



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 09:52 PM BST

PDB ID : 4DR2
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

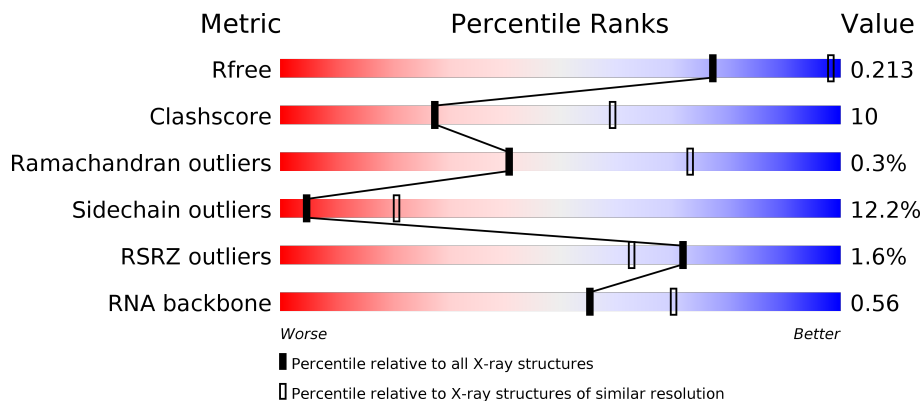
1 Overall quality at a glance

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.









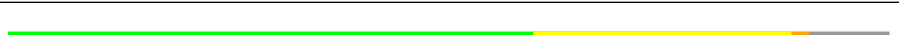
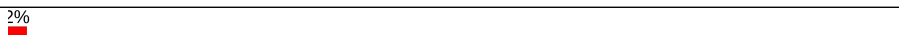
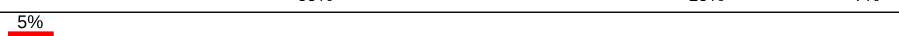








Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1619 (3.28-3.20)
Clashscore	141614	1755 (3.28-3.20)
Ramachandran outliers	138981	1728 (3.28-3.20)
Sidechain outliers	138945	1727 (3.28-3.20)
RSRZ outliers	127900	1567 (3.28-3.20)
RNA backbone	3102	1034 (3.58-2.90)

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

Mol	Chain	Length	Quality of chain
1	A	1522	
2	B	256	
3	C	239	
4	D	209	

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

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
22	PAR	A	1613	-	-	-	X
23	MG	A	1691	-	-	-	X
23	MG	A	1718	-	-	-	X
23	MG	A	1797	-	-	-	X
23	MG	A	1798	-	-	-	X
23	MG	A	1799	-	-	-	X
23	MG	A	1801	-	-	-	X
23	MG	A	1805	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	MG	A	1807	-	-	-	X
23	MG	A	1823	-	-	-	X
23	MG	A	1847	-	-	-	X
23	MG	A	1851	-	-	-	X
23	MG	A	1854	-	-	-	X
23	MG	A	1861	-	-	-	X
23	MG	A	1862	-	-	-	X
23	MG	A	1864	-	-	-	X
23	MG	A	1866	-	-	-	X
23	MG	A	1867	-	-	-	X
23	MG	A	1874	-	-	-	X
23	MG	A	1881	-	-	-	X
23	MG	A	1882	-	-	-	X
23	MG	A	1884	-	-	-	X
23	MG	A	1888	-	-	-	X
23	MG	A	1889	-	-	-	X
23	MG	A	1896	-	-	-	X
23	MG	A	1899[A]	-	-	-	X
23	MG	A	1899[B]	-	-	-	X
23	MG	A	1900	-	-	-	X
23	MG	A	1915	-	-	-	X
23	MG	N	102	-	-	-	X

2 Entry composition i

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
			Total	C	N	O	P			
1	A	1512	32504	14477	6011	10505	1511	0	0	0

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
			Total	C	N	O	S			
2	B	236	1896	1211	337	343	5	0	0	1

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	207	1613	1016	315	281	1	0	0	1

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	151	1147	724	218	201	4	0	0	1

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
9	I	127	1010	639	197	174	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	J	99	793	498	157	137	1	0	0	1

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	K	117	873	543	166	161	3	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	L	125	973	612	196	163	2	0	0	1

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	N	60	491	311	104	72	4	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
16	P	84	701	443	140	117	1	0	0	1

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
17	Q	101	838	536	157	143	2	0	0	0

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
			Total	C	N	O			
18	R	73	598	381	118	99	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
19	S	81	Total 648	C 414	N 120	O 112	S 2	0	0	1

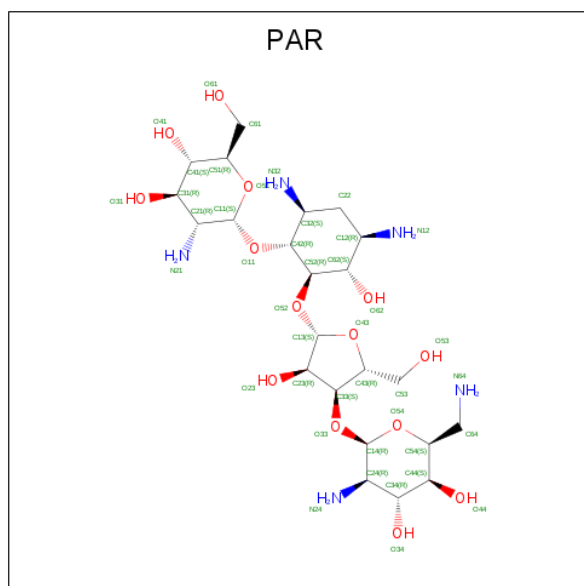
- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
20	T	99	Total 763	C 470	N 162	O 129	S 2	0	0	0

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

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

- Molecule 22 is PAROMOMYCIN (three-letter code: PAR) (formula: $C_{23}H_{45}N_5O_{14}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
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

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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		
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		
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		

- Molecule 23 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	P	1	Total	Mg	0	0
			1	1		
23	Q	1	Total	Mg	0	0
			1	1		
23	D	2	Total	Mg	0	0
			2	2		
23	E	2	Total	Mg	0	0
			2	2		
23	H	2	Total	Mg	0	0
			2	2		
23	I	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	A	305	Total Mg 311 311	0	6
23	T	2	Total Mg 2 2	0	0
23	N	1	Total Mg 1 1	0	0
23	O	1	Total Mg 1 1	0	0
23	L	1	Total Mg 1 1	0	0
23	S	1	Total Mg 1 1	0	0
23	F	1	Total Mg 1 1	0	0

- Molecule 24 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

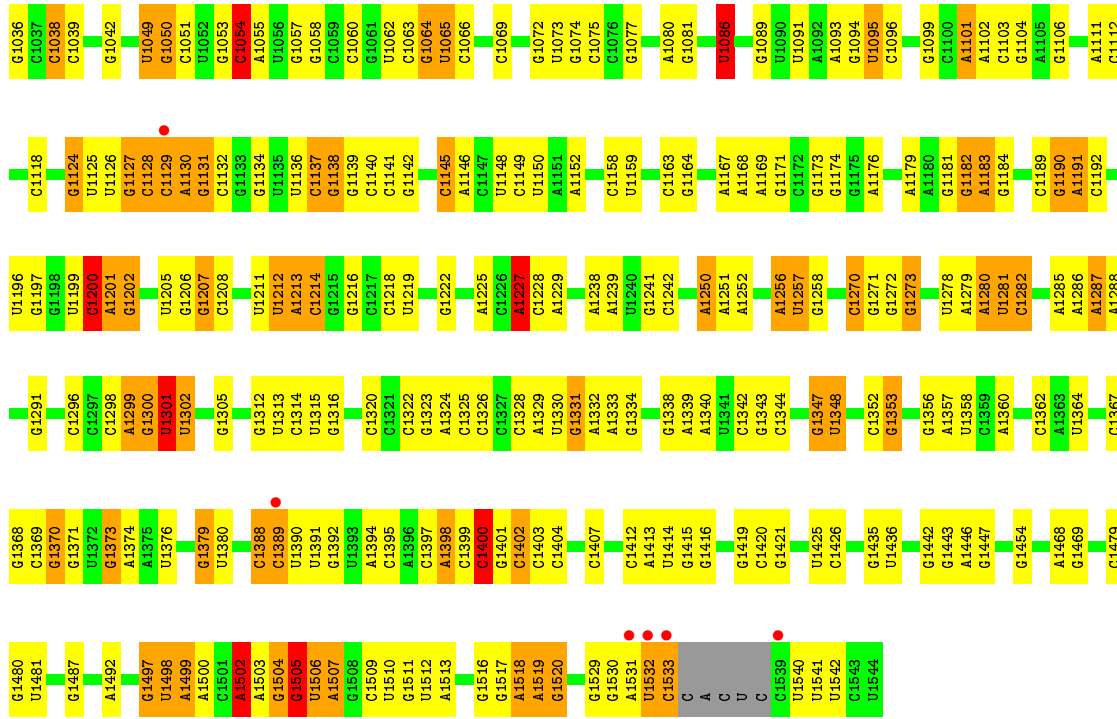
- Molecule 25 is water.

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

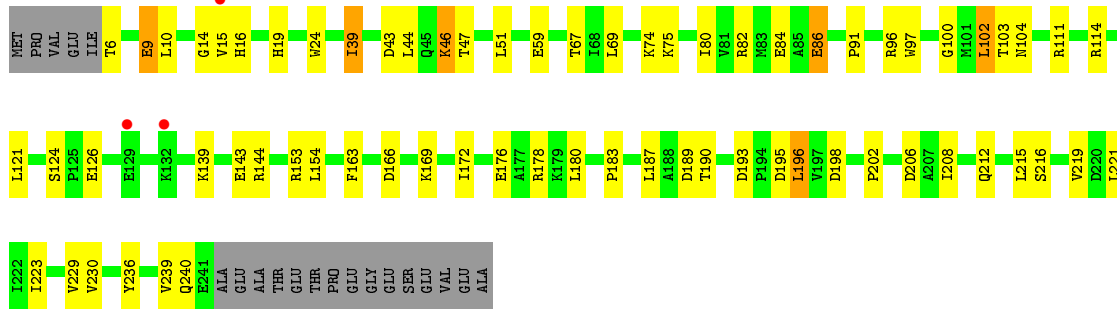
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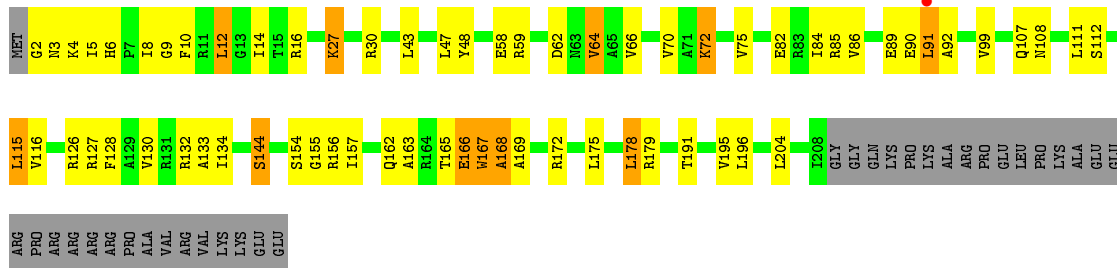
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	U	1	Total	O	0	0
			1	1		



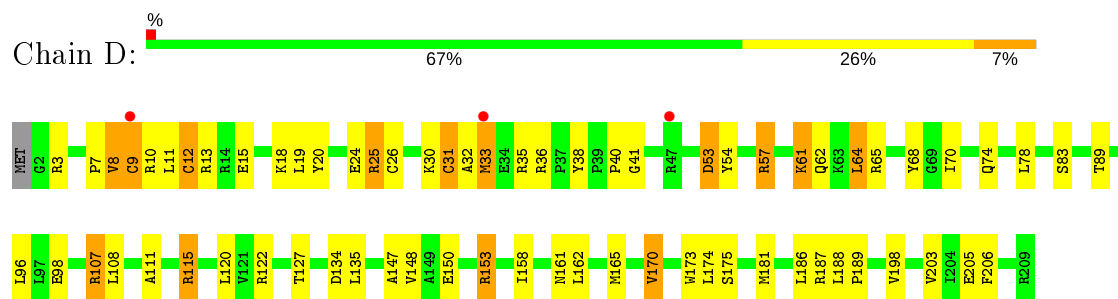
• Molecule 2: 30S ribosomal protein S2



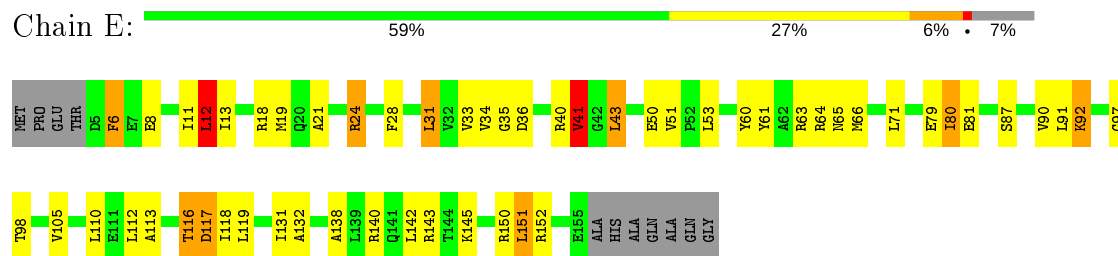
• Molecule 3: 30S ribosomal protein S3



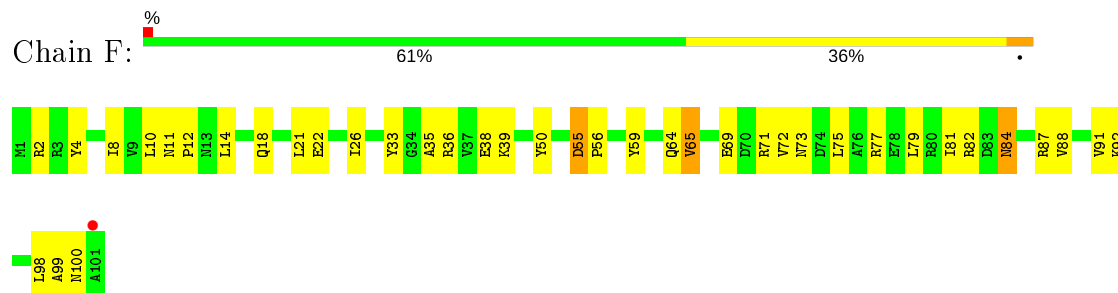
• Molecule 4: 30S ribosomal protein S4



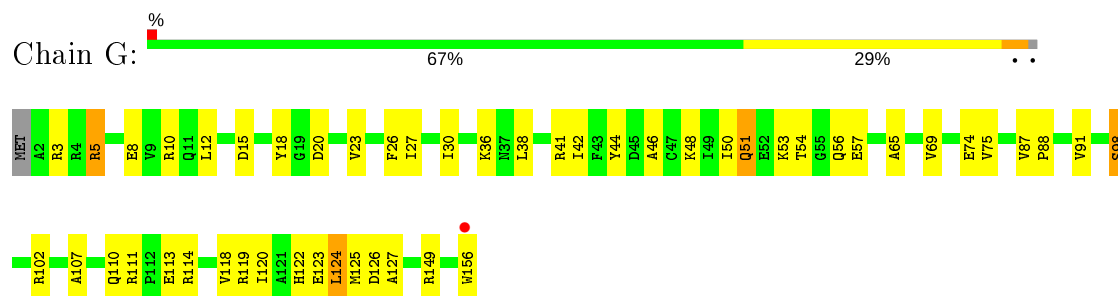
- Molecule 5: 30S ribosomal protein S5



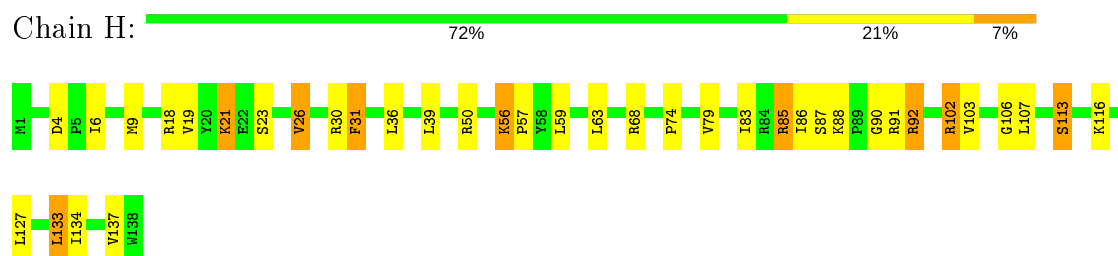
- Molecule 6: 30S ribosomal protein S6



- Molecule 7: 30S ribosomal protein S7

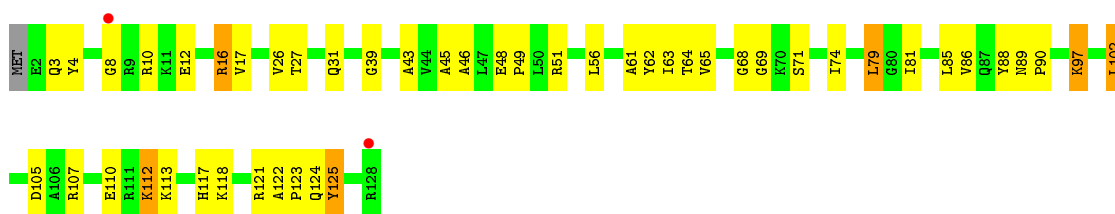


- Molecule 8: 30S ribosomal protein S8



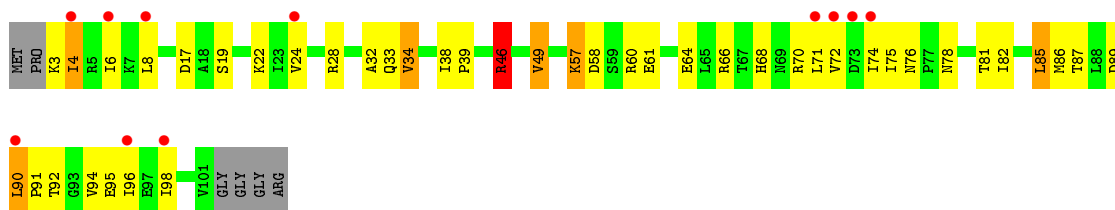
- Molecule 9: 30S ribosomal protein S9

Chain I: 2% 62% 33% 5%



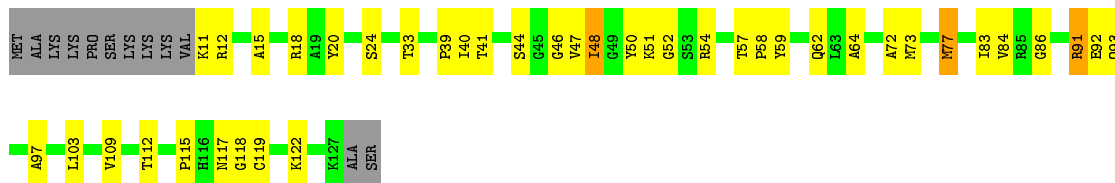
- Molecule 10: 30S ribosomal protein S10

Chain J: 10% 53% 34% 6% 6%



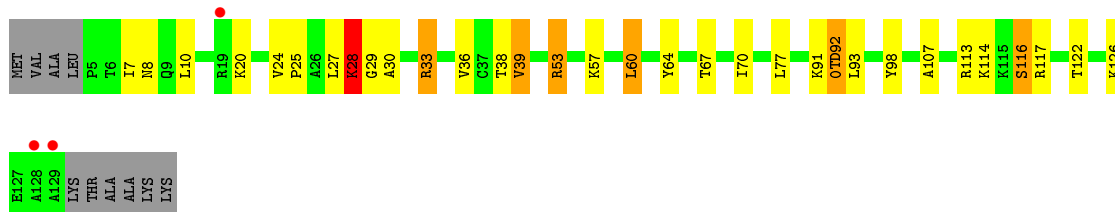
- Molecule 11: 30S ribosomal protein S11

Chain K: 59% 29% 9%



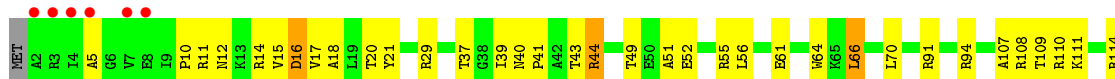
- Molecule 12: 30S ribosomal protein S12

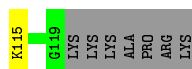
Chain L: 2% 69% 19% 7%



- Molecule 13: 30S ribosomal protein S13

Chain M: 5% 65% 26% 6%

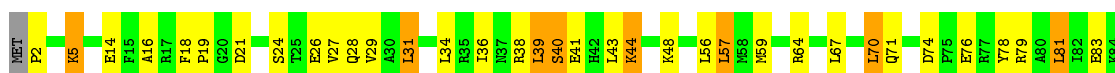




- Molecule 14: 30S ribosomal protein S14



- Molecule 15: 30S ribosomal protein S15



- Molecule 16: 30S ribosomal protein S16



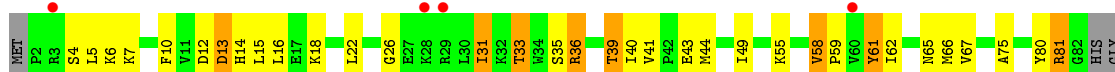
- Molecule 17: 30S ribosomal protein S17



- Molecule 18: 30S ribosomal protein S18



- Molecule 19: 30S ribosomal protein S19



LYS
GLU
ALA
LYS
ALA
THR
LYS
LYS
LYS

- Molecule 20: 30S ribosomal protein S20



MET
ALA
GLN
LYS
LYS
PRO
LYS
R8
R9
L10
S11
A12
R15
H16
R17
Q18
S19
L20
K34
T35
Q42
L43
L44
Q45
E46
G47
K48
A49
E50
E51
K54
I55
M56
R57
R58
A59
E60
S61
L62
I63
A67
K68
G69
R73
K74
N75
A76
A77
A78
R79
R80
K81
L84

M85
E93
I99
I100
G101
G102
G103
A106

- Molecule 21: 30S ribosomal protein THX



MET
G2
F3
G4
D5
R6
R7
T8
G11
K12
R15
G16
T17
Y18
R22
P23
R24
R25
R26
LYS

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) 99.4 (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)	Xtrriage
Refinement program	PHENIX dev_978	Depositor
R, R_{free}	0.171 , 0.211 0.173 , 0.213	Depositor DCC
R_{free} test set	11415 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	88.7	Xtrriage
Anisotropy	0.297	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 65.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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 i

5.1 Standard geometry i

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

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	0.63	3/36037 (0.0%)	1.03	121/56239 (0.2%)
2	B	0.41	0/1931	0.65	0/2607
3	C	0.42	0/1637	0.63	0/2207
4	D	0.49	3/1733 (0.2%)	0.63	1/2318 (0.0%)
5	E	0.51	0/1163	0.75	2/1566 (0.1%)
6	F	0.37	0/856	0.59	0/1154
7	G	0.37	0/1276	0.55	0/1709
8	H	0.50	0/1136	0.71	0/1527
9	I	0.39	0/1029	0.66	0/1379
10	J	0.38	0/806	0.68	1/1084 (0.1%)
11	K	0.43	0/888	0.69	0/1198
12	L	0.49	0/978	0.70	0/1308
13	M	0.38	0/947	0.59	0/1270
14	N	0.43	0/500	0.67	0/663
15	O	0.41	0/745	0.61	0/992
16	P	0.48	0/717	0.71	0/965
17	Q	0.52	0/851	0.74	0/1136
18	R	0.40	0/604	0.60	0/801
19	S	0.34	0/662	0.61	0/892
20	T	0.48	0/765	0.70	0/1007
21	U	0.44	0/213	0.69	0/279
All	All	0.57	6/55474 (0.0%)	0.93	125/82301 (0.2%)

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

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

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

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	975	A	N9-C4	-6.19	1.34	1.37
4	D	31	CYS	CB-SG	6.06	1.92	1.82
1	A	1502	A	N9-C4	-5.34	1.34	1.37
1	A	1502	A	N7-C5	-5.24	1.36	1.39
4	D	9	CYS	CB-SG	5.06	1.90	1.82
4	D	12	CYS	CB-SG	5.04	1.90	1.82

