



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 12:00 am BST

PDB ID : 4LF8  
Title : Crystal Structure of 30S ribosomal subunit from *Thermus thermophilus*  
Authors : Demirci, H.; Belardinelli, R.; Carr, J.; Murphy IV, F.; Jogl, G.; Dahlberg, A.E.; Gregory, S.T.  
Deposited on : 2013-06-26  
Resolution : 3.15 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

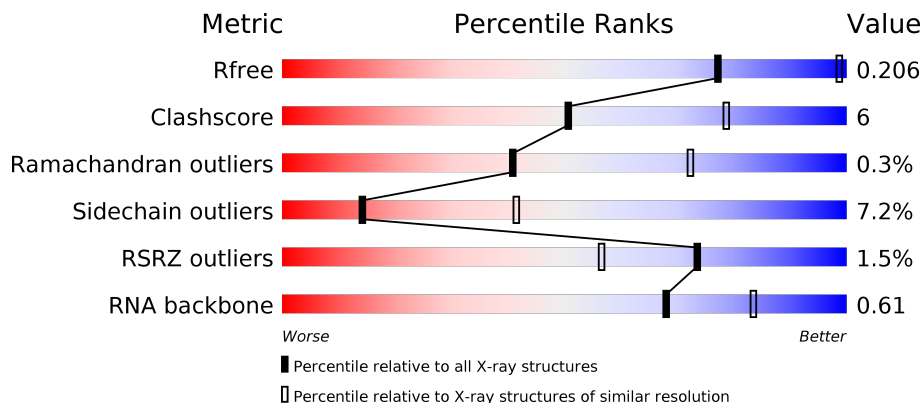
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.15 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.



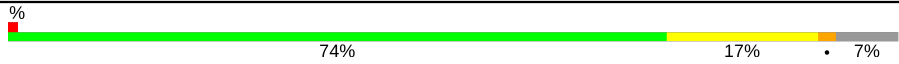





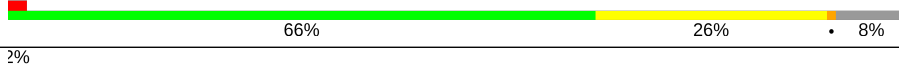

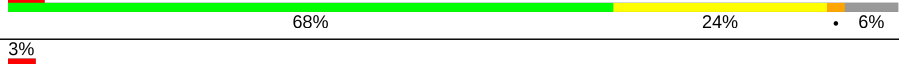


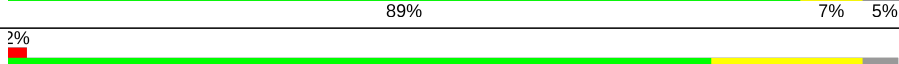

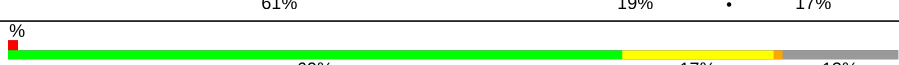

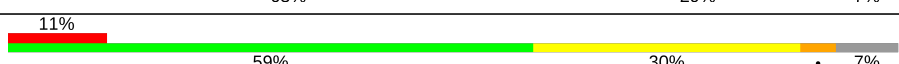

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1626 (3.18-3.10)
Clashscore	141614	1735 (3.18-3.10)
Ramachandran outliers	138981	1677 (3.18-3.10)
Sidechain outliers	138945	1677 (3.18-3.10)
RSRZ outliers	127900	1588 (3.18-3.10)
RNA backbone	3102	1000 (3.46-2.82)

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

Mol	Chain	Length	Quality of chain
1	A	1522	 69% 26% . .
2	B	256	 70% 22% 8%
3	C	239	 64% 22% . 13%
4	D	209	 79% 18% .

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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
1	PSU	A	1541	-	-	-	X
22	MG	A	1607	-	-	-	X
22	MG	A	1610	-	-	-	X
22	MG	A	1617	-	-	-	X
22	MG	A	1636	-	-	-	X
22	MG	A	1658	-	-	-	X
22	MG	A	1666	-	-	-	X
22	MG	A	1668	-	-	-	X

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<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
22	MG	A	1671	-	-	-	X
22	MG	A	1678	-	-	-	X
22	MG	A	1685	-	-	-	X
22	MG	A	1760	-	-	-	X
22	MG	A	1766	-	-	-	X
22	MG	A	1767	-	-	-	X
22	MG	A	1768	-	-	-	X
22	MG	A	1771	-	-	-	X
22	MG	A	1772	-	-	-	X
22	MG	A	1773	-	-	-	X
22	MG	A	1774	-	-	-	X
22	MG	A	1779	-	-	-	X
22	MG	A	1788	-	-	-	X
22	MG	A	1791	-	-	-	X
22	MG	A	1796	-	-	-	X
22	MG	D	304	-	-	-	X
23	K	A	1739	-	-	-	X
23	K	A	1754	-	-	-	X
23	K	A	1757	-	-	-	X

## 2 Entry composition i

There are 26 unique types of molecules in this entry. The entry contains 52220 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	1510	32460	14455	6006	10490	1509	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 ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	236	1874	1195	336	338	5	0	0	1

- Molecule 3 is a protein called 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 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 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 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 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 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 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 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 ribosomal protein S11.

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

- Molecule 12 is a protein called 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 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 ribosomal protein S14.

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

- Molecule 15 is a protein called 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 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 ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
17	Q	101	838	536	156	144	2	0	0	0

- Molecule 18 is a protein called 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 ribosomal protein S19.

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

- Molecule 20 is a protein called ribosomal protein S20.

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

- Molecule 21 is a protein called ribosomal protein THX.

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

- Molecule 22 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

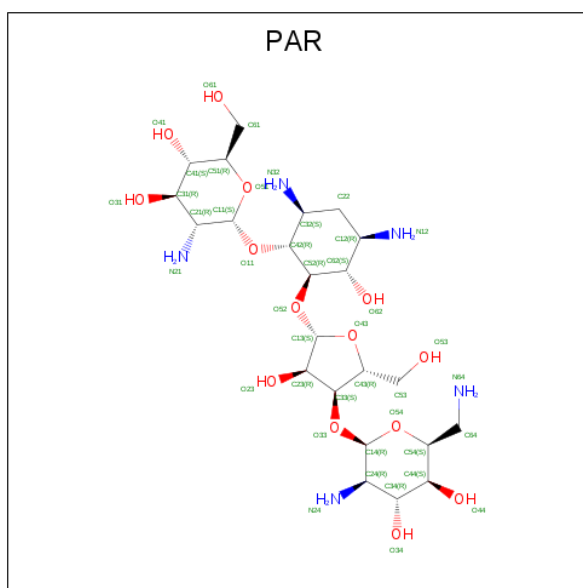
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	G	1	Total 1	Mg 1	0	0
22	D	3	Total 3	Mg 3	0	0
22	E	1	Total 1	Mg 1	0	0
22	H	1	Total 1	Mg 1	0	0
22	B	1	Total 1	Mg 1	0	0
22	C	1	Total 1	Mg 1	0	0
22	A	190	Total 190	Mg 190	0	0
22	T	1	Total 1	Mg 1	0	0
22	N	1	Total 1	Mg 1	0	0
22	L	1	Total 1	Mg 1	0	0
22	M	1	Total 1	Mg 1	0	0

- Molecule 23 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	A	19	Total 19	K 19	0	0
23	E	1	Total 1	K 1	0	0



- Molecule 24 is PAROMOMYCIN (three-letter code: PAR) (formula:  $C_{23}H_{45}N_5O_{14}$ ).



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

- Molecule 25 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

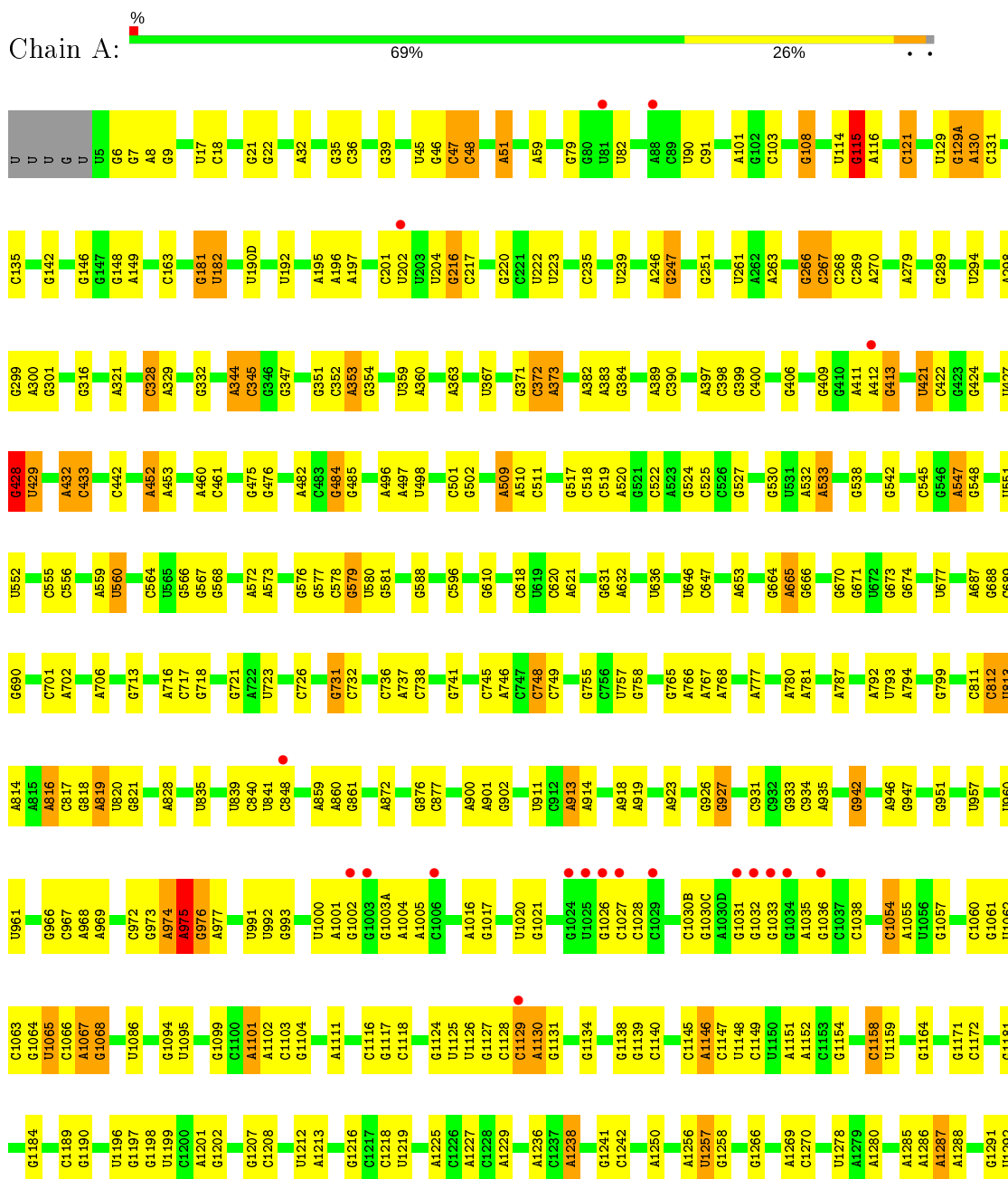
- Molecule 26 is water.

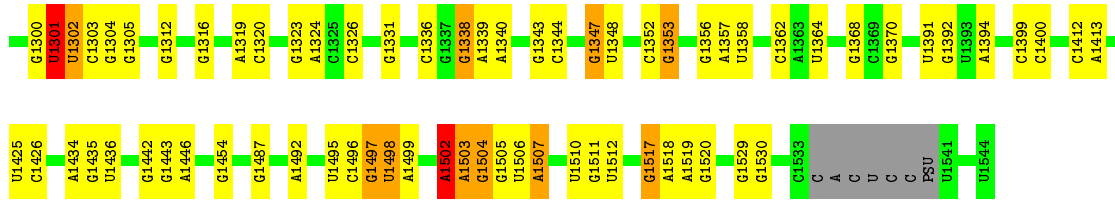
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
26	A	20	Total 20	O 20	0	0
26	H	4	Total 4	O 4	0	0

### 3 Residue-property plots

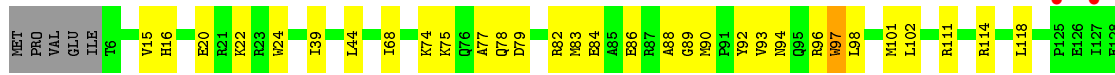
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

- Molecule 1: 16S rRNA

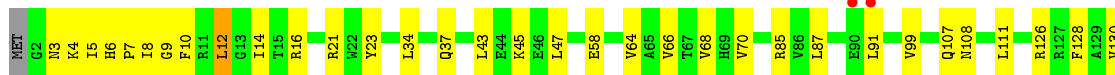




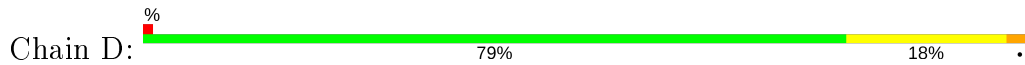
● Molecule 2: ribosomal protein S2



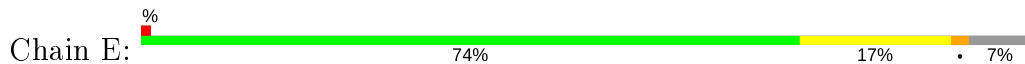
● Molecule 3: ribosomal protein S3

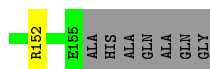


● Molecule 4: ribosomal protein S4

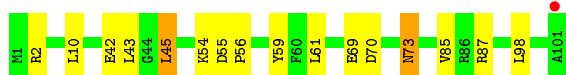
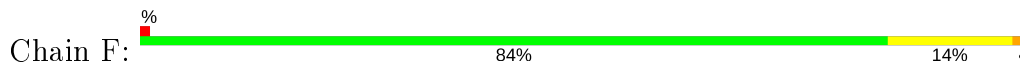


● Molecule 5: ribosomal protein S5

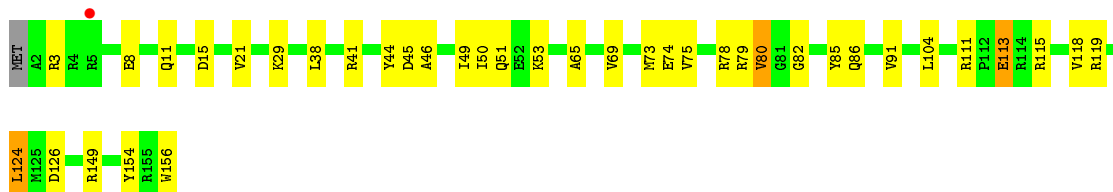
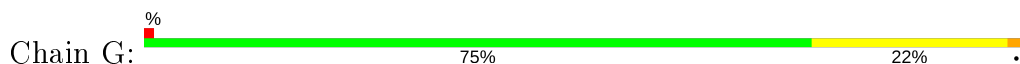




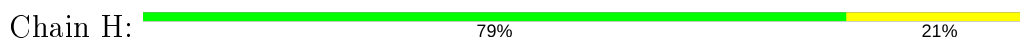
- Molecule 6: ribosomal protein S6



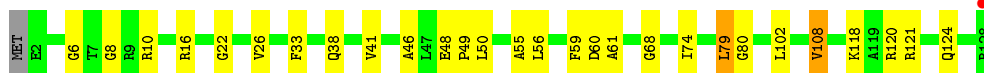
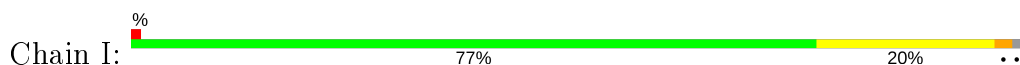
- Molecule 7: ribosomal protein S7



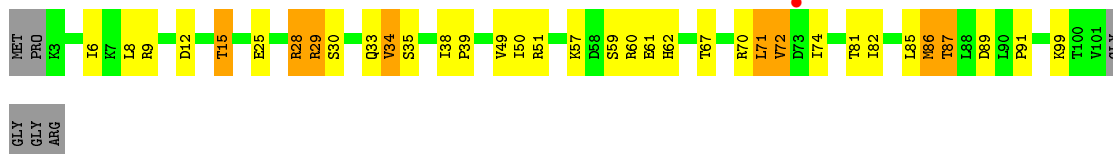
- Molecule 8: ribosomal protein S8



- Molecule 9: ribosomal protein S9



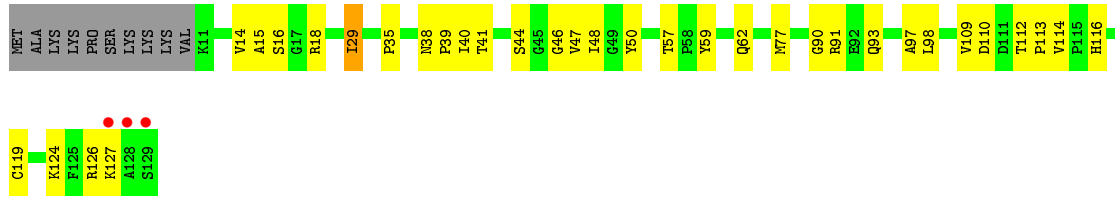
- Molecule 10: ribosomal protein S10



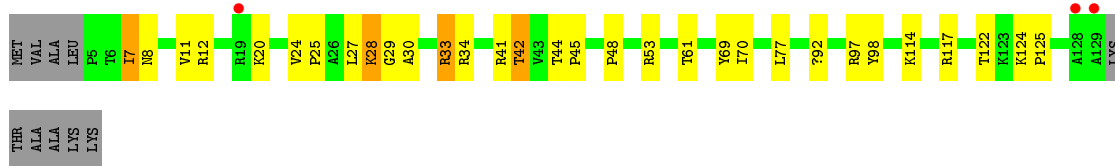
- Molecule 11: ribosomal protein S11



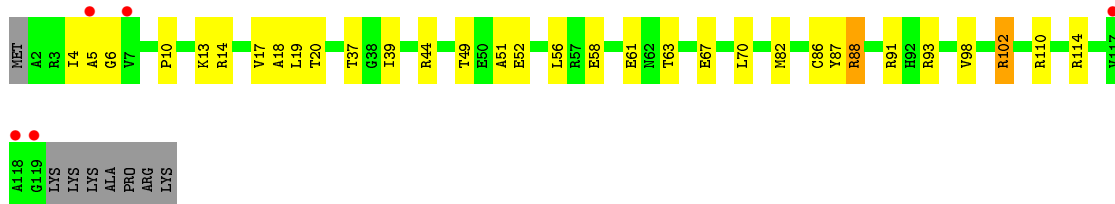
GLY  
GLY  
ARG



• Molecule 12: ribosomal protein S12



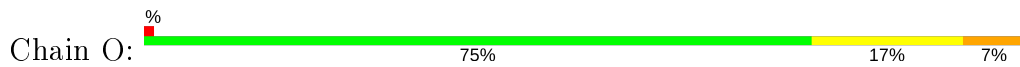
• Molecule 13: ribosomal protein S13



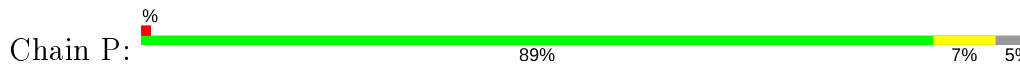
• Molecule 14: ribosomal protein S14



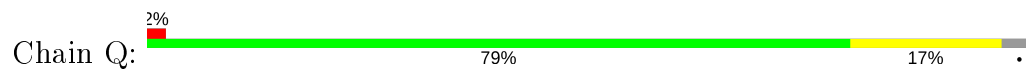
• Molecule 15: ribosomal protein S15



• Molecule 16: ribosomal protein S16



- Molecule 17: ribosomal protein S17



- Molecule 18: ribosomal protein S18



- Molecule 19: ribosomal protein S19



- Molecule 20: ribosomal protein S20



- Molecule 21: ribosomal protein THX



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	402.44Å 402.44Å 176.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.62 – 3.15 34.61 – 3.15	Depositor EDS
% Data completeness (in resolution range)	98.2 (34.62-3.15) 98.0 (34.61-3.15)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.72 (at 3.12Å)	Xtrriage
Refinement program	PHENIX dev_1119	Depositor
R, $R_{free}$	0.168 , 0.205 0.170 , 0.206	Depositor DCC
$R_{free}$ test set	12364 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	89.8	Xtrriage
Anisotropy	0.318	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 68.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	52220	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	105.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.92% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, K, 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	0.35	0/36067	0.82	27/56291 (0.0%)
2	B	0.28	0/1909	0.51	0/2579
3	C	0.28	0/1637	0.48	0/2207
4	D	0.32	0/1733	0.49	0/2318
5	E	0.34	0/1163	0.55	0/1566
6	F	0.25	0/856	0.46	0/1154
7	G	0.26	0/1276	0.45	0/1709
8	H	0.33	0/1136	0.52	0/1527
9	I	0.27	0/1029	0.51	0/1379
10	J	0.29	0/806	0.57	0/1084
11	K	0.28	0/900	0.54	0/1213
12	L	0.32	0/978	0.60	0/1308
13	M	0.25	0/947	0.48	0/1270
14	N	0.29	0/501	0.49	0/664
15	O	0.28	0/745	0.47	0/992
16	P	0.30	0/717	0.50	0/965
17	Q	0.32	0/851	0.58	0/1136
18	R	0.27	0/604	0.51	0/801
19	S	0.24	0/662	0.48	0/892
20	T	0.32	0/765	0.54	0/1007
21	U	0.25	0/213	0.46	0/279
All	All	0.33	0/55495	0.73	27/82341 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
8	H	0	1
10	J	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
18	R	0	1
All	All	0	3

