



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 05:29 am BST

PDB ID : 4X64
Title : Crystal Structure of 30S ribosomal subunit from *Thermus thermophilus*
Authors : Demirci, H.; Chen, J.; Choi, J.; Soltis, M.; Puglisi, J.D.
Deposited on : 2014-12-06
Resolution : 3.35 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

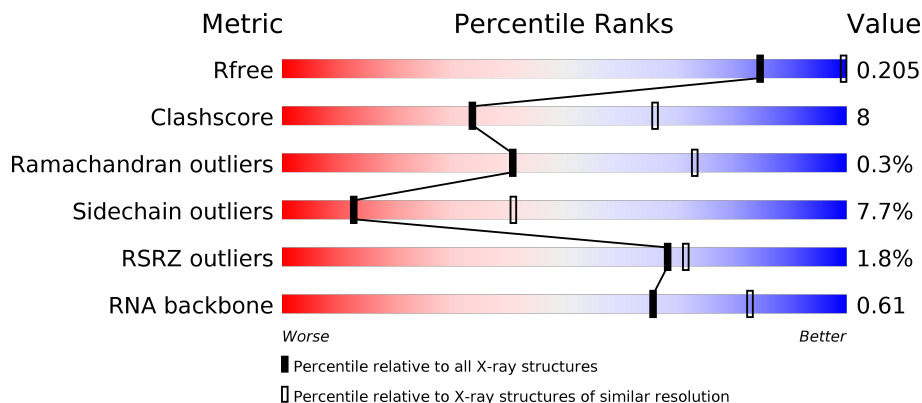
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



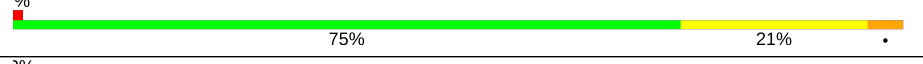

The reported resolution of this entry is 3.35 Å.

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.













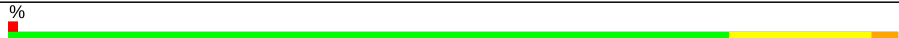








Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1558 (3.42-3.30)
Clashscore	141614	1627 (3.42-3.30)
Ramachandran outliers	138981	1599 (3.42-3.30)
Sidechain outliers	138945	1598 (3.42-3.30)
RSRZ outliers	127900	1507 (3.42-3.30)
RNA backbone	3102	1023 (3.80-2.92)

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

Mol	Chain	Length	Quality of chain
1	A	1522	 55% 36% 7% ..
2	B	236	 73% 25% . 3%
3	C	207	 75% 21% .
4	D	208	 74% 22% . 2%

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Mol	Chain	Length	Quality of chain
5	E	151	
6	F	101	
7	G	155	
8	H	138	
9	I	127	
10	J	99	
11	K	119	
12	L	125	
13	M	118	
14	N	60	
15	O	88	
16	P	84	
17	Q	99	
18	R	73	
19	S	81	
20	T	99	
21	U	25	
22	a	6	
23	b	11	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	MG	A	1639	-	-	-	X
25	MG	A	1717	-	-	-	X
25	MG	A	1742	-	-	-	X
25	MG	A	1782	-	-	-	X
25	MG	A	1787	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	MG	A	1802	-	-	-	X
25	MG	A	1803	-	-	-	X
25	MG	A	1829	-	-	-	X
25	MG	A	1832	-	-	-	X
25	MG	A	1833	-	-	-	X
25	MG	A	1844	-	-	-	X
25	MG	A	1868	-	-	-	X
25	MG	A	1871	-	-	-	X
25	MG	Q	202	-	-	-	X
26	K	A	1901	-	-	-	X
26	K	A	1909	-	-	-	X
26	K	A	1910	-	-	-	X
26	K	A	1919	-	-	-	X
26	K	A	1926	-	-	-	X
26	K	A	1927	-	-	-	X
26	K	E	202	-	-	-	X

2 Entry composition i

There are 28 unique types of molecules in this entry. The entry contains 52825 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	A	1512	32504	14477	6011	10505	1511	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1534	C	A	conflict	GB 55771382
A	1535	A	C	conflict	GB 55771382

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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 30S ribosomal protein S15.

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
17	Q	99	823	528	151	142	2	0	0	0

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
18	R	73	598	381	118	99	0	0	0

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

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

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

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

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

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

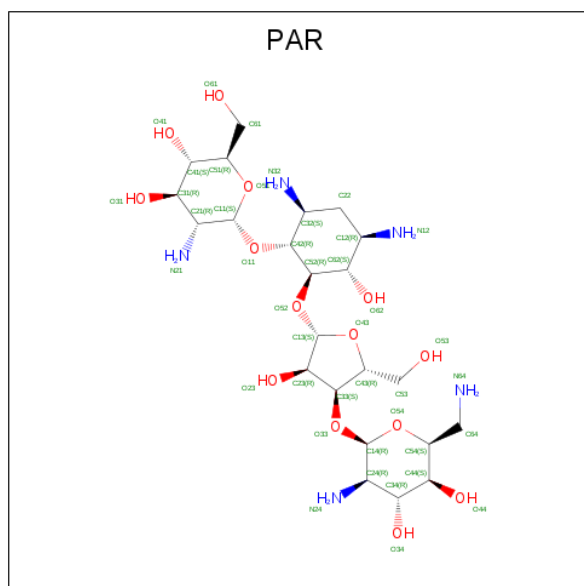
- Molecule 22 is a RNA chain called RNA (5'-D*(MA6)P*AP*AP*UP*UP*U)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
22	a	6	124	58	21	40	5	0	0	0

- Molecule 23 is a RNA chain called RNA (5'-D(P*GP*AP*CP*UP*(70U)P*UP*UP*(12A)P*AP*(PSU)P*C)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
23	b	11	247	112	37	85	11	2	0	0	0

- Molecule 24 is PAROMOMYCIN (three-letter code: PAR) (formula: C₂₃H₄₅N₅O₁₄).



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

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

- Molecule 25 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	P	4	Total	Mg	0	0
			4	4		
25	G	2	Total	Mg	0	0
			2	2		
25	Q	2	Total	Mg	0	0
			2	2		
25	D	1	Total	Mg	0	0
			1	1		
25	E	1	Total	Mg	0	0
			1	1		
25	H	4	Total	Mg	0	0
			4	4		
25	b	2	Total	Mg	0	0
			2	2		
25	C	1	Total	Mg	0	0
			1	1		
25	a	2	Total	Mg	0	0
			2	2		
25	A	284	Total	Mg	0	0
			284	284		
25	T	1	Total	Mg	0	0
			1	1		
25	N	1	Total	Mg	0	0
			1	1		
25	L	2	Total	Mg	0	0
			2	2		
25	S	3	Total	Mg	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	F	1	Total	Mg	0	0
			1	1		

- Molecule 26 is POTASSIUM ION (three-letter code: K) (formula: K).

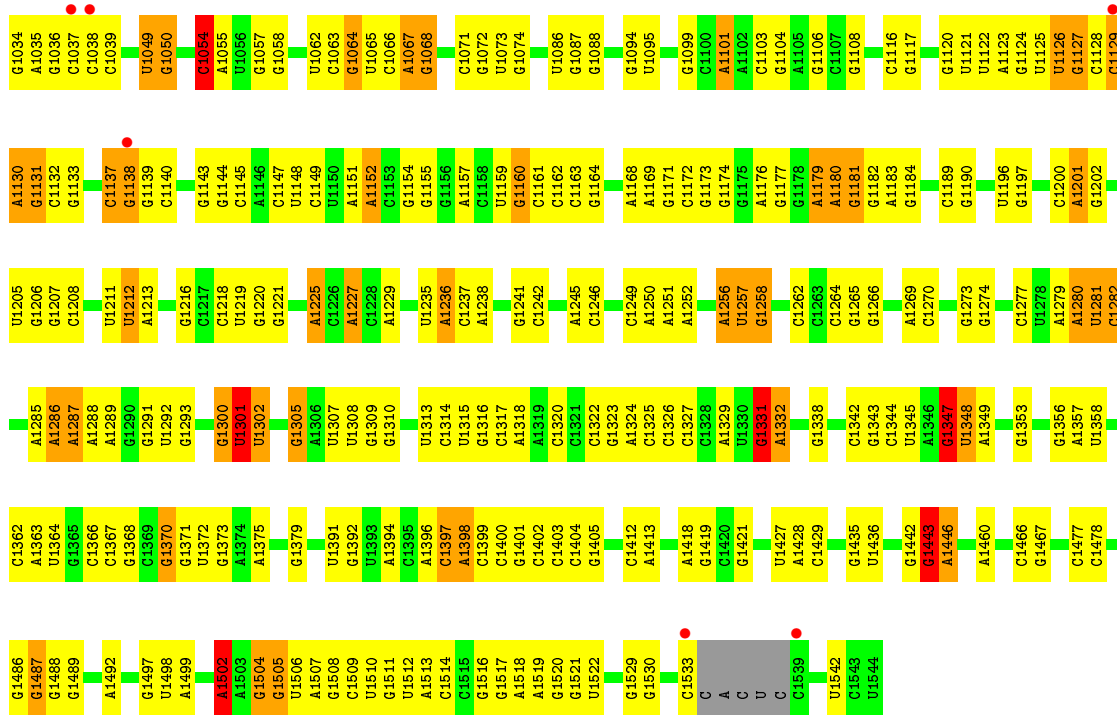
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
26	G	1	Total	K	0	0
			1	1		
26	A	38	Total	K	0	0
			38	38		
26	M	1	Total	K	0	0
			1	1		
26	E	1	Total	K	0	0
			1	1		

- Molecule 27 is ZINC ION (three-letter code: ZN) (formula: Zn).

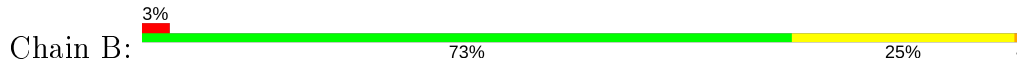
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
27	D	1	Total	Zn	0	0
			1	1		
27	N	1	Total	Zn	0	0
			1	1		

- Molecule 28 is water.

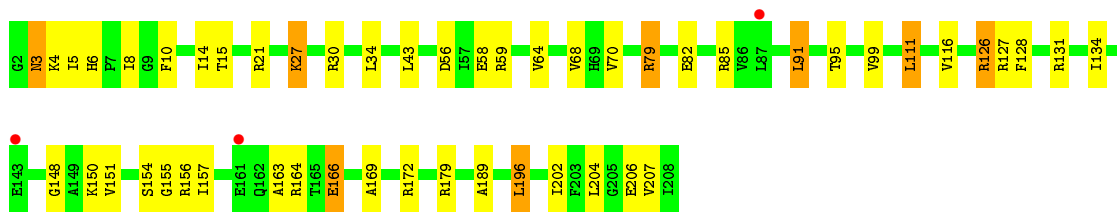
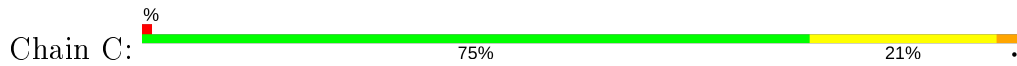
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	A	213	Total	O	0	0
			213	213		
28	D	2	Total	O	0	0
			2	2		
28	E	5	Total	O	0	0
			5	5		
28	L	3	Total	O	0	0
			3	3		
28	T	1	Total	O	0	0
			1	1		
28	U	1	Total	O	0	0
			1	1		



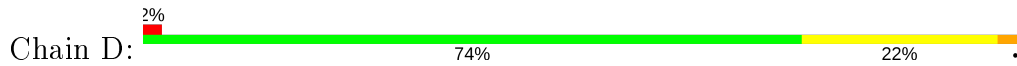
• Molecule 2: 30S ribosomal protein S2

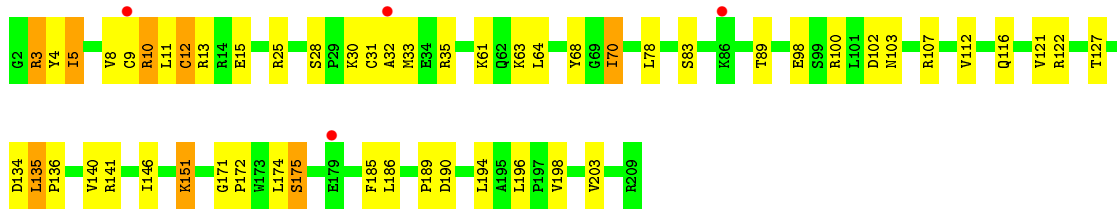


• Molecule 3: 30S ribosomal protein S3

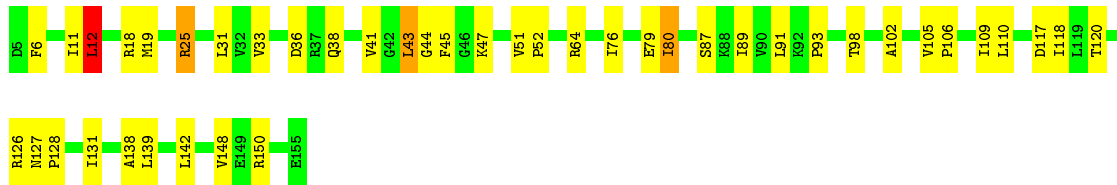


• Molecule 4: 30S ribosomal protein S4

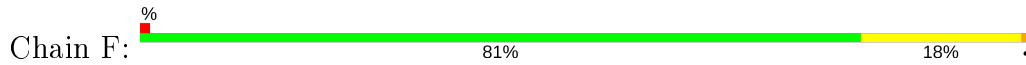




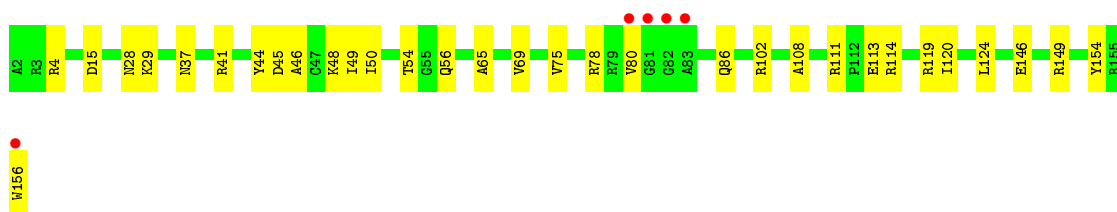
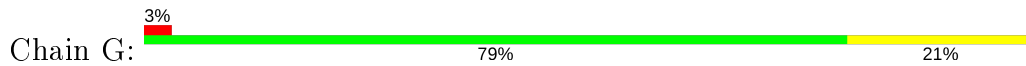
• Molecule 5: 30S ribosomal protein S5



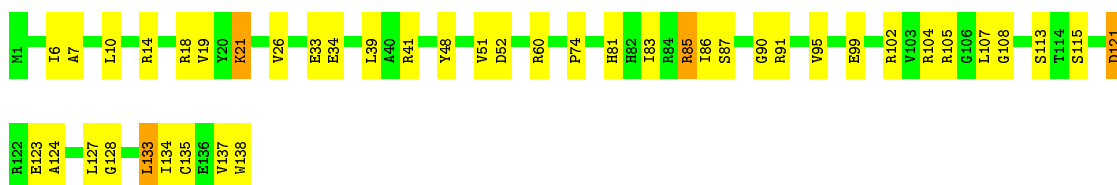
• Molecule 6: 30S ribosomal protein S6



• Molecule 7: 30S ribosomal protein S7

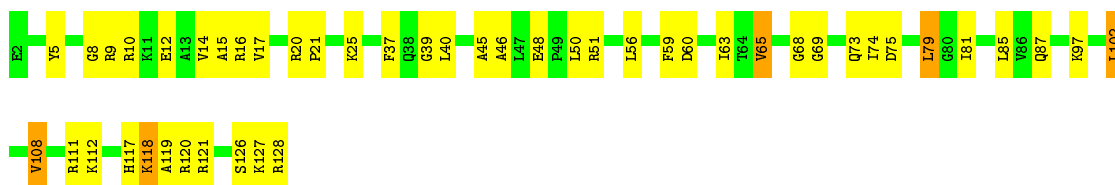


• Molecule 8: 30S ribosomal protein S8

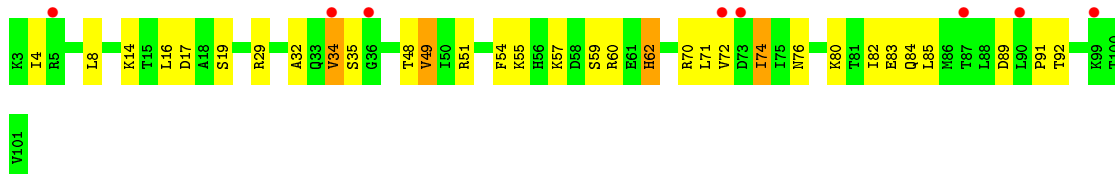


• Molecule 9: 30S ribosomal protein S9

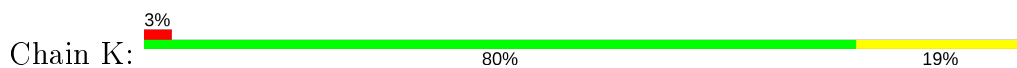




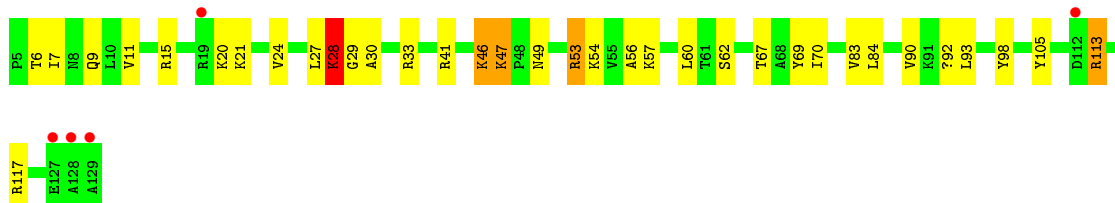
- Molecule 10: 30S ribosomal protein S10



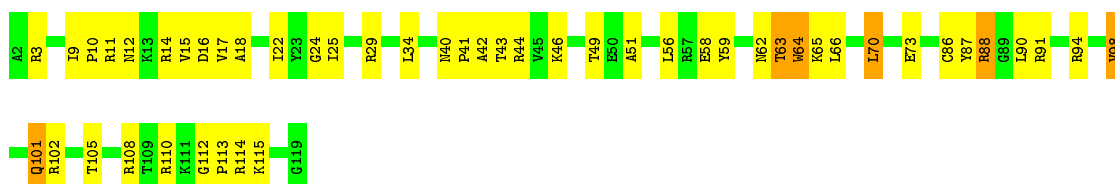
- Molecule 11: 30S ribosomal protein S11



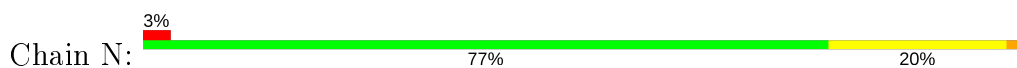
- Molecule 12: 30S ribosomal protein S12



- Molecule 13: 30S ribosomal protein S13

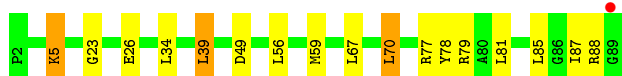
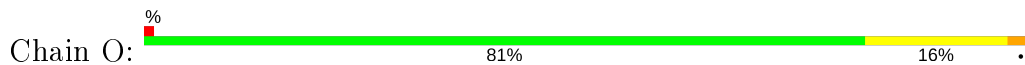


- Molecule 14: 30S ribosomal protein S14 type Z

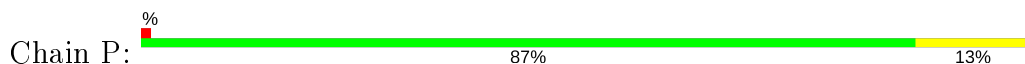




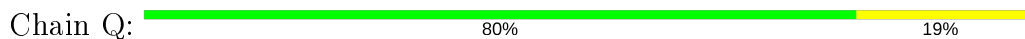
- Molecule 15: 30S ribosomal protein S15



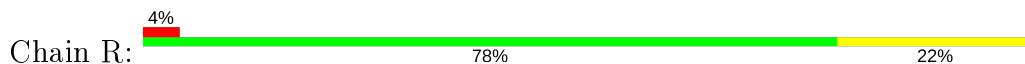
- Molecule 16: 30S ribosomal protein S16



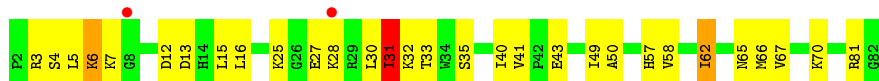
- Molecule 17: 30S ribosomal protein S17



- Molecule 18: 30S ribosomal protein S18



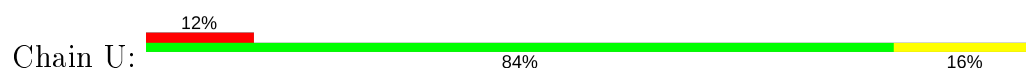
- Molecule 19: 30S ribosomal protein S19



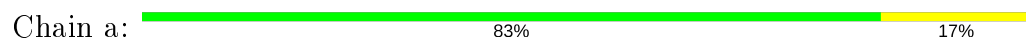
- Molecule 20: 30S ribosomal protein S20



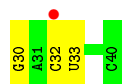
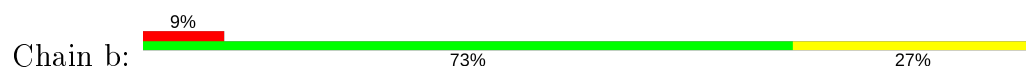
- Molecule 21: 30S ribosomal protein Thx



- Molecule 22: RNA (5'-D(*(MA6)P*AP*AP*UP*UP*U)-3')



- Molecule 23: RNA (5'-D(P*GP*AP*CP*UP*(70U)P*UP*UP*(12A)P*AP*(PSU)P*C)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	400.50Å 400.50Å 175.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.88 – 3.35 34.88 – 3.35	Depositor EDS
% Data completeness (in resolution range)	84.4 (34.88-3.35) 79.9 (34.88-3.35)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 3.32Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: dev_1938)	Depositor
R, R_{free}	0.165 , 0.205 0.165 , 0.205	Depositor DCC
R_{free} test set	8617 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	55.8	Xtrriage
Anisotropy	0.051	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 78.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	52825	wwPDB-VP
Average B, all atoms (Å ²)	92.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 12A, PAR, MA6, ZN, 70U, K, 0TD, MG, 2MG, 5MC, UR3, 4OC, M2G, 7MG, 6MD, 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	0.36	0/36037	0.87	32/56239 (0.1%)
2	B	0.26	0/1909	0.44	0/2579
3	C	0.28	0/1637	0.45	0/2207
4	D	0.32	0/1733	0.47	1/2318 (0.0%)
5	E	0.32	0/1163	0.52	1/1566 (0.1%)
6	F	0.25	0/856	0.43	0/1154
7	G	0.26	0/1276	0.45	0/1709
8	H	0.31	0/1136	0.48	0/1527
9	I	0.26	0/1029	0.47	0/1379
10	J	0.29	0/806	0.50	0/1084
11	K	0.30	0/900	0.51	0/1213
12	L	0.32	0/978	0.55	0/1308
13	M	0.26	0/947	0.46	0/1270
14	N	0.30	0/501	0.44	0/664
15	O	0.26	0/745	0.45	0/992
16	P	0.30	0/717	0.49	0/965
17	Q	0.33	0/836	0.51	0/1117
18	R	0.27	0/604	0.43	0/801
19	S	0.24	0/662	0.51	0/892
20	T	0.29	0/765	0.53	0/1007
21	U	0.25	0/213	0.42	0/279
22	a	0.29	0/115	0.83	0/176
23	b	0.83	1/184 (0.5%)	0.80	0/277
All	All	0.34	1/55749 (0.0%)	0.76	34/82723 (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
12	L	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	30	G	OP3-P	-10.49	1.48	1.61