All (125) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	108	G	C4-C5-N7	10.01	114.81	110.80
1	A	108	G	C5-N7-C8	-9.95	99.32	104.30
1	A	1128	C	C6-N1-C2	-9.70	116.42	120.30
1	A	328	C	N1-C2-O2	9.68	124.71	118.90
1	A	1502	A	C5-N7-C8	-9.64	99.08	103.90
1	A	1054	C	N1-C2-O2	9.01	124.31	118.90
1	A	1502	A	C2-N3-C4	-8.94	106.13	110.60
1	A	1054	C	C2-N1-C1'	8.79	128.47	118.80
1	A	927	G	C4-N9-C1'	8.77	137.90	126.50
1	A	108	G	N7-C8-N9	8.49	117.34	113.10
1	A	1502	A	N7-C8-N9	8.30	117.95	113.80
1	A	1502	A	C6-C5-N7	-8.19	126.57	132.30
1	A	266	G	C8-N9-C4	-8.07	103.17	106.40
1	A	929	G	C8-N9-C4	7.98	109.59	106.40
1	A	1200	C	N1-C2-O2	7.92	123.65	118.90
1	A	975	A	C5-N7-C8	-7.86	99.97	103.90
1	A	1502	A	C4-C5-N7	7.72	114.56	110.70
1	A	1502	A	N1-C6-N6	7.67	123.20	118.60
1	A	204	U	C2-N1-C1'	7.65	126.89	117.70
1	A	1532	U	C5-C6-N1	7.53	126.47	122.70
1	A	204	U	N3-C2-O2	-7.41	117.01	122.20
1	A	328	C	N3-C2-O2	-7.32	116.77	121.90
1	A	204	U	N1-C2-O2	7.31	127.92	122.80
1	A	124	G	C5-C6-N1	7.30	115.15	111.50
1	A	1054	C	C6-N1-C1'	-7.23	112.12	120.80
1	A	839	U	C2-N1-C1'	7.23	126.38	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	927	G	C8-N9-C1'	-7.23	117.60	127.00
1	A	328	C	C2-N1-C1'	7.12	126.63	118.80
1	A	299	G	C4-C5-N7	6.96	113.58	110.80
1	A	108	G	C6-C5-N7	-6.84	126.30	130.40
1	A	1389	C	C6-N1-C2	-6.83	117.57	120.30
1	A	108	G	C4-N9-C1'	6.74	135.26	126.50
1	A	812	C	C2-N1-C1'	6.73	126.21	118.80
1	A	1502	A	N1-C2-N3	6.63	132.62	129.30
1	A	266	G	N7-C8-N9	6.61	116.40	113.10
1	A	299	G	N9-C4-C5	-6.58	102.77	105.40
1	A	1505	G	C8-N9-C4	-6.56	103.78	106.40
1	A	1128	C	C5-C6-N1	6.55	124.28	121.00
1	A	1388	C	C6-N1-C2	6.50	122.90	120.30
1	A	1388	C	C5-C6-N1	-6.50	117.75	121.00
1	A	372	C	N1-C2-O2	6.48	122.79	118.90
1	A	108	G	N1-C6-O6	6.47	123.78	119.90
1	A	722	A	N1-C6-N6	6.42	122.45	118.60
1	A	235	C	C6-N1-C2	6.34	122.84	120.30
1	A	975	A	C2-N3-C4	-6.32	107.44	110.60
1	A	927	G	N7-C8-N9	6.28	116.24	113.10
1	A	1064	G	N9-C4-C5	6.27	107.91	105.40
1	A	1505	G	C5-C6-O6	6.21	132.33	128.60
1	A	839	U	N1-C2-O2	6.19	127.13	122.80
1	A	117	G	N1-C6-O6	6.19	123.61	119.90
1	A	303	A	C8-N9-C4	6.17	108.27	105.80
1	A	1390	U	C5-C4-O4	-6.13	122.22	125.90
10	J	46	ARG	NE-CZ-NH1	6.12	123.36	120.30
5	E	12	LEU	CA-CB-CG	6.11	129.35	115.30
5	E	41	VAL	CB-CA-C	-6.11	99.80	111.40
1	A	328	C	N3-C4-N4	-6.08	113.74	118.00
1	A	839	U	N3-C2-O2	-6.04	117.97	122.20
1	A	135	C	N1-C2-O2	-5.98	115.31	118.90
1	A	1227	A	C5-N7-C8	-5.97	100.92	103.90
1	A	1416	G	N1-C6-O6	5.97	123.48	119.90
1	A	559	A	C8-N9-C4	-5.96	103.42	105.80
1	A	570	G	C8-N9-C4	-5.95	104.02	106.40
1	A	24	U	C5-C6-N1	-5.92	119.74	122.70
1	A	266	G	C5-N7-C8	-5.90	101.35	104.30
1	A	1054	C	C5-C6-N1	5.89	123.94	121.00
1	A	328	C	C6-N1-C1'	-5.88	113.74	120.80
1	A	1227	A	N7-C8-N9	5.86	116.73	113.80
1	A	1389	C	N3-C4-C5	-5.83	119.57	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	12	CYS	CA-CB-SG	5.78	124.41	114.00
1	A	232	G	N9-C4-C5	-5.78	103.09	105.40
1	A	975	A	N1-C6-N6	5.77	122.06	118.60
1	A	927	G	C8-N9-C4	-5.76	104.10	106.40
1	A	372	C	C6-N1-C2	5.75	122.60	120.30
1	A	299	G	C5-C6-O6	-5.71	125.17	128.60
1	A	929	G	N3-C4-C5	5.69	131.44	128.60
1	A	1227	A	C8-N9-C4	-5.68	103.53	105.80
1	A	1200	C	C2-N1-C1'	5.68	125.05	118.80
1	A	1503	A	C2-N3-C4	5.68	113.44	110.60
1	A	1299	A	C6-C5-N7	-5.67	128.33	132.30
1	A	981	U	N3-C4-O4	5.67	123.37	119.40
1	A	372	C	N1-C2-N3	-5.66	115.24	119.20
1	A	232	G	C8-N9-C4	5.66	108.66	106.40
1	A	108	G	C5-C6-O6	-5.64	125.21	128.60
1	A	181	G	C8-N9-C4	-5.64	104.14	106.40
1	A	812	C	N1-C2-O2	5.61	122.27	118.90
1	A	266	G	N3-C4-N9	-5.60	122.64	126.00
1	A	722	A	C2-N3-C4	-5.60	107.80	110.60
1	A	328	C	C5-C4-N4	5.58	124.11	120.20
1	A	128	G	C8-N9-C4	5.57	108.63	106.40
1	A	1301	U	P-O3'-C3'	5.56	126.37	119.70
1	A	15	G	C4-N9-C1'	5.52	133.68	126.50
1	A	752	G	C8-N9-C4	5.50	108.60	106.40
1	A	975	A	C4-C5-N7	5.48	113.44	110.70
1	A	1509	C	C6-N1-C2	5.47	122.49	120.30
1	A	929	G	C4-N9-C1'	-5.47	119.39	126.50
1	A	108	G	C8-N9-C1'	-5.47	119.89	127.00
1	A	817	C	C6-N1-C2	5.45	122.48	120.30
1	A	15	G	C8-N9-C1'	-5.45	119.92	127.00
1	A	1158	C	C2-N1-C1'	5.44	124.79	118.80
1	A	1299	A	N7-C8-N9	5.44	116.52	113.80
1	A	6	G	C4-N9-C1'	5.42	133.54	126.50
1	A	1222	G	C5-C6-N1	-5.41	108.79	111.50
1	A	1200	C	C6-N1-C1'	-5.41	114.31	120.80
1	A	960	U	C2-N1-C1'	5.38	124.16	117.70
1	A	325	A	N1-C6-N6	-5.34	115.40	118.60
1	A	948	C	N3-C2-O2	5.33	125.64	121.90
1	A	975	A	N7-C8-N9	5.33	116.46	113.80
1	A	706	A	N1-C6-N6	5.28	121.77	118.60
1	A	812	C	C6-N1-C1'	-5.26	114.48	120.80
1	A	1502	A	C8-N9-C4	-5.26	103.69	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	328	C	P-O3'-C3'	5.21	125.96	119.70
1	A	1086	U	C5-C6-N1	5.21	125.31	122.70
1	A	1322	C	C6-N1-C2	5.20	122.38	120.30
1	A	199	G	C8-N9-C4	5.18	108.47	106.40
1	A	295	C	C6-N1-C2	5.14	122.36	120.30
1	A	1373	G	C5-C6-O6	5.13	131.68	128.60
1	A	481	G	N1-C6-O6	5.11	122.96	119.90
1	A	131	C	N3-C2-O2	-5.09	118.33	121.90
1	A	1502	A	C5-C6-N1	-5.09	115.16	117.70
1	A	1299	A	C4-N9-C1'	5.06	135.40	126.30
1	A	108	G	C8-N9-C4	-5.04	104.38	106.40
1	A	686	U	C2-N1-C1'	-5.04	111.65	117.70
1	A	881	G	C8-N9-C4	5.03	108.41	106.40
1	A	819	A	N7-C8-N9	5.03	116.31	113.80
1	A	20	U	C5-C4-O4	-5.01	122.89	125.90

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32504	0	16434	451	0
2	B	1896	0	1936	33	0
3	C	1613	0	1677	44	0
4	D	1703	0	1763	50	0
5	E	1147	0	1207	35	0
6	F	843	0	857	25	0
7	G	1257	0	1296	30	0
8	H	1116	0	1177	26	0
9	I	1010	0	1037	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	J	793	0	835	33	0
11	K	873	0	894	21	0
12	L	973	0	1058	24	0
13	M	937	0	995	21	0
14	N	491	0	524	18	0
15	O	734	0	771	26	0
16	P	701	0	720	13	0
17	Q	838	0	909	22	0
18	R	598	0	670	16	0
19	S	648	0	673	20	0
20	T	763	0	861	30	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
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	888	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 (888) 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:N	20:T:75:ASN:OD1	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1127:G:N2	1:A:1145:C:N3	2.37	0.68
1:A:261:U:OP2	20:T:79:ARG:NH2	2.26	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:H241	22:A:1610:PAR:H33	1.58	0.67
1:A:976:G:H5'	1:A:1358:U:O2'	1.95	0.67
1:A:673:G:H2'	1:A:674:G:C8	2.30	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
19:S:36:ARG:NH2	19:S:75:ALA:O	2.28	0.65
22:A:1614:PAR:O44	22:A:1614:PAR:N64	2.30	0.65
6:F:84:ASN:OD1	6:F:84:ASN:N	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:152:ARG:NH2	8:H:107:LEU:O	2.30	0.64
5:E:24:ARG:HH11	5:E:24:ARG:HB3	1.62	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:933:G:O6	7:G:3:ARG:NH2	2.31	0.64
7:G:111:ARG:HB2	7:G:119:ARG:HG2	1.79	0.64
1:A:1131:G:OP1	9:I:3:GLN:NE2	2.31	0.64
1:A:1388:C:H2'	1:A:1389:C:O4'	1.97	0.64
1:A:452:A:HO2'	1:A:453:A:H8	1.45	0.63
9:I:16:ARG:HG3	9:I:64:THR:HB	1.79	0.63
1:A:1326:C:OP1	21:U:12:LYS:NZ	2.29	0.63
1:A:1281:U:O2'	1:A:1282:C:OP1	2.16	0.63
1:A:1152:A:OP1	10:J:68:HIS:ND1	2.28	0.63
1:A:353:A:H5'	1:A:353:A:H8	1.63	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:1399:C:H4'	1:A:1400:5MC:H5''	1.82	0.62
1:A:538:G:H5''	12:L:114:LYS:HB2	1.80	0.62
1:A:619:U:N3	4:D:134:ASP:OD2	2.25	0.62
1:A:235:C:H5'	17:Q:70:ARG:HG2	1.80	0.62
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
20:T:56:MET:HE1	20:T:85:MET:HA	1.81	0.61
1:A:1479:C:H2'	1:A:1480:G:H8	1.65	0.61
1:A:474:G:H2'	1:A:475:G:H8	1.64	0.61
9:I:46:ALA:HB2	9:I:74:ILE:HG23	1.82	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:359:U:H2'	1:A:360:A:C8	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:G:H5''	4:D:115:ARG:HB3	1.82	0.61
1:A:103:C:OP1	20:T:17:ARG:NH1	2.32	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
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
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:776:G:O6	22:A:1614:PAR:N24	2.35	0.60
1:A:98:U:O4	22:A:1613:PAR:N12	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:H	3:C:27:LYS:HD3	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
7:G:15:ASP:OD2	7:G:44:TYR:OH	2.15	0.59
3:C:12:LEU:HD11	14:N:51:GLY:HA2	1.82	0.59
1:A:1435:G:H2'	1:A:1436:U:C6	2.36	0.59
7:G:15:ASP:OD1	7:G:18:TYR:N	2.24	0.59
7:G:5:ARG:HH12	7:G:8:GLU:HG2	1.67	0.59
13:M:5:ALA:HB1	13:M:66:LEU:HD12	1.84	0.59
15:O:36:ILE:HG13	15:O:59:MET:HE2	1.85	0.59
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
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
1:A:130:A:OP2	1:A:190(E):U:O2'	2.18	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:1024:G:N1	25:A:2509:HOH:O	2.29	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:765:G:H5''	1:A:766:A:OP1	2.03	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: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:580:U:H2'	1:A:581:G:O4'	2.04	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: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
1:A:17:U:H2'	1:A:18:C:C6	2.39	0.57
15:O:70:LEU:HD13	15:O:78:TYR:HA	1.87	0.57
19:S:10:PHE:O	19:S:39:THR:OG1	2.19	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:1347:G:O2'	1:A:1348:U:P	2.62	0.57
1:A:182:U:OP2	1:A:182:U:H6	1.87	0.57
1:A:974:A:H8	1:A:974:A:OP1	1.88	0.57
1:A:1168:A:H2'	1:A:1169:A:C8	2.39	0.57
11:K:58:PRO:HB3	11:K:93:GLN:HG3	1.86	0.57
1:A:974:A:P	14:N:41:ARG:HH12	2.28	0.57
1:A:1305:G:H5''	21:U:4:GLY:HA3	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
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
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
12:L:25:PRO:C	12:L:27:LEU:H	2.08	0.56
1:A:1392:G:N2	1:A:1502:A:H8	2.03	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
22:A:1607:PAR:N64	22:A:1607:PAR:O44	2.38	0.56
1:A:141:A:H1'	1:A:182:U:O2	2.05	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
7:G:122:HIS:HA	7:G:125:MET:HE2	1.86	0.56
1:A:581:G:O3'	15:O:64:ARG:NH2	2.38	0.56
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
1:A:328:C:O2	1:A:328:C:H2'	2.06	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:1129:C:OP1	9:I:62:TYR:OH	2.22	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: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
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
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
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: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:1328:C:H2'	1:A:1329:A:H8	1.73	0.54
1:A:151:A:H2'	1:A:152:A:O4'	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1532:U:O5'	1:A:1532:U:H6	1.91	0.54
1:A:7:G:H5'	1:A:298:A:O4'	2.06	0.54
1:A:353:A:H5'	1:A:353:A:C8	2.43	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
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
4:D:170:VAL:HG13	4:D:174:LEU:HB2	1.89	0.53
18:R:47:THR:HG22	18:R:48:GLY:H	1.73	0.53
1:A:1250:A:H4'	9:I:68:GLY:N	2.23	0.53
1:A:371:G:O2'	1:A:372:C:H5'	2.08	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: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
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
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: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:933:G:OP2	7:G:3:ARG:HB3	2.09	0.52
1:A:432:A:HO2'	1:A:433:C:P	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1389:C:O5'	1:A:1389:C:H6	1.92	0.52
8:H:102:ARG:HE	8:H:102:ARG:H	1.57	0.52
1:A:1296:C:H4'	1:A:1302:U:C5	2.44	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
4:D:61:LYS:HE2	4:D:206:PHE:CE2	2.45	0.52
1:A:1367:C:H5'	10:J:60:ARG:NH1	2.23	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:610:G:OP1	22:A:1606:PAR:H641	2.10	0.52
1:A:116:A:H61	1:A:313:A:H1'	1.75	0.52
1:A:1347:G:N7	9:I:10:ARG:NH2	2.57	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
13:M:107:ALA:O	13:M:111:LYS:HB2	2.10	0.52
1:A:974:A:OP2	14:N:41:ARG:NH1	2.43	0.52
1:A:1182:G:H4'	1:A:1183:A:O5'	2.10	0.52
1:A:149:A:H2'	1:A:150:C:C6	2.45	0.52
2:B:195:ASP:O	8:H:68:ARG:NH2	2.42	0.52
2:B:47:THR:HA	2:B:202:PRO:HG2	1.92	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
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:1128:C:H6	1:A:1128:C:O5'	1.93	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
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:1516:G:H2'	1:A:1518:MA6:OP2	2.11	0.51
1:A:559:A:H4'	1:A:560:U:O5'	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
4:D:31:CYS:C	4:D:33:MET:H	2.14	0.50
11:K:62:GLN:HG3	11:K:97:ALA:HB2	1.92	0.50
15:O:5:LYS:HD2	15:O:5:LYS:H	1.75	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:413:G:N2	1:A:428:G:H1'	2.26	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:1031:G:H2'	1:A:1032:G:H8	1.75	0.50
1:A:299:G:H2'	1:A:300:A:C8	2.47	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:1060:C:C5	3:C:2:GLY:HA3	2.46	0.50
1:A:129:U:O3'	1:A:129(A):G:H3'	2.11	0.50
4:D:153:ARG:HD3	4:D:181:MET:HG3	1.93	0.50
1:A:1342:C:O2'	9:I:124:GLN:HB2	2.11	0.50
1:A:1216:G:H5''	14:N:5:ALA:HB2	1.93	0.50
15:O:41:GLU:O	15:O:44:LYS:HB2	2.11	0.50
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
22:A:1616:PAR:HN61	22:A:1616:PAR:H33	1.77	0.49
1:A:457:C:H2'	1:A:458:C:H6	1.78	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1285:A:H4'	1:A:1286:A:O5'	2.13	0.49
1:A:376:G:OP2	16:P:67:THR:HG21	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:22:LYS:HZ3	10:J:90:LEU:H	1.61	0.49
10:J:6:ILE:HG12	10:J:98:ILE:HG23	1.93	0.49
1:A:1190:G:O2'	1:A:1191:A:P	2.70	0.49
1:A:452:A:O2'	1:A:453:A:H8	1.95	0.49
2:B:100:GLY:O	2:B:104:ASN:N	2.46	0.49
4:D:173:TRP:CG	4:D:189:PRO:HG3	2.48	0.49
4:D:32:ALA:O	4:D:36:ARG:N	2.33	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: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
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
7:G:51:GLN:C	7:G:53:LYS:H	2.17	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: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
1:A:190(F):G:H4'	1:A:190(G):G:OP2	2.13	0.48
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: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
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
3:C:86:VAL:O	3:C:90:GLU:HG3	2.13	0.48
1:A:1402:4OC:O2	1:A:1500:A:N1	2.46	0.48
1:A:45:U:H2'	1:A:46:G:C8	2.48	0.48
1:A:1053:G:C3'	1:A:1054:C:H5'	2.44	0.48
1:A:539:A:H2'	1:A:540:G:C8	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:42:GLN:O	20:T:45:GLN:HB2	2.14	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:107:G:N7	20:T:15:ARG:NH2	2.62	0.48
1:A:1333:A:H2'	1:A:1334:G:O4'	2.13	0.48
1:A:266:G:H5''	1:A:267:C:C5	2.48	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:N	7:G:113:GLU:OE1	2.46	0.47
1:A:1347:G:N2	1:A:1373:G:H2'	2.29	0.47
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:61:G:O2'	25:A:2002:HOH:O	2.20	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:1167:A:H8	1:A:1167:A:OP1	1.97	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
9:I:112:LYS:HD2	9:I:113:LYS:N	2.29	0.47
1:A:1371:G:O3'	9:I:69:GLY:HA3	2.13	0.47
1:A:384:G:H2'	1:A:385:C:C6	2.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1216:G:H5''	14:N:5:ALA:CB	2.44	0.47
15:O:29:VAL:HG11	15:O:67:LEU:HD21	1.97	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
1:A:474:G:H2'	1:A:475:G:C8	2.47	0.47
5:E:80:ILE:HD12	5:E:142:LEU:HD21	1.95	0.47
5:E:24:ARG:HB3	5:E:24:ARG:NH1	2.28	0.47
14:N:34:TYR:N	14:N:39:LEU:O	2.48	0.47
1:A:247:G:OP2	17:Q:100:LYS:HG3	2.14	0.47
19:S:40:ILE:HG22	19:S:67:VAL:HA	1.96	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:828:A:H4'	1:A:828:A:OP1	2.15	0.47
1:A:1419:G:H1	1:A:1481:U:H3	1.63	0.47
1:A:179:A:H2'	1:A:180:U:C6	2.50	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:299:G:C6	1:A:300:A:C6	3.03	0.46
1:A:46:G:O2'	1:A:365:U:H1'	2.15	0.46
1:A:509:A:H3'	1:A:509:A:C8	2.50	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
1:A:657:G:H4'	15:O:28:GLN:HG2	1.98	0.46
1:A:114:U:OP1	22:A:1604:PAR:H32	2.15	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:100:LYS:HB2	17:Q:101:ARG:CZ	2.45	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
1:A:447:G:H2'	1:A:485:G:N2	2.31	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: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
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
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:HA	4:D:78:LEU:HD23	1.73	0.46
12:L:38:THR:HG22	12:L:39:VAL:HG22	1.98	0.46
15:O:57:LEU:HA	15:O:57:LEU:HD12	1.67	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:1425:U:H2'	1:A:1426:C:H6	1.80	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
1:A:977:A:H2'	1:A:978:A:H5''	1.98	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:H	9:I:56:LEU:HD12	1.81	0.46
1:A:1316:G:H4'	14:N:18:VAL:HG11	1.98	0.46
4:D:35:ARG:C	4:D:36:ARG:HG3	2.34	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:1504:G:C3'	1:A:1505:G:H5'	2.46	0.45
1:A:267:C:H2'	1:A:268:C:C6	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HA	18:R:18:ARG:HD3	1.80	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:556:C:H2'	1:A:557:G:O4'	2.17	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
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
1:A:107:G:H2'	1:A:108:G:H5'	1.99	0.45
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
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: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
1:A:517:G:N1	1:A:533:A:OP2	2.33	0.45
10:J:4:ILE:HG13	10:J:4:ILE:H	1.54	0.45
1:A:501:C:OP1	12:L:117:ARG:NH2	2.50	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:877:C:OP1	8:H:88:LYS:NZ	2.34	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: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
1:A:325:A:H2'	1:A:326:G:O4'	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1129:C:H4'	1:A:1130:A:OP2	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
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:986:A:O2'	19:S:55:LYS:O	2.35	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:HD13	5:E:80:ILE:N	2.32	0.44
6:F:100:ASN:OD1	18:R:23:LYS:HE2	2.17	0.44
9:I:17:VAL:HG11	9:I:81:ILE:HA	1.99	0.44
1:A:130:A:C8	17:Q:63:ARG:HG3	2.53	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:1347:G:C2'	1:A:1348:U:OP2	2.66	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
4:D:120:LEU:HD23	4:D:120:LEU:HA	1.82	0.44
9:I:26:VAL:HG13	9:I:61:ALA:HB3	1.99	0.44
6:F:50:TYR:CE1	18:R:77:GLY:HA2	2.52	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:189:ASP:OD2	2:B:190:THR:N	2.41	0.44
2:B:183:PRO:HA	2:B:198:ASP:OD2	2.17	0.44
1:A:620:C:N1	4:D:135:LEU:HD13	2.31	0.44
15:O:85:LEU:HB3	15:O:87:ILE:HD11	2.00	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
1:A:707:C:H2'	1:A:708:C:C6	2.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1064:G:H1'	1:A:1190:G:N2	2.32	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
2:B:124:SER:OG	2:B:126:GLU:HG2	2.18	0.44
1:A:1330:U:H2'	1:A:1331:G:H5'	1.99	0.44
22:A:1601:PAR:O52	22:A:1601:PAR:H11	2.17	0.44
1:A:633:G:OP2	22:A:1612:PAR:H11	2.18	0.44
1:A:109:A:C6	1:A:326:G:C6	3.06	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:1074:G:O2'	1:A:1101:A:N1	2.45	0.43
1:A:1343:G:H4'	9:I:122:ALA:HB3	2.00	0.43
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
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
13:M:108:ARG:NH2	13:M:111:LYS:HE2	2.32	0.43
20:T:62:LEU:HD23	20:T:62:LEU:HA	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:1001:A:H2'	1:A:1002:G:H8	1.83	0.43
1:A:1228:C:OP1	13:M:115:LYS:NZ	2.49	0.43
1:A:179:A:H2'	1:A:180:U:H6	1.83	0.43
7:G:120:ILE:O	7:G:124:LEU:HB2	2.18	0.43
7:G:23:VAL:O	7:G:27:ILE:HG13	2.19	0.43
9:I:125:TYR:HD2	9:I:125:TYR:H	1.65	0.43
11:K:46:GLY:HA2	11:K:50:TYR:O	2.17	0.43
1:A:1086:U:O5'	1:A:1086:U:H6	2.00	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:309:G:H1'	1:A:608:A:C2	2.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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:1141:C:H2'	1:A:1142:G:H8	1.84	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
2:B:103:THR:HG23	2:B:176:GLU:OE1	2.17	0.43
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:HA	12:L:7:ILE:HD13	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:117:G:P	25:A:2020:HOH:O	2.77	0.43
1:A:1425:U:H2'	1:A:1426:C:C6	2.54	0.43
1:A:90:U:H2'	1:A:91: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
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
6:F:69:GLU:CD	6:F:69:GLU:H	2.22	0.43
13:M:49:THR:HG22	13:M:51:ALA:N	2.29	0.43
1:A:390:C:H6	1:A:390:C:O5'	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:O	3:C:5:ILE:HD12	2.19	0.42
5:E:87:SER:HB3	5:E:131:ILE:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1518:MA6:H8	1:A:1518:MA6:O5'	2.18	0.42
1:A:269:C:H2'	1:A:270:A:C8	2.54	0.42
1:A:62:U:H2'	1:A:63:C:C6	2.54	0.42
14:N:40:CYS:O	14:N:44:LEU:HB3	2.19	0.42
1:A:1498:UR3:H6	1:A:1498:UR3:O5'	2.19	0.42
22:A:1613:PAR:H11	22:A:1613:PAR:H52	1.82	0.42
1:A:64:G:C6	22:A:1613:PAR:N32	2.88	0.42
1:A:570:G:H1'	1:A:820:U:C4	2.53	0.42
1:A:993:G:H2'	1:A:995:C:H41	1.84	0.42
12:L:117:ARG:HD2	12:L:122:THR:HG22	2.01	0.42
12:L:53:ARG:NH1	12:L:92:0TD:OD1	2.52	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:411:A:OP1	4:D:30:LYS:NZ	2.51	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
1:A:109:A:C6	1:A:327:A:C6	3.07	0.42
1:A:1190:G:O2'	1:A:1191:A:O5'	2.36	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
8:H:56:LYS:HA	8:H:57:PRO:HD3	1.78	0.42
1:A:695:A:OP1	11:K:52:GLY:HA3	2.19	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:H	4:D:57:ARG:HG2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:954:G:N2	1:A:1227:A:H62	2.13	0.42
1:A:224:C:H2'	1:A:225:C:H6	1.84	0.42
1:A:217:C:O2'	1:A:461:C:N4	2.53	0.42
1:A:946:A:H2'	1:A:947:G:H8	1.78	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
1:A:542:G:H5'	4:D:41:GLY:HA3	2.02	0.42
6:F:8:ILE:HD11	6:F:79:LEU:HD13	2.01	0.42
10:J:71:LEU:HA	10:J:71:LEU:HD23	1.88	0.42
20:T:59:ALA:O	20:T:63:ILE:HG13	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
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
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: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
1:A:857:C:H2'	1:A:858:G:O4'	2.20	0.41
2:B:102:LEU:HB3	2:B:180:LEU:HD12	2.01	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: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
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
1:A:1360:A:OP2	14:N:35:ARG:NH2	2.53	0.41
16:P:58:TYR:O	16:P:62:VAL:HG22	2.20	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:728:A:O5'	1:A:728:A:H8	2.03	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:D:24:GLU:C	4:D:26:CYS:H	2.23	0.41
5:E:13:ILE:HD12	5:E:13:ILE:HG23	1.81	0.41
5:E:6:PHE:HE2	5:E:36:ASP:HB3	1.86	0.41
9:I:105:ASP:OD2	9:I:107:ARG:HG3	2.20	0.41
9:I:49:PRO:HB2	9:I:81:ILE:HG22	2.02	0.41
11:K:44:SER:H	11:K:47:VAL:HB	1.85	0.41
20:T:74:LYS:HB3	20:T:74:LYS:HE3	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:80:TYR:CE1	19:S:81:ARG:HD2	2.55	0.41
1:A:1003:G:H22	1:A:1039:C:H1'	1.85	0.41
1:A:295:C:H2'	1:A:296:U:O4'	2.20	0.41
1:A:6:G:H4'	1:A:298:A:H4'	2.03	0.41
1:A:658:G:H2'	1:A:659:U:C6	2.55	0.41
3:C:43:LEU:HD21	3:C:91:LEU:HD13	2.02	0.41
12:L:33:ARG:HD2	12:L:33:ARG:HA	1.64	0.41
15:O:71:GLN:HB2	15:O:78:TYR:CE1	2.56	0.41
19:S:22:LEU:HA	19:S:22:LEU:HD23	1.94	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
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
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
11:K:115:PRO:C	11:K:117:ASN:H	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:C:O2	1:A:379:C:H4'	2.21	0.41
1:A:1072:G:H2'	1:A:1073:U:C6	2.55	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: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: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
1:A:1251:A:H4'	9:I:12:GLU:OE1	2.20	0.41
1:A:526:C:OP2	12:L:91:LYS:HE3	2.21	0.41
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: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
3:C:92:ALA:HB2	3:C:99:VAL:HG22	2.02	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:1391:U:H2'	1:A:1392:G:C8	2.56	0.41
22:A:1613:PAR:H42	22:A:1613:PAR:H13	1.60	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
5:E:117:ASP:OD2	5:E:117:ASP:N	2.54	0.41
11:K:72:ALA:HB1	11:K:77:MET:HE2	2.02	0.41
1:A:1029:C:H2'	1:A:1030:C:C6	2.56	0.40
1:A:116:A:C8	1:A:116:A:OP2	2.75	0.40
1:A:1190:G:HO2'	1:A:1191:A:P	2.44	0.40
1:A:1347:G:HO2'	1:A:1348:U:H5	1.64	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
6:F:75:LEU:HD23	6:F:79:LEU:HG	2.02	0.40
15:O:81:LEU:HA	15:O:81:LEU:HD23	1.88	0.40
1:A:1251:A:H2'	1:A:1252:A:O4'	2.21	0.40
22:A:1606:PAR:O52	22:A:1606:PAR:H11	2.21	0.40
22:A:1608:PAR:H13	22:A:1608:PAR:H42	1.74	0.40
3:C:178:LEU:HD13	3:C:178:LEU:HA	1.80	0.40
4:D:108:LEU:HA	4:D:108:LEU:HD23	1.83	0.40
4:D:175:SER:HB3	4:D:186:LEU:HD11	2.02	0.40
4:D:68:TYR:OH	4:D:98:GLU:OE1	2.30	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:107:ALA:O	7:G:110:GLN:HB2	2.21	0.40
1:A:932:C:H5''	7:G:3:ARG:HG2	2.03	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:1020:U:H2'	1:A:1021:G:H8	1.85	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
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
5:E:116:THR:HB	5:E:117:ASP:OD2	2.21	0.40
10:J:57:LYS:HG2	10:J:58:ASP:CG	2.42	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:1531:A:O5'	1:A:1531:A:H8	2.04	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
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
1:A:1128:C:C4'	9:I:16:ARG:HH22	2.35	0.40
13:M:18:ALA:O	13:M:21:TYR:HB2	2.22	0.40
13:M:91:ARG:HD2	13:M:91:ARG:HA	1.91	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	234/256 (91%)	218 (93%)	15 (6%)	1 (0%)	34	68
3	C	205/239 (86%)	187 (91%)	16 (8%)	2 (1%)	15	50
4	D	206/209 (99%)	198 (96%)	7 (3%)	1 (0%)	29	64
5	E	149/162 (92%)	143 (96%)	6 (4%)	0	100	100
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%)	15	50
11	K	115/129 (89%)	109 (95%)	6 (5%)	0	100	100
12	L	122/135 (90%)	111 (91%)	10 (8%)	1 (1%)	19	55
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%)	12	44
20	T	97/106 (92%)	88 (91%)	8 (8%)	1 (1%)	15	50
21	U	23/27 (85%)	22 (96%)	1 (4%)	0	100	100
All	All	2352/2541 (93%)	2203 (94%)	141 (6%)	8 (0%)	41	73