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1054	C	N1-C2-O2	7.33	123.30	118.90
1	A	1054	C	C2-N1-C1'	6.98	126.48	118.80
1	A	328	C	N1-C2-O2	6.50	122.80	118.90
1	A	108	G	C4-C5-N7	6.35	113.34	110.80
1	A	1301	U	P-O3'-C3'	6.17	127.10	119.70
1	A	108	G	C5-N7-C8	-5.83	101.39	104.30
1	A	328	C	C2-N1-C1'	5.76	125.14	118.80
1	A	108	G	O4'-C1'-N9	5.74	112.80	108.20
1	A	108	G	C6-C5-N7	-5.60	127.04	130.40
1	A	913	A	P-O3'-C3'	5.48	126.27	119.70
1	A	432	A	OP1-P-O3'	5.40	117.07	105.20
1	A	975	A	O4'-C1'-N9	-5.39	103.89	108.20
1	A	484	G	P-O3'-C3'	5.33	126.10	119.70
1	A	1054	C	C6-N1-C1'	-5.31	114.43	120.80
1	A	108	G	C4-N9-C1'	5.30	133.39	126.50
1	A	1158	C	C2-N1-C1'	5.25	124.57	118.80
1	A	428	G	P-O3'-C3'	5.23	125.97	119.70
1	A	328	C	N3-C2-O2	-5.21	118.25	121.90
1	A	812	C	P-O3'-C3'	5.18	125.92	119.70
1	A	328	C	P-O3'-C3'	5.17	125.91	119.70
1	A	432	A	P-O3'-C3'	5.15	125.89	119.70
1	A	748	C	P-O3'-C3'	5.13	125.86	119.70
1	A	1067	A	P-O3'-C3'	5.10	125.81	119.70
1	A	1065	U	P-O3'-C3'	5.07	125.79	119.70
1	A	1502	A	C6-C5-N7	-5.05	128.77	132.30
1	A	108	G	N1-C6-O6	5.02	122.91	119.90
1	A	115	G	P-O3'-C3'	5.01	125.71	119.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	H	90	GLY	Peptide
10	J	87	THR	Peptide

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Mol	Chain	Res	Type	Group
18	R	20	ALA	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	32460	0	16405	221	0
2	B	1874	0	1887	28	0
3	C	1613	0	1677	33	0
4	D	1703	0	1763	25	0
5	E	1147	0	1207	17	0
6	F	843	0	857	10	0
7	G	1257	0	1296	20	0
8	H	1116	0	1177	14	0
9	I	1010	0	1037	17	0
10	J	793	0	835	30	0
11	K	885	0	904	19	0
12	L	973	0	1058	19	0
13	M	937	0	995	19	0
14	N	492	0	529	12	0
15	O	734	0	771	12	0
16	P	701	0	720	5	0
17	Q	838	0	907	10	0
18	R	598	0	670	15	0
19	S	648	0	673	8	0
20	T	763	0	861	20	0
21	U	209	0	221	9	0
22	A	190	0	0	0	0
22	B	1	0	0	0	0
22	C	1	0	0	0	0
22	D	3	0	0	0	0
22	E	1	0	0	0	0
22	G	1	0	0	0	0
22	H	1	0	0	0	0
22	L	1	0	0	0	0
22	M	1	0	0	0	0
22	N	1	0	0	0	0
22	T	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	A	19	0	0	0	0
23	E	1	0	0	0	0
24	A	378	0	405	16	0
25	D	1	0	0	0	0
25	N	1	0	0	0	0
26	A	20	0	0	0	0
26	H	4	0	0	0	0
All	All	52220	0	36855	498	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 6.