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	328	C	N1-C2-O2	8.72	124.14	118.90
1	A	328	C	C2-N1-C1'	8.07	127.68	118.80
1	A	839	U	C2-N1-C1'	7.07	126.18	117.70
1	A	1301	U	P-O3'-C3'	6.86	127.93	119.70
1	A	839	U	N1-C2-O2	6.59	127.42	122.80
1	A	254	G	O5'-P-OP1	-6.49	99.86	105.70
1	A	60	A	P-O3'-C3'	6.46	127.46	119.70
1	A	243	A	P-O3'-C3'	6.36	127.33	119.70
1	A	328	C	N3-C2-O2	-6.17	117.58	121.90
1	A	108	G	O4'-C1'-N9	6.08	113.06	108.20
1	A	204	U	C2-N1-C1'	6.04	124.95	117.70
4	D	12	CYS	CA-CB-SG	5.89	124.61	114.00
1	A	328	C	C6-N1-C1'	-5.82	113.82	120.80
1	A	839	U	N3-C2-O2	-5.67	118.23	122.20
1	A	913	A	P-O3'-C3'	5.62	126.45	119.70
1	A	1054	C	O4'-C1'-N1	5.61	112.69	108.20
1	A	1502	A	N1-C6-N6	5.54	121.93	118.60
1	A	433	C	C5-C6-N1	5.52	123.76	121.00
1	A	812	C	P-O3'-C3'	5.44	126.22	119.70
1	A	433	C	C2-N1-C1'	5.40	124.74	118.80
1	A	1067	A	P-O3'-C3'	5.40	126.18	119.70
1	A	1347	G	P-O3'-C3'	5.36	126.13	119.70
1	A	687	A	P-O3'-C3'	5.33	126.09	119.70
1	A	328	C	P-O3'-C3'	5.29	126.05	119.70
1	A	328	C	C5-C6-N1	5.21	123.61	121.00
1	A	432	A	P-O3'-C3'	5.21	125.96	119.70
1	A	484	G	P-O3'-C3'	5.21	125.95	119.70
1	A	1331	G	O4'-C1'-N9	5.18	112.34	108.20
1	A	117	G	N1-C6-O6	5.17	123.00	119.90
1	A	1443	G	P-O3'-C3'	5.16	125.89	119.70
5	E	12	LEU	CA-CB-CG	5.15	127.14	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	701	C	P-O3'-C3'	5.12	125.85	119.70
1	A	1502	A	C6-C5-N7	-5.09	128.74	132.30
1	A	1347	G	OP2-P-O3'	5.00	116.21	105.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	H	90	GLY	Peptide
12	L	46	LYS	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32504	0	16434	433	0
2	B	1874	0	1887	34	0
3	C	1613	0	1677	34	0
4	D	1703	0	1763	31	0
5	E	1147	0	1207	24	0
6	F	843	0	857	8	0
7	G	1257	0	1296	19	0
8	H	1116	0	1177	28	0
9	I	1010	0	1037	36	0
10	J	793	0	835	19	0
11	K	885	0	904	12	0
12	L	973	0	1058	28	0
13	M	937	0	995	28	0
14	N	492	0	529	10	0
15	O	734	0	771	12	0
16	P	701	0	720	5	0
17	Q	823	0	891	12	0
18	R	598	0	670	9	0
19	S	648	0	673	17	0
20	T	763	0	861	19	0
21	U	209	0	221	1	0
22	a	124	0	67	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	b	247	0	129	0	0
24	A	252	0	270	13	0
25	A	284	0	0	0	0
25	C	1	0	0	0	0
25	D	1	0	0	0	0
25	E	1	0	0	0	0
25	F	1	0	0	0	0
25	G	2	0	0	0	0
25	H	4	0	0	0	0
25	L	2	0	0	0	0
25	N	1	0	0	0	0
25	P	4	0	0	0	0
25	Q	2	0	0	0	0
25	S	3	0	0	0	0
25	T	1	0	0	0	0
25	a	2	0	0	0	0
25	b	2	0	0	0	0
26	A	38	0	0	0	0
26	E	1	0	0	0	0
26	G	1	0	0	0	0
26	M	1	0	0	0	0
27	D	1	0	0	0	0
27	N	1	0	0	0	0
28	A	213	0	0	3	0
28	D	2	0	0	1	0
28	E	5	0	0	0	0
28	L	3	0	0	0	0
28	T	1	0	0	0	0
28	U	1	0	0	0	0
All	All	52825	0	36929	744	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 8.