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 [i](#)

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%)	177 (88%)	24 (12%)	5	21
3	C	160/188 (85%)	134 (84%)	26 (16%)	2	10
4	D	180/181 (99%)	162 (90%)	18 (10%)	7	28
5	E	115/123 (94%)	96 (84%)	19 (16%)	2	10
6	F	90/90 (100%)	82 (91%)	8 (9%)	9	34
7	G	126/127 (99%)	112 (89%)	14 (11%)	6	24
8	H	119/119 (100%)	103 (87%)	16 (13%)	4	17
9	I	98/99 (99%)	87 (89%)	11 (11%)	6	24
10	J	87/92 (95%)	79 (91%)	8 (9%)	9	32
11	K	89/99 (90%)	79 (89%)	10 (11%)	6	24
12	L	103/110 (94%)	92 (89%)	11 (11%)	6	26
13	M	94/101 (93%)	85 (90%)	9 (10%)	8	30
14	N	48/50 (96%)	43 (90%)	5 (10%)	7	27
15	O	79/80 (99%)	66 (84%)	13 (16%)	2	10
16	P	72/74 (97%)	64 (89%)	8 (11%)	6	24
17	Q	95/97 (98%)	84 (88%)	11 (12%)	5	23
18	R	64/77 (83%)	61 (95%)	3 (5%)	26	60
19	S	71/80 (89%)	58 (82%)	13 (18%)	1	7
20	T	76/82 (93%)	63 (83%)	13 (17%)	2	9
21	U	19/22 (86%)	17 (90%)	2 (10%)	7	26
All	All	1986/2111 (94%)	1744 (88%)	242 (12%)	5	21

All (242) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	9	GLU
2	B	16	HIS
2	B	24	TRP

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Mol	Chain	Res	Type
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	114	ARG
2	B	121	LEU
2	B	144	ARG
2	B	153	ARG
2	B	163	PHE
2	B	169	LYS
2	B	172	ILE
2	B	187	LEU
2	B	196	LEU
2	B	206	ASP
2	B	208	ILE
2	B	236	TYR
3	C	3	ASN
3	C	12	LEU
3	C	14	ILE
3	C	27	LYS
3	C	48	TYR
3	C	62	ASP
3	C	64	VAL
3	C	70	VAL
3	C	72	LYS
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	127	ARG
3	C	144	SER
3	C	162	GLN
3	C	165	THR
3	C	167	TRP
3	C	175	LEU

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Mol	Chain	Res	Type
3	C	178	LEU
3	C	191	THR
3	C	195	VAL
3	C	196	LEU
3	C	204	LEU
4	D	8	VAL
4	D	15	GLU
4	D	19	LEU
4	D	25	ARG
4	D	33	MET
4	D	53	ASP
4	D	57	ARG
4	D	61	LYS
4	D	64	LEU
4	D	70	ILE
4	D	74	GLN
4	D	96	LEU
4	D	107	ARG
4	D	115	ARG
4	D	122	ARG
4	D	150	GLU
4	D	153	ARG
4	D	170	VAL
5	E	6	PHE
5	E	12	LEU
5	E	18	ARG
5	E	24	ARG
5	E	31	LEU
5	E	41	VAL
5	E	43	LEU
5	E	50	GLU
5	E	53	LEU
5	E	64	ARG
5	E	65	ASN
5	E	79	GLU
5	E	80	ILE
5	E	92	LYS
5	E	116	THR
5	E	117	ASP
5	E	145	LYS
5	E	150	ARG
5	E	151	LEU

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Mol	Chain	Res	Type
6	F	21	LEU
6	F	36	ARG
6	F	55	ASP
6	F	65	VAL
6	F	82	ARG
6	F	84	ASN
6	F	87	ARG
6	F	98	LEU
7	G	5	ARG
7	G	10	ARG
7	G	12	LEU
7	G	36	LYS
7	G	41	ARG
7	G	48	LYS
7	G	51	GLN
7	G	57	GLU
7	G	75	VAL
7	G	98	SER
7	G	114	ARG
7	G	124	LEU
7	G	149	ARG
7	G	156	TRP
8	H	18	ARG
8	H	21	LYS
8	H	23	SER
8	H	26	VAL
8	H	30	ARG
8	H	31	PHE
8	H	39	LEU
8	H	50	ARG
8	H	56	LYS
8	H	63	LEU
8	H	85	ARG
8	H	91	ARG
8	H	92	ARG
8	H	102	ARG
8	H	113	SER
8	H	133	LEU
9	I	16	ARG
9	I	65	VAL
9	I	71	SER
9	I	79	LEU

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Mol	Chain	Res	Type
9	I	86	VAL
9	I	97	LYS
9	I	102	LEU
9	I	112	LYS
9	I	118	LYS
9	I	121	ARG
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	85	LEU
10	J	90	LEU
10	J	95	GLU
11	K	11	LYS
11	K	18	ARG
11	K	24	SER
11	K	48	ILE
11	K	51	LYS
11	K	77	MET
11	K	84	VAL
11	K	91	ARG
11	K	119	CYS
11	K	122	LYS
12	L	20	LYS
12	L	28	LYS
12	L	33	ARG
12	L	36	VAL
12	L	39	VAL
12	L	53	ARG
12	L	60	LEU
12	L	67	THR
12	L	93	LEU
12	L	116	SER
12	L	126	LYS
13	M	16	ASP
13	M	44	ARG
13	M	56	LEU
13	M	64	TRP
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	9	LYS
14	N	23	ARG
14	N	29	ARG
14	N	31	ARG
15	O	5	LYS
15	O	14	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	48	LYS
15	O	57	LEU
15	O	70	LEU
15	O	81	LEU
15	O	88	ARG
16	P	2	VAL
16	P	8	ARG
16	P	27	LYS
16	P	31	LYS
16	P	42	ARG
16	P	54	GLU
16	P	55	ARG
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	96	GLN
17	Q	97	SER
17	Q	98	LEU
17	Q	99	SER
17	Q	101	ARG
18	R	46	GLU
18	R	85	LEU

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Mol	Chain	Res	Type
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	33	THR
19	S	36	ARG
19	S	39	THR
19	S	58	VAL
19	S	61	TYR
19	S	65	ASN
19	S	81	ARG
20	T	8	ARG
20	T	15	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	93	GLU
21	U	8	THR
21	U	15	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	6	HIS
3	C	108	ASN
4	D	42	GLN
6	F	73	ASN
17	Q	96	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1507/1522 (99%)	256 (16%)	35 (2%)

All (256) 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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
1	A	1038	C
1	A	1042	G
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
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

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Mol	Chain	Res	Type
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
1	A	1397	C
1	A	1398	A
1	A	1400	5MC
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	1499	A
1	A	1502	A
1	A	1504	G

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Mol	Chain	Res	Type
1	A	1505	G
1	A	1506	U
1	A	1507	A
1	A	1517	G
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
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

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Mol	Chain	Res	Type
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
1	MA6	A	1518	1	19,26,27	0.97	1 (5%)	18,38,41	0.84	1 (5%)
12	0TD	L	92	12	4,9,10	1.06	0	3,11,13	3.85	1 (33%)
1	UR3	A	1498	1	14,22,23	0.77	0	15,32,35	1.07	1 (6%)
1	7MG	A	527	1,23	22,26,27	2.40	6 (27%)	28,39,42	1.58	5 (17%)
1	MA6	A	1519	1	19,26,27	0.71	0	18,38,41	1.01	1 (5%)
1	2MG	A	1207	1	19,26,27	2.39	3 (15%)	21,38,41	2.04	3 (14%)
1	5MC	A	1407	1	15,22,23	0.92	0	19,32,35	0.98	1 (5%)
1	5MC	A	1404	1	15,22,23	1.13	2 (13%)	19,32,35	1.07	2 (10%)
1	5MC	A	1400	1	15,22,23	1.13	1 (6%)	19,32,35	0.92	0
1	PSU	A	516	1,23	17,21,22	1.05	2 (11%)	20,30,33	2.99	6 (30%)
1	PSU	A	1541	1,23	17,21,22	1.06	2 (11%)	20,30,33	3.13	6 (30%)
1	5MC	A	967	1	15,22,23	0.88	1 (6%)	19,32,35	1.01	0
1	PSU	A	1540	1	17,21,22	1.01	1 (5%)	20,30,33	3.10	5 (25%)
1	4OC	A	1402	1	16,23,24	0.99	1 (6%)	17,32,35	0.68	0
1	M2G	A	966	1	20,27,28	1.52	3 (15%)	22,40,43	2.29	2 (9%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

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

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1207	2MG	C2-N2	8.06	1.40	1.34
1	A	527	7MG	C4-N3	7.16	1.43	1.34
1	A	1207	2MG	C6-N1	5.49	1.42	1.33
1	A	966	M2G	C6-N1	5.13	1.42	1.33
1	A	527	7MG	C2-N2	4.86	1.43	1.33
1	A	527	7MG	C8-N9	-4.81	1.34	1.45
1	A	1541	PSU	C4-N3	3.31	1.38	1.33
1	A	527	7MG	C6-N1	3.30	1.38	1.33
1	A	1540	PSU	C4-N3	3.21	1.38	1.33
1	A	966	M2G	C2-N2	2.92	1.39	1.34
1	A	1404	5MC	C2-N3	2.90	1.43	1.38
1	A	527	7MG	CM7-N7	-2.63	1.41	1.46
1	A	1400	5MC	C5-C4	2.50	1.45	1.41
1	A	516	PSU	C4-N3	2.49	1.37	1.33
1	A	1518	MA6	C6-N1	2.49	1.36	1.33
1	A	1207	2MG	C2-N1	2.47	1.42	1.34
1	A	516	PSU	C5-C1'	-2.20	1.50	1.52
1	A	1402	4OC	C4-N4	2.16	1.40	1.36
1	A	527	7MG	C6-C5	2.09	1.44	1.41
1	A	1541	PSU	O4'-C1'	-2.08	1.41	1.44
1	A	1404	5MC	C4-N4	2.06	1.39	1.34
1	A	966	M2G	C2-N1	2.03	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	967	5MC	C4-N4	2.02	1.39	1.34

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1540	PSU	N1-C2-N3	-10.91	119.76	128.43
1	A	1541	PSU	N1-C2-N3	-10.78	119.86	128.43
1	A	516	PSU	N1-C2-N3	-9.54	120.85	128.43
1	A	966	M2G	C5-C6-N1	-8.21	112.21	123.43
1	A	1207	2MG	C5-C6-N1	-7.55	113.11	123.43
12	L	92	0TD	CSB-SB-CB	-6.45	89.17	101.85
1	A	516	PSU	C4-N3-C2	5.88	120.10	115.14
1	A	1541	PSU	C4-N3-C2	5.82	120.06	115.14
1	A	1540	PSU	C4-N3-C2	5.70	119.96	115.14
1	A	966	M2G	C6-N1-C2	5.56	122.80	116.18
1	A	516	PSU	C5-C4-N3	-4.79	119.19	125.36
1	A	527	7MG	N3-C4-N9	4.34	132.48	126.91
1	A	1541	PSU	C5-C4-N3	-4.24	119.90	125.36
1	A	1540	PSU	C5-C4-N3	-3.87	120.38	125.36
1	A	1207	2MG	C6-N1-C2	3.57	121.57	115.18
1	A	527	7MG	C5-C4-N3	-3.37	120.99	126.49
1	A	516	PSU	C5-C6-N1	-3.36	120.31	124.44
1	A	1541	PSU	C6-N1-C2	3.09	120.46	115.36
1	A	1540	PSU	C6-N1-C2	3.07	120.43	115.36
1	A	1404	5MC	CM5-C5-C4	-3.06	118.62	121.72
1	A	527	7MG	N7-C8-N9	2.96	107.61	103.38
1	A	1541	PSU	C5-C6-N1	-2.92	120.85	124.44
1	A	527	7MG	C6-N1-C2	2.66	120.15	115.93
1	A	516	PSU	C6-N1-C2	2.58	119.61	115.36
1	A	1540	PSU	C5-C6-N1	-2.55	121.30	124.44
1	A	1519	MA6	N1-C6-N6	-2.46	114.47	117.06
1	A	1498	UR3	C3'-C2'-C1'	2.36	104.53	100.98
1	A	1518	MA6	C1'-N9-C4	-2.17	122.82	126.64
1	A	527	7MG	N1-C2-N3	-2.14	122.06	125.42
1	A	1407	5MC	CM5-C5-C6	2.14	123.19	118.68
1	A	1207	2MG	C4-C5-N7	2.13	111.62	109.40
1	A	1404	5MC	CM5-C5-C6	2.10	123.10	118.68
1	A	516	PSU	O4'-C1'-C2'	2.05	107.99	104.66
1	A	1541	PSU	O4'-C1'-C2'	2.00	107.91	104.66

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	L	92	0TD	CG-CB-SB-CSB
1	A	527	7MG	O4'-C4'-C5'-O5'
1	A	527	7MG	C3'-C4'-C5'-O5'
1	A	1400	5MC	O4'-C4'-C5'-O5'
1	A	967	5MC	O4'-C4'-C5'-O5'
1	A	1400	5MC	C3'-C4'-C5'-O5'
1	A	1402	4OC	O4'-C4'-C5'-O5'
1	A	967	5MC	C3'-C4'-C5'-O5'
1	A	1402	4OC	C3'-C4'-C5'-O5'
1	A	1519	MA6	C4'-C5'-O5'-P
1	A	966	M2G	C4'-C5'-O5'-P
1	A	1541	PSU	O4'-C1'-C5-C4

There are no ring outliers.

8 monomers are involved in 16 short contacts:

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

5.5 Carbohydrates [i](#)

There are no monosaccharides 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	1617	-	45,45,45	1.38	6 (13%)	64,67,67	1.63	12 (18%)
22	PAR	A	1607	-	45,45,45	1.35	5 (11%)	64,67,67	1.62	13 (20%)
22	PAR	A	1606	-	45,45,45	1.30	6 (13%)	64,67,67	1.60	17 (26%)
22	PAR	A	1604	-	45,45,45	1.25	3 (6%)	64,67,67	1.62	13 (20%)
22	PAR	A	1603	-	45,45,45	1.36	4 (8%)	64,67,67	1.57	10 (15%)
22	PAR	A	1614	-	45,45,45	1.56	10 (22%)	64,67,67	1.67	13 (20%)
22	PAR	A	1609	-	45,45,45	1.24	6 (13%)	64,67,67	1.57	13 (20%)
22	PAR	A	1615	-	45,45,45	1.57	8 (17%)	64,67,67	1.63	13 (20%)
22	PAR	A	1610	-	45,45,45	1.61	8 (17%)	64,67,67	1.69	12 (18%)
22	PAR	A	1611	-	45,45,45	1.94	11 (24%)	64,67,67	1.63	10 (15%)
22	PAR	A	1616	-	45,45,45	1.41	6 (13%)	64,67,67	1.63	12 (18%)
22	PAR	A	1601	-	45,45,45	1.10	5 (11%)	64,67,67	1.51	12 (18%)
22	PAR	A	1608	-	45,45,45	1.22	4 (8%)	64,67,67	1.66	13 (20%)
22	PAR	A	1612	-	45,45,45	1.67	8 (17%)	64,67,67	1.72	12 (18%)
22	PAR	A	1602	-	45,45,45	1.13	4 (8%)	64,67,67	1.72	13 (20%)
22	PAR	A	1605	-	45,45,45	1.28	4 (8%)	64,67,67	1.67	12 (18%)
22	PAR	A	1613	-	45,45,45	1.70	10 (22%)	64,67,67	1.66	13 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	PAR	A	1617	-	-	3/18/94/94	1/4/4/4
22	PAR	A	1607	-	-	4/18/94/94	0/4/4/4
22	PAR	A	1606	-	-	7/18/94/94	0/4/4/4
22	PAR	A	1604	-	-	6/18/94/94	0/4/4/4
22	PAR	A	1603	-	-	3/18/94/94	0/4/4/4
22	PAR	A	1614	-	-	6/18/94/94	0/4/4/4
22	PAR	A	1609	-	-	2/18/94/94	0/4/4/4
22	PAR	A	1615	-	-	11/18/94/94	1/4/4/4
22	PAR	A	1610	-	-	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	-	-	5/18/94/94	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	PAR	A	1608	-	-	8/18/94/94	0/4/4/4
22	PAR	A	1612	-	-	8/18/94/94	0/4/4/4
22	PAR	A	1602	-	-	7/18/94/94	0/4/4/4
22	PAR	A	1605	-	-	3/18/94/94	0/4/4/4
22	PAR	A	1613	-	-	11/18/94/94	0/4/4/4

All (108) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	1611	PAR	C13-C23	5.16	1.59	1.52
22	A	1611	PAR	C52-C42	4.86	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	C64-C54	4.50	1.58	1.52
22	A	1612	PAR	C14-C24	4.34	1.60	1.52
22	A	1614	PAR	C13-C23	4.26	1.58	1.52
22	A	1612	PAR	O43-C13	4.24	1.49	1.41
22	A	1604	PAR	C52-C42	4.17	1.60	1.52
22	A	1610	PAR	C34-C24	4.16	1.58	1.53
22	A	1613	PAR	C13-C23	4.13	1.58	1.52
22	A	1617	PAR	O43-C13	4.08	1.49	1.41
22	A	1613	PAR	C31-C21	3.74	1.58	1.53
22	A	1605	PAR	C64-C54	3.61	1.57	1.52
22	A	1613	PAR	C52-C42	3.60	1.59	1.52
22	A	1607	PAR	O43-C13	3.57	1.48	1.41
22	A	1607	PAR	C64-C54	3.56	1.56	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	1610	PAR	C52-C42	3.52	1.59	1.52
22	A	1612	PAR	C34-C24	3.50	1.57	1.53
22	A	1611	PAR	C14-C24	3.41	1.59	1.52
22	A	1613	PAR	C34-C24	3.38	1.57	1.53
22	A	1607	PAR	C13-C23	3.36	1.57	1.52
22	A	1615	PAR	C52-C42	3.33	1.59	1.52
22	A	1615	PAR	C64-C54	3.30	1.56	1.52
22	A	1610	PAR	C14-C24	3.30	1.58	1.52
22	A	1616	PAR	O43-C13	3.29	1.47	1.41
22	A	1602	PAR	C64-C54	3.29	1.56	1.52
22	A	1614	PAR	C64-C54	3.27	1.56	1.52
22	A	1611	PAR	C64-C54	3.26	1.56	1.52
22	A	1603	PAR	C52-C42	3.26	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	1612	PAR	C52-C42	3.22	1.58	1.52
22	A	1617	PAR	C52-C42	3.19	1.58	1.52
22	A	1614	PAR	C14-C24	3.18	1.58	1.52
22	A	1614	PAR	C52-C42	3.17	1.58	1.52
22	A	1610	PAR	O43-C13	3.17	1.47	1.41
22	A	1609	PAR	C64-C54	3.16	1.56	1.52
22	A	1612	PAR	C13-C23	3.15	1.56	1.52
22	A	1606	PAR	C52-C42	3.11	1.58	1.52
22	A	1617	PAR	C34-C24	3.07	1.57	1.53
22	A	1604	PAR	C64-C54	3.05	1.56	1.52
22	A	1611	PAR	C62-C52	3.05	1.60	1.52
22	A	1611	PAR	C34-C24	3.05	1.57	1.53
22	A	1616	PAR	C52-C42	3.04	1.58	1.52
22	A	1606	PAR	C64-C54	3.03	1.56	1.52
22	A	1616	PAR	C31-C21	3.01	1.57	1.53
22	A	1611	PAR	O33-C14	3.00	1.50	1.41
22	A	1601	PAR	C64-C54	3.00	1.56	1.52
22	A	1608	PAR	C64-C54	2.98	1.56	1.52
22	A	1615	PAR	C13-C23	2.97	1.56	1.52
22	A	1613	PAR	C62-C52	2.97	1.60	1.52
22	A	1605	PAR	C13-C23	2.94	1.56	1.52
22	A	1613	PAR	C64-C54	2.92	1.56	1.52
22	A	1615	PAR	C14-C24	2.92	1.58	1.52
22	A	1617	PAR	C64-C54	2.88	1.56	1.52
22	A	1606	PAR	C31-C21	2.85	1.57	1.53
22	A	1616	PAR	C64-C54	2.83	1.55	1.52
22	A	1613	PAR	C14-C24	2.83	1.57	1.52
22	A	1608	PAR	O43-C13	2.79	1.46	1.41
22	A	1608	PAR	C34-C24	2.78	1.57	1.53
22	A	1603	PAR	C64-C54	2.76	1.55	1.52
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	1610	PAR	C64-C54	2.69	1.55	1.52
22	A	1609	PAR	C52-C42	2.68	1.57	1.52
22	A	1606	PAR	O43-C13	2.67	1.46	1.41
22	A	1611	PAR	O52-C52	2.67	1.50	1.43
22	A	1610	PAR	O33-C14	2.66	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	2.58	1.57	1.52
22	A	1616	PAR	C13-C23	2.54	1.56	1.52
22	A	1601	PAR	C52-C42	2.50	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	1609	PAR	C33-C43	2.49	1.59	1.52
22	A	1614	PAR	C33-C43	2.46	1.59	1.52
22	A	1602	PAR	C11-C21	2.44	1.57	1.52
22	A	1609	PAR	C31-C21	2.43	1.56	1.53
22	A	1607	PAR	C52-C42	2.42	1.57	1.52
22	A	1612	PAR	O33-C14	2.39	1.48	1.41
22	A	1613	PAR	O43-C13	2.38	1.45	1.41
22	A	1616	PAR	O33-C14	2.34	1.48	1.41
22	A	1606	PAR	C33-C43	2.34	1.59	1.52
22	A	1615	PAR	C33-C43	2.33	1.59	1.52
22	A	1604	PAR	C33-C43	2.31	1.59	1.52
22	A	1602	PAR	O43-C13	2.28	1.45	1.41
22	A	1614	PAR	C31-C21	2.27	1.56	1.53
22	A	1614	PAR	C62-C52	2.27	1.58	1.52
22	A	1601	PAR	C33-C43	2.24	1.58	1.52
22	A	1611	PAR	C22-C12	-2.24	1.48	1.53
22	A	1602	PAR	C33-C43	2.23	1.58	1.52
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	1610	PAR	C44-C54	2.19	1.57	1.53
22	A	1608	PAR	C13-C23	2.18	1.55	1.52
22	A	1611	PAR	O33-C33	2.18	1.49	1.43
22	A	1615	PAR	O52-C52	2.12	1.49	1.43
22	A	1614	PAR	O52-C52	2.12	1.49	1.43
22	A	1603	PAR	O43-C13	2.11	1.45	1.41
22	A	1605	PAR	O43-C13	2.10	1.45	1.41
22	A	1609	PAR	C13-C23	2.10	1.55	1.52
22	A	1612	PAR	C41-C51	2.08	1.57	1.53
22	A	1613	PAR	C11-C21	2.07	1.56	1.52
22	A	1613	PAR	O11-C42	2.06	1.49	1.43
22	A	1614	PAR	C34-C24	2.04	1.56	1.53
22	A	1615	PAR	O43-C13	2.02	1.45	1.41
22	A	1601	PAR	C14-C24	2.02	1.56	1.52
22	A	1614	PAR	C11-C21	2.00	1.56	1.52

