631	1/1	0.99	0.04	78,78,78,78	0
23	MG	A	1623	1/1	0.99	0.07	62,62,62,62	0
23	MG	A	1772	1/1	0.99	0.06	67,67,67,67	0
23	MG	A	1695	1/1	0.99	0.04	62,62,62,62	0
23	MG	A	1648	1/1	0.99	0.05	86,86,86,86	0
24	ZN	N	101	1/1	0.99	0.10	141,141,141,141	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.

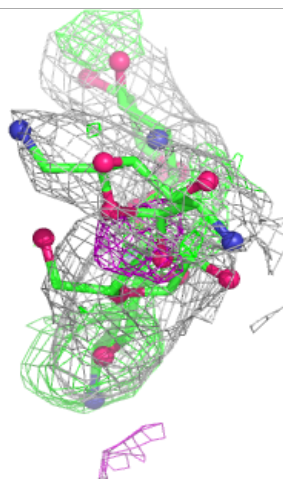
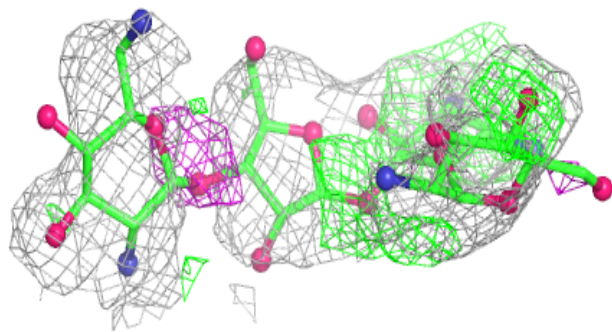
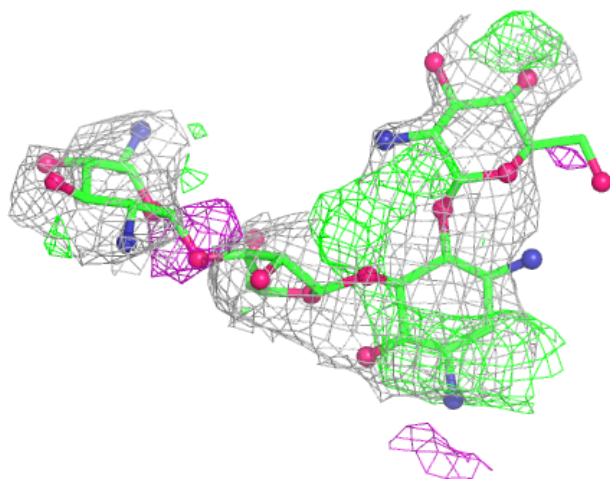
Electron density around PAR A 1614:

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



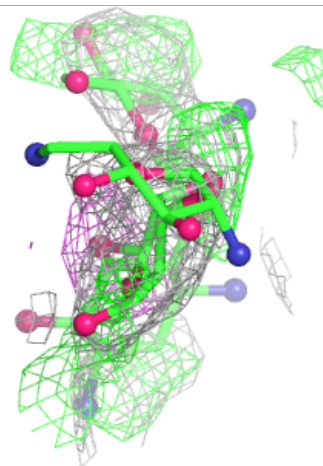
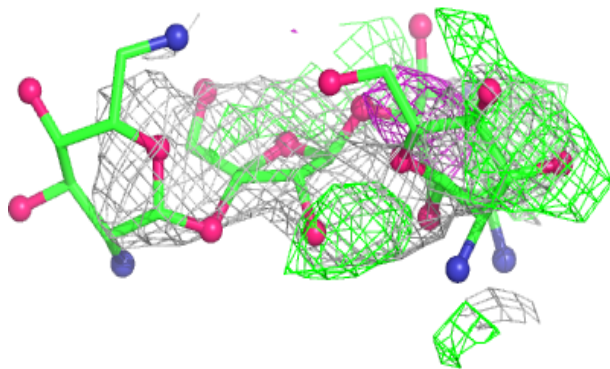
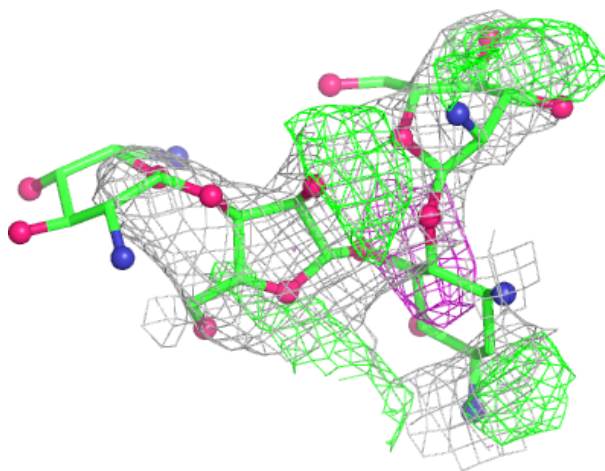
Electron density around PAR A 1611:

