Full wwPDB X-ray Structure Validation Report (i)

Jun 23, 2024 – 08:09 PM EDT

PDB ID	:	4X66
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	:	3.45 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

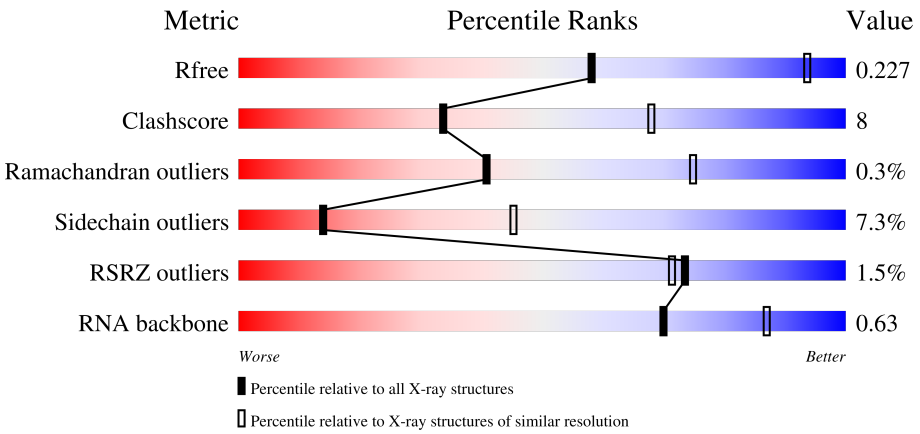
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.45 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	1278 (3.50-3.38)
Clashscore	141614	1361 (3.50-3.38)
Ramachandran outliers	138981	1327 (3.50-3.38)
Sidechain outliers	138945	1328 (3.50-3.38)
RSRZ outliers	127900	1192 (3.50-3.38)
RNA backbone	3102	1024 (3.92-2.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	54% 37% 8% •
2	B	236	3% 77% 23%
3	C	207	77% 21% •
4	D	208	% 80% 18% •

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Mol	Chain	Length	Quality of chain
5	E	151	74% 23%
6	F	101	% 77% 22%
7	G	155	% 75% 25%
8	H	138	75% 22%
9	I	127	3% 65% 31%
10	J	99	13% 65% 31%
11	K	119	3% 82% 17%
12	L	125	6% 67% 30%
13	M	118	4% 75% 22%
14	N	60	3% 75% 23%
15	O	88	2% 76% 20%
16	P	84	76% 24%
17	Q	99	82% 17%
18	R	73	3% 81% 18%
19	S	81	2% 65% 30%
20	T	99	2% 78% 18%
21	U	25	4% 72% 28%
22	a	6	67% 33%
23	b	11	45% 55%

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
24	PAR	A	1602	-	-	-	X
25	MG	A	1607	-	-	-	X
25	MG	A	1639	-	-	-	X
25	MG	A	1667	-	-	-	X
25	MG	A	1709	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	MG	A	1720	-	-	-	X
25	MG	A	1735	-	-	-	X
25	MG	A	1748	-	-	-	X
25	MG	A	1753	-	-	-	X
25	MG	A	1765	-	-	-	X
25	MG	A	1770	-	-	-	X
25	MG	A	1772	-	-	-	X
25	MG	A	1775	-	-	-	X
25	MG	A	1782	-	-	-	X
25	MG	A	1788	-	-	-	X
25	MG	A	1797	-	-	-	X
25	MG	A	1808	-	-	-	X
25	MG	A	1819	-	-	-	X
25	MG	A	1820	-	-	-	X
25	MG	A	1822	-	-	-	X
25	MG	A	1824	-	-	-	X
25	MG	A	1830	-	-	-	X
25	MG	A	1847	-	-	-	X
25	MG	A	1848	-	-	-	X
25	MG	A	1852	-	-	-	X
25	MG	A	1855	-	-	-	X
25	MG	A	1864	-	-	-	X
25	MG	A	1866	-	-	-	X
25	MG	A	1885	-	-	-	X
25	MG	C	301	-	-	-	X
25	MG	G	201	-	-	-	X
25	MG	H	201	-	-	-	X
25	MG	L	201	-	-	-	X
25	MG	Q	202	-	-	-	X
26	K	A	1888	-	-	-	X
26	K	A	1891	-	-	-	X
26	K	A	1904	-	-	-	X
26	K	A	1905	-	-	-	X
26	K	A	1907	-	-	-	X
26	K	A	1912	-	-	-	X
26	K	A	1913	-	-	-	X

2 Entry composition (i)

There are 28 unique types of molecules in this entry. The entry contains 52822 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

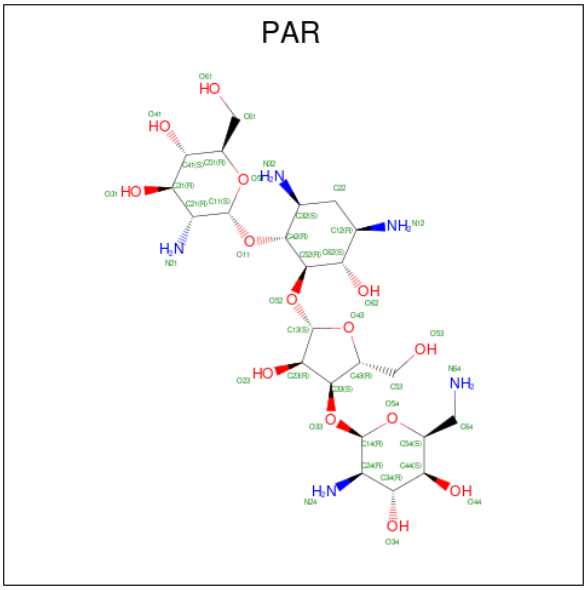
- Molecule 22 is a RNA chain called RNA (5'-D(*AP*AP*(MA6)P*UP*UP*U)-3').

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: $C_{23}H_{45}N_5O_{14}$).



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
			Total	C	N	O		
24	A	1	42	23	5	14	0	0
24	A	1	42	23	5	14	0	0
24	A	1	42	23	5	14	0	0
24	A	1	42	23	5	14	0	0
24	A	1	42	23	5	14	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
25	A	280	280	280	0	0
25	C	1	1	1	0	0
25	D	1	1	1	0	0
25	E	1	1	1	0	0
25	F	1	1	1	0	0
25	G	1	1	1	0	0
25	H	2	2	2	0	0
25	L	2	2	2	0	0
25	P	4	4	4	0	0
25	Q	2	2	2	0	0
25	S	3	3	3	0	0
25	T	1	1	1	0	0
25	a	1	1	1	0	0
25	b	1	1	1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	44	Total K 44 44	0	0
26	E	1	Total K 1 1	0	0
26	G	1	Total K 1 1	0	0

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

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

- Molecule 28 is water.

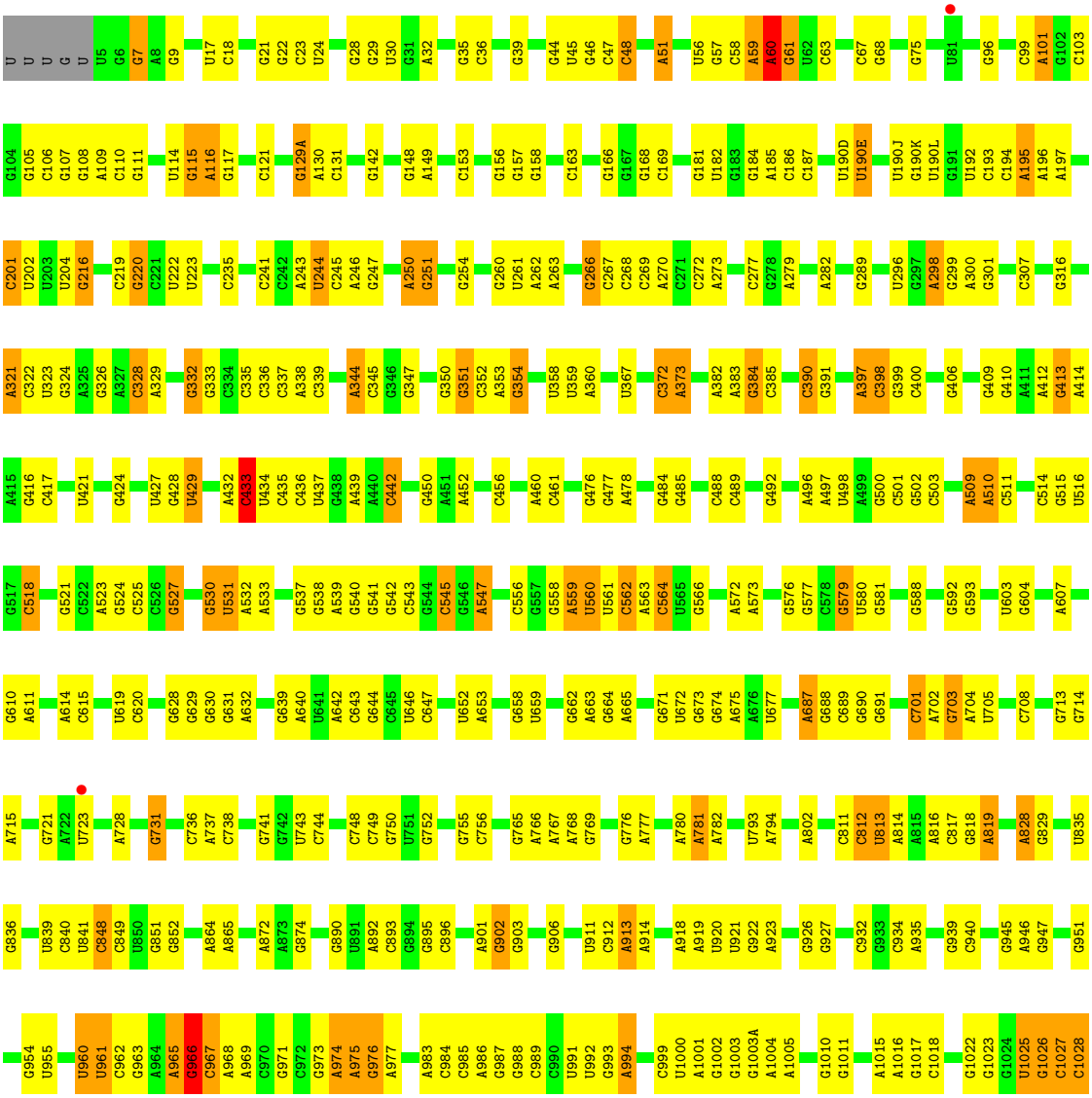
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	212	Total O 212 212	0	0
28	D	2	Total O 2 2	0	0
28	E	5	Total O 5 5	0	0
28	K	1	Total O 1 1	0	0
28	L	4	Total O 4 4	0	0
28	O	1	Total O 1 1	0	0
28	T	1	Total O 1 1	0	0
28	a	1	Total O 1 1	0	0

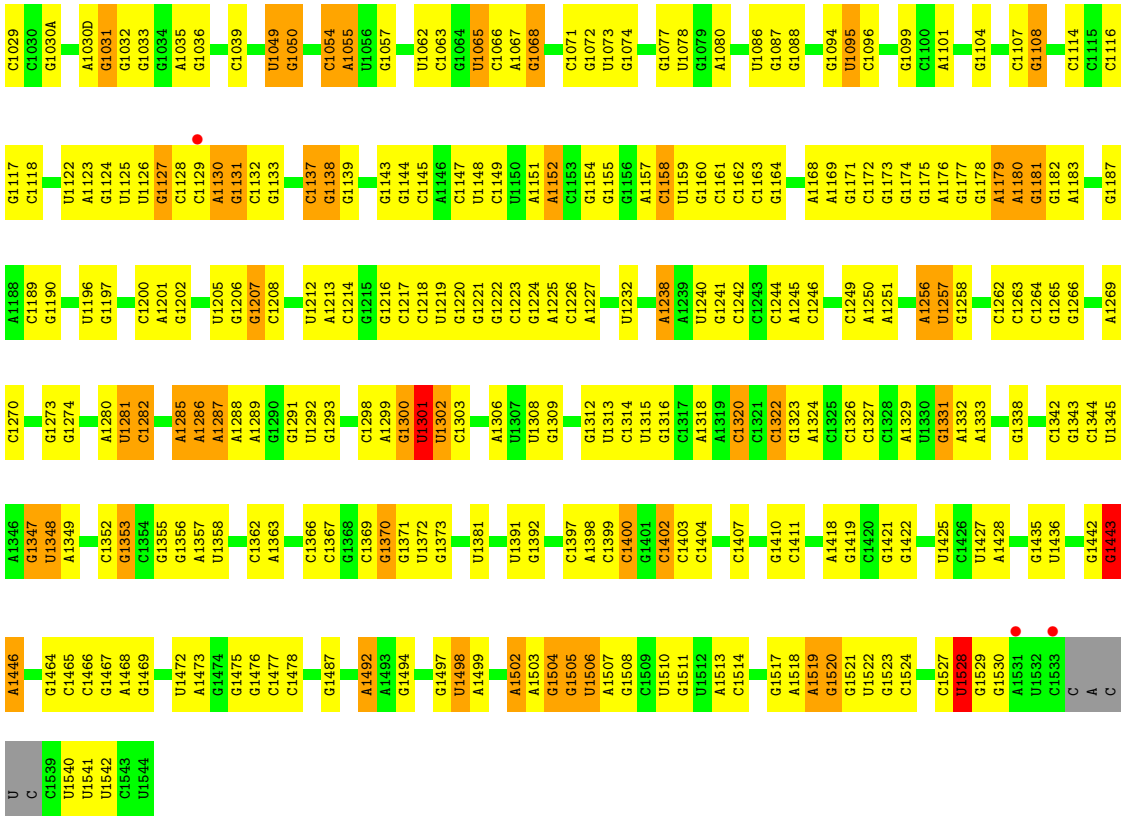
3 Residue-property plots (i)