All (213) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1612	PAR	O33-C14-C24	7.38	120.94	108.22
22	A	1610	PAR	O33-C14-C24	7.07	120.40	108.22
22	A	1602	PAR	O33-C14-C24	6.82	119.96	108.22
22	A	1611	PAR	O33-C14-C24	6.53	119.46	108.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1605	PAR	O33-C14-C24	6.49	119.40	108.22
22	A	1616	PAR	O33-C14-C24	6.48	119.38	108.22
22	A	1617	PAR	O33-C14-C24	6.43	119.29	108.22
22	A	1608	PAR	O33-C14-C24	6.42	119.28	108.22
22	A	1613	PAR	O33-C14-C24	6.18	118.86	108.22
22	A	1614	PAR	O33-C14-C24	6.11	118.73	108.22
22	A	1607	PAR	O33-C14-C24	6.05	118.64	108.22
22	A	1615	PAR	O33-C14-C24	5.96	118.47	108.22
22	A	1604	PAR	O33-C14-C24	5.62	117.89	108.22
22	A	1606	PAR	O33-C14-C24	5.37	117.46	108.22
22	A	1601	PAR	O33-C14-C24	5.24	117.25	108.22
22	A	1603	PAR	O33-C14-C24	5.16	117.11	108.22
22	A	1609	PAR	O33-C14-C24	5.04	116.90	108.22
22	A	1602	PAR	O43-C13-C23	-3.91	99.94	104.98
22	A	1606	PAR	O52-C13-C23	3.86	115.95	107.96
22	A	1602	PAR	O52-C13-O43	-3.83	107.29	111.43
22	A	1613	PAR	C13-C23-C33	3.82	106.69	102.10
22	A	1609	PAR	O52-C13-C23	3.76	115.74	107.96
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	1614	PAR	O52-C13-C23	3.59	115.39	107.96
22	A	1611	PAR	C13-C23-C33	3.57	106.39	102.10
22	A	1603	PAR	O52-C13-C23	3.56	115.34	107.96
22	A	1615	PAR	O52-C13-C23	3.56	115.33	107.96
22	A	1611	PAR	O52-C13-C23	3.47	115.15	107.96
22	A	1602	PAR	O34-C34-C44	-3.41	102.46	110.35
22	A	1617	PAR	C14-O33-C33	-3.34	109.69	117.96
22	A	1601	PAR	O52-C13-C23	3.28	114.76	107.96
22	A	1605	PAR	C14-O33-C33	-3.27	109.87	117.96
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
22	A	1606	PAR	C34-C24-N24	-3.23	104.43	111.05
22	A	1608	PAR	O52-C13-C23	3.21	114.62	107.96
22	A	1612	PAR	O34-C34-C44	-3.21	102.93	110.35
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	1610	PAR	O52-C13-C23	3.14	114.47	107.96
22	A	1611	PAR	C34-C24-N24	-3.13	104.65	111.05
22	A	1609	PAR	O34-C34-C44	-3.10	103.18	110.35
22	A	1604	PAR	O52-C13-C23	3.09	114.37	107.96
22	A	1616	PAR	O52-C13-C23	3.09	114.37	107.96
22	A	1603	PAR	O34-C34-C44	-3.07	103.25	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1605	PAR	O52-C13-C23	3.07	114.32	107.96
22	A	1601	PAR	O34-C34-C44	-3.06	103.27	110.35
22	A	1613	PAR	O52-C13-O43	-3.05	108.13	111.43
22	A	1616	PAR	C14-O33-C33	-3.02	110.49	117.96
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	C34-C24-N24	-3.01	104.89	111.05
22	A	1607	PAR	O34-C34-C44	-3.00	103.41	110.35
22	A	1613	PAR	C14-O33-C33	-3.00	110.54	117.96
22	A	1604	PAR	C34-C24-N24	-3.00	104.91	111.05
22	A	1614	PAR	O11-C11-O51	2.98	119.01	110.67
22	A	1607	PAR	C14-O33-C33	-2.98	110.59	117.96
22	A	1607	PAR	C34-C24-N24	-2.98	104.95	111.05
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	1608	PAR	O34-C34-C44	-2.96	103.50	110.35
22	A	1617	PAR	C34-C24-N24	-2.95	105.00	111.05
22	A	1617	PAR	O34-C34-C44	-2.94	103.56	110.35
22	A	1606	PAR	O11-C11-O51	2.94	118.88	110.67
22	A	1605	PAR	O34-C34-C44	-2.93	103.57	110.35
22	A	1607	PAR	O52-C13-C23	2.91	114.00	107.96
22	A	1616	PAR	C34-C24-N24	-2.91	105.09	111.05
22	A	1612	PAR	O52-C13-O43	-2.91	108.28	111.43
22	A	1605	PAR	O54-C54-C44	2.90	114.96	109.69
22	A	1615	PAR	O11-C11-O51	2.89	118.75	110.67
22	A	1610	PAR	O52-C13-O43	-2.88	108.31	111.43
22	A	1604	PAR	O34-C34-C44	-2.86	103.74	110.35
22	A	1613	PAR	O52-C13-C23	2.86	113.88	107.96
22	A	1603	PAR	C13-O52-C52	-2.84	110.93	117.96
22	A	1611	PAR	O11-C11-O51	2.84	118.61	110.67
22	A	1612	PAR	O52-C13-C23	2.84	113.85	107.96
22	A	1608	PAR	O52-C13-O43	-2.84	108.36	111.43
22	A	1612	PAR	O54-C54-C44	2.84	114.85	109.69
22	A	1616	PAR	O11-C11-O51	2.83	118.58	110.67
22	A	1611	PAR	O34-C34-C44	-2.82	103.84	110.35
22	A	1615	PAR	C34-C24-N24	-2.81	105.30	111.05
22	A	1602	PAR	C14-O33-C33	-2.81	111.02	117.96
22	A	1616	PAR	O34-C34-C44	-2.80	103.88	110.35
22	A	1613	PAR	O11-C11-O51	2.79	118.47	110.67
22	A	1613	PAR	O34-C34-C44	-2.79	103.90	110.35
22	A	1615	PAR	C13-C23-C33	2.77	105.44	102.10
22	A	1614	PAR	O34-C34-C44	-2.75	103.98	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1609	PAR	C13-O52-C52	-2.74	111.17	117.96
22	A	1607	PAR	O51-C51-C61	2.72	113.21	106.44
22	A	1604	PAR	O11-C11-O51	2.71	118.24	110.67
22	A	1617	PAR	O52-C13-C23	2.71	113.57	107.96
22	A	1604	PAR	C13-C23-C33	2.71	105.36	102.10
22	A	1615	PAR	O34-C34-C44	-2.71	104.09	110.35
22	A	1617	PAR	O11-C11-O51	2.70	118.22	110.67
22	A	1612	PAR	O11-C11-O51	2.70	118.22	110.67
22	A	1603	PAR	O11-C11-O51	2.69	118.20	110.67
22	A	1616	PAR	O54-C54-C44	2.69	114.58	109.69
22	A	1609	PAR	O11-C11-O51	2.68	118.15	110.67
22	A	1613	PAR	O11-C42-C52	2.66	114.25	107.48
22	A	1602	PAR	C34-C24-N24	-2.66	105.61	111.05
22	A	1608	PAR	C22-C12-C62	2.65	114.04	110.04
22	A	1612	PAR	C14-O33-C33	-2.64	111.42	117.96
22	A	1608	PAR	C14-O33-C33	-2.63	111.45	117.96
22	A	1610	PAR	O11-C11-O51	2.62	118.00	110.67
22	A	1610	PAR	O34-C34-C44	-2.62	104.30	110.35
22	A	1606	PAR	O34-C34-C44	-2.61	104.31	110.35
22	A	1607	PAR	O11-C11-O51	2.61	117.96	110.67
22	A	1615	PAR	C14-O33-C33	-2.60	111.52	117.96
22	A	1604	PAR	O54-C54-C44	2.60	114.42	109.69
22	A	1611	PAR	C14-O33-C33	-2.60	111.54	117.96
22	A	1601	PAR	O11-C11-O51	2.58	117.87	110.67
22	A	1616	PAR	O52-C13-O43	-2.57	108.65	111.43
22	A	1607	PAR	O52-C13-O43	-2.57	108.65	111.43
22	A	1604	PAR	C13-O52-C52	-2.57	111.62	117.96
22	A	1605	PAR	O11-C11-O51	2.56	117.82	110.67
22	A	1610	PAR	O51-C51-C61	2.55	112.78	106.44
22	A	1608	PAR	C13-C23-C33	2.55	105.17	102.10
22	A	1604	PAR	O11-C11-C21	-2.55	103.83	108.22
22	A	1606	PAR	C13-O52-C52	-2.54	111.67	117.96
22	A	1606	PAR	O43-C13-C23	-2.53	101.72	104.98
22	A	1614	PAR	C14-O33-C33	-2.52	111.72	117.96
22	A	1616	PAR	O51-C51-C61	2.52	112.70	106.44
22	A	1604	PAR	O52-C13-O43	-2.52	108.70	111.43
22	A	1615	PAR	C13-O52-C52	-2.52	111.74	117.96
22	A	1614	PAR	C11-O51-C51	2.50	118.60	113.69
22	A	1607	PAR	C22-C12-C62	2.50	113.81	110.04
22	A	1606	PAR	C31-C41-C51	2.49	114.69	110.24
22	A	1610	PAR	C14-O33-C33	-2.49	111.80	117.96
22	A	1614	PAR	C22-C12-C62	2.49	113.80	110.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1610	PAR	C11-O51-C51	2.47	118.54	113.69
22	A	1602	PAR	O11-C11-O51	2.46	117.55	110.67
22	A	1610	PAR	O54-C54-C44	2.46	114.16	109.69
22	A	1608	PAR	O11-C11-O51	2.46	117.55	110.67
22	A	1605	PAR	C13-O52-C52	-2.46	111.88	117.96
22	A	1601	PAR	C13-O52-C52	-2.45	111.89	117.96
22	A	1603	PAR	O52-C13-O43	-2.45	108.77	111.43
22	A	1609	PAR	O43-C13-C23	-2.44	101.83	104.98
22	A	1602	PAR	O34-C34-C24	-2.44	105.84	110.22
22	A	1613	PAR	O52-C52-C42	2.43	113.65	107.48
22	A	1605	PAR	O52-C13-O43	-2.42	108.81	111.43
22	A	1609	PAR	C14-O33-C33	-2.42	111.98	117.96
22	A	1613	PAR	C22-C12-C62	2.42	113.69	110.04
22	A	1612	PAR	C23-C33-C43	-2.41	98.96	103.22
22	A	1608	PAR	O51-C51-C61	2.40	112.40	106.44
22	A	1611	PAR	C11-O51-C51	2.40	118.39	113.69
22	A	1607	PAR	C13-C23-C33	2.38	104.96	102.10
22	A	1608	PAR	C13-O52-C52	-2.37	112.09	117.96
22	A	1605	PAR	O51-C51-C61	2.37	112.33	106.44
22	A	1616	PAR	C13-O52-C52	-2.37	112.11	117.96
22	A	1614	PAR	C13-O52-C52	-2.37	112.11	117.96
22	A	1604	PAR	C14-O33-C33	-2.36	112.12	117.96
22	A	1610	PAR	C13-O52-C52	-2.36	112.13	117.96
22	A	1613	PAR	O51-C51-C61	2.35	112.28	106.44
22	A	1601	PAR	C23-C33-C43	-2.34	99.07	103.22
22	A	1617	PAR	C22-C12-C62	2.34	113.57	110.04
22	A	1615	PAR	O51-C51-C61	2.33	112.23	106.44
22	A	1601	PAR	O43-C13-C23	-2.32	101.99	104.98
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	1611	PAR	O51-C51-C61	2.29	112.14	106.44
22	A	1606	PAR	C23-C33-C43	-2.29	99.17	103.22
22	A	1617	PAR	C13-O52-C52	-2.28	112.31	117.96
22	A	1617	PAR	O52-C13-O43	-2.28	108.96	111.43
22	A	1612	PAR	C11-O51-C51	2.27	118.14	113.69
22	A	1606	PAR	O11-C11-C21	-2.27	104.31	108.22
22	A	1609	PAR	C22-C12-C62	2.26	113.45	110.04
22	A	1617	PAR	O51-C51-C61	2.26	112.05	106.44
22	A	1601	PAR	O51-C51-C61	2.26	112.05	106.44
22	A	1610	PAR	C13-C23-C33	2.26	104.82	102.10
22	A	1617	PAR	O54-C54-C44	2.25	113.79	109.69
22	A	1614	PAR	O51-C51-C61	2.25	112.02	106.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1603	PAR	O51-C51-C61	2.24	112.00	106.44
22	A	1602	PAR	C23-C33-C43	-2.23	99.27	103.22
22	A	1602	PAR	O52-C13-C23	2.23	112.58	107.96
22	A	1617	PAR	C11-O51-C51	2.23	118.06	113.69
22	A	1604	PAR	O51-C51-C61	2.22	111.95	106.44
22	A	1606	PAR	O51-C51-C41	2.20	113.69	109.69
22	A	1601	PAR	C14-O33-C33	-2.20	112.53	117.96
22	A	1607	PAR	O54-C54-C44	2.19	113.68	109.69
22	A	1608	PAR	O54-C54-C44	2.19	113.67	109.69
22	A	1606	PAR	O54-C54-C44	2.18	113.66	109.69
22	A	1603	PAR	C14-O33-C33	-2.18	112.56	117.96
22	A	1607	PAR	C13-O52-C52	-2.16	112.62	117.96
22	A	1602	PAR	C11-O51-C51	2.16	117.92	113.69
22	A	1609	PAR	O51-C51-C61	2.16	111.80	106.44
22	A	1616	PAR	C22-C12-C62	2.15	113.28	110.04
22	A	1615	PAR	C22-C12-C62	2.15	113.28	110.04
22	A	1612	PAR	O51-C51-C61	2.14	111.76	106.44
22	A	1602	PAR	O51-C51-C61	2.14	111.76	106.44
22	A	1616	PAR	C13-C23-C33	2.12	104.66	102.10
22	A	1601	PAR	O33-C14-O54	-2.12	104.76	110.67
22	A	1606	PAR	O51-C51-C61	2.11	111.69	106.44
22	A	1607	PAR	C11-O51-C51	2.10	117.82	113.69
22	A	1615	PAR	O54-C54-C44	2.10	113.51	109.69
22	A	1609	PAR	O33-C14-O54	-2.10	104.82	110.67
22	A	1612	PAR	C13-O52-C52	-2.09	112.79	117.96
22	A	1606	PAR	O52-C13-O43	-2.09	109.17	111.43
22	A	1614	PAR	O52-C13-O43	-2.09	109.17	111.43
22	A	1602	PAR	O54-C54-C44	2.09	113.48	109.69
22	A	1606	PAR	C11-O51-C51	2.09	117.78	113.69
22	A	1608	PAR	C11-O51-C51	2.08	117.76	113.69
22	A	1609	PAR	O43-C43-C53	2.07	113.69	109.21
22	A	1609	PAR	C11-O51-C51	2.07	117.76	113.69
22	A	1615	PAR	O52-C13-O43	-2.07	109.19	111.43
22	A	1605	PAR	C22-C12-C62	2.06	113.14	110.04
22	A	1606	PAR	C22-C32-C42	2.05	114.72	109.53
22	A	1613	PAR	C13-O52-C52	-2.05	112.89	117.96
22	A	1604	PAR	C11-O51-C51	2.05	117.70	113.69
22	A	1614	PAR	O54-C54-C44	2.03	113.39	109.69
22	A	1615	PAR	O52-C52-C42	2.02	112.61	107.48
22	A	1606	PAR	C14-O33-C33	-2.02	112.97	117.96
22	A	1611	PAR	O54-C54-C44	2.01	113.34	109.69

There are no chirality outliers.

All (107) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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	1604	PAR	C23-C13-O52-C52
22	A	1604	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
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	1612	PAR	C23-C13-O52-C52
22	A	1612	PAR	C24-C14-O33-C33
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	1614	PAR	O43-C13-O52-C52
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	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	1605	PAR	O54-C54-C64-N64
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	1617	PAR	C44-C54-C64-N64
22	A	1613	PAR	C42-C52-O52-C13
22	A	1616	PAR	O51-C11-O11-C42
22	A	1612	PAR	O54-C14-O33-C33
22	A	1616	PAR	O54-C14-O33-C33
22	A	1614	PAR	O54-C14-O33-C33
22	A	1613	PAR	O54-C14-O33-C33
22	A	1608	PAR	O54-C14-O33-C33
22	A	1613	PAR	C52-C42-O11-C11
22	A	1608	PAR	O51-C11-O11-C42

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Mol	Chain	Res	Type	Atoms
22	A	1615	PAR	O43-C43-C53-O53
22	A	1602	PAR	C33-C43-C53-O53
22	A	1615	PAR	O51-C11-O11-C42
22	A	1606	PAR	O43-C43-C53-O53
22	A	1602	PAR	O43-C43-C53-O53
22	A	1613	PAR	C33-C43-C53-O53
22	A	1605	PAR	O54-C14-O33-C33
22	A	1613	PAR	O43-C43-C53-O53
22	A	1616	PAR	C33-C43-C53-O53
22	A	1616	PAR	O51-C51-C61-O61
22	A	1614	PAR	O51-C51-C61-O61
22	A	1606	PAR	O54-C14-O33-C33
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	1608	PAR	C42-C52-O52-C13
22	A	1615	PAR	O51-C51-C61-O61
22	A	1610	PAR	O51-C51-C61-O61
22	A	1614	PAR	C41-C51-C61-O61
22	A	1608	PAR	O51-C51-C61-O61
22	A	1603	PAR	O51-C11-O11-C42
22	A	1604	PAR	O54-C14-O33-C33
22	A	1604	PAR	C52-C42-O11-C11
22	A	1615	PAR	C41-C51-C61-O61
22	A	1612	PAR	O51-C51-C61-O61
22	A	1616	PAR	C41-C51-C61-O61
22	A	1601	PAR	O43-C43-C53-O53
22	A	1611	PAR	C62-C52-O52-C13
22	A	1615	PAR	O43-C13-O52-C52
22	A	1612	PAR	O43-C13-O52-C52
22	A	1613	PAR	O43-C13-O52-C52
22	A	1611	PAR	C42-C52-O52-C13
22	A	1605	PAR	C41-C51-C61-O61
22	A	1601	PAR	O54-C14-O33-C33
22	A	1610	PAR	O54-C14-O33-C33
22	A	1608	PAR	C62-C52-O52-C13
22	A	1617	PAR	O54-C14-O33-C33
22	A	1603	PAR	O43-C43-C53-O53
22	A	1606	PAR	C52-C42-O11-C11
22	A	1608	PAR	O43-C13-O52-C52
22	A	1611	PAR	C23-C13-O52-C52
22	A	1608	PAR	C23-C13-O52-C52

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

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:

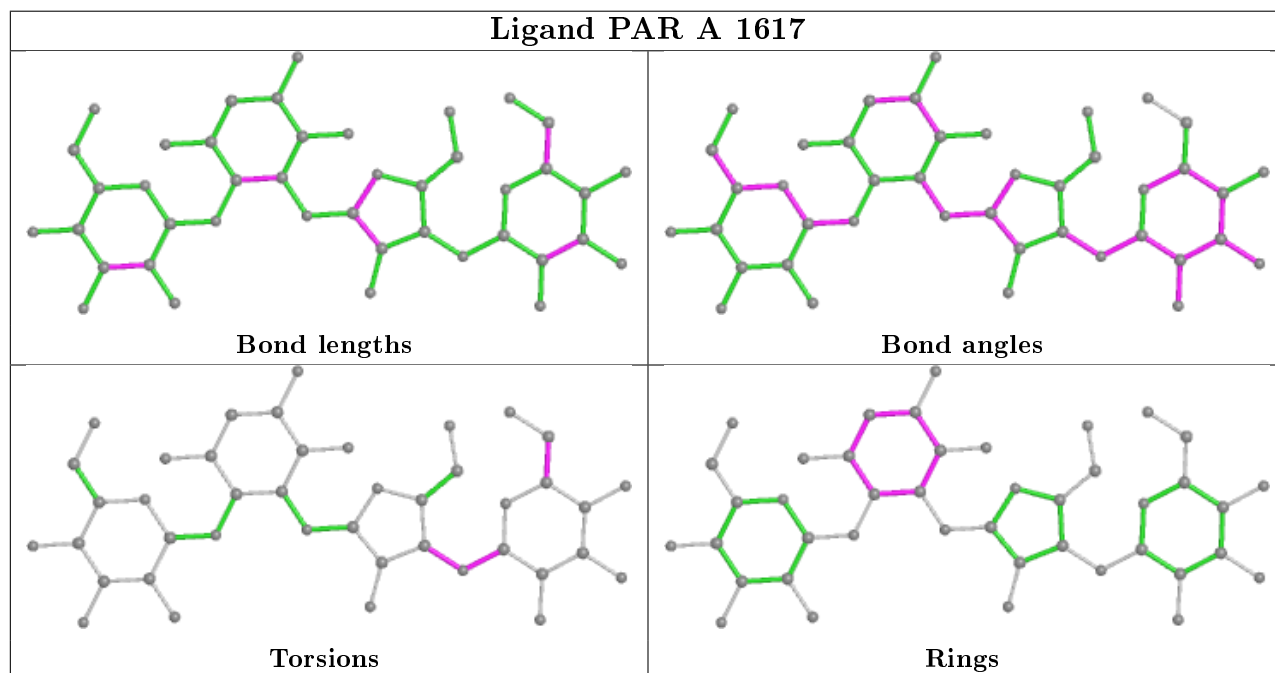
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	1617	PAR	2	0
22	A	1607	PAR	2	0
22	A	1606	PAR	2	0
22	A	1604	PAR	3	0
22	A	1614	PAR	3	0
22	A	1609	PAR	1	0
22	A	1615	PAR	1	0
22	A	1610	PAR	3	0