All (744) 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:235:C:H5'	17:Q:70:ARG:HG2	1.53	0.91
1:A:48:C:OP1	24:A:1603:PAR:N12	2.11	0.83
4:D:32:ALA:HA	4:D:35:ARG:HG2	1.61	0.81
1:A:266:G:H5'	1:A:268:C:H41	1.47	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:662:G:N7	24:A:1604:PAR:N12	2.32	0.78
12:L:53:ARG:NH1	12:L:92:0TD:OD2	2.17	0.78
1:A:1502:A:H2	1:A:1505:G:H1	1.31	0.77
1:A:537:G:OP1	12:L:113:ARG:NH2	2.18	0.77
1:A:951:G:OP2	13:M:102:ARG:NH2	2.18	0.76
24:A:1602:PAR:HN21	24:A:1602:PAR:H23	1.49	0.76
19:S:50:ALA:HB1	19:S:57:HIS:HB3	1.69	0.75
1:A:1345:U:OP1	9:I:120:ARG:NH1	2.19	0.75
1:A:664:G:H22	1:A:741:G:H1	1.34	0.74
15:O:56:LEU:HA	15:O:59:MET:HE2	1.69	0.74
1:A:713:G:H2'	1:A:714:G:C8	2.22	0.74
11:K:15:ALA:HA	11:K:77:MET:HA	1.68	0.74
12:L:41:ARG:HE	12:L:57:LYS:HE2	1.53	0.73
3:C:14:ILE:HG22	3:C:15:THR:HG23	1.71	0.72
8:H:10:LEU:HD22	8:H:83:ILE:HD11	1.72	0.72
9:I:51:ARG:HG3	9:I:56:LEU:HD21	1.70	0.72
1:A:1003:G:N2	1:A:1039:C:O2	2.22	0.71
5:E:80:ILE:HD13	5:E:138:ALA:HB1	1.72	0.71
1:A:542:G:OP1	4:D:10:ARG:NH2	2.23	0.71
5:E:79:GLU:HG3	5:E:93:PRO:HD2	1.72	0.71
1:A:975:A:H4'	1:A:976:G:H5''	1.73	0.71
1:A:677:U:H3	1:A:713:G:H22	1.40	0.70
11:K:57:THR:HG22	11:K:59:TYR:H	1.56	0.70
1:A:1301:U:O2'	1:A:1302:U:O5'	2.07	0.70
10:J:82:ILE:HA	10:J:85:LEU:HB2	1.72	0.70
1:A:1391:U:H2'	1:A:1392:G:C8	2.26	0.70
1:A:673:G:H2'	1:A:674:G:C8	2.26	0.69
1:A:298:A:N6	28:A:2150:HOH:O	2.18	0.69
8:H:85:ARG:NE	8:H:87:SER:O	2.26	0.69
1:A:243:A:H4'	1:A:244:U:O5'	1.93	0.69
1:A:1086:U:H3	1:A:1099:G:H22	1.38	0.69
1:A:1347:G:O6	9:I:10:ARG:NH2	2.25	0.69
1:A:21:G:H2'	1:A:22:G:C8	2.28	0.69
1:A:1122:U:O4	1:A:1123:A:N6	2.27	0.68
5:E:80:ILE:HD12	5:E:91:LEU:HB2	1.75	0.68
1:A:153:C:H42	1:A:168:G:H1	1.41	0.68
12:L:24:VAL:HG13	12:L:98:TYR:HE1	1.58	0.67
3:C:27:LYS:H	3:C:27:LYS:HD3	1.60	0.67
3:C:156:ARG:H	3:C:163:ALA:HA	1.59	0.67
15:O:87:ILE:HG22	15:O:88:ARG:H	1.58	0.67
1:A:946:A:H2'	1:A:947:G:C8	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1435:G:H2'	1:A:1436:U:C6	2.29	0.66
1:A:60:A:H4'	1:A:61:G:O5'	1.95	0.66
10:J:8:LEU:HB2	10:J:70:ARG:HB2	1.77	0.66
19:S:33:THR:HG22	19:S:35:SER:H	1.58	0.66
1:A:1200:C:O2'	1:A:1205:U:O4	2.14	0.66
19:S:5:LEU:HD21	19:S:70:LYS:HZ1	1.61	0.66
1:A:1427:U:H2'	1:A:1428:A:H8	1.59	0.66
17:Q:67:LYS:HA	17:Q:70:ARG:HH12	1.59	0.66
3:C:64:VAL:HG23	3:C:99:VAL:HG11	1.79	0.65
1:A:427:U:OP1	4:D:13:ARG:NH2	2.29	0.65
10:J:48:THR:HA	10:J:62:HIS:HB3	1.77	0.65
1:A:974:A:OP2	14:N:41:ARG:NH1	2.29	0.65
1:A:1124:G:N7	1:A:1145:C:O2'	2.27	0.64
1:A:670:G:N7	24:A:1606:PAR:O44	2.29	0.64
7:G:113:GLU:HB2	7:G:119:ARG:HG2	1.78	0.64
1:A:1250:A:H2'	1:A:1251:A:C8	2.32	0.64
10:J:32:ALA:HB2	10:J:76:ASN:HB2	1.80	0.64
7:G:78:ARG:NH1	7:G:154:TYR:O	2.31	0.63
7:G:146:GLU:HA	7:G:149:ARG:HG2	1.81	0.63
1:A:279:A:OP2	17:Q:95:TYR:OH	2.15	0.63
1:A:983:A:O2'	1:A:1050:G:OP2	2.16	0.62
13:M:91:ARG:HB2	13:M:98:VAL:HG13	1.80	0.62
1:A:1356:G:H2'	1:A:1357:A:C8	2.34	0.62
12:L:33:ARG:HG2	12:L:62:SER:HB2	1.81	0.62
1:A:1010:G:H2'	1:A:1011:G:H8	1.65	0.62
1:A:328:C:H4'	1:A:329:A:H5'	1.81	0.62
4:D:102:ASP:OD1	4:D:103:ASN:N	2.32	0.62
2:B:223:ILE:HD13	2:B:230:VAL:H	1.65	0.61
2:B:84:GLU:OE2	2:B:233:SER:OG	2.16	0.61
8:H:113:SER:HB2	8:H:134:ILE:HD11	1.82	0.61
1:A:560:U:H5'	1:A:566:G:N2	2.14	0.61
1:A:1071:C:H2'	1:A:1072:G:H8	1.66	0.61
10:J:19:SER:HB3	10:J:91:PRO:HG3	1.81	0.61
5:E:98:THR:HB	5:E:117:ASP:HB3	1.83	0.61
8:H:121:ASP:OD1	8:H:121:ASP:N	2.33	0.61
1:A:390:C:O3'	16:P:28:ARG:NH2	2.34	0.61
5:E:110:LEU:HD13	5:E:118:ILE:HG21	1.82	0.60
13:M:10:PRO:HB2	13:M:18:ALA:HB1	1.83	0.60
1:A:1026:G:H3'	1:A:1027:C:H5''	1.83	0.60
10:J:51:ARG:HD2	10:J:59:SER:HB2	1.84	0.60
1:A:114:U:H5''	24:A:1603:PAR:H52	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:46:ALA:HB2	9:I:74:ILE:HG23	1.84	0.60
1:A:835:U:OP1	18:R:64:ARG:NH2	2.35	0.59
5:E:93:PRO:HG2	8:H:105:ARG:HH11	1.67	0.59
1:A:975:A:H5'	1:A:975:A:H8	1.67	0.59
1:A:501:C:OP1	12:L:117:ARG:NH2	2.34	0.59
5:E:33:VAL:HG22	5:E:43:LEU:HD23	1.83	0.59
1:A:359:U:H2'	1:A:360:A:C8	2.38	0.59
17:Q:24:GLU:HG2	17:Q:39:SER:HB3	1.85	0.59
20:T:10:LEU:HD12	20:T:11:SER:H	1.68	0.59
1:A:1427:U:H2'	1:A:1428:A:C8	2.38	0.58
1:A:440:A:H3'	1:A:442:C:H6	1.68	0.58
4:D:25:ARG:HA	4:D:28:SER:HB2	1.85	0.58
1:A:527:7MG:O2'	1:A:535:A:N1	2.33	0.58
8:H:86:ILE:HD12	8:H:133:LEU:HD22	1.83	0.58
1:A:1291:G:H4'	9:I:39:GLY:HA3	1.83	0.58
1:A:523:A:N6	12:L:92:0TD:OD1	2.35	0.58
1:A:1004:A:OP1	1:A:1025:U:N3	2.29	0.58
1:A:875:C:O2'	8:H:14:ARG:NH1	2.37	0.58
1:A:646:U:H2'	1:A:647:C:C6	2.38	0.58
1:A:1391:U:H2'	1:A:1392:G:H8	1.69	0.58
1:A:1504:G:OP1	1:A:1507:A:H4'	2.04	0.58
1:A:1057:G:H5''	3:C:154:SER:HB2	1.86	0.58
3:C:126:ARG:HE	3:C:128:PHE:HD2	1.49	0.58
20:T:10:LEU:HG	20:T:12:ALA:H	1.68	0.58
1:A:1035:A:H2'	1:A:1036:G:H8	1.68	0.57
5:E:12:LEU:HD13	5:E:31:LEU:HB2	1.86	0.57
6:F:10:LEU:HD12	6:F:59:TYR:HB3	1.86	0.57
19:S:13:ASP:HA	19:S:16:LEU:HB3	1.86	0.57
1:A:920:U:H2'	1:A:921:U:C6	2.38	0.57
1:A:250:A:H4'	1:A:251:G:O5'	2.04	0.57
1:A:642:A:H2'	1:A:643:C:H6	1.70	0.57
4:D:140:VAL:HG11	4:D:146:ILE:HD11	1.86	0.57
1:A:360:A:H61	24:A:1603:PAR:H44	1.69	0.57
1:A:1049:U:O2'	14:N:3:ARG:NH1	2.37	0.57
1:A:1147:C:O2'	9:I:5:TYR:OH	2.23	0.57
1:A:17:U:H2'	1:A:18:C:C6	2.40	0.56
3:C:189:ALA:HB3	3:C:196:LEU:HB2	1.86	0.56
11:K:110:ASP:OD2	18:R:88:LYS:NZ	2.35	0.56
15:O:26:GLU:OE1	15:O:77:ARG:NH1	2.38	0.56
1:A:1502:A:H2	1:A:1505:G:N1	2.02	0.56
1:A:1062:U:H2'	1:A:1063:C:C6	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1396:A:H4'	1:A:1397:C:H5''	1.88	0.56
1:A:1266:G:N2	1:A:1269:A:OP2	2.30	0.56
13:M:108:ARG:HD2	13:M:114:ARG:HE	1.71	0.56
1:A:116:A:H5''	28:A:2017:HOH:O	2.05	0.56
1:A:1229:A:OP2	13:M:114:ARG:HD3	2.06	0.56
1:A:714:G:H2'	1:A:715:A:C8	2.41	0.56
1:A:736:C:H2'	1:A:737:A:C8	2.41	0.56
4:D:98:GLU:OE2	4:D:107:ARG:NE	2.35	0.56
12:L:53:ARG:HG2	12:L:69:TYR:HE2	1.70	0.56
1:A:235:C:N4	28:A:2087:HOH:O	2.38	0.56
12:L:28:LYS:HB3	12:L:30:ALA:HB2	1.88	0.56
1:A:1510:U:H2'	1:A:1511:G:C8	2.41	0.56
9:I:118:LYS:O	9:I:120:ARG:N	2.33	0.56
17:Q:66:SER:O	17:Q:70:ARG:NH1	2.39	0.56
1:A:976:G:H5'	1:A:1358:U:O2'	2.06	0.55
3:C:116:VAL:HG21	3:C:202:ILE:HD11	1.88	0.55
1:A:1286:A:H2'	1:A:1287:A:H4'	1.87	0.55
1:A:981:U:H5	1:A:982:U:HO2'	1.54	0.55
20:T:89:ARG:NH2	20:T:105:SER:O	2.37	0.55
1:A:110:C:H2'	1:A:111:G:O4'	2.07	0.55
1:A:1287:A:H2'	1:A:1288:A:C8	2.41	0.55
1:A:1132:C:H2'	1:A:1133:G:H8	1.70	0.55
2:B:122:PHE:HA	2:B:127:ILE:HG12	1.88	0.55
3:C:64:VAL:HB	3:C:99:VAL:HG21	1.88	0.55
8:H:18:ARG:NH2	8:H:81:HIS:O	2.40	0.55
1:A:103:C:OP1	20:T:17:ARG:NH1	2.40	0.55
1:A:1250:A:H4'	9:I:68:GLY:N	2.21	0.55
1:A:1392:G:N2	1:A:1502:A:H8	2.05	0.55
1:A:524:G:H2'	1:A:525:C:C6	2.42	0.55
9:I:15:ALA:HB2	9:I:65:VAL:HG13	1.88	0.54
1:A:269:C:H2'	1:A:270:A:C8	2.42	0.54
1:A:1072:G:H2'	1:A:1073:U:C6	2.43	0.54
1:A:851:G:H2'	1:A:852:G:H8	1.71	0.54
3:C:79:ARG:HE	3:C:82:GLU:HG2	1.73	0.54
9:I:50:LEU:HB3	9:I:56:LEU:H	1.72	0.54
17:Q:83:ASP:N	17:Q:83:ASP:OD1	2.39	0.54
1:A:359:U:H2'	1:A:360:A:H8	1.71	0.54
1:A:1313:U:O4	19:S:4:SER:OG	2.19	0.54
7:G:54:THR:HG22	7:G:56:GLN:H	1.71	0.54
1:A:646:U:H2'	1:A:647:C:H6	1.73	0.54
7:G:75:VAL:HG21	7:G:86:GLN:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1162:C:H42	1:A:1174:G:H1	1.54	0.54
7:G:37:ASN:ND2	9:I:39:GLY:O	2.34	0.54
9:I:25:LYS:N	9:I:60:ASP:OD1	2.41	0.54
10:J:4:ILE:HD11	10:J:74:ILE:HD12	1.90	0.54
1:A:1251:A:H2'	1:A:1252:A:C8	2.42	0.54
1:A:35:G:H2'	1:A:36:C:C6	2.43	0.54
18:R:32:ARG:HA	18:R:69:THR:HG21	1.90	0.54
1:A:1301:U:HO2'	1:A:1302:U:P	2.31	0.54
10:J:51:ARG:HG3	10:J:60:ARG:O	2.08	0.54
1:A:562:C:H1'	12:L:15:ARG:HG3	1.89	0.54
12:L:6:THR:OG1	12:L:9:GLN:HG3	2.08	0.54
1:A:750:G:N3	15:O:23:GLY:HA3	2.23	0.54
1:A:1189:C:H5''	3:C:5:ILE:HG12	1.90	0.53
1:A:1513:A:H2'	1:A:1514:C:C6	2.43	0.53
1:A:745:C:H2'	1:A:746:A:C8	2.44	0.53
16:P:57:ARG:NH1	16:P:79:VAL:O	2.42	0.53
1:A:337:C:H2'	1:A:338:A:H8	1.72	0.53
3:C:91:LEU:HD21	3:C:99:VAL:HG22	1.91	0.53
4:D:10:ARG:HG2	4:D:11:LEU:HD23	1.90	0.53
14:N:16:PHE:HB2	14:N:19:ARG:HG3	1.89	0.53
1:A:1323:G:H2'	1:A:1324:A:C8	2.44	0.53
1:A:337:C:H2'	1:A:338:A:C8	2.43	0.53
9:I:8:GLY:HA2	9:I:79:LEU:HD13	1.90	0.53
1:A:851:G:H2'	1:A:852:G:C8	2.44	0.53
13:M:15:VAL:HG23	13:M:43:THR:O	2.09	0.53
1:A:376:G:H5''	16:P:5:ARG:HD2	1.91	0.53
24:A:1602:PAR:H23	24:A:1602:PAR:N21	2.22	0.52
1:A:421:U:H3	3:C:127:ARG:CZ	2.22	0.52
1:A:666:G:N7	24:A:1604:PAR:N64	2.57	0.52
1:A:895:G:H2'	1:A:896:C:C6	2.44	0.52
11:K:33:THR:HA	11:K:39:PRO:HA	1.91	0.52
1:A:975:A:H5'	1:A:975:A:C8	2.44	0.52
8:H:86:ILE:HG13	8:H:135:CYS:HA	1.90	0.52
13:M:63:THR:HG23	13:M:64:TRP:H	1.74	0.52
1:A:1329:A:H5'	13:M:29:ARG:HD2	1.91	0.52
1:A:419:C:H42	1:A:424:G:H1	1.56	0.52
1:A:59:A:H1'	1:A:354:G:N2	2.24	0.52
1:A:1124:G:H5'	10:J:35:SER:HB3	1.91	0.52
4:D:151:LYS:H	4:D:151:LYS:HD2	1.75	0.52
14:N:27:CYS:SG	14:N:29:ARG:HB2	2.50	0.52
1:A:1028:C:H2'	1:A:1029:C:H6	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1305:G:N2	1:A:1331:G:H1'	2.24	0.52
1:A:190(J):U:H2'	1:A:190(K):G:H8	1.74	0.52
1:A:501:C:H2'	1:A:502:G:H8	1.74	0.52
1:A:1218:C:H2'	1:A:1219:U:C6	2.45	0.52
1:A:161:A:H2'	1:A:162:A:C8	2.45	0.52
1:A:757:U:H2'	1:A:758:G:O4'	2.10	0.52
1:A:1012:U:H2'	1:A:1013:G:C8	2.45	0.52
1:A:1460:A:OP1	20:T:27:LYS:NZ	2.43	0.52
1:A:946:A:H2'	1:A:947:G:H8	1.71	0.52
1:A:954:G:H21	1:A:1227:A:H62	1.58	0.51
15:O:39:LEU:HD13	15:O:56:LEU:HB2	1.92	0.51
21:U:5:ASP:O	21:U:11:GLY:HA3	2.10	0.51
20:T:67:ALA:O	20:T:73:HIS:ND1	2.43	0.51
5:E:102:ALA:HB1	5:E:106:PRO:HG2	1.92	0.51
10:J:49:VAL:HG23	14:N:41:ARG:HB2	1.92	0.51
5:E:87:SER:HB3	5:E:131:ILE:HD13	1.93	0.51
12:L:60:LEU:HB3	12:L:62:SER:HB3	1.92	0.51
13:M:16:ASP:OD1	13:M:17:VAL:N	2.39	0.51
1:A:1305:G:N2	1:A:1332:A:OP2	2.44	0.51
1:A:190(K):G:H2'	1:A:190(L):U:C6	2.46	0.51
1:A:436:C:H2'	1:A:437:U:H6	1.74	0.51
1:A:611:A:H2	1:A:629:G:H22	1.58	0.51
2:B:88:ALA:HB1	2:B:226:ARG:HH22	1.75	0.51
7:G:15:ASP:OD1	7:G:44:TYR:OH	2.28	0.51
1:A:501:C:H2'	1:A:502:G:C8	2.45	0.51
2:B:48:MET:HA	2:B:51:LEU:HB2	1.91	0.51
19:S:5:LEU:HD21	19:S:70:LYS:NZ	2.25	0.51
1:A:738:C:OP2	6:F:92:LYS:NZ	2.41	0.51
11:K:57:THR:HG22	11:K:59:TYR:N	2.26	0.51
12:L:56:ALA:HB2	12:L:70:ILE:HD11	1.93	0.51
11:K:69:ALA:O	11:K:73:MET:HG2	2.11	0.51
1:A:1087:G:H2'	1:A:1088:G:H8	1.76	0.50
1:A:1179:A:O2'	1:A:1180:A:OP1	2.30	0.50
1:A:1399:C:H4'	1:A:1400:5MC:H5''	1.93	0.50
8:H:19:VAL:HG23	8:H:21:LYS:HD3	1.93	0.50
1:A:642:A:H2'	1:A:643:C:C6	2.46	0.50
9:I:112:LYS:HE3	9:I:117:HIS:O	2.12	0.50
11:K:80:VAL:HG21	11:K:103:LEU:HD13	1.94	0.50
13:M:65:LYS:NZ	13:M:73:GLU:OE2	2.37	0.50
1:A:523:A:H61	12:L:92:0TD:CG	2.24	0.50
1:A:811:C:O2'	1:A:901:A:N1	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:973:G:H3'	1:A:974:A:H5''	1.94	0.50
6:F:33:TYR:HB2	6:F:75:LEU:HD12	1.93	0.50
8:H:6:ILE:HB	8:H:85:ARG:HH12	1.77	0.50
12:L:27:LEU:O	12:L:29:GLY:N	2.44	0.50
1:A:603:U:H2'	1:A:604:G:H8	1.77	0.50
1:A:662:G:H2'	1:A:663:A:C8	2.46	0.50
6:F:4:TYR:CZ	6:F:72:VAL:HG21	2.46	0.50
1:A:360:A:N6	24:A:1603:PAR:H44	2.25	0.50
3:C:157:ILE:HD13	3:C:166:GLU:HB2	1.93	0.50
17:Q:40:LYS:HD2	17:Q:42:TYR:CZ	2.46	0.50
1:A:1207:2MG:H2'	1:A:1208:C:H6	1.75	0.50
1:A:1402:4OC:HM22	1:A:1403:C:H5'	1.94	0.50
1:A:397:A:H5'	1:A:398:C:OP1	2.12	0.50
1:A:1017:G:H2'	1:A:1018:C:C6	2.47	0.50
1:A:1028:C:H2'	1:A:1029:C:C6	2.47	0.50
1:A:269:C:H2'	1:A:270:A:H8	1.76	0.50
1:A:335:C:H2'	1:A:336:C:C6	2.46	0.50
1:A:1307:U:OP1	13:M:101:GLN:NE2	2.45	0.50
20:T:50:GLU:H	20:T:99:LEU:HD12	1.77	0.50
1:A:1347:G:O2'	1:A:1348:U:P	2.70	0.50
12:L:41:ARG:HH21	12:L:57:LYS:NZ	2.09	0.50
1:A:1148:U:H2'	1:A:1149:C:O4'	2.12	0.49
1:A:1157:A:C2	1:A:1181:G:C4	3.00	0.49
1:A:560:U:H4'	1:A:561:U:H5''	1.94	0.49
1:A:864:A:H2'	1:A:865:A:C8	2.47	0.49
19:S:31:ILE:HG22	19:S:49:ILE:HA	1.93	0.49
9:I:21:PRO:HA	9:I:59:PHE:HA	1.94	0.49
9:I:97:LYS:HA	9:I:102:LEU:HD11	1.93	0.49
1:A:1131:G:O2'	1:A:1132:C:O4'	2.23	0.49
1:A:194:C:H2'	1:A:195:A:H5''	1.95	0.49
1:A:610:G:C4	1:A:611:A:C8	3.00	0.49
3:C:148:GLY:HA3	3:C:172:ARG:O	2.13	0.49
3:C:3:ASN:N	3:C:3:ASN:OD1	2.45	0.49
1:A:670:G:OP2	24:A:1606:PAR:N24	2.44	0.49
2:B:87:ARG:NH2	2:B:233:SER:HB2	2.28	0.49
3:C:131:ARG:HH11	3:C:166:GLU:HG3	1.78	0.49
1:A:7:G:H5'	1:A:298:A:O4'	2.12	0.49
1:A:57:G:H2'	1:A:58:C:C6	2.48	0.49
10:J:57:LYS:HG3	10:J:60:ARG:HH21	1.77	0.49
1:A:1035:A:H2'	1:A:1036:G:C8	2.47	0.49
1:A:1342:C:H2'	1:A:1343:G:C8	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1349:A:OP1	9:I:120:ARG:HB2	2.12	0.49
4:D:175:SER:HB3	4:D:186:LEU:HD21	1.95	0.49
1:A:153:C:N4	1:A:168:G:H1	2.08	0.49
8:H:7:ALA:HB2	8:H:85:ARG:HD2	1.95	0.49
1:A:1137:C:H4'	1:A:1138:G:C2	2.47	0.48
1:A:179:A:H2'	1:A:180:U:C6	2.48	0.48
1:A:222:U:H2'	1:A:223:U:C6	2.48	0.48
1:A:328:C:O2	1:A:328:C:H2'	2.12	0.48
1:A:1466:C:H2'	1:A:1467:G:O4'	2.13	0.48
1:A:299:G:H2'	1:A:300:A:C8	2.48	0.48
6:F:2:ARG:CZ	6:F:69:GLU:HG2	2.44	0.48
1:A:1521:G:H2'	1:A:1522:U:C6	2.49	0.48
13:M:88:ARG:HH11	19:S:3:ARG:HH21	1.61	0.48
1:A:1316:G:H4'	14:N:18:VAL:HG11	1.95	0.48
1:A:820:U:H4'	1:A:821:G:OP2	2.12	0.48
1:A:1256:A:O2'	1:A:1257:U:O5'	2.30	0.48
1:A:677:U:O2	1:A:777:A:O2'	2.32	0.48
1:A:818:G:H3'	1:A:819:A:H5''	1.94	0.48
1:A:1396:A:O4'	1:A:1398:A:H1'	2.14	0.48
4:D:63:LYS:HD2	4:D:198:VAL:HG22	1.96	0.48
13:M:11:ARG:HG3	13:M:12:ASN:HB2	1.95	0.48
1:A:1310:G:OP2	13:M:88:ARG:NH2	2.47	0.48
1:A:372:C:H4'	1:A:373:A:O5'	2.13	0.48
1:A:939:G:H2'	1:A:940:C:C6	2.48	0.48
3:C:134:ILE:HG23	3:C:151:VAL:HB	1.94	0.48
8:H:108:GLY:HA3	8:H:138:TRP:HB3	1.95	0.48
1:A:192:U:H1'	20:T:103:GLY:HA2	1.96	0.48
2:B:114:ARG:HH11	2:B:118:LEU:HD11	1.79	0.48
1:A:1014:A:H2'	1:A:1015:A:C8	2.48	0.48
1:A:378:G:H2'	1:A:379:C:C6	2.48	0.48
1:A:390:C:H2'	1:A:391:G:C8	2.49	0.48
1:A:399:G:H2'	1:A:400:C:C6	2.49	0.48
4:D:9:CYS:O	4:D:12:CYS:HB2	2.14	0.48
8:H:86:ILE:HG21	8:H:133:LEU:HD13	1.95	0.48
13:M:90:LEU:O	13:M:94:ARG:HG2	2.12	0.48
1:A:1015:A:H2'	1:A:1016:A:C8	2.49	0.48
1:A:1405:G:H21	1:A:1518:MA6:H1'	1.79	0.48
1:A:1516:G:N2	1:A:1519:MA6:OP2	2.46	0.48
3:C:59:ARG:HG2	3:C:64:VAL:HG22	1.94	0.48
1:A:1315:U:H2'	1:A:1316:G:O4'	2.14	0.47
1:A:666:G:H5'	1:A:726:C:H1'	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:674:G:H2'	1:A:675:A:H8	1.79	0.47
1:A:939:G:H5''	7:G:102:ARG:NH1	2.29	0.47
7:G:46:ALA:O	7:G:50:ILE:HG12	2.13	0.47
1:A:563:A:H2'	1:A:567:G:C8	2.49	0.47
2:B:24:TRP:HB2	2:B:190:THR:HG22	1.96	0.47
5:E:11:ILE:HG21	5:E:105:VAL:HG22	1.95	0.47
1:A:1147:C:O2	9:I:16:ARG:NH1	2.46	0.47
19:S:50:ALA:HA	19:S:58:VAL:O	2.14	0.47
1:A:1343:G:H2'	1:A:1344:C:C6	2.49	0.47
2:B:73:THR:HG23	2:B:95:GLN:O	2.13	0.47
6:F:9:VAL:HB	6:F:87:ARG:HB2	1.95	0.47
1:A:192:U:C1'	20:T:103:GLY:HA2	2.43	0.47
1:A:409:G:H1	1:A:433:C:H42	1.62	0.47
1:A:603:U:H2'	1:A:604:G:C8	2.50	0.47
1:A:625:G:O6	24:A:1605:PAR:N24	2.48	0.47
1:A:836:G:C6	1:A:851:G:C6	3.03	0.47
1:A:962:C:H2'	1:A:963:G:O4'	2.15	0.47
1:A:580:U:H2'	1:A:581:G:O4'	2.15	0.47
4:D:61:LYS:HB2	4:D:203:VAL:HG13	1.95	0.47
1:A:691:G:H3'	11:K:26:ASN:HD21	1.80	0.47
12:L:46:LYS:HG3	12:L:92:0TD:H8	1.97	0.47
1:A:222:U:H2'	1:A:223:U:H6	1.79	0.47
1:A:279:A:C5	17:Q:98:LEU:HD12	2.49	0.47
1:A:344:A:H5'	1:A:345:C:C5	2.50	0.47
1:A:678:U:H2'	1:A:679:C:C6	2.50	0.47
1:A:839:U:O2	1:A:839:U:H2'	2.14	0.47
19:S:41:VAL:HG23	19:S:43:GLU:HG2	1.96	0.47
1:A:1317:C:H2'	1:A:1318:A:O4'	2.15	0.47
1:A:1399:C:C2	1:A:1502:A:N6	2.83	0.47
1:A:400:C:H2'	1:A:401:C:C6	2.50	0.47
1:A:452:A:HO2'	1:A:453:A:H8	1.60	0.47
1:A:814:A:H2'	1:A:816:A:H5''	1.97	0.47
12:L:53:ARG:HG2	12:L:93:LEU:HD11	1.96	0.47
1:A:1017:G:H2'	1:A:1018:C:H6	1.78	0.47
1:A:860:A:H2'	1:A:861:G:O4'	2.15	0.47
1:A:412:A:C6	4:D:35:ARG:HB2	2.50	0.47
5:E:18:ARG:HG2	5:E:25:ARG:HB2	1.96	0.47
1:A:1016:A:H2'	1:A:1017:G:O4'	2.14	0.47
1:A:1172:C:H2'	1:A:1173:G:H8	1.79	0.47
1:A:928:G:O2'	1:A:1533:C:OP1	2.32	0.47
4:D:30:LYS:HA	4:D:35:ARG:HH11	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:87:THR:HG23	11:K:91:ARG:HH22	1.80	0.47
1:A:187:C:O2	20:T:105:SER:HB3	2.14	0.47
1:A:892:A:H2'	1:A:893:C:C6	2.51	0.46
2:B:36:ARG:HD2	2:B:41:ILE:HD12	1.97	0.46
1:A:1049:U:H4'	1:A:1050:G:O5'	2.15	0.46
10:J:32:ALA:O	10:J:34:VAL:HG23	2.15	0.46
13:M:49:THR:HG22	13:M:51:ALA:H	1.79	0.46
18:R:47:THR:HG22	18:R:48:GLY:H	1.81	0.46
20:T:59:ALA:O	20:T:63:ILE:HG13	2.15	0.46
1:A:1370:G:C2	1:A:1371:G:C8	3.04	0.46
1:A:895:G:H2'	1:A:896:C:H6	1.80	0.46
13:M:3:ARG:HA	13:M:9:ILE:HG13	1.98	0.46
1:A:1225:A:N3	1:A:1225:A:H2'	2.31	0.46
1:A:1401:G:C2	1:A:1402:4OC:H1'	2.50	0.46
1:A:539:A:H2'	1:A:540:G:C8	2.51	0.46
1:A:1064:G:N2	1:A:1190:G:O2'	2.49	0.46
1:A:1498:UR3:O4'	1:A:1519:MA6:H2	2.15	0.46
1:A:358:U:H2'	1:A:359:U:C6	2.51	0.46
1:A:663:A:H5''	18:R:61:LYS:HE3	1.98	0.46
1:A:749:C:H2'	1:A:750:G:H8	1.81	0.46
10:J:14:LYS:HB3	10:J:14:LYS:HE2	1.62	0.46
1:A:1288:A:H2'	1:A:1289:A:C8	2.51	0.46
1:A:1443:G:H4'	1:A:1446:A:C5'	2.46	0.46
1:A:1498:UR3:OP2	1:A:1542:U:O2'	2.33	0.46
1:A:190(J):U:H2'	1:A:190(K):G:C8	2.50	0.46
1:A:382:A:H2'	1:A:383:A:C8	2.51	0.46
2:B:8:LYS:H	2:B:217:ARG:HH12	1.64	0.46
1:A:1034:G:H2'	1:A:1035:A:H8	1.80	0.46
1:A:1301:U:HO2'	1:A:1302:U:C5'	2.23	0.46
1:A:1428:A:H2'	1:A:1429:C:C6	2.51	0.46
1:A:195:A:H1'	1:A:222:U:O2'	2.16	0.46
5:E:139:LEU:HA	5:E:142:LEU:HD12	1.96	0.46
1:A:1371:G:O3'	9:I:69:GLY:HA3	2.16	0.46
1:A:1127:G:H21	1:A:1147:C:N4	2.15	0.45
1:A:973:G:O5'	1:A:973:G:H8	1.99	0.45
12:L:7:ILE:O	12:L:11:VAL:HG23	2.16	0.45
1:A:1443:G:H4'	1:A:1446:A:O5'	2.15	0.45
1:A:49:U:C2	1:A:361:G:N2	2.84	0.45
1:A:639:G:H2'	1:A:640:A:H8	1.82	0.45
1:A:678:U:H2'	1:A:679:C:H6	1.81	0.45
1:A:932:C:H4'	7:G:4:ARG:NH2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:41:ARG:NH2	9:I:39:GLY:HA2	2.32	0.45
2:B:88:ALA:HB1	2:B:226:ARG:NH2	2.31	0.45
1:A:1068:G:H8	1:A:1068:G:OP2	1.99	0.45
1:A:200:G:H2'	1:A:201:C:O4'	2.16	0.45
1:A:1435:G:H2'	1:A:1436:U:H6	1.77	0.45
1:A:918:A:H2'	1:A:919:A:C8	2.52	0.45
4:D:3:ARG:NH2	4:D:5:ILE:HD11	2.31	0.45
4:D:98:GLU:HG2	4:D:189:PRO:HG3	1.98	0.45
1:A:1375:A:P	7:G:28:ASN:HD22	2.38	0.45
10:J:89:ASP:HB2	10:J:91:PRO:HD2	1.97	0.45
12:L:54:LYS:N	12:L:54:LYS:HD2	2.32	0.45
1:A:1326:C:H2'	1:A:1327:C:H6	1.81	0.45
1:A:500:G:H2'	1:A:501:C:C6	2.51	0.45
8:H:127:LEU:HA	8:H:127:LEU:HD23	1.81	0.45
1:A:1154:G:H2'	1:A:1155:G:H8	1.82	0.45
8:H:124:ALA:O	8:H:128:GLY:N	2.50	0.45
11:K:120:ARG:HA	11:K:121:PRO:HD3	1.82	0.45
3:C:30:ARG:HB3	14:N:36:PHE:O	2.16	0.45
15:O:5:LYS:HD2	15:O:5:LYS:H	1.82	0.45
17:Q:59:ILE:HG23	17:Q:71:PHE:HB3	1.97	0.45
20:T:45:GLN:HB2	20:T:91:LEU:HD13	1.99	0.45
1:A:1486:G:H2'	1:A:1487:G:O4'	2.16	0.45
1:A:1392:G:H21	1:A:1502:A:H8	1.64	0.45
1:A:186:C:H2'	1:A:187:C:C6	2.52	0.45
1:A:46:G:H2'	1:A:366:C:C5	2.52	0.45
1:A:665:A:N3	1:A:732:C:H2'	2.32	0.45
5:E:36:ASP:OD2	5:E:38:GLN:HB2	2.15	0.45
1:A:1116:C:O2'	9:I:108:VAL:HG21	2.16	0.45
19:S:62:ILE:HA	19:S:66:MET:SD	2.56	0.45
1:A:1073:U:C2	1:A:1074:G:C8	3.05	0.45
1:A:994:A:N7	1:A:1216:G:H4'	2.32	0.45
14:N:3:ARG:HB3	14:N:6:LEU:HD23	1.99	0.45
19:S:5:LEU:O	19:S:6:LYS:HB2	2.17	0.45
1:A:999:C:H2'	1:A:1000:U:H6	1.82	0.45
1:A:719:C:O2'	18:R:49:LYS:HB3	2.16	0.45
1:A:737:A:H2'	1:A:738:C:H6	1.82	0.45
1:A:965:A:H4'	1:A:966:M2G:OP1	2.15	0.45
4:D:112:VAL:HG12	4:D:116:GLN:OE1	2.17	0.45
20:T:76:ALA:O	20:T:80:ARG:HG3	2.17	0.45
1:A:435:C:H2'	1:A:436:C:H6	1.81	0.44
13:M:12:ASN:OD1	13:M:46:LYS:NZ	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1277:C:O2'	1:A:1279:A:H1'	2.17	0.44
1:A:266:G:H5''	1:A:267:C:C5	2.52	0.44
1:A:631:G:O3'	1:A:632:A:H8	2.00	0.44
2:B:124:SER:HB2	2:B:125:PRO:HD2	1.99	0.44
4:D:78:LEU:HA	4:D:78:LEU:HD23	1.72	0.44
4:D:83:SER:HA	4:D:89:THR:HG23	1.99	0.44
13:M:34:LEU:HD13	13:M:41:PRO:HA	1.98	0.44
1:A:1031:G:H2'	1:A:1032:G:H8	1.82	0.44
1:A:1236:A:H2'	1:A:1237:C:C6	2.52	0.44
1:A:186:C:H2'	1:A:187:C:H6	1.81	0.44
1:A:398:C:H2'	1:A:399:G:H8	1.82	0.44
1:A:1037:C:H2'	1:A:1038:C:C6	2.52	0.44
1:A:1163:C:C2	1:A:1164:G:C8	3.05	0.44
1:A:335:C:H2'	1:A:336:C:H6	1.80	0.44
1:A:477:G:H2'	1:A:478:A:H8	1.82	0.44
1:A:674:G:H2'	1:A:675:A:C8	2.52	0.44
1:A:966:M2G:HM22	1:A:967:5MC:O2	2.17	0.44
7:G:45:ASP:O	7:G:49:ILE:HG13	2.17	0.44
1:A:1372:U:H2'	1:A:1373:G:O4'	2.18	0.44
1:A:892:A:H2'	1:A:893:C:H6	1.81	0.44
15:O:26:GLU:OE1	15:O:77:ARG:HD2	2.16	0.44
2:B:114:ARG:O	2:B:117:GLU:HB3	2.18	0.44
13:M:24:GLY:HA3	13:M:66:LEU:HD22	2.00	0.44
19:S:5:LEU:HD11	19:S:70:LYS:HZ1	1.83	0.44
1:A:767:A:H2'	1:A:768:A:O4'	2.18	0.44
2:B:180:LEU:HD23	2:B:180:LEU:HA	1.81	0.44
3:C:155:GLY:HA2	3:C:164:ARG:H	1.82	0.44
4:D:31:CYS:C	4:D:33:MET:H	2.21	0.44
8:H:19:VAL:CG2	8:H:21:LYS:HD3	2.48	0.44
9:I:17:VAL:HG11	9:I:81:ILE:HA	1.99	0.44
1:A:1031:G:H2'	1:A:1032:G:C8	2.53	0.44
1:A:1120:G:H2'	1:A:1121:U:H6	1.82	0.44
1:A:381:C:H2'	1:A:382:A:O4'	2.18	0.44
2:B:47:THR:HA	2:B:202:PRO:HG2	2.00	0.44
12:L:24:VAL:HG13	12:L:98:TYR:CE1	2.44	0.44
12:L:60:LEU:HB3	12:L:62:SER:H	1.82	0.44
1:A:1245:A:H2'	1:A:1246:C:C6	2.53	0.44
1:A:1347:G:O2'	1:A:1348:U:OP2	2.35	0.44
1:A:321:A:H2'	1:A:322:C:C6	2.53	0.44
1:A:339:C:H2'	1:A:340:U:H6	1.83	0.44
1:A:743:U:H2'	1:A:744:C:C6	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:922:G:C6	1:A:923:A:C6	3.06	0.44
9:I:81:ILE:O	9:I:85:LEU:HB2	2.18	0.44
1:A:263:A:OP2	20:T:79:ARG:NH1	2.51	0.44
1:A:1172:C:H2'	1:A:1173:G:C8	2.53	0.43
1:A:1241:G:H2'	1:A:1242:C:H6	1.83	0.43
1:A:1418:A:H2'	1:A:1419:G:O4'	2.17	0.43
1:A:620:C:C2	4:D:135:LEU:HD22	2.53	0.43
1:A:824:C:H2'	1:A:825:G:H8	1.83	0.43
2:B:174:VAL:O	2:B:178:ARG:HG2	2.17	0.43
2:B:90:MET:HA	2:B:91:PRO:HD3	1.79	0.43
8:H:51:VAL:HG11	8:H:60:ARG:HG3	2.00	0.43
12:L:69:TYR:CD2	12:L:90:VAL:HG21	2.53	0.43
1:A:1314:C:H2'	1:A:1315:U:H6	1.83	0.43
1:A:280:C:O2	17:Q:38:ARG:HG3	2.18	0.43
2:B:155:LEU:HA	2:B:155:LEU:HD23	1.91	0.43
2:B:80:ILE:HD11	2:B:208:ILE:HG22	2.00	0.43
15:O:85:LEU:HD13	15:O:87:ILE:HD11	2.00	0.43
1:A:1163:C:H2'	1:A:1164:G:H8	1.83	0.43
1:A:399:G:H2'	1:A:400:C:H6	1.83	0.43
1:A:555:C:H2'	1:A:556:C:C6	2.54	0.43
6:F:25:ILE:HG21	6:F:82:ARG:HD2	2.01	0.43
9:I:56:LEU:HA	9:I:56:LEU:HD23	1.83	0.43
1:A:559:A:P	5:E:126:ARG:HH22	2.41	0.43
1:A:668:G:O4'	15:O:49:ASP:HB2	2.18	0.43
1:A:1002:G:H2'	1:A:1003:G:C8	2.54	0.43
1:A:1130:A:OP1	9:I:20:ARG:NH2	2.51	0.43
1:A:168:G:C2	1:A:169:C:C5	3.06	0.43
1:A:456:C:H2'	1:A:457:C:H6	1.82	0.43
1:A:669:U:H2'	1:A:670:G:C8	2.53	0.43
1:A:691:G:H2'	1:A:692:U:C6	2.54	0.43
2:B:103:THR:HG23	2:B:176:GLU:HB2	1.99	0.43
13:M:59:TYR:O	13:M:63:THR:HG22	2.18	0.43
14:N:9:LYS:C	14:N:9:LYS:HD2	2.38	0.43
18:R:47:THR:HG23	18:R:83:GLU:O	2.18	0.43
1:A:1132:C:H2'	1:A:1133:G:C8	2.53	0.43
1:A:628:G:H2'	1:A:629:G:C8	2.53	0.43
1:A:731:G:H5'	1:A:766:A:H4'	2.00	0.43
7:G:65:ALA:O	7:G:69:VAL:HG23	2.17	0.43
9:I:10:ARG:HG2	9:I:75:ASP:HB2	2.00	0.43
3:C:58:GLU:HB3	10:J:92:THR:HG21	1.99	0.43
13:M:86:CYS:SG	13:M:87:TYR:N	2.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:42:ARG:NH1	18:R:42:ARG:HB3	2.34	0.43
1:A:826:C:H2'	1:A:827:U:C6	2.53	0.43
1:A:911:U:H2'	1:A:912:C:C6	2.53	0.43
2:B:114:ARG:NH1	2:B:118:LEU:HD21	2.33	0.43
2:B:178:ARG:NH2	8:H:74:PRO:HB3	2.33	0.43
7:G:80:VAL:HG11	7:G:154:TYR:CE1	2.53	0.43
1:A:1326:C:H2'	1:A:1327:C:C6	2.54	0.43
1:A:1512:U:H2'	1:A:1513:A:C8	2.53	0.43
1:A:511:C:C2	1:A:512:U:C5	3.07	0.43
1:A:642:A:N7	8:H:115:SER:HA	2.33	0.43
20:T:67:ALA:HA	20:T:73:HIS:H	1.84	0.43
1:A:1428:A:H2'	1:A:1429:C:H6	1.83	0.43
1:A:45:U:H2'	1:A:46:G:C8	2.53	0.43
2:B:42:ILE:HG21	2:B:202:PRO:O	2.18	0.43
13:M:40:ASN:HD21	13:M:42:ALA:HB3	1.83	0.43
18:R:51:LEU:HA	18:R:52:PRO:HD3	1.85	0.43
1:A:1151:A:C2	1:A:1152:A:C5	3.06	0.43
1:A:1190:G:OP1	3:C:4:LYS:HA	2.19	0.43
1:A:1508:G:H2'	1:A:1509:C:H6	1.84	0.43
3:C:64:VAL:H	3:C:99:VAL:HB	1.83	0.43
4:D:174:LEU:HD23	4:D:185:PHE:HA	2.00	0.43
15:O:79:ARG:HD2	15:O:79:ARG:HA	1.83	0.43
1:A:1057:G:H5''	3:C:154:SER:CB	2.47	0.42
1:A:1264:C:H2'	1:A:1265:G:H8	1.84	0.42
1:A:1292:U:H2'	1:A:1293:G:C8	2.54	0.42
1:A:1521:G:H2'	1:A:1522:U:H6	1.84	0.42
1:A:190(K):G:H2'	1:A:190(L):U:H6	1.83	0.42
1:A:677:U:H2'	1:A:678:U:H6	1.84	0.42
1:A:765:G:N2	1:A:813:U:OP2	2.47	0.42
2:B:197:VAL:HB	2:B:200:ILE:HG12	2.01	0.42
1:A:1235:U:H2'	1:A:1236:A:O4'	2.18	0.42
1:A:1262:C:H42	1:A:1273:G:H1	1.67	0.42
1:A:57:G:H2'	1:A:58:C:H6	1.84	0.42
1:A:792:A:H4'	1:A:793:U:O5'	2.19	0.42
2:B:193:ASP:HA	2:B:194:PRO:HD3	1.89	0.42
13:M:3:ARG:HD2	13:M:9:ILE:HD11	2.01	0.42
1:A:1176:A:H2'	1:A:1177:G:C8	2.53	0.42
1:A:1308:U:H2'	1:A:1309:G:H8	1.83	0.42
3:C:179:ARG:HD2	3:C:206:GLU:HG2	2.01	0.42
19:S:30:LEU:HB3	19:S:31:ILE:H	1.39	0.42
1:A:1087:G:H2'	1:A:1088:G:C8	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1241:G:H2'	1:A:1242:C:C6	2.54	0.42
1:A:328:C:H4'	1:A:329:A:C5'	2.47	0.42
1:A:677:U:H2'	1:A:678:U:C6	2.54	0.42
1:A:925:G:H1	1:A:1391:U:H3	1.66	0.42
7:G:120:ILE:O	7:G:124:LEU:HB2	2.19	0.42
9:I:102:LEU:HD12	9:I:102:LEU:H	1.84	0.42
1:A:1126:U:H1'	1:A:1280:A:C6	2.55	0.42
1:A:270:A:H2'	1:A:271:C:C6	2.55	0.42
1:A:6:G:H4'	1:A:298:A:H4'	2.01	0.42
1:A:994:A:N3	1:A:994:A:H2'	2.35	0.42
1:A:999:C:H2'	1:A:1000:U:C6	2.53	0.42
1:A:1106:G:H5''	3:C:172:ARG:HG2	2.01	0.42
3:C:68:VAL:HG12	3:C:70:VAL:HG23	2.01	0.42
5:E:31:LEU:HD23	5:E:31:LEU:HA	1.80	0.42
9:I:69:GLY:O	9:I:73:GLN:HG3	2.19	0.42
12:L:84:LEU:HB2	12:L:105:TYR:CE2	2.55	0.42
1:A:1314:C:H2'	1:A:1315:U:C6	2.54	0.42
1:A:413:G:N2	1:A:429:U:OP2	2.47	0.42
1:A:687:A:N3	1:A:688:G:H1'	2.35	0.42
7:G:29:LYS:HD2	7:G:29:LYS:HA	1.90	0.42
20:T:53:LEU:HD12	20:T:100:ILE:HG22	2.02	0.42
1:A:321:A:H2'	1:A:322:C:H6	1.85	0.42
1:A:456:C:C2	1:A:457:C:C5	3.08	0.42
1:A:542:G:H2'	1:A:543:C:C6	2.55	0.42
1:A:651:C:O2'	1:A:652:U:H5'	2.19	0.42
1:A:741:G:OP2	24:A:1604:PAR:O41	2.26	0.42
1:A:976:G:OP2	1:A:1358:U:O2'	2.34	0.42
9:I:126:SER:C	9:I:128:ARG:H	2.23	0.42
9:I:45:ALA:O	9:I:48:GLU:HB2	2.19	0.42
15:O:67:LEU:HA	15:O:67:LEU:HD23	1.82	0.42
1:A:1072:G:H2'	1:A:1073:U:H6	1.84	0.42
1:A:1180:A:H5''	1:A:1181:G:OP2	2.19	0.42
1:A:766:A:C8	1:A:814:A:C6	3.08	0.42
4:D:3:ARG:HB2	4:D:3:ARG:HE	1.76	0.42
5:E:33:VAL:HG11	5:E:109:ILE:HA	2.01	0.42
8:H:41:ARG:NH1	8:H:123:GLU:OE2	2.53	0.42
1:A:114:U:O2'	1:A:115:G:H5'	2.19	0.42
1:A:1160:G:C6	1:A:1161:C:C5	3.08	0.42
1:A:1256:A:H5'	1:A:1258:G:H1'	2.00	0.42
1:A:1404:5MC:H2'	1:A:1405:G:C8	2.55	0.42
24:A:1606:PAR:H322	24:A:1606:PAR:HN21	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:U:H2'	1:A:21:G:O4'	2.20	0.42
1:A:323:U:H2'	1:A:324:G:O4'	2.18	0.42
9:I:8:GLY:HA3	9:I:79:LEU:HB3	2.01	0.42
10:J:54:PHE:CD2	10:J:55:LYS:HG2	2.54	0.42
12:L:21:LYS:HG2	12:L:21:LYS:H	1.72	0.42
13:M:65:LYS:HE3	13:M:65:LYS:HB2	1.86	0.42
1:A:1054:C:H2'	1:A:1054:C:H6	1.61	0.42
1:A:1207:2MG:H2'	1:A:1208:C:C6	2.53	0.42
1:A:1273:G:H2'	1:A:1274:G:O4'	2.20	0.42
1:A:771:G:H2'	1:A:772:U:C6	2.55	0.42
1:A:84:U:H2'	1:A:88:A:C8	2.55	0.42
1:A:985:C:H2'	1:A:986:A:H8	1.84	0.42
4:D:141:ARG:NH2	28:D:401:HOH:O	2.53	0.42
4:D:70:ILE:HD11	4:D:100:ARG:CZ	2.50	0.42
1:A:277:C:H5''	17:Q:68:ARG:NH2	2.35	0.42
1:A:1168:A:H2'	1:A:1169:A:C8	2.55	0.41
1:A:1049:U:H5'	1:A:1201:A:OP2	2.20	0.41
1:A:204:U:H4'	1:A:216:G:C8	2.55	0.41
2:B:221:LEU:HD22	2:B:221:LEU:HA	1.88	0.41
7:G:108:ALA:O	7:G:111:ARG:HB2	2.19	0.41
1:A:1128:C:H42	1:A:1143:G:H1	1.68	0.41
1:A:737:A:H2'	1:A:738:C:C6	2.54	0.41
1:A:921:U:O2	5:E:19:MET:HB2	2.20	0.41
5:E:43:LEU:HD22	5:E:44:GLY:N	2.35	0.41
10:J:57:LYS:HE2	10:J:60:ARG:NH2	2.35	0.41
13:M:70:LEU:HD23	13:M:70:LEU:HA	1.84	0.41
15:O:70:LEU:HD13	15:O:78:TYR:HA	2.02	0.41
1:A:1064:G:H1'	1:A:1190:G:H21	1.85	0.41
1:A:1211:U:H5'	1:A:1212:U:OP1	2.20	0.41
1:A:1218:C:H2'	1:A:1219:U:H6	1.85	0.41
1:A:1366:C:H2'	1:A:1367:C:C6	2.56	0.41
1:A:1488:G:H2'	1:A:1489:G:C8	2.55	0.41
2:B:71:VAL:HG22	2:B:93:VAL:HB	2.02	0.41
3:C:150:LYS:HG3	3:C:169:ALA:HB2	2.02	0.41
5:E:45:PHE:CD2	5:E:47:LYS:HD2	2.55	0.41
8:H:6:ILE:HB	8:H:85:ARG:NH1	2.35	0.41
8:H:83:ILE:HG13	8:H:137:VAL:HG22	2.02	0.41
9:I:16:ARG:O	9:I:63:ILE:HA	2.19	0.41
1:A:522:C:OP2	12:L:69:TYR:OH	2.30	0.41
1:A:630:G:H5'	1:A:631:G:OP2	2.20	0.41
3:C:5:ILE:HD13	3:C:10:PHE:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:111:ARG:NH1	7:G:113:GLU:OE2	2.54	0.41
8:H:33:GLU:HG3	8:H:48:TYR:CE2	2.55	0.41
1:A:1120:G:H2'	1:A:1121:U:C6	2.56	0.41
1:A:33:A:H2'	1:A:34:C:C6	2.56	0.41
1:A:538:G:H2'	1:A:539:A:H8	1.83	0.41
1:A:872:A:C4	1:A:874:G:N7	2.88	0.41
3:C:111:LEU:HD22	3:C:111:LEU:HA	1.87	0.41
3:C:6:HIS:HD2	3:C:8:ILE:H	1.68	0.41
10:J:16:LEU:HD13	10:J:70:ARG:HG2	2.02	0.41
12:L:47:LYS:HD3	12:L:47:LYS:HA	1.97	0.41
20:T:43:LEU:HD11	20:T:55:ILE:HD12	2.02	0.41
1:A:1220:G:H2'	1:A:1221:G:C8	2.55	0.41
1:A:16:A:N1	1:A:919:A:H2	2.18	0.41
1:A:28:G:O2'	1:A:296:U:OP1	2.35	0.41
1:A:538:G:H2'	1:A:539:A:C8	2.55	0.41
1:A:923:A:H2'	1:A:924:C:C6	2.56	0.41
1:A:985:C:H2'	1:A:986:A:C8	2.56	0.41
2:B:33:TYR:HB2	2:B:43:ASP:HA	2.03	0.41
9:I:118:LYS:C	9:I:120:ARG:H	2.18	0.41
16:P:23:ASP:OD2	16:P:25:ARG:HB2	2.21	0.41
1:A:1143:G:H2'	1:A:1144:G:C8	2.56	0.41
1:A:407:G:H2'	1:A:408:A:C8	2.56	0.41
2:B:74:LYS:C	2:B:76:GLN:H	2.24	0.41
13:M:112:GLY:HA3	13:M:113:PRO:HD2	1.95	0.41
13:M:22:ILE:HB	13:M:25:ILE:HB	2.03	0.41
1:A:1477:C:H2'	1:A:1478:C:H6	1.86	0.41
1:A:419:C:N4	1:A:424:G:H1	2.19	0.41
2:B:130:ARG:NH2	3:C:207:VAL:HG21	2.36	0.41
5:E:51:VAL:HB	5:E:52:PRO:HD3	2.02	0.41
10:J:29:ARG:HB2	10:J:84:GLN:HE22	1.85	0.41
19:S:40:ILE:HG22	19:S:67:VAL:HA	2.03	0.41
1:A:791:G:C6	1:A:792:A:N7	2.89	0.41
9:I:9:ARG:HG3	9:I:14:VAL:HG12	2.01	0.41
20:T:53:LEU:O	20:T:57:ARG:HD2	2.21	0.41
1:A:1057:G:H2'	1:A:1058:G:O4'	2.21	0.41
1:A:1071:C:H2'	1:A:1072:G:C8	2.49	0.41
1:A:1074:G:O2'	1:A:1101:A:N1	2.47	0.41
1:A:1129:C:H4'	1:A:1130:A:OP2	2.19	0.41
1:A:1324:A:H2'	1:A:1325:C:H6	1.85	0.41
1:A:179:A:H2'	1:A:180:U:H6	1.85	0.41
1:A:477:G:H2'	1:A:478:A:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:983:A:H5'	1:A:984:C:OP2	2.21	0.41
2:B:55:PHE:HD2	2:B:221:LEU:HG	1.86	0.41
3:C:155:GLY:HA3	3:C:163:ALA:HB1	2.03	0.41
5:E:148:VAL:HG21	8:H:107:LEU:HD13	2.03	0.41
11:K:126:ARG:HB3	11:K:127:LYS:H	1.76	0.41
19:S:31:ILE:HD13	19:S:32:LYS:H	1.86	0.41
1:A:62:U:O2'	1:A:379:C:O2	2.37	0.41
1:A:728:A:H2'	1:A:729:A:C8	2.57	0.41
1:A:88:A:H2'	1:A:89:C:O4'	2.21	0.41
14:N:14:PRO:O	14:N:15:LYS:HB3	2.21	0.41
1:A:1281:U:O2'	1:A:1282:C:OP1	2.36	0.40
1:A:488:C:H2'	1:A:489:C:H6	1.85	0.40
1:A:642:A:C8	8:H:115:SER:HA	2.56	0.40
4:D:9:CYS:O	4:D:13:ARG:HG3	2.21	0.40
4:D:68:TYR:OH	4:D:196:LEU:HD11	2.20	0.40
6:F:23:LYS:O	6:F:27:GLN:HG2	2.21	0.40
8:H:95:VAL:HB	8:H:99:GLU:HB2	2.03	0.40
1:A:1368:G:OP2	9:I:112:LYS:HD3	2.21	0.40
1:A:1511:G:H2'	1:A:1512:U:O4'	2.21	0.40
1:A:704:A:C5	1:A:705:U:C5	3.09	0.40
1:A:715:A:H2'	1:A:716:A:C8	2.55	0.40
1:A:987:G:H2'	1:A:988:G:C8	2.56	0.40
2:B:101:MET:HA	2:B:108:ILE:HG13	2.03	0.40
4:D:121:VAL:O	4:D:134:ASP:HA	2.21	0.40
5:E:127:ASN:HA	5:E:128:PRO:HD3	1.85	0.40
5:E:79:GLU:O	8:H:104:ARG:NH1	2.55	0.40
9:I:37:PHE:HD1	9:I:40:LEU:HD12	1.86	0.40
2:B:140:HIS:HA	2:B:143:GLU:HB3	2.03	0.40
1:A:403:C:OP1	4:D:136:PRO:HD2	2.21	0.40
17:Q:45:HIS:HB3	17:Q:72:ARG:HG2	2.03	0.40
20:T:89:ARG:HE	20:T:104:LEU:HD22	1.87	0.40
1:A:1206:G:C6	1:A:1207:2MG:C5	3.09	0.40
1:A:1300:G:O2'	1:A:1301:U:P	2.79	0.40
1:A:156:G:C6	1:A:166:G:C6	3.10	0.40
1:A:689:C:H2'	1:A:690:G:O4'	2.21	0.40
1:A:89:C:H2'	1:A:90:U:O4'	2.21	0.40
4:D:171:GLY:HA2	4:D:172:PRO:HD3	1.91	0.40
1:A:1103:C:H2'	1:A:1104:G:O4'	2.22	0.40
1:A:1412:C:H2'	1:A:1413:A:C8	2.56	0.40
11:K:12:ARG:HD2	11:K:14:VAL:HG22	2.03	0.40
12:L:49:ASN:ND2	12:L:92:0TD:SB	2.95	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:26:ARG:HD2	16:P:31:LYS:O	2.22	0.40
19:S:27:GLU:HG2	19:S:28:LYS:N	2.36	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	234/236 (99%)	205 (88%)	28 (12%)	1 (0%)	34	68
3	C	205/207 (99%)	189 (92%)	16 (8%)	0	100	100
4	D	206/208 (99%)	201 (98%)	4 (2%)	1 (0%)	29	63
5	E	149/151 (99%)	145 (97%)	4 (3%)	0	100	100
6	F	99/101 (98%)	96 (97%)	3 (3%)	0	100	100
7	G	153/155 (99%)	144 (94%)	9 (6%)	0	100	100
8	H	136/138 (99%)	134 (98%)	2 (2%)	0	100	100
9	I	125/127 (98%)	112 (90%)	12 (10%)	1 (1%)	19	53
10	J	97/99 (98%)	80 (82%)	15 (16%)	2 (2%)	7	32
11	K	117/119 (98%)	106 (91%)	11 (9%)	0	100	100
12	L	122/125 (98%)	114 (93%)	7 (6%)	1 (1%)	19	53
13	M	116/118 (98%)	110 (95%)	6 (5%)	0	100	100
14	N	58/60 (97%)	54 (93%)	4 (7%)	0	100	100
15	O	86/88 (98%)	83 (96%)	3 (4%)	0	100	100
16	P	82/84 (98%)	77 (94%)	5 (6%)	0	100	100
17	Q	97/99 (98%)	95 (98%)	2 (2%)	0	100	100
18	R	71/73 (97%)	68 (96%)	3 (4%)	0	100	100
19	S	79/81 (98%)	71 (90%)	6 (8%)	2 (2%)	5	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	T	97/99 (98%)	84 (87%)	13 (13%)	0	100	100
21	U	23/25 (92%)	22 (96%)	1 (4%)	0	100	100
All	All	2352/2393 (98%)	2190 (93%)	154 (6%)	8 (0%)	41	73