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

- Molecule 1: 16S rRNA

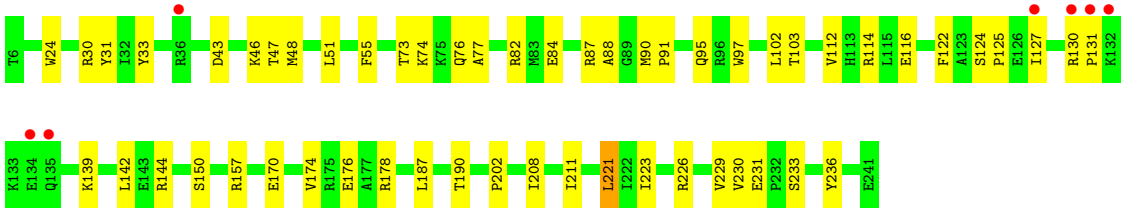
Chain A: 54% 37% 8%





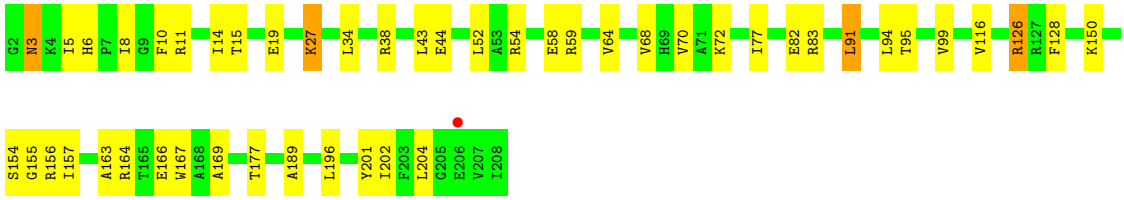
- Molecule 2: 30S ribosomal protein S2

Chain B:



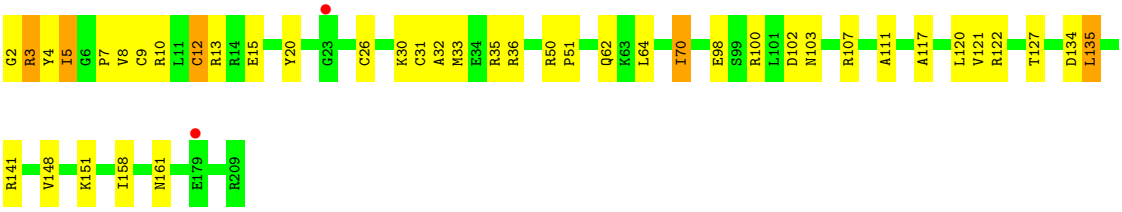
- Molecule 3: 30S ribosomal protein S3

Chain C:



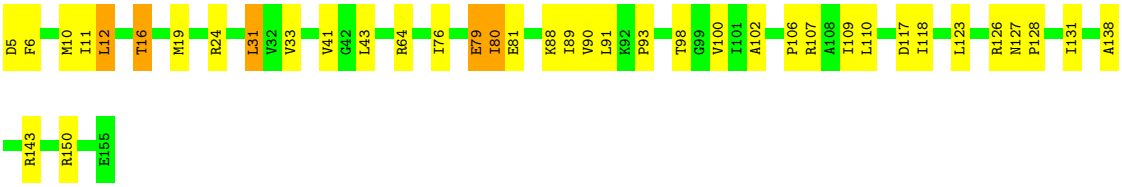
- Molecule 4: 30S ribosomal protein S4

Chain D:



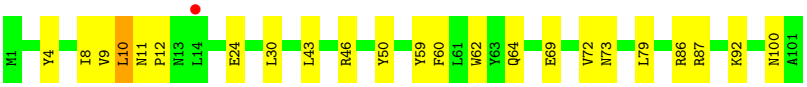
• Molecule 5: 30S ribosomal protein S5

Chain E: 74% 23%



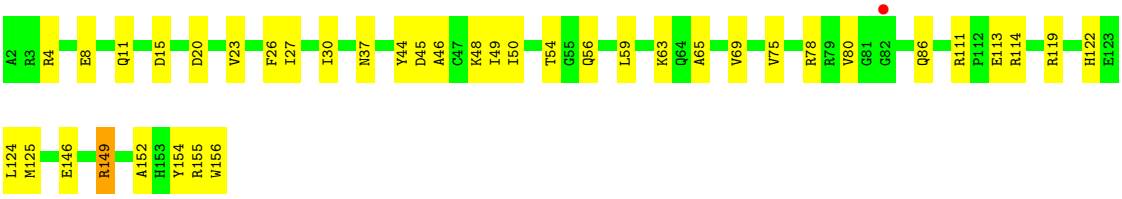
• Molecule 6: 30S ribosomal protein S6

Chain F: % 77% 22%



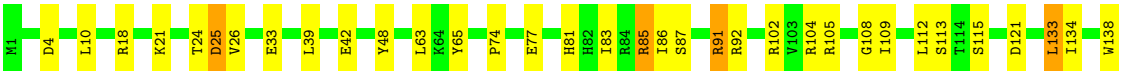
• Molecule 7: 30S ribosomal protein S7

Chain G: % 75% 25%



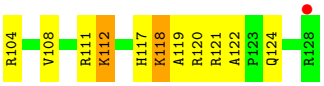
• Molecule 8: 30S ribosomal protein S8

Chain H: 75% 22%



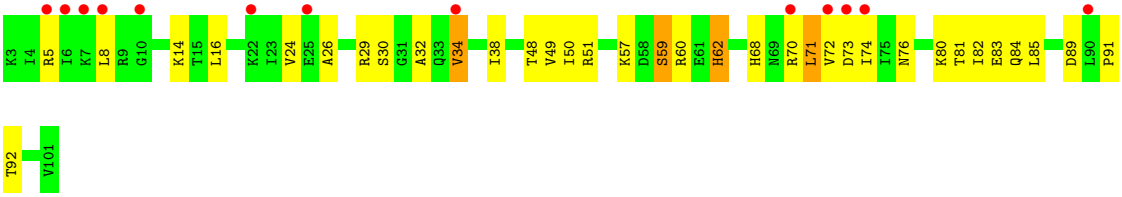
• Molecule 9: 30S ribosomal protein S9

Chain I: 3% 65% 31%



• Molecule 10: 30S ribosomal protein S10

Chain J:

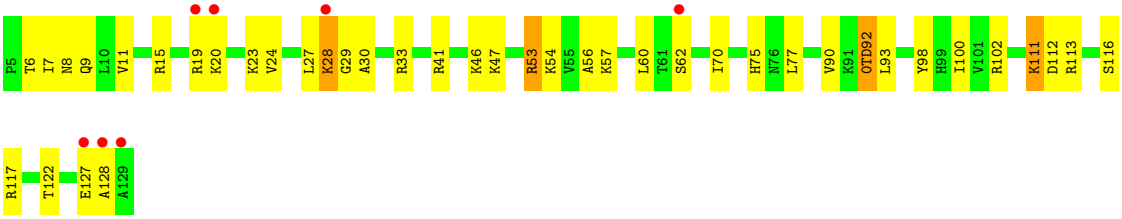


• Molecule 11: 30S ribosomal protein S11

Chain K:

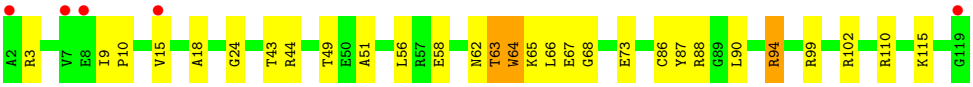
• Molecule 12: 30S ribosomal protein S12

Chain L:



• Molecule 13: 30S ribosomal protein S13

Chain M:

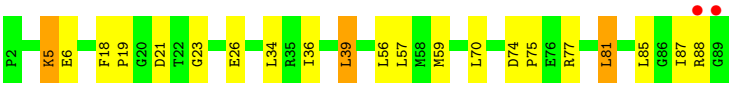


• Molecule 14: 30S ribosomal protein S14 type Z

Chain N:

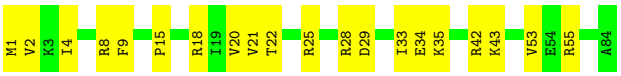
• Molecule 15: 30S ribosomal protein S15

Chain O:



• Molecule 16: 30S ribosomal protein S16

Chain P:



• Molecule 17: 30S ribosomal protein S17

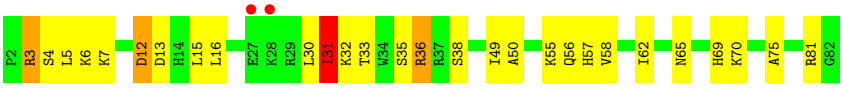
Chain Q:

• Molecule 18: 30S ribosomal protein S18

Chain R:

• Molecule 19: 30S ribosomal protein S19

Chain S:



• Molecule 20: 30S ribosomal protein S20

Chain T:

• Molecule 21: 30S ribosomal protein Thx

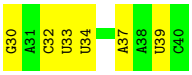
Chain U:

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

Chain a:

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

Chain b:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	401.32Å 401.32Å 175.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.78 – 3.45 49.78 – 3.45	Depositor EDS
% Data completeness (in resolution range)	96.4 (49.78-3.45) 90.7 (49.78-3.45)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.58 (at 3.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1938)	Depositor
R, R_{free}	0.194 , 0.227 0.194 , 0.227	Depositor DCC
R_{free} test set	9121 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	82.3	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 73.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	52822	wwPDB-VP
Average B, all atoms (Å^2)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.89% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PAR, M2G, 2MG, PSU, K, MG, 5MC, 0TD, 4OC, 6MZ, ZN, 70U, 7MG, UR3, 12A, MA6

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	0.48	0/36037	0.83	13/56239 (0.0%)
2	B	0.25	0/1909	0.40	0/2579
3	C	0.28	0/1637	0.43	0/2207
4	D	0.31	0/1733	0.45	1/2318 (0.0%)
5	E	0.33	0/1163	0.50	0/1566
6	F	0.25	0/856	0.40	0/1154
7	G	0.27	0/1276	0.43	0/1709
8	H	0.36	0/1136	0.44	0/1527
9	I	0.27	0/1029	0.44	0/1379
10	J	0.27	0/806	0.48	0/1084
11	K	0.32	0/900	0.47	0/1213
12	L	0.33	0/978	0.50	0/1308
13	M	0.27	0/947	0.43	0/1270
14	N	0.31	0/501	0.41	0/664
15	O	0.26	0/745	0.41	0/992
16	P	0.34	0/717	0.46	0/965
17	Q	0.35	0/836	0.47	0/1117
18	R	0.28	0/604	0.41	0/801
19	S	0.25	0/662	0.49	0/892
20	T	0.29	0/765	0.50	0/1007
21	U	0.26	0/213	0.42	0/279
22	a	0.32	0/111	0.80	0/168
23	b	0.82	1/184 (0.5%)	0.78	0/277
All	All	0.42	1/55745 (0.0%)	0.73	14/82715 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	30	G	OP3-P	-10.52	1.48	1.61