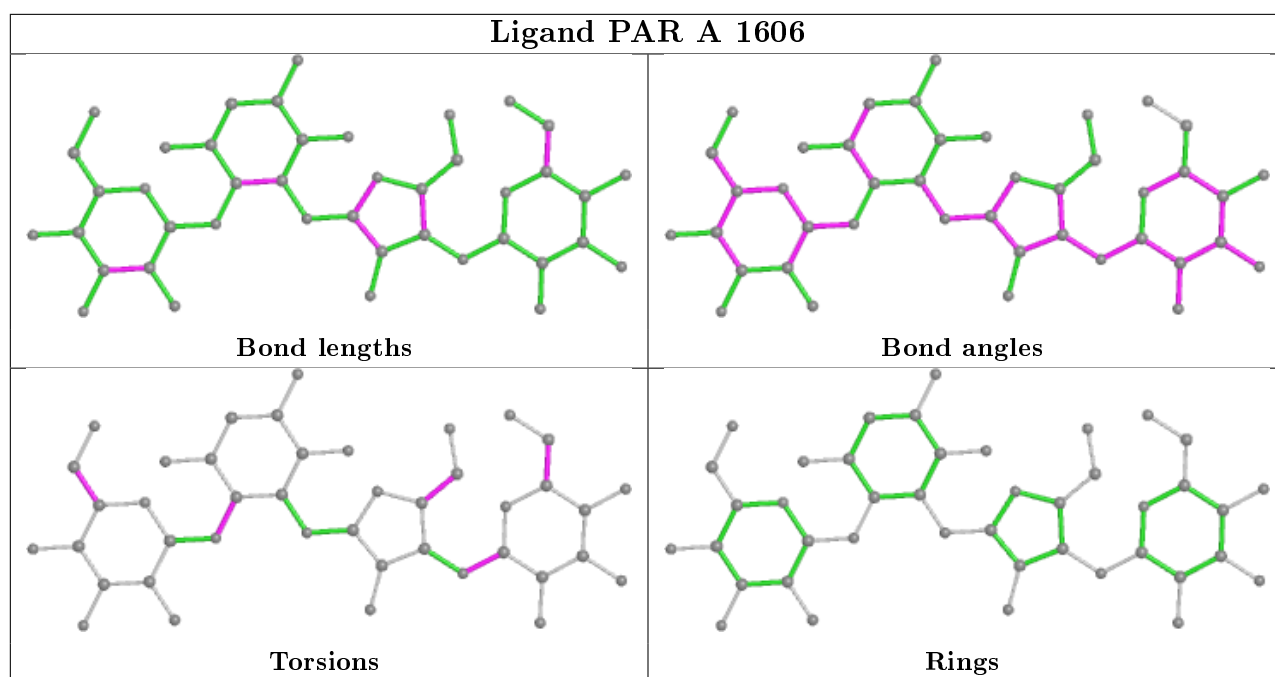
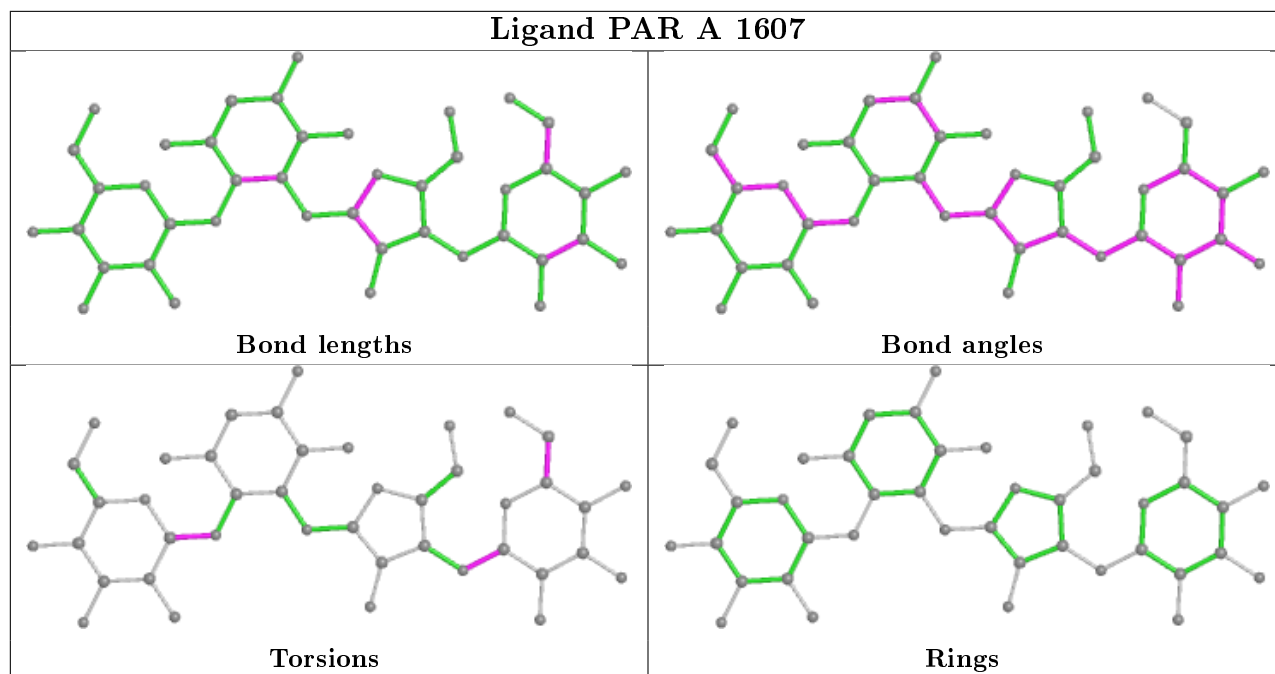
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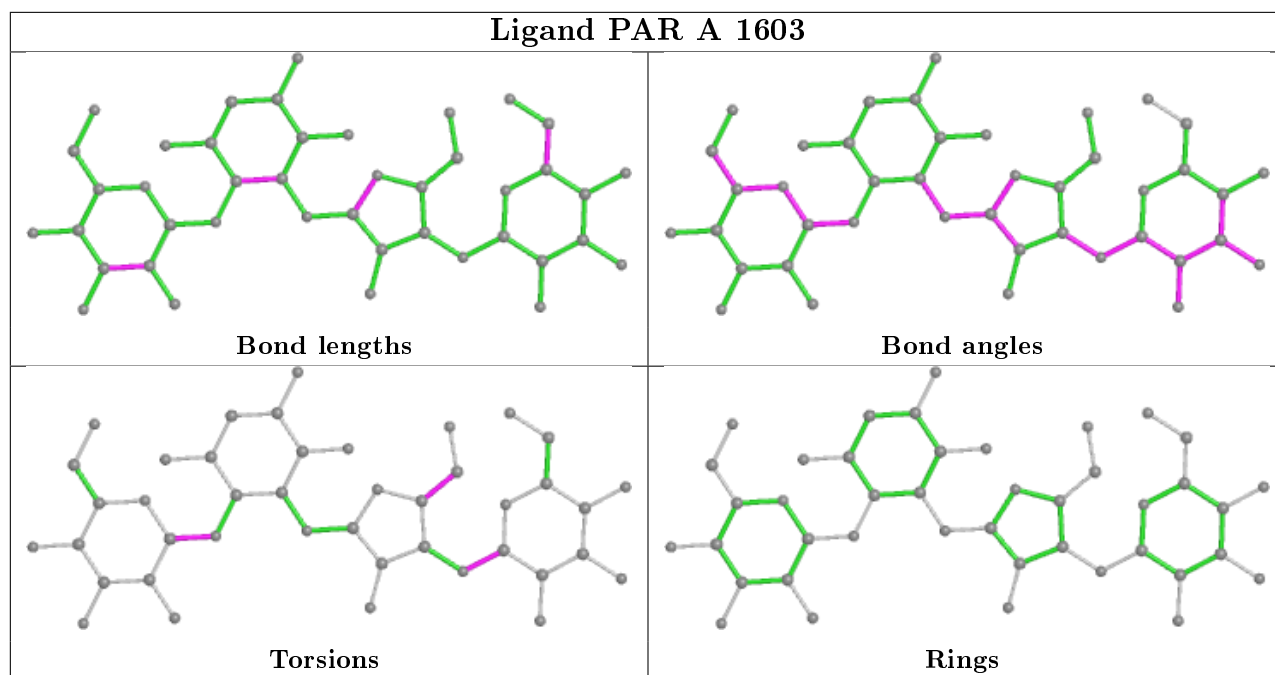
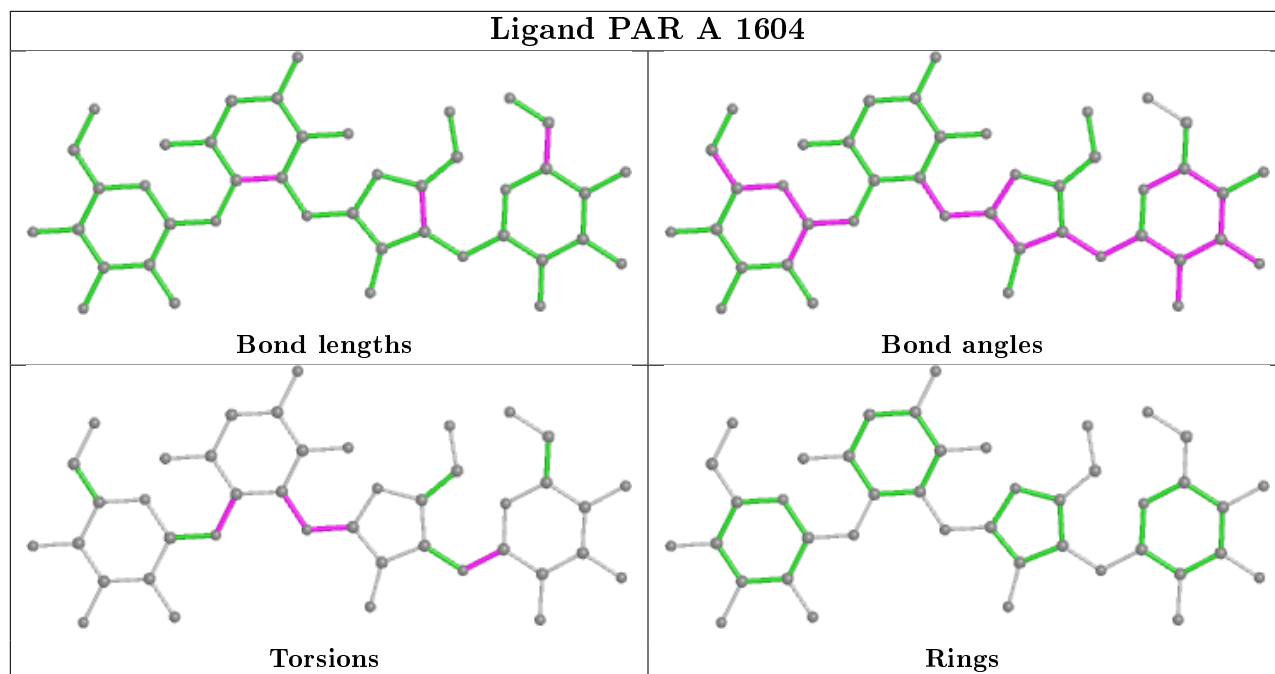
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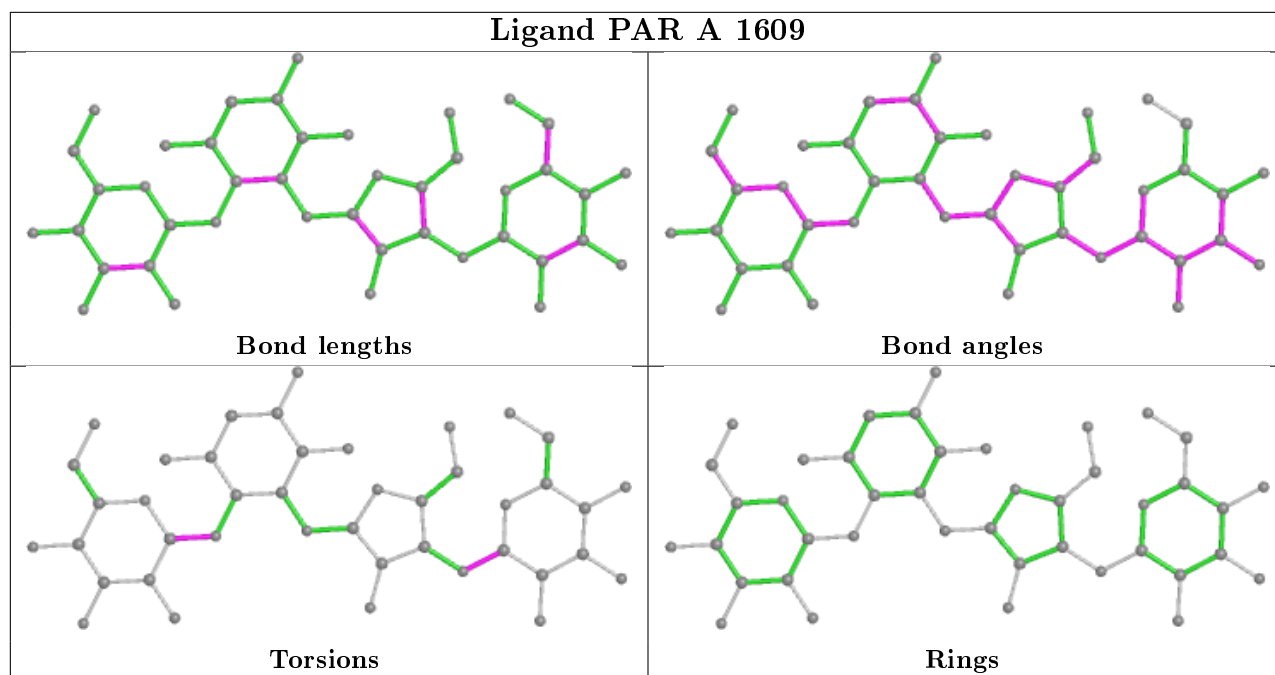
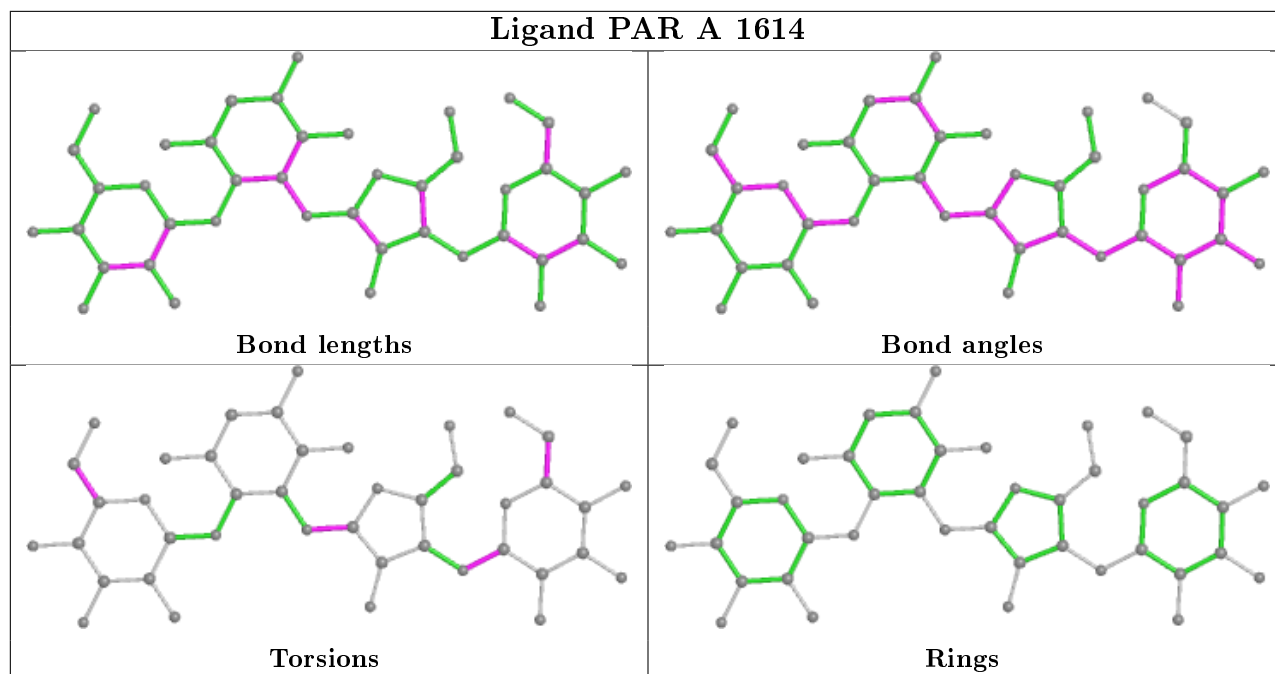
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	1611	PAR	1	0
22	A	1616	PAR	3	0
22	A	1601	PAR	1	0
22	A	1608	PAR	1	0
22	A	1612	PAR	4	0
22	A	1602	PAR	1	0
22	A	1613	PAR	6	0

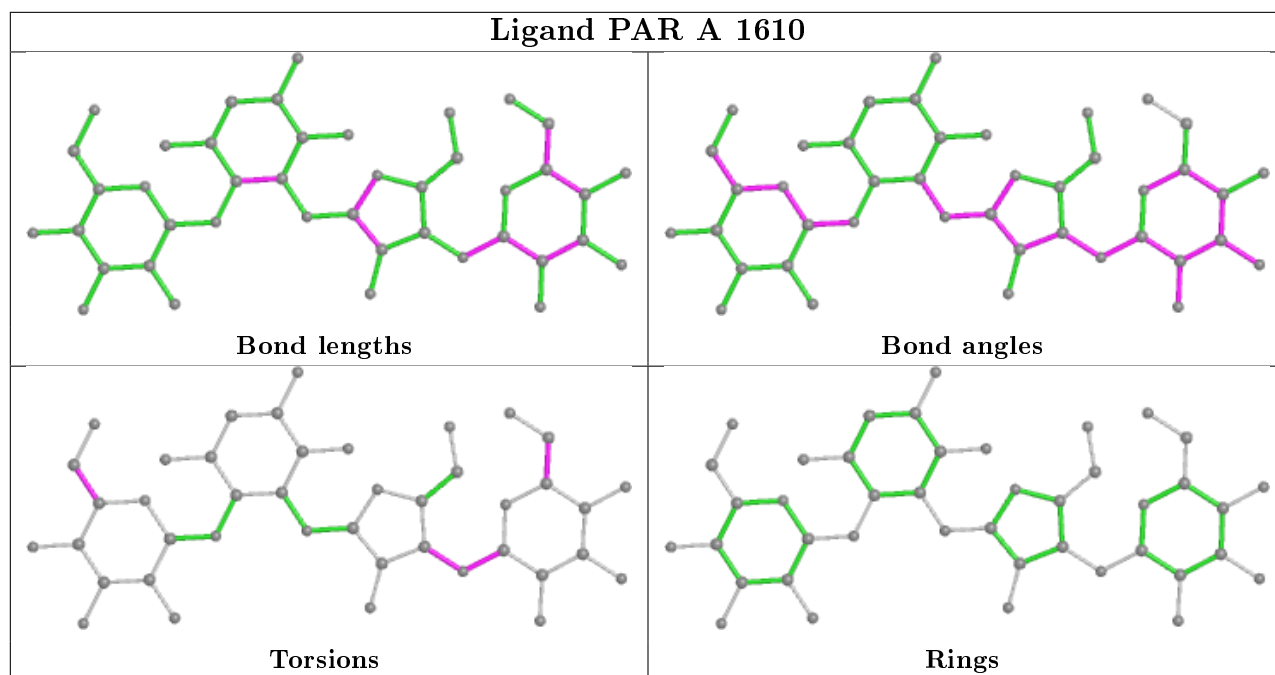
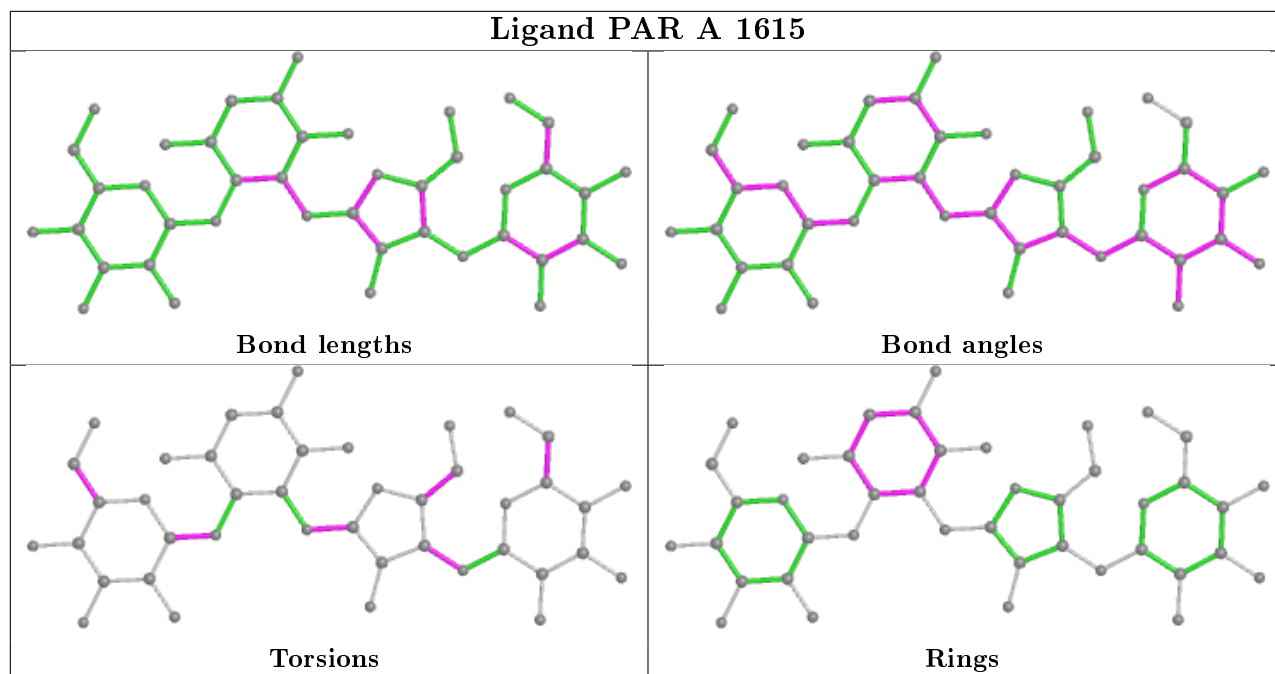
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

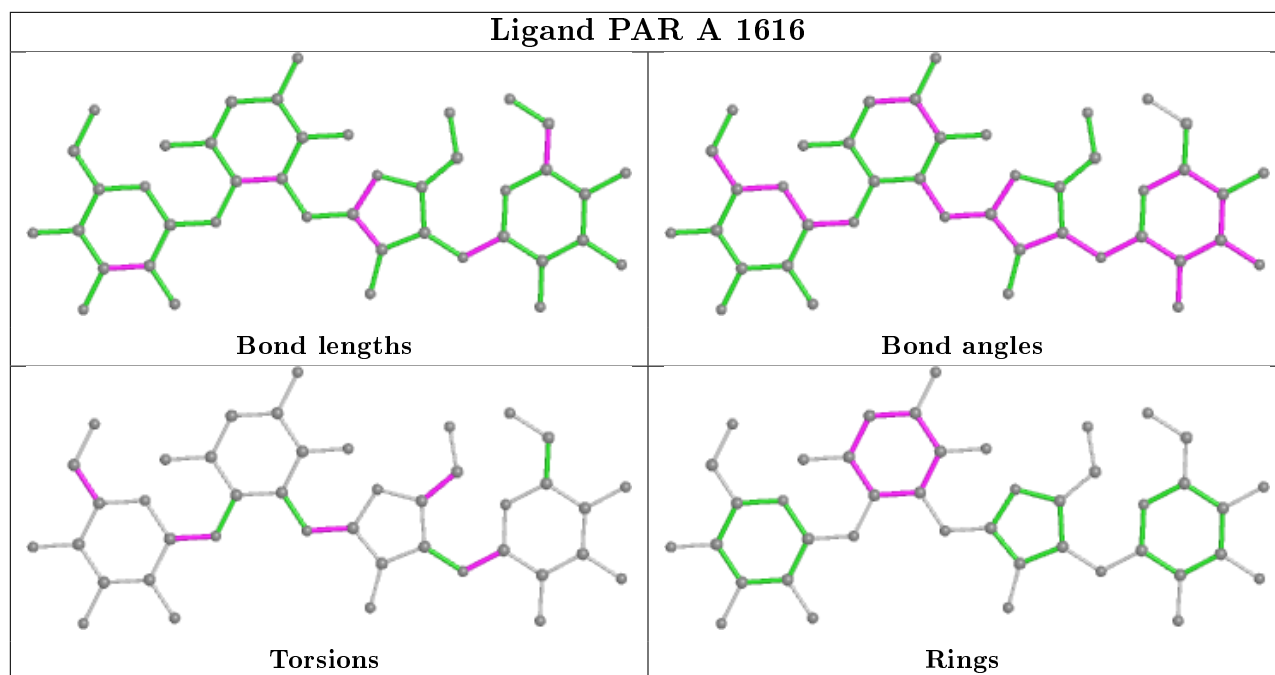
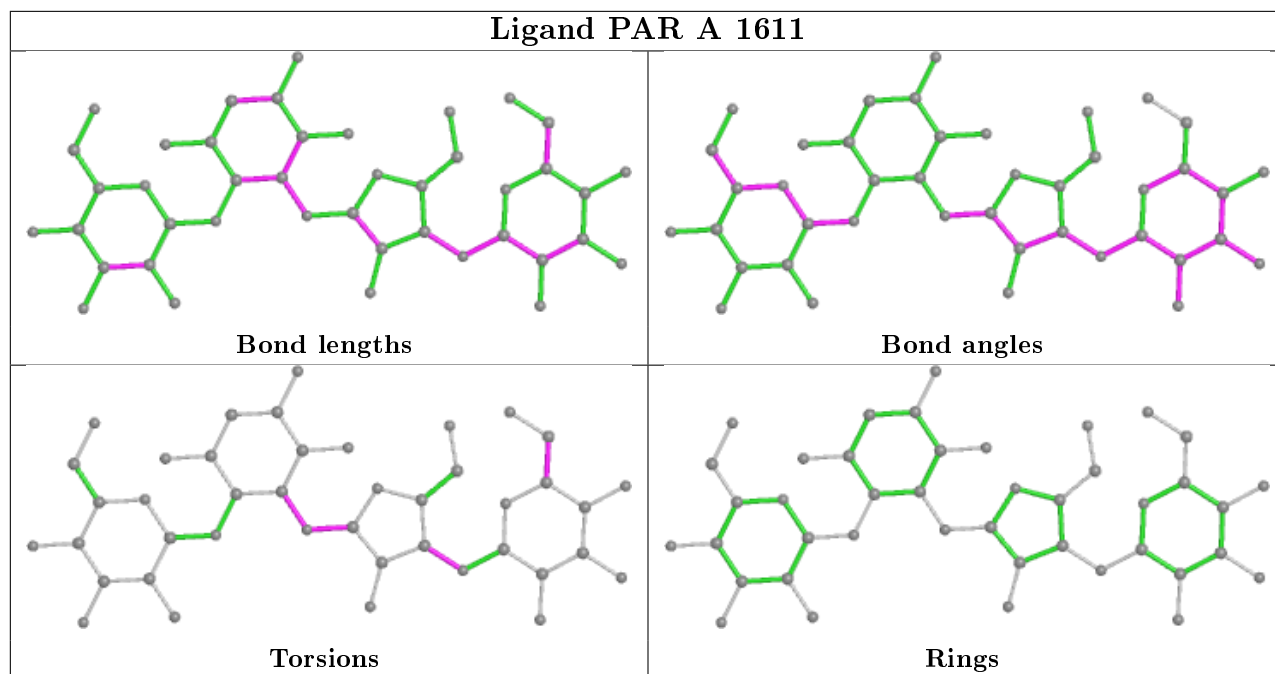


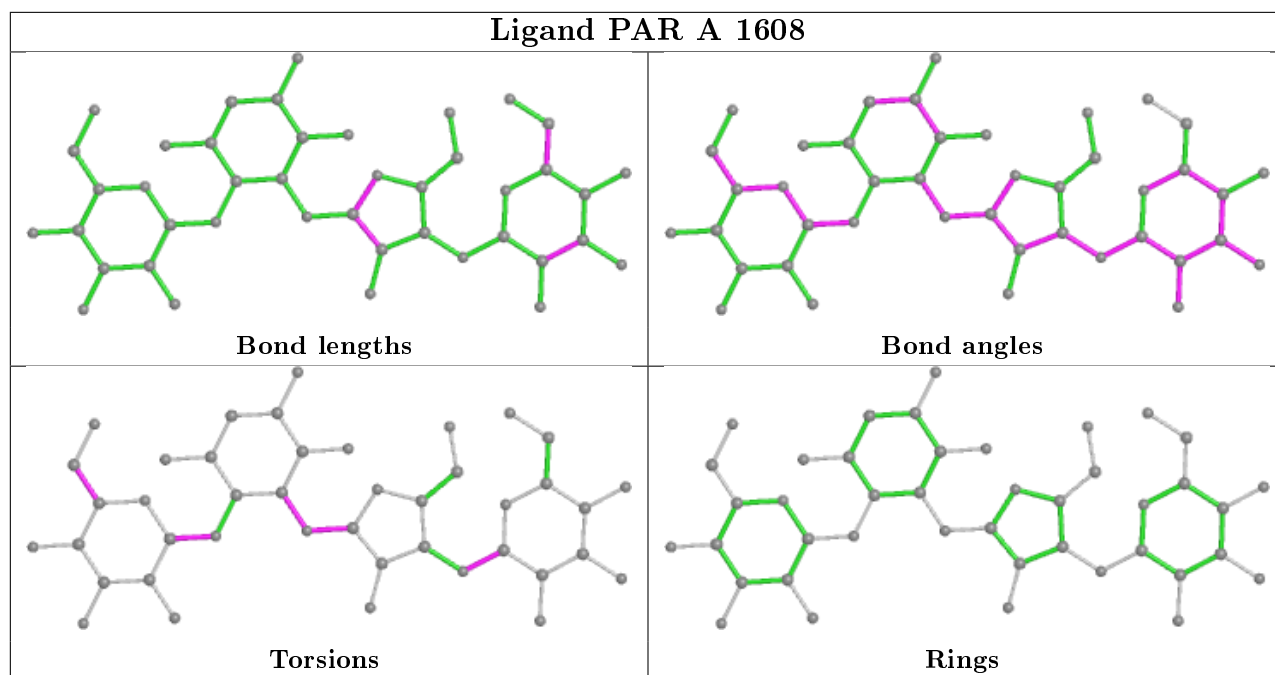
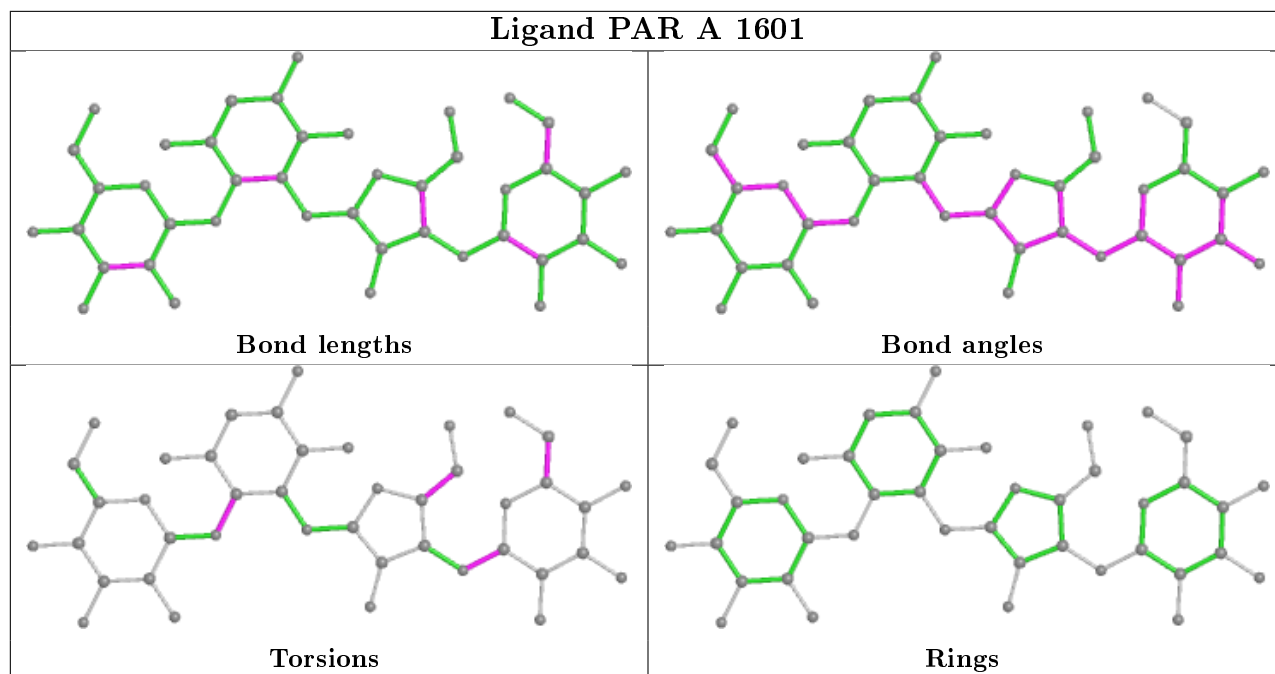