All (498) 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)
1:A:1086:U:H3	1:A:1099:G:H22	1.20	0.85
1:A:235:C:H5'	17:Q:70:ARG:HG2	1.59	0.83
1:A:1502:A:H2	1:A:1505:G:H1	1.25	0.81
2:B:75:LYS:HA	2:B:78:GLN:HB2	1.61	0.81
10:J:34:VAL:HG12	10:J:35:SER:H	1.44	0.81
5:E:78:HIS:HD2	8:H:107:LEU:HD12	1.42	0.81
1:A:975:A:H4'	1:A:976:G:H5''	1.63	0.81
1:A:279:A:OP2	17:Q:95:TYR:OH	2.01	0.79
4:D:32:ALA:HA	4:D:35:ARG:HB2	1.66	0.78
10:J:25:GLU:HA	10:J:28:ARG:HG2	1.65	0.77
11:K:15:ALA:HA	11:K:77:MET:HA	1.68	0.75
13:M:10:PRO:HB2	13:M:18:ALA:HB1	1.67	0.74
12:L:48:PRO:HD2	12:L:92:OTD:H8	1.69	0.74
1:A:427:U:OP1	4:D:13:ARG:NH2	2.21	0.73
18:R:21:LYS:HB3	18:R:24:ALA:HB3	1.70	0.73
1:A:821:G:N7	24:A:1811:PAR:H641	2.03	0.72
15:O:87:ILE:HG22	15:O:88:ARG:H	1.54	0.72
20:T:65:LYS:HA	20:T:68:LYS:HD3	1.71	0.72
9:I:46:ALA:HB2	9:I:74:ILE:HG23	1.71	0.71
1:A:664:G:H22	1:A:741:G:H1	1.38	0.71
2:B:84:GLU:HG2	2:B:215:LEU:HB3	1.71	0.70
1:A:835:U:OP1	18:R:64:ARG:NH2	2.24	0.70
1:A:542:G:OP1	4:D:10:ARG:NH2	2.23	0.70
24:A:1811:PAR:H241	24:A:1811:PAR:H43	1.58	0.69
1:A:266:G:H5'	1:A:268:C:H41	1.55	0.69
15:O:26:GLU:OE1	15:O:77:ARG:NH1	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:155:GLY:HA3	3:C:163:ALA:HB1	1.75	0.68
1:A:1326:C:OP2	21:U:6:ARG:NH2	2.27	0.68
11:K:57:THR:HG22	11:K:59:TYR:H	1.58	0.68
5:E:81:GLU:HG2	5:E:90:VAL:HG22	1.76	0.68
1:A:1028:C:H42	1:A:1033:G:H1	1.40	0.68
3:C:6:HIS:HD2	3:C:9:GLY:H	1.43	0.67
1:A:517:G:N1	1:A:533:A:OP2	2.26	0.67
15:O:39:LEU:HD12	15:O:56:LEU:HB2	1.74	0.67
10:J:34:VAL:HG13	10:J:74:ILE:HA	1.76	0.67
20:T:75:ASN:N	20:T:75:ASN:OD1	2.27	0.67
1:A:560:U:H5'	1:A:566:G:N2	2.10	0.67
1:A:1128:C:O2'	1:A:1130:A:OP1	2.13	0.66
3:C:21:ARG:HB2	3:C:58:GLU:HG2	1.78	0.65
3:C:91:LEU:HB3	3:C:99:VAL:HG21	1.78	0.65
1:A:1189:C:H5''	3:C:5:ILE:HG12	1.78	0.65
24:A:1818:PAR:H241	24:A:1818:PAR:H33	1.61	0.64
3:C:177:THR:HG23	3:C:180:ALA:HB2	1.78	0.64
3:C:156:ARG:H	3:C:163:ALA:HA	1.61	0.64
1:A:818:G:H3'	1:A:819:A:H5''	1.79	0.64
13:M:13:LYS:HA	13:M:44:ARG:HH11	1.63	0.64
1:A:946:A:H2'	1:A:947:G:C8	2.33	0.63
14:N:12:ARG:H	14:N:12:ARG:HD2	1.63	0.63
9:I:22:GLY:HA3	9:I:60:ASP:HB2	1.81	0.62
9:I:8:GLY:HA2	9:I:79:LEU:HD13	1.81	0.62
1:A:372:C:H4'	1:A:373:A:O5'	1.98	0.62
1:A:580:U:H2'	1:A:581:G:O4'	2.00	0.62
1:A:975:A:H5'	1:A:975:A:H8	1.64	0.62
5:E:98:THR:HB	5:E:117:ASP:HB3	1.80	0.61
1:A:1278:U:O4	10:J:99:LYS:NZ	2.30	0.61
13:M:6:GLY:HA3	13:M:67:GLU:HG3	1.80	0.61
1:A:1502:A:H2	1:A:1505:G:N1	1.97	0.61
3:C:6:HIS:CD2	3:C:8:ILE:HB	2.36	0.61
7:G:15:ASP:OD2	7:G:44:TYR:OH	2.17	0.61
1:A:1392:G:H21	1:A:1502:A:H8	1.47	0.61
1:A:1003(A):G:N2	1:A:1038:C:O2	2.34	0.60
13:M:4:ILE:HG22	13:M:5:ALA:H	1.67	0.60
20:T:50:GLU:HA	20:T:100:ILE:HB	1.84	0.60
1:A:664:G:OP1	18:R:64:ARG:NH1	2.35	0.60
1:A:1151:A:HO2'	1:A:1152:A:H8	1.50	0.60
1:A:1392:G:N2	1:A:1502:A:H8	2.01	0.59
1:A:266:G:H5''	1:A:267:C:C5	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:10:LEU:HD22	8:H:83:ILE:HD11	1.85	0.59
10:J:89:ASP:HB2	10:J:91:PRO:HD3	1.85	0.58
18:R:22:VAL:HB	18:R:56:THR:HA	1.83	0.58
2:B:77:ALA:HB2	2:B:211:ILE:HD13	1.83	0.58
5:E:102:ALA:O	5:E:107:ARG:NH1	2.36	0.58
11:K:90:GLY:HA2	11:K:93:GLN:HB2	1.84	0.58
3:C:150:LYS:HG3	3:C:169:ALA:HB2	1.84	0.58
7:G:113:GLU:HG2	7:G:119:ARG:HG2	1.85	0.58
9:I:26:VAL:HB	9:I:33:PHE:HB2	1.84	0.58
11:K:18:ARG:NH1	11:K:35:PRO:O	2.37	0.57
4:D:57:ARG:HB3	4:D:206:PHE:HB2	1.86	0.57
8:H:83:ILE:HG13	8:H:137:VAL:HG22	1.86	0.57
1:A:344:A:H5'	1:A:345:C:H5	1.70	0.57
1:A:353:A:H5'	1:A:353:A:H8	1.70	0.57
3:C:134:ILE:HG22	3:C:168:ALA:HB3	1.85	0.57
3:C:8:ILE:HG23	3:C:16:ARG:HG2	1.84	0.57
20:T:92:LEU:O	20:T:96:GLY:HA2	2.04	0.57
1:A:1250:A:H4'	9:I:68:GLY:N	2.20	0.57
1:A:51:A:OP2	24:A:1813:PAR:H24	2.04	0.57
2:B:24:TRP:HB2	2:B:190:THR:HG22	1.85	0.57
1:A:670:G:H21	6:F:73:ASN:HD21	1.53	0.56
10:J:50:ILE:HD11	10:J:57:LYS:HD2	1.87	0.56
20:T:67:ALA:HA	20:T:73:HIS:H	1.69	0.56
5:E:152:ARG:NH2	8:H:107:LEU:O	2.38	0.56
12:L:8:ASN:O	12:L:12:ARG:HG3	2.06	0.56
12:L:24:VAL:HG13	12:L:98:TYR:HE2	1.70	0.56
3:C:12:LEU:HD11	14:N:51:GLY:HA2	1.88	0.56
20:T:10:LEU:HG	20:T:12:ALA:H	1.71	0.56
1:A:316:G:OP2	1:A:351:G:O2'	2.24	0.56
5:E:50:GLU:HG3	5:E:52:PRO:HD2	1.87	0.56
18:R:38:GLU:HA	18:R:41:LYS:HE2	1.88	0.56
1:A:967:5MC:H2'	1:A:968:A:N7	2.21	0.55
6:F:70:ASP:N	6:F:70:ASP:OD1	2.39	0.55
11:K:40:ILE:HG22	11:K:41:THR:HG23	1.87	0.55
1:A:1435:G:H2'	1:A:1436:U:C6	2.40	0.55
13:M:37:THR:HG23	13:M:39:ILE:HG13	1.87	0.55
3:C:131:ARG:NE	3:C:166:GLU:OE2	2.40	0.55
4:D:49:ARG:HD2	4:D:49:ARG:H	1.70	0.55
1:A:716:A:OP2	24:A:1816:PAR:O61	2.22	0.55
1:A:522:C:OP2	12:L:69:TYR:OH	2.22	0.55
19:S:50:ALA:HB1	19:S:57:HIS:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1518:A:H2'	1:A:1519:A:C8	2.42	0.55
2:B:15:VAL:HG13	2:B:203:GLY:HA2	1.89	0.54
1:A:1236:A:H4'	1:A:1304:G:H4'	1.90	0.54
3:C:5:ILE:HD13	3:C:10:PHE:HB2	1.89	0.54
12:L:24:VAL:HG13	12:L:98:TYR:CE2	2.42	0.54
16:P:18:ARG:HD3	16:P:35:LYS:HD2	1.90	0.54
1:A:1190:G:N7	24:A:1817:PAR:H642	2.23	0.54
1:A:1266:G:N2	1:A:1269:A:OP2	2.38	0.54
1:A:538:G:H5''	12:L:114:LYS:HB2	1.89	0.54
1:A:8:A:C6	4:D:209:ARG:HB2	2.43	0.54
12:L:27:LEU:O	12:L:29:GLY:N	2.41	0.54
14:N:16:PHE:HB2	14:N:19:ARG:HG3	1.89	0.54
10:J:49:VAL:HG13	14:N:41:ARG:HB2	1.90	0.54
24:A:1813:PAR:O44	24:A:1813:PAR:N64	2.41	0.53
2:B:193:ASP:HB3	2:B:196:LEU:HD12	1.90	0.53
4:D:4:TYR:HB3	4:D:115:ARG:HH12	1.73	0.53
1:A:581:G:O3'	15:O:64:ARG:NH2	2.42	0.53
1:A:1104:G:O5'	2:B:111:ARG:HD2	2.08	0.53
1:A:48:C:OP1	24:A:1813:PAR:H62	2.09	0.53
1:A:1127:G:H21	1:A:1147:C:N4	2.06	0.53
1:A:1510:U:H2'	1:A:1511:G:C8	2.43	0.53
1:A:427:U:OP2	4:D:36:ARG:NH2	2.38	0.53
1:A:382:A:H2'	1:A:383:A:C8	2.44	0.53
1:A:413:G:N2	1:A:429:U:OP2	2.23	0.53
1:A:1347:G:N7	9:I:10:ARG:NH2	2.56	0.53
1:A:299:G:H2'	1:A:300:A:C8	2.44	0.53
1:A:718:G:C8	11:K:116:HIS:HB3	2.44	0.53
1:A:673:G:H2'	1:A:674:G:C8	2.43	0.53
1:A:923:A:OP1	5:E:21:ALA:HB2	2.08	0.53
1:A:1001:A:H2'	1:A:1002:G:C8	2.44	0.52
1:A:45:U:H2'	1:A:46:G:C8	2.43	0.52
10:J:6:ILE:HB	10:J:72:VAL:HB	1.91	0.52
16:P:81:ARG:HE	16:P:83:GLU:HG3	1.75	0.52
4:D:64:LEU:HG	4:D:198:VAL:HG11	1.91	0.52
3:C:174:PRO:HB2	3:C:177:THR:HG22	1.92	0.52
8:H:113:SER:HB2	8:H:134:ILE:HD11	1.91	0.52
14:N:33:VAL:HA	14:N:40:CYS:HA	1.91	0.52
1:A:390:C:H4'	16:P:28:ARG:HH21	1.75	0.52
2:B:20:GLU:HA	2:B:39:ILE:HD13	1.91	0.52
1:A:17:U:H2'	1:A:18:C:C6	2.45	0.52
1:A:35:G:H2'	1:A:36:C:C6	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:88:ARG:HG3	13:M:98:VAL:HB	1.92	0.52
7:G:111:ARG:NH2	7:G:126:ASP:OD2	2.43	0.52
17:Q:41:LYS:NZ	17:Q:88:TYR:OH	2.43	0.52
1:A:363:A:H62	12:L:28:LYS:HE3	1.75	0.52
2:B:83:MET:HA	2:B:86:GLU:HB2	1.92	0.52
10:J:8:LEU:HB2	10:J:70:ARG:HB2	1.91	0.52
1:A:1064:G:H1'	1:A:1190:G:N2	2.25	0.52
2:B:88:ALA:O	2:B:90:MET:N	2.42	0.52
1:A:942:G:H21	9:I:124:GLN:NE2	2.08	0.52
1:A:1190:G:OP1	3:C:4:LYS:HA	2.10	0.51
1:A:951:G:OP2	13:M:102:ARG:NH2	2.43	0.51
8:H:6:ILE:HD11	8:H:31:PHE:HD2	1.75	0.51
2:B:223:ILE:HD13	2:B:230:VAL:H	1.74	0.51
15:O:11:VAL:HG11	15:O:34:LEU:HD12	1.93	0.51
2:B:212:GLN:HE21	2:B:235:SER:HB2	1.75	0.51
4:D:175:SER:HB3	4:D:186:LEU:HD11	1.92	0.51
1:A:860:A:H2'	1:A:861:G:O4'	2.11	0.51
5:E:76:ILE:HG23	5:E:78:HIS:H	1.76	0.51
18:R:18:ARG:HA	18:R:18:ARG:HH11	1.76	0.51
5:E:12:LEU:HD13	5:E:31:LEU:HB2	1.92	0.51
18:R:47:THR:HG22	18:R:48:GLY:H	1.76	0.51
1:A:1218:C:H2'	1:A:1219:U:C6	2.46	0.51
2:B:84:GLU:HG3	2:B:219:VAL:HG21	1.92	0.51
7:G:79:ARG:NH2	7:G:82:GLY:H	2.09	0.51
1:A:1035:A:H2'	1:A:1036:G:H8	1.77	0.50
4:D:9:CYS:HA	4:D:12:CYS:HB2	1.93	0.50
1:A:1323:G:H2'	1:A:1324:A:C8	2.47	0.50
24:A:1817:PAR:O43	24:A:1817:PAR:N21	2.44	0.50
1:A:933:G:O6	7:G:3:ARG:NH2	2.44	0.50
1:A:1225:A:N3	1:A:1225:A:H2'	2.25	0.50
1:A:1305:G:N2	1:A:1331:G:H1'	2.26	0.50
11:K:110:ASP:HB2	18:R:88:LYS:HE2	1.92	0.50
1:A:1145:C:H4'	1:A:1146:A:H5'	1.93	0.50
1:A:765:G:N2	1:A:813:U:OP2	2.40	0.50
2:B:129:GLU:O	2:B:130:ARG:HB2	2.11	0.50
3:C:126:ARG:HE	3:C:128:PHE:HD1	1.60	0.50
1:A:181:G:H4'	1:A:182:U:H5'	1.94	0.50
12:L:117:ARG:HB3	12:L:122:THR:HB	1.94	0.50
1:A:47:C:OP1	24:A:1813:PAR:N32	2.45	0.49
4:D:102:ASP:OD1	4:D:103:ASN:N	2.46	0.49
19:S:36:ARG:NH2	19:S:75:ALA:O	2.36	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1001:A:H2'	1:A:1002:G:H8	1.77	0.49
1:A:371:G:O2'	1:A:372:C:H5'	2.12	0.49
20:T:65:LYS:O	20:T:68:LYS:HB2	2.12	0.49
2:B:98:LEU:HB2	2:B:101:MET:HG3	1.93	0.49
1:A:1291:G:O2'	9:I:38:GLN:HG3	2.13	0.49
6:F:10:LEU:HB2	6:F:59:TYR:HB3	1.95	0.49
10:J:12:ASP:O	10:J:15:THR:HG22	2.12	0.49
21:U:14:TRP:HE3	21:U:15:ARG:HG3	1.78	0.49
2:B:132:LYS:HD2	2:B:136:VAL:HG23	1.95	0.49
2:B:74:LYS:HD2	2:B:166:ASP:HB2	1.95	0.49
5:E:78:HIS:CD2	8:H:107:LEU:HD12	2.34	0.49
1:A:409:G:H1	1:A:433:C:H42	1.61	0.49
4:D:32:ALA:O	4:D:36:ARG:N	2.36	0.49
1:A:269:C:H2'	1:A:270:A:C8	2.47	0.48
1:A:820:U:H4'	1:A:821:G:OP2	2.12	0.48
7:G:78:ARG:NH1	7:G:154:TYR:O	2.46	0.48
13:M:5:ALA:HB2	13:M:61:GLU:HG2	1.95	0.48
1:A:646:U:H2'	1:A:647:C:C6	2.48	0.48
7:G:115:ARG:HD2	7:G:118:VAL:HG23	1.95	0.48
1:A:390:C:O3'	16:P:28:ARG:NH2	2.46	0.48
1:A:7:G:H5'	1:A:298:A:O4'	2.13	0.48
1:A:1497:G:H2'	1:A:1498:UR3:H5'	1.95	0.48
1:A:1068:G:OP2	1:A:1068:G:H8	1.97	0.48
3:C:68:VAL:HG12	3:C:70:VAL:HG23	1.95	0.48
12:L:25:PRO:C	12:L:27:LEU:H	2.18	0.48
1:A:665:A:H2'	1:A:732:C:O2	2.13	0.48
20:T:67:ALA:O	20:T:73:HIS:ND1	2.47	0.48
24:A:1818:PAR:N24	24:A:1818:PAR:H33	2.27	0.47
2:B:132:LYS:HD3	2:B:135:GLN:HB2	1.94	0.47
1:A:452:A:HO2'	1:A:453:A:H8	1.62	0.47
3:C:155:GLY:O	3:C:196:LEU:HD22	2.14	0.47
1:A:1164:G:H1	1:A:1172:C:H42	1.61	0.47
24:A:1813:PAR:O52	24:A:1813:PAR:H11	2.14	0.47
1:A:1216:G:H5''	14:N:5:ALA:HB2	1.95	0.47
1:A:1031:G:H2'	1:A:1032:G:H8	1.79	0.47
1:A:1207:2MG:HM23	1:A:1208:C:H1'	1.97	0.47
10:J:34:VAL:HG12	10:J:35:SER:N	2.22	0.47
15:O:85:LEU:HD13	15:O:87:ILE:HD11	1.95	0.47
1:A:620:C:C2	4:D:135:LEU:HD13	2.49	0.47
1:A:421:U:H5'	1:A:422:C:H5	1.80	0.47
1:A:911:U:OP2	12:L:97:ARG:NH1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:967:5MC:H2'	1:A:968:A:C8	2.50	0.47
12:L:41:ARG:HG2	12:L:42:THR:H	1.80	0.47
15:O:45:VAL:HG12	15:O:46:HIS:H	1.80	0.47
1:A:1111:A:N1	3:C:177:THR:HB	2.30	0.47
1:A:1287:A:H2'	1:A:1288:A:C8	2.50	0.47
3:C:43:LEU:HD12	3:C:47:LEU:HD22	1.96	0.47
1:A:767:A:H2'	1:A:768:A:O4'	2.15	0.47
10:J:6:ILE:HD12	10:J:72:VAL:HG11	1.97	0.47
1:A:222:U:H2'	1:A:223:U:C6	2.50	0.47
11:K:38:ASN:HA	11:K:39:PRO:HD3	1.84	0.47
5:E:43:LEU:HD11	5:E:132:ALA:HB1	1.97	0.46
7:G:38:LEU:HA	7:G:41:ARG:HB2	1.98	0.46
9:I:60:ASP:OD2	9:I:61:ALA:N	2.48	0.46
1:A:1241:G:H2'	1:A:1242:C:C6	2.50	0.46
1:A:975:A:H5'	1:A:975:A:C8	2.47	0.46
1:A:976:G:H5'	1:A:1358:U:O2'	2.15	0.46
1:A:359:U:H2'	1:A:360:A:C8	2.50	0.46
6:F:2:ARG:NH2	6:F:69:GLU:HG2	2.30	0.46
6:F:45:LEU:HD23	6:F:45:LEU:H	1.81	0.46
7:G:46:ALA:O	7:G:50:ILE:HG12	2.15	0.46
1:A:1343:G:H2'	1:A:1344:C:C6	2.51	0.46
1:A:1412:C:H2'	1:A:1413:A:C8	2.50	0.46
1:A:519:C:H2'	1:A:520:A:C8	2.50	0.46
4:D:150:GLU:N	4:D:150:GLU:OE2	2.44	0.46
19:S:15:LEU:HA	19:S:18:LYS:HD2	1.96	0.46
1:A:142:G:O2'	1:A:196:A:N1	2.43	0.46
12:L:27:LEU:HG	12:L:28:LYS:H	1.81	0.46
1:A:524:G:H2'	1:A:525:C:C6	2.51	0.46
7:G:45:ASP:O	7:G:49:ILE:HG13	2.16	0.46
5:E:140:ARG:O	5:E:143:ARG:NH2	2.49	0.46
7:G:78:ARG:HH11	7:G:154:TYR:HB3	1.80	0.46
10:J:28:ARG:HD3	10:J:28:ARG:HA	1.58	0.46
17:Q:27:PHE:CE1	17:Q:36:ILE:HD11	2.51	0.46
1:A:1057:G:H5'	3:C:154:SER:CB	2.46	0.46
1:A:1356:G:H2'	1:A:1357:A:C8	2.50	0.46
1:A:1292:U:OP1	7:G:41:ARG:NH2	2.49	0.46
13:M:91:ARG:HB2	13:M:98:VAL:HG12	1.97	0.46
13:M:82:MET:HB3	13:M:93:ARG:NH2	2.31	0.46
3:C:130:VAL:O	3:C:134:ILE:HG13	2.15	0.46
11:K:109:VAL:HG11	18:R:84:LYS:HD3	1.98	0.46
7:G:51:GLN:C	7:G:53:LYS:H	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:49:THR:HB	13:M:52:GLU:HG2	1.98	0.45
1:A:239:U:O4	24:A:1812:PAR:H642	2.17	0.45
1:A:509:A:H5'	4:D:54:TYR:HD2	1.80	0.45
8:H:64:LYS:HG2	8:H:79:VAL:HG21	1.98	0.45
1:A:1148:U:H2'	1:A:1149:C:O4'	2.16	0.45
1:A:927:G:O2'	1:A:1503:A:N7	2.38	0.45
14:N:58:LYS:HB3	14:N:58:LYS:HE2	1.74	0.45
1:A:1425:U:H2'	1:A:1426:C:C6	2.52	0.45
1:A:1301:U:O2'	1:A:1302:U:O5'	2.33	0.45
1:A:1103:C:OP1	2:B:96:ARG:NH1	2.49	0.45
1:A:1504:G:OP1	1:A:1507:A:H4'	2.17	0.45
1:A:738:C:H5''	6:F:69:GLU:HB3	1.99	0.45
10:J:51:ARG:CZ	10:J:61:GLU:HB2	2.46	0.45
1:A:399:G:H2'	1:A:400:C:C6	2.51	0.45
1:A:677:U:H3	1:A:713:G:H22	1.65	0.45
1:A:706:A:H1'	11:K:29:ILE:HD11	1.98	0.45
11:K:14:VAL:HG21	11:K:40:ILE:HD11	1.99	0.45
1:A:6:G:H4'	1:A:298:A:H4'	1.99	0.45
2:B:16:HIS:HB3	2:B:44:LEU:HD21	1.99	0.45
1:A:1348:U:H4'	9:I:120:ARG:HG3	1.98	0.45
17:Q:100:LYS:HE2	17:Q:100:LYS:HB3	1.75	0.45
8:H:34:GLU:OE2	8:H:37:ARG:NH1	2.50	0.44
1:A:1303:C:H2'	1:A:1304:G:H5'	1.98	0.44
9:I:6:GLY:HA3	9:I:80:GLY:O	2.18	0.44
10:J:57:LYS:HG3	10:J:60:ARG:HH21	1.82	0.44
10:J:82:ILE:HA	10:J:85:LEU:HB2	1.98	0.44
15:O:27:VAL:HG12	15:O:31:LEU:HD22	2.00	0.44
1:A:1339:A:H2'	1:A:1340:A:O4'	2.17	0.44
21:U:6:ARG:CZ	21:U:15:ARG:HH22	2.30	0.44
17:Q:64:PRO:HB3	17:Q:70:ARG:NE	2.33	0.44
1:A:976:G:OP2	1:A:1358:U:O2'	2.32	0.44
3:C:6:HIS:HA	3:C:7:PRO:HD3	1.84	0.44
6:F:2:ARG:CZ	6:F:69:GLU:HG2	2.48	0.44
2:B:178:ARG:NH2	8:H:74:PRO:HG3	2.33	0.44
11:K:44:SER:H	11:K:47:VAL:HB	1.82	0.44
15:O:70:LEU:HD13	15:O:78:TYR:HA	1.99	0.44
20:T:59:ALA:O	20:T:63:ILE:HG13	2.16	0.44
11:K:112:THR:HA	11:K:113:PRO:HD3	1.80	0.44
1:A:1229:A:OP2	13:M:114:ARG:HD3	2.18	0.44
19:S:5:LEU:HG	19:S:6:LYS:H	1.83	0.44
1:A:1285:A:H4'	1:A:1286:A:O5'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1497:G:C2'	1:A:1498:UR3:H5'	2.47	0.43
2:B:74:LYS:NZ	2:B:206:ASP:HA	2.33	0.43
17:Q:67:LYS:HA	17:Q:70:ARG:HH12	1.83	0.43
18:R:47:THR:HA	18:R:83:GLU:HB2	2.00	0.43
20:T:40:ALA:HB2	20:T:55:ILE:HG22	1.99	0.43
1:A:1101:A:H4'	1:A:1102:A:O5'	2.18	0.43
1:A:1111:A:H4'	2:B:133:LYS:HE2	2.00	0.43
3:C:178:LEU:HA	3:C:178:LEU:HD13	1.80	0.43
14:N:26:ARG:NH2	14:N:46:GLU:OE1	2.52	0.43
1:A:192:U:O4'	20:T:103:GLY:HA2	2.19	0.43
1:A:130:A:H1'	1:A:263:A:O2'	2.18	0.43
3:C:155:GLY:HA2	3:C:164:ARG:H	1.83	0.43
1:A:620:C:N1	4:D:135:LEU:HD13	2.34	0.43
10:J:57:LYS:HE2	10:J:60:ARG:NH2	2.33	0.43
12:L:33:ARG:HA	12:L:33:ARG:HD2	1.73	0.43
13:M:39:ILE:HD12	13:M:56:LEU:HD12	2.00	0.43
19:S:25:LYS:HE3	19:S:25:LYS:HB2	1.87	0.43
19:S:80:TYR:CE1	19:S:81:ARG:HD3	2.53	0.43
4:D:162:LEU:HD23	4:D:162:LEU:HA	1.85	0.43
11:K:16:SER:O	11:K:35:PRO:HD3	2.18	0.43
1:A:1316:G:H4'	14:N:18:VAL:HG11	2.00	0.43
1:A:1020:U:H2'	1:A:1021:G:H8	1.83	0.43
1:A:1030(B):C:H2'	1:A:1030(C):G:O4'	2.19	0.43
1:A:192:U:C1'	20:T:103:GLY:HA2	2.48	0.43
5:E:33:VAL:HG11	5:E:109:ILE:HA	2.00	0.43
7:G:74:GLU:HG2	7:G:91:VAL:HG22	2.00	0.43
12:L:34:ARG:O	12:L:61:THR:HG23	2.18	0.43
14:N:5:ALA:O	14:N:8:GLU:HG3	2.18	0.43
15:O:5:LYS:HA	15:O:5:LYS:HE3	2.01	0.43
5:E:45:PHE:CE2	5:E:47:LYS:HD2	2.54	0.43
8:H:20:TYR:CE2	8:H:75:ARG:HD2	2.53	0.43
10:J:38:ILE:HB	10:J:71:LEU:HB2	2.01	0.43
20:T:36:LEU:HA	20:T:36:LEU:HD23	1.78	0.43
1:A:114:U:O2'	1:A:115:G:H5'	2.19	0.43
1:A:266:G:H5''	1:A:267:C:H5	1.81	0.43
13:M:19:LEU:HD21	13:M:56:LEU:HD21	2.01	0.43
13:M:87:TYR:CZ	13:M:91:ARG:HD3	2.54	0.43
1:A:129:U:O3'	1:A:129(A):G:H3'	2.18	0.43
1:A:192:U:H4'	20:T:57:ARG:HD3	2.00	0.43
1:A:501:C:H2'	1:A:502:G:C8	2.54	0.43
1:A:578:C:H2'	1:A:579:G:O4'	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1147:C:O2	9:I:16:ARG:NH1	2.52	0.43
9:I:56:LEU:O	9:I:59:PHE:N	2.35	0.43
1:A:736:C:H2'	1:A:737:A:C8	2.54	0.43
1:A:973:G:H3'	1:A:974:A:H5''	2.01	0.43
3:C:6:HIS:NE2	3:C:8:ILE:HB	2.34	0.43
19:S:22:LEU:HD11	19:S:31:ILE:HD11	2.01	0.43
1:A:1054:C:O2'	1:A:1055:A:H5''	2.19	0.43
1:A:1062:U:H2'	1:A:1063:C:C6	2.54	0.43
1:A:389:A:C6	1:A:390:C:H1'	2.54	0.43
1:A:818:G:C3'	1:A:819:A:H5''	2.46	0.42
1:A:1124:G:H4'	10:J:38:ILE:HD11	2.00	0.42
1:A:1425:U:H2'	1:A:1426:C:H6	1.83	0.42
2:B:92:TYR:CE1	2:B:94:ASN:HB2	2.55	0.42
10:J:38:ILE:HA	10:J:39:PRO:HD3	1.88	0.42
11:K:62:GLN:HG3	11:K:97:ALA:HB2	2.02	0.42
13:M:49:THR:HG22	13:M:51:ALA:H	1.84	0.42
18:R:21:LYS:NZ	18:R:21:LYS:HA	2.34	0.42
1:A:1304:G:C6	1:A:1305:G:N1	2.87	0.42
1:A:1517:G:H3'	1:A:1518:A:H8	1.84	0.42
1:A:877:C:H5''	8:H:88:LYS:HD3	2.01	0.42
2:B:68:ILE:O	2:B:90:MET:HB3	2.19	0.42
15:O:67:LEU:HD23	15:O:67:LEU:HA	1.88	0.42
21:U:25:LYS:HA	21:U:25:LYS:HD3	1.74	0.42
1:A:1511:G:H2'	1:A:1512:U:O4'	2.20	0.42
1:A:731:G:OP1	1:A:766:A:H1'	2.18	0.42
1:A:974:A:P	14:N:29:ARG:HH22	2.43	0.42
17:Q:64:PRO:HB3	17:Q:70:ARG:HE	1.84	0.42
1:A:1127:G:N2	1:A:1145:C:C2	2.88	0.42
1:A:547:A:H4'	1:A:548:G:O5'	2.20	0.42
1:A:551:U:H2'	1:A:552:U:C6	2.54	0.42
1:A:1057:G:H5''	3:C:154:SER:HB2	2.01	0.42
18:R:21:LYS:H	18:R:21:LYS:HD2	1.83	0.42
21:U:14:TRP:CE3	21:U:15:ARG:HG3	2.55	0.42
4:D:135:LEU:HA	4:D:136:PRO:HD3	1.85	0.42
5:E:112:LEU:HA	5:E:112:LEU:HD23	1.84	0.42
1:A:972:C:O3'	10:J:57:LYS:HD3	2.20	0.42
1:A:1020:U:H2'	1:A:1021:G:C8	2.55	0.42
1:A:216:G:O2'	1:A:217:C:O4'	2.37	0.42
1:A:8:A:N6	4:D:209:ARG:HB2	2.35	0.42
11:K:98:LEU:HA	11:K:98:LEU:HD23	1.87	0.42
15:O:10:LYS:HA	15:O:10:LYS:HD2	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:757:U:H2'	1:A:758:G:O4'	2.20	0.42
1:A:972:C:OP2	10:J:57:LYS:NZ	2.51	0.42
3:C:111:LEU:HD23	3:C:111:LEU:HA	1.91	0.42
3:C:195:VAL:C	3:C:196:LEU:HD23	2.39	0.42
7:G:29:LYS:HD3	7:G:29:LYS:HA	1.94	0.42
12:L:124:LYS:HA	12:L:125:PRO:HD2	1.77	0.42
1:A:1257:U:H4'	1:A:1257:U:OP2	2.20	0.42
1:A:1352:C:H2'	1:A:1353:G:C8	2.54	0.42
1:A:1190:G:O6	24:A:1817:PAR:H43	2.20	0.42
4:D:78:LEU:HD23	4:D:78:LEU:HA	1.83	0.42
10:J:28:ARG:HH12	10:J:33:GLN:HG3	1.84	0.42
2:B:179:LYS:HE3	2:B:179:LYS:HB2	1.88	0.42
6:F:55:ASP:HA	6:F:56:PRO:HD3	1.78	0.42
7:G:124:LEU:HA	7:G:124:LEU:HD13	1.89	0.42
12:L:45:PRO:HB2	12:L:92:OTD:SB	2.60	0.42
14:N:3:ARG:O	14:N:7:ILE:HG13	2.19	0.42
20:T:10:LEU:HD12	20:T:11:SER:H	1.84	0.42
1:A:666:G:H5'	1:A:726:C:H1'	2.02	0.41
7:G:65:ALA:O	7:G:69:VAL:HG23	2.19	0.41
1:A:689:C:H2'	1:A:690:G:O4'	2.20	0.41
9:I:8:GLY:HA3	9:I:79:LEU:HB3	2.02	0.41
12:L:70:ILE:HD13	12:L:77:LEU:HD12	2.01	0.41
18:R:23:LYS:HD2	18:R:58:LEU:HD23	2.02	0.41
1:A:957:U:H4'	19:S:79:THR:HB	2.02	0.41
1:A:1391:U:H2'	1:A:1392:G:C8	2.55	0.41
7:G:69:VAL:HG21	7:G:104:LEU:HD21	2.01	0.41
24:A:1817:PAR:O34	10:J:59:SER:HA	2.20	0.41
13:M:17:VAL:O	13:M:20:THR:HB	2.19	0.41
1:A:1016:A:H2'	1:A:1017:G:O4'	2.20	0.41
1:A:1134:G:H1	1:A:1140:C:H42	1.68	0.41
1:A:567:G:H2'	1:A:568:G:O4'	2.20	0.41
1:A:90:U:H2'	1:A:91:C:C6	2.56	0.41
3:C:148:GLY:HA3	3:C:172:ARG:O	2.20	0.41
4:D:100:ARG:O	4:D:104:VAL:HG23	2.19	0.41
8:H:98:LYS:HE3	8:H:98:LYS:HB2	1.93	0.41
10:J:38:ILE:HB	10:J:71:LEU:CB	2.51	0.41
1:A:1326:C:OP1	21:U:12:LYS:NZ	2.47	0.41
1:A:900:A:H2'	1:A:901:A:C8	2.56	0.41
8:H:28:ALA:HB3	8:H:57:PRO:HB2	2.02	0.41
21:U:3:LYS:HD3	21:U:14:TRP:CD1	2.56	0.41
1:A:1116:C:O2'	9:I:108:VAL:HG21	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:118:LEU:HB3	2:B:142:LEU:HD12	2.02	0.41
10:J:29:ARG:H	10:J:29:ARG:NH1	2.18	0.41
11:K:46:GLY:HA2	11:K:50:TYR:O	2.20	0.41
13:M:98:VAL:HG13	13:M:110:ARG:HH12	1.85	0.41
1:A:1000:U:H2'	1:A:1001:A:C8	2.55	0.41
1:A:1035:A:H2'	1:A:1036:G:C8	2.55	0.41
1:A:1495:U:H2'	1:A:1496:C:C6	2.56	0.41
7:G:80:VAL:HG21	7:G:85:TYR:CG	2.55	0.41
10:J:30:SER:HB3	10:J:81:THR:OG1	2.21	0.41
1:A:261:U:OP2	20:T:79:ARG:NH2	2.53	0.41
5:E:34:VAL:HG12	5:E:62:ALA:HB1	2.03	0.41
11:K:126:ARG:HB3	11:K:127:LYS:H	1.75	0.41
1:A:298:A:H2'	1:A:299:G:O4'	2.21	0.41
18:R:76:LEU:HD23	18:R:76:LEU:HA	1.83	0.41
1:A:421:U:H5'	1:A:422:C:C5	2.56	0.41
1:A:475:G:H2'	1:A:476:G:H8	1.85	0.41
1:A:501:C:H2'	1:A:502:G:H8	1.86	0.41
1:A:745:C:H2'	1:A:746:A:C8	2.56	0.41
1:A:811:C:O2'	1:A:901:A:N1	2.49	0.41
3:C:87:LEU:HA	3:C:87:LEU:HD23	1.94	0.41
4:D:111:ALA:HB2	4:D:120:LEU:HD12	2.01	0.41
7:G:75:VAL:HG21	7:G:86:GLN:HB3	2.03	0.41
1:A:246:A:O3'	1:A:247:G:H4'	2.21	0.41
1:A:555:C:H2'	1:A:556:C:C6	2.56	0.41
5:E:31:LEU:HA	5:E:31:LEU:HD23	1.87	0.41
17:Q:3:LYS:HD3	17:Q:61:GLU:O	2.21	0.41
1:A:103:C:OP1	20:T:17:ARG:NH1	2.53	0.40
1:A:1060:C:H2'	1:A:1061:G:H8	1.87	0.40
1:A:121:C:C6	24:A:1812:PAR:H44	2.56	0.40
1:A:413:G:N2	1:A:428:G:H1'	2.36	0.40
1:A:636:U:H5'	17:Q:2:PRO:HG3	2.03	0.40
4:D:31:CYS:C	4:D:33:MET:H	2.24	0.40
9:I:48:GLU:N	9:I:49:PRO:HD2	2.35	0.40
10:J:38:ILE:HD12	10:J:71:LEU:HD12	2.03	0.40
4:D:25:ARG:HG2	4:D:25:ARG:O	2.21	0.40
6:F:42:GLU:HG3	6:F:61:LEU:HD23	2.04	0.40
1:A:192:U:H1'	20:T:103:GLY:HA2	2.03	0.40
1:A:1338:G:H2'	1:A:1339:A:C8	2.56	0.40
1:A:135:C:O2	16:P:1:MET:HB2	2.21	0.40
1:A:1434:A:H2'	1:A:1435:G:O4'	2.21	0.40
1:A:148:G:H2'	1:A:149:A:C8	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:U:OP1	1:A:610:G:O2'	2.29	0.40
1:A:814:A:H2'	1:A:816:A:H5'	2.04	0.40
3:C:23:TYR:OH	10:J:9:ARG:HD3	2.20	0.40
9:I:50:LEU:HB3	9:I:55:ALA:HB3	2.03	0.40
11:K:124:LYS:HB3	11:K:124:LYS:HE2	1.89	0.40
12:L:7:ILE:O	12:L:11:VAL:HG23	2.20	0.40
13:M:86:CYS:SG	13:M:87:TYR:N	2.94	0.40
20:T:14:LYS:O	20:T:18:GLN:HG3	2.20	0.40
21:U:5:ASP:O	21:U:11:GLY:HA3	2.21	0.40
1:A:1129:C:H1'	1:A:1131:G:OP2	2.21	0.40
1:A:21:G:H2'	1:A:22:G:C8	2.57	0.40
1:A:620:C:H2'	1:A:621:A:O4'	2.21	0.40
1:A:918:A:H2'	1:A:919:A:C8	2.56	0.40
6:F:10:LEU:HD23	6:F:85:VAL:HA	2.03	0.40
10:J:86:MET:HB3	10:J:87:THR:H	1.64	0.40
18:R:21:LYS:N	18:R:21:LYS:HD2	2.36	0.40
20:T:67:ALA:HB2	20:T:77:ALA:HB2	2.04	0.40
21:U:6:ARG:HG2	21:U:6:ARG:H	1.65	0.40
1:A:1198:G:H2'	1:A:1199:U:C6	2.56	0.40
1:A:1238:A:H5'	1:A:1336:C:H41	1.87	0.40
2:B:93:VAL:HG11	2:B:97:TRP:CD1	2.56	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%)	211 (90%)	22 (9%)	1 (0%)	34 67
3	C	205/239 (86%)	190 (93%)	14 (7%)	1 (0%)	29 63
4	D	206/209 (99%)	199 (97%)	6 (3%)	1 (0%)	29 63
5	E	149/162 (92%)	144 (97%)	5 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	99/101 (98%)	95 (96%)	4 (4%)	0	100	100
7	G	153/156 (98%)	144 (94%)	9 (6%)	0	100	100
8	H	136/138 (99%)	133 (98%)	3 (2%)	0	100	100
9	I	125/128 (98%)	113 (90%)	12 (10%)	0	100	100
10	J	97/105 (92%)	80 (82%)	15 (16%)	2 (2%)	7	28
11	K	117/129 (91%)	105 (90%)	12 (10%)	0	100	100
12	L	122/135 (90%)	112 (92%)	8 (7%)	2 (2%)	9	35
13	M	116/126 (92%)	110 (95%)	6 (5%)	0	100	100
14	N	58/61 (95%)	54 (93%)	4 (7%)	0	100	100
15	O	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
16	P	82/88 (93%)	81 (99%)	1 (1%)	0	100	100
17	Q	99/105 (94%)	93 (94%)	6 (6%)	0	100	100
18	R	71/88 (81%)	65 (92%)	6 (8%)	0	100	100
19	S	79/93 (85%)	72 (91%)	7 (9%)	0	100	100
20	T	97/106 (92%)	87 (90%)	10 (10%)	0	100	100
21	U	23/27 (85%)	22 (96%)	1 (4%)	0	100	100
All	All	2354/2541 (93%)	2191 (93%)	156 (7%)	7 (0%)	41	72