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	254	G	O5'-P-OP1	-7.51	98.94	105.70
1	A	1301	U	P-O3'-C3'	6.86	127.94	119.70
1	A	60	A	P-O3'-C3'	6.17	127.11	119.70
1	A	1528	U	P-O3'-C3'	5.93	126.82	119.70
1	A	328	C	C2-N1-C1'	5.61	124.97	118.80
4	D	12	CYS	CA-CB-SG	5.49	123.88	114.00
1	A	913	A	P-O3'-C3'	5.42	126.20	119.70
1	A	328	C	P-O3'-C3'	5.36	126.14	119.70
1	A	812	C	P-O3'-C3'	5.25	126.00	119.70
1	A	433	C	C2-N1-C1'	5.24	124.56	118.80
1	A	1285	A	P-O3'-C3'	5.09	125.81	119.70
1	A	1065	U	P-O3'-C3'	5.08	125.79	119.70
1	A	108	G	O4'-C1'-N9	5.06	112.25	108.20
1	A	1443	G	P-O3'-C3'	5.03	125.73	119.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32504	0	16434	455	0
2	B	1874	0	1887	29	0
3	C	1613	0	1677	33	0
4	D	1703	0	1763	25	0
5	E	1147	0	1207	25	0
6	F	843	0	857	10	0
7	G	1257	0	1296	20	0
8	H	1116	0	1177	22	0
9	I	1010	0	1037	34	0
10	J	793	0	835	25	0
11	K	885	0	904	10	0
12	L	973	0	1058	31	0
13	M	937	0	995	15	0
14	N	492	0	529	13	0
15	O	734	0	771	11	0
16	P	701	0	720	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	Q	823	0	891	12	0
18	R	598	0	670	9	0
19	S	648	0	672	18	0
20	T	763	0	861	12	0
21	U	209	0	221	5	0
22	a	124	0	67	0	0
23	b	247	0	129	0	0
24	A	252	0	270	13	0
25	A	280	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	1	0	0	0	0
25	H	2	0	0	0	0
25	L	2	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	1	0	0	0	0
25	b	1	0	0	0	0
26	A	44	0	0	0	0
26	E	1	0	0	0	0
26	G	1	0	0	0	0
27	D	1	0	0	0	0
27	N	1	0	0	0	0
28	A	212	0	0	3	0
28	D	2	0	0	1	0
28	E	5	0	0	0	0
28	K	1	0	0	0	0
28	L	4	0	0	0	0
28	O	1	0	0	0	0
28	T	1	0	0	0	0
28	a	1	0	0	0	0
All	All	52822	0	36928	740	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 (740) 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:1028:C:H42	1:A:1033:G:H1	1.13	0.96
1:A:153:C:H42	1:A:168:G:H1	1.20	0.89
1:A:235:C:H5'	17:Q:70:ARG:HG2	1.53	0.88
1:A:48:C:OP1	24:A:1603:PAR:N12	2.07	0.87
1:A:664:G:H22	1:A:741:G:H1	1.22	0.86
1:A:1306:A:H61	1:A:1331:G:H1'	1.39	0.85
11:K:15:ALA:HA	11:K:77:MET:HA	1.61	0.82
1:A:1422:G:N2	1:A:1478:C:N3	2.32	0.78
1:A:442:C:H42	1:A:492:G:H1	1.30	0.77
1:A:1391:U:H2'	1:A:1392:G:C8	2.19	0.77
1:A:677:U:H3	1:A:713:G:H22	1.32	0.76
1:A:1028:C:N4	1:A:1033:G:H1	1.84	0.75
1:A:103:C:OP1	20:T:17:ARG:NH1	2.19	0.74
2:B:223:ILE:HD13	2:B:230:VAL:H	1.52	0.74
20:T:10:LEU:HG	20:T:12:ALA:H	1.53	0.74
13:M:88:ARG:HH11	19:S:3:ARG:HH21	1.33	0.73
19:S:33:THR:HG22	19:S:35:SER:H	1.50	0.73
1:A:951:G:OP2	13:M:102:ARG:NH2	2.22	0.73
1:A:537:G:OP1	12:L:113:ARG:NH2	2.21	0.72
1:A:975:A:H4'	1:A:976:G:H5"	1.71	0.72
7:G:146:GLU:HA	7:G:149:ARG:HG2	1.73	0.71
10:J:82:ILE:HA	10:J:85:LEU:HB2	1.72	0.71
9:I:46:ALA:HB2	9:I:74:ILE:HG23	1.74	0.70
1:A:501:C:OP1	12:L:117:ARG:NH2	2.24	0.70
9:I:44:VAL:HG12	9:I:51:ARG:HH22	1.55	0.70
1:A:413:G:N2	1:A:429:U:OP2	2.24	0.70
1:A:409:G:H1	1:A:433:C:H42	1.40	0.69
10:J:8:LEU:HB2	10:J:70:ARG:HB2	1.75	0.69
3:C:14:ILE:HG22	3:C:15:THR:HG23	1.73	0.69
1:A:673:G:H2'	1:A:674:G:C8	2.27	0.69
1:A:153:C:N4	1:A:168:G:H1	1.89	0.69
1:A:974:A:OP2	14:N:41:ARG:NH1	2.26	0.69
1:A:1502:A:H2	1:A:1505:G:H1	1.39	0.69
1:A:713:G:H2'	1:A:714:G:C8	2.28	0.69
1:A:1162:C:H42	1:A:1174:G:H1	1.39	0.69
1:A:1435:G:H2'	1:A:1436:U:C6	2.29	0.68
1:A:1391:U:H2'	1:A:1392:G:H8	1.59	0.68
1:A:1249:C:O2'	9:I:73:GLN:NE2	2.26	0.68
9:I:51:ARG:HG3	9:I:56:LEU:HD21	1.73	0.68
4:D:32:ALA:HA	4:D:35:ARG:HG2	1.75	0.68
8:H:10:LEU:HD22	8:H:83:ILE:HD11	1.74	0.68
13:M:10:PRO:HB2	13:M:18:ALA:HB1	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1004:A:OP1	1:A:1025:U:N3	2.25	0.68
1:A:1422:G:H1	1:A:1478:C:H42	1.40	0.67
4:D:102:ASP:OD1	4:D:103:ASN:N	2.26	0.67
19:S:36:ARG:NH2	19:S:75:ALA:O	2.28	0.66
1:A:1086:U:H3	1:A:1099:G:H22	1.42	0.66
3:C:156:ARG:H	3:C:163:ALA:HA	1.60	0.66
5:E:80:ILE:HD12	5:E:91:LEU:HB2	1.76	0.66
1:A:1306:A:N6	1:A:1331:G:H1'	2.08	0.66
1:A:60:A:H4'	1:A:61:G:O5'	1.96	0.66
3:C:64:VAL:HB	3:C:99:VAL:HG21	1.78	0.65
1:A:1200:C:O2'	1:A:1205:U:O4	2.13	0.65
1:A:1427:U:H2'	1:A:1428:A:H8	1.61	0.65
4:D:7:PRO:HB2	4:D:10:ARG:HD2	1.78	0.65
1:A:21:G:H2'	1:A:22:G:C8	2.31	0.65
3:C:11:ARG:NH1	3:C:177:THR:O	2.29	0.65
1:A:1152:A:OP1	10:J:68:HIS:ND1	2.30	0.65
1:A:1250:A:H2'	1:A:1251:A:C8	2.32	0.64
17:Q:66:SER:O	17:Q:70:ARG:NH1	2.31	0.64
6:F:10:LEU:HD12	6:F:59:TYR:HB3	1.80	0.64
14:N:11:LYS:HG3	14:N:13:THR:H	1.61	0.64
1:A:984:C:H42	1:A:1221:G:H1	1.46	0.64
1:A:1347:G:O6	9:I:10:ARG:NH2	2.28	0.64
10:J:48:THR:HA	10:J:62:HIS:HB3	1.80	0.64
1:A:756:C:N4	28:A:2075:HOH:O	2.30	0.64
1:A:1345:U:OP1	9:I:120:ARG:NH1	2.31	0.64
9:I:9:ARG:HG2	9:I:14:VAL:HG12	1.78	0.64
12:L:53:ARG:NH1	12:L:92:0TD:OD2	2.31	0.64
16:P:4:ILE:HG12	16:P:21:VAL:HG22	1.80	0.63
3:C:70:VAL:HG12	3:C:72:LYS:H	1.63	0.63
1:A:201:C:H42	1:A:216:G:H1	1.46	0.62
1:A:652:U:O4	1:A:752:G:O2'	2.17	0.62
1:A:1281:U:H5"	1:A:1282:C:H5	1.64	0.62
1:A:674:G:H2'	1:A:675:A:H8	1.64	0.62
3:C:64:VAL:HG23	3:C:99:VAL:HG11	1.81	0.62
1:A:1026:G:H3'	1:A:1027:C:H5"	1.81	0.62
1:A:1147:C:O2'	9:I:5:TYR:OH	2.17	0.62
1:A:662:G:N7	24:A:1604:PAR:N12	2.48	0.62
13:M:65:LYS:NZ	13:M:73:GLU:OE2	2.33	0.62
1:A:1286:A:H2'	1:A:1287:A:H4'	1.81	0.62
1:A:269:C:H2'	1:A:270:A:H8	1.65	0.61
8:H:86:ILE:HD12	8:H:133:LEU:HD22	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1122:U:O4	1:A:1123:A:N6	2.33	0.61
1:A:542:G:OP1	4:D:10:ARG:NH2	2.33	0.61
1:A:1137:C:H4'	1:A:1138:G:C2	2.35	0.61
5:E:81:GLU:HG3	5:E:90:VAL:HG22	1.81	0.61
7:G:54:THR:HG22	7:G:56:GLN:H	1.64	0.61
9:I:25:LYS:N	9:I:60:ASP:OD1	2.34	0.61
1:A:1301:U:HO2'	1:A:1302:U:P	2.23	0.61
1:A:201:C:N3	1:A:216:G:N2	2.37	0.60
1:A:1003:G:N2	1:A:1039:C:O2	2.34	0.60
1:A:1301:U:O2'	1:A:1302:U:O5'	2.18	0.60
24:A:1602:PAR:H23	24:A:1602:PAR:HN21	1.67	0.60
9:I:97:LYS:HA	9:I:102:LEU:HD11	1.84	0.60
10:J:49:VAL:HG23	14:N:41:ARG:HB2	1.82	0.60
19:S:50:ALA:HB1	19:S:57:HIS:HB3	1.83	0.60
2:B:48:MET:HA	2:B:51:LEU:HB2	1.81	0.60
1:A:51:A:OP2	24:A:1603:PAR:N24	2.35	0.60
3:C:189:ALA:HB3	3:C:196:LEU:HB2	1.83	0.60
1:A:427:U:OP1	4:D:13:ARG:NH2	2.33	0.60
1:A:1356:G:H2'	1:A:1357:A:C8	2.37	0.60
20:T:75:ASN:OD1	20:T:75:ASN:N	2.34	0.60
1:A:1313:U:O4	19:S:4:SER:OG	2.18	0.60
1:A:1435:G:H2'	1:A:1436:U:H6	1.66	0.60
1:A:714:G:H2'	1:A:715:A:C8	2.37	0.59
1:A:243:A:H4'	1:A:244:U:H5'	1.84	0.59
1:A:1402:4OC:HM22	1:A:1403:C:H5'	1.84	0.59
19:S:55:LYS:HG2	19:S:56:GLN:HG3	1.84	0.59
2:B:77:ALA:HB2	2:B:211:ILE:HD13	1.84	0.59
5:E:33:VAL:HG22	5:E:43:LEU:HD23	1.83	0.59
15:O:87:ILE:HG22	15:O:88:ARG:H	1.67	0.59
3:C:44:GLU:HG2	3:C:52:LEU:HD11	1.84	0.59
1:A:1323:G:H2'	1:A:1324:A:C8	2.38	0.59
1:A:442:C:N4	1:A:492:G:H1	2.00	0.58
1:A:1010:G:H2'	1:A:1011:G:H8	1.68	0.58
1:A:1222:G:OP2	1:A:1322:C:N4	2.31	0.58
15:O:26:GLU:HA	15:O:81:LEU:HD11	1.85	0.58
1:A:279:A:OP2	17:Q:95:TYR:OH	2.19	0.58
1:A:1504:G:OP1	1:A:1507:A:H4'	2.03	0.58
10:J:89:ASP:HB2	10:J:91:PRO:HD2	1.86	0.58
1:A:28:G:O2'	1:A:296:U:OP1	2.21	0.58
3:C:157:ILE:HD13	3:C:166:GLU:HB2	1.85	0.58
6:F:9:VAL:HB	6:F:87:ARG:HB2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1520:G:H2'	1:A:1521:G:H8	1.69	0.57
7:G:78:ARG:NH1	7:G:154:TYR:O	2.37	0.57
17:Q:67:LYS:HA	17:Q:70:ARG:HH12	1.69	0.57
1:A:390:C:H2'	1:A:391:G:C8	2.39	0.57
5:E:98:THR:HB	5:E:117:ASP:HB3	1.85	0.57
1:A:250:A:H4'	1:A:251:G:O5'	2.03	0.57
1:A:1143:G:H2'	1:A:1144:G:C8	2.38	0.57
1:A:1392:G:H21	1:A:1502:A:H8	1.50	0.57
20:T:10:LEU:HD12	20:T:11:SER:H	1.69	0.57
1:A:241:C:H4'	12:L:19:ARG:HH22	1.70	0.57
1:A:266:G:H5'	1:A:268:C:H41	1.68	0.57
7:G:122:HIS:HA	7:G:125:MET:HE2	1.86	0.57
1:A:1343:G:H2'	1:A:1344:C:C6	2.40	0.57
4:D:141:ARG:NH2	28:D:401:HOH:O	2.36	0.57
5:E:12:LEU:HD13	5:E:31:LEU:HB2	1.86	0.57
1:A:1250:A:H4'	9:I:68:GLY:N	2.20	0.57
3:C:155:GLY:HA2	3:C:164:ARG:H	1.70	0.57
1:A:765:G:N2	1:A:813:U:OP2	2.36	0.56
1:A:811:C:O2'	1:A:901:A:N1	2.37	0.56
1:A:946:A:H2'	1:A:947:G:C8	2.40	0.56
1:A:1124:G:N7	1:A:1145:C:O2'	2.30	0.56
1:A:1291:G:H4'	9:I:39:GLY:HA3	1.86	0.56
4:D:98:GLU:OE2	4:D:107:ARG:NE	2.30	0.56
3:C:6:HIS:HD2	3:C:8:ILE:H	1.51	0.56
1:A:1494:G:OP1	24:A:1601:PAR:N32	2.39	0.56
8:H:42:GLU:HG3	8:H:109:ILE:HD13	1.87	0.56
1:A:646:U:H2'	1:A:647:C:C6	2.40	0.56
1:A:114:U:H5"	24:A:1603:PAR:H52	1.86	0.56
2:B:174:VAL:O	2:B:178:ARG:HG2	2.05	0.56
3:C:19:GLU:HG2	3:C:54:ARG:HE	1.71	0.56
5:E:80:ILE:HD13	5:E:138:ALA:HB1	1.87	0.56
2:B:88:ALA:HB1	2:B:226:ARG:HH21	1.71	0.56
3:C:3:ASN:OD1	3:C:3:ASN:N	2.38	0.56
5:E:102:ALA:O	5:E:107:ARG:NH1	2.38	0.55
17:Q:68:ARG:O	17:Q:68:ARG:HG3	2.06	0.55
1:A:17:U:H2'	1:A:18:C:C6	2.41	0.55
1:A:619:U:N3	4:D:134:ASP:OD1	2.27	0.55
11:K:110:ASP:OD2	18:R:88:LYS:NZ	2.39	0.55
1:A:372:C:H4'	1:A:373:A:O5'	2.06	0.55
1:A:1071:C:H42	1:A:1104:G:H1	1.54	0.55
1:A:1510:U:H2'	1:A:1511:G:C8	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:56:ALA:HB2	12:L:70:ILE:HD11	1.87	0.55
1:A:390:C:O3'	16:P:28:ARG:NH2	2.40	0.55
10:J:57:LYS:HE2	10:J:60:ARG:NH2	2.21	0.55
1:A:975:A:H5'	1:A:975:A:H8	1.72	0.55
1:A:1326:C:OP1	21:U:12:LYS:NZ	2.39	0.55
4:D:111:ALA:HB2	4:D:120:LEU:HD12	1.88	0.55
10:J:57:LYS:HG3	10:J:60:ARG:HH21	1.72	0.55
1:A:523:A:N6	12:L:92:0TD:OD1	2.40	0.55
1:A:918:A:H2'	1:A:919:A:C8	2.42	0.55
20:T:67:ALA:O	20:T:73:HIS:ND1	2.40	0.55
1:A:1287:A:H2'	1:A:1288:A:C8	2.41	0.54
13:M:88:ARG:NH1	19:S:3:ARG:HH21	2.04	0.54
13:M:49:THR:HG22	13:M:51:ALA:H	1.72	0.54
18:R:32:ARG:HA	18:R:69:THR:HG21	1.89	0.54
1:A:864:A:H2'	1:A:865:A:C8	2.42	0.54
12:L:75:HIS:HA	12:L:102:ARG:HH22	1.72	0.54
1:A:1057:G:H5"	3:C:154:SER:HB2	1.90	0.54
2:B:33:TYR:HB2	2:B:43:ASP:HA	1.89	0.54
1:A:983:A:O2'	1:A:1050:G:OP2	2.26	0.54
1:A:1392:G:N2	1:A:1502:A:H8	2.05	0.54
5:E:110:LEU:HD13	5:E:118:ILE:HG21	1.89	0.54
13:M:63:THR:HG23	13:M:64:TRP:H	1.73	0.54
1:A:1049:U:H4'	1:A:1050:G:O5'	2.07	0.54
10:J:51:ARG:HB2	10:J:59:SER:HB2	1.90	0.54
14:N:27:CYS:SG	14:N:29:ARG:HB2	2.48	0.54
3:C:58:GLU:HB3	10:J:92:THR:HG21	1.90	0.53
8:H:18:ARG:NH2	8:H:81:HIS:O	2.42	0.53
1:A:1266:G:N2	1:A:1269:A:OP2	2.35	0.53
12:L:24:VAL:HG13	12:L:98:TYR:HE1	1.72	0.53
1:A:559:A:OP1	5:E:126:ARG:NH2	2.34	0.53
9:I:28:VAL:HG22	9:I:63:ILE:HB	1.90	0.53
1:A:262:A:H2'	1:A:263:A:C8	2.44	0.53
1:A:580:U:H2'	1:A:581:G:O4'	2.09	0.53
1:A:390:C:H2'	1:A:391:G:H8	1.72	0.53
1:A:1187:G:O2'	9:I:111:ARG:NH1	2.42	0.53
1:A:1349:A:OP2	9:I:118:LYS:NZ	2.42	0.53
7:G:15:ASP:HB3	7:G:20:ASP:H	1.75	0.52
1:A:1288:A:H2'	1:A:1289:A:C8	2.45	0.52
5:E:79:GLU:O	8:H:104:ARG:NH1	2.41	0.52
1:A:1314:C:H2'	1:A:1315:U:H6	1.75	0.52
1:A:835:U:OP1	18:R:64:ARG:NH2	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1035:A:H2'	1:A:1036:G:H8	1.73	0.52
5:E:79:GLU:HG3	5:E:93:PRO:HD2	1.91	0.52
14:N:9:LYS:HD3	14:N:21:TYR:O	2.09	0.52
1:A:190(J):U:H2'	1:A:190(K):G:H8	1.74	0.52
14:N:24:CYS:SG	14:N:40:CYS:N	2.82	0.52
1:A:35:G:H2'	1:A:36:C:C6	2.45	0.52
1:A:477:G:H2'	1:A:478:A:H8	1.75	0.52
1:A:1425:U:H3	1:A:1475:G:H1	1.58	0.52
24:A:1601:PAR:O44	24:A:1601:PAR:N64	2.42	0.52
8:H:85:ARG:NE	8:H:87:SER:O	2.43	0.52
1:A:1016:A:H2'	1:A:1017:G:O4'	2.10	0.52
1:A:1163:C:H2'	1:A:1164:G:H8	1.75	0.52
1:A:1062:U:H2'	1:A:1063:C:C6	2.44	0.52
1:A:1128:C:N3	1:A:1144:G:N2	2.58	0.51
1:A:1245:A:H2'	1:A:1246:C:C6	2.45	0.51
1:A:1371:G:O3'	9:I:69:GLY:HA3	2.10	0.51
7:G:15:ASP:OD1	7:G:44:TYR:OH	2.26	0.51
7:G:113:GLU:HB2	7:G:119:ARG:HG3	1.91	0.51
8:H:21:LYS:O	8:H:65:TYR:OH	2.17	0.51
12:L:41:ARG:HH21	12:L:57:LYS:NZ	2.08	0.51
1:A:1162:C:N4	1:A:1174:G:H1	2.07	0.51
5:E:88:LYS:HB3	5:E:123:LEU:HB2	1.91	0.51
1:A:1015:A:H2'	1:A:1016:A:C8	2.46	0.51
1:A:524:G:H2'	1:A:525:C:C6	2.45	0.51
1:A:116:A:H5"	28:A:2018:HOH:O	2.10	0.51
1:A:501:C:H2'	1:A:502:G:H8	1.75	0.51
16:P:22:THR:HA	16:P:33:ILE:HG13	1.92	0.51
1:A:1095:U:H2'	1:A:1096:C:C6	2.46	0.51
2:B:84:GLU:OE2	2:B:233:SER:OG	2.20	0.51
2:B:122:PHE:HA	2:B:127:ILE:HG12	1.91	0.51
2:B:124:SER:HB2	2:B:125:PRO:HD2	1.93	0.51
7:G:75:VAL:HG21	7:G:86:GLN:HB3	1.93	0.51
10:J:26:ALA:O	10:J:84:GLN:NE2	2.44	0.51
1:A:1262:C:H42	1:A:1273:G:H1	1.59	0.51
1:A:24:U:OP1	12:L:23:LYS:NZ	2.37	0.51
1:A:750:G:N3	15:O:23:GLY:HA3	2.26	0.51
1:A:999:C:H2'	1:A:1000:U:C6	2.46	0.51
1:A:1505:G:O2'	1:A:1506:U:OP2	2.27	0.51
9:I:8:GLY:HA2	9:I:79:LEU:HD13	1.92	0.51
1:A:976:G:H5'	1:A:1358:U:O2'	2.10	0.50
1:A:1443:G:H4'	1:A:1446:A:O5'	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:73:THR:HG23	2:B:95:GLN:O	2.11	0.50
5:E:102:ALA:HB1	5:E:106:PRO:HG2	1.93	0.50
7:G:46:ALA:O	7:G:50:ILE:HG12	2.11	0.50
1:A:1475:G:H2'	1:A:1476:G:H8	1.76	0.50
1:A:1498:UR3:OP2	1:A:1542:U:O2'	2.27	0.50
3:C:64:VAL:H	3:C:99:VAL:HB	1.77	0.50
5:E:98:THR:N	5:E:117:ASP:OD2	2.44	0.50
1:A:192:U:H2'	1:A:193:C:H6	1.77	0.50
1:A:192:U:H1'	20:T:103:GLY:HA2	1.92	0.50
1:A:359:U:H2'	1:A:360:A:H8	1.76	0.50
10:J:24:VAL:HG13	10:J:34:VAL:HG11	1.93	0.50
1:A:190(K):G:H2'	1:A:190(L):U:H6	1.75	0.50
2:B:97:TRP:HZ2	2:B:102:LEU:HD13	1.77	0.50
9:I:112:LYS:HE3	9:I:117:HIS:O	2.11	0.50
10:J:29:ARG:NH1	10:J:84:GLN:OE1	2.44	0.50
19:S:13:ASP:HA	19:S:16:LEU:HB3	1.93	0.50
1:A:241:C:H4'	12:L:19:ARG:NH2	2.26	0.50
1:A:639:G:H2'	1:A:640:A:H8	1.75	0.50
1:A:973:G:H3'	1:A:974:A:H5"	1.94	0.50
2:B:223:ILE:HD13	2:B:230:VAL:N	2.24	0.50
8:H:24:THR:HG22	8:H:63:LEU:HD21	1.94	0.50
1:A:603:U:H2'	1:A:604:G:H8	1.77	0.50
1:A:646:U:H2'	1:A:647:C:H6	1.75	0.50
1:A:1513:A:H2'	1:A:1514:C:C6	2.47	0.50
11:K:27:ASN:OD1	11:K:28:THR:N	2.45	0.50
13:M:86:CYS:SG	13:M:87:TYR:N	2.84	0.50
1:A:1002:G:H2'	1:A:1003:G:C8	2.47	0.50
5:E:143:ARG:NH1	8:H:77:GLU:OE2	2.43	0.50
10:J:32:ALA:HB2	10:J:76:ASN:HB2	1.94	0.50
1:A:1132:C:H2'	1:A:1133:G:H8	1.77	0.49
1:A:1352:C:OP1	21:U:3:LYS:NZ	2.29	0.49
3:C:34:LEU:HG	14:N:25:VAL:HG21	1.93	0.49
1:A:1287:A:H2	1:A:1353:G:H1'	1.77	0.49
24:A:1602:PAR:H23	24:A:1602:PAR:N21	2.27	0.49
8:H:25:ASP:N	8:H:25:ASP:OD1	2.44	0.49
1:A:736:C:H2'	1:A:737:A:C8	2.47	0.49
13:M:90:LEU:O	13:M:94:ARG:HG2	2.13	0.49
1:A:1343:G:H4'	9:I:122:ALA:HB3	1.94	0.49
10:J:48:THR:O	14:N:34:TYR:OH	2.30	0.49
1:A:976:G:OP2	1:A:1358:U:O2'	2.26	0.49
5:E:80:ILE:HG23	8:H:104:ARG:HH22	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:C:H2'	1:A:273:A:H8	1.78	0.49
1:A:501:C:H2'	1:A:502:G:C8	2.47	0.49
1:A:558:G:OP2	1:A:559:A:O2'	2.28	0.49
1:A:614:A:H2'	1:A:615:C:C6	2.48	0.49
1:A:1178:G:OP1	9:I:93:ARG:NH1	2.45	0.49
1:A:335:C:H2'	1:A:336:C:C6	2.48	0.49
2:B:47:THR:HA	2:B:202:PRO:HG2	1.94	0.49
15:O:39:LEU:HD13	15:O:56:LEU:HB2	1.94	0.49
1:A:743:U:H2'	1:A:744:C:C6	2.48	0.49
1:A:1157:A:C2	1:A:1181:G:C4	3.00	0.49
1:A:1219:U:P	14:N:19:ARG:HH22	2.36	0.49
2:B:73:THR:N	2:B:170:GLU:OE1	2.37	0.49
3:C:5:ILE:HD13	3:C:10:PHE:HB2	1.94	0.49
3:C:38:ARG:HB3	3:C:94:LEU:HD21	1.94	0.49
12:L:41:ARG:HH21	12:L:57:LYS:HZ1	1.61	0.49
1:A:851:G:H2'	1:A:852:G:H8	1.77	0.49
1:A:1256:A:HO2'	1:A:1257:U:P	2.36	0.49
8:H:108:GLY:HA3	8:H:138:TRP:HB3	1.94	0.49
1:A:45:U:H2'	1:A:46:G:C8	2.48	0.48
1:A:920:U:H2'	1:A:921:U:C6	2.47	0.48
1:A:1189:C:OP1	10:J:51:ARG:NH2	2.34	0.48
17:Q:83:ASP:OD1	17:Q:83:ASP:N	2.46	0.48
1:A:59:A:H1'	1:A:354:G:N2	2.28	0.48
24:A:1604:PAR:O53	24:A:1604:PAR:N21	2.43	0.48
8:H:121:ASP:OD1	8:H:121:ASP:N	2.44	0.48
10:J:51:ARG:HG3	10:J:60:ARG:O	2.14	0.48
1:A:186:C:H2'	1:A:187:C:C6	2.48	0.48
1:A:186:C:H2'	1:A:187:C:H6	1.78	0.48
1:A:737:A:H2'	1:A:738:C:H6	1.78	0.48
1:A:1218:C:H2'	1:A:1219:U:C6	2.49	0.48
1:A:1288:A:H2'	1:A:1289:A:H8	1.78	0.48
1:A:1298:C:H4'	1:A:1299:A:C4	2.49	0.48
1:A:1347:G:O2'	1:A:1348:U:P	2.71	0.48
9:I:50:LEU:HB3	9:I:56:LEU:H	1.79	0.48
1:A:456:C:H42	1:A:476:G:H1	1.61	0.48
1:A:538:G:H2'	1:A:539:A:H8	1.77	0.48
3:C:59:ARG:HG2	3:C:64:VAL:HG22	1.96	0.48
21:U:6:ARG:HB2	21:U:15:ARG:NH1	2.28	0.48
1:A:105:G:H2'	1:A:106:C:C6	2.48	0.48
7:G:23:VAL:O	7:G:27:ILE:HG12	2.13	0.48
1:A:737:A:H2'	1:A:738:C:C6	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1001:A:H2'	1:A:1002:G:C8	2.49	0.48
1:A:1072:G:H2'	1:A:1073:U:C6	2.48	0.48
1:A:523:A:H61	12:L:92:0TD:CG	2.27	0.48
1:A:966:M2G:H8	1:A:966:M2G:OP2	1.97	0.48
1:A:427:U:OP2	4:D:36:ARG:NH2	2.40	0.48
1:A:767:A:O2'	1:A:1524:C:O2	2.27	0.48
3:C:116:VAL:HG21	3:C:202:ILE:HD11	1.96	0.48
4:D:70:ILE:HD11	4:D:100:ARG:CZ	2.44	0.48
19:S:3:ARG:HH22	19:S:69:HIS:CE1	2.32	0.48
1:A:344:A:H5'	1:A:345:C:C5	2.49	0.47
1:A:434:U:H2'	1:A:435:C:C6	2.49	0.47
1:A:1028:C:H2'	1:A:1029:C:H6	1.78	0.47
3:C:27:LYS:HD3	3:C:27:LYS:H	1.79	0.47
6:F:8:ILE:HD11	6:F:79:LEU:HD13	1.96	0.47
1:A:360:A:N6	24:A:1603:PAR:H44	2.30	0.47
1:A:190(K):G:H2'	1:A:190(L):U:C6	2.49	0.47
1:A:642:A:C8	8:H:115:SER:HA	2.50	0.47
10:J:5:ARG:HA	10:J:73:ASP:OD1	2.14	0.47
1:A:382:A:H2'	1:A:383:A:C8	2.49	0.47
1:A:610:G:OP1	24:A:1605:PAR:N64	2.48	0.47
1:A:1320:C:O2	19:S:36:ARG:NH1	2.47	0.47
8:H:113:SER:HB2	8:H:134:ILE:HD11	1.96	0.47
9:I:32:ASP:OD1	9:I:33:PHE:N	2.47	0.47
11:K:72:ALA:HB1	11:K:77:MET:HE2	1.96	0.47
1:A:384:G:H2'	1:A:385:C:C6	2.50	0.47
1:A:1154:G:H2'	1:A:1155:G:H8	1.79	0.47
1:A:1520:G:H2'	1:A:1521:G:C8	2.49	0.47
9:I:15:ALA:HB2	9:I:65:VAL:HG13	1.96	0.47
16:P:34:GLU:OE2	16:P:55:ARG:HD3	2.15	0.47