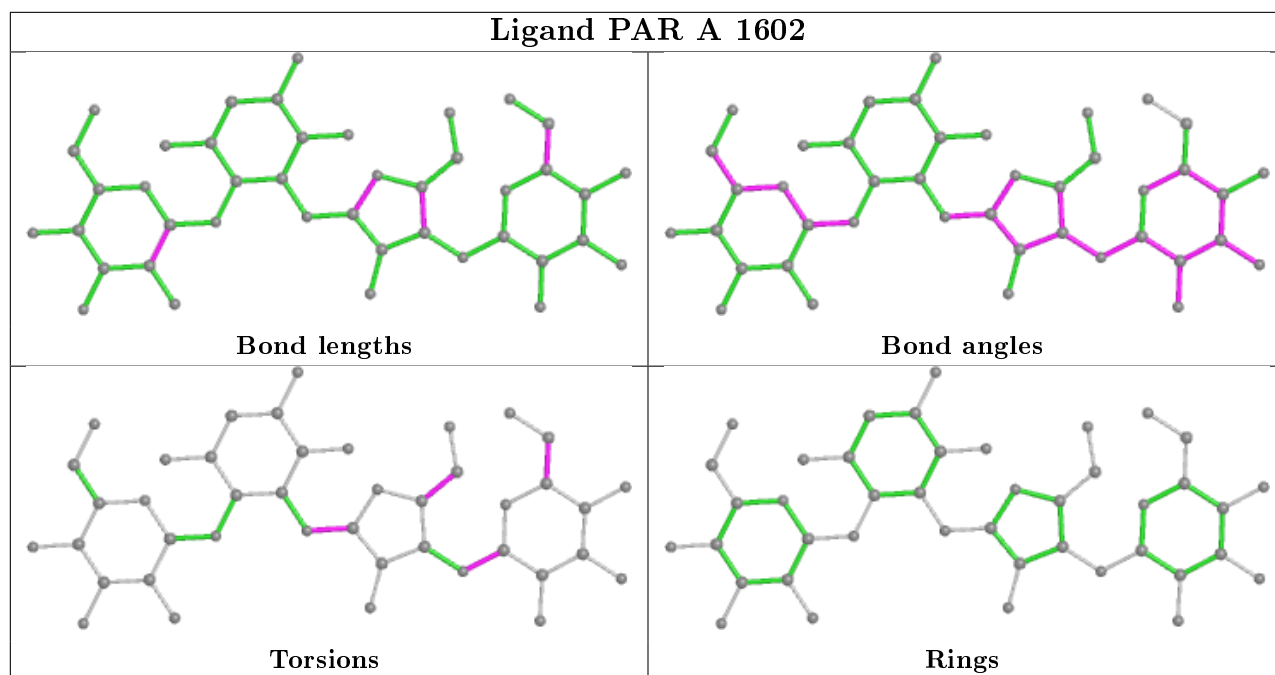
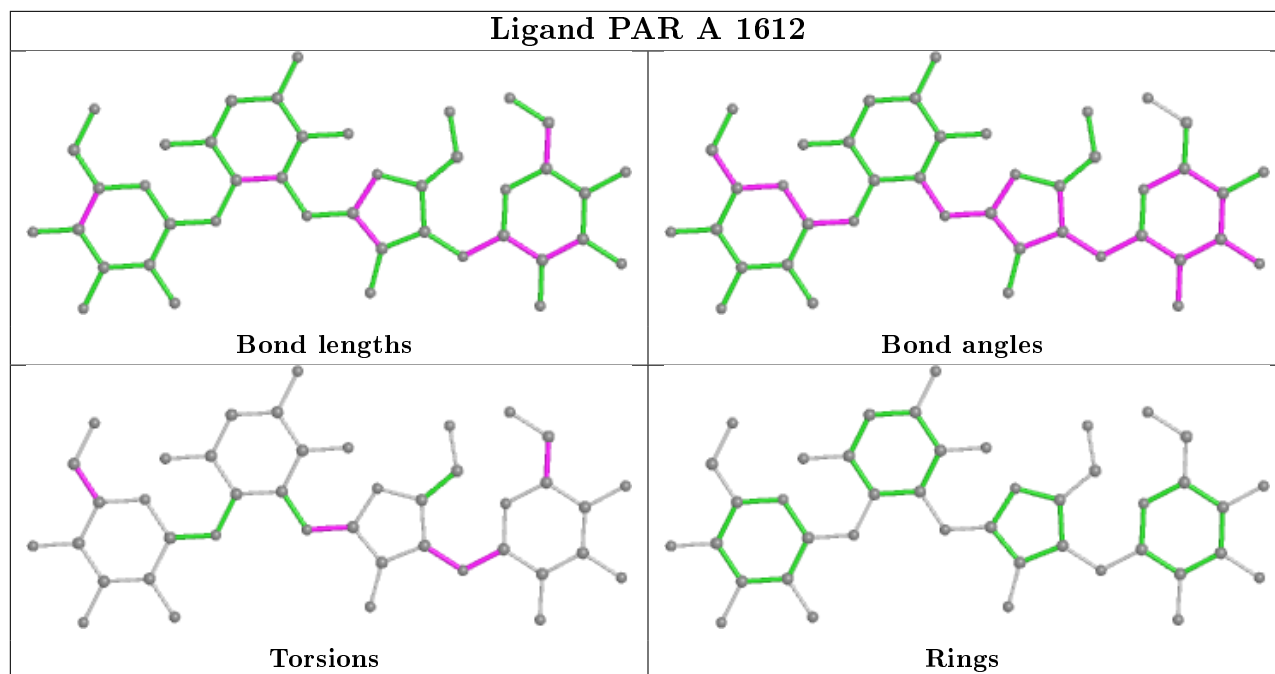


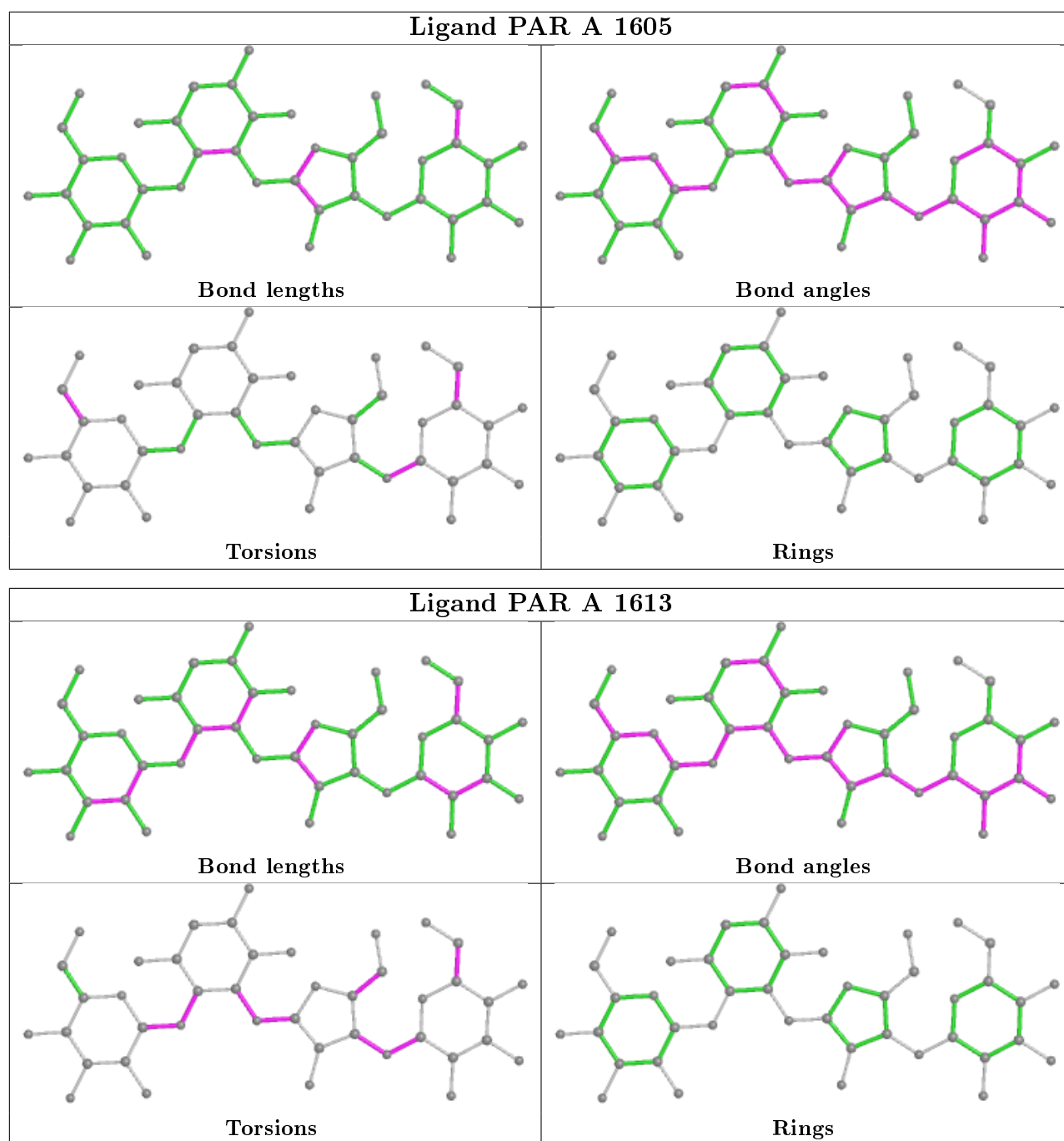












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.27	16 (1%) 80 73	48, 81, 183, 551	0
2	B	236/256 (92%)	-0.19	3 (1%) 77 68	60, 104, 154, 168	0
3	C	207/239 (86%)	-0.28	1 (0%) 91 87	69, 106, 153, 184	0
4	D	208/209 (99%)	-0.27	3 (1%) 75 66	53, 86, 123, 147	0
5	E	151/162 (93%)	-0.42	0 100 100	50, 70, 105, 144	0
6	F	101/101 (100%)	-0.13	1 (0%) 82 75	73, 111, 136, 155	0
7	G	155/156 (99%)	-0.29	1 (0%) 89 85	66, 100, 155, 187	0
8	H	138/138 (100%)	-0.43	0 100 100	45, 68, 95, 127	0
9	I	127/128 (99%)	0.09	2 (1%) 72 63	67, 110, 140, 169	0
10	J	99/105 (94%)	0.61	11 (11%) 5 4	69, 133, 194, 209	0
11	K	117/129 (90%)	-0.12	0 100 100	57, 85, 120, 137	0
12	L	124/135 (91%)	-0.07	3 (2%) 59 47	47, 87, 123, 166	0
13	M	118/126 (93%)	0.15	6 (5%) 28 18	72, 106, 131, 151	0
14	N	60/61 (98%)	-0.13	2 (3%) 46 34	76, 97, 143, 194	0
15	O	88/89 (98%)	-0.14	1 (1%) 80 73	67, 87, 119, 163	0
16	P	84/88 (95%)	-0.22	0 100 100	61, 77, 109, 166	0
17	Q	101/105 (96%)	-0.22	1 (0%) 82 75	54, 74, 108, 154	0
18	R	73/88 (82%)	0.06	2 (2%) 54 42	65, 87, 190, 221	0
19	S	81/93 (87%)	0.14	4 (4%) 29 19	93, 124, 165, 187	0
20	T	99/106 (93%)	-0.09	2 (2%) 65 54	61, 85, 130, 156	0
21	U	25/27 (92%)	0.98	4 (16%) 1 1	77, 95, 129, 151	0
All	All	3890/4063 (95%)	-0.18	63 (1%) 72 63	45, 89, 156, 551	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
14	N	12	ARG	7.0
12	L	129	ALA	6.5
1	A	1002	G	6.3
21	U	26	LYS	6.1
9	I	128	ARG	5.7
1	A	1129	C	5.6
19	S	29	ARG	5.0
1	A	1003	G	5.0
12	L	128	ALA	4.3
10	J	71	LEU	4.2
13	M	5	ALA	4.1
18	R	17	SER	4.0
1	A	1532	U	3.8
1	A	930	C	3.7
10	J	73	ASP	3.7
10	J	72	VAL	3.7
10	J	6	ILE	3.5
1	A	1533	C	3.4
10	J	74	ILE	3.3
13	M	7	VAL	3.3
13	M	8	GLU	3.3
10	J	8	LEU	3.2
4	D	47	ARG	3.2
19	S	28	LYS	3.1
1	A	841	U	3.1
14	N	13	THR	3.1
6	F	101	ALA	3.0
7	G	156	TRP	3.0
20	T	9	ASN	2.9
19	S	3	ARG	2.9
10	J	24	VAL	2.9
2	B	132	LYS	2.9
10	J	4	ILE	2.9
1	A	1531	A	2.8
13	M	4	ILE	2.7
1	A	1389	C	2.7
10	J	96	ILE	2.7
18	R	88	LYS	2.6
21	U	18	TYR	2.6
9	I	8	GLY	2.5
1	A	1539	C	2.5
12	L	19	ARG	2.5
1	A	1032	G	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	202	U	2.5
10	J	98	ILE	2.4
2	B	129	GLU	2.4
4	D	33	MET	2.3
17	Q	102	GLY	2.3
1	A	1001	A	2.3
2	B	15	VAL	2.3
21	U	24	ARG	2.3
4	D	9	CYS	2.3
13	M	2	ALA	2.2
3	C	91	LEU	2.2
1	A	929	G	2.2
13	M	3	ARG	2.1
20	T	99	LEU	2.1
21	U	12	LYS	2.1
19	S	60	VAL	2.1
10	J	90	LEU	2.1
15	O	89	GLY	2.1
1	A	1030(B)	C	2.0
1	A	1031	G	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	0.81	0.51	197,257,265,266	0
1	PSU	A	1541	20/21	0.87	0.30	205,208,212,214	0
1	7MG	A	527	24/25	0.97	0.17	60,65,76,80	0
1	MA6	A	1519	24/25	0.97	0.21	50,57,68,73	0
1	5MC	A	1407	21/22	0.97	0.20	58,69,78,82	0
1	5MC	A	1404	21/22	0.97	0.18	52,62,70,73	0
1	5MC	A	1400	21/22	0.97	0.17	56,78,91,92	0
1	PSU	A	516	20/21	0.97	0.16	91,99,107,112	0
1	MA6	A	1518	24/25	0.97	0.18	57,62,73,74	0
1	2MG	A	1207	24/25	0.97	0.16	84,91,99,100	0
12	0TD	L	92	10/11	0.97	0.28	47,89,101,397	0
1	UR3	A	1498	21/22	0.98	0.19	57,68,78,81	0
1	5MC	A	967	21/22	0.98	0.12	53,66,76,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	4OC	A	1402	22/23	0.98	0.17	56,67,76,80	0
1	M2G	A	966	25/26	0.98	0.14	65,74,83,93	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
23	MG	A	1792	1/1	0.33	0.30	100,100,100,100	0
23	MG	A	1899[A]	1/1	0.40	0.55	45,45,45,45	1
23	MG	A	1899[B]	1/1	0.40	0.55	45,45,45,45	1
23	MG	A	1882	1/1	0.43	0.95	94,94,94,94	0
23	MG	A	1864	1/1	0.43	1.86	96,96,96,96	0
23	MG	A	1851	1/1	0.45	0.49	89,89,89,89	0
23	MG	A	1881	1/1	0.46	0.63	102,102,102,102	0
23	MG	A	1824	1/1	0.54	0.29	92,92,92,92	0
23	MG	A	1861	1/1	0.56	1.02	75,75,75,75	0
23	MG	A	1758	1/1	0.57	0.28	149,149,149,149	0
23	MG	A	1730	1/1	0.58	0.20	98,98,98,98	0
23	MG	A	1885	1/1	0.58	0.34	96,96,96,96	0
23	MG	A	1749	1/1	0.58	0.21	138,138,138,138	0
23	MG	A	1756	1/1	0.62	0.20	158,158,158,158	0
23	MG	A	1900	1/1	0.62	0.47	77,77,77,77	0
23	MG	A	1889	1/1	0.63	1.16	92,92,92,92	0
23	MG	A	1797	1/1	0.64	0.44	85,85,85,85	0
23	MG	A	1805	1/1	0.64	1.29	83,83,83,83	0
23	MG	I	201	1/1	0.66	0.23	92,92,92,92	0
23	MG	A	1884	1/1	0.67	0.63	85,85,85,85	0
23	MG	A	1854	1/1	0.67	0.46	76,76,76,76	0
23	MG	A	1637	1/1	0.68	0.29	90,90,90,90	0
23	MG	A	1852	1/1	0.68	0.19	65,65,65,65	0
23	MG	A	1847	1/1	0.69	0.70	70,70,70,70	0
23	MG	A	1798	1/1	0.69	0.67	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
22	PAR	A	1613	42/42	0.69	0.48	152,152,152,152	0
23	MG	A	1820	1/1	0.70	0.17	88,88,88,88	0
23	MG	A	1799	1/1	0.70	0.46	74,74,74,74	0
23	MG	A	1691	1/1	0.71	0.57	118,118,118,118	0
23	MG	A	1674	1/1	0.71	0.22	96,96,96,96	0
23	MG	A	1880	1/1	0.71	0.27	96,96,96,96	0
23	MG	N	102	1/1	0.72	0.55	76,76,76,76	0
23	MG	A	1828	1/1	0.72	0.18	100,100,100,100	0
22	PAR	A	1611	42/42	0.72	0.37	130,130,130,130	0
23	MG	A	1742	1/1	0.72	0.26	146,146,146,146	0
23	MG	A	1888	1/1	0.72	0.42	71,71,71,71	0
23	MG	A	1866	1/1	0.73	0.53	83,83,83,83	0
23	MG	A	1823	1/1	0.73	0.60	82,82,82,82	0
23	MG	A	1915	1/1	0.73	0.43	101,101,101,101	0
23	MG	A	1801	1/1	0.73	0.70	87,87,87,87	0
23	MG	A	1718	1/1	0.73	0.53	89,89,89,89	0
23	MG	A	1862	1/1	0.73	0.80	70,70,70,70	0
23	MG	A	1872	1/1	0.73	0.17	59,59,59,59	0
23	MG	A	1894	1/1	0.75	0.34	64,64,64,64	0
23	MG	A	1858[B]	1/1	0.76	0.37	32,32,32,32	1
23	MG	A	1859[B]	1/1	0.76	0.40	59,59,59,59	1
23	MG	A	1859[A]	1/1	0.76	0.40	59,59,59,59	1
23	MG	A	1736	1/1	0.76	0.23	138,138,138,138	0
23	MG	A	1731	1/1	0.76	0.20	140,140,140,140	0
23	MG	A	1827	1/1	0.76	0.37	91,91,91,91	0
23	MG	A	1916[A]	1/1	0.76	0.25	50,50,50,50	1
23	MG	A	1916[B]	1/1	0.76	0.25	50,50,50,50	1
23	MG	A	1858[A]	1/1	0.76	0.37	32,32,32,32	1
23	MG	A	1883	1/1	0.76	0.29	68,68,68,68	0
23	MG	A	1678	1/1	0.77	0.18	101,101,101,101	0
23	MG	A	1896	1/1	0.78	0.58	89,89,89,89	0
23	MG	A	1909	1/1	0.78	0.12	91,91,91,91	0
23	MG	A	1815	1/1	0.78	0.27	71,71,71,71	0
23	MG	A	1733	1/1	0.79	0.12	142,142,142,142	0
23	MG	A	1867	1/1	0.79	0.40	75,75,75,75	0
22	PAR	A	1614	42/42	0.79	0.33	147,147,147,147	0
23	MG	A	1874	1/1	0.79	0.46	90,90,90,90	0
23	MG	A	1856	1/1	0.79	0.20	90,90,90,90	0
23	MG	A	1807	1/1	0.79	1.01	96,96,96,96	0
23	MG	Q	201	1/1	0.79	0.13	86,86,86,86	0
23	MG	A	1621	1/1	0.79	0.08	131,131,131,131	0
23	MG	A	1826	1/1	0.79	0.30	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
23	MG	A	1709	1/1	0.80	0.33	87,87,87,87	0
23	MG	A	1755	1/1	0.80	0.28	96,96,96,96	0
23	MG	A	1796	1/1	0.80	0.55	94,94,94,94	0
23	MG	A	1825	1/1	0.80	0.33	88,88,88,88	0
23	MG	A	1692	1/1	0.80	0.08	98,98,98,98	0
23	MG	A	1673	1/1	0.80	0.13	70,70,70,70	0
23	MG	A	1788	1/1	0.81	0.59	75,75,75,75	0
23	MG	A	1918	1/1	0.81	0.48	90,90,90,90	0
23	MG	A	1837	1/1	0.81	0.63	84,84,84,84	0
23	MG	A	1850	1/1	0.81	0.18	60,60,60,60	0
23	MG	A	1727	1/1	0.81	0.09	117,117,117,117	0
23	MG	F	201	1/1	0.81	0.59	80,80,80,80	0
23	MG	A	1920	1/1	0.82	0.27	72,72,72,72	0
23	MG	A	1830	1/1	0.82	0.45	92,92,92,92	0
23	MG	A	1814	1/1	0.82	0.27	85,85,85,85	0
23	MG	A	1770	1/1	0.82	0.20	101,101,101,101	0
23	MG	A	1768	1/1	0.82	0.70	122,122,122,122	0
23	MG	A	1759	1/1	0.82	0.31	79,79,79,79	0
23	MG	A	1767	1/1	0.82	0.15	113,113,113,113	0
23	MG	A	1902	1/1	0.82	0.39	93,93,93,93	0
22	PAR	A	1615	42/42	0.82	0.29	169,169,169,169	0
23	MG	A	1795	1/1	0.83	0.12	101,101,101,101	0
23	MG	A	1811	1/1	0.83	0.81	87,87,87,87	0
22	PAR	A	1616	42/42	0.83	0.42	126,126,126,126	42
23	MG	A	1836	1/1	0.83	0.30	86,86,86,86	0
23	MG	A	1714	1/1	0.83	0.09	115,115,115,115	0
23	MG	A	1786	1/1	0.83	0.14	154,154,154,154	0
23	MG	A	1846	1/1	0.83	0.72	81,81,81,81	0
23	MG	A	1813	1/1	0.84	0.27	55,55,55,55	0
23	MG	A	1890	1/1	0.84	0.19	86,86,86,86	0
23	MG	A	1737	1/1	0.84	0.23	105,105,105,105	0
23	MG	A	1913	1/1	0.84	0.30	69,69,69,69	0
23	MG	E	201	1/1	0.84	0.12	110,110,110,110	0
23	MG	A	1671	1/1	0.84	0.34	68,68,68,68	0
23	MG	A	1723	1/1	0.84	0.17	103,103,103,103	0
23	MG	A	1656	1/1	0.84	0.20	124,124,124,124	0
23	MG	A	1712	1/1	0.85	0.09	112,112,112,112	0
23	MG	A	1804	1/1	0.85	1.15	103,103,103,103	0
23	MG	A	1831	1/1	0.85	0.45	85,85,85,85	0
23	MG	A	1848	1/1	0.85	0.31	71,71,71,71	0
23	MG	A	1710	1/1	0.85	0.33	92,92,92,92	0
23	MG	A	1632	1/1	0.85	0.10	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
23	MG	A	1860	1/1	0.85	1.26	102,102,102,102	0
23	MG	A	1877	1/1	0.85	0.24	105,105,105,105	0
23	MG	A	1794	1/1	0.85	0.55	80,80,80,80	0
23	MG	A	1922	1/1	0.85	0.28	77,77,77,77	0
23	MG	P	101	1/1	0.85	0.50	63,63,63,63	0
23	MG	E	202	1/1	0.85	0.53	74,74,74,74	0
23	MG	A	1817	1/1	0.85	0.49	99,99,99,99	0
23	MG	L	201	1/1	0.85	0.16	81,81,81,81	0
23	MG	A	1728	1/1	0.85	0.17	144,144,144,144	0
23	MG	A	1871	1/1	0.86	0.80	85,85,85,85	0
23	MG	A	1809	1/1	0.86	0.36	58,58,58,58	0
23	MG	A	1700	1/1	0.86	0.10	90,90,90,90	0
23	MG	A	1697	1/1	0.86	0.65	66,66,66,66	0
23	MG	A	1717	1/1	0.86	0.22	110,110,110,110	0
23	MG	A	1643	1/1	0.86	0.40	74,74,74,74	0
23	MG	A	1802	1/1	0.86	0.35	71,71,71,71	0
23	MG	H	201	1/1	0.87	0.19	85,85,85,85	0
23	MG	A	1747	1/1	0.87	0.49	166,166,166,166	0
23	MG	A	1735	1/1	0.87	0.21	92,92,92,92	0
23	MG	A	1738	1/1	0.87	0.53	116,116,116,116	0
23	MG	A	1893	1/1	0.87	0.36	71,71,71,71	0
23	MG	A	1699	1/1	0.87	0.17	112,112,112,112	0
23	MG	A	1855	1/1	0.87	0.35	74,74,74,74	0
23	MG	A	1740	1/1	0.87	0.12	96,96,96,96	0
23	MG	A	1751	1/1	0.87	0.23	81,81,81,81	0
23	MG	A	1819	1/1	0.87	1.07	96,96,96,96	0
23	MG	A	1785	1/1	0.87	0.28	142,142,142,142	0
23	MG	A	1783	1/1	0.87	0.31	132,132,132,132	0
23	MG	A	1789	1/1	0.87	0.15	100,100,100,100	0
23	MG	A	1744	1/1	0.88	0.14	99,99,99,99	0
23	MG	A	1766	1/1	0.88	0.18	118,118,118,118	0
23	MG	A	1791	1/1	0.88	0.40	84,84,84,84	0
23	MG	A	1843	1/1	0.88	0.14	62,62,62,62	0
23	MG	A	1790	1/1	0.88	0.25	89,89,89,89	0
23	MG	H	202	1/1	0.88	0.18	72,72,72,72	0
22	PAR	A	1610	42/42	0.88	0.33	111,111,111,111	0
23	MG	A	1652	1/1	0.88	0.41	86,86,86,86	0
23	MG	A	1919	1/1	0.88	0.24	85,85,85,85	0
23	MG	A	1863	1/1	0.88	0.36	90,90,90,90	0
23	MG	A	1761	1/1	0.88	0.14	103,103,103,103	0
22	PAR	A	1617	42/42	0.88	0.30	137,137,137,137	0
23	MG	A	1774	1/1	0.88	0.17	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
23	MG	A	1887	1/1	0.88	0.23	93,93,93,93	0
23	MG	A	1629	1/1	0.89	0.21	96,96,96,96	0
23	MG	A	1901	1/1	0.89	0.25	81,81,81,81	0
23	MG	A	1679	1/1	0.89	0.28	73,73,73,73	0
23	MG	A	1800	1/1	0.89	0.17	83,83,83,83	0
23	MG	A	1669	1/1	0.89	0.17	76,76,76,76	0
23	MG	A	1895[A]	1/1	0.89	0.55	30,30,30,30	1
23	MG	A	1725	1/1	0.89	0.09	94,94,94,94	0
23	MG	A	1752	1/1	0.89	0.23	105,105,105,105	0
23	MG	A	1895[B]	1/1	0.89	0.55	30,30,30,30	1
23	MG	A	1838	1/1	0.89	0.42	80,80,80,80	0
23	MG	A	1687	1/1	0.89	0.22	92,92,92,92	0
23	MG	A	1769	1/1	0.89	0.09	108,108,108,108	0
23	MG	A	1839	1/1	0.89	0.32	84,84,84,84	0
23	MG	A	1704	1/1	0.89	0.17	87,87,87,87	0
23	MG	A	1693	1/1	0.89	0.26	129,129,129,129	0
23	MG	A	1808	1/1	0.89	0.58	93,93,93,93	0
23	MG	A	1686	1/1	0.89	0.14	73,73,73,73	0
23	MG	A	1720	1/1	0.89	0.08	94,94,94,94	0
23	MG	S	101	1/1	0.89	0.11	83,83,83,83	0
22	PAR	A	1612	42/42	0.89	0.27	69,69,69,69	42
23	MG	A	1651	1/1	0.89	0.56	61,61,61,61	0
23	MG	A	1787	1/1	0.89	0.19	165,165,165,165	0
23	MG	A	1914	1/1	0.90	0.25	81,81,81,81	0
23	MG	A	1703	1/1	0.90	0.12	85,85,85,85	0
23	MG	A	1654	1/1	0.90	0.16	104,104,104,104	0
23	MG	A	1873	1/1	0.90	0.60	59,59,59,59	0
23	MG	A	1675	1/1	0.90	0.39	101,101,101,101	0
23	MG	A	1869	1/1	0.90	0.28	71,71,71,71	0
23	MG	A	1857	1/1	0.90	0.30	59,59,59,59	0
23	MG	A	1879	1/1	0.90	0.27	79,79,79,79	0
23	MG	D	302	1/1	0.90	0.10	112,112,112,112	0
23	MG	A	1628	1/1	0.90	0.20	44,44,44,44	0
23	MG	A	1670	1/1	0.90	0.12	84,84,84,84	0
23	MG	A	1793	1/1	0.90	1.43	84,84,84,84	0
23	MG	A	1715	1/1	0.90	0.19	107,107,107,107	0
23	MG	A	1870	1/1	0.90	0.53	75,75,75,75	0
23	MG	A	1865	1/1	0.90	0.13	66,66,66,66	0
23	MG	A	1841	1/1	0.90	0.19	74,74,74,74	0
23	MG	A	1844	1/1	0.90	0.28	71,71,71,71	0
23	MG	A	1665	1/1	0.91	0.20	90,90,90,90	0
23	MG	A	1655	1/1	0.91	0.11	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
23	MG	O	101	1/1	0.91	0.30	104,104,104,104	0
23	MG	A	1763	1/1	0.91	0.34	102,102,102,102	0
23	MG	A	1832	1/1	0.91	0.34	68,68,68,68	0
22	PAR	A	1607	42/42	0.91	0.24	92,92,92,92	42
23	MG	A	1779	1/1	0.91	0.15	70,70,70,70	0
23	MG	A	1638	1/1	0.91	0.32	93,93,93,93	0
23	MG	A	1743	1/1	0.91	0.17	145,145,145,145	0
23	MG	A	1849	1/1	0.92	0.35	63,63,63,63	0
23	MG	A	1620	1/1	0.92	0.18	91,91,91,91	0
23	MG	A	1732	1/1	0.92	0.48	86,86,86,86	0
23	MG	A	1781	1/1	0.92	0.29	104,104,104,104	0
23	MG	A	1892	1/1	0.92	0.19	58,58,58,58	0
23	MG	A	1907	1/1	0.92	0.57	81,81,81,81	0
24	ZN	D	301	1/1	0.92	0.54	194,194,194,194	0
23	MG	A	1694	1/1	0.92	0.34	97,97,97,97	0
23	MG	A	1640	1/1	0.92	0.27	78,78,78,78	0
23	MG	A	1680	1/1	0.92	0.07	85,85,85,85	0
23	MG	A	1775	1/1	0.92	0.14	83,83,83,83	0
23	MG	A	1829	1/1	0.92	0.26	90,90,90,90	0
22	PAR	A	1608	42/42	0.92	0.22	97,97,97,97	0
23	MG	A	1653	1/1	0.92	0.17	96,96,96,96	0
23	MG	A	1771	1/1	0.92	0.08	67,67,67,67	0
23	MG	A	1891	1/1	0.92	0.46	70,70,70,70	0
23	MG	A	1685	1/1	0.92	0.20	90,90,90,90	0
23	MG	A	1689	1/1	0.92	0.13	87,87,87,87	0
23	MG	A	1622	1/1	0.92	0.17	111,111,111,111	0
23	MG	A	1834	1/1	0.92	0.20	77,77,77,77	0
23	MG	A	1910	1/1	0.92	0.11	80,80,80,80	0
22	PAR	A	1605	42/42	0.92	0.24	93,93,93,93	0
23	MG	A	1636	1/1	0.93	0.20	72,72,72,72	0
23	MG	A	1627	1/1	0.93	0.13	70,70,70,70	0
22	PAR	A	1609	42/42	0.93	0.21	77,77,77,77	42
23	MG	A	1842	1/1	0.93	0.27	70,70,70,70	0
23	MG	A	1650	1/1	0.93	0.15	106,106,106,106	0
23	MG	A	1753	1/1	0.93	0.10	109,109,109,109	0
23	MG	A	1822	1/1	0.93	0.56	69,69,69,69	0
23	MG	A	1634	1/1	0.93	0.19	44,44,44,44	0
23	MG	A	1748	1/1	0.93	0.11	115,115,115,115	0
23	MG	A	1897	1/1	0.93	0.25	47,47,47,47	0
23	MG	A	1641	1/1	0.93	0.28	92,92,92,92	0
23	MG	A	1623	1/1	0.93	0.11	62,62,62,62	0
23	MG	A	1777	1/1	0.93	0.27	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
23	MG	A	1816	1/1	0.93	0.32	75,75,75,75	0
23	MG	A	1625	1/1	0.93	0.09	90,90,90,90	0
23	MG	A	1921[B]	1/1	0.93	0.15	28,28,28,28	1
23	MG	A	1688	1/1	0.93	0.16	115,115,115,115	0
23	MG	A	1875	1/1	0.93	0.07	55,55,55,55	0
23	MG	A	1921[A]	1/1	0.93	0.15	28,28,28,28	1
23	MG	A	1778	1/1	0.93	0.15	107,107,107,107	0
23	MG	A	1780	1/1	0.94	0.07	66,66,66,66	0
23	MG	A	1630	1/1	0.94	0.16	87,87,87,87	0
23	MG	A	1690	1/1	0.94	0.07	108,108,108,108	0
23	MG	A	1835	1/1	0.94	0.56	72,72,72,72	0
23	MG	A	1706	1/1	0.94	0.27	123,123,123,123	0
23	MG	A	1917	1/1	0.94	0.55	68,68,68,68	0
23	MG	A	1762	1/1	0.94	0.05	127,127,127,127	0
23	MG	A	1784	1/1	0.94	0.12	127,127,127,127	0
23	MG	A	1642	1/1	0.94	0.16	77,77,77,77	0
22	PAR	A	1603	42/42	0.94	0.19	83,83,83,83	3
23	MG	A	1764	1/1	0.94	0.20	107,107,107,107	0
23	MG	A	1745	1/1	0.94	0.17	79,79,79,79	0
23	MG	A	1765	1/1	0.94	0.14	107,107,107,107	0
23	MG	A	1649	1/1	0.94	0.13	90,90,90,90	0
23	MG	A	1886	1/1	0.94	0.17	86,86,86,86	0
23	MG	A	1711	1/1	0.94	0.10	102,102,102,102	0
23	MG	A	1806	1/1	0.94	0.25	81,81,81,81	0
23	MG	A	1663	1/1	0.94	0.34	92,92,92,92	0
23	MG	A	1803	1/1	0.94	0.28	62,62,62,62	0
23	MG	A	1644	1/1	0.94	0.09	50,50,50,50	0
23	MG	A	1903	1/1	0.94	0.25	46,46,46,46	0
23	MG	A	1682	1/1	0.95	0.15	33,33,33,33	0
23	MG	A	1661	1/1	0.95	0.31	112,112,112,112	0
23	MG	A	1708	1/1	0.95	0.10	77,77,77,77	0
23	MG	A	1782	1/1	0.95	0.14	62,62,62,62	0
23	MG	A	1668	1/1	0.95	0.10	92,92,92,92	0
23	MG	A	1677	1/1	0.95	0.09	70,70,70,70	0
23	MG	D	303	1/1	0.95	0.10	63,63,63,63	0
23	MG	A	1701	1/1	0.95	0.34	83,83,83,83	0
23	MG	A	1754	1/1	0.95	0.08	111,111,111,111	0
23	MG	A	1667	1/1	0.95	0.16	78,78,78,78	0
23	MG	A	1878	1/1	0.95	0.15	49,49,49,49	0
23	MG	A	1659	1/1	0.95	0.15	84,84,84,84	0
23	MG	A	1658	1/1	0.95	0.17	103,103,103,103	0
23	MG	A	1739	1/1	0.95	0.40	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
23	MG	A	1906	1/1	0.95	0.59	75,75,75,75	0
23	MG	A	1696	1/1	0.95	0.07	84,84,84,84	0
22	PAR	A	1602	42/42	0.95	0.18	58,58,58,58	0
23	MG	A	1664	1/1	0.95	0.10	94,94,94,94	0
23	MG	A	1840	1/1	0.95	0.29	79,79,79,79	0
22	PAR	A	1604	42/42	0.95	0.21	70,70,70,70	0
23	MG	A	1760	1/1	0.95	0.30	77,77,77,77	0
23	MG	A	1713	1/1	0.95	0.20	95,95,95,95	0
23	MG	A	1722	1/1	0.95	0.11	100,100,100,100	0
23	MG	A	1908	1/1	0.96	0.11	69,69,69,69	0
23	MG	A	1904	1/1	0.96	0.10	80,80,80,80	0
23	MG	A	1631	1/1	0.96	0.05	78,78,78,78	0
23	MG	A	1684	1/1	0.96	0.17	81,81,81,81	0
22	PAR	A	1606	42/42	0.96	0.17	64,64,64,64	42
23	MG	A	1707	1/1	0.96	0.20	112,112,112,112	0
23	MG	A	1911	1/1	0.96	0.14	62,62,62,62	0
23	MG	A	1633	1/1	0.96	0.14	64,64,64,64	0
23	MG	A	1773	1/1	0.96	0.36	91,91,91,91	0
23	MG	A	1721	1/1	0.96	0.09	93,93,93,93	0
23	MG	A	1821	1/1	0.96	0.24	82,82,82,82	0
23	MG	A	1912	1/1	0.96	0.17	70,70,70,70	0
23	MG	A	1833	1/1	0.96	0.18	58,58,58,58	0
23	MG	A	1619	1/1	0.96	0.15	79,79,79,79	0
23	MG	T	201	1/1	0.96	0.18	100,100,100,100	0
22	PAR	A	1601	42/42	0.96	0.20	70,70,70,70	0
23	MG	A	1746	1/1	0.96	0.13	88,88,88,88	0
23	MG	A	1726	1/1	0.96	0.04	91,91,91,91	0
23	MG	A	1729	1/1	0.96	0.11	93,93,93,93	0
23	MG	A	1853	1/1	0.96	0.24	55,55,55,55	0
23	MG	A	1868	1/1	0.96	0.18	73,73,73,73	0
23	MG	A	1845	1/1	0.96	0.21	63,63,63,63	0
23	MG	A	1776	1/1	0.96	0.08	86,86,86,86	0
23	MG	A	1716	1/1	0.97	0.17	74,74,74,74	0
23	MG	T	202	1/1	0.97	0.24	56,56,56,56	0
23	MG	A	1810	1/1	0.97	0.13	63,63,63,63	0
23	MG	A	1741	1/1	0.97	0.10	76,76,76,76	0
23	MG	A	1898	1/1	0.97	0.22	55,55,55,55	0
23	MG	A	1660	1/1	0.97	0.06	66,66,66,66	0
23	MG	A	1695	1/1	0.97	0.11	62,62,62,62	0
23	MG	A	1624	1/1	0.97	0.09	95,95,95,95	0
23	MG	A	1635	1/1	0.97	0.16	65,65,65,65	0
23	MG	A	1698	1/1	0.97	0.11	91,91,91,91	0