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	L	28	LYS
19	S	31	ILE
9	I	119	ALA
10	J	72	VAL
19	S	6	LYS
10	J	34	VAL
2	B	229	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	194/204 (95%)	183 (94%)	11 (6%)	20	52
3	C	160/161 (99%)	145 (91%)	15 (9%)	8	31
4	D	180/180 (100%)	166 (92%)	14 (8%)	12	40
5	E	115/116 (99%)	104 (90%)	11 (10%)	8	30
6	F	90/90 (100%)	85 (94%)	5 (6%)	21	53
7	G	126/126 (100%)	123 (98%)	3 (2%)	49	74
8	H	119/119 (100%)	109 (92%)	10 (8%)	11	37
9	I	98/98 (100%)	88 (90%)	10 (10%)	7	28
10	J	87/89 (98%)	80 (92%)	7 (8%)	12	39
11	K	90/90 (100%)	85 (94%)	5 (6%)	21	53
12	L	103/103 (100%)	96 (93%)	7 (7%)	16	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	M	94/94 (100%)	80 (85%)	14 (15%)	3	13
14	N	49/49 (100%)	45 (92%)	4 (8%)	11	38
15	O	79/79 (100%)	74 (94%)	5 (6%)	18	49
16	P	72/72 (100%)	69 (96%)	3 (4%)	30	60
17	Q	94/94 (100%)	89 (95%)	5 (5%)	22	54
18	R	64/64 (100%)	60 (94%)	4 (6%)	18	49
19	S	71/71 (100%)	63 (89%)	8 (11%)	6	23
20	T	76/76 (100%)	67 (88%)	9 (12%)	5	21
21	U	19/20 (95%)	17 (90%)	2 (10%)	7	26
All	All	1980/1995 (99%)	1828 (92%)	152 (8%)	13	41

All (152) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	46	LYS
2	B	69	LEU
2	B	82	ARG
2	B	114	ARG
2	B	121	LEU
2	B	144	ARG
2	B	157	ARG
2	B	206	ASP
2	B	208	ILE
2	B	221	LEU
2	B	236	TYR
3	C	3	ASN
3	C	21	ARG
3	C	27	LYS
3	C	34	LEU
3	C	43	LEU
3	C	56	ASP
3	C	79	ARG
3	C	85	ARG
3	C	91	LEU
3	C	95	THR
3	C	111	LEU
3	C	126	ARG
3	C	166	GLU
3	C	196	LEU

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Mol	Chain	Res	Type
3	C	204	LEU
4	D	3	ARG
4	D	4	TYR
4	D	8	VAL
4	D	10	ARG
4	D	15	GLU
4	D	64	LEU
4	D	70	ILE
4	D	122	ARG
4	D	127	THR
4	D	135	LEU
4	D	151	LYS
4	D	175	SER
4	D	190	ASP
4	D	194	LEU
5	E	6	PHE
5	E	12	LEU
5	E	25	ARG
5	E	41	VAL
5	E	43	LEU
5	E	64	ARG
5	E	76	ILE
5	E	80	ILE
5	E	89	ILE
5	E	120	THR
5	E	150	ARG
6	F	10	LEU
6	F	24	GLU
6	F	73	ASN
6	F	83	ASP
6	F	86	ARG
7	G	48	LYS
7	G	114	ARG
7	G	156	TRP
8	H	21	LYS
8	H	26	VAL
8	H	34	GLU
8	H	39	LEU
8	H	52	ASP
8	H	85	ARG
8	H	91	ARG
8	H	102	ARG

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Mol	Chain	Res	Type
8	H	121	ASP
8	H	133	LEU
9	I	12	GLU
9	I	65	VAL
9	I	79	LEU
9	I	87	GLN
9	I	102	LEU
9	I	108	VAL
9	I	111	ARG
9	I	118	LYS
9	I	121	ARG
9	I	127	LYS
10	J	17	ASP
10	J	49	VAL
10	J	62	HIS
10	J	71	LEU
10	J	74	ILE
10	J	80	LYS
10	J	83	GLU
11	K	11	LYS
11	K	29	ILE
11	K	48	ILE
11	K	109	VAL
11	K	120	ARG
12	L	20	LYS
12	L	28	LYS
12	L	47	LYS
12	L	53	ARG
12	L	67	THR
12	L	83	VAL
12	L	113	ARG
13	M	14	ARG
13	M	44	ARG
13	M	56	LEU
13	M	58	GLU
13	M	62	ASN
13	M	63	THR
13	M	64	TRP
13	M	70	LEU
13	M	88	ARG
13	M	98	VAL
13	M	101	GLN

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Mol	Chain	Res	Type
13	M	105	THR
13	M	110	ARG
13	M	115	LYS
14	N	6	LEU
14	N	9	LYS
14	N	11	LYS
14	N	33	VAL
15	O	5	LYS
15	O	34	LEU
15	O	39	LEU
15	O	70	LEU
15	O	81	LEU
16	P	2	VAL
16	P	53	VAL
16	P	54	GLU
17	Q	52	LYS
17	Q	74	LEU
17	Q	78	GLU
17	Q	91	ARG
17	Q	98	LEU
18	R	25	THR
18	R	38	GLU
18	R	39	VAL
18	R	86	VAL
19	S	7	LYS
19	S	12	ASP
19	S	15	LEU
19	S	25	LYS
19	S	31	ILE
19	S	62	ILE
19	S	65	ASN
19	S	81	ARG
20	T	8	ARG
20	T	42	GLN
20	T	48	LYS
20	T	56	MET
20	T	57	ARG
20	T	73	HIS
20	T	74	LYS
20	T	75	ASN
20	T	84	LEU
21	U	9	ARG