1:A:1131:G:H2'	1:A:1132:C:C6	2.49	0.47
1:A:1179:A:O2'	1:A:1180:A:OP1	2.33	0.47
4:D:121:VAL:O	4:D:134:ASP:HA	2.15	0.47
1:A:266:G:O3'	17:Q:67:LYS:HB2	2.15	0.47
1:A:1028:C:N3	1:A:1033:G:N2	2.50	0.47
1:A:776:G:N2	1:A:802:A:OP2	2.39	0.47
1:A:1292:U:H2'	1:A:1293:G:C8	2.50	0.47
1:A:1399:C:C2	1:A:1502:A:N6	2.83	0.47
4:D:9:CYS:O	4:D:12:CYS:HB2	2.15	0.47
1:A:975:A:H5'	1:A:975:A:C8	2.49	0.47
1:A:1399:C:H4'	1:A:1400:5MC:H5"	1.97	0.47
1:A:1466:C:H2'	1:A:1467:G:O4'	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:46:GLU:CD	18:R:46:GLU:H	2.17	0.47
1:A:1168:A:H2'	1:A:1169:A:C8	2.49	0.46
1:A:1427:U:H2'	1:A:1428:A:C8	2.45	0.46
10:J:32:ALA:O	10:J:34:VAL:HG23	2.16	0.46
1:A:359:U:H2'	1:A:360:A:C8	2.50	0.46
1:A:545:C:OP2	4:D:62:GLN:NE2	2.48	0.46
1:A:560:U:H5'	1:A:566:G:C2	2.50	0.46
1:A:1148:U:H2'	1:A:1149:C:O4'	2.16	0.46
1:A:1369:C:H2'	1:A:1370:G:C8	2.50	0.46
15:O:26:GLU:OE1	15:O:77:ARG:HD2	2.14	0.46
19:S:31:ILE:HG22	19:S:49:ILE:HA	1.98	0.46
1:A:190(J):U:H2'	1:A:190(K):G:C8	2.50	0.46
1:A:399:G:H2'	1:A:400:C:C6	2.51	0.46
14:N:27:CYS:HB3	14:N:43:CYS:SG	2.54	0.46
18:R:47:THR:HG22	18:R:48:GLY:H	1.81	0.46
1:A:44:G:N2	1:A:399:G:C4	2.83	0.46
1:A:1238:A:N7	1:A:1303:C:H1'	2.30	0.46
1:A:1367:C:OP2	9:I:112:LYS:NZ	2.47	0.46
1:A:1372:U:H2'	1:A:1373:G:O4'	2.15	0.46
1:A:1477:C:H2'	1:A:1478:C:H6	1.80	0.46
4:D:148:VAL:HG11	4:D:158:ILE:HD13	1.97	0.46
5:E:33:VAL:HG11	5:E:109:ILE:HA	1.96	0.46
18:R:51:LEU:HA	18:R:52:PRO:HD3	1.80	0.46
1:A:148:G:H2'	1:A:149:A:C8	2.50	0.46
1:A:662:G:H2'	1:A:663:A:C8	2.50	0.46
1:A:1118:C:H1'	1:A:1179:A:C5	2.51	0.46
2:B:103:THR:HG23	2:B:176:GLU:OE1	2.16	0.46
21:U:5:ASP:O	21:U:11:GLY:HA3	2.16	0.46
1:A:321:A:H2'	1:A:322:C:H6	1.81	0.46
1:A:509:A:N3	1:A:543:C:O2'	2.42	0.46
1:A:851:G:H2'	1:A:852:G:C8	2.51	0.46
1:A:895:G:H2'	1:A:896:C:C6	2.49	0.46
1:A:1086:U:H3	1:A:1099:G:N2	2.12	0.46
3:C:155:GLY:HA3	3:C:163:ALA:HB1	1.98	0.46
1:A:337:C:H2'	1:A:338:A:H8	1.81	0.46
1:A:708:C:OP1	11:K:85:ARG:NH2	2.41	0.46
1:A:1264:C:H2'	1:A:1265:G:H8	1.81	0.46
1:A:1507:A:H2'	1:A:1508:G:C8	2.51	0.46
9:I:8:GLY:HA3	9:I:79:LEU:HB3	1.97	0.46
19:S:30:LEU:HB3	19:S:31:ILE:H	1.41	0.46
1:A:530:G:HO2'	1:A:531:U:P	2.38	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:547:A:OP2	4:D:2:GLY:N	2.48	0.46
2:B:55:PHE:HD2	2:B:221:LEU:HG	1.80	0.46
4:D:151:LYS:H	4:D:151:LYS:HD2	1.80	0.46
5:E:100:VAL:O	5:E:107:ARG:NH2	2.47	0.46
1:A:450:G:OP1	16:P:43:LYS:NZ	2.49	0.46
1:A:984:C:N4	1:A:1221:G:H1	2.13	0.46
3:C:68:VAL:HG12	3:C:70:VAL:HG23	1.97	0.46
4:D:3:ARG:NH2	4:D:5:ILE:HD11	2.31	0.46
1:A:848:C:H2'	1:A:849:C:H6	1.80	0.46
1:A:1292:U:H2'	1:A:1293:G:H8	1.80	0.46
17:Q:10:VAL:HG13	17:Q:19:VAL:HB	1.98	0.46
1:A:658:G:H2'	1:A:659:U:H6	1.80	0.45
6:F:50:TYR:CE2	18:R:77:GLY:HA2	2.52	0.45
21:U:6:ARG:HB2	21:U:15:ARG:HH12	1.82	0.45
1:A:190(D):U:O2'	1:A:190(E):U:H5'	2.16	0.45
1:A:620:C:C2	4:D:135:LEU:HD22	2.51	0.45
1:A:965:A:H4'	1:A:966:M2G:OP1	2.14	0.45
1:A:56:U:H2'	1:A:57:G:H8	1.80	0.45
1:A:954:G:H2'	1:A:955:U:C6	2.51	0.45
1:A:1190:G:OP1	3:C:5:ILE:HG13	2.16	0.45
1:A:1244:C:H42	1:A:1293:G:H1	1.63	0.45
3:C:150:LYS:HB3	3:C:201:TYR:HB2	1.97	0.45
8:H:4:ASP:OD2	8:H:85:ARG:NH1	2.50	0.45
9:I:7:THR:HB	9:I:83:ARG:HH11	1.82	0.45
1:A:922:G:C6	1:A:923:A:C6	3.05	0.45
1:A:1342:C:H2'	1:A:1343:G:C8	2.51	0.45
15:O:56:LEU:HA	15:O:59:MET:HE2	1.98	0.45
1:A:219:C:C4	1:A:220:G:C8	3.04	0.45
1:A:769:G:H4'	1:A:1513:A:H4'	1.98	0.45
1:A:1073:U:C2	1:A:1074:G:C8	3.04	0.45
1:A:1219:U:OP1	14:N:19:ARG:NH2	2.33	0.45
3:C:70:VAL:HG12	3:C:72:LYS:N	2.30	0.45
4:D:111:ALA:HA	4:D:161:ASN:ND2	2.31	0.45
7:G:78:ARG:HG2	7:G:80:VAL:HG23	1.99	0.45
15:O:85:LEU:HD23	15:O:85:LEU:HA	1.81	0.45
1:A:110:C:O2'	16:P:25:ARG:O	2.34	0.45
1:A:316:G:OP2	1:A:351:G:O2'	2.35	0.45
1:A:436:C:H2'	1:A:437:U:H6	1.82	0.45
1:A:538:G:H2'	1:A:539:A:C8	2.52	0.45
1:A:628:G:H2'	1:A:629:G:C8	2.51	0.45
1:A:1342:C:H2'	1:A:1343:G:H8	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:50:ALA:HA	19:S:58:VAL:O	2.17	0.45
1:A:360:A:H61	24:A:1603:PAR:H44	1.81	0.45
1:A:539:A:H2'	1:A:540:G:C8	2.52	0.45
6:F:62:TRP:CH2	6:F:64:GLN:HB2	2.52	0.45
19:S:12:ASP:HB2	19:S:38:SER:HB3	1.99	0.45
20:T:53:LEU:O	20:T:57:ARG:HD2	2.17	0.45
1:A:939:G:H2'	1:A:940:C:C6	2.52	0.45
7:G:26:PHE:CE2	7:G:30:ILE:HD11	2.52	0.45
9:I:8:GLY:H	9:I:83:ARG:NH1	2.15	0.45
1:A:902:G:H2'	1:A:903:G:H8	1.82	0.45
2:B:178:ARG:NH2	8:H:74:PRO:HB3	2.32	0.45
16:P:8:ARG:NH2	16:P:15:PRO:HB3	2.31	0.45
1:A:384:G:H2'	1:A:385:C:H6	1.80	0.44
1:A:434:U:H2'	1:A:435:C:H6	1.82	0.44
1:A:999:C:H2'	1:A:1000:U:H6	1.82	0.44
1:A:1074:G:O2'	2:B:103:THR:OG1	2.35	0.44
1:A:1320:C:N3	19:S:36:ARG:HD3	2.31	0.44
6:F:4:TYR:CZ	6:F:72:VAL:HG21	2.51	0.44
7:G:45:ASP:O	7:G:49:ILE:HG13	2.17	0.44
9:I:118:LYS:O	9:I:120:ARG:N	2.45	0.44
1:A:261:U:OP2	20:T:79:ARG:NH2	2.51	0.44
1:A:1224:G:O2'	1:A:1322:C:OP1	2.29	0.44
1:A:1355:G:H2'	1:A:1356:G:C8	2.52	0.44
4:D:20:TYR:HD2	4:D:26:CYS:HB3	1.83	0.44
17:Q:59:ILE:HD13	17:Q:73:VAL:HA	1.99	0.44
1:A:960:U:H1'	1:A:1223:C:H5'	1.98	0.44
1:A:1028:C:H2'	1:A:1029:C:C6	2.53	0.44
1:A:1127:G:H21	1:A:1147:C:N4	2.14	0.44
2:B:231:GLU:CD	2:B:231:GLU:H	2.21	0.44
5:E:5:ASP:OD1	5:E:5:ASP:N	2.50	0.44
13:M:67:GLU:HB3	13:M:68:GLY:H	1.44	0.44
1:A:277:C:OP1	17:Q:68:ARG:NH2	2.25	0.44
1:A:537:G:H2'	1:A:538:G:C8	2.53	0.44
1:A:1035:A:H2'	1:A:1036:G:C8	2.53	0.44
1:A:1172:C:H2'	1:A:1173:G:H8	1.82	0.44
1:A:1240:U:OP1	7:G:119:ARG:NH1	2.49	0.44
18:R:21:LYS:O	18:R:25:THR:OG1	2.31	0.44
20:T:92:LEU:O	20:T:96:GLY:N	2.49	0.44
1:A:129(A):G:N2	1:A:190(E):U:H5"	2.33	0.44
12:L:60:LEU:HB3	12:L:62:SER:H	1.83	0.44
1:A:260:G:H2'	1:A:261:U:C6	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1163:C:H2'	1:A:1164:G:C8	2.52	0.44
1:A:1316:G:N2	1:A:1318:A:H3'	2.32	0.44
5:E:11:ILE:HB	5:E:31:LEU:HB3	2.00	0.44
12:L:127:GLU:HB2	12:L:128:ALA:H	1.57	0.44
1:A:142:G:O2'	1:A:196:A:N1	2.46	0.44
12:L:70:ILE:HD13	12:L:77:LEU:HD12	2.00	0.44
1:A:503:C:OP2	12:L:116:SER:OG	2.23	0.44
1:A:610:G:C4	1:A:611:A:C8	3.05	0.44
1:A:643:C:C2	1:A:644:G:C8	3.06	0.44
1:A:1031:G:H2'	1:A:1032:G:H8	1.83	0.44
1:A:1300:G:O2'	1:A:1301:U:O5'	2.35	0.44
1:A:1521:G:H2'	1:A:1522:U:C6	2.53	0.44
2:B:87:ARG:CZ	2:B:233:SER:HB2	2.47	0.44
3:C:91:LEU:HD21	3:C:99:VAL:HG22	1.98	0.44
4:D:117:ALA:O	4:D:121:VAL:HG23	2.18	0.44
1:A:358:U:H2'	1:A:359:U:C6	2.53	0.44
1:A:1323:G:H2'	1:A:1324:A:H8	1.82	0.44
2:B:90:MET:HA	2:B:91:PRO:HD3	1.80	0.44
13:M:3:ARG:HA	13:M:9:ILE:HG13	2.00	0.44
1:A:321:A:H2'	1:A:322:C:C6	2.53	0.43
1:A:542:G:H2'	1:A:543:C:H6	1.82	0.43
1:A:603:U:H2'	1:A:604:G:C8	2.53	0.43
1:A:872:A:C4	1:A:874:G:N7	2.86	0.43
1:A:1077:G:N2	1:A:1080:A:OP2	2.46	0.43
1:A:1315:U:H2'	1:A:1316:G:O4'	2.18	0.43
1:A:114:U:O2'	1:A:115:G:H5'	2.19	0.43
1:A:350:G:O2'	1:A:351:G:H5'	2.18	0.43
1:A:690:G:H2'	1:A:691:G:C8	2.54	0.43
1:A:731:G:OP1	1:A:766:A:H1'	2.19	0.43
1:A:1418:A:H2'	1:A:1419:G:O4'	2.18	0.43
10:J:30:SER:HB2	10:J:81:THR:HA	2.00	0.43
1:A:7:G:H5'	1:A:298:A:O4'	2.17	0.43
1:A:57:G:H2'	1:A:58:C:C6	2.53	0.43
1:A:109:A:C6	1:A:326:G:C6	3.07	0.43
1:A:1072:G:H2'	1:A:1073:U:H6	1.84	0.43
1:A:1128:C:H42	1:A:1143:G:H1	1.65	0.43
20:T:50:GLU:O	20:T:54:LYS:HB2	2.18	0.43
1:A:168:G:C2	1:A:169:C:C5	3.06	0.43
1:A:399:G:H2'	1:A:400:C:H6	1.83	0.43
1:A:562:C:H1'	12:L:15:ARG:HG3	2.01	0.43
1:A:946:A:O2'	1:A:1333:A:N3	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1160:G:C6	1:A:1161:C:C5	3.07	0.43
5:E:131:ILE:HD13	5:E:131:ILE:HA	1.92	0.43
10:J:49:VAL:HG23	14:N:41:ARG:HD2	2.00	0.43
11:K:33:THR:HA	11:K:39:PRO:HA	2.00	0.43
1:A:56:U:H2'	1:A:57:G:C8	2.54	0.43
1:A:323:U:H2'	1:A:324:G:O4'	2.18	0.43
1:A:921:U:O2	5:E:19:MET:HB2	2.19	0.43
1:A:1220:G:H2'	1:A:1221:G:C8	2.53	0.43
1:A:1527:C:O2'	1:A:1528:U:H5'	2.19	0.43
12:L:54:LYS:HD2	12:L:54:LYS:N	2.34	0.43
13:M:65:LYS:O	13:M:66:LEU:HD23	2.18	0.43
1:A:768:A:H4'	1:A:1523:G:N2	2.33	0.43
1:A:1003(A):G:H2'	1:A:1004:A:H4'	2.01	0.43
1:A:1256:A:O2'	1:A:1257:U:O5'	2.36	0.43
4:D:31:CYS:C	4:D:33:MET:H	2.22	0.43
11:K:54:ARG:O	11:K:57:THR:OG1	2.27	0.43
12:L:46:LYS:HG3	12:L:92:0TD:H5	2.00	0.43
1:A:29:G:O2'	1:A:30:U:H5'	2.19	0.43
1:A:335:C:H2'	1:A:336:C:H6	1.82	0.43
1:A:1017:G:H2'	1:A:1018:C:C6	2.53	0.43
1:A:1068:G:H8	1:A:1068:G:OP2	2.01	0.43
7:G:65:ALA:O	7:G:69:VAL:HG23	2.19	0.43
1:A:296:U:O2'	1:A:556:C:O2	2.35	0.43
1:A:518:C:H2'	1:A:530:G:N3	2.34	0.43
1:A:818:G:H3'	1:A:819:A:H5"	2.00	0.43
1:A:1087:G:H2'	1:A:1088:G:H8	1.84	0.43
15:O:18:PHE:HB2	15:O:19:PRO:HD2	2.00	0.43
16:P:34:GLU:HG2	16:P:35:LYS:N	2.34	0.43
1:A:222:U:H2'	1:A:223:U:H6	1.84	0.43
1:A:736:C:H2'	1:A:737:A:H8	1.84	0.43
1:A:743:U:H2'	1:A:744:C:H6	1.82	0.43
10:J:50:ILE:H	10:J:50:ILE:HG13	1.68	0.43
12:L:7:ILE:O	12:L:11:VAL:HG23	2.19	0.43
15:O:36:ILE:HG12	15:O:59:MET:HE3	2.01	0.43
1:A:67:C:H2'	1:A:68:G:C8	2.54	0.43
1:A:246:A:C2	1:A:282:A:C5	3.07	0.43
1:A:397:A:H5'	1:A:398:C:OP1	2.17	0.43
1:A:836:G:C6	1:A:851:G:C6	3.07	0.43
1:A:1189:C:H5"	3:C:5:ILE:HG12	2.01	0.43
1:A:1521:G:H2'	1:A:1522:U:H6	1.84	0.43
1:A:129(A):G:C2	1:A:190(E):U:H5"	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:658:G:H2'	1:A:659:U:C6	2.54	0.42
1:A:895:G:H2'	1:A:896:C:H6	1.84	0.42
1:A:1031:G:H2'	1:A:1032:G:C8	2.54	0.42
3:C:150:LYS:HG3	3:C:169:ALA:HB2	2.01	0.42
1:A:110:C:H2'	1:A:111:G:O4'	2.18	0.42
1:A:780:A:O2'	1:A:781:A:H5"	2.19	0.42
1:A:848:C:H2'	1:A:849:C:C6	2.54	0.42
1:A:983:A:H5'	1:A:984:C:OP2	2.19	0.42
1:A:1130:A:OP1	9:I:20:ARG:NH2	2.52	0.42
1:A:1157:A:H4'	1:A:1158:C:O5'	2.19	0.42
1:A:1410:G:H2'	1:A:1411:C:C6	2.55	0.42
9:I:65:VAL:HG11	9:I:73:GLN:HB3	2.01	0.42
12:L:8:ASN:OD1	17:Q:34:LYS:HE2	2.19	0.42
12:L:24:VAL:HG13	12:L:98:TYR:CE1	2.52	0.42
16:P:15:PRO:HD2	16:P:42:ARG:HD3	2.01	0.42
1:A:192:U:C1'	20:T:103:GLY:HA2	2.48	0.42
1:A:332:G:C2	1:A:333:G:C8	3.07	0.42
1:A:509:A:O2'	1:A:510:A:OP1	2.35	0.42
1:A:1114:C:H1'	14:N:60:SER:OG	2.19	0.42
6:F:46:ARG:HB2	6:F:60:PHE:CE2	2.55	0.42
13:M:15:VAL:HG23	13:M:43:THR:O	2.19	0.42
15:O:5:LYS:H	15:O:5:LYS:HD2	1.84	0.42
1:A:156:G:C6	1:A:166:G:C6	3.08	0.42
1:A:235:C:N4	28:A:2086:HOH:O	2.52	0.42
1:A:560:U:H4'	1:A:561:U:H5"	1.99	0.42
1:A:945:G:C2	1:A:946:A:C8	3.07	0.42
1:A:1216:G:H2'	1:A:1217:C:H6	1.85	0.42
7:G:59:LEU:HD11	7:G:63:LYS:HE3	2.00	0.42
1:A:45:U:OP1	1:A:307:C:O2'	2.36	0.42
1:A:1017:G:H2'	1:A:1018:C:H6	1.83	0.42
1:A:1175:G:H2'	1:A:1176:A:H8	1.83	0.42
1:A:1177:G:O5'	9:I:97:LYS:NZ	2.52	0.42
3:C:77:ILE:O	3:C:83:ARG:HB3	2.19	0.42
10:J:16:LEU:HD12	10:J:68:HIS:HB2	2.01	0.42
1:A:542:G:H2'	1:A:543:C:C6	2.54	0.42
1:A:1273:G:H2'	1:A:1274:G:O4'	2.19	0.42
2:B:130:ARG:HB3	2:B:131:PRO:HD2	2.01	0.42
12:L:117:ARG:HB3	12:L:122:THR:O	2.19	0.42
13:M:24:GLY:HA3	13:M:66:LEU:HD22	2.02	0.42
1:A:514:C:H2'	1:A:515:G:H8	1.83	0.42
1:A:642:A:H2'	1:A:643:C:H6	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:704:A:C5	1:A:705:U:C5	3.08	0.42
1:A:828:A:H2'	1:A:829:G:O4'	2.20	0.42
1:A:974:A:H8	1:A:974:A:OP1	2.03	0.42
1:A:1206:G:C6	1:A:1207:2MG:C5	3.07	0.42
1:A:1475:G:H2'	1:A:1476:G:C8	2.54	0.42
5:E:127:ASN:HA	5:E:128:PRO:HD3	1.94	0.42
7:G:111:ARG:HB2	7:G:119:ARG:HG2	2.02	0.42
1:A:184:G:H2'	1:A:185:A:H8	1.84	0.42
1:A:477:G:H2'	1:A:478:A:C8	2.54	0.42
1:A:1472:U:H2'	1:A:1473:A:H8	1.84	0.42
1:A:1492:A:OP1	12:L:47:LYS:N	2.53	0.42
4:D:50:ARG:HA	4:D:51:PRO:HD3	1.80	0.42
11:K:40:ILE:HG22	11:K:41:THR:HG23	2.00	0.42
12:L:6:THR:OG1	12:L:9:GLN:HG3	2.19	0.42
12:L:90:VAL:HG12	12:L:92:0TD:OD1	2.18	0.42
1:A:192:U:H2'	1:A:193:C:C6	2.55	0.42
1:A:1366:C:H2'	1:A:1367:C:C6	2.55	0.42
7:G:152:ALA:O	7:G:155:ARG:NH1	2.52	0.42
1:A:194:C:H2'	1:A:195:A:H5"	2.02	0.42
1:A:911:U:H2'	1:A:912:C:C6	2.55	0.42
1:A:986:A:H2'	1:A:987:G:C8	2.55	0.42
1:A:1054:C:H2'	1:A:1055:A:H5"	2.02	0.42
3:C:126:ARG:HE	3:C:128:PHE:HD1	1.67	0.42
1:A:671:G:H2'	1:A:672:U:O4'	2.20	0.41
1:A:932:C:H4'	7:G:4:ARG:NH2	2.35	0.41
12:L:111:LYS:HE3	12:L:112:ASP:H	1.85	0.41
1:A:962:C:H2'	1:A:963:G:O4'	2.20	0.41
1:A:1464:G:H2'	1:A:1465:C:C6	2.55	0.41
19:S:5:LEU:O	19:S:6:LYS:HB2	2.20	0.41
1:A:372:C:H1'	1:A:373:A:OP2	2.20	0.41
1:A:592:G:H2'	1:A:593:G:H8	1.85	0.41
1:A:1080:A:H5"	5:E:16:THR:HG21	2.03	0.41
11:K:120:ARG:HA	11:K:121:PRO:HD3	1.89	0.41
12:L:28:LYS:HB3	12:L:30:ALA:HB2	2.02	0.41
12:L:127:GLU:OE1	12:L:128:ALA:N	2.53	0.41
1:A:674:G:H2'	1:A:675:A:C8	2.49	0.41
1:A:987:G:H2'	1:A:988:G:C8	2.56	0.41
1:A:1291:G:OP1	7:G:37:ASN:ND2	2.52	0.41
1:A:1498:UR3:O4'	1:A:1519:MA6:H2	2.21	0.41
11:K:117:ASN:OD1	11:K:117:ASN:N	2.53	0.41
17:Q:27:PHE:CE2	17:Q:36:ILE:HD11	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:G:H2'	1:A:23:C:C6	2.55	0.41
1:A:57:G:H2'	1:A:58:C:H6	1.85	0.41
1:A:99:C:H2'	1:A:101:A:O4'	2.21	0.41
1:A:338:A:H2'	1:A:339:C:H6	1.86	0.41
1:A:488:C:H2'	1:A:489:C:H6	1.85	0.41
1:A:687:A:C2	1:A:704:A:C5	3.08	0.41
1:A:741:G:OP2	24:A:1604:PAR:O41	2.36	0.41
1:A:1035:A:C2	1:A:1036:G:C5	3.09	0.41
1:A:1151:A:C2	1:A:1152:A:C5	3.09	0.41
1:A:1207:2MG:H2'	1:A:1208:C:H6	1.86	0.41
1:A:1262:C:H2'	1:A:1263:C:H6	1.86	0.41
1:A:1370:G:C2	1:A:1371:G:C8	3.08	0.41
1:A:299:G:H2'	1:A:300:A:C8	2.56	0.41
1:A:540:G:H2'	1:A:541:G:O4'	2.20	0.41
1:A:579:G:H5'	1:A:728:A:H1'	2.01	0.41
1:A:890:G:O2'	1:A:906:G:O6	2.28	0.41
1:A:1030(A):G:N2	1:A:1030(D):A:OP2	2.52	0.41
1:A:1241:G:H2'	1:A:1242:C:C6	2.55	0.41
3:C:5:ILE:HG13	3:C:5:ILE:H	1.70	0.41
5:E:31:LEU:HD23	5:E:31:LEU:HA	1.83	0.41
12:L:27:LEU:O	12:L:29:GLY:N	2.53	0.41
16:P:28:ARG:HG3	16:P:29:ASP:OD1	2.21	0.41
1:A:410:G:OP1	4:D:30:LYS:NZ	2.33	0.41
1:A:664:G:OP1	18:R:64:ARG:HD2	2.21	0.41
1:A:994:A:OP1	1:A:994:A:C8	2.74	0.41
1:A:1225:A:H5"	1:A:1226:C:OP2	2.20	0.41
1:A:1281:U:O2'	1:A:1282:C:OP1	2.33	0.41
2:B:127:ILE:H	2:B:127:ILE:HG13	1.67	0.41
2:B:178:ARG:HH22	8:H:74:PRO:HB3	1.85	0.41
16:P:9:PHE:CE1	16:P:18:ARG:HD2	2.54	0.41
16:P:28:ARG:NH1	16:P:29:ASP:OD1	2.54	0.41
1:A:22:G:H2'	1:A:23:C:H6	1.84	0.41
1:A:416:G:H2'	1:A:417:C:H6	1.86	0.41
1:A:560:U:H5'	1:A:566:G:N2	2.35	0.41
1:A:564:C:O2'	8:H:91:ARG:NH2	2.54	0.41
1:A:642:A:N7	8:H:115:SER:HA	2.36	0.41
1:A:1326:C:H2'	1:A:1327:C:H6	1.85	0.41
2:B:74:LYS:C	2:B:76:GLN:H	2.24	0.41
6:F:11:ASN:HA	6:F:12:PRO:HD2	1.94	0.41
19:S:31:ILE:HD13	19:S:32:LYS:H	1.85	0.41
1:A:105:G:H2'	1:A:106:C:H6	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:960:U:H4'	1:A:961:U:C5'	2.50	0.41
1:A:1073:U:H2'	1:A:1074:G:H8	1.86	0.41
1:A:1116:C:O2'	9:I:108:VAL:HG21	2.21	0.41
1:A:1241:G:H2'	1:A:1242:C:H6	1.86	0.41
1:A:1309:G:C6	1:A:1329:A:C2	3.09	0.41
2:B:130:ARG:HD3	2:B:130:ARG:HA	1.75	0.41
15:O:74:ASP:HA	15:O:75:PRO:HD2	1.91	0.41
1:A:75:G:C6	1:A:96:G:C6	3.08	0.41
1:A:537:G:H2'	1:A:538:G:H8	1.86	0.41
1:A:701:C:H5"	1:A:703:G:O4'	2.21	0.41
2:B:43:ASP:O	2:B:47:THR:OG1	2.38	0.41
1:A:106:C:H2'	1:A:107:G:O4'	2.21	0.40
1:A:222:U:H2'	1:A:223:U:C6	2.56	0.40
1:A:409:G:H1	1:A:433:C:N4	2.14	0.40
1:A:689:C:H2'	1:A:690:G:O4'	2.21	0.40
1:A:922:G:H2'	1:A:923:A:C8	2.56	0.40
1:A:985:C:H2'	1:A:986:A:H8	1.86	0.40
19:S:5:LEU:HD21	19:S:70:LYS:NZ	2.36	0.40
1:A:1468:A:H2'	1:A:1469:G:O4'	2.21	0.40
2:B:30:ARG:HG3	2:B:31:TYR:CD1	2.56	0.40
9:I:97:LYS:HB3	9:I:98:PRO:HD3	2.03	0.40
10:J:38:ILE:H	10:J:71:LEU:CB	2.33	0.40
1:A:614:A:H2'	1:A:615:C:H6	1.86	0.40
1:A:1022:G:C2	1:A:1023:G:C8	3.08	0.40
1:A:1107:C:C4	1:A:1108:G:C8	3.09	0.40
1:A:1117:G:H5'	1:A:1118:C:OP2	2.22	0.40
1:A:1163:C:C2	1:A:1164:G:C8	3.08	0.40
1:A:1232:U:P	9:I:124:GLN:HE21	2.44	0.40
6:F:4:TYR:CE2	6:F:92:LYS:HG2	2.57	0.40
6:F:30:LEU:HA	6:F:30:LEU:HD23	1.87	0.40
1:A:814:A:H2'	1:A:816:A:H5"	2.04	0.40
1:A:892:A:H2'	1:A:893:C:H6	1.87	0.40
8:H:33:GLU:HG3	8:H:48:TYR:CE2	2.57	0.40
20:T:81:LYS:O	20:T:85:MET:HG3	2.22	0.40
1:A:157:G:C2	1:A:158:G:C8	3.09	0.40
1:A:500:G:H2'	1:A:501:C:C6	2.56	0.40
1:A:865:A:H5'	1:A:1078:U:O4	2.22	0.40
1:A:1308:U:OP2	13:M:99:ARG:HG3	2.21	0.40
1:A:1464:G:H2'	1:A:1465:C:H6	1.85	0.40
2:B:112:VAL:O	2:B:116:GLU:HG2	2.21	0.40
8:H:112:LEU:HD23	8:H:133:LEU:HA	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:14:LYS:HE2	10:J:14:LYS:HB3	1.84	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	70
3	C	205/207 (99%)	190 (93%)	15 (7%)	0	100	100
4	D	206/208 (99%)	200 (97%)	5 (2%)	1 (0%)	29	66
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%)	133 (98%)	3 (2%)	0	100	100
9	I	125/127 (98%)	114 (91%)	10 (8%)	1 (1%)	19	57
10	J	97/99 (98%)	78 (80%)	17 (18%)	2 (2%)	7	36
11	K	117/119 (98%)	105 (90%)	12 (10%)	0	100	100
12	L	122/125 (98%)	111 (91%)	10 (8%)	1 (1%)	19	57
13	M	116/118 (98%)	109 (94%)	7 (6%)	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%)	78 (95%)	4 (5%)	0	100	100
17	Q	97/99 (98%)	94 (97%)	3 (3%)	0	100	100
18	R	71/73 (97%)	67 (94%)	4 (6%)	0	100	100
19	S	79/81 (98%)	71 (90%)	7 (9%)	1 (1%)	12	46
20	T	97/99 (98%)	85 (88%)	12 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	U	23/25 (92%)	22 (96%)	1 (4%)	0	100	100
All	All	2352/2393 (98%)	2184 (93%)	161 (7%)	7 (0%)	41	75