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



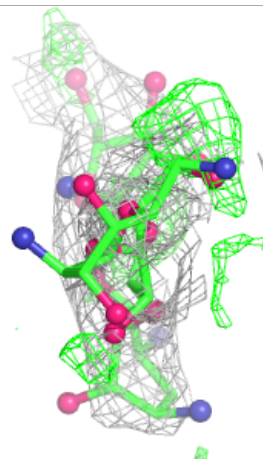
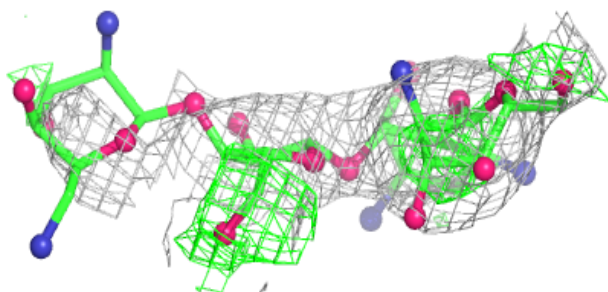
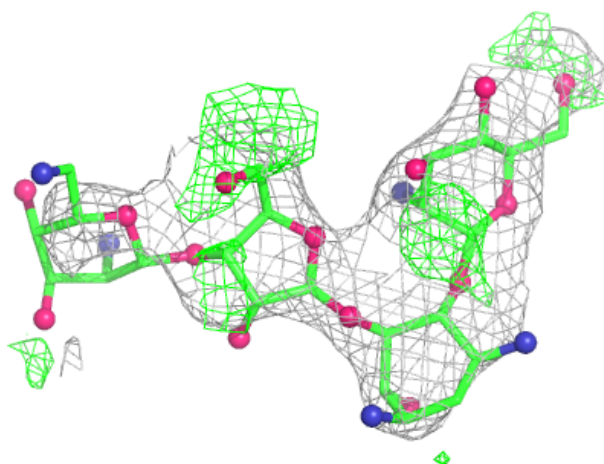
Electron density around PAR A 1613:

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



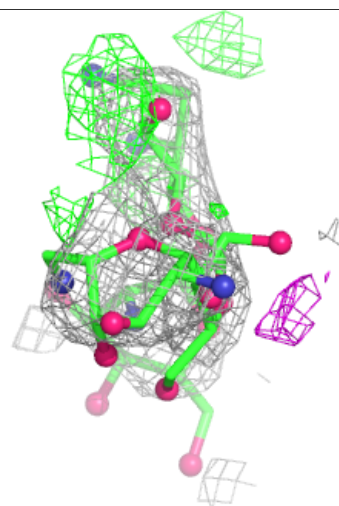
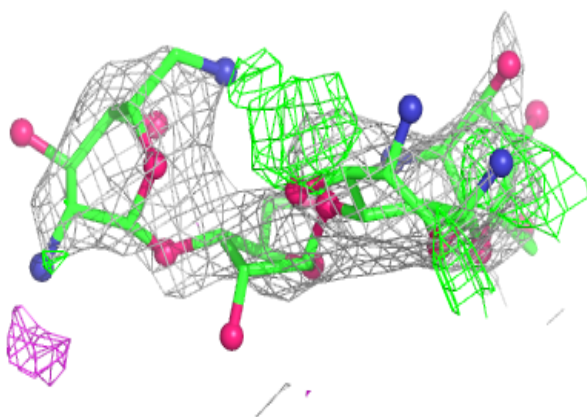
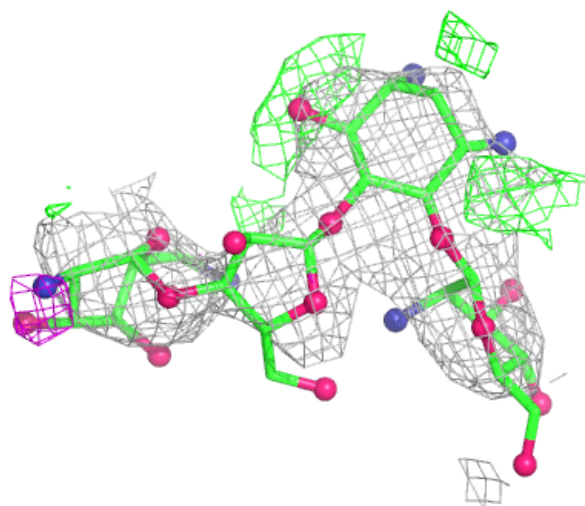
Electron density around PAR A 1615:

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



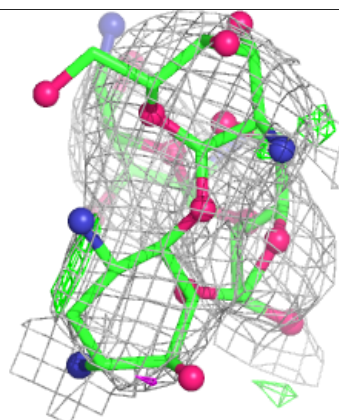
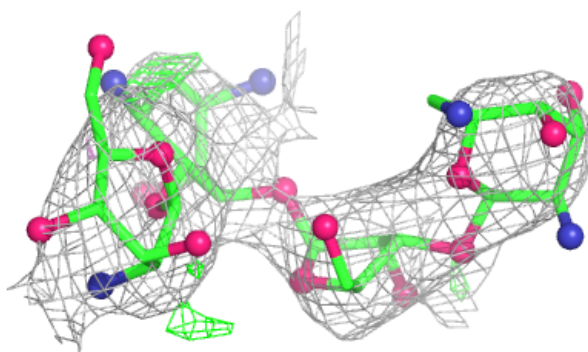
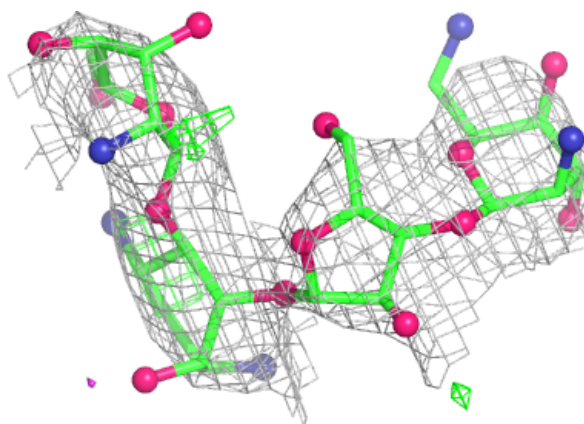
Electron density around PAR A 1616:

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



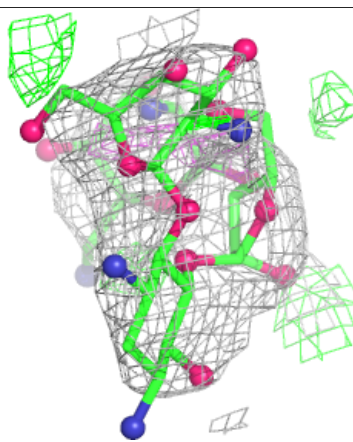
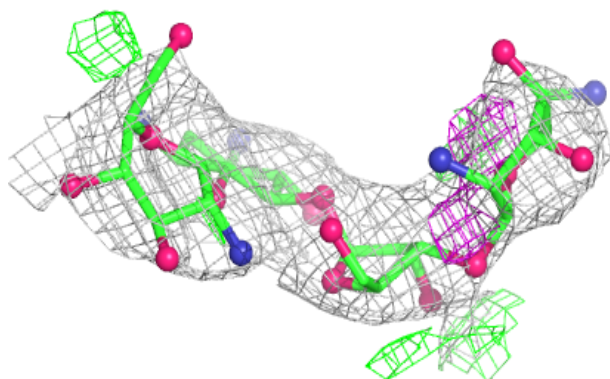
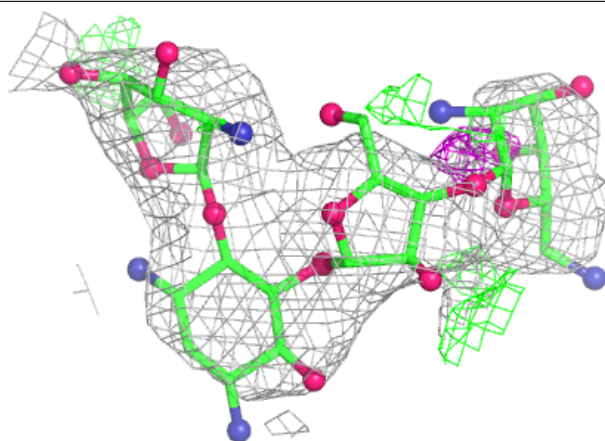
Electron density around PAR A 1617:

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



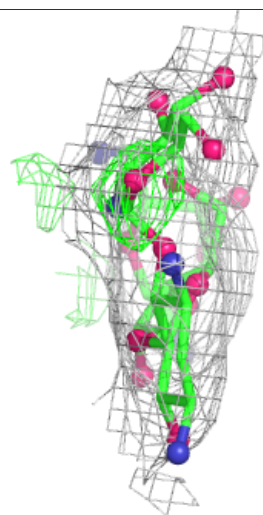
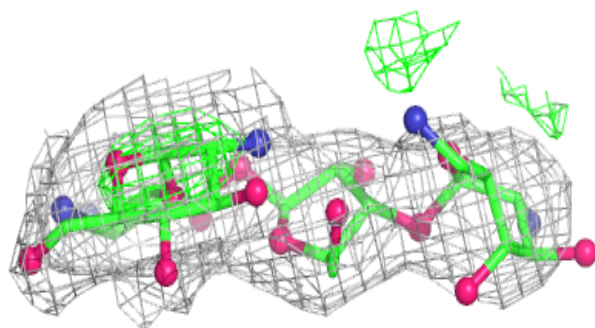
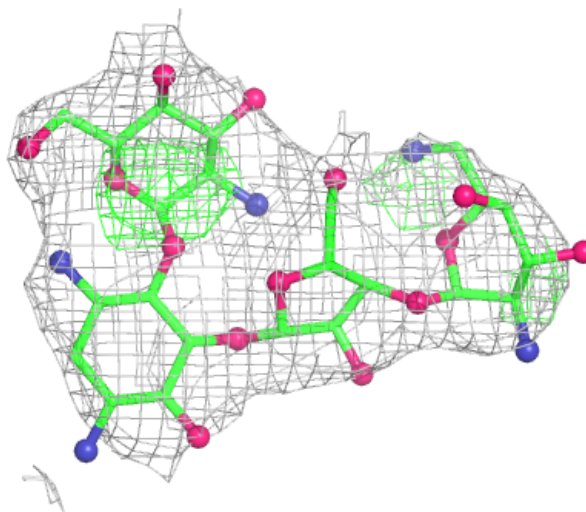
Electron density around PAR A 1610:

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



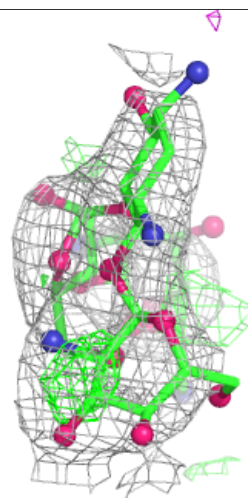
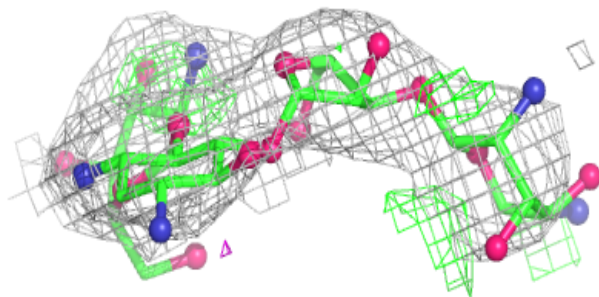
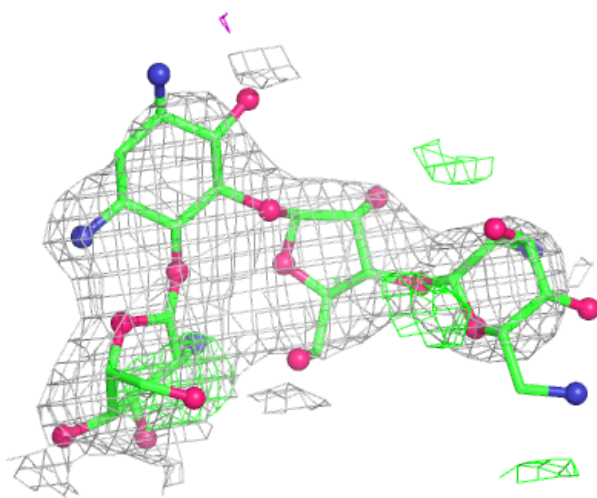
Electron density around PAR A 1605:

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



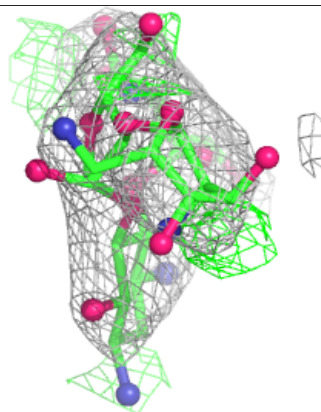
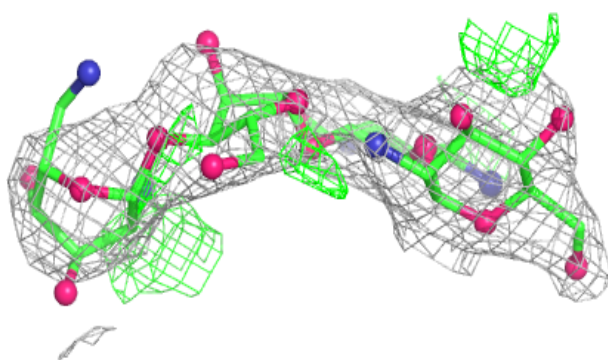
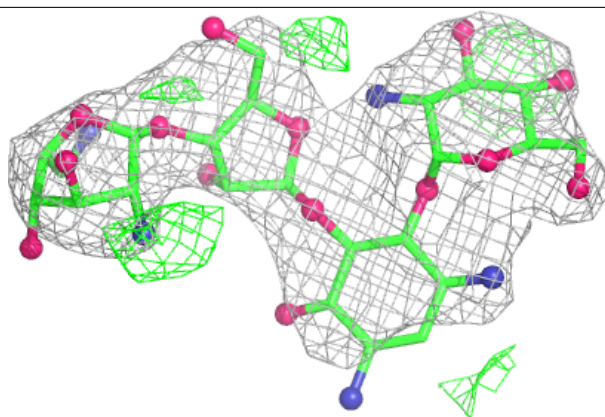
Electron density around PAR A 1607:

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



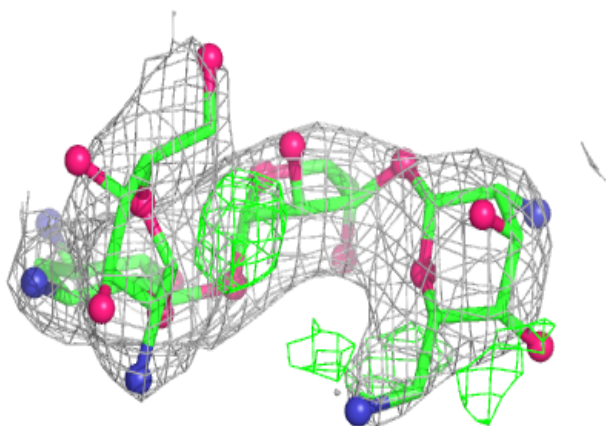
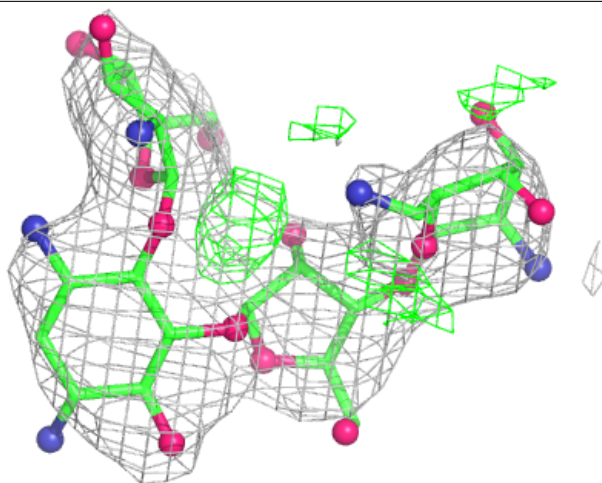
Electron density around PAR A 1612:

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



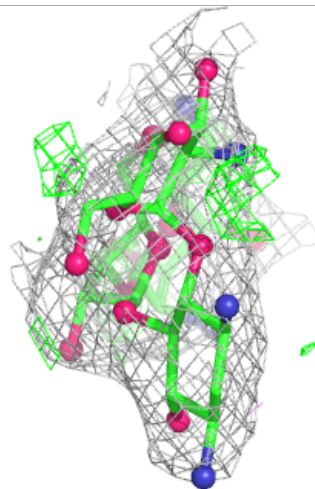
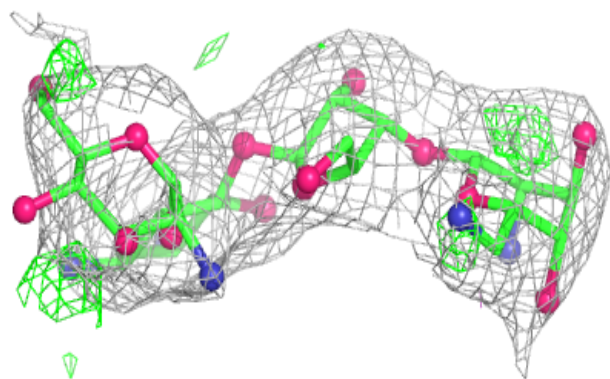
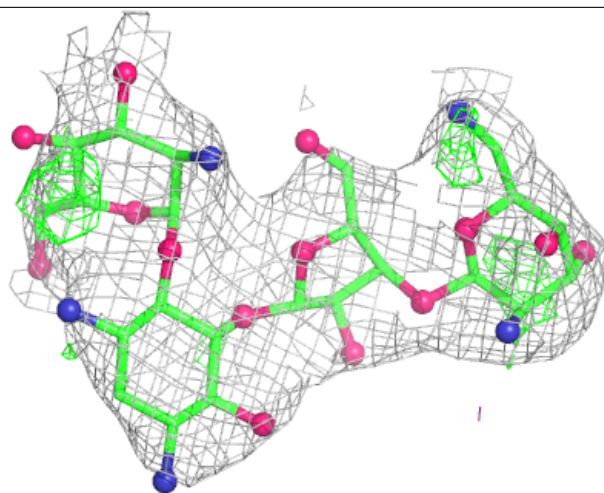
Electron density around PAR A 1608:

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and green (positive)



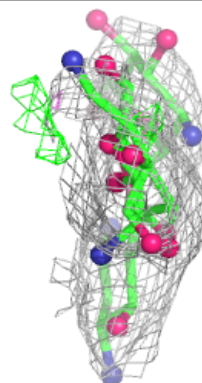
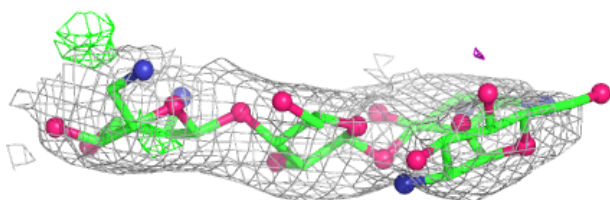
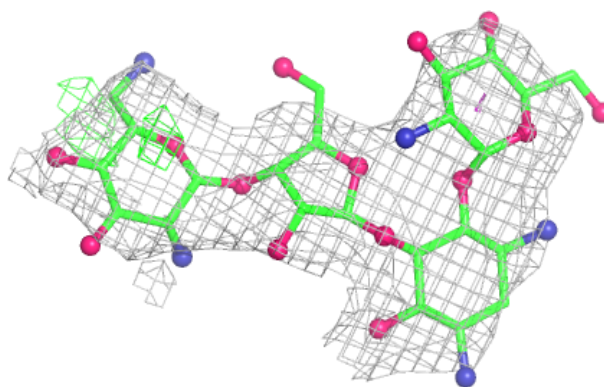
Electron density around PAR A 1603:

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

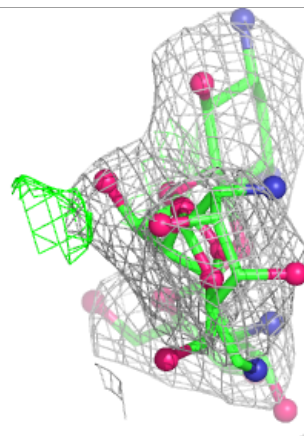
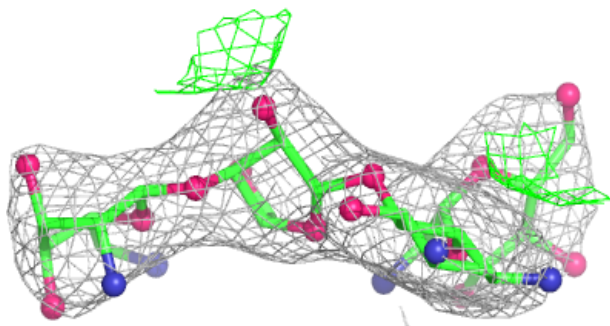


Electron density around PAR A 1609:

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

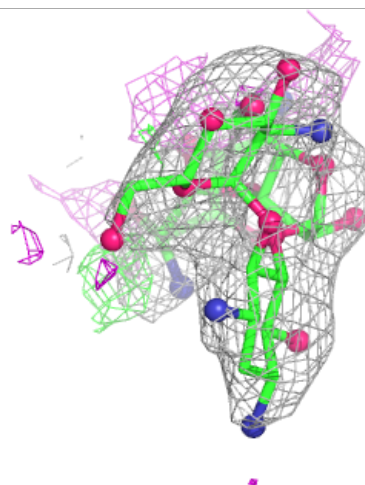
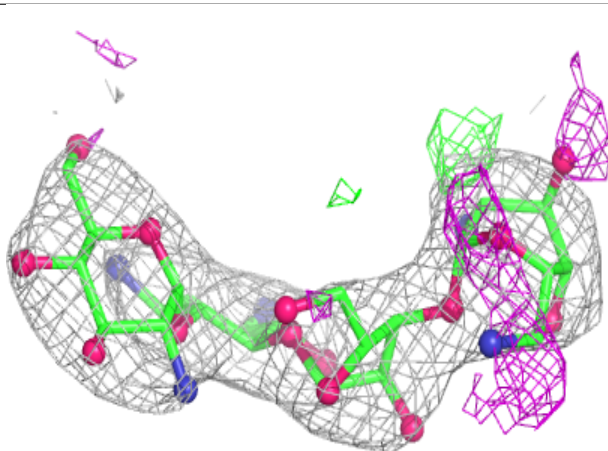
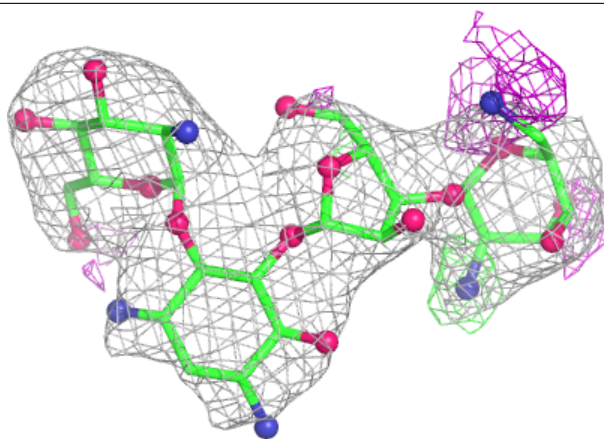
**Electron density around PAR A 1606:**