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Mol	Chain	Res	Type
21	U	12	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
9	I	73	GLN
13	M	106	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1507/1522 (99%)	236 (15%)	42 (2%)
22	a	4/6 (66%)	1 (25%)	0
23	b	8/11 (72%)	2 (25%)	0
All	All	1519/1539 (98%)	239 (15%)	42 (2%)

All (239) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	9	G
1	A	32	A
1	A	39	G
1	A	44	G
1	A	47	C
1	A	48	C
1	A	50	A
1	A	51	A
1	A	54	C
1	A	59	A
1	A	61	G
1	A	63	C
1	A	101	A
1	A	116	A
1	A	117	G
1	A	121	C
1	A	129(A)	G
1	A	130	A
1	A	131	C
1	A	163	C
1	A	182	U

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Mol	Chain	Res	Type
1	A	190(E)	U
1	A	195	A
1	A	197	A
1	A	202	U
1	A	204	U
1	A	216	G
1	A	220	G
1	A	231	G
1	A	244	U
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	351	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	390	C
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	414	A
1	A	419	C
1	A	421	U
1	A	422	C
1	A	424	G
1	A	429	U
1	A	430	A

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Mol	Chain	Res	Type
1	A	433	C
1	A	439	A
1	A	442	C
1	A	452	A
1	A	461	C
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	531	U
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	562	C
1	A	563	A
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	607	A
1	A	618	C
1	A	630	G
1	A	631	G
1	A	632	A
1	A	653	A
1	A	665	A
1	A	666	G
1	A	687	A
1	A	688	G
1	A	702	A

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Mol	Chain	Res	Type
1	A	721	G
1	A	723	U
1	A	731	G
1	A	749	C
1	A	755	G
1	A	777	A
1	A	781	A
1	A	782	A
1	A	793	U
1	A	794	A
1	A	813	U
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	874	G
1	A	902	G
1	A	914	A
1	A	926	G
1	A	927	G
1	A	934	C
1	A	935	A
1	A	960	U
1	A	966	M2G
1	A	967	5MC
1	A	968	A
1	A	969	A
1	A	971	G
1	A	972	C
1	A	974	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	978	A
1	A	989	C
1	A	991	U
1	A	992	U
1	A	993	G
1	A	994	A

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Mol	Chain	Res	Type
1	A	1005	A
1	A	1025	U
1	A	1026	G
1	A	1027	C
1	A	1028	C
1	A	1031	G
1	A	1050	G
1	A	1054	C
1	A	1055	A
1	A	1064	G
1	A	1065	U
1	A	1066	C
1	A	1068	G
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1108	G
1	A	1117	G
1	A	1125	U
1	A	1126	U
1	A	1127	G
1	A	1129	C
1	A	1130	A
1	A	1131	G
1	A	1137	C
1	A	1138	G
1	A	1139	G
1	A	1140	C
1	A	1152	A
1	A	1159	U
1	A	1160	G
1	A	1171	G
1	A	1180	A
1	A	1181	G
1	A	1183	A
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

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Mol	Chain	Res	Type
1	A	1225	A
1	A	1227	A
1	A	1236	A
1	A	1238	A
1	A	1249	C
1	A	1257	U
1	A	1258	G
1	A	1270	C
1	A	1280	A
1	A	1281	U
1	A	1282	C
1	A	1286	A
1	A	1287	A
1	A	1300	G
1	A	1301	U
1	A	1302	U
1	A	1305	G
1	A	1320	C
1	A	1322	C
1	A	1332	A
1	A	1338	G
1	A	1348	U
1	A	1353	G
1	A	1362	C
1	A	1363	A
1	A	1364	U
1	A	1370	G
1	A	1379	G
1	A	1394	A
1	A	1397	C
1	A	1398	A
1	A	1421	G
1	A	1442	G
1	A	1443	G
1	A	1446	A
1	A	1487	G
1	A	1492	A
1	A	1497	G
1	A	1499	A
1	A	1502	A
1	A	1504	G
1	A	1505	G

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Mol	Chain	Res	Type
1	A	1506	U
1	A	1517	G
1	A	1520	G
1	A	1529	G
1	A	1530	G
22	a	6	U
23	b	32	C
23	b	33	U

All (42) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	60	A
1	A	115	G
1	A	129(A)	G
1	A	181	G
1	A	243	A
1	A	250	A
1	A	266	G
1	A	328	C
1	A	372	C
1	A	428	G
1	A	429	U
1	A	432	A
1	A	484	G
1	A	496	A
1	A	509	A
1	A	532	A
1	A	559	A
1	A	575	G
1	A	687	A
1	A	701	C
1	A	748	C
1	A	793	U
1	A	812	C
1	A	913	A
1	A	965	A
1	A	1049	U
1	A	1065	U
1	A	1067	A
1	A	1129	C
1	A	1179	A

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Mol	Chain	Res	Type
1	A	1182	G
1	A	1201	A
1	A	1212	U
1	A	1256	A
1	A	1281	U
1	A	1285	A
1	A	1300	G
1	A	1301	U
1	A	1331	G
1	A	1347	G
1	A	1443	G
1	A	1505	G

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

18 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	0.92	0	19,32,35	1.10	2 (10%)
1	MA6	A	1519	1	19,26,27	1.18	2 (10%)	18,38,41	0.77	0
1	M2G	A	966	1	20,27,28	1.88	4 (20%)	22,40,43	2.51	5 (22%)
1	PSU	A	1541	1,25	17,21,22	1.33	4 (23%)	20,30,33	3.47	5 (25%)
23	12A	b	37	25,23	26,36,37	2.97	4 (15%)	29,52,55	2.69	8 (27%)
1	7MG	A	527	1	22,26,27	2.23	6 (27%)	28,39,42	1.65	7 (25%)
1	PSU	A	516	1,25	17,21,22	1.37	4 (23%)	20,30,33	3.66	5 (25%)
1	PSU	A	1540	1	17,21,22	1.34	3 (17%)	20,30,33	3.46	5 (25%)
12	0TD	L	92	12	4,9,10	1.06	0	3,11,13	2.23	2 (66%)
1	5MC	A	967	1	15,22,23	0.89	0	19,32,35	1.03	1 (5%)
1	UR3	A	1498	1	14,22,23	0.88	1 (7%)	15,32,35	1.20	1 (6%)
23	PSU	b	39	23	17,21,22	1.29	3 (17%)	20,30,33	3.58	6 (30%)
1	2MG	A	1207	1	19,26,27	2.13	3 (15%)	21,38,41	2.02	3 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MC	A	1400	1	15,22,23	0.88	0	19,32,35	1.03	2 (10%)
1	MA6	A	1518	1	19,26,27	1.06	1 (5%)	18,38,41	0.75	0
23	70U	b	34	22,23	19,26,27	2.78	6 (31%)	21,37,40	2.05	3 (14%)
1	4OC	A	1402	1	16,23,24	0.80	0	17,32,35	0.79	0
1	5MC	A	1404	1	15,22,23	0.75	0	19,32,35	0.98	1 (5%)

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	MA6	A	1519	1	-	3/7/29/30	0/3/3/3
1	M2G	A	966	1	-	7/7/29/30	0/3/3/3
1	PSU	A	1541	1,25	-	1/7/25/26	0/2/2/2
23	12A	b	37	25,23	-	4/17/43/44	0/3/3/3
1	7MG	A	527	1	-	2/7/37/38	0/3/3/3
1	PSU	A	516	1,25	-	0/7/25/26	0/2/2/2
1	PSU	A	1540	1	-	0/7/25/26	0/2/2/2
12	0TD	L	92	12	-	2/3/12/14	-
1	5MC	A	967	1	-	2/5/25/26	0/2/2/2
1	UR3	A	1498	1	-	0/5/25/26	0/2/2/2
23	PSU	b	39	23	-	2/7/25/26	0/2/2/2
1	2MG	A	1207	1	-	0/5/27/28	0/3/3/3
1	5MC	A	1400	1	-	2/5/25/26	0/2/2/2
1	MA6	A	1518	1	-	2/7/29/30	0/3/3/3
23	70U	b	34	22,23	-	6/11/31/32	0/2/2/2
1	4OC	A	1402	1	-	3/9/29/30	0/2/2/2
1	5MC	A	1404	1	-	0/5/25/26	0/2/2/2

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	37	12A	C2-S2	10.53	1.84	1.75
23	b	34	70U	C2-S2	7.26	1.81	1.66
1	A	1207	2MG	C2-N2	6.58	1.39	1.34
23	b	37	12A	C6-N6	6.43	1.47	1.36
23	b	37	12A	CC-N	6.42	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	34	70U	O4-C4	6.33	1.40	1.24
1	A	527	7MG	C4-N3	5.77	1.41	1.34
1	A	966	M2G	C6-N1	5.66	1.42	1.33
1	A	1207	2MG	C6-N1	5.42	1.42	1.33
1	A	527	7MG	C2-N2	5.20	1.44	1.33
23	b	37	12A	CC-N6	4.82	1.47	1.37
1	A	527	7MG	C8-N9	-4.58	1.34	1.45
23	b	34	70U	C5M-C5	3.91	1.57	1.51
23	b	34	70U	O9-C8	3.73	1.44	1.33
1	A	966	M2G	C2-N1	3.46	1.40	1.34
1	A	966	M2G	C4-N3	3.36	1.40	1.35
23	b	34	70U	O9-C9	-3.25	1.37	1.45
1	A	966	M2G	C2-N2	3.24	1.40	1.34
1	A	1540	PSU	C2-N3	-3.05	1.32	1.38
1	A	516	PSU	C2-N1	-3.04	1.32	1.38
1	A	527	7MG	C6-N1	3.00	1.38	1.33
23	b	39	PSU	C2-N1	-2.99	1.32	1.38
1	A	1541	PSU	C2-N1	-2.95	1.32	1.38
23	b	39	PSU	C2-N3	-2.94	1.32	1.38
1	A	516	PSU	C2-N3	-2.92	1.32	1.38
1	A	1540	PSU	C2-N1	-2.91	1.32	1.38
1	A	1541	PSU	C2-N3	-2.86	1.32	1.38
1	A	1519	MA6	C6-N1	2.85	1.37	1.33
1	A	1518	MA6	C6-N1	2.76	1.37	1.33
1	A	527	7MG	C6-C5	2.59	1.45	1.41
23	b	34	70U	C6-C5	2.54	1.42	1.37
1	A	527	7MG	CM7-N7	-2.41	1.41	1.46
1	A	1207	2MG	C4-N3	2.40	1.39	1.35
1	A	516	PSU	O4-C4	-2.39	1.18	1.24
1	A	1540	PSU	O4-C4	-2.29	1.18	1.24
1	A	1541	PSU	O4-C4	-2.21	1.19	1.24
1	A	1519	MA6	C2-N1	2.19	1.38	1.33
23	b	39	PSU	O4-C4	-2.19	1.19	1.24
1	A	516	PSU	O4'-C1'	-2.13	1.41	1.44
1	A	1541	PSU	O4'-C1'	-2.06	1.41	1.44
1	A	1498	UR3	C6-N1	2.03	1.38	1.35

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	516	PSU	N1-C2-N3	-11.41	119.36	128.43
1	A	1541	PSU	N1-C2-N3	-10.67	119.94	128.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1540	PSU	N1-C2-N3	-10.53	120.06	128.43
23	b	39	PSU	N1-C2-N3	-10.53	120.06	128.43
23	b	37	12A	C2M-S2-C2	9.21	109.15	102.27
1	A	516	PSU	C4-N3-C2	8.83	122.60	115.14
1	A	966	M2G	C5-C6-N1	-8.34	112.02	123.43
23	b	39	PSU	C4-N3-C2	8.06	121.95	115.14
1	A	1541	PSU	C4-N3-C2	8.04	121.93	115.14
1	A	1540	PSU	C4-N3-C2	7.88	121.80	115.14
1	A	1207	2MG	C5-C6-N1	-7.53	113.13	123.43
23	b	37	12A	CA-N-CC	6.86	130.07	122.75
1	A	966	M2G	C6-N1-C2	6.00	123.33	116.18
23	b	34	70U	O9-C8-C5M	5.96	119.71	111.45
23	b	34	70U	C2-N3-C4	5.11	121.16	115.93
23	b	37	12A	N6-CC-N	4.85	120.53	113.76
23	b	39	PSU	C5-C4-N3	-4.83	119.14	125.36
1	A	516	PSU	C5-C4-N3	-4.66	119.35	125.36
1	A	1541	PSU	C5-C4-N3	-4.58	119.46	125.36
1	A	1540	PSU	C5-C4-N3	-4.49	119.58	125.36
23	b	39	PSU	C5-C6-N1	-4.19	119.29	124.44
1	A	1540	PSU	C5-C6-N1	-4.16	119.32	124.44
23	b	34	70U	C5-C4-N3	-4.08	119.27	125.25
23	b	39	PSU	C6-N1-C2	4.04	122.02	115.36
1	A	1540	PSU	C6-N1-C2	4.04	122.02	115.36
1	A	516	PSU	C6-N1-C2	4.00	121.96	115.36
1	A	1541	PSU	C6-N1-C2	4.00	121.96	115.36
1	A	1541	PSU	C5-C6-N1	-3.98	119.54	124.44
1	A	1207	2MG	C6-N1-C2	3.86	122.10	115.18
23	b	39	PSU	C5-C1'-C2'	-3.82	108.50	115.32
23	b	37	12A	OO-CC-N6	-3.77	117.24	123.62
1	A	527	7MG	N3-C4-N9	3.74	131.72	126.91
1	A	516	PSU	C5-C6-N1	-3.67	119.93	124.44
1	A	527	7MG	C5-C4-N3	-3.60	120.62	126.49
1	A	527	7MG	N7-C8-N9	3.47	108.34	103.38
23	b	37	12A	C2-N3-C4	3.37	119.97	115.32
1	A	527	7MG	C6-N1-C2	2.82	120.41	115.93
1	A	966	M2G	N3-C2-N2	2.79	120.01	117.18
23	b	37	12A	N3-C2-N1	-2.62	122.17	126.98
1	A	966	M2G	N1-C2-N2	-2.59	114.56	117.19
12	L	92	0TD	CSB-SB-CB	-2.54	96.86	101.85
23	b	37	12A	C4-C5-N7	-2.48	106.81	109.40
1	A	527	7MG	N1-C2-N3	-2.45	121.58	125.42
12	L	92	0TD	CB-CA-N	-2.45	103.88	109.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	527	7MG	C2-N3-C4	2.43	120.61	113.89
1	A	1498	UR3	C3'-C2'-C1'	2.35	104.52	100.98
1	A	1407	5MC	N4-C4-N3	-2.34	113.73	117.03
1	A	966	M2G	C2-N3-C4	-2.27	112.70	115.28
1	A	1400	5MC	N4-C4-N3	-2.19	113.94	117.03
1	A	1207	2MG	C4-C5-N7	2.11	111.60	109.40
23	b	37	12A	C2-N1-C6	2.10	120.94	117.19
1	A	967	5MC	C2-N3-C4	2.07	118.52	116.02
1	A	527	7MG	C4-N9-C1'	-2.06	121.70	126.60
1	A	1400	5MC	C2-N3-C4	2.06	118.50	116.02
1	A	1404	5MC	C2-N3-C4	2.05	118.50	116.02
1	A	1407	5MC	C2-N3-C4	2.04	118.48	116.02

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1519	MA6	C3'-C4'-C5'-O5'
1	A	966	M2G	N1-C2-N2-CM1
1	A	966	M2G	N1-C2-N2-CM2
1	A	966	M2G	N3-C2-N2-CM1
23	b	37	12A	N1-C2-S2-C2M
23	b	37	12A	N3-C2-S2-C2M
23	b	37	12A	CB-CA-N-CC
12	L	92	0TD	O-C-CA-CB
12	L	92	0TD	CG-CB-SB-CSB
1	A	967	5MC	O4'-C4'-C5'-O5'
1	A	967	5MC	C3'-C4'-C5'-O5'
23	b	34	70U	C5M-C8-O9-C9
23	b	34	70U	O8-C8-O9-C9
1	A	966	M2G	C4'-C5'-O5'-P
1	A	966	M2G	N3-C2-N2-CM2
1	A	1519	MA6	O4'-C4'-C5'-O5'
1	A	1402	4OC	O4'-C4'-C5'-O5'
1	A	527	7MG	O4'-C4'-C5'-O5'
1	A	1400	5MC	O4'-C4'-C5'-O5'
1	A	1402	4OC	C3'-C4'-C5'-O5'
1	A	527	7MG	C3'-C4'-C5'-O5'
1	A	966	M2G	O4'-C4'-C5'-O5'
1	A	1400	5MC	C3'-C4'-C5'-O5'
1	A	1518	MA6	O4'-C4'-C5'-O5'
1	A	1519	MA6	C5-C6-N6-C9

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Mol	Chain	Res	Type	Atoms
1	A	1518	MA6	C3'-C4'-C5'-O5'
1	A	966	M2G	C3'-C4'-C5'-O5'
1	A	1402	4OC	C5-C4-N4-CM4
23	b	34	70U	C6-C5-C5M-C8
23	b	39	PSU	O4'-C4'-C5'-O5'
23	b	37	12A	C-CA-CB-OG1
1	A	1541	PSU	O4'-C1'-C5-C4
23	b	34	70U	C3'-C4'-C5'-O5'
23	b	34	70U	O4'-C4'-C5'-O5'
23	b	39	PSU	C3'-C4'-C5'-O5'
23	b	34	70U	C4-C5-C5M-C8

There are no ring outliers.

11 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1519	MA6	2	0
1	A	966	M2G	2	0
1	A	527	7MG	1	0
12	L	92	0TD	5	0
1	A	967	5MC	1	0
1	A	1498	UR3	2	0
1	A	1207	2MG	3	0
1	A	1400	5MC	1	0
1	A	1518	MA6	1	0
1	A	1402	4OC	2	0
1	A	1404	5MC	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 360 ligands modelled in this entry, 354 are monoatomic - leaving 6 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	1605	-	45,45,45	1.32	7 (15%)	64,67,67	1.62	13 (20%)
24	PAR	A	1604	-	45,45,45	1.34	6 (13%)	64,67,67	1.65	13 (20%)
24	PAR	A	1601	-	45,45,45	1.37	8 (17%)	64,67,67	1.62	11 (17%)
24	PAR	A	1603	-	45,45,45	1.46	6 (13%)	64,67,67	1.65	13 (20%)
24	PAR	A	1606	-	45,45,45	1.39	5 (11%)	64,67,67	1.65	12 (18%)
24	PAR	A	1602	-	45,45,45	1.35	8 (17%)	64,67,67	1.68	11 (17%)

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	1605	-	-	10/18/94/94	1/4/4/4
24	PAR	A	1604	-	-	7/18/94/94	1/4/4/4
24	PAR	A	1601	-	-	9/18/94/94	0/4/4/4
24	PAR	A	1603	-	-	8/18/94/94	1/4/4/4
24	PAR	A	1606	-	-	10/18/94/94	1/4/4/4
24	PAR	A	1602	-	-	7/18/94/94	0/4/4/4

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1603	PAR	C13-C23	4.73	1.59	1.52
24	A	1601	PAR	C52-C42	3.95	1.60	1.52
24	A	1603	PAR	C52-C42	3.62	1.59	1.52
24	A	1602	PAR	C13-C23	3.58	1.57	1.52
24	A	1606	PAR	C13-C23	3.49	1.57	1.52
24	A	1604	PAR	C52-C42	3.38	1.59	1.52
24	A	1603	PAR	O43-C13	3.13	1.47	1.41
24	A	1601	PAR	C64-C54	3.10	1.56	1.52
24	A	1606	PAR	C52-C42	3.06	1.58	1.52
24	A	1605	PAR	C52-C42	2.99	1.58	1.52
24	A	1606	PAR	C64-C54	2.99	1.56	1.52
24	A	1604	PAR	C64-C54	2.94	1.56	1.52
24	A	1604	PAR	C34-C24	2.88	1.57	1.53
24	A	1602	PAR	C34-C24	2.88	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1605	PAR	C34-C24	2.87	1.57	1.53
24	A	1606	PAR	C34-C24	2.85	1.57	1.53
24	A	1606	PAR	C31-C21	2.84	1.57	1.53
24	A	1603	PAR	C64-C54	2.82	1.55	1.52
24	A	1604	PAR	C13-C23	2.80	1.56	1.52
24	A	1605	PAR	C13-C23	2.70	1.56	1.52
24	A	1605	PAR	C64-C54	2.66	1.55	1.52
24	A	1602	PAR	C64-C54	2.63	1.55	1.52
24	A	1601	PAR	C13-C23	2.57	1.56	1.52
24	A	1601	PAR	C31-C21	2.52	1.56	1.53
24	A	1603	PAR	C14-C24	2.42	1.57	1.52
24	A	1605	PAR	C33-C43	2.41	1.59	1.52
24	A	1602	PAR	C14-C24	2.37	1.57	1.52
24	A	1605	PAR	C14-C24	2.29	1.56	1.52
24	A	1601	PAR	C33-C43	2.27	1.59	1.52
24	A	1602	PAR	C31-C21	2.25	1.56	1.53
24	A	1601	PAR	C62-C52	2.24	1.58	1.52
24	A	1604	PAR	C33-C43	2.19	1.58	1.52
24	A	1602	PAR	C33-C43	2.18	1.58	1.52
24	A	1603	PAR	C34-C24	2.15	1.56	1.53
24	A	1602	PAR	C52-C42	2.14	1.56	1.52
24	A	1601	PAR	C22-C12	-2.09	1.49	1.53
24	A	1604	PAR	C14-C24	2.08	1.56	1.52
24	A	1602	PAR	C11-C21	2.06	1.56	1.52
24	A	1605	PAR	C31-C21	2.06	1.56	1.53
24	A	1601	PAR	C11-C21	2.06	1.56	1.52