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	L	28	LYS
19	S	31	ILE
10	J	72	VAL
9	I	119	ALA
10	J	34	VAL
4	D	5	ILE
2	B	229	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	194/204 (95%)	180 (93%)	14 (7%)	14	46
3	C	160/161 (99%)	151 (94%)	9 (6%)	21	53
4	D	180/180 (100%)	171 (95%)	9 (5%)	24	57
5	E	115/116 (99%)	102 (89%)	13 (11%)	6	25
6	F	90/90 (100%)	83 (92%)	7 (8%)	12	42
7	G	126/126 (100%)	119 (94%)	7 (6%)	21	53
8	H	119/119 (100%)	110 (92%)	9 (8%)	13	43
9	I	98/98 (100%)	90 (92%)	8 (8%)	11	40
10	J	87/89 (98%)	81 (93%)	6 (7%)	15	47
11	K	90/90 (100%)	84 (93%)	6 (7%)	16	48
12	L	103/103 (100%)	97 (94%)	6 (6%)	20	52
13	M	94/94 (100%)	85 (90%)	9 (10%)	8	33
14	N	49/49 (100%)	47 (96%)	2 (4%)	30	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	O	79/79 (100%)	71 (90%)	8 (10%)	7	31
16	P	72/72 (100%)	68 (94%)	4 (6%)	21	53
17	Q	94/94 (100%)	88 (94%)	6 (6%)	17	50
18	R	64/64 (100%)	61 (95%)	3 (5%)	26	59
19	S	71/71 (100%)	62 (87%)	9 (13%)	4	20
20	T	76/76 (100%)	67 (88%)	9 (12%)	5	23
21	U	19/20 (95%)	18 (95%)	1 (5%)	22	55
All	All	1980/1995 (99%)	1835 (93%)	145 (7%)	14	45