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	L	28	LYS
10	J	34	VAL
10	J	72	VAL
12	L	30	ALA
2	B	89	GLY
3	C	66	VAL
4	D	5	ILE

### 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	194/220 (88%)	184 (95%)	10 (5%)	23	53
3	C	160/188 (85%)	145 (91%)	15 (9%)	8	30
4	D	180/181 (99%)	164 (91%)	16 (9%)	9	32
5	E	115/123 (94%)	105 (91%)	10 (9%)	10	34
6	F	90/90 (100%)	84 (93%)	6 (7%)	16	44
7	G	126/127 (99%)	117 (93%)	9 (7%)	14	42
8	H	119/119 (100%)	110 (92%)	9 (8%)	13	39
9	I	98/99 (99%)	92 (94%)	6 (6%)	18	47
10	J	87/92 (95%)	80 (92%)	7 (8%)	12	37
11	K	90/99 (91%)	85 (94%)	5 (6%)	21	50
12	L	103/110 (94%)	97 (94%)	6 (6%)	20	49
13	M	94/101 (93%)	88 (94%)	6 (6%)	17	46
14	N	49/50 (98%)	44 (90%)	5 (10%)	7	25
15	O	79/80 (99%)	71 (90%)	8 (10%)	7	26
16	P	72/74 (97%)	72 (100%)	0	100	100
17	Q	95/97 (98%)	89 (94%)	6 (6%)	18	46
18	R	64/77 (83%)	60 (94%)	4 (6%)	18	46
19	S	71/80 (89%)	67 (94%)	4 (6%)	21	50
20	T	76/82 (93%)	67 (88%)	9 (12%)	5	20
21	U	19/22 (86%)	17 (90%)	2 (10%)	7	24
All	All	1981/2111 (94%)	1838 (93%)	143 (7%)	14	41

All (143) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	22	LYS
2	B	79	ASP
2	B	82	ARG
2	B	97	TRP
2	B	102	LEU
2	B	114	ARG
2	B	144	ARG
2	B	157	ARG
2	B	213	LEU
2	B	221	LEU
3	C	3	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	C	12	LEU
3	C	14	ILE
3	C	34	LEU
3	C	37	GLN
3	C	45	LYS
3	C	64	VAL
3	C	85	ARG
3	C	107	GLN
3	C	108	ASN
3	C	167	TRP
3	C	178	LEU
3	C	188	LEU
3	C	196	LEU
3	C	204	LEU
4	D	3	ARG
4	D	8	VAL
4	D	10	ARG
4	D	12	CYS
4	D	19	LEU
4	D	34	GLU
4	D	49	ARG
4	D	64	LEU
4	D	78	LEU
4	D	83	SER
4	D	96	LEU
4	D	115	ARG
4	D	122	ARG
4	D	127	THR
4	D	170	VAL
4	D	194	LEU
5	E	12	LEU
5	E	19	MET
5	E	41	VAL
5	E	43	LEU
5	E	64	ARG
5	E	65	ASN
5	E	76	ILE
5	E	78	HIS
5	E	79	GLU
5	E	80	ILE
6	F	43	LEU
6	F	45	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
6	F	54	LYS
6	F	73	ASN
6	F	87	ARG
6	F	98	LEU
7	G	8	GLU
7	G	11	GLN
7	G	21	VAL
7	G	73	MET
7	G	80	VAL
7	G	113	GLU
7	G	124	LEU
7	G	149	ARG
7	G	156	TRP
8	H	21	LYS
8	H	39	LEU
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	133	LEU
9	I	41	VAL
9	I	79	LEU
9	I	102	LEU
9	I	108	VAL
9	I	118	LYS
9	I	121	ARG
10	J	15	THR
10	J	28	ARG
10	J	29	ARG
10	J	62	HIS
10	J	67	THR
10	J	71	LEU
10	J	86	MET
11	K	29	ILE
11	K	48	ILE
11	K	91	ARG
11	K	114	VAL
11	K	119	CYS
12	L	7	ILE
12	L	20	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
12	L	33	ARG
12	L	42	THR
12	L	44	THR
12	L	53	ARG
13	M	14	ARG
13	M	58	GLU
13	M	63	THR
13	M	70	LEU
13	M	88	ARG
13	M	102	ARG
14	N	9	LYS
14	N	26	ARG
14	N	33	VAL
14	N	35	ARG
14	N	41	ARG
15	O	5	LYS
15	O	10	LYS
15	O	31	LEU
15	O	34	LEU
15	O	39	LEU
15	O	57	LEU
15	O	70	LEU
15	O	81	LEU
17	Q	38	ARG
17	Q	53	LEU
17	Q	59	ILE
17	Q	74	LEU
17	Q	83	ASP
17	Q	98	LEU
18	R	18	ARG
18	R	21	LYS
18	R	46	GLU
18	R	85	LEU
19	S	7	LYS
19	S	43	GLU
19	S	70	LYS
19	S	81	ARG
20	T	8	ARG
20	T	19	SER
20	T	27	LYS
20	T	42	GLN
20	T	56	MET

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Mol	Chain	Res	Type
20	T	71	THR
20	T	74	LYS
20	T	75	ASN
20	T	84	LEU
21	U	10	ARG
21	U	25	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	6	HIS
5	E	78	HIS
6	F	73	ASN
9	I	38	GLN
9	I	124	GLN
13	M	106	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1507/1522 (99%)	211 (14%)	26 (1%)

All (211) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	9	G
1	A	32	A
1	A	39	G
1	A	47	C
1	A	48	C
1	A	51	A
1	A	59	A
1	A	79	G
1	A	82	U
1	A	101	A
1	A	116	A
1	A	121	C
1	A	129(A)	G
1	A	130	A
1	A	131	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	146	G
1	A	163	C
1	A	182	U
1	A	190(D)	U
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	289	G
1	A	301	G
1	A	321	A
1	A	328	C
1	A	329	A
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	373	A
1	A	384	G
1	A	397	A
1	A	398	C
1	A	406	G
1	A	411	A
1	A	412	A
1	A	413	G
1	A	421	U
1	A	424	G
1	A	429	U
1	A	433	C
1	A	442	C
1	A	452	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	460	A
1	A	461	C
1	A	482	A
1	A	484	G
1	A	485	G
1	A	497	A
1	A	498	U
1	A	509	A
1	A	510	A
1	A	511	C
1	A	518	C
1	A	527	7MG
1	A	530	G
1	A	532	A
1	A	533	A
1	A	545	C
1	A	547	A
1	A	559	A
1	A	560	U
1	A	564	C
1	A	572	A
1	A	573	A
1	A	576	G
1	A	577	G
1	A	579	G
1	A	588	G
1	A	596	C
1	A	618	C
1	A	631	G
1	A	632	A
1	A	653	A
1	A	665	A
1	A	671	G
1	A	687	A
1	A	688	G
1	A	702	A
1	A	717	C
1	A	721	G
1	A	723	U
1	A	731	G
1	A	749	C
1	A	755	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	777	A
1	A	780	A
1	A	781	A
1	A	787	A
1	A	792	A
1	A	793	U
1	A	794	A
1	A	799	G
1	A	813	U
1	A	816	A
1	A	817	C
1	A	819	A
1	A	828	A
1	A	839	U
1	A	840	C
1	A	841	U
1	A	848	C
1	A	859	A
1	A	872	A
1	A	876	G
1	A	902	G
1	A	914	A
1	A	926	G
1	A	927	G
1	A	931	C
1	A	934	C
1	A	935	A
1	A	942	G
1	A	960	U
1	A	961	U
1	A	966	M2G
1	A	969	A
1	A	974	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	991	U
1	A	992	U
1	A	993	G
1	A	1004	A
1	A	1005	A
1	A	1026	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	1027	C
1	A	1065	U
1	A	1066	C
1	A	1068	G
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1117	G
1	A	1118	C
1	A	1125	U
1	A	1126	U
1	A	1129	C
1	A	1130	A
1	A	1138	G
1	A	1139	G
1	A	1146	A
1	A	1154	G
1	A	1158	C
1	A	1159	U
1	A	1171	G
1	A	1181	G
1	A	1184	G
1	A	1196	U
1	A	1197	G
1	A	1201	A
1	A	1202	G
1	A	1212	U
1	A	1213	A
1	A	1227	A
1	A	1238	A
1	A	1256	A
1	A	1257	U
1	A	1258	G
1	A	1270	C
1	A	1280	A
1	A	1287	A
1	A	1300	G
1	A	1301	U
1	A	1302	U
1	A	1312	G
1	A	1319	A
1	A	1320	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	1338	G
1	A	1347	G
1	A	1353	G
1	A	1362	C
1	A	1364	U
1	A	1368	G
1	A	1370	G
1	A	1394	A
1	A	1399	C
1	A	1400	5MC
1	A	1442	G
1	A	1443	G
1	A	1446	A
1	A	1454	G
1	A	1487	G
1	A	1492	A
1	A	1497	G
1	A	1498	UR3
1	A	1499	A
1	A	1502	A
1	A	1503	A
1	A	1504	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

All (26) RNA pucker outliers are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	108	G
1	A	115	G
1	A	129(A)	G
1	A	181	G
1	A	266	G
1	A	328	C
1	A	329	A
1	A	372	C
1	A	428	G
1	A	432	A

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Mol	Chain	Res	Type
1	A	484	G
1	A	496	A
1	A	509	A
1	A	559	A
1	A	687	A
1	A	701	C
1	A	748	C
1	A	812	C
1	A	913	A
1	A	960	U
1	A	1065	U
1	A	1067	A
1	A	1129	C
1	A	1201	A
1	A	1256	A
1	A	1301	U

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

12 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	5MC	A	1407	1	15,22,23	0.93	1 (6%)	19,32,35	1.14	2 (10%)
1	PSU	A	1541	1	17,21,22	1.07	2 (11%)	20,30,33	3.12	5 (25%)
1	7MG	A	527	1	22,26,27	2.27	6 (27%)	28,39,42	1.77	7 (25%)
1	PSU	A	516	1,22	17,21,22	1.00	1 (5%)	20,30,33	3.14	5 (25%)
1	M2G	A	966	1	20,27,28	1.87	4 (20%)	22,40,43	2.26	3 (13%)
12	0TD	L	92	12	4,9,10	0.80	0	3,11,13	1.87	2 (66%)
1	5MC	A	967	1	15,22,23	0.88	0	19,32,35	1.03	1 (5%)
1	UR3	A	1498	1	14,22,23	0.73	0	15,32,35	1.19	1 (6%)
1	5MC	A	1400	1	15,22,23	0.92	0	19,32,35	1.04	1 (5%)
1	2MG	A	1207	1	19,26,27	2.26	4 (21%)	21,38,41	2.00	3 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	4OC	A	1402	1	16,23,24	0.90	0	17,32,35	0.68	0
1	5MC	A	1404	1	15,22,23	0.81	0	19,32,35	1.08	2 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	A	1407	1	-	0/5/25/26	0/2/2/2
1	PSU	A	1541	1	-	0/7/25/26	0/2/2/2
1	7MG	A	527	1	-	2/7/37/38	0/3/3/3
1	PSU	A	516	1,22	-	0/7/25/26	0/2/2/2
1	M2G	A	966	1	-	2/7/29/30	0/3/3/3
12	0TD	L	92	12	-	1/3/12/14	-
1	5MC	A	967	1	-	0/5/25/26	0/2/2/2
1	UR3	A	1498	1	-	0/5/25/26	0/2/2/2
1	5MC	A	1400	1	-	2/5/25/26	0/2/2/2
1	2MG	A	1207	1	-	0/5/27/28	0/3/3/3
1	4OC	A	1402	1	-	2/9/29/30	0/2/2/2
1	5MC	A	1404	1	-	0/5/25/26	0/2/2/2

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1207	2MG	C2-N2	6.94	1.40	1.34
1	A	527	7MG	C4-N3	6.46	1.42	1.34
1	A	1207	2MG	C6-N1	5.94	1.43	1.33
1	A	966	M2G	C6-N1	5.70	1.43	1.33
1	A	527	7MG	C2-N2	5.16	1.44	1.33
1	A	527	7MG	C8-N9	-4.60	1.34	1.45
1	A	966	M2G	C2-N2	3.46	1.40	1.34
1	A	966	M2G	C2-N1	3.38	1.40	1.34
1	A	516	PSU	C4-N3	3.11	1.38	1.33
1	A	1541	PSU	C4-N3	3.05	1.38	1.33
1	A	527	7MG	C6-N1	2.89	1.38	1.33
1	A	966	M2G	C4-N3	2.88	1.40	1.35
1	A	527	7MG	C6-C5	2.36	1.44	1.41
1	A	1207	2MG	C4-N3	2.27	1.39	1.35
1	A	1207	2MG	C2-N1	2.27	1.41	1.34
1	A	527	7MG	CM7-N7	-2.25	1.42	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1407	5MC	C5-C4	2.19	1.44	1.41
1	A	1541	PSU	O4'-C1'	-2.03	1.41	1.44

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	516	PSU	N1-C2-N3	-10.86	119.80	128.43
1	A	1541	PSU	N1-C2-N3	-10.53	120.06	128.43
1	A	966	M2G	C5-C6-N1	-7.98	112.51	123.43
1	A	1207	2MG	C5-C6-N1	-7.38	113.34	123.43
1	A	516	PSU	C4-N3-C2	5.78	120.02	115.14
1	A	966	M2G	C6-N1-C2	5.60	122.85	116.18
1	A	1541	PSU	C4-N3-C2	5.56	119.84	115.14
1	A	527	7MG	N3-C4-N9	4.95	133.27	126.91
1	A	1541	PSU	C5-C4-N3	-4.41	119.68	125.36
1	A	516	PSU	C5-C4-N3	-4.32	119.80	125.36
1	A	527	7MG	C5-C4-N3	-4.10	119.80	126.49
1	A	527	7MG	N7-C8-N9	3.68	108.64	103.38
1	A	1207	2MG	C6-N1-C2	3.68	121.76	115.18
1	A	1541	PSU	C5-C6-N1	-3.33	120.35	124.44
1	A	516	PSU	C6-N1-C2	3.16	120.57	115.36
1	A	1541	PSU	C6-N1-C2	3.14	120.54	115.36
1	A	516	PSU	C5-C6-N1	-3.03	120.71	124.44
1	A	527	7MG	C6-N1-C2	2.73	120.26	115.93
1	A	1498	UR3	C3'-C2'-C1'	2.50	104.74	100.98
12	L	92	0TD	CSB-SB-CB	-2.41	97.12	101.85
1	A	1407	5MC	N4-C4-N3	-2.38	113.67	117.03
1	A	1207	2MG	C4-C5-N7	2.33	111.83	109.40
1	A	527	7MG	C2-N3-C4	2.30	120.26	113.89
1	A	1400	5MC	C2-N3-C4	2.27	118.75	116.02
1	A	527	7MG	C6-C5-C4	2.26	117.62	115.20
1	A	527	7MG	N1-C2-N3	-2.23	121.92	125.42
1	A	967	5MC	C2-N3-C4	2.16	118.63	116.02
12	L	92	0TD	O-C-CA	-2.16	119.12	124.78
1	A	1407	5MC	C2-N3-C4	2.12	118.58	116.02
1	A	1404	5MC	C2-N3-C4	2.06	118.50	116.02
1	A	1404	5MC	CM5-C5-C6	2.06	123.02	118.68
1	A	966	M2G	N3-C2-N2	2.05	119.26	117.18

There are no chirality outliers.