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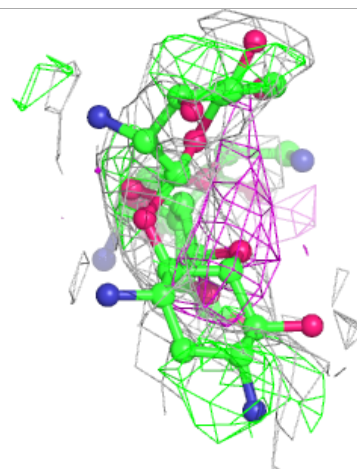
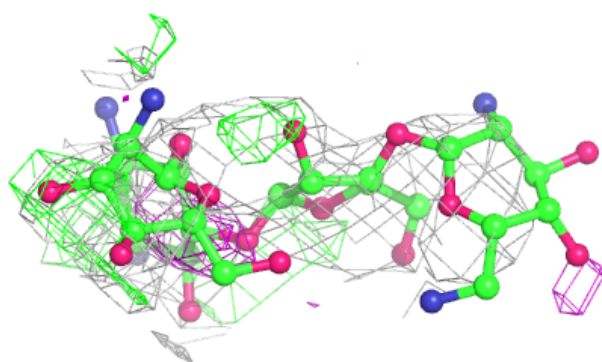
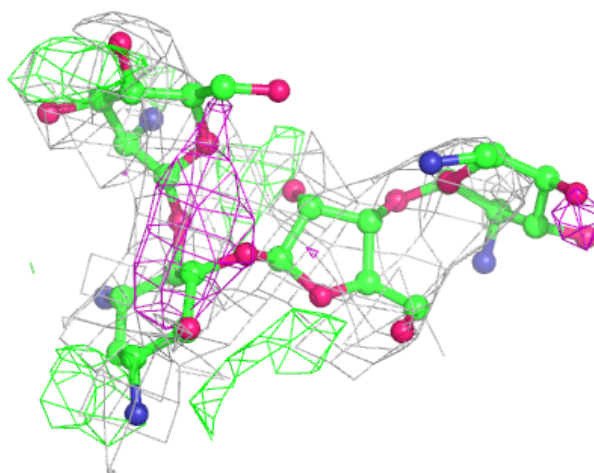
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
23	MG	A	1705	1/1	0.97	0.06	76,76,76,76	0
23	MG	A	1666	1/1	0.97	0.09	54,54,54,54	0
23	MG	A	1645	1/1	0.97	0.31	64,64,64,64	0
23	MG	A	1734	1/1	0.97	0.21	96,96,96,96	0
23	MG	A	1647	1/1	0.97	0.17	101,101,101,101	0
23	MG	A	1812	1/1	0.97	0.99	77,77,77,77	0
23	MG	A	1683	1/1	0.97	0.16	73,73,73,73	0
23	MG	A	1618	1/1	0.97	0.29	79,79,79,79	0
23	MG	A	1702	1/1	0.97	0.16	68,68,68,68	0
23	MG	A	1676	1/1	0.97	0.22	82,82,82,82	0
23	MG	A	1876	1/1	0.97	0.12	60,60,60,60	0
23	MG	A	1724	1/1	0.98	0.03	97,97,97,97	0
23	MG	A	1719	1/1	0.98	0.10	71,71,71,71	0
23	MG	A	1681	1/1	0.98	0.13	89,89,89,89	0
23	MG	A	1750	1/1	0.98	0.16	100,100,100,100	0
23	MG	A	1672	1/1	0.98	0.14	58,58,58,58	0
23	MG	A	1657	1/1	0.98	0.10	54,54,54,54	0
23	MG	A	1639	1/1	0.98	0.21	72,72,72,72	0
24	ZN	N	101	1/1	0.98	0.24	141,141,141,141	0
23	MG	A	1772	1/1	0.98	0.11	67,67,67,67	0
23	MG	A	1757	1/1	0.98	0.26	61,61,61,61	0
23	MG	A	1662	1/1	0.99	0.21	59,59,59,59	0
23	MG	A	1818	1/1	0.99	0.20	79,79,79,79	0
23	MG	A	1648	1/1	0.99	0.10	86,86,86,86	0
23	MG	A	1646	1/1	0.99	0.10	85,85,85,85	0
23	MG	A	1905	1/1	0.99	0.40	100,100,100,100	0
23	MG	A	1626	1/1	1.00	0.17	53,53,53,53	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.

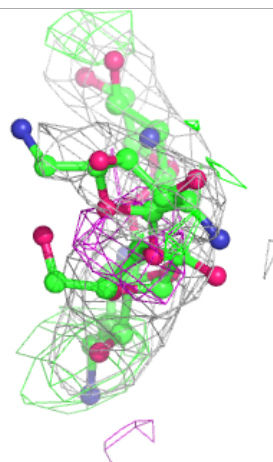
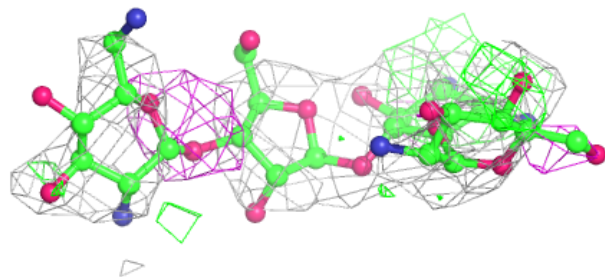
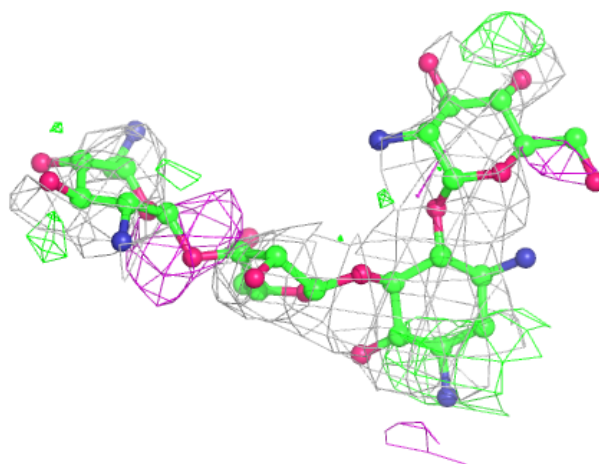
Electron density around PAR A 1613:

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



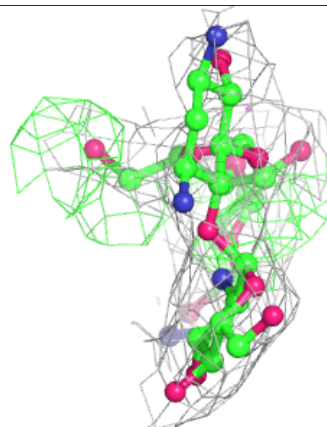
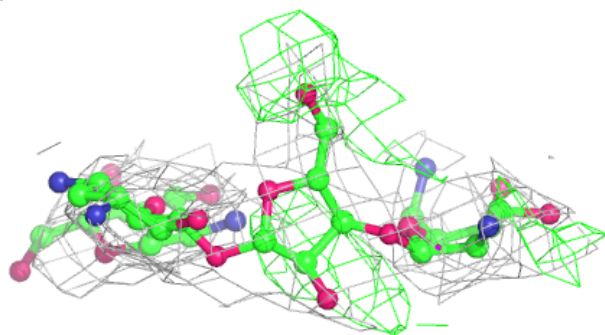
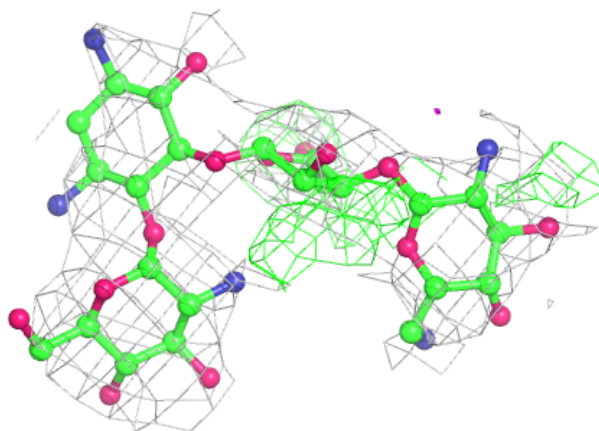
Electron density around PAR A 1611:

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



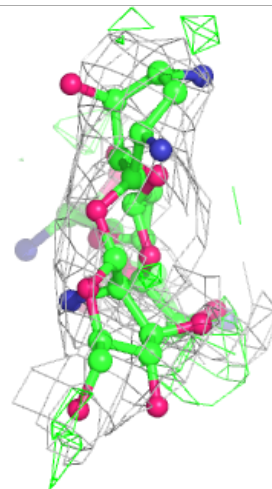
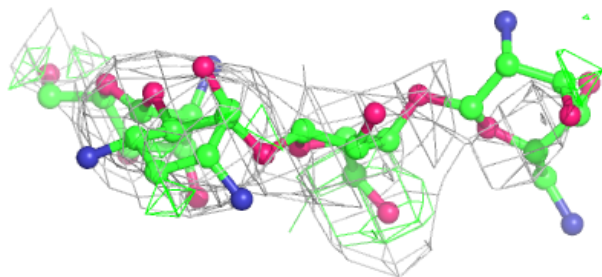
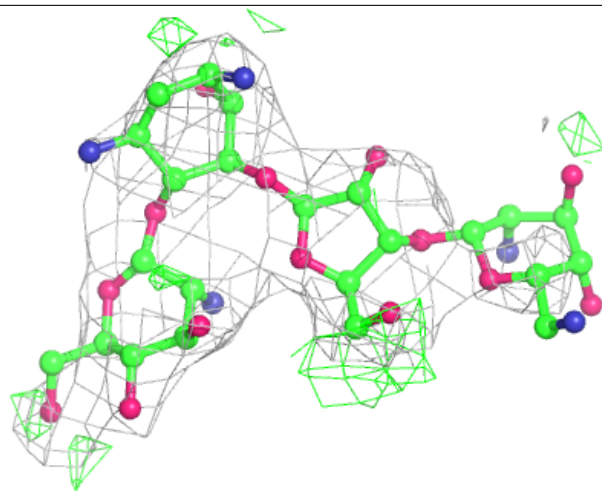
Electron density around PAR A 1614:

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



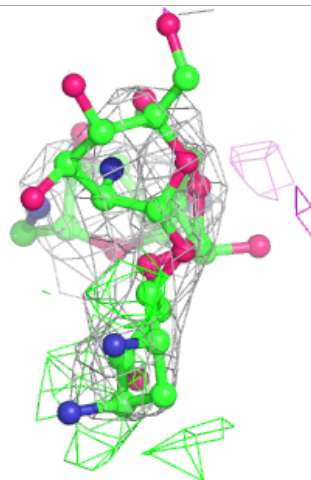
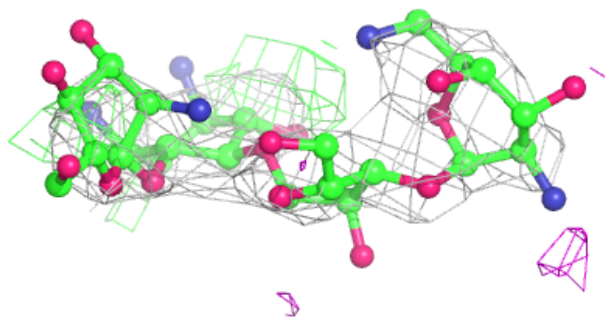
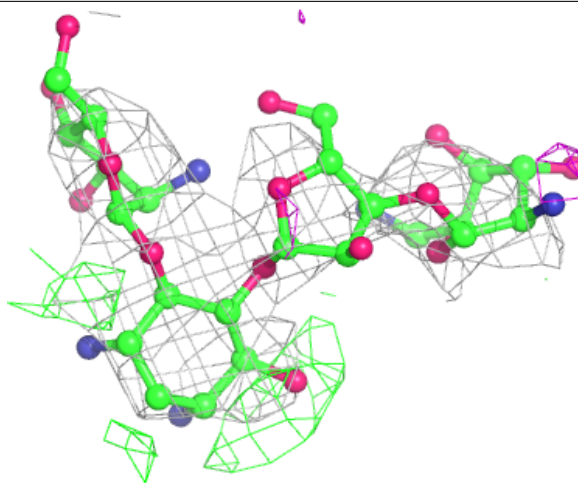
Electron density around PAR A 1615:

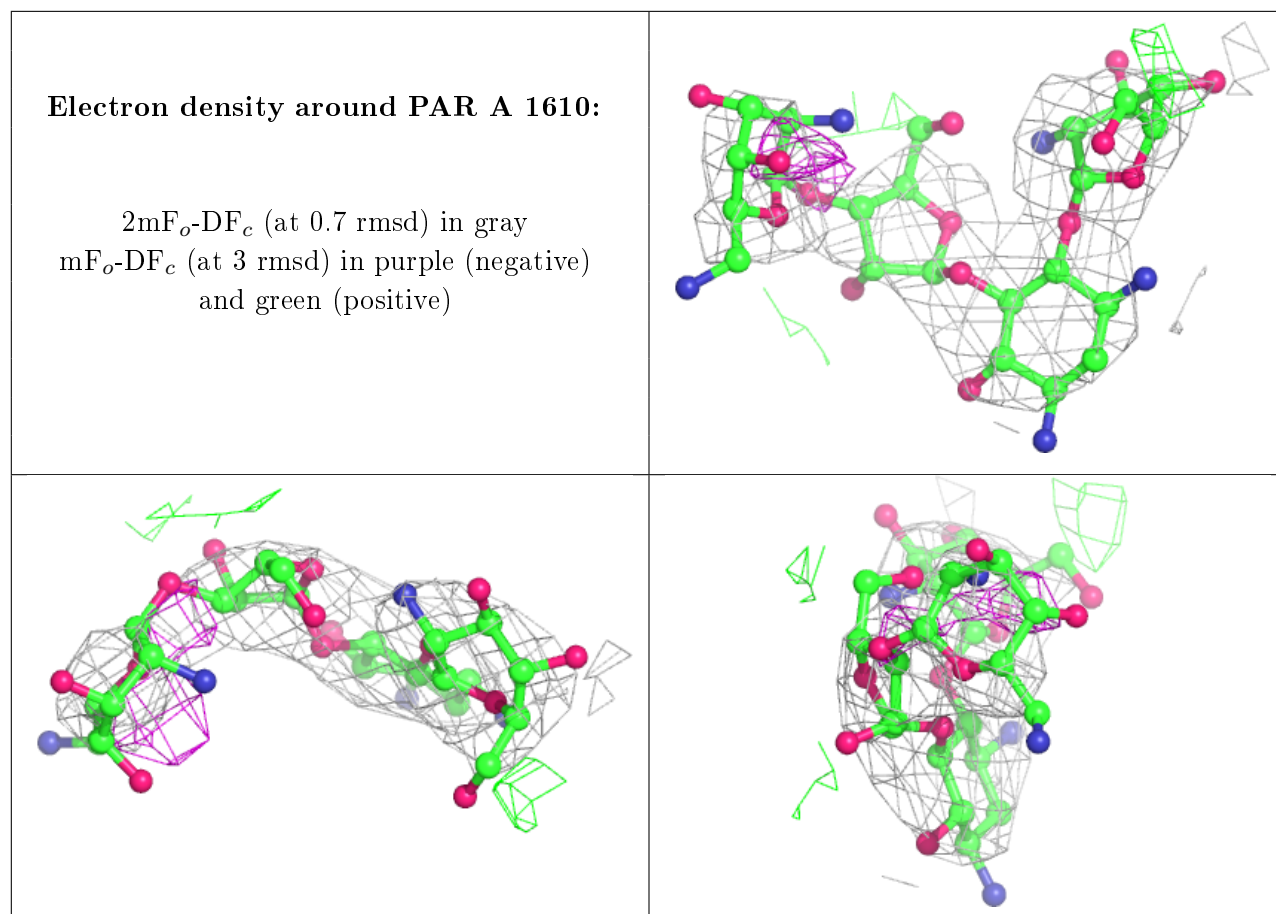
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around PAR A 1616:

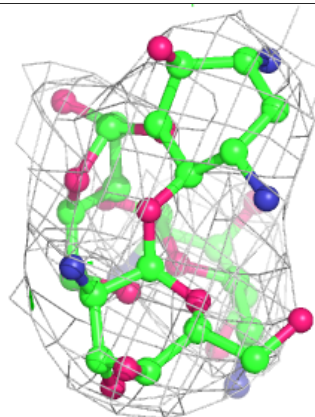
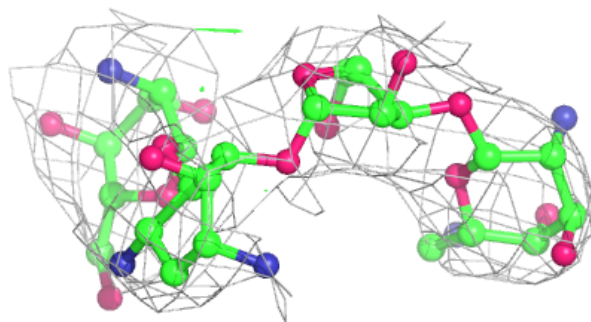
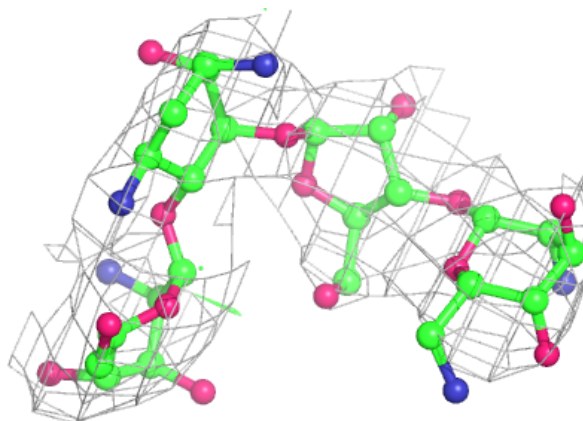
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





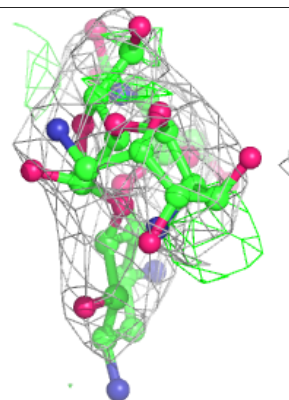
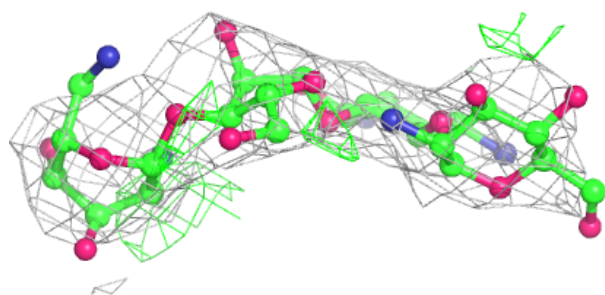
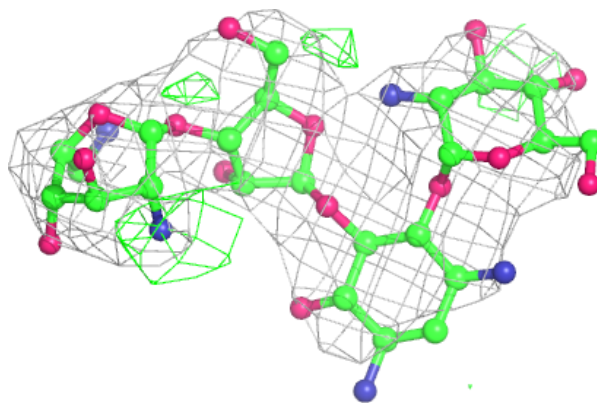
Electron density around PAR A 1617:

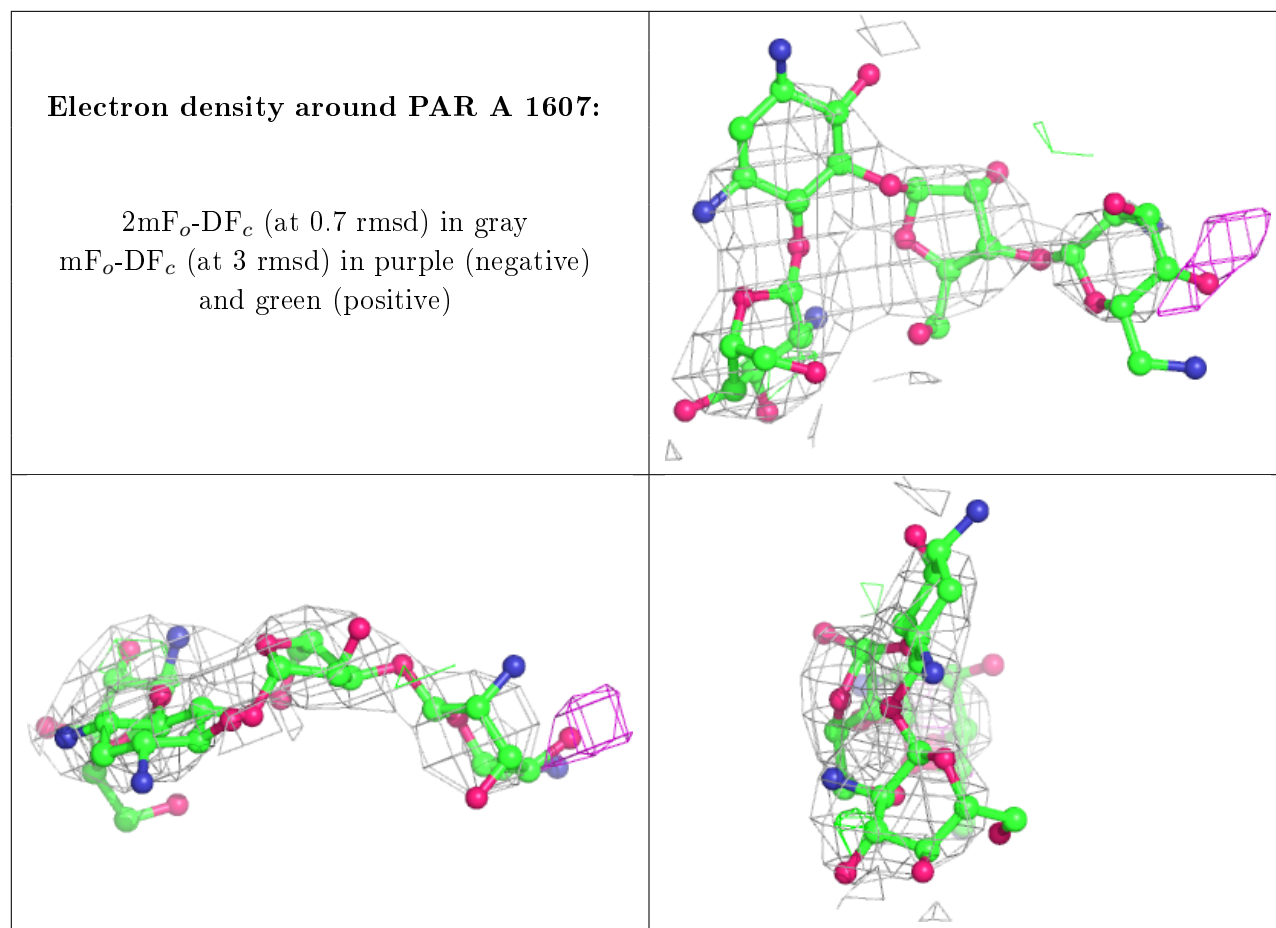
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around PAR A 1612:

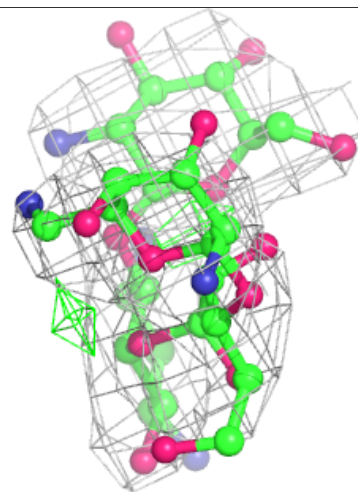
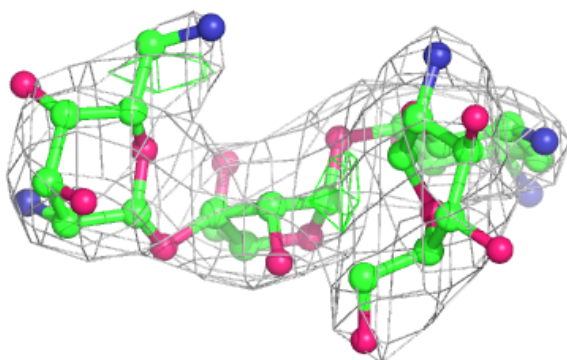
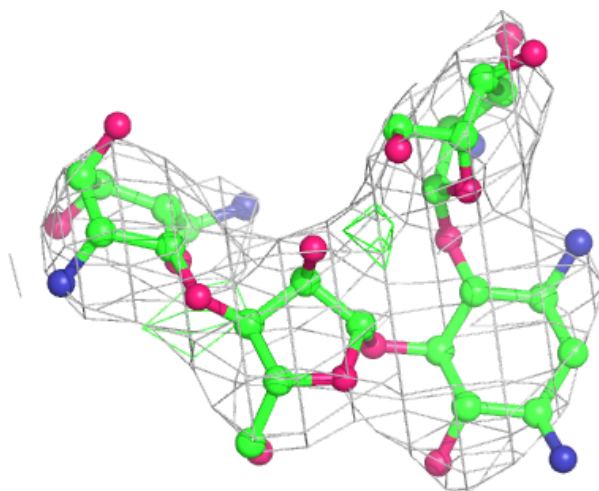
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





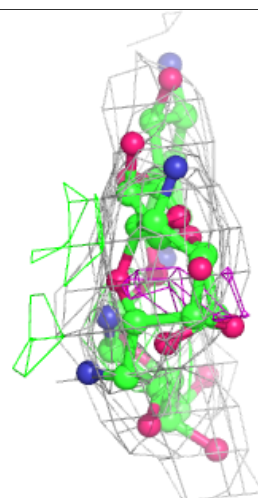
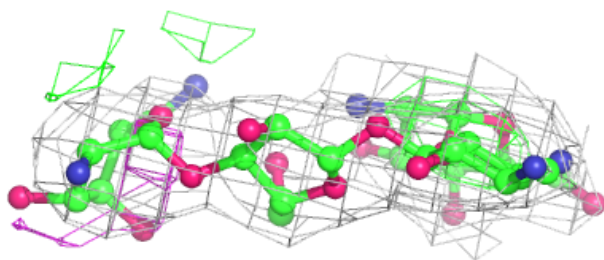
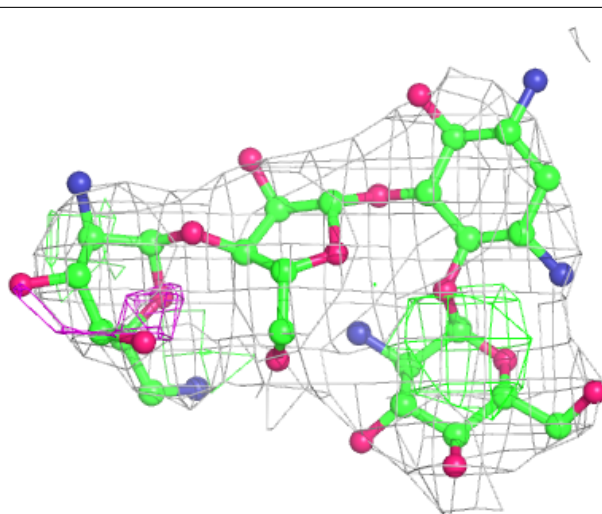
Electron density around PAR A 1608:

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



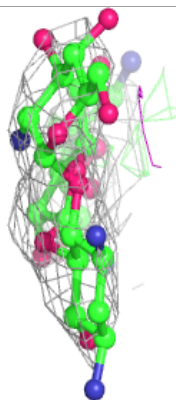
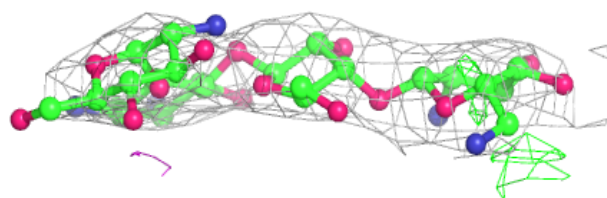
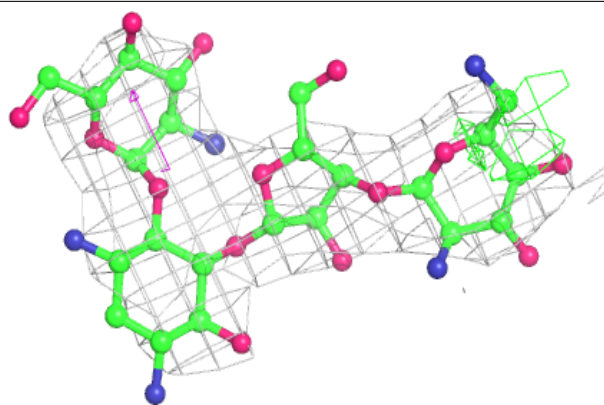
Electron density around PAR A 1605:

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

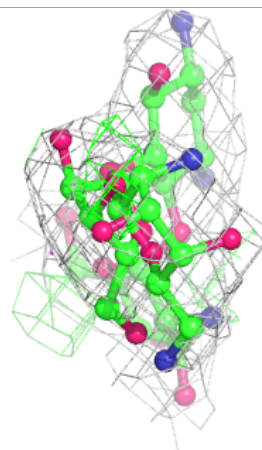
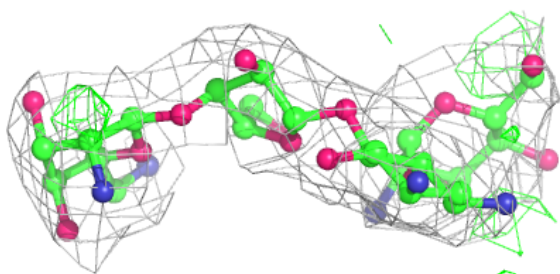
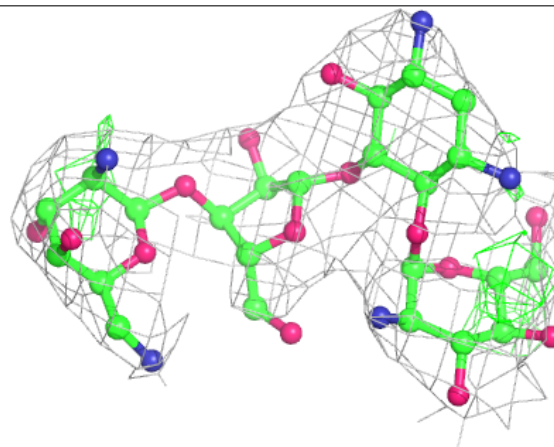


Electron density around PAR A 1609:

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

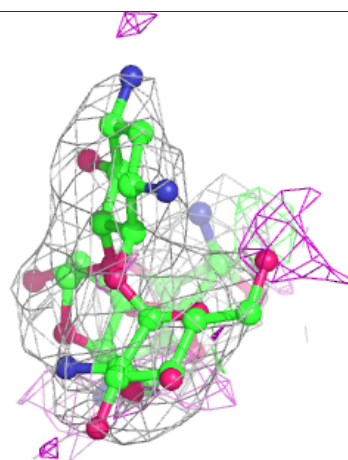
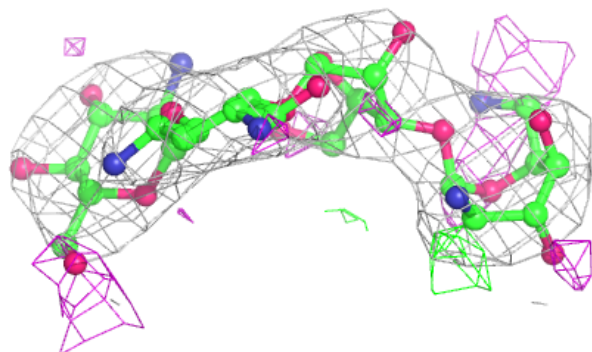
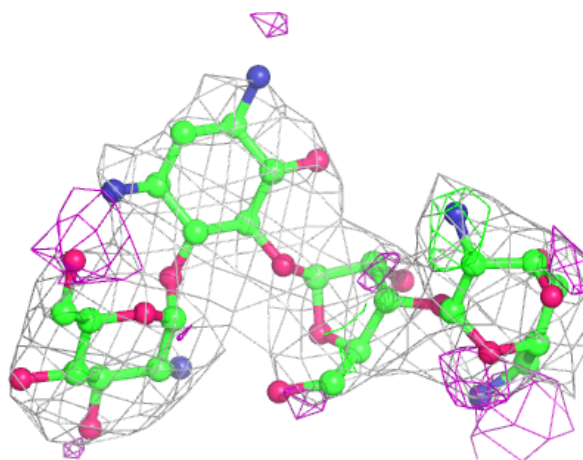
**Electron density around PAR A 1603:**

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



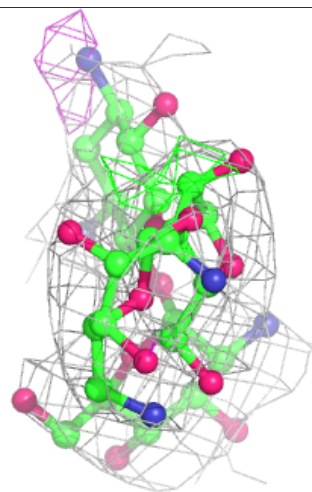
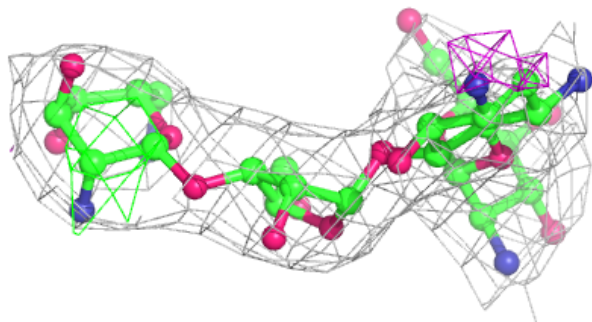
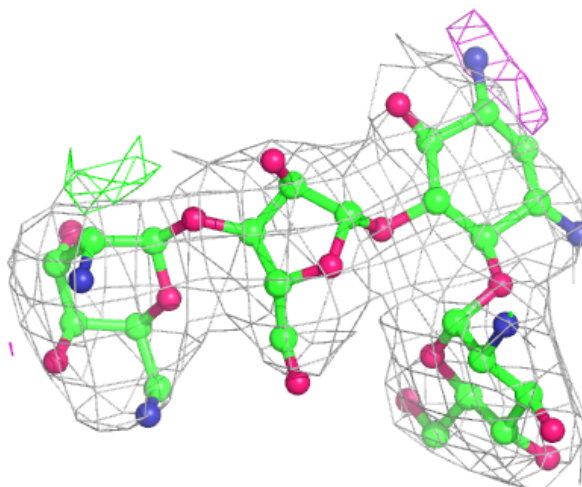
Electron density around PAR A 1602:

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



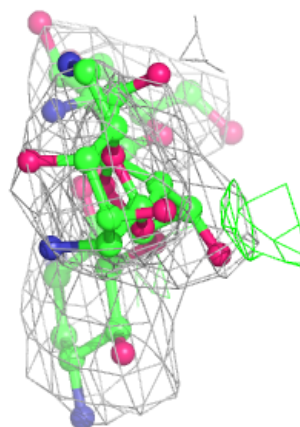
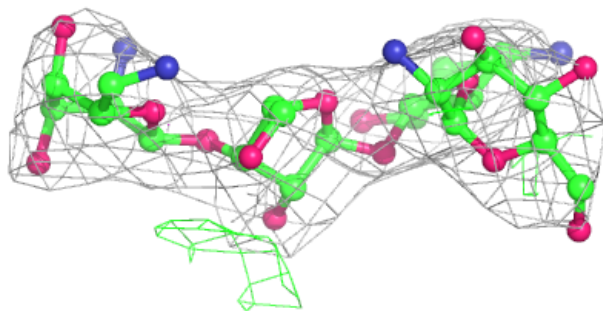
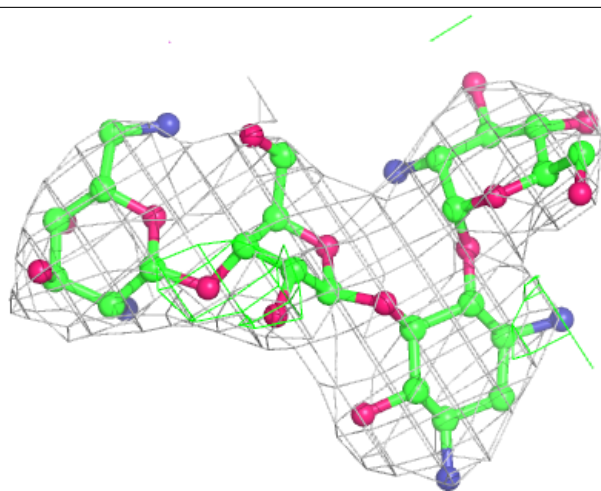
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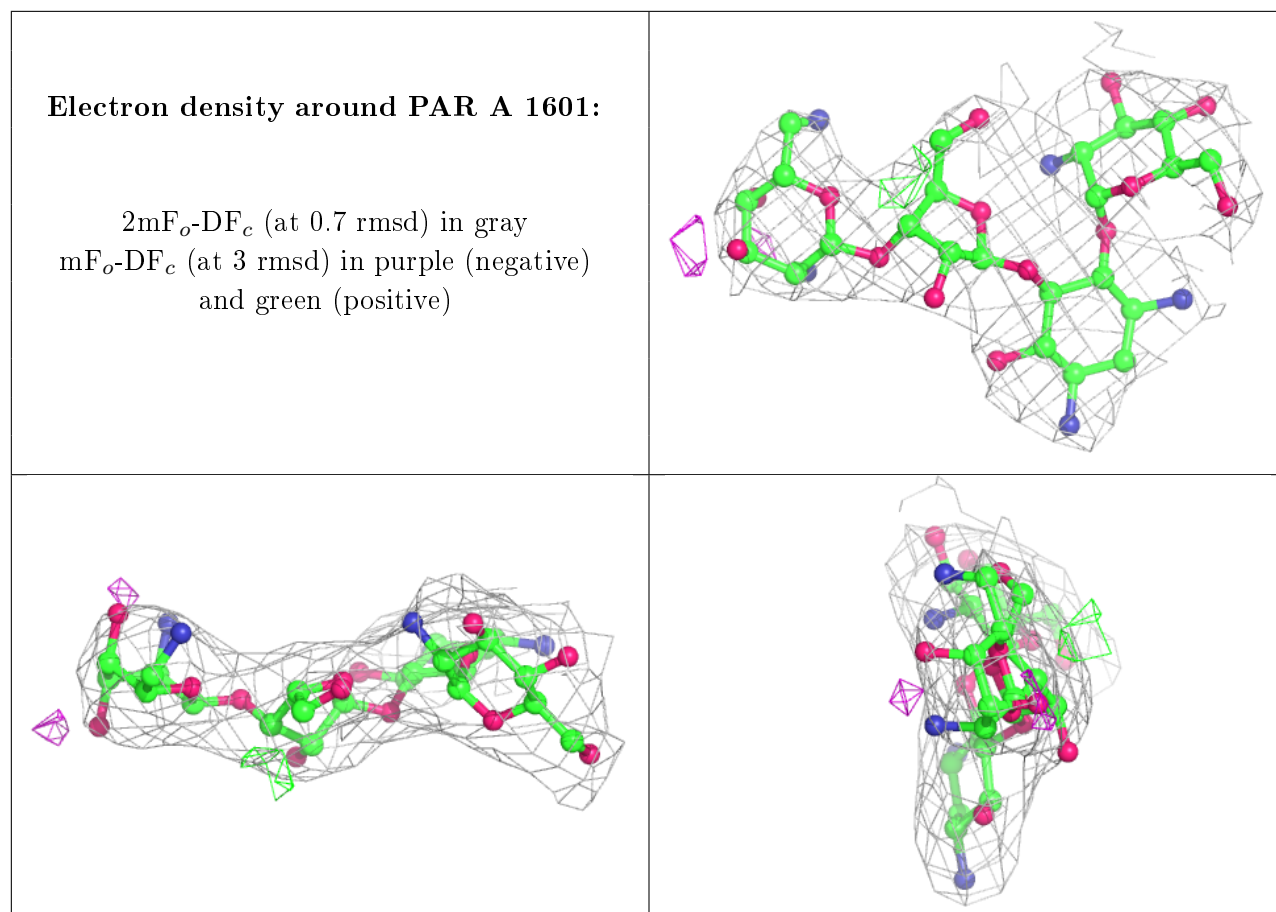
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around PAR A 1606:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.