All (145) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	24	TRP
2	B	46	LYS
2	B	82	ARG
2	B	114	ARG
2	B	139	LYS
2	B	142	LEU
2	B	144	ARG
2	B	150	SER
2	B	157	ARG
2	B	187	LEU
2	B	190	THR
2	B	208	ILE
2	B	221	LEU
2	B	236	TYR
3	C	3	ASN
3	C	27	LYS
3	C	43	LEU
3	C	82	GLU
3	C	91	LEU
3	C	95	THR
3	C	126	ARG
3	C	167	TRP
3	C	204	LEU
4	D	3	ARG
4	D	4	TYR
4	D	8	VAL
4	D	15	GLU
4	D	64	LEU

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Mol	Chain	Res	Type
4	D	70	ILE
4	D	122	ARG
4	D	127	THR
4	D	135	LEU
5	E	6	PHE
5	E	10	MET
5	E	12	LEU
5	E	16	THR
5	E	24	ARG
5	E	31	LEU
5	E	41	VAL
5	E	64	ARG
5	E	76	ILE
5	E	79	GLU
5	E	80	ILE
5	E	89	ILE
5	E	150	ARG
6	F	10	LEU
6	F	24	GLU
6	F	43	LEU
6	F	69	GLU
6	F	73	ASN
6	F	86	ARG
6	F	100	ASN
7	G	8	GLU
7	G	11	GLN
7	G	48	LYS
7	G	114	ARG
7	G	124	LEU
7	G	149	ARG
7	G	156	TRP
8	H	25	ASP
8	H	26	VAL
8	H	39	LEU
8	H	85	ARG
8	H	91	ARG
8	H	92	ARG
8	H	102	ARG
8	H	105	ARG
8	H	133	LEU
9	I	12	GLU
9	I	35	GLU