All (9) torsion outliers are listed below:

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

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	L	92	0TD	2	0
1	A	967	5MC	2	0
1	A	1498	UR3	2	0
1	A	1207	2MG	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 233 ligands modelled in this entry, 224 are monoatomic - leaving 9 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
24	PAR	A	1813	-	45,45,45	1.35	5 (11%)	64,67,67	1.63	13 (20%)
24	PAR	A	1818	-	45,45,45	1.50	9 (20%)	64,67,67	1.65	12 (18%)
24	PAR	A	1817	-	45,45,45	1.42	9 (20%)	64,67,67	1.63	11 (17%)
24	PAR	A	1810	-	45,45,45	1.29	7 (15%)	64,67,67	1.58	12 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	PAR	A	1811	-	45,45,45	1.38	6 (13%)	64,67,67	1.69	14 (21%)
24	PAR	A	1814	-	45,45,45	1.39	7 (15%)	64,67,67	1.62	11 (17%)
24	PAR	A	1815	-	45,45,45	1.26	6 (13%)	64,67,67	1.58	11 (17%)
24	PAR	A	1812	-	45,45,45	1.25	6 (13%)	64,67,67	1.61	10 (15%)
24	PAR	A	1816	-	45,45,45	1.33	7 (15%)	64,67,67	1.64	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
24	PAR	A	1813	-	-	7/18/94/94	0/4/4/4
24	PAR	A	1818	-	-	5/18/94/94	0/4/4/4
24	PAR	A	1817	-	-	9/18/94/94	0/4/4/4
24	PAR	A	1810	-	-	7/18/94/94	0/4/4/4
24	PAR	A	1811	-	-	3/18/94/94	1/4/4/4
24	PAR	A	1814	-	-	2/18/94/94	0/4/4/4
24	PAR	A	1815	-	-	8/18/94/94	0/4/4/4
24	PAR	A	1812	-	-	6/18/94/94	0/4/4/4
24	PAR	A	1816	-	-	10/18/94/94	0/4/4/4

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1811	PAR	C34-C24	4.46	1.59	1.53
24	A	1813	PAR	C52-C42	4.22	1.61	1.52
24	A	1814	PAR	C13-C23	4.04	1.58	1.52
24	A	1818	PAR	C52-C42	3.81	1.60	1.52
24	A	1811	PAR	C14-C24	3.58	1.59	1.52
24	A	1817	PAR	C52-C42	3.52	1.59	1.52
24	A	1815	PAR	C52-C42	3.41	1.59	1.52
24	A	1816	PAR	C34-C24	3.39	1.57	1.53
24	A	1818	PAR	C34-C24	3.36	1.57	1.53
24	A	1817	PAR	C13-C23	3.20	1.57	1.52
24	A	1810	PAR	C52-C42	3.19	1.58	1.52
24	A	1812	PAR	C52-C42	3.12	1.58	1.52
24	A	1818	PAR	C13-C23	3.07	1.56	1.52
24	A	1810	PAR	C64-C54	3.00	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1818	PAR	O43-C13	2.99	1.47	1.41
24	A	1815	PAR	C64-C54	2.98	1.56	1.52
24	A	1814	PAR	C64-C54	2.95	1.56	1.52
24	A	1814	PAR	C52-C42	2.95	1.58	1.52
24	A	1810	PAR	C34-C24	2.87	1.57	1.53
24	A	1812	PAR	C64-C54	2.86	1.55	1.52
24	A	1813	PAR	O43-C13	2.86	1.46	1.41
24	A	1817	PAR	C64-C54	2.85	1.55	1.52
24	A	1816	PAR	C31-C21	2.77	1.57	1.53
24	A	1813	PAR	C13-C23	2.74	1.56	1.52
24	A	1816	PAR	O43-C13	2.73	1.46	1.41
24	A	1814	PAR	C14-C24	2.67	1.57	1.52
24	A	1818	PAR	C64-C54	2.66	1.55	1.52
24	A	1814	PAR	C34-C24	2.65	1.56	1.53
24	A	1816	PAR	C13-C23	2.62	1.56	1.52
24	A	1818	PAR	C14-C24	2.62	1.57	1.52
24	A	1816	PAR	C64-C54	2.60	1.55	1.52
24	A	1813	PAR	C64-C54	2.54	1.55	1.52
24	A	1817	PAR	C34-C24	2.53	1.56	1.53
24	A	1817	PAR	C14-C24	2.51	1.57	1.52
24	A	1812	PAR	C14-C24	2.50	1.57	1.52
24	A	1815	PAR	C31-C21	2.50	1.56	1.53
24	A	1810	PAR	C31-C21	2.48	1.56	1.53
24	A	1811	PAR	O43-C13	2.47	1.46	1.41
24	A	1818	PAR	C31-C21	2.46	1.56	1.53
24	A	1815	PAR	C33-C43	2.37	1.59	1.52
24	A	1812	PAR	C33-C43	2.35	1.59	1.52
24	A	1815	PAR	O43-C13	2.34	1.45	1.41
24	A	1812	PAR	C34-C24	2.33	1.56	1.53
24	A	1810	PAR	C33-C43	2.27	1.59	1.52
24	A	1811	PAR	O52-C52	2.23	1.49	1.43
24	A	1813	PAR	C62-C52	2.22	1.58	1.52
24	A	1817	PAR	C33-C43	2.22	1.58	1.52
24	A	1815	PAR	C13-C23	2.21	1.55	1.52
24	A	1818	PAR	O33-C14	2.20	1.47	1.41
24	A	1814	PAR	C31-C21	2.19	1.56	1.53
24	A	1817	PAR	C31-C21	2.19	1.56	1.53
24	A	1810	PAR	C13-C23	2.15	1.55	1.52
24	A	1817	PAR	C11-C21	2.14	1.56	1.52
24	A	1810	PAR	C14-C24	2.07	1.56	1.52
24	A	1811	PAR	C31-C21	2.07	1.56	1.53
24	A	1817	PAR	C62-C52	2.06	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1812	PAR	C31-C21	2.06	1.56	1.53
24	A	1814	PAR	O43-C13	2.05	1.45	1.41
24	A	1818	PAR	C11-C21	2.05	1.56	1.52
24	A	1816	PAR	C14-C24	2.04	1.56	1.52
24	A	1816	PAR	C52-C42	2.04	1.56	1.52
24	A	1811	PAR	C33-C43	2.01	1.58	1.52

All (107) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1818	PAR	O33-C14-C24	6.69	119.73	108.22
24	A	1811	PAR	O33-C14-C24	6.62	119.63	108.22
24	A	1816	PAR	O33-C14-C24	6.22	118.92	108.22
24	A	1814	PAR	O33-C14-C24	6.19	118.88	108.22
24	A	1817	PAR	O33-C14-C24	5.96	118.48	108.22
24	A	1810	PAR	O33-C14-C24	5.93	118.44	108.22
24	A	1813	PAR	O33-C14-C24	5.83	118.27	108.22
24	A	1812	PAR	O33-C14-C24	5.76	118.13	108.22
24	A	1815	PAR	O33-C14-C24	5.55	117.78	108.22
24	A	1815	PAR	O52-C13-C23	3.86	115.97	107.96
24	A	1814	PAR	C13-C23-C33	3.85	106.73	102.10
24	A	1812	PAR	O52-C13-C23	3.63	115.49	107.96
24	A	1811	PAR	O52-C13-C23	3.43	115.08	107.96
24	A	1817	PAR	C13-C23-C33	3.38	106.17	102.10
24	A	1814	PAR	O52-C13-C23	3.36	114.93	107.96
24	A	1810	PAR	O52-C13-C23	3.33	114.86	107.96
24	A	1817	PAR	O52-C13-C23	3.32	114.85	107.96
24	A	1813	PAR	O52-C13-C23	3.23	114.65	107.96
24	A	1818	PAR	O52-C13-C23	3.18	114.55	107.96
24	A	1818	PAR	C34-C24-N24	-3.15	104.61	111.05
24	A	1815	PAR	C34-C24-N24	-3.14	104.62	111.05
24	A	1816	PAR	O52-C13-C23	3.11	114.40	107.96
24	A	1810	PAR	O34-C34-C44	-3.08	103.23	110.35
24	A	1817	PAR	C34-C24-N24	-3.06	104.77	111.05
24	A	1814	PAR	C34-C24-N24	-3.06	104.78	111.05
24	A	1813	PAR	C34-C24-N24	-3.05	104.80	111.05
24	A	1813	PAR	C13-C23-C33	3.05	105.77	102.10
24	A	1811	PAR	O34-C34-C44	-3.03	103.35	110.35
24	A	1812	PAR	C34-C24-N24	-3.03	104.85	111.05
24	A	1816	PAR	C34-C24-N24	-2.99	104.92	111.05
24	A	1813	PAR	O34-C34-C44	-2.97	103.48	110.35
24	A	1813	PAR	O11-C11-O51	2.97	118.96	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1811	PAR	C34-C24-N24	-2.96	105.00	111.05
24	A	1812	PAR	O34-C34-C44	-2.95	103.54	110.35
24	A	1816	PAR	O34-C34-C44	-2.94	103.55	110.35
24	A	1810	PAR	C34-C24-N24	-2.92	105.06	111.05
24	A	1817	PAR	O11-C11-O51	2.91	118.80	110.67
24	A	1817	PAR	O34-C34-C44	-2.88	103.68	110.35
24	A	1818	PAR	O34-C34-C44	-2.88	103.69	110.35
24	A	1814	PAR	C14-O33-C33	-2.88	110.84	117.96
24	A	1811	PAR	O43-C13-C23	-2.87	101.28	104.98
24	A	1814	PAR	O34-C34-C44	-2.87	103.72	110.35
24	A	1812	PAR	O11-C11-O51	2.85	118.63	110.67
24	A	1815	PAR	O11-C11-O51	2.82	118.55	110.67
24	A	1815	PAR	O34-C34-C44	-2.80	103.88	110.35
24	A	1816	PAR	C22-C12-C62	2.80	114.26	110.04
24	A	1812	PAR	C13-O52-C52	-2.76	111.13	117.96
24	A	1816	PAR	O52-C13-O43	-2.76	108.44	111.43
24	A	1810	PAR	O11-C11-O51	2.76	118.37	110.67
24	A	1818	PAR	O52-C13-O43	-2.75	108.45	111.43
24	A	1815	PAR	C13-O52-C52	-2.72	111.23	117.96
24	A	1811	PAR	C14-O33-C33	-2.70	111.27	117.96
24	A	1816	PAR	C14-O33-C33	-2.70	111.29	117.96
24	A	1817	PAR	O52-C13-O43	-2.67	108.54	111.43
24	A	1818	PAR	O11-C11-O51	2.66	118.11	110.67
24	A	1817	PAR	C14-O33-C33	-2.66	111.38	117.96
24	A	1811	PAR	O11-C11-O51	2.63	118.01	110.67
24	A	1816	PAR	O11-C11-O51	2.63	118.01	110.67
24	A	1810	PAR	C14-O33-C33	-2.60	111.52	117.96
24	A	1818	PAR	C14-O33-C33	-2.60	111.53	117.96
24	A	1813	PAR	C14-O33-C33	-2.57	111.61	117.96
24	A	1812	PAR	C14-O33-C33	-2.54	111.67	117.96
24	A	1814	PAR	C13-O52-C52	-2.54	111.69	117.96
24	A	1818	PAR	C13-C23-C33	2.53	105.15	102.10
24	A	1810	PAR	C13-O52-C52	-2.53	111.71	117.96
24	A	1814	PAR	O11-C11-O51	2.47	117.58	110.67
24	A	1813	PAR	O52-C13-O43	-2.47	108.76	111.43
24	A	1818	PAR	O51-C51-C61	2.46	112.54	106.44
24	A	1817	PAR	C13-O52-C52	-2.46	111.89	117.96
24	A	1811	PAR	O52-C13-O43	-2.44	108.79	111.43
24	A	1811	PAR	O52-C52-C42	2.42	113.62	107.48
24	A	1811	PAR	C23-C33-C43	-2.40	98.97	103.22
24	A	1813	PAR	C11-O51-C51	2.39	118.38	113.69
24	A	1818	PAR	C13-O52-C52	-2.39	112.05	117.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1813	PAR	C13-O52-C52	-2.39	112.05	117.96
24	A	1815	PAR	O43-C13-C23	-2.37	101.92	104.98
24	A	1810	PAR	O52-C13-O43	-2.34	108.89	111.43
24	A	1814	PAR	O52-C13-O43	-2.34	108.90	111.43
24	A	1816	PAR	C13-C23-C33	2.33	104.90	102.10
24	A	1816	PAR	O51-C51-C61	2.33	112.22	106.44
24	A	1817	PAR	C11-O51-C51	2.31	118.23	113.69
24	A	1811	PAR	C22-C12-C62	2.30	113.52	110.04
24	A	1814	PAR	O51-C51-C61	2.30	112.15	106.44
24	A	1810	PAR	O51-C51-C61	2.29	112.12	106.44
24	A	1811	PAR	O51-C51-C61	2.28	112.10	106.44
24	A	1818	PAR	C11-O51-C51	2.27	118.15	113.69
24	A	1817	PAR	O51-C51-C61	2.25	112.03	106.44
24	A	1815	PAR	O51-C51-C61	2.25	112.02	106.44
24	A	1815	PAR	O54-C54-C44	2.23	113.75	109.69
24	A	1816	PAR	C13-O52-C52	-2.23	112.44	117.96
24	A	1812	PAR	O51-C51-C61	2.22	111.96	106.44
24	A	1815	PAR	C14-O33-C33	-2.22	112.48	117.96
24	A	1816	PAR	O54-C54-C44	2.21	113.71	109.69
24	A	1818	PAR	O54-C54-C44	2.21	113.70	109.69
24	A	1813	PAR	O51-C51-C61	2.20	111.91	106.44
24	A	1811	PAR	O33-C14-O54	-2.20	104.54	110.67
24	A	1810	PAR	C13-C23-C33	2.13	104.67	102.10
24	A	1812	PAR	O43-C13-C23	-2.13	102.24	104.98
24	A	1810	PAR	O54-C54-C44	2.11	113.53	109.69
24	A	1815	PAR	O52-C13-O43	-2.07	109.19	111.43
24	A	1812	PAR	C11-O51-C51	2.07	117.75	113.69
24	A	1811	PAR	C13-O52-C52	-2.05	112.88	117.96
24	A	1813	PAR	O54-C54-C44	2.04	113.40	109.69
24	A	1814	PAR	C22-C12-C62	2.03	113.10	110.04
24	A	1813	PAR	O11-C11-C21	-2.02	104.73	108.22
24	A	1816	PAR	O52-C52-C42	2.02	112.61	107.48
24	A	1810	PAR	C11-O51-C51	2.01	117.63	113.69

There are no chirality outliers.

All (57) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	1811	PAR	C24-C14-O33-C33
24	A	1813	PAR	C23-C13-O52-C52
24	A	1818	PAR	C24-C14-O33-C33
24	A	1810	PAR	C44-C54-C64-N64

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Mol	Chain	Res	Type	Atoms
24	A	1810	PAR	O54-C54-C64-N64
24	A	1815	PAR	C33-C43-C53-O53
24	A	1815	PAR	C44-C54-C64-N64
24	A	1815	PAR	O54-C54-C64-N64
24	A	1816	PAR	C44-C54-C64-N64
24	A	1816	PAR	O54-C54-C64-N64
24	A	1817	PAR	C21-C11-O11-C42
24	A	1817	PAR	C44-C54-C64-N64
24	A	1817	PAR	O54-C54-C64-N64
24	A	1811	PAR	O54-C14-O33-C33
24	A	1816	PAR	O51-C11-O11-C42
24	A	1816	PAR	O54-C14-O33-C33
24	A	1815	PAR	O43-C43-C53-O53
24	A	1817	PAR	O43-C43-C53-O53
24	A	1812	PAR	O43-C43-C53-O53
24	A	1814	PAR	O54-C14-O33-C33
24	A	1811	PAR	C62-C52-O52-C13
24	A	1817	PAR	C33-C43-C53-O53
24	A	1812	PAR	C33-C43-C53-O53
24	A	1815	PAR	O51-C51-C61-O61
24	A	1815	PAR	O54-C14-O33-C33
24	A	1816	PAR	O51-C51-C61-O61
24	A	1816	PAR	C42-C52-O52-C13
24	A	1815	PAR	C41-C51-C61-O61
24	A	1818	PAR	O54-C14-O33-C33
24	A	1810	PAR	O43-C43-C53-O53
24	A	1810	PAR	C33-C43-C53-O53
24	A	1813	PAR	C52-C42-O11-C11
24	A	1818	PAR	O51-C51-C61-O61
24	A	1813	PAR	O43-C13-O52-C52
24	A	1812	PAR	O43-C13-O52-C52
24	A	1813	PAR	O54-C14-O33-C33
24	A	1816	PAR	C62-C52-O52-C13
24	A	1816	PAR	O43-C13-O52-C52
24	A	1817	PAR	O43-C13-O52-C52
24	A	1816	PAR	C23-C13-O52-C52
24	A	1817	PAR	C23-C13-O52-C52
24	A	1813	PAR	C32-C42-O11-C11
24	A	1810	PAR	C52-C42-O11-C11
24	A	1813	PAR	C44-C54-C64-N64
24	A	1814	PAR	C43-C33-O33-C14
24	A	1816	PAR	C41-C51-C61-O61

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Mol	Chain	Res	Type	Atoms
24	A	1812	PAR	C52-C42-O11-C11
24	A	1815	PAR	C52-C42-O11-C11
24	A	1812	PAR	O51-C11-O11-C42
24	A	1810	PAR	O43-C13-O52-C52
24	A	1818	PAR	C23-C13-O52-C52
24	A	1810	PAR	C23-C13-O52-C52
24	A	1812	PAR	C23-C13-O52-C52
24	A	1813	PAR	C23-C33-O33-C14
24	A	1818	PAR	C43-C33-O33-C14
24	A	1817	PAR	C23-C33-O33-C14
24	A	1817	PAR	C24-C14-O33-C33

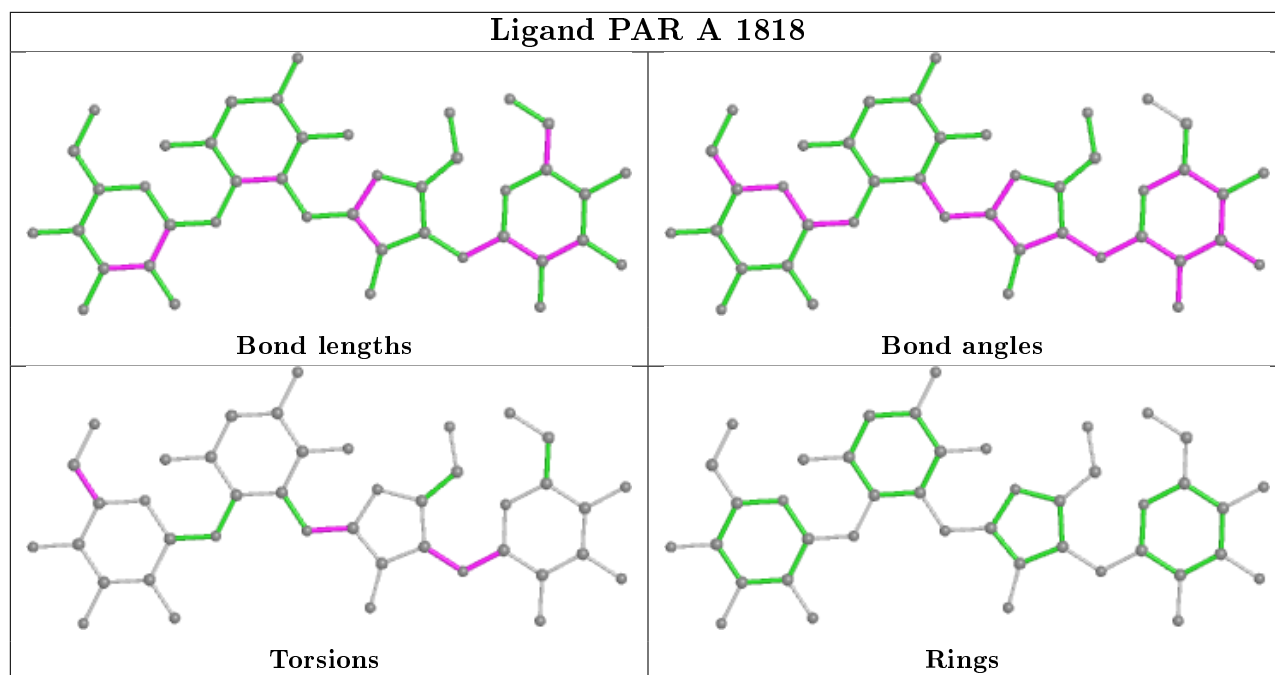
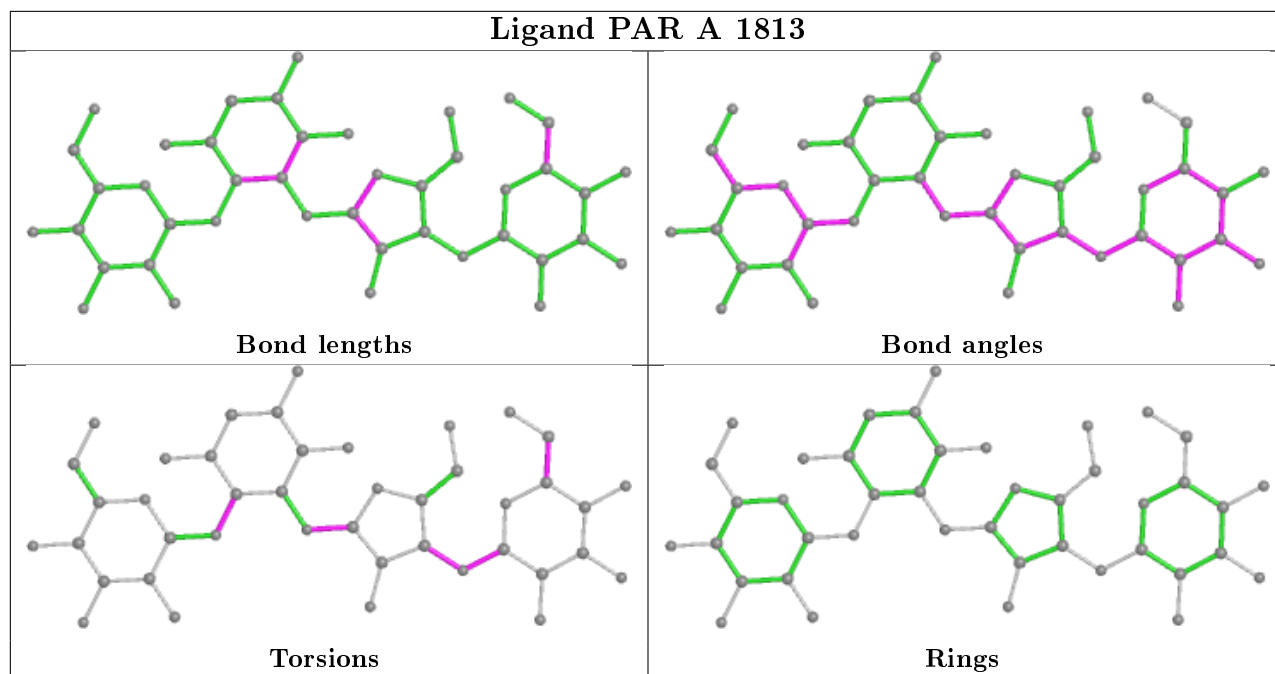
All (1) ring outliers are listed below:

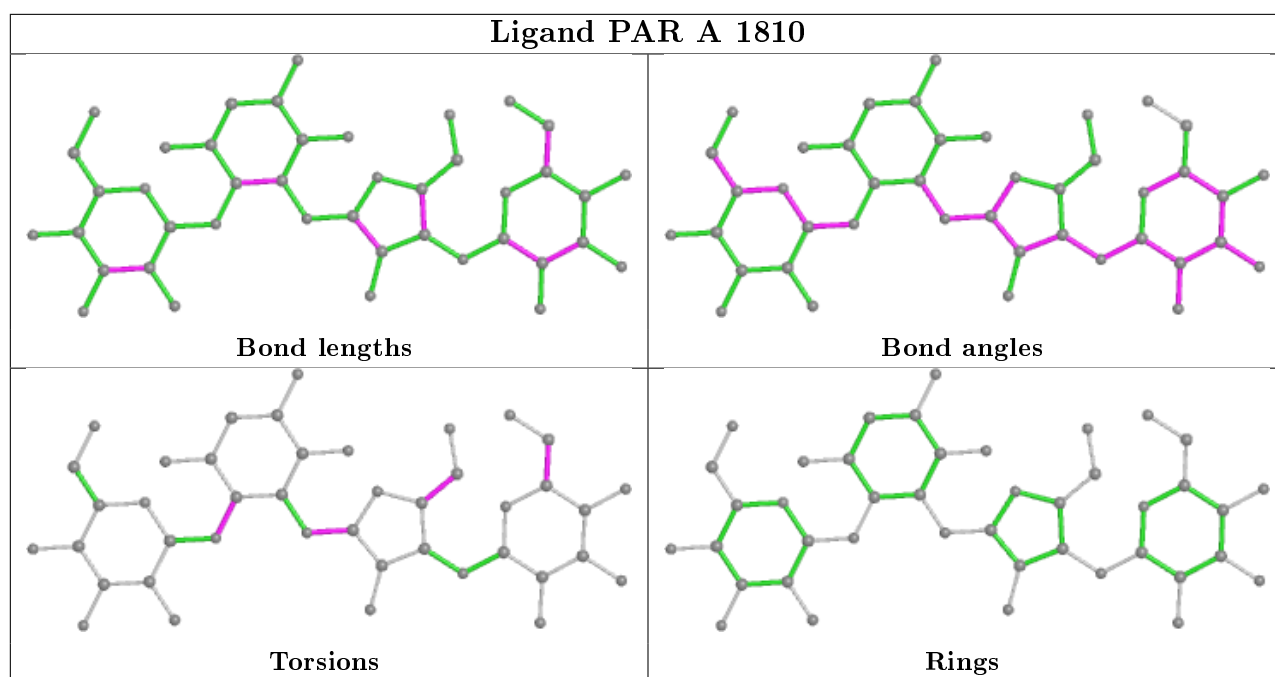
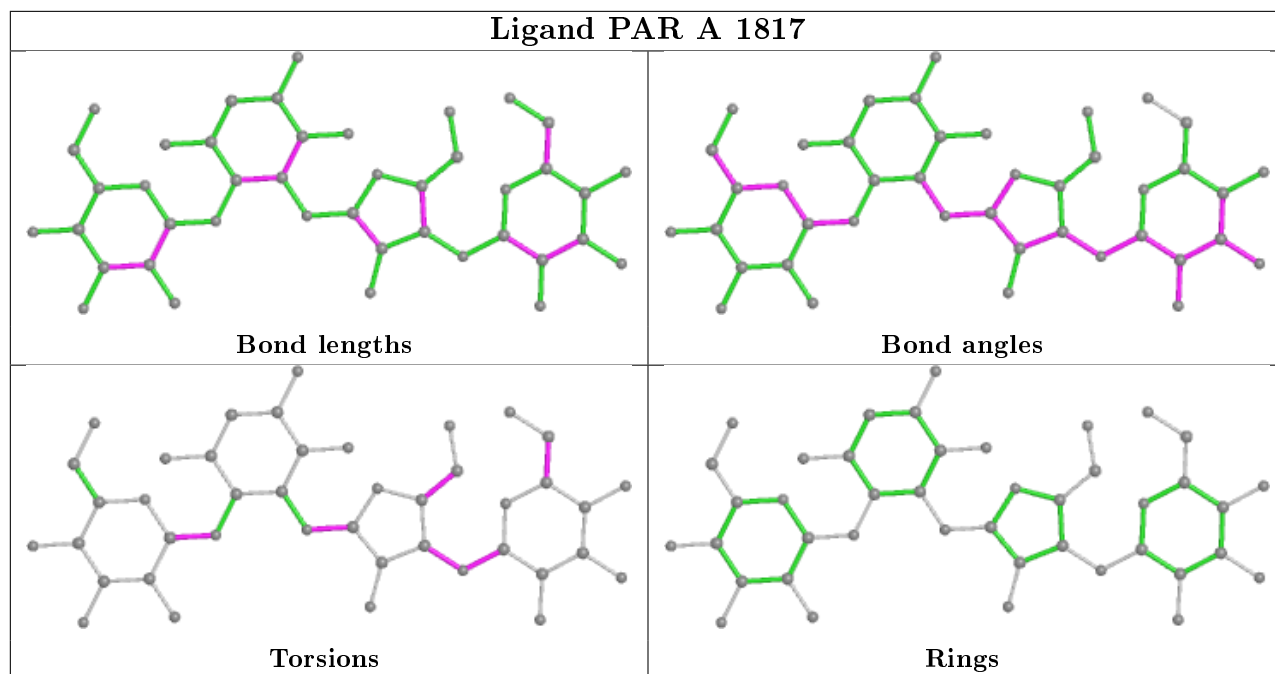
Mol	Chain	Res	Type	Atoms
24	A	1811	PAR	C12-C22-C32-C42-C52-C62

6 monomers are involved in 16 short contacts:

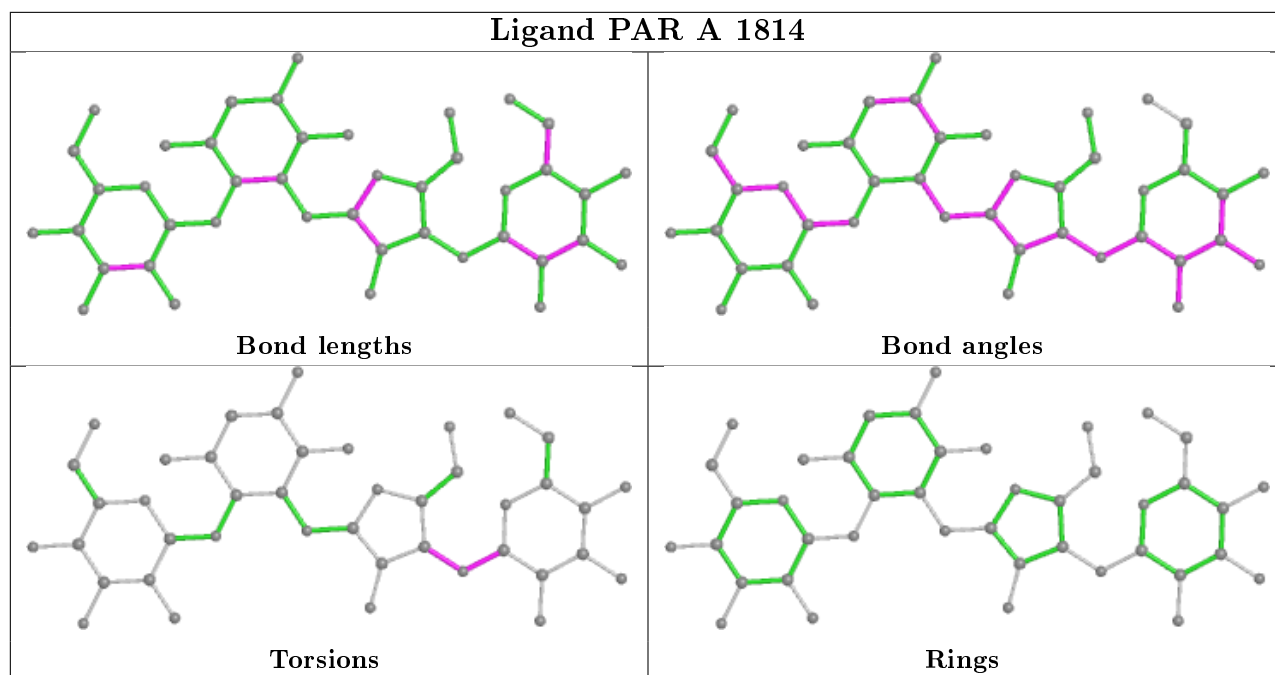
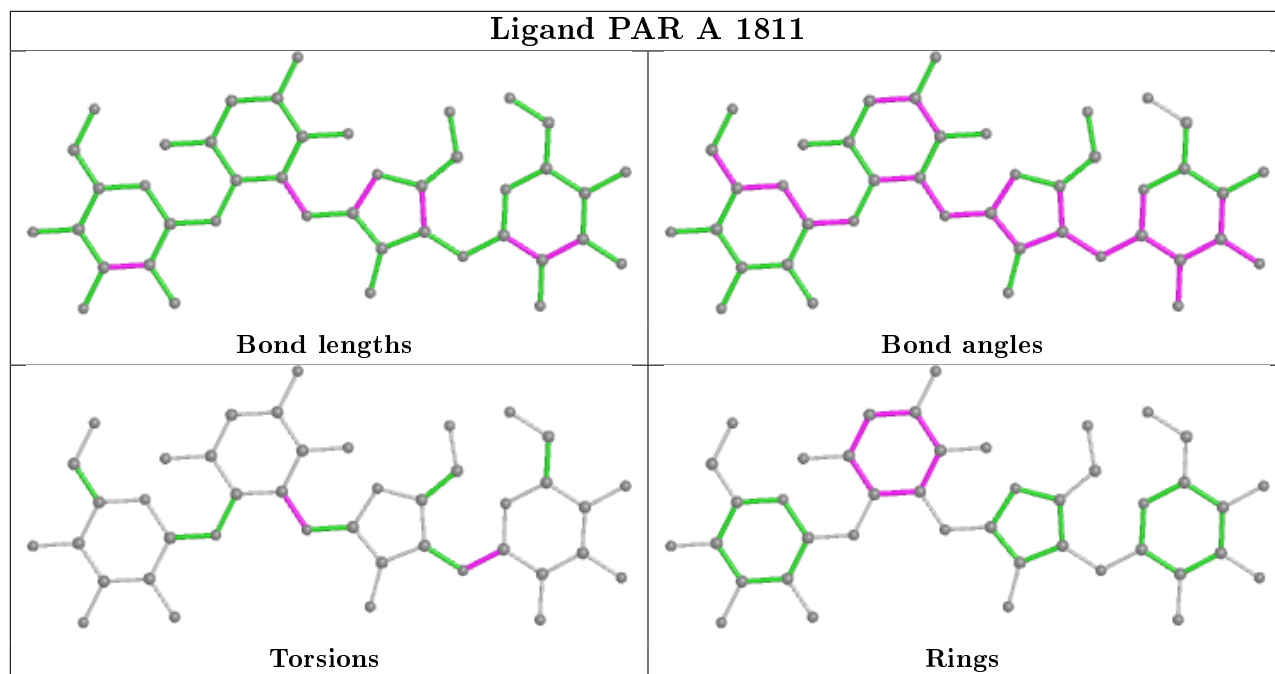
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A	1813	PAR	5	0
24	A	1818	PAR	2	0
24	A	1817	PAR	4	0
24	A	1811	PAR	2	0
24	A	1812	PAR	2	0
24	A	1816	PAR	1	0

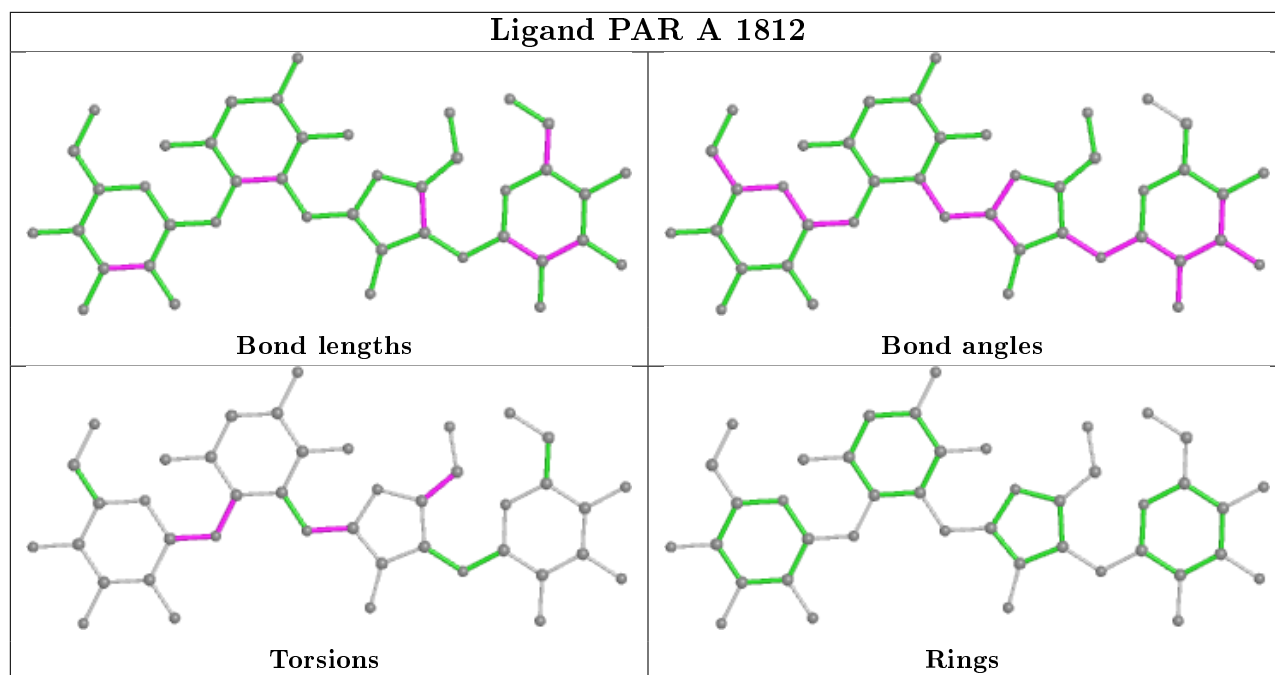
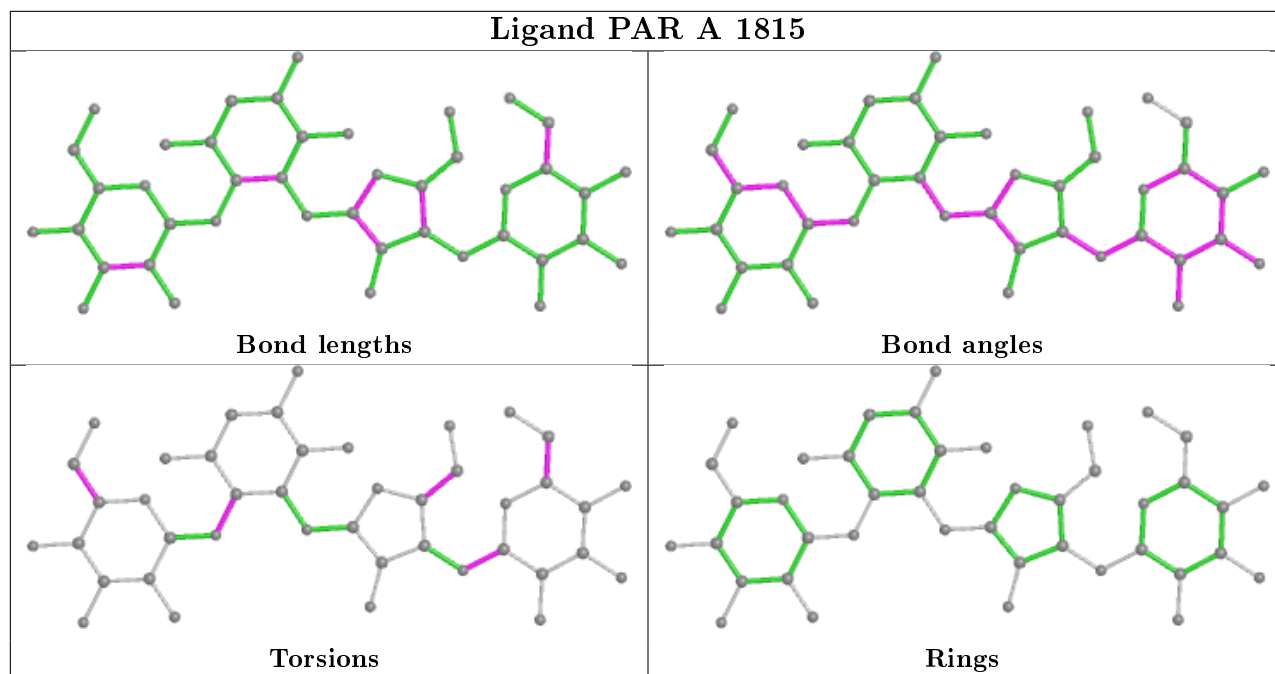
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