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



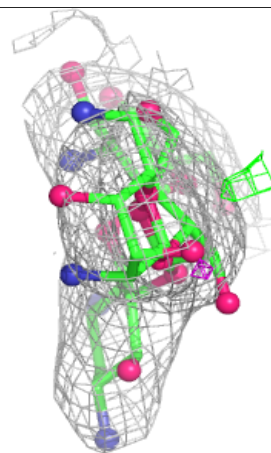
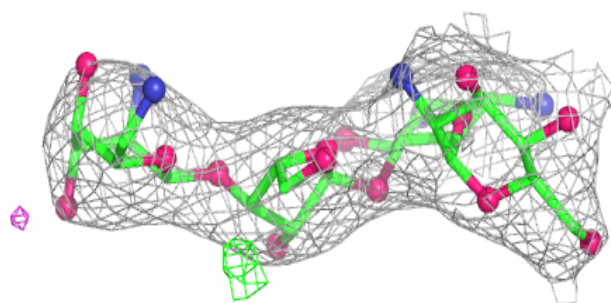
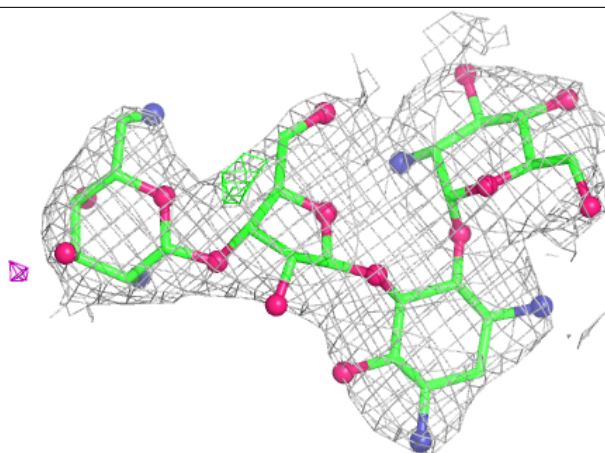
Electron density around PAR A 1602:

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



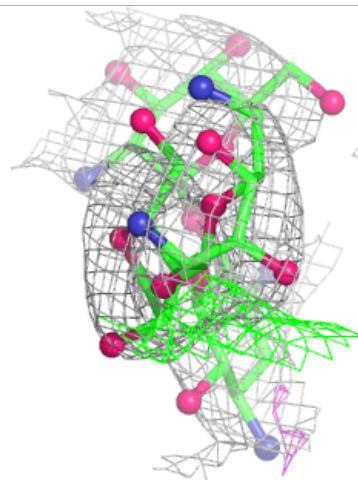
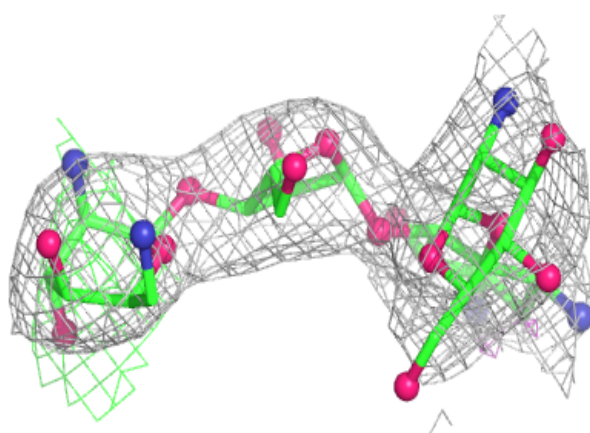
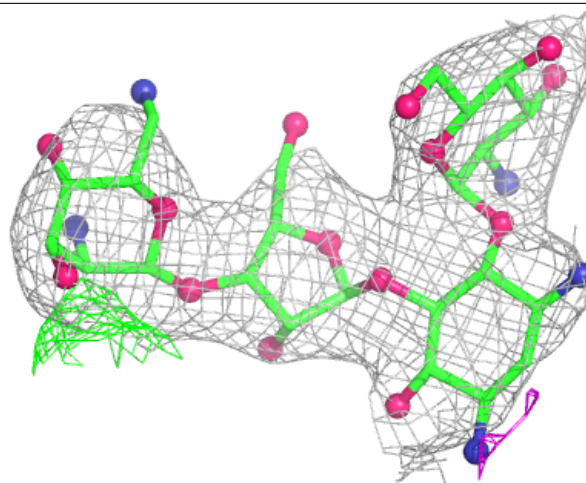
Electron density around PAR A 1601:

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



Electron density around PAR A 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.