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Mol	Chain	Res	Type
9	I	79	LEU
9	I	102	LEU
9	I	104	ARG
9	I	112	LYS
9	I	118	LYS
9	I	121	ARG
10	J	59	SER
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	91	ARG
11	K	92	GLU
11	K	117	ASN
12	L	20	LYS
12	L	33	ARG
12	L	53	ARG
12	L	93	LEU
12	L	100	ILE
12	L	111	LYS
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	94	ARG
13	M	110	ARG
13	M	115	LYS
14	N	9	LYS
14	N	22	THR
15	O	5	LYS
15	O	6	GLU
15	O	21	ASP
15	O	34	LEU
15	O	39	LEU
15	O	57	LEU
15	O	70	LEU

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Mol	Chain	Res	Type
15	O	81	LEU
16	P	1	MET
16	P	2	VAL
16	P	20	VAL
16	P	53	VAL
17	Q	38	ARG
17	Q	52	LYS
17	Q	68	ARG
17	Q	74	LEU
17	Q	78	GLU
17	Q	98	LEU
18	R	39	VAL
18	R	47	THR
18	R	66	LEU
19	S	3	ARG
19	S	7	LYS
19	S	12	ASP
19	S	15	LEU
19	S	31	ILE
19	S	36	ARG
19	S	62	ILE
19	S	65	ASN
19	S	81	ARG
20	T	8	ARG
20	T	48	LYS
20	T	54	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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	6	HIS
4	D	119	GLN
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%)	223 (14%)	42 (2%)
22	a	4/6 (66%)	1 (25%)	0
23	b	8/11 (72%)	2 (25%)	0
All	All	1519/1539 (98%)	226 (14%)	42 (2%)