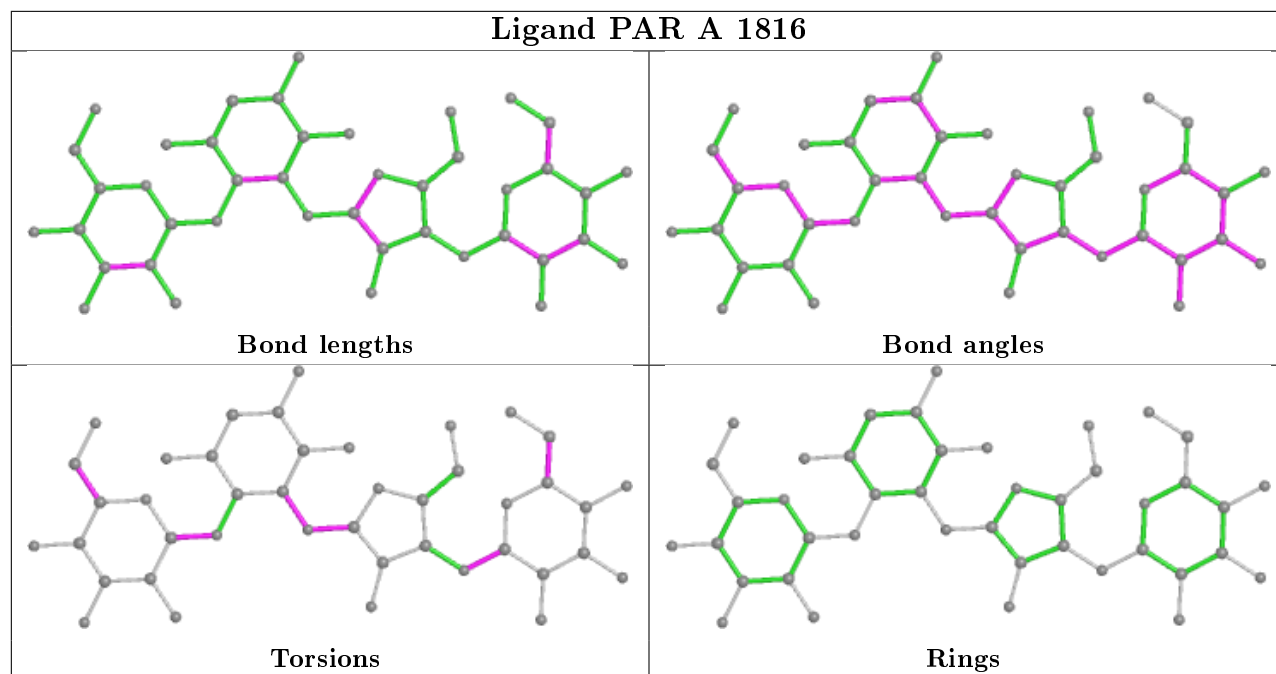












## 5.7 Other polymers [i](#)

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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	1499/1522 (98%)	-0.24	19 (1%) 77 61	60, 89, 179, 289	0
2	B	236/256 (92%)	-0.29	4 (1%) 70 51	72, 117, 215, 241	0
3	C	207/239 (86%)	-0.24	2 (0%) 82 70	71, 121, 166, 205	0
4	D	208/209 (99%)	-0.30	2 (0%) 82 70	68, 101, 148, 172	0
5	E	151/162 (93%)	-0.37	1 (0%) 87 77	58, 82, 128, 181	0
6	F	101/101 (100%)	-0.40	1 (0%) 82 70	90, 127, 160, 185	0
7	G	155/156 (99%)	-0.36	1 (0%) 89 80	81, 110, 167, 204	0
8	H	138/138 (100%)	-0.53	0 100 100	54, 80, 109, 148	0
9	I	127/128 (99%)	-0.27	1 (0%) 86 74	85, 124, 167, 189	0
10	J	99/105 (94%)	-0.02	1 (1%) 82 70	78, 150, 227, 265	0
11	K	119/129 (92%)	-0.06	3 (2%) 57 37	74, 96, 145, 181	0
12	L	124/135 (91%)	-0.22	3 (2%) 59 38	61, 94, 126, 212	0
13	M	118/126 (93%)	-0.14	5 (4%) 36 18	83, 119, 160, 191	0
14	N	60/61 (98%)	-0.02	2 (3%) 46 25	78, 110, 152, 248	0
15	O	88/89 (98%)	-0.27	1 (1%) 80 66	64, 97, 141, 190	0
16	P	84/88 (95%)	-0.36	1 (1%) 79 64	68, 88, 121, 206	0
17	Q	101/105 (96%)	-0.29	2 (1%) 65 46	67, 86, 127, 191	0
18	R	73/88 (82%)	-0.10	3 (4%) 37 19	75, 101, 171, 228	0
19	S	81/93 (87%)	-0.02	1 (1%) 79 64	64, 152, 205, 231	0
20	T	99/106 (93%)	-0.25	1 (1%) 82 70	70, 96, 158, 187	0
21	U	25/27 (92%)	0.44	3 (12%) 4 2	88, 113, 141, 201	0
All	All	3893/4063 (95%)	-0.25	57 (1%) 73 56	54, 100, 176, 289	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	K	129	SER	14.9
11	K	128	ALA	10.7
1	A	1129	C	9.8
12	L	129	ALA	8.2
18	R	17	SER	5.1
13	M	7	VAL	4.3
1	A	1025	U	4.1
2	B	125	PRO	4.1
17	Q	102	GLY	4.1
1	A	1027	C	4.0
14	N	13	THR	4.0
1	A	202	U	3.8
9	I	128	ARG	3.5
3	C	91	LEU	3.3
1	A	1033	G	3.2
10	J	73	ASP	3.2
16	P	84	ALA	3.1
6	F	101	ALA	3.1
2	B	231	GLU	3.0
11	K	127	LYS	3.0
1	A	1003	G	2.9
7	G	5	ARG	2.9
1	A	1036	G	2.8
17	Q	101	ARG	2.8
12	L	128	ALA	2.8
19	S	29	ARG	2.6
18	R	88	LYS	2.6
4	D	33	MET	2.6
14	N	12	ARG	2.6
13	M	118	ALA	2.6
1	A	1002	G	2.6
21	U	18	TYR	2.6
1	A	1032	G	2.5
21	U	26	LYS	2.5
2	B	127	ILE	2.5
2	B	131	PRO	2.5
13	M	117	VAL	2.5
18	R	16	PRO	2.5
1	A	1024	G	2.5
1	A	1026	G	2.4
1	A	88	A	2.4
15	O	88	ARG	2.4
13	M	5	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
13	M	119	GLY	2.4
1	A	412	A	2.3
1	A	1006	C	2.3
1	A	81	U	2.3
4	D	35	ARG	2.2
1	A	1029	C	2.2
1	A	1034	G	2.2
12	L	19	ARG	2.2
5	E	5	ASP	2.1
20	T	99	LEU	2.1
1	A	848	C	2.1
21	U	25	LYS	2.1
3	C	90	GLU	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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	PSU	A	1541	20/21	0.75	0.59	227,258,272,273	0
1	PSU	A	516	20/21	0.94	0.14	97,107,116,119	0
1	5MC	A	1407	21/22	0.95	0.22	90,117,131,134	0
12	0TD	L	92	10/11	0.95	0.32	87,102,191,361	0
1	UR3	A	1498	21/22	0.97	0.20	73,85,98,111	0
1	2MG	A	1207	24/25	0.97	0.13	101,109,115,119	0
1	5MC	A	1404	21/22	0.97	0.16	66,80,105,108	0
1	M2G	A	966	25/26	0.98	0.12	69,82,96,109	0
1	5MC	A	1400	21/22	0.98	0.15	64,90,122,129	0
1	7MG	A	527	24/25	0.98	0.15	67,80,93,111	0
1	4OC	A	1402	22/23	0.98	0.16	73,79,89,94	0
1	5MC	A	967	21/22	0.98	0.15	67,79,98,104	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands i

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
22	MG	A	1601	1/1	0.38	0.15	91,91,91,91	0
22	MG	A	1774	1/1	0.54	0.89	93,93,93,93	0
22	MG	A	1809	1/1	0.55	0.15	100,100,100,100	0
23	K	A	1757	1/1	0.56	0.72	180,180,180,180	0
22	MG	A	1617	1/1	0.58	0.85	85,85,85,85	0
22	MG	A	1760	1/1	0.59	0.82	93,93,93,93	0
22	MG	A	1678	1/1	0.61	1.01	91,91,91,91	0
22	MG	D	303	1/1	0.62	0.22	95,95,95,95	0
22	MG	A	1666	1/1	0.63	0.76	93,93,93,93	0
22	MG	A	1658	1/1	0.64	0.43	93,93,93,93	0
23	K	A	1739	1/1	0.67	0.51	159,159,159,159	0
22	MG	A	1772	1/1	0.69	0.44	96,96,96,96	0
22	MG	A	1788	1/1	0.69	0.47	80,80,80,80	0
22	MG	A	1798	1/1	0.70	0.19	93,93,93,93	0
22	MG	A	1610	1/1	0.71	1.05	114,114,114,114	0
22	MG	D	304	1/1	0.71	1.09	117,117,117,117	0
22	MG	A	1792	1/1	0.71	0.16	98,98,98,98	0
22	MG	A	1615	1/1	0.72	0.37	99,99,99,99	0
22	MG	A	1768	1/1	0.72	0.76	100,100,100,100	0
22	MG	A	1738	1/1	0.73	0.29	102,102,102,102	0
22	MG	A	1791	1/1	0.73	0.46	76,76,76,76	0
22	MG	A	1607	1/1	0.74	0.71	72,72,72,72	0
23	K	A	1754	1/1	0.74	0.89	166,166,166,166	0
22	MG	A	1636	1/1	0.74	1.08	95,95,95,95	0
22	MG	A	1773	1/1	0.75	0.44	96,96,96,96	0
23	K	A	1750	1/1	0.75	0.10	166,166,166,166	0
22	MG	A	1778	1/1	0.76	0.25	79,79,79,79	0
22	MG	A	1767	1/1	0.76	0.53	96,96,96,96	0
22	MG	A	1668	1/1	0.76	0.42	93,93,93,93	0
22	MG	A	1618	1/1	0.77	0.25	76,76,76,76	0
22	MG	A	1775	1/1	0.77	0.38	98,98,98,98	0
22	MG	A	1611	1/1	0.78	0.22	78,78,78,78	0
22	MG	A	1671	1/1	0.78	0.40	105,105,105,105	0
22	MG	A	1779	1/1	0.78	1.16	95,95,95,95	0
22	MG	A	1620	1/1	0.78	0.30	117,117,117,117	0
22	MG	H	201	1/1	0.78	0.20	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
22	MG	A	1790	1/1	0.79	0.35	91,91,91,91	0
22	MG	A	1612	1/1	0.79	0.35	65,65,65,65	0
22	MG	A	1766	1/1	0.79	0.46	90,90,90,90	0
22	MG	A	1796	1/1	0.79	0.52	111,111,111,111	0
22	MG	A	1685	1/1	0.80	0.44	103,103,103,103	0
22	MG	A	1656	1/1	0.80	0.24	111,111,111,111	0
22	MG	A	1696	1/1	0.80	0.55	86,86,86,86	0
22	MG	A	1771	1/1	0.80	0.68	86,86,86,86	0
22	MG	A	1801	1/1	0.80	0.31	111,111,111,111	0
22	MG	A	1782	1/1	0.81	0.14	311,311,311,311	0
22	MG	A	1694	1/1	0.81	0.55	83,83,83,83	0
23	K	A	1752	1/1	0.81	0.55	158,158,158,158	0
22	MG	A	1793	1/1	0.81	0.76	96,96,96,96	0
22	MG	A	1613	1/1	0.81	0.97	92,92,92,92	0
22	MG	A	1693	1/1	0.81	0.89	78,78,78,78	0
22	MG	L	201	1/1	0.82	0.13	102,102,102,102	0
22	MG	A	1623	1/1	0.82	1.08	89,89,89,89	0
22	MG	A	1641	1/1	0.82	0.38	81,81,81,81	0
22	MG	A	1758	1/1	0.83	0.84	97,97,97,97	0
22	MG	A	1643	1/1	0.83	0.65	86,86,86,86	0
22	MG	A	1765	1/1	0.83	0.35	92,92,92,92	0
22	MG	A	1640	1/1	0.83	0.30	75,75,75,75	0
22	MG	A	1794	1/1	0.83	0.10	91,91,91,91	0
22	MG	C	301	1/1	0.83	0.25	81,81,81,81	0
22	MG	A	1803	1/1	0.84	0.17	78,78,78,78	0
22	MG	A	1648	1/1	0.84	0.77	89,89,89,89	0
22	MG	A	1692	1/1	0.84	0.54	89,89,89,89	0
22	MG	A	1616	1/1	0.84	0.71	78,78,78,78	0
22	MG	A	1776	1/1	0.84	0.23	114,114,114,114	0
22	MG	A	1777	1/1	0.85	0.68	91,91,91,91	0
22	MG	A	1609	1/1	0.85	0.27	78,78,78,78	0
22	MG	A	1719	1/1	0.85	0.25	97,97,97,97	0
22	MG	A	1781	1/1	0.85	0.69	90,90,90,90	0
22	MG	A	1659	1/1	0.85	0.47	86,86,86,86	0
22	MG	A	1614	1/1	0.85	0.48	79,79,79,79	0
22	MG	A	1807	1/1	0.85	0.94	97,97,97,97	0
22	MG	A	1732	1/1	0.85	0.65	87,87,87,87	0
22	MG	A	1681	1/1	0.85	0.76	67,67,67,67	0
22	MG	A	1606	1/1	0.86	0.52	78,78,78,78	0
22	MG	A	1652	1/1	0.86	0.59	86,86,86,86	0
24	PAR	A	1812	42/42	0.86	0.27	70,135,158,165	4
22	MG	A	1720	1/1	0.86	0.69	110,110,110,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
22	MG	A	1603	1/1	0.86	0.15	94,94,94,94	0
22	MG	A	1661	1/1	0.86	0.33	65,65,65,65	0
23	K	A	1744	1/1	0.86	0.18	155,155,155,155	0
22	MG	A	1764	1/1	0.86	0.43	88,88,88,88	0
22	MG	A	1737	1/1	0.86	1.05	90,90,90,90	0
22	MG	A	1728	1/1	0.86	0.38	74,74,74,74	0
22	MG	G	201	1/1	0.87	1.16	108,108,108,108	0
22	MG	A	1663	1/1	0.87	0.48	76,76,76,76	0
22	MG	A	1682	1/1	0.87	0.37	93,93,93,93	0
22	MG	A	1723	1/1	0.87	0.93	81,81,81,81	0
23	K	A	1756	1/1	0.87	0.15	145,145,145,145	0
22	MG	A	1736	1/1	0.87	0.21	96,96,96,96	0
22	MG	A	1715	1/1	0.88	0.26	95,95,95,95	0
22	MG	A	1691	1/1	0.88	1.45	73,73,73,73	0
22	MG	A	1714	1/1	0.88	0.50	82,82,82,82	0
22	MG	A	1695	1/1	0.88	0.26	79,79,79,79	0
22	MG	A	1621	1/1	0.88	0.63	91,91,91,91	0
23	K	A	1753	1/1	0.88	0.23	136,136,136,136	0
22	MG	A	1645	1/1	0.88	0.33	76,76,76,76	0
22	MG	N	102	1/1	0.88	0.30	74,74,74,74	0
23	K	A	1742	1/1	0.88	0.42	145,145,145,145	0
23	K	A	1747	1/1	0.88	0.37	136,136,136,136	0
22	MG	A	1808	1/1	0.88	0.16	92,92,92,92	0
22	MG	A	1664	1/1	0.88	0.44	85,85,85,85	0
22	MG	A	1676	1/1	0.88	0.18	67,67,67,67	0
22	MG	A	1686	1/1	0.89	0.33	83,83,83,83	0
22	MG	A	1724	1/1	0.89	0.41	89,89,89,89	0
22	MG	A	1627	1/1	0.89	0.66	68,68,68,68	0
22	MG	A	1799	1/1	0.89	0.16	114,114,114,114	0
22	MG	A	1635	1/1	0.89	0.12	75,75,75,75	0
22	MG	A	1725	1/1	0.89	0.23	87,87,87,87	0
22	MG	A	1797	1/1	0.89	0.40	73,73,73,73	0
22	MG	A	1665	1/1	0.89	0.53	75,75,75,75	0
23	K	A	1740	1/1	0.89	0.15	131,131,131,131	0
22	MG	A	1675	1/1	0.89	0.92	92,92,92,92	0
22	MG	A	1654	1/1	0.90	0.64	64,64,64,64	0
22	MG	A	1644	1/1	0.90	0.50	59,59,59,59	0
22	MG	A	1763	1/1	0.90	0.18	73,73,73,73	0
24	PAR	A	1817	42/42	0.90	0.29	78,116,126,131	42
22	MG	A	1780	1/1	0.90	0.80	82,82,82,82	0
22	MG	A	1632	1/1	0.90	0.48	117,117,117,117	0
24	PAR	A	1818	42/42	0.90	0.29	76,116,186,287	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
22	MG	A	1787	1/1	0.90	0.33	73,73,73,73	0
22	MG	A	1800	1/1	0.90	0.31	90,90,90,90	0
23	K	A	1751	1/1	0.90	0.24	153,153,153,153	0
22	MG	A	1608	1/1	0.90	0.60	85,85,85,85	0
22	MG	A	1735	1/1	0.90	0.14	64,64,64,64	0
22	MG	A	1684	1/1	0.91	0.56	63,63,63,63	0
22	MG	A	1642	1/1	0.91	0.16	56,56,56,56	0
22	MG	A	1677	1/1	0.91	0.95	78,78,78,78	0
22	MG	A	1770	1/1	0.91	1.19	76,76,76,76	0
22	MG	A	1657	1/1	0.91	0.24	92,92,92,92	0
22	MG	A	1713	1/1	0.91	0.24	86,86,86,86	0
23	K	A	1741	1/1	0.91	0.40	149,149,149,149	0
22	MG	A	1631	1/1	0.91	0.46	81,81,81,81	0
22	MG	A	1726	1/1	0.91	0.24	72,72,72,72	0
22	MG	A	1702	1/1	0.92	0.11	83,83,83,83	0
24	PAR	A	1811	42/42	0.92	0.23	48,80,116,129	0
22	MG	A	1733	1/1	0.92	0.19	58,58,58,58	0
22	MG	A	1619	1/1	0.92	0.83	62,62,62,62	0
22	MG	A	1698	1/1	0.92	0.90	91,91,91,91	0
23	K	A	1748	1/1	0.92	0.78	137,137,137,137	0
22	MG	A	1672	1/1	0.92	0.42	63,63,63,63	0
24	PAR	A	1814	42/42	0.92	0.20	90,115,162,164	0
24	PAR	A	1816	42/42	0.92	0.26	65,100,113,117	42
22	MG	A	1670	1/1	0.92	0.41	64,64,64,64	0
22	MG	A	1680	1/1	0.93	0.63	73,73,73,73	0
22	MG	A	1721	1/1	0.93	0.36	64,64,64,64	0
22	MG	A	1687	1/1	0.93	0.17	65,65,65,65	0
22	MG	A	1795	1/1	0.93	0.13	81,81,81,81	0
22	MG	A	1653	1/1	0.93	0.60	82,82,82,82	0
22	MG	A	1806	1/1	0.93	0.45	81,81,81,81	0
22	MG	A	1709	1/1	0.93	0.61	67,67,67,67	0
22	MG	A	1789	1/1	0.93	0.38	69,69,69,69	0
22	MG	A	1727	1/1	0.93	0.08	51,51,51,51	0
22	MG	A	1717	1/1	0.93	0.89	112,112,112,112	0
22	MG	A	1802	1/1	0.93	0.41	80,80,80,80	0
22	MG	A	1718	1/1	0.93	0.09	73,73,73,73	0
22	MG	A	1730	1/1	0.94	0.11	63,63,63,63	0
22	MG	A	1629	1/1	0.94	0.48	60,60,60,60	0
22	MG	E	201	1/1	0.94	0.41	77,77,77,77	0
22	MG	A	1669	1/1	0.94	0.12	73,73,73,73	0
22	MG	B	301	1/1	0.94	0.06	98,98,98,98	0
22	MG	A	1634	1/1	0.94	0.42	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
23	K	A	1749	1/1	0.94	0.55	145,145,145,145	0
22	MG	A	1705	1/1	0.94	0.38	59,59,59,59	0
22	MG	A	1688	1/1	0.94	1.44	73,73,73,73	0
22	MG	A	1729	1/1	0.94	0.21	121,121,121,121	0
22	MG	A	1769	1/1	0.94	0.60	75,75,75,75	0
23	K	A	1755	1/1	0.95	0.39	156,156,156,156	0
22	MG	A	1704	1/1	0.95	0.31	52,52,52,52	0
22	MG	A	1689	1/1	0.95	0.54	51,51,51,51	0
22	MG	A	1683	1/1	0.95	0.52	80,80,80,80	0
22	MG	A	1625	1/1	0.95	0.67	61,61,61,61	0
22	MG	A	1784	1/1	0.95	0.06	275,275,275,275	0
24	PAR	A	1810	42/42	0.95	0.17	57,91,136,144	0
22	MG	A	1759	1/1	0.95	0.39	87,87,87,87	0
23	K	A	1743	1/1	0.95	0.28	138,138,138,138	0
22	MG	A	1785	1/1	0.95	0.15	307,307,307,307	0
22	MG	A	1602	1/1	0.95	0.58	77,77,77,77	0
24	PAR	A	1813	42/42	0.96	0.24	58,82,93,107	0
22	MG	A	1674	1/1	0.96	0.21	63,63,63,63	0
22	MG	A	1646	1/1	0.96	0.76	77,77,77,77	0
23	K	E	202	1/1	0.96	0.21	149,149,149,149	0
22	MG	A	1731	1/1	0.96	0.44	69,69,69,69	0
22	MG	A	1711	1/1	0.96	0.41	80,80,80,80	0
22	MG	A	1722	1/1	0.96	0.19	81,81,81,81	0
25	ZN	D	301	1/1	0.96	0.34	99,99,99,99	0
22	MG	T	201	1/1	0.96	0.23	68,68,68,68	0
22	MG	A	1660	1/1	0.96	0.35	71,71,71,71	0
22	MG	A	1690	1/1	0.96	0.37	81,81,81,81	0
22	MG	A	1716	1/1	0.96	0.48	56,56,56,56	0
22	MG	A	1626	1/1	0.96	0.11	106,106,106,106	0
22	MG	A	1647	1/1	0.96	0.53	54,54,54,54	0
24	PAR	A	1815	42/42	0.96	0.18	51,78,86,90	42
22	MG	A	1649	1/1	0.96	0.64	69,69,69,69	0
22	MG	A	1700	1/1	0.96	0.23	53,53,53,53	0
23	K	A	1745	1/1	0.96	0.68	167,167,167,167	0
22	MG	A	1637	1/1	0.97	0.17	37,37,37,37	0
22	MG	A	1805	1/1	0.97	0.18	91,91,91,91	0
22	MG	A	1667	1/1	0.97	0.45	64,64,64,64	0
22	MG	A	1624	1/1	0.97	0.57	48,48,48,48	0
22	MG	A	1651	1/1	0.97	0.23	51,51,51,51	0
22	MG	A	1734	1/1	0.97	0.51	71,71,71,71	0
22	MG	A	1673	1/1	0.97	0.44	82,82,82,82	0
22	MG	A	1786	1/1	0.97	0.26	79,79,79,79	0