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1602	PAR	O33-C14-C24	6.27	119.02	108.22
24	A	1603	PAR	O33-C14-C24	6.18	118.87	108.22
24	A	1601	PAR	O33-C14-C24	6.15	118.81	108.22
24	A	1606	PAR	O33-C14-C24	6.14	118.79	108.22
24	A	1604	PAR	O33-C14-C24	6.12	118.76	108.22
24	A	1605	PAR	O33-C14-C24	5.93	118.44	108.22
24	A	1603	PAR	C13-C23-C33	3.64	106.48	102.10
24	A	1602	PAR	O52-C13-C23	3.62	115.47	107.96
24	A	1605	PAR	O52-C13-C23	3.59	115.39	107.96
24	A	1604	PAR	O52-C13-C23	3.56	115.34	107.96
24	A	1606	PAR	C13-C23-C33	3.46	106.27	102.10
24	A	1606	PAR	O52-C13-C23	3.41	115.03	107.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1603	PAR	O52-C13-C23	3.33	114.86	107.96
24	A	1602	PAR	C13-C23-C33	3.29	106.06	102.10
24	A	1601	PAR	C34-C24-N24	-3.24	104.41	111.05
24	A	1601	PAR	O52-C13-C23	3.23	114.65	107.96
24	A	1605	PAR	C34-C24-N24	-3.13	104.63	111.05
24	A	1601	PAR	C13-C23-C33	3.12	105.86	102.10
24	A	1602	PAR	O34-C34-C44	-3.12	103.13	110.35
24	A	1602	PAR	C34-C24-N24	-3.11	104.69	111.05
24	A	1603	PAR	C34-C24-N24	-3.06	104.79	111.05
24	A	1604	PAR	C34-C24-N24	-3.05	104.81	111.05
24	A	1603	PAR	O34-C34-C44	-3.04	103.33	110.35
24	A	1604	PAR	C13-C23-C33	3.01	105.73	102.10
24	A	1606	PAR	C34-C24-N24	-3.00	104.90	111.05
24	A	1606	PAR	O34-C34-C44	-2.97	103.49	110.35
24	A	1604	PAR	O34-C34-C44	-2.95	103.53	110.35
24	A	1601	PAR	O34-C34-C44	-2.93	103.57	110.35
24	A	1605	PAR	O34-C34-C44	-2.90	103.65	110.35
24	A	1602	PAR	O11-C11-O51	2.88	118.73	110.67
24	A	1603	PAR	C14-O33-C33	-2.88	110.84	117.96
24	A	1605	PAR	O11-C11-O51	2.82	118.54	110.67
24	A	1604	PAR	C14-O33-C33	-2.78	111.08	117.96
24	A	1601	PAR	O11-C11-O51	2.75	118.35	110.67
24	A	1604	PAR	C13-O52-C52	-2.74	111.18	117.96
24	A	1606	PAR	C14-O33-C33	-2.73	111.20	117.96
24	A	1603	PAR	O11-C11-O51	2.71	118.23	110.67
24	A	1602	PAR	C22-C12-C62	2.68	114.09	110.04
24	A	1602	PAR	C14-O33-C33	-2.66	111.37	117.96
24	A	1604	PAR	O11-C11-O51	2.64	118.05	110.67
24	A	1606	PAR	O52-C13-O43	-2.63	108.58	111.43
24	A	1601	PAR	C14-O33-C33	-2.61	111.50	117.96
24	A	1605	PAR	C13-O52-C52	-2.59	111.55	117.96
24	A	1605	PAR	C14-O33-C33	-2.55	111.66	117.96
24	A	1606	PAR	C13-O52-C52	-2.54	111.68	117.96
24	A	1604	PAR	O52-C13-O43	-2.53	108.69	111.43
24	A	1606	PAR	O11-C11-O51	2.50	117.67	110.67
24	A	1601	PAR	O52-C13-O43	-2.50	108.72	111.43
24	A	1603	PAR	C13-O52-C52	-2.47	111.85	117.96
24	A	1605	PAR	C13-C23-C33	2.40	104.99	102.10
24	A	1603	PAR	O51-C51-C61	2.37	112.33	106.44
24	A	1605	PAR	O51-C51-C61	2.35	112.27	106.44
24	A	1601	PAR	C13-O52-C52	-2.33	112.19	117.96
24	A	1603	PAR	O52-C13-O43	-2.30	108.94	111.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1606	PAR	O51-C51-C61	2.30	112.14	106.44
24	A	1602	PAR	C11-O51-C51	2.28	118.17	113.69
24	A	1601	PAR	O51-C51-C61	2.28	112.11	106.44
24	A	1602	PAR	C13-O52-C52	-2.26	112.36	117.96
24	A	1606	PAR	C22-C12-C62	2.26	113.46	110.04
24	A	1602	PAR	O51-C51-C61	2.25	112.03	106.44
24	A	1604	PAR	O51-C51-C61	2.20	111.92	106.44
24	A	1606	PAR	O54-C54-C44	2.17	113.63	109.69
24	A	1604	PAR	O54-C54-C44	2.13	113.57	109.69
24	A	1604	PAR	C22-C12-C62	2.12	113.23	110.04
24	A	1601	PAR	O54-C54-C44	2.11	113.52	109.69
24	A	1605	PAR	O52-C13-O43	-2.08	109.18	111.43
24	A	1603	PAR	C11-O51-C51	2.07	117.75	113.69
24	A	1605	PAR	O54-C54-C44	2.07	113.45	109.69
24	A	1604	PAR	O52-C52-C42	2.03	112.65	107.48
24	A	1603	PAR	O54-C54-C44	2.03	113.38	109.69
24	A	1605	PAR	O52-C52-C42	2.02	112.60	107.48
24	A	1605	PAR	O43-C13-C23	-2.01	102.39	104.98
24	A	1603	PAR	C22-C32-C42	2.01	114.60	109.53

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	1603	PAR	C44-C54-C64-N64
24	A	1603	PAR	O54-C54-C64-N64
24	A	1604	PAR	C21-C11-O11-C42
24	A	1604	PAR	C44-C54-C64-N64
24	A	1604	PAR	O54-C54-C64-N64
24	A	1606	PAR	O51-C11-O11-C42
24	A	1606	PAR	C23-C13-O52-C52
24	A	1605	PAR	C21-C11-O11-C42
24	A	1605	PAR	C44-C54-C64-N64
24	A	1605	PAR	O54-C54-C64-N64
24	A	1602	PAR	C23-C13-O52-C52
24	A	1602	PAR	O43-C13-O52-C52
24	A	1602	PAR	C44-C54-C64-N64
24	A	1602	PAR	O54-C54-C64-N64
24	A	1601	PAR	C43-C33-O33-C14
24	A	1601	PAR	O54-C54-C64-N64
24	A	1605	PAR	O51-C11-O11-C42
24	A	1602	PAR	O54-C14-O33-C33

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Mol	Chain	Res	Type	Atoms
24	A	1604	PAR	O54-C14-O33-C33
24	A	1606	PAR	O54-C14-O33-C33
24	A	1601	PAR	C33-C43-C53-O53
24	A	1601	PAR	O43-C43-C53-O53
24	A	1605	PAR	C33-C43-C53-O53
24	A	1603	PAR	O51-C11-O11-C42
24	A	1603	PAR	C41-C51-C61-O61
24	A	1606	PAR	C41-C51-C61-O61
24	A	1601	PAR	C41-C51-C61-O61
24	A	1605	PAR	O51-C51-C61-O61
24	A	1606	PAR	O43-C43-C53-O53
24	A	1606	PAR	C33-C43-C53-O53
24	A	1605	PAR	O43-C43-C53-O53
24	A	1604	PAR	O43-C13-O52-C52
24	A	1603	PAR	O43-C43-C53-O53
24	A	1604	PAR	O51-C51-C61-O61
24	A	1601	PAR	C44-C54-C64-N64
24	A	1606	PAR	O51-C51-C61-O61
24	A	1601	PAR	O51-C51-C61-O61
24	A	1603	PAR	O51-C51-C61-O61
24	A	1606	PAR	O54-C54-C64-N64
24	A	1601	PAR	C52-C42-O11-C11
24	A	1601	PAR	C24-C14-O33-C33
24	A	1603	PAR	C33-C43-C53-O53
24	A	1602	PAR	O51-C11-O11-C42
24	A	1605	PAR	C62-C52-O52-C13
24	A	1605	PAR	C41-C51-C61-O61
24	A	1605	PAR	C52-C42-O11-C11
24	A	1603	PAR	C23-C33-O33-C14
24	A	1604	PAR	C23-C33-O33-C14
24	A	1606	PAR	C43-C33-O33-C14
24	A	1602	PAR	C43-C33-O33-C14
24	A	1606	PAR	C21-C11-O11-C42

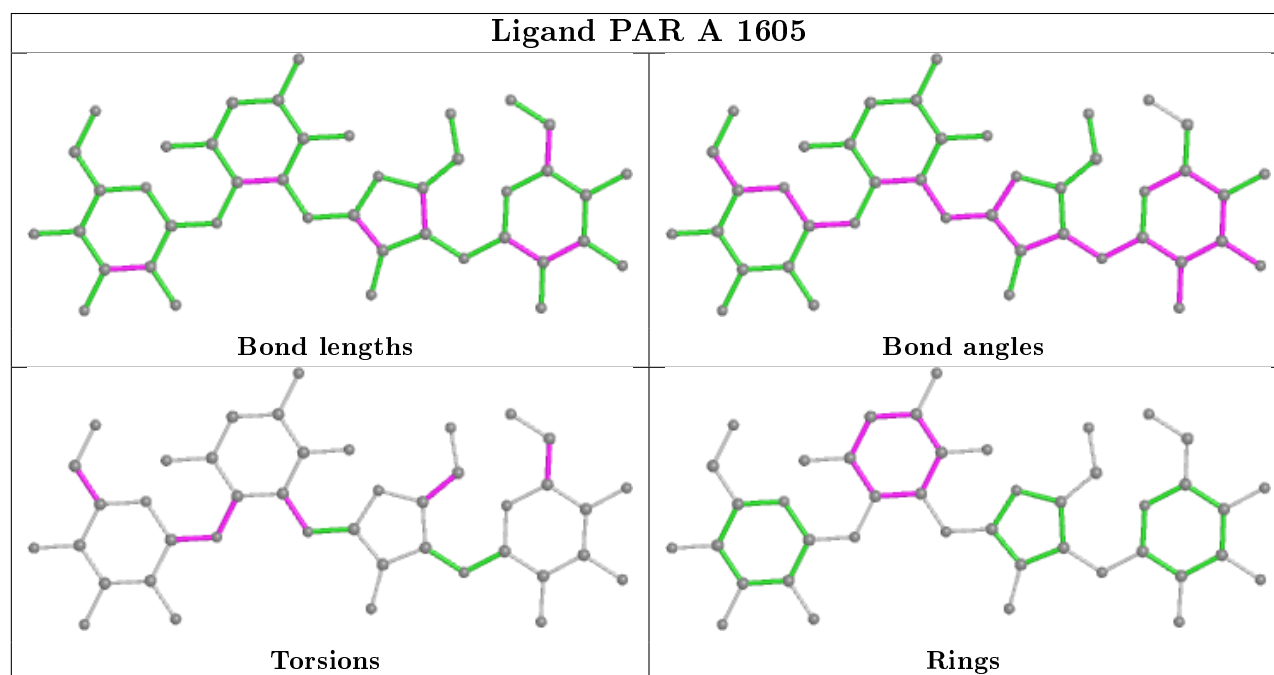
All (4) ring outliers are listed below:

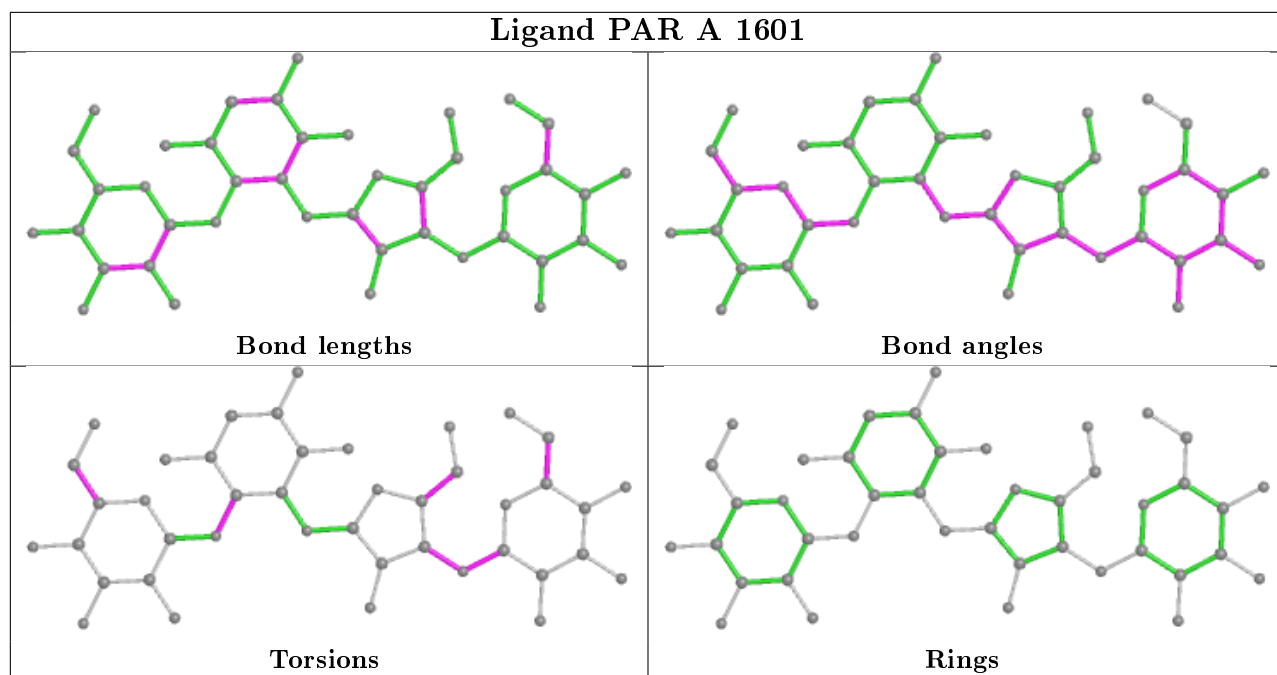
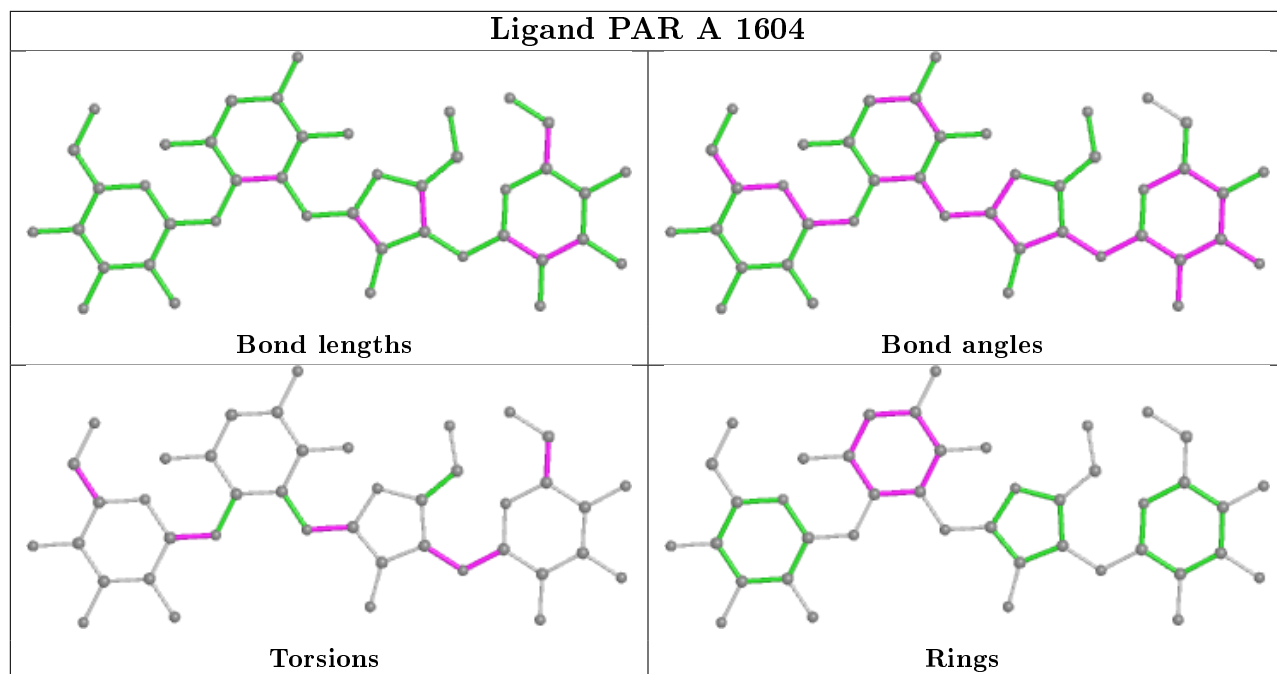
Mol	Chain	Res	Type	Atoms
24	A	1603	PAR	C12-C22-C32-C42-C52-C62
24	A	1605	PAR	C12-C22-C32-C42-C52-C62
24	A	1604	PAR	C12-C22-C32-C42-C52-C62
24	A	1606	PAR	C12-C22-C32-C42-C52-C62

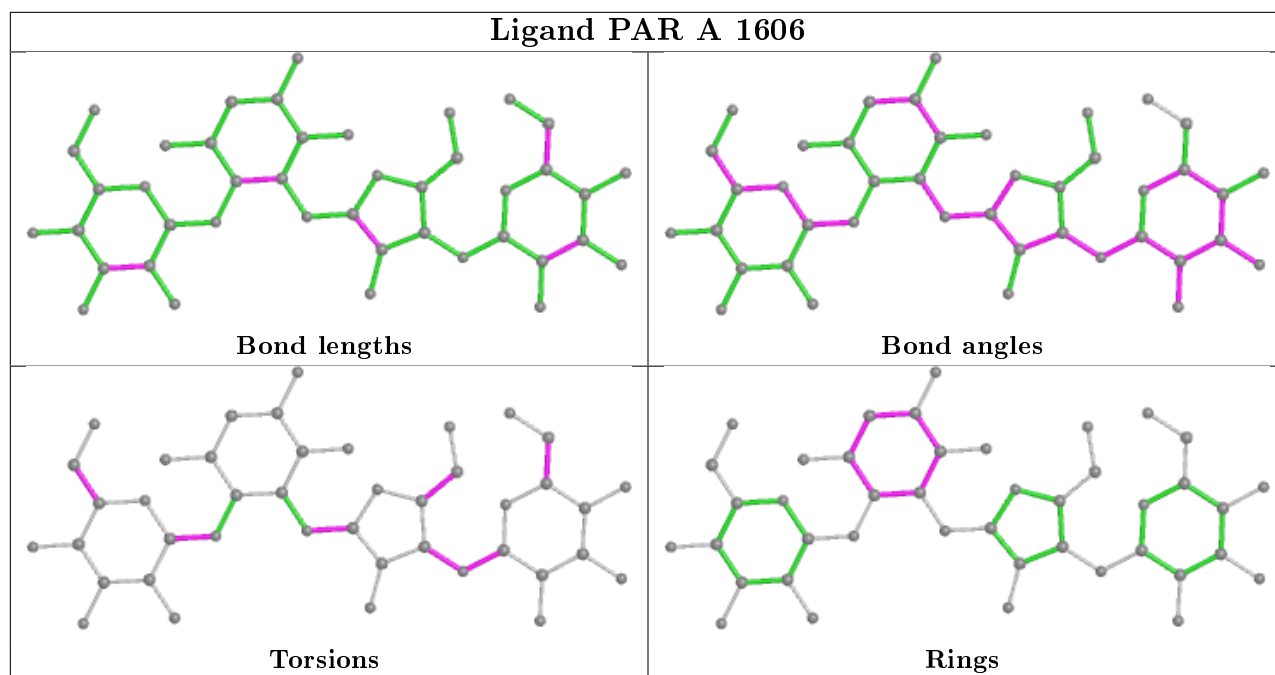
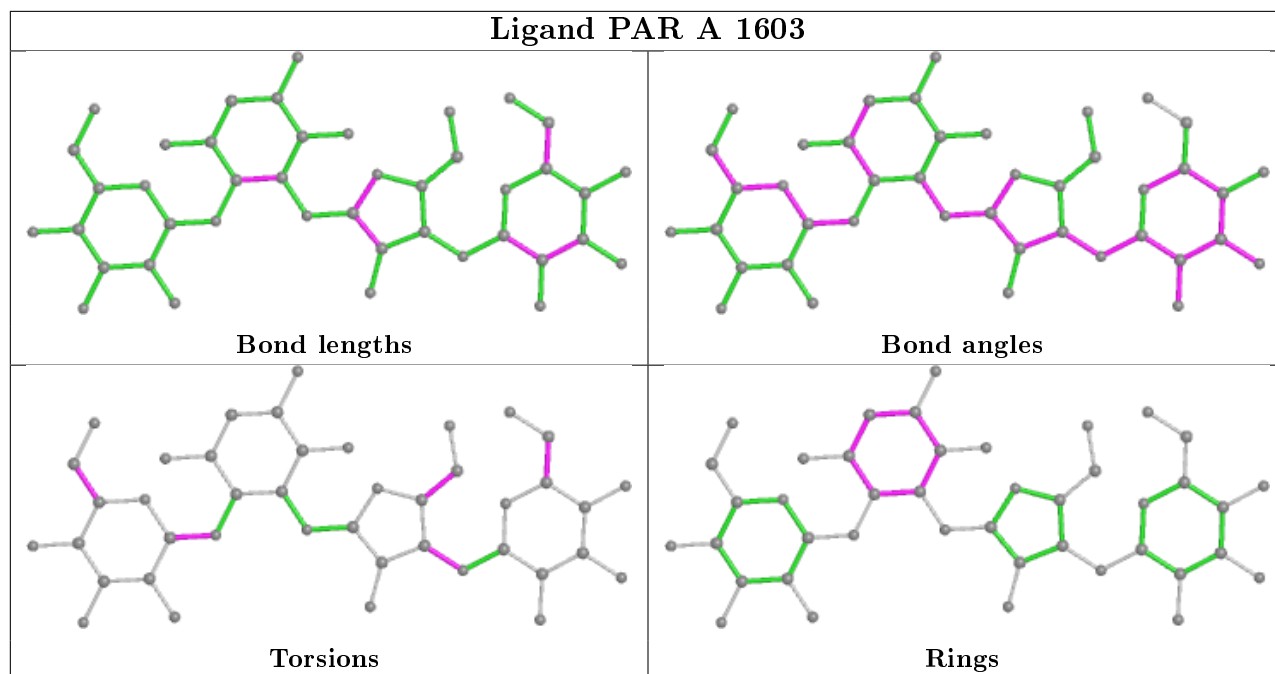
5 monomers are involved in 13 short contacts:

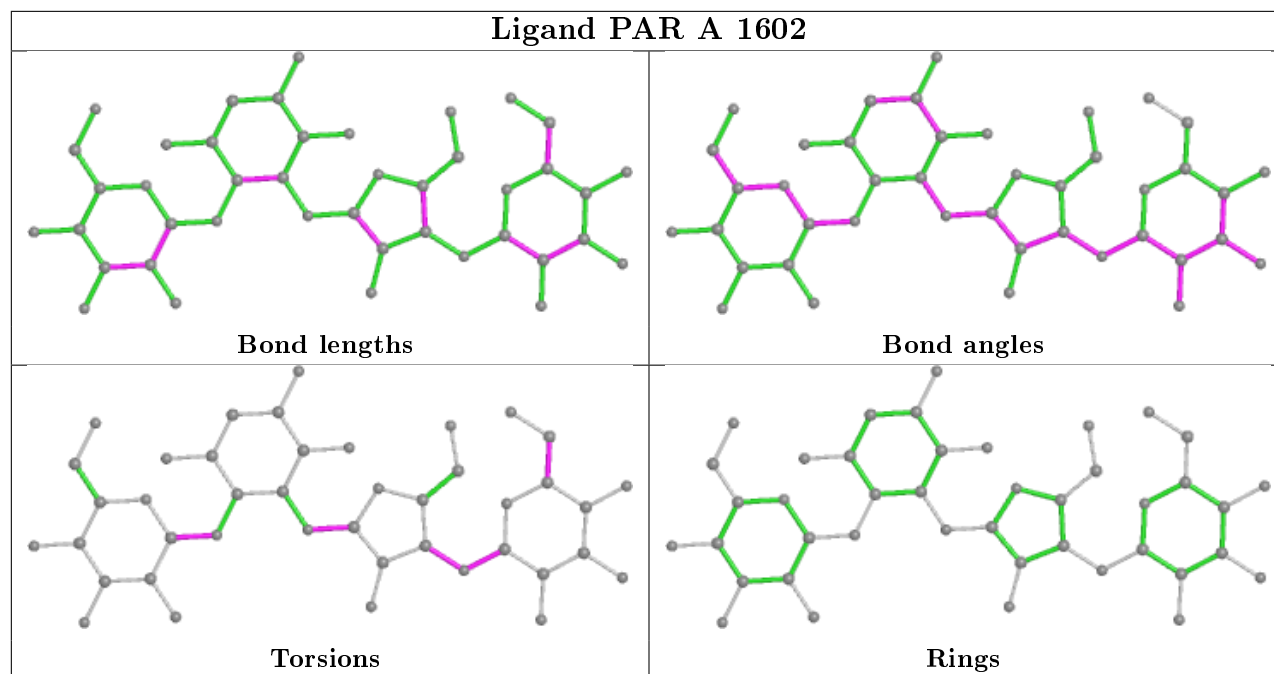
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A	1605	PAR	1	0
24	A	1604	PAR	3	0
24	A	1603	PAR	4	0
24	A	1606	PAR	3	0
24	A	1602	PAR	2	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1498/1522 (98%)	-0.21	18 (1%) 79 82	42, 76, 161, 281	0
2	B	236/236 (100%)	-0.07	7 (2%) 50 53	74, 121, 209, 250	0
3	C	207/207 (100%)	-0.02	3 (1%) 75 78	52, 115, 164, 212	0
4	D	208/208 (100%)	-0.25	4 (1%) 66 70	50, 87, 136, 163	0
5	E	151/151 (100%)	-0.37	0 100 100	49, 73, 114, 185	0
6	F	101/101 (100%)	-0.26	1 (0%) 82 86	72, 112, 142, 179	0
7	G	155/155 (100%)	-0.27	5 (3%) 47 50	66, 97, 165, 208	0
8	H	138/138 (100%)	-0.50	0 100 100	48, 70, 100, 143	0
9	I	127/127 (100%)	-0.07	0 100 100	78, 112, 161, 181	0
10	J	99/99 (100%)	0.41	8 (8%) 12 13	55, 135, 220, 317	0
11	K	119/119 (100%)	-0.05	4 (3%) 45 47	52, 78, 120, 164	0
12	L	124/125 (99%)	-0.19	5 (4%) 38 40	44, 78, 129, 273	0
13	M	118/118 (100%)	-0.13	0 100 100	68, 103, 144, 210	0
14	N	60/60 (100%)	-0.10	2 (3%) 46 48	73, 96, 147, 225	0
15	O	88/88 (100%)	-0.15	1 (1%) 80 84	49, 88, 137, 201	0
16	P	84/84 (100%)	-0.39	1 (1%) 79 82	42, 74, 100, 190	0
17	Q	99/99 (100%)	-0.35	0 100 100	49, 73, 123, 134	0
18	R	73/73 (100%)	-0.10	3 (4%) 37 39	56, 91, 163, 223	0
19	S	81/81 (100%)	0.08	2 (2%) 57 59	37, 124, 185, 246	0
20	T	99/99 (100%)	-0.27	3 (3%) 50 53	57, 76, 122, 195	0
21	U	25/25 (100%)	0.87	3 (12%) 4 5	72, 95, 139, 157	0
22	a	5/6 (83%)	0.49	0 100 100	82, 87, 122, 145	0
23	b	8/11 (72%)	0.86	1 (12%) 3 4	93, 123, 178, 205	0
All	All	3903/3932 (99%)	-0.17	71 (1%) 68 71	37, 88, 164, 317	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	K	128	ALA	9.6
11	K	129	SER	8.8
12	L	129	ALA	6.9
1	A	1129	C	4.4
7	G	80	VAL	4.2
1	A	216	G	4.2
1	A	217	C	4.2
2	B	136	VAL	3.9
11	K	127	LYS	3.8
14	N	12	ARG	3.8
12	L	128	ALA	3.7
21	U	26	LYS	3.7
21	U	25	LYS	3.7
14	N	13	THR	3.6
2	B	134	GLU	3.6
23	b	32	C	3.5
15	O	89	GLY	3.4
1	A	82	U	3.3
2	B	131	PRO	3.2
20	T	9	ASN	3.2
12	L	19	ARG	3.1
10	J	87	THR	3.1
12	L	112	ASP	3.1
18	R	17	SER	2.9
2	B	133	LYS	2.8
3	C	143	GLU	2.8
1	A	1006	C	2.7
2	B	132	LYS	2.7
1	A	993	G	2.7
6	F	101	ALA	2.6
7	G	156	TRP	2.6
20	T	100	ILE	2.6
4	D	86	LYS	2.6
4	D	32	ALA	2.6
10	J	5	ARG	2.6
3	C	87	LEU	2.5
7	G	82	GLY	2.5
4	D	179	GLU	2.4
1	A	1138	G	2.4
11	K	126	ARG	2.4
1	A	1005	A	2.4
10	J	73	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	461	C	2.4
18	R	16	PRO	2.3
7	G	81	GLY	2.3
7	G	83	ALA	2.3
10	J	36	GLY	2.3
10	J	99	LYS	2.3
19	S	28	LYS	2.3
10	J	34	VAL	2.2
2	B	135	GLN	2.2
10	J	72	VAL	2.2
10	J	90	LEU	2.2
1	A	1004	A	2.2
12	L	127	GLU	2.2
3	C	161	GLU	2.2
2	B	127	ILE	2.1
1	A	1533	C	2.1
20	T	8	ARG	2.1
18	R	85	LEU	2.1
1	A	631	G	2.1
1	A	1038	C	2.1
1	A	204	U	2.1
1	A	1037	C	2.1
1	A	1539	C	2.1
1	A	202	U	2.1
1	A	994	A	2.1
21	U	18	TYR	2.1
19	S	8	GLY	2.1
16	P	46	PRO	2.0
4	D	9	CYS	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	PSU	A	1540	20/21	0.90	0.39	155,164,169,173	0
1	PSU	A	1541	20/21	0.91	0.25	150,156,164,181	0
23	PSU	b	39	20/21	0.92	0.29	104,126,140,145	0
12	0TD	L	92	10/11	0.93	0.26	62,88,113,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	PSU	A	516	20/21	0.94	0.16	77,89,103,106	0
23	70U	b	34	25/26	0.94	0.20	85,105,133,143	0
23	12A	b	37	34/35	0.95	0.26	84,103,128,134	0
1	2MG	A	1207	24/25	0.95	0.17	96,105,108,110	0
1	M2G	A	966	25/26	0.95	0.23	68,84,96,100	0
1	5MC	A	1400	21/22	0.96	0.25	52,66,88,95	0
1	4OC	A	1402	22/23	0.96	0.16	56,61,71,74	0
1	MA6	A	1518	24/25	0.97	0.19	44,51,59,60	0
1	5MC	A	967	21/22	0.97	0.14	68,77,89,91	0
1	7MG	A	527	24/25	0.97	0.16	54,64,75,84	0
1	5MC	A	1407	21/22	0.98	0.19	49,56,64,69	0
1	MA6	A	1519	24/25	0.98	0.19	43,50,64,70	0
1	UR3	A	1498	21/22	0.98	0.15	44,54,60,78	0
1	5MC	A	1404	21/22	0.98	0.14	45,49,62,65	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
26	K	E	202	1/1	0.20	0.88	169,169,169,169	0
25	MG	A	1862	1/1	0.51	0.40	81,81,81,81	0
26	K	A	1901	1/1	0.54	0.72	180,180,180,180	0
26	K	A	1896	1/1	0.57	0.16	152,152,152,152	0
25	MG	A	1607	1/1	0.60	0.38	86,86,86,86	0
25	MG	A	1869	1/1	0.63	0.30	93,93,93,93	0
26	K	A	1910	1/1	0.64	0.66	160,160,160,160	0
25	MG	A	1787	1/1	0.64	0.65	66,66,66,66	0
25	MG	A	1790	1/1	0.66	0.19	92,92,92,92	0
25	MG	A	1639	1/1	0.67	0.54	64,64,64,64	0
25	MG	A	1747	1/1	0.67	0.30	87,87,87,87	0
26	K	A	1902	1/1	0.69	0.34	130,130,130,130	0
25	MG	Q	201	1/1	0.69	0.19	92,92,92,92	0
26	K	A	1919	1/1	0.69	0.46	125,125,125,125	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
26	K	A	1921	1/1	0.70	0.33	133,133,133,133	0
25	MG	A	1832	1/1	0.70	0.67	70,70,70,70	0
25	MG	A	1717	1/1	0.70	0.44	94,94,94,94	0
25	MG	A	1829	1/1	0.71	0.79	81,81,81,81	0
25	MG	A	1746	1/1	0.72	0.16	84,84,84,84	0
25	MG	A	1742	1/1	0.72	1.04	106,106,106,106	0
25	MG	A	1687	1/1	0.72	0.28	74,74,74,74	0
26	K	A	1909	1/1	0.73	0.62	153,153,153,153	0
26	K	A	1905	1/1	0.74	0.37	148,148,148,148	0
25	MG	A	1802	1/1	0.74	0.41	90,90,90,90	0
26	K	A	1900	1/1	0.75	0.33	135,135,135,135	0
26	K	A	1911	1/1	0.75	0.36	165,165,165,165	0
25	MG	a	101	1/1	0.75	0.39	97,97,97,97	0
25	MG	A	1629	1/1	0.76	0.33	77,77,77,77	0
25	MG	A	1871	1/1	0.76	0.41	47,47,47,47	0
25	MG	Q	202	1/1	0.76	0.45	79,79,79,79	0
25	MG	A	1729	1/1	0.76	0.26	80,80,80,80	0
26	K	A	1926	1/1	0.77	0.81	161,161,161,161	0
26	K	M	201	1/1	0.77	0.32	152,152,152,152	0
25	MG	A	1692	1/1	0.77	0.17	109,109,109,109	0
25	MG	A	1803	1/1	0.77	0.46	67,67,67,67	0
26	K	A	1897	1/1	0.78	0.30	126,126,126,126	0
25	MG	A	1822	1/1	0.79	0.34	88,88,88,88	0
25	MG	A	1758	1/1	0.79	0.36	64,64,64,64	0
26	K	A	1912	1/1	0.79	0.39	177,177,177,177	0
26	K	A	1927	1/1	0.79	0.57	134,134,134,134	0
25	MG	A	1833	1/1	0.79	0.51	91,91,91,91	0
25	MG	A	1740	1/1	0.79	0.14	81,81,81,81	0
25	MG	A	1782	1/1	0.79	0.46	75,75,75,75	0
26	K	A	1891	1/1	0.79	0.36	144,144,144,144	0
25	MG	A	1800	1/1	0.79	0.39	102,102,102,102	0
25	MG	A	1749	1/1	0.80	0.38	74,74,74,74	0
25	MG	A	1844	1/1	0.80	0.57	87,87,87,87	0
25	MG	A	1868	1/1	0.80	0.44	89,89,89,89	0
25	MG	A	1777	1/1	0.80	0.32	88,88,88,88	0
26	K	A	1914	1/1	0.80	0.24	122,122,122,122	0
25	MG	A	1882	1/1	0.80	0.30	73,73,73,73	0
25	MG	A	1885	1/1	0.81	0.47	78,78,78,78	0
25	MG	A	1769	1/1	0.81	0.70	93,93,93,93	0
25	MG	A	1648	1/1	0.81	0.20	77,77,77,77	0
25	MG	C	301	1/1	0.81	0.27	76,76,76,76	0
25	MG	A	1843	1/1	0.81	0.34	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
25	MG	A	1704	1/1	0.81	0.15	164,164,164,164	0
25	MG	G	202	1/1	0.81	0.27	104,104,104,104	0
26	K	A	1890	1/1	0.82	0.19	132,132,132,132	0
25	MG	A	1823	1/1	0.82	0.44	91,91,91,91	0
25	MG	A	1875	1/1	0.82	0.14	74,74,74,74	0
25	MG	A	1702	1/1	0.82	0.15	34,34,34,34	0
25	MG	A	1855	1/1	0.82	0.35	93,93,93,93	0
25	MG	A	1824	1/1	0.82	0.43	98,98,98,98	0
26	K	A	1913	1/1	0.82	0.30	162,162,162,162	0
25	MG	A	1752	1/1	0.82	0.21	95,95,95,95	0
26	K	A	1925	1/1	0.82	0.26	155,155,155,155	0
26	K	A	1916	1/1	0.83	0.51	188,188,188,188	0
25	MG	A	1734	1/1	0.83	0.39	84,84,84,84	0
25	MG	A	1799	1/1	0.83	0.33	151,151,151,151	0
25	MG	A	1846	1/1	0.83	0.29	78,78,78,78	0
25	MG	A	1609	1/1	0.83	0.14	109,109,109,109	0
25	MG	A	1781	1/1	0.84	0.26	75,75,75,75	0
25	MG	A	1625	1/1	0.84	0.28	75,75,75,75	0
25	MG	A	1774	1/1	0.84	0.23	62,62,62,62	0
24	PAR	A	1605	42/42	0.84	0.28	123,142,151,159	0
25	MG	A	1663	1/1	0.84	0.58	68,68,68,68	0
25	MG	A	1772	1/1	0.84	0.47	76,76,76,76	0
25	MG	A	1826	1/1	0.84	0.39	82,82,82,82	0
25	MG	A	1738	1/1	0.85	0.25	83,83,83,83	0
25	MG	A	1757	1/1	0.85	0.26	87,87,87,87	0
25	MG	A	1874	1/1	0.85	0.33	87,87,87,87	0
25	MG	A	1828	1/1	0.85	0.30	81,81,81,81	0
25	MG	A	1700	1/1	0.85	0.34	86,86,86,86	0
26	K	A	1922	1/1	0.85	0.28	137,137,137,137	0
25	MG	H	202	1/1	0.85	0.11	62,62,62,62	0
25	MG	A	1827	1/1	0.85	0.33	68,68,68,68	0
25	MG	A	1733	1/1	0.85	0.27	74,74,74,74	0
26	K	A	1907	1/1	0.86	0.33	140,140,140,140	0
24	PAR	A	1602	42/42	0.86	0.32	76,129,171,179	0
25	MG	H	203	1/1	0.86	0.20	89,89,89,89	0
25	MG	A	1820	1/1	0.86	0.27	72,72,72,72	0
25	MG	A	1726	1/1	0.86	0.28	86,86,86,86	0
25	MG	A	1831	1/1	0.86	0.27	87,87,87,87	0
25	MG	A	1727	1/1	0.86	0.24	97,97,97,97	0
25	MG	A	1850	1/1	0.86	0.42	78,78,78,78	0
25	MG	A	1888	1/1	0.86	0.26	77,77,77,77	0
25	MG	P	103	1/1	0.86	0.15	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
25	MG	A	1732	1/1	0.87	0.22	71,71,71,71	0
25	MG	A	1763	1/1	0.87	0.37	50,50,50,50	0
25	MG	A	1872	1/1	0.87	0.21	75,75,75,75	0
25	MG	A	1728	1/1	0.87	0.37	61,61,61,61	0
25	MG	A	1805	1/1	0.87	0.20	77,77,77,77	0
25	MG	A	1879	1/1	0.87	0.20	128,128,128,128	0
25	MG	A	1760	1/1	0.87	0.25	69,69,69,69	0
25	MG	A	1712	1/1	0.87	0.21	66,66,66,66	0
25	MG	A	1783	1/1	0.87	0.51	73,73,73,73	0
26	K	A	1895	1/1	0.87	0.36	154,154,154,154	0
25	MG	A	1715	1/1	0.87	0.28	82,82,82,82	0
25	MG	A	1814	1/1	0.87	0.19	273,273,273,273	0
25	MG	A	1673	1/1	0.87	0.36	66,66,66,66	0
25	MG	A	1881	1/1	0.87	0.26	78,78,78,78	0
25	MG	A	1766	1/1	0.87	0.27	73,73,73,73	0
25	MG	A	1889	1/1	0.88	0.28	75,75,75,75	0
25	MG	A	1737	1/1	0.88	0.19	65,65,65,65	0
25	MG	A	1851	1/1	0.88	0.31	85,85,85,85	0
25	MG	A	1883	1/1	0.88	0.25	63,63,63,63	0
26	K	A	1899	1/1	0.88	0.27	149,149,149,149	0
25	MG	A	1821	1/1	0.88	0.20	71,71,71,71	0
25	MG	L	201	1/1	0.88	0.34	79,79,79,79	0
25	MG	A	1886	1/1	0.88	0.17	73,73,73,73	0
25	MG	A	1616	1/1	0.88	0.38	80,80,80,80	0
25	MG	A	1768	1/1	0.88	0.18	73,73,73,73	0
25	MG	A	1839	1/1	0.88	0.33	85,85,85,85	0
25	MG	A	1681	1/1	0.88	0.22	93,93,93,93	0
25	MG	A	1679	1/1	0.88	0.39	70,70,70,70	0
25	MG	A	1809	1/1	0.88	0.31	78,78,78,78	0
25	MG	a	102	1/1	0.88	0.19	70,70,70,70	0
24	PAR	A	1604	42/42	0.88	0.24	100,133,205,209	0
25	MG	A	1854	1/1	0.88	0.29	69,69,69,69	0
25	MG	A	1696	1/1	0.89	0.30	55,55,55,55	0
26	K	A	1920	1/1	0.89	0.54	133,133,133,133	0
26	K	A	1918	1/1	0.89	0.20	139,139,139,139	0
25	MG	A	1731	1/1	0.89	0.28	61,61,61,61	0
25	MG	H	201	1/1	0.89	0.18	58,58,58,58	0
25	MG	A	1635	1/1	0.89	0.35	49,49,49,49	0
25	MG	A	1703	1/1	0.89	0.73	84,84,84,84	0
25	MG	b	101	1/1	0.89	0.23	84,84,84,84	0
25	MG	A	1878	1/1	0.89	0.25	79,79,79,79	0
25	MG	A	1834	1/1	0.89	0.85	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
25	MG	A	1776	1/1	0.89	0.19	88,88,88,88	0
25	MG	A	1884	1/1	0.89	0.25	112,112,112,112	0
26	K	A	1923	1/1	0.89	0.41	102,102,102,102	0
25	MG	A	1709	1/1	0.89	0.15	130,130,130,130	0
25	MG	A	1613	1/1	0.90	0.30	67,67,67,67	0
25	MG	A	1722	1/1	0.90	0.29	52,52,52,52	0
25	MG	L	202	1/1	0.90	0.09	59,59,59,59	0
25	MG	A	1745	1/1	0.90	0.23	52,52,52,52	0
25	MG	A	1645	1/1	0.90	0.14	210,210,210,210	0
25	MG	A	1767	1/1	0.90	0.59	64,64,64,64	0
24	PAR	A	1606	42/42	0.90	0.32	96,119,131,139	0
25	MG	A	1676	1/1	0.90	0.49	80,80,80,80	0
25	MG	A	1789	1/1	0.90	0.18	56,56,56,56	0
25	MG	A	1793	1/1	0.90	0.21	85,85,85,85	0
25	MG	A	1637	1/1	0.90	0.36	69,69,69,69	0
25	MG	A	1840	1/1	0.90	0.25	74,74,74,74	0
25	MG	A	1856	1/1	0.90	0.36	71,71,71,71	0
25	MG	H	204	1/1	0.90	0.17	43,43,43,43	0
24	PAR	A	1603	42/42	0.90	0.30	78,105,140,150	0
25	MG	A	1807	1/1	0.90	0.10	83,83,83,83	0
25	MG	A	1765	1/1	0.91	0.27	59,59,59,59	0
25	MG	A	1816	1/1	0.91	0.23	62,62,62,62	0
26	K	G	203	1/1	0.91	0.13	178,178,178,178	0
25	MG	A	1759	1/1	0.91	0.11	42,42,42,42	0
25	MG	A	1736	1/1	0.91	0.54	74,74,74,74	0
25	MG	A	1835	1/1	0.91	0.21	62,62,62,62	0
25	MG	A	1618	1/1	0.91	0.14	118,118,118,118	0
26	K	A	1898	1/1	0.91	0.48	134,134,134,134	0
25	MG	A	1650	1/1	0.91	0.31	71,71,71,71	0
25	MG	A	1680	1/1	0.91	0.21	247,247,247,247	0
25	MG	A	1873	1/1	0.91	0.22	80,80,80,80	0
25	MG	A	1857	1/1	0.91	0.21	44,44,44,44	0
25	MG	A	1877	1/1	0.92	0.22	76,76,76,76	0
25	MG	A	1721	1/1	0.92	0.11	49,49,49,49	0
25	MG	A	1870	1/1	0.92	0.15	43,43,43,43	0
25	MG	G	201	1/1	0.92	0.17	55,55,55,55	0
25	MG	A	1614	1/1	0.92	0.10	89,89,89,89	0
25	MG	A	1672	1/1	0.92	0.16	69,69,69,69	0
25	MG	A	1688	1/1	0.92	0.10	131,131,131,131	0
25	MG	A	1753	1/1	0.92	0.26	48,48,48,48	0
25	MG	A	1815	1/1	0.92	0.14	56,56,56,56	0
25	MG	A	1858	1/1	0.92	0.24	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
25	MG	A	1817	1/1	0.92	0.27	58,58,58,58	0
25	MG	A	1667	1/1	0.92	0.43	55,55,55,55	0
25	MG	A	1671	1/1	0.92	0.66	52,52,52,52	0
25	MG	A	1685	1/1	0.92	0.23	71,71,71,71	0
25	MG	A	1714	1/1	0.92	0.13	41,41,41,41	0
25	MG	A	1849	1/1	0.92	0.45	56,56,56,56	0
26	K	A	1894	1/1	0.92	0.48	126,126,126,126	0
25	MG	A	1693	1/1	0.92	0.21	80,80,80,80	0
25	MG	A	1876	1/1	0.93	0.15	59,59,59,59	0
25	MG	A	1641	1/1	0.93	0.20	60,60,60,60	0
25	MG	A	1647	1/1	0.93	0.27	98,98,98,98	0
25	MG	A	1847	1/1	0.93	0.25	82,82,82,82	0
25	MG	A	1837	1/1	0.93	0.19	69,69,69,69	0
25	MG	A	1691	1/1	0.93	0.20	58,58,58,58	0
25	MG	A	1719	1/1	0.93	0.18	66,66,66,66	0
25	MG	A	1791	1/1	0.93	0.27	52,52,52,52	0
25	MG	A	1842	1/1	0.93	0.15	55,55,55,55	0
25	MG	D	302	1/1	0.93	0.09	71,71,71,71	0
25	MG	A	1804	1/1	0.93	0.12	88,88,88,88	0
25	MG	A	1863	1/1	0.93	0.22	56,56,56,56	0
25	MG	S	103	1/1	0.93	0.10	62,62,62,62	0
25	MG	A	1818	1/1	0.93	0.34	74,74,74,74	0
25	MG	A	1710	1/1	0.93	0.23	64,64,64,64	0
25	MG	S	102	1/1	0.93	0.13	58,58,58,58	0
25	MG	A	1770	1/1	0.93	0.42	69,69,69,69	0
25	MG	A	1841	1/1	0.93	0.21	74,74,74,74	0
25	MG	A	1611	1/1	0.93	0.18	66,66,66,66	0
25	MG	A	1865	1/1	0.93	0.17	90,90,90,90	0
25	MG	A	1788	1/1	0.93	0.48	88,88,88,88	0
25	MG	A	1634	1/1	0.93	0.12	102,102,102,102	0
25	MG	A	1762	1/1	0.93	0.15	65,65,65,65	0
25	MG	A	1880	1/1	0.93	0.14	67,67,67,67	0
25	MG	A	1845	1/1	0.93	0.24	55,55,55,55	0
25	MG	A	1666	1/1	0.94	0.09	89,89,89,89	0
25	MG	E	201	1/1	0.94	0.10	119,119,119,119	0
25	MG	A	1756	1/1	0.94	0.30	73,73,73,73	0
25	MG	A	1741	1/1	0.94	0.22	65,65,65,65	0
25	MG	A	1619	1/1	0.94	0.08	66,66,66,66	0
25	MG	N	102	1/1	0.94	0.27	73,73,73,73	0
25	MG	A	1755	1/1	0.94	0.26	73,73,73,73	0
25	MG	A	1860	1/1	0.94	0.15	67,67,67,67	0
25	MG	P	102	1/1	0.94	0.17	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
25	MG	A	1830	1/1	0.94	0.26	54,54,54,54	0
25	MG	A	1720	1/1	0.94	0.21	51,51,51,51	0
25	MG	A	1751	1/1	0.94	0.14	67,67,67,67	0
25	MG	A	1670	1/1	0.94	0.16	58,58,58,58	0
25	MG	A	1861	1/1	0.94	0.20	86,86,86,86	0
25	MG	A	1786	1/1	0.94	0.43	63,63,63,63	0
25	MG	A	1743	1/1	0.94	0.21	35,35,35,35	0
25	MG	A	1797	1/1	0.94	0.18	118,118,118,118	0
25	MG	A	1867	1/1	0.94	0.38	70,70,70,70	0
25	MG	A	1665	1/1	0.94	0.15	70,70,70,70	0
25	MG	A	1610	1/1	0.94	0.23	106,106,106,106	0
25	MG	A	1838	1/1	0.94	0.33	72,72,72,72	0
25	MG	A	1644	1/1	0.94	0.21	124,124,124,124	0
25	MG	A	1623	1/1	0.94	0.12	42,42,42,42	0
25	MG	A	1808	1/1	0.94	0.23	56,56,56,56	0
25	MG	A	1819	1/1	0.94	0.16	52,52,52,52	0
25	MG	A	1739	1/1	0.94	0.23	63,63,63,63	0
25	MG	A	1725	1/1	0.94	0.22	36,36,36,36	0
26	K	A	1906	1/1	0.94	0.22	109,109,109,109	0
25	MG	A	1836	1/1	0.94	0.16	72,72,72,72	0
26	K	A	1917	1/1	0.95	0.30	148,148,148,148	0
25	MG	A	1656	1/1	0.95	0.12	100,100,100,100	0
25	MG	A	1794	1/1	0.95	0.14	60,60,60,60	0
25	MG	A	1748	1/1	0.95	0.39	84,84,84,84	0
25	MG	A	1813	1/1	0.95	0.08	179,179,179,179	0
25	MG	A	1711	1/1	0.95	0.14	143,143,143,143	0
25	MG	A	1668	1/1	0.95	0.45	38,38,38,38	0
25	MG	A	1887	1/1	0.95	0.28	67,67,67,67	0
25	MG	A	1718	1/1	0.95	0.26	84,84,84,84	0
25	MG	A	1708	1/1	0.95	0.13	51,51,51,51	0
26	K	A	1903	1/1	0.95	0.31	128,128,128,128	0
25	MG	A	1771	1/1	0.95	0.19	55,55,55,55	0
25	MG	A	1682	1/1	0.95	0.15	98,98,98,98	0
25	MG	A	1657	1/1	0.95	0.11	22,22,22,22	0
26	K	A	1892	1/1	0.95	0.20	115,115,115,115	0
24	PAR	A	1601	42/42	0.95	0.21	41,62,103,110	0
25	MG	A	1764	1/1	0.95	0.17	52,52,52,52	0
25	MG	A	1694	1/1	0.95	0.09	86,86,86,86	0
25	MG	A	1801	1/1	0.95	0.22	84,84,84,84	0
25	MG	S	101	1/1	0.95	0.12	46,46,46,46	0
26	K	A	1915	1/1	0.95	0.16	167,167,167,167	0
25	MG	A	1669	1/1	0.95	0.14	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
25	MG	A	1658	1/1	0.95	0.21	41,41,41,41	0
25	MG	A	1852	1/1	0.95	0.18	78,78,78,78	0
25	MG	A	1706	1/1	0.95	0.29	71,71,71,71	0
25	MG	A	1750	1/1	0.95	0.14	58,58,58,58	0
25	MG	A	1723	1/1	0.95	0.22	136,136,136,136	0
25	MG	A	1775	1/1	0.95	0.69	82,82,82,82	0
25	MG	A	1632	1/1	0.95	0.57	39,39,39,39	0
25	MG	A	1779	1/1	0.95	0.34	96,96,96,96	0
25	MG	A	1653	1/1	0.95	0.16	136,136,136,136	0
25	MG	A	1780	1/1	0.95	0.40	75,75,75,75	0
25	MG	A	1859	1/1	0.95	0.39	83,83,83,83	0
25	MG	A	1642	1/1	0.96	0.16	46,46,46,46	0
25	MG	A	1651	1/1	0.96	0.12	49,49,49,49	0
25	MG	A	1730	1/1	0.96	0.09	44,44,44,44	0
25	MG	A	1636	1/1	0.96	0.17	39,39,39,39	0
25	MG	A	1640	1/1	0.96	0.22	83,83,83,83	0
25	MG	A	1825	1/1	0.96	0.29	48,48,48,48	0
25	MG	A	1652	1/1	0.96	0.14	70,70,70,70	0
25	MG	A	1864	1/1	0.96	0.21	81,81,81,81	0
25	MG	A	1811	1/1	0.96	0.18	64,64,64,64	0
25	MG	A	1810	1/1	0.96	0.12	47,47,47,47	0
25	MG	T	201	1/1	0.96	0.27	64,64,64,64	0
25	MG	A	1674	1/1	0.96	0.22	85,85,85,85	0
25	MG	A	1795	1/1	0.96	0.20	206,206,206,206	0
25	MG	A	1724	1/1	0.96	0.31	29,29,29,29	0
25	MG	A	1798	1/1	0.96	0.15	228,228,228,228	0
25	MG	A	1695	1/1	0.96	0.13	88,88,88,88	0
25	MG	A	1659	1/1	0.96	0.10	106,106,106,106	0
25	MG	A	1848	1/1	0.96	0.24	40,40,40,40	0
25	MG	A	1633	1/1	0.96	0.20	58,58,58,58	0
26	K	A	1904	1/1	0.96	0.14	120,120,120,120	0
25	MG	A	1735	1/1	0.96	0.27	61,61,61,61	0
25	MG	A	1707	1/1	0.96	0.13	97,97,97,97	0
25	MG	A	1928	1/1	0.97	0.32	60,60,60,60	0
25	MG	P	104	1/1	0.97	0.16	80,80,80,80	0
25	MG	b	102	1/1	0.97	0.09	77,77,77,77	0
25	MG	A	1773	1/1	0.97	0.15	56,56,56,56	0
25	MG	A	1716	1/1	0.97	0.17	194,194,194,194	0
25	MG	A	1675	1/1	0.97	0.16	107,107,107,107	0
25	MG	A	1617	1/1	0.97	0.17	33,33,33,33	0
25	MG	A	1796	1/1	0.97	0.05	124,124,124,124	0
26	K	A	1893	1/1	0.97	0.12	125,125,125,125	0