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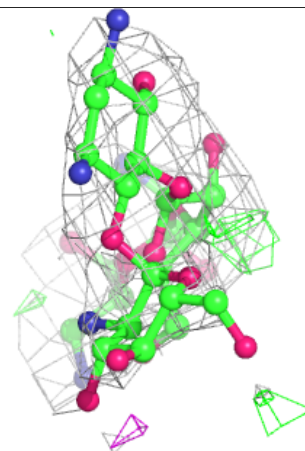
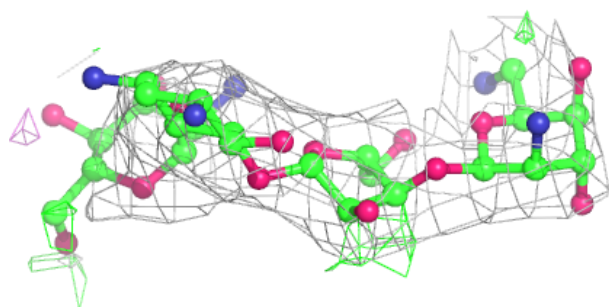
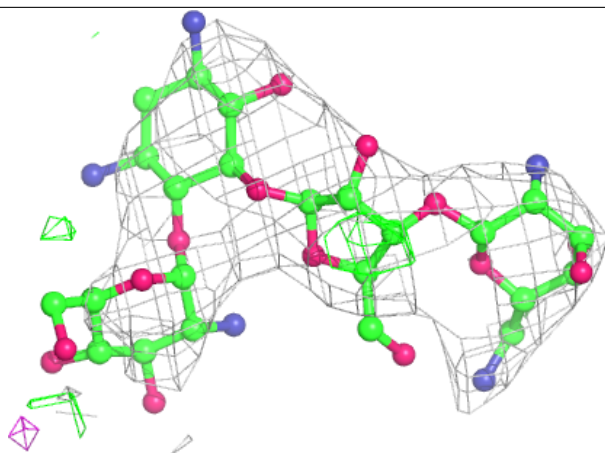
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
22	MG	A	1706	1/1	0.97	0.29	59,59,59,59	0
22	MG	A	1699	1/1	0.97	0.58	59,59,59,59	0
22	MG	A	1783	1/1	0.97	0.07	96,96,96,96	0
22	MG	A	1605	1/1	0.97	1.00	70,70,70,70	0
22	MG	A	1628	1/1	0.97	0.59	55,55,55,55	0
22	MG	M	201	1/1	0.97	0.29	83,83,83,83	0
22	MG	A	1697	1/1	0.98	0.34	73,73,73,73	0
22	MG	A	1638	1/1	0.98	0.24	51,51,51,51	0
22	MG	A	1639	1/1	0.98	0.81	54,54,54,54	0
23	K	A	1746	1/1	0.98	0.19	152,152,152,152	0
22	MG	A	1622	1/1	0.98	0.25	92,92,92,92	0
22	MG	A	1708	1/1	0.98	0.69	60,60,60,60	0
22	MG	A	1662	1/1	0.98	0.28	65,65,65,65	0
22	MG	A	1604	1/1	0.98	0.63	49,49,49,49	0
22	MG	A	1761	1/1	0.98	1.09	79,79,79,79	0
22	MG	A	1762	1/1	0.98	0.64	78,78,78,78	0
22	MG	A	1630	1/1	0.98	0.43	69,69,69,69	0
22	MG	A	1707	1/1	0.98	0.58	67,67,67,67	0
22	MG	A	1633	1/1	0.98	0.34	50,50,50,50	0
22	MG	D	302	1/1	0.98	0.07	66,66,66,66	0
22	MG	A	1712	1/1	0.99	0.52	63,63,63,63	0
25	ZN	N	101	1/1	0.99	0.21	104,104,104,104	0
22	MG	A	1650	1/1	0.99	0.53	55,55,55,55	0
22	MG	A	1679	1/1	0.99	0.28	51,51,51,51	0
22	MG	A	1655	1/1	0.99	0.19	65,65,65,65	0
22	MG	A	1703	1/1	0.99	0.12	55,55,55,55	0
22	MG	A	1701	1/1	0.99	0.72	53,53,53,53	0
22	MG	A	1804	1/1	0.99	0.42	72,72,72,72	0
22	MG	A	1710	1/1	1.00	0.23	80,80,80,80	0

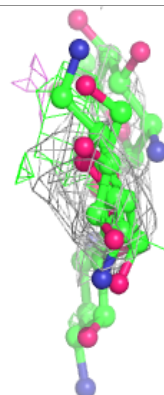
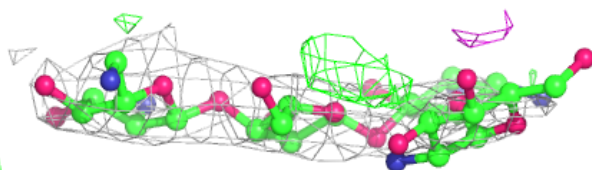
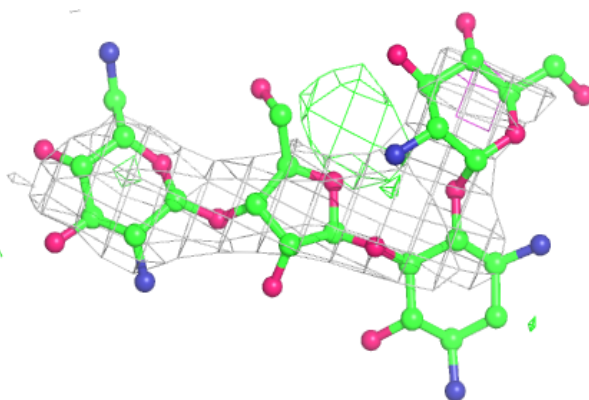
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around PAR A 1812:**

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

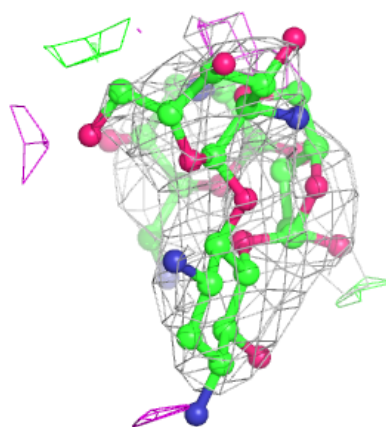
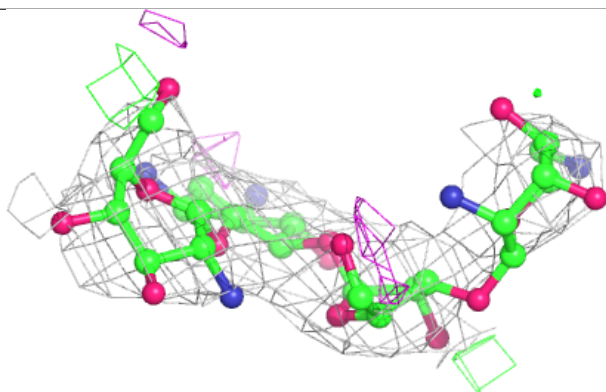
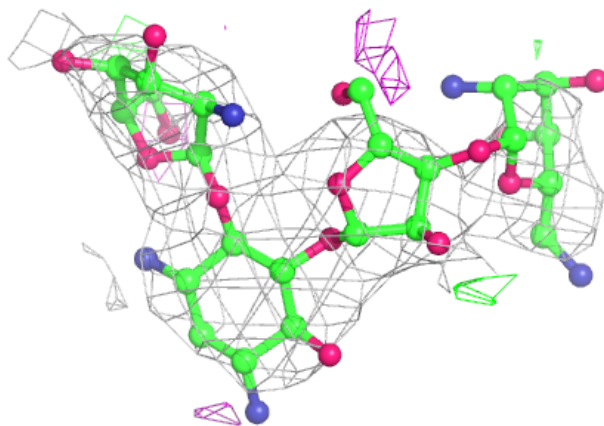
**Electron density around PAR A 1817:**

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



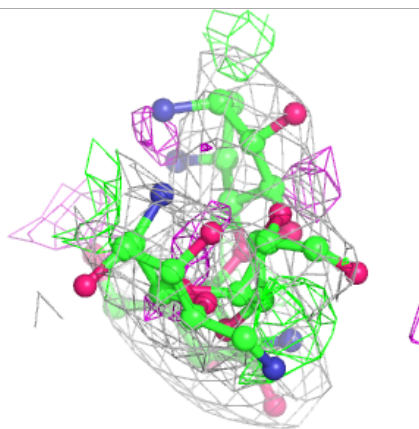
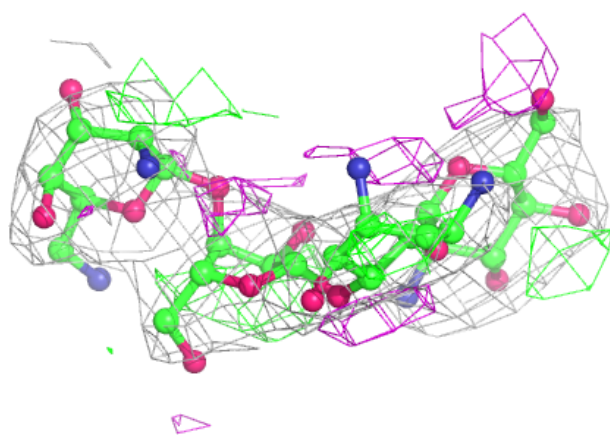
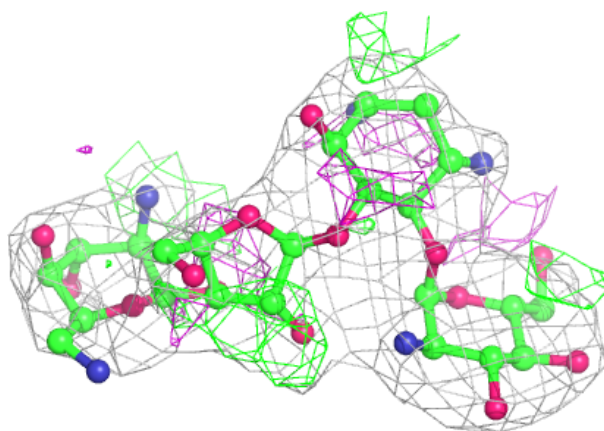
**Electron density around PAR A 1818:**

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



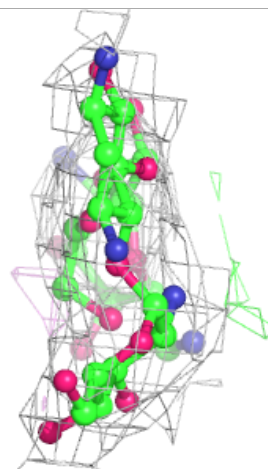
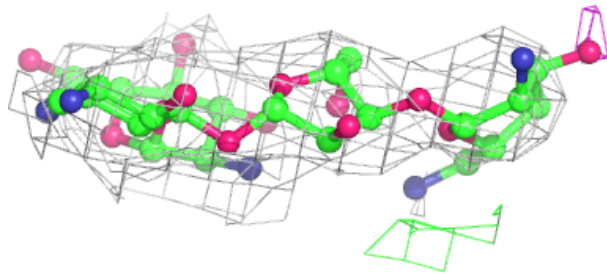
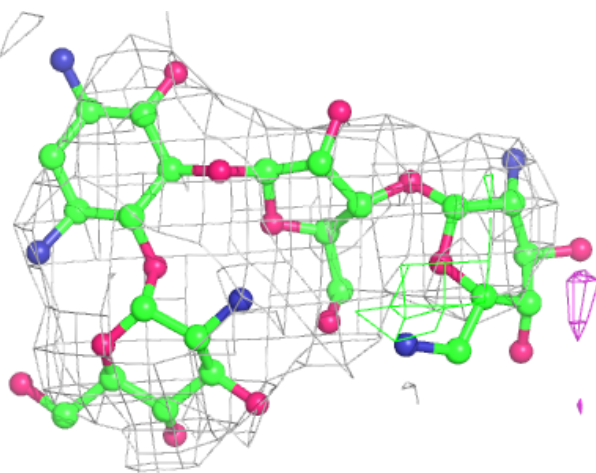
**Electron density around PAR A 1811:**

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



**Electron density around PAR A 1814:**

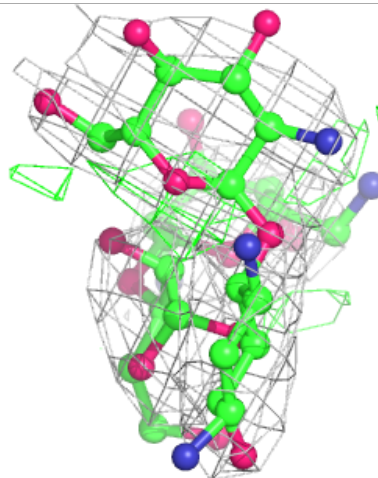
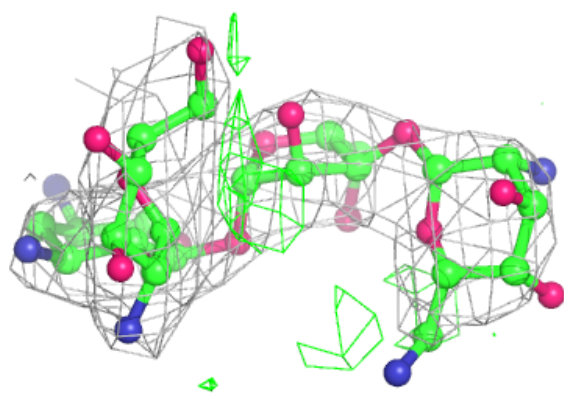
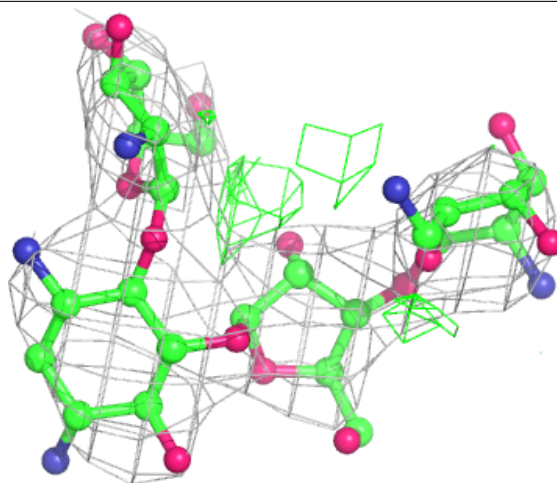
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





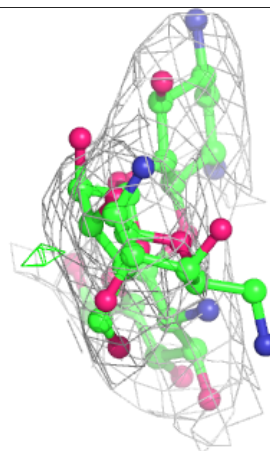
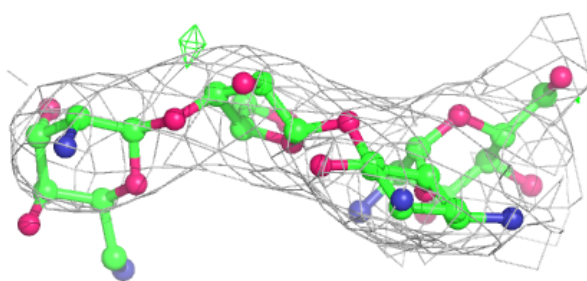
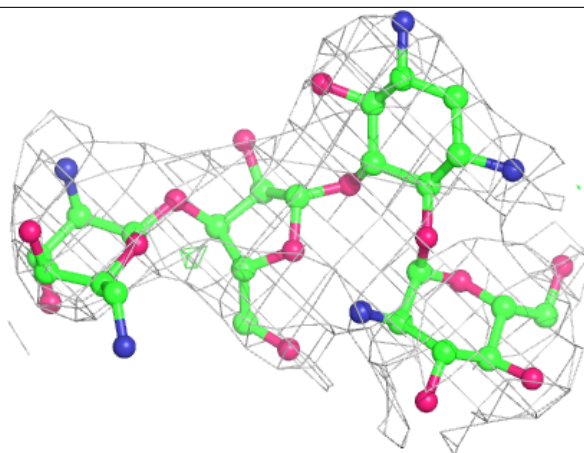
**Electron density around PAR A 1816:**

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



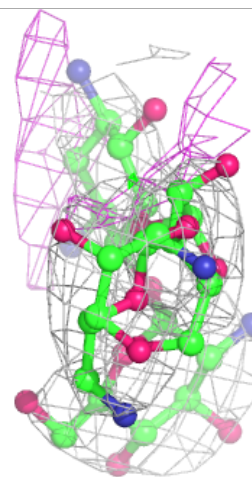
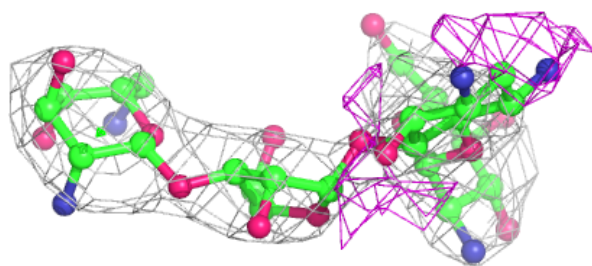
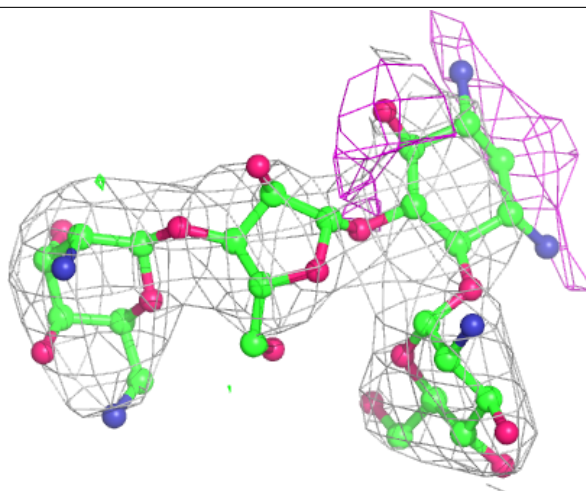
**Electron density around PAR A 1810:**

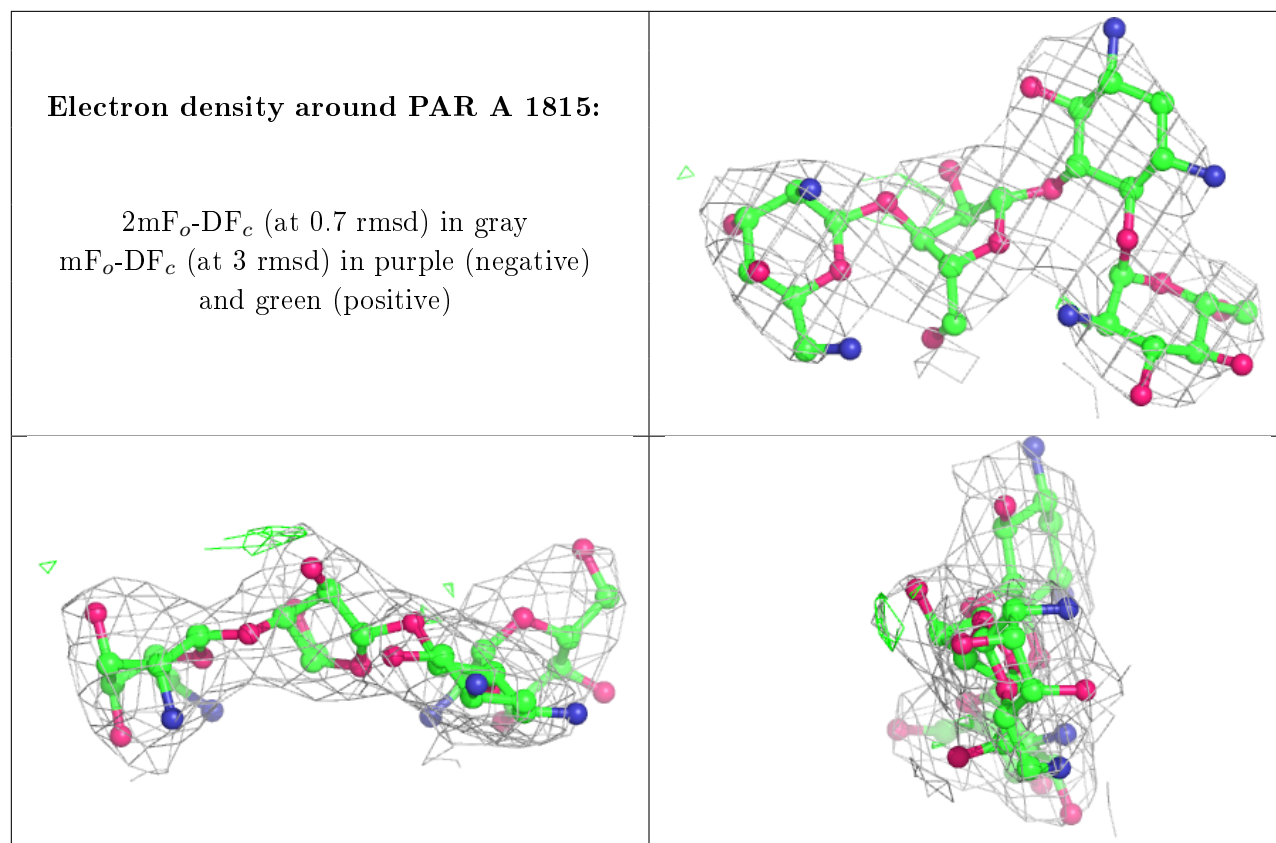
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around PAR A 1813:**

$2mF_o-DF_c$  (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.