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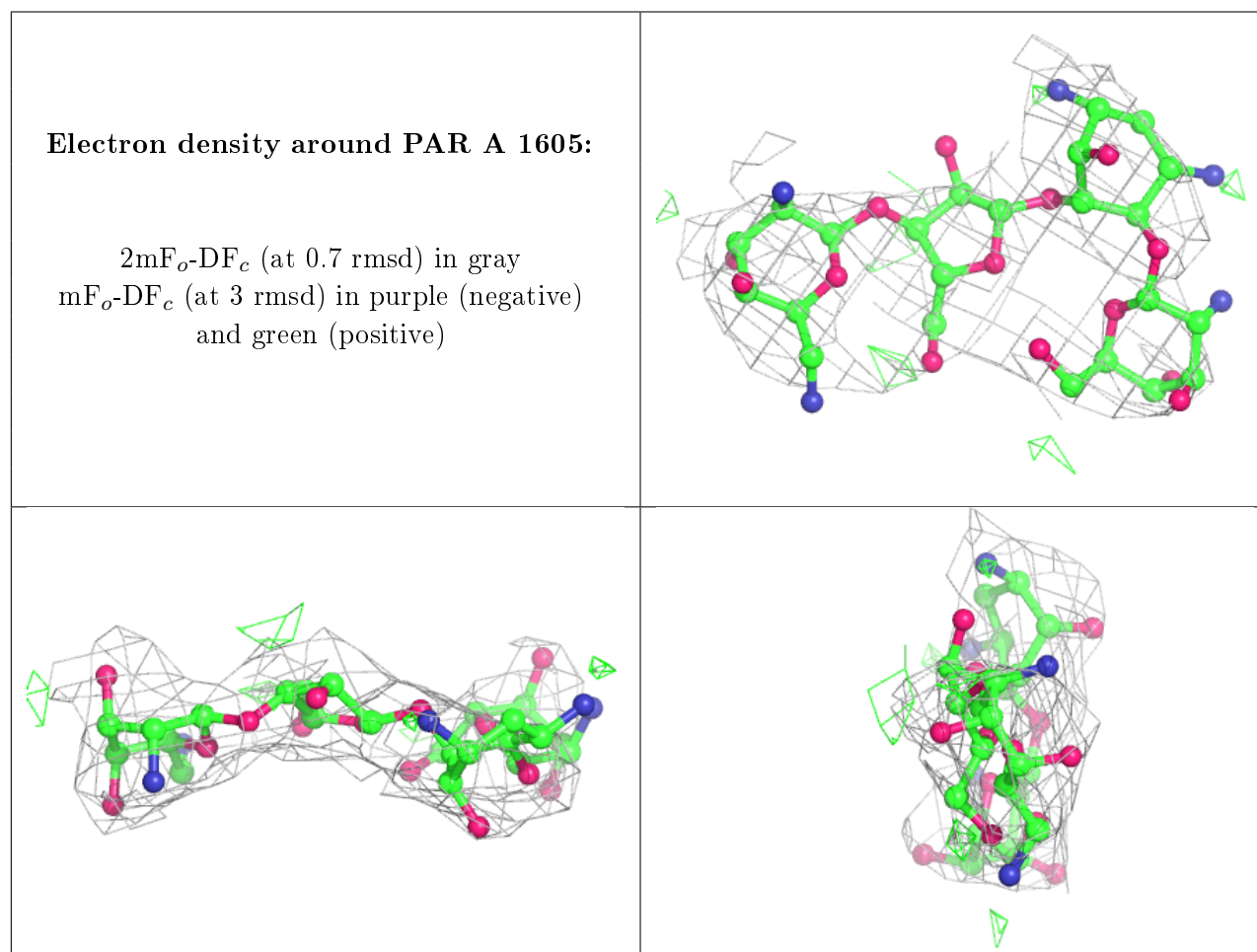
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
25	MG	A	1697	1/1	0.97	0.14	226,226,226,226	0
25	MG	A	1677	1/1	0.97	0.09	87,87,87,87	0
25	MG	A	1701	1/1	0.97	0.34	38,38,38,38	0
25	MG	A	1684	1/1	0.97	0.10	87,87,87,87	0
25	MG	A	1806	1/1	0.97	0.35	72,72,72,72	0
25	MG	A	1754	1/1	0.97	0.15	53,53,53,53	0
25	MG	A	1778	1/1	0.97	0.15	38,38,38,38	0
25	MG	A	1622	1/1	0.97	0.17	60,60,60,60	0
26	K	A	1924	1/1	0.97	0.13	127,127,127,127	0
25	MG	A	1853	1/1	0.97	0.11	37,37,37,37	0
25	MG	A	1784	1/1	0.97	0.30	35,35,35,35	0
25	MG	A	1626	1/1	0.97	0.17	57,57,57,57	0
25	MG	A	1649	1/1	0.98	0.14	44,44,44,44	0
25	MG	A	1713	1/1	0.98	0.24	74,74,74,74	0
25	MG	A	1664	1/1	0.98	0.16	80,80,80,80	0
25	MG	A	1643	1/1	0.98	0.31	83,83,83,83	0
25	MG	A	1792	1/1	0.98	0.34	51,51,51,51	0
25	MG	A	1628	1/1	0.98	0.12	58,58,58,58	0
25	MG	A	1630	1/1	0.98	0.29	32,32,32,32	0
26	K	A	1908	1/1	0.98	0.23	101,101,101,101	0
25	MG	A	1761	1/1	0.98	0.21	48,48,48,48	0
25	MG	A	1661	1/1	0.98	0.09	96,96,96,96	0
25	MG	A	1678	1/1	0.98	0.20	53,53,53,53	0
25	MG	A	1744	1/1	0.98	0.12	60,60,60,60	0
25	MG	A	1638	1/1	0.98	0.11	73,73,73,73	0
25	MG	A	1683	1/1	0.98	0.11	62,62,62,62	0
25	MG	A	1866	1/1	0.98	0.26	76,76,76,76	0
25	MG	A	1690	1/1	0.98	0.26	127,127,127,127	0
25	MG	A	1699	1/1	0.98	0.17	69,69,69,69	0
25	MG	A	1654	1/1	0.98	0.21	91,91,91,91	0
25	MG	A	1631	1/1	0.98	0.08	89,89,89,89	0
25	MG	A	1660	1/1	0.98	0.17	11,11,11,11	0
25	MG	A	1689	1/1	0.98	0.24	163,163,163,163	0
25	MG	A	1655	1/1	0.98	0.11	69,69,69,69	0
25	MG	A	1615	1/1	0.98	0.15	49,49,49,49	0
27	ZN	N	101	1/1	0.98	0.12	89,89,89,89	0
25	MG	A	1698	1/1	0.98	0.31	54,54,54,54	0
25	MG	A	1686	1/1	0.98	0.30	41,41,41,41	0
25	MG	A	1621	1/1	0.98	0.15	86,86,86,86	0
25	MG	A	1785	1/1	0.98	0.13	56,56,56,56	0
25	MG	A	1705	1/1	0.98	0.04	62,62,62,62	0
25	MG	F	201	1/1	0.98	0.06	69,69,69,69	0

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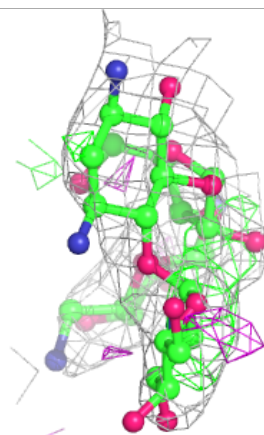
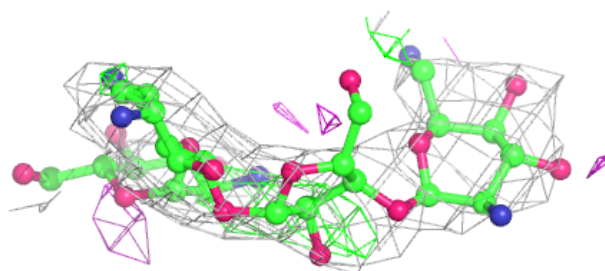
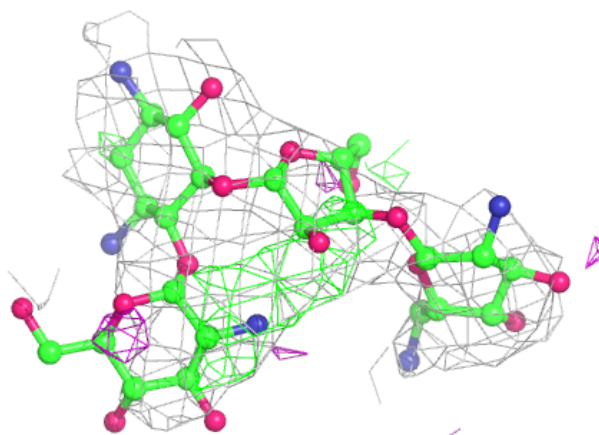
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
25	MG	A	1812	1/1	0.98	0.22	46,46,46,46	0
27	ZN	D	301	1/1	0.99	0.31	55,55,55,55	0
25	MG	A	1620	1/1	0.99	0.07	76,76,76,76	0
25	MG	A	1624	1/1	0.99	0.11	62,62,62,62	0
25	MG	A	1646	1/1	0.99	0.11	44,44,44,44	0
25	MG	A	1608	1/1	0.99	0.14	63,63,63,63	0
25	MG	A	1627	1/1	0.99	0.26	90,90,90,90	0
25	MG	A	1662	1/1	0.99	0.26	115,115,115,115	0
25	MG	P	101	1/1	0.99	0.10	34,34,34,34	0
25	MG	A	1612	1/1	0.99	0.11	54,54,54,54	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.



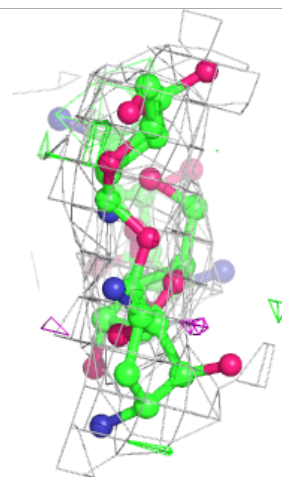
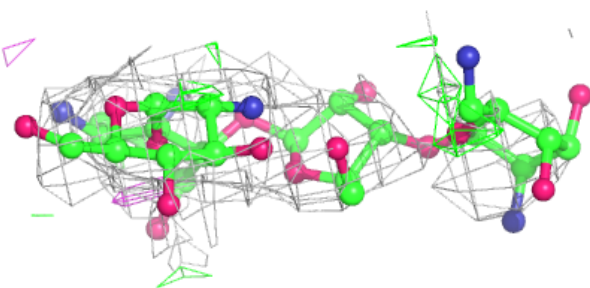
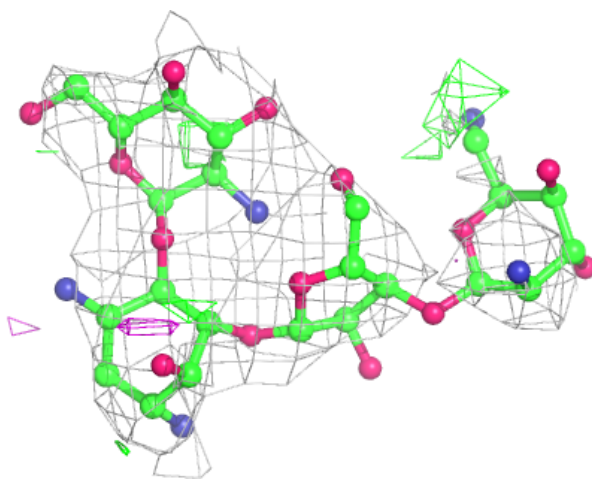
Electron density around PAR A 1602:

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



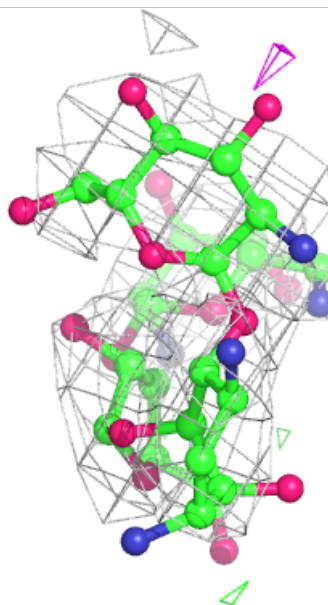
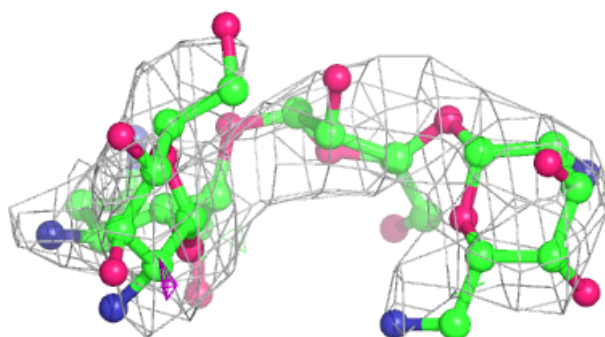
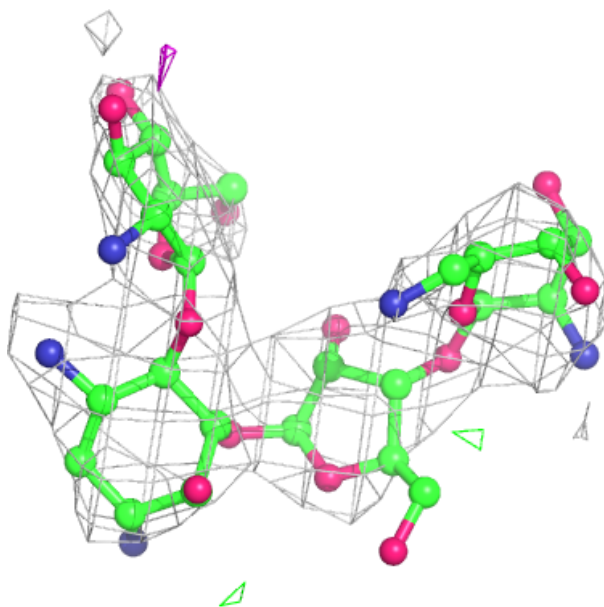
Electron density around PAR A 1604:

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



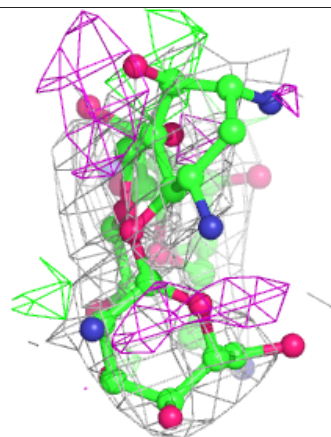
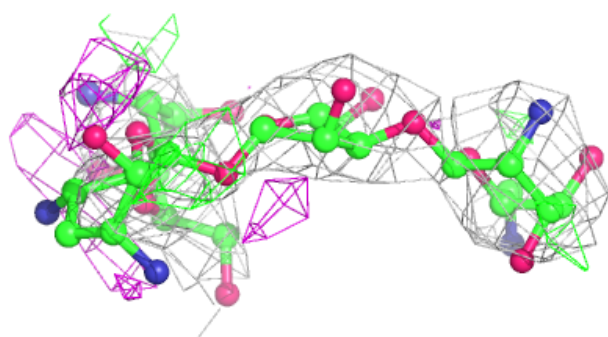
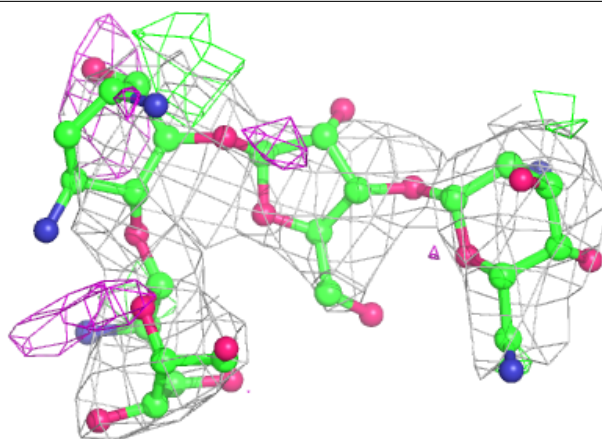
Electron density around PAR A 1606:

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

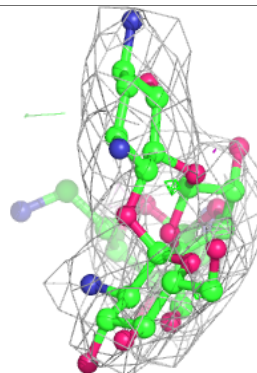
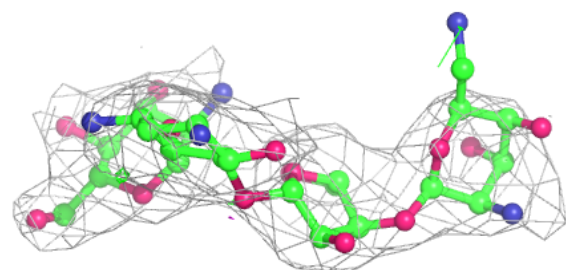
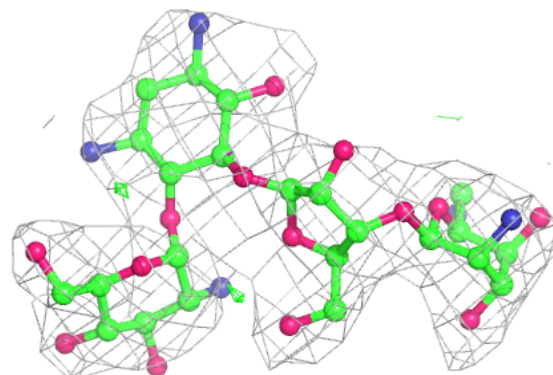


Electron density around PAR A 1603:

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

**Electron density around PAR A 1601:**

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



6.5 Other polymers

There are no such residues in this entry.