All (226) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	7	G
1	A	9	G
1	A	32	A
1	A	39	G
1	A	47	C
1	A	48	C
1	A	51	A
1	A	59	A
1	A	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
1	A	190(E)	U
1	A	195	A
1	A	197	A
1	A	201	C
1	A	202	U
1	A	204	U
1	A	216	G
1	A	220	G
1	A	244	U
1	A	245	C
1	A	247	G
1	A	251	G
1	A	267	C
1	A	289	G

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Mol	Chain	Res	Type
1	A	298	A
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	347	G
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	412	A
1	A	413	G
1	A	414	A
1	A	421	U
1	A	424	G
1	A	429	U
1	A	433	C
1	A	439	A
1	A	442	C
1	A	452	A
1	A	460	A
1	A	461	C
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	521	G
1	A	527	7MG
1	A	531	U
1	A	532	A

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Mol	Chain	Res	Type
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	607	A
1	A	630	G
1	A	631	G
1	A	632	A
1	A	653	A
1	A	665	A
1	A	687	A
1	A	688	G
1	A	702	A
1	A	703	G
1	A	721	G
1	A	723	U
1	A	731	G
1	A	748	C
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

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Mol	Chain	Res	Type
1	A	848	C
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	961	U
1	A	965	A
1	A	966	M2G
1	A	967	5MC
1	A	968	A
1	A	969	A
1	A	971	G
1	A	974	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	989	C
1	A	991	U
1	A	992	U
1	A	993	G
1	A	994	A
1	A	1005	A
1	A	1025	U
1	A	1026	G
1	A	1027	C
1	A	1028	C
1	A	1031	G
1	A	1050	G
1	A	1054	C
1	A	1055	A
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	1125	U
1	A	1126	U

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Mol	Chain	Res	Type
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	1152	A
1	A	1158	C
1	A	1159	U
1	A	1171	G
1	A	1180	A
1	A	1181	G
1	A	1183	A
1	A	1196	U
1	A	1197	G
1	A	1201	A
1	A	1202	G
1	A	1212	U
1	A	1213	A
1	A	1214	C
1	A	1227	A
1	A	1238	A
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	1312	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

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Mol	Chain	Res	Type
1	A	1363	A
1	A	1370	G
1	A	1381	U
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	1503	A
1	A	1504	G
1	A	1505	G
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	250	A
1	A	266	G
1	A	328	C
1	A	329	A
1	A	372	C
1	A	428	G
1	A	432	A
1	A	484	G
1	A	496	A

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Mol	Chain	Res	Type
1	A	509	A
1	A	530	G
1	A	532	A
1	A	559	A
1	A	687	A
1	A	701	C
1	A	748	C
1	A	812	C
1	A	913	A
1	A	960	U
1	A	965	A
1	A	1049	U
1	A	1065	U
1	A	1067	A
1	A	1129	C
1	A	1179	A
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
1	A	1528	U

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

19 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	1404	1	18,22,23	0.85	0	26,32,35	0.87	1 (3%)
1	5MC	A	1400	1	18,22,23	1.01	2 (11%)	26,32,35	1.01	2 (7%)
1	PSU	A	1541	25,1	18,21,22	1.89	7 (38%)	22,30,33	1.52	3 (13%)
1	5MC	A	1407	1	18,22,23	0.98	0	26,32,35	1.05	2 (7%)
23	12A	b	37	23,25	29,36,37	2.81	4 (13%)	34,52,55	2.36	8 (23%)
1	MA6	A	1518	1	18,26,27	0.72	0	19,38,41	0.83	1 (5%)
1	2MG	A	1207	1	18,26,27	1.31	4 (22%)	16,38,41	1.42	2 (12%)
1	MA6	A	1519	26,1	18,26,27	0.90	1 (5%)	19,38,41	0.69	0
1	M2G	A	966	1	20,27,28	1.44	4 (20%)	22,40,43	1.42	3 (13%)
1	PSU	A	1540	1	18,21,22	1.90	7 (38%)	22,30,33	1.50	3 (13%)
22	6MZ	a	3	22	18,25,26	1.17	2 (11%)	16,36,39	0.62	0
1	UR3	A	1498	1	19,22,23	0.71	1 (5%)	26,32,35	1.03	1 (3%)
23	70U	b	34	23	22,26,27	3.55	10 (45%)	28,37,40	1.52	5 (17%)
1	4OC	A	1402	1	20,23,24	0.99	2 (10%)	26,32,35	0.79	1 (3%)
1	7MG	A	527	1	22,26,27	5.07	4 (18%)	29,39,42	2.09	9 (31%)
23	PSU	b	39	23	18,21,22	1.93	7 (38%)	22,30,33	1.51	3 (13%)
12	0TD	L	92	12	7,9,10	0.99	0	6,11,13	2.10	4 (66%)
1	PSU	A	516	25,1	18,21,22	2.00	7 (38%)	22,30,33	1.44	4 (18%)
1	5MC	A	967	1	18,22,23	1.06	2 (11%)	26,32,35	0.95	2 (7%)

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	1404	1	-	0/7/25/26	0/2/2/2
1	5MC	A	1400	1	-	2/7/25/26	0/2/2/2
1	PSU	A	1541	25,1	-	1/7/25/26	0/2/2/2
1	5MC	A	1407	1	-	0/7/25/26	0/2/2/2
23	12A	b	37	23,25	-	7/21/43/44	0/3/3/3
1	MA6	A	1518	1	-	2/7/29/30	0/3/3/3
1	2MG	A	1207	1	-	0/5/27/28	0/3/3/3
1	MA6	A	1519	26,1	-	5/7/29/30	0/3/3/3
1	M2G	A	966	1	-	3/7/29/30	0/3/3/3
1	PSU	A	1540	1	-	0/7/25/26	0/2/2/2
22	6MZ	a	3	22	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	UR3	A	1498	1	-	0/7/25/26	0/2/2/2
23	70U	b	34	23	-	5/13/31/32	0/2/2/2
1	4OC	A	1402	1	-	2/9/29/30	0/2/2/2
1	7MG	A	527	1	-	2/7/37/38	0/3/3/3
23	PSU	b	39	23	-	0/7/25/26	0/2/2/2
12	0TD	L	92	12	-	3/7/12/14	-
1	PSU	A	516	25,1	-	0/7/25/26	0/2/2/2
1	5MC	A	967	1	-	2/7/25/26	0/2/2/2

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	527	7MG	C8-N9	-22.99	1.33	1.46
23	b	37	12A	C2-S2	10.79	1.84	1.75
23	b	34	70U	O4-C4	8.67	1.40	1.23
23	b	34	70U	C2-S2	8.47	1.81	1.67
23	b	37	12A	C6-N6	6.18	1.47	1.36
23	b	37	12A	CC-N	6.15	1.48	1.35
23	b	34	70U	C6-N1	-5.88	1.28	1.38
23	b	34	70U	C4-N3	-5.06	1.29	1.38
23	b	37	12A	CC-N6	4.40	1.46	1.37
1	A	527	7MG	C2-N2	3.87	1.43	1.34
23	b	34	70U	C5M-C5	3.68	1.57	1.50
1	A	516	PSU	C2-N1	-3.62	1.31	1.36
23	b	34	70U	O9-C8	3.60	1.44	1.33
23	b	34	70U	C4-C5	-3.56	1.37	1.45
1	A	516	PSU	C6-C5	3.43	1.39	1.35
23	b	39	PSU	C2-N1	-3.42	1.32	1.36
23	b	39	PSU	C4-N3	-3.39	1.32	1.38
1	A	1540	PSU	C6-C5	3.37	1.39	1.35
1	A	516	PSU	C4-N3	-3.37	1.32	1.38
23	b	39	PSU	C6-C5	3.36	1.39	1.35
1	A	1540	PSU	C4-N3	-3.35	1.32	1.38
1	A	1541	PSU	C6-C5	3.35	1.39	1.35
23	b	34	70U	O9-C9	-3.29	1.37	1.45
1	A	1541	PSU	C4-N3	-3.28	1.32	1.38
1	A	966	M2G	C6-N1	3.24	1.42	1.37
1	A	1541	PSU	C2-N1	-3.24	1.32	1.36
1	A	1540	PSU	C2-N1	-3.20	1.32	1.36
1	A	516	PSU	C2-N3	-3.16	1.32	1.37
1	A	966	M2G	C2-N3	3.14	1.34	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	3	6MZ	C6-N6	3.14	1.40	1.35
23	b	39	PSU	C2-N3	-3.05	1.32	1.37
1	A	1540	PSU	C2-N3	-3.05	1.32	1.37
23	b	34	70U	C6-C5	3.02	1.43	1.34
1	A	1541	PSU	C2-N3	-3.02	1.32	1.37
1	A	966	M2G	C2-N2	2.80	1.40	1.35
1	A	1207	2MG	C2-N2	2.79	1.39	1.33
1	A	1207	2MG	C6-N1	2.75	1.42	1.37
1	A	527	7MG	C5-N7	2.71	1.38	1.35
1	A	516	PSU	O4-C4	-2.69	1.18	1.23
1	A	1207	2MG	C5-C6	-2.64	1.42	1.47
1	A	1400	5MC	C2-N1	2.62	1.45	1.40
23	b	34	70U	C2-N3	-2.61	1.31	1.37
1	A	966	M2G	C5-C6	-2.56	1.42	1.47
23	b	39	PSU	O4-C4	-2.50	1.18	1.23
1	A	1540	PSU	O4-C4	-2.46	1.18	1.23
1	A	967	5MC	C2-N1	2.43	1.45	1.40
1	A	1402	4OC	C2-N3	2.42	1.41	1.36
1	A	1541	PSU	O4-C4	-2.42	1.19	1.23
1	A	1207	2MG	C2-N1	2.36	1.40	1.36
1	A	967	5MC	C2-N3	2.30	1.41	1.36
1	A	527	7MG	C4-N3	2.27	1.39	1.34
1	A	1541	PSU	C6-N1	-2.22	1.32	1.36
23	b	39	PSU	C6-N1	-2.21	1.32	1.36
1	A	516	PSU	O2-C2	-2.19	1.18	1.23
23	b	39	PSU	O2-C2	-2.19	1.18	1.23
1	A	1540	PSU	O2-C2	-2.14	1.18	1.23
1	A	1541	PSU	O2-C2	-2.14	1.18	1.23
1	A	1540	PSU	C6-N1	-2.14	1.32	1.36
1	A	1519	MA6	C6-N1	2.13	1.36	1.33
1	A	1498	UR3	C2-N1	2.11	1.41	1.38
22	a	3	6MZ	C6-N1	2.08	1.36	1.34
1	A	1400	5MC	C2-N3	2.07	1.40	1.36
1	A	516	PSU	C6-N1	-2.05	1.32	1.36
1	A	1402	4OC	O2-C2	-2.01	1.20	1.23

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	37	12A	C2M-S2-C2	10.17	109.86	102.27
1	A	527	7MG	C5-C6-N1	4.92	119.66	110.99
23	b	34	70U	O9-C8-C5M	4.76	120.08	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	527	7MG	C2-N3-C4	4.59	120.48	112.30
23	b	37	12A	N6-CC-N	4.51	120.06	113.76
1	A	527	7MG	N9-C4-N3	4.35	131.97	125.47
1	A	1540	PSU	N1-C2-N3	4.24	119.93	115.13
1	A	1541	PSU	N1-C2-N3	4.22	119.91	115.13
1	A	1207	2MG	O6-C6-N1	-4.21	115.68	120.65
23	b	39	PSU	N1-C2-N3	4.19	119.87	115.13
1	A	527	7MG	C5-C4-N3	-4.06	120.40	128.13
1	A	966	M2G	N1-C2-N2	-4.00	114.63	118.04
1	A	516	PSU	N1-C2-N3	3.80	119.44	115.13
23	b	37	12A	C2-N3-C4	3.55	120.21	115.32
1	A	527	7MG	N9-C8-N7	3.53	108.42	103.38
1	A	1207	2MG	O6-C6-C5	3.43	131.07	124.37
1	A	966	M2G	O6-C6-C5	3.20	130.61	124.37
23	b	34	70U	C5-C4-N3	3.16	119.40	114.97
1	A	1541	PSU	C4-N3-C2	-3.10	121.87	126.34
23	b	37	12A	OO-CC-N6	-3.10	118.39	123.62
1	A	1540	PSU	C4-N3-C2	-3.06	121.92	126.34
23	b	39	PSU	C4-N3-C2	-2.98	122.04	126.34
12	L	92	0TD	CSB-SB-CB	-2.94	97.12	102.44
23	b	37	12A	N3-C2-N1	-2.88	121.69	126.98
23	b	34	70U	C5-C6-N1	-2.80	119.14	122.91
1	A	527	7MG	C2-N1-C6	-2.75	120.08	125.10
1	A	527	7MG	O6-C6-C5	-2.73	120.84	127.54
23	b	39	PSU	O2-C2-N1	-2.71	119.81	122.79
1	A	966	M2G	O6-C6-N1	-2.69	117.47	120.65
1	A	1498	UR3	C6-N1-C2	-2.68	119.39	121.79
23	b	37	12A	CA-N-CC	2.67	126.38	121.94
12	L	92	0TD	OD1-CG-CB	-2.62	116.95	122.44
1	A	516	PSU	C4-N3-C2	-2.62	122.56	126.34
1	A	1541	PSU	O2-C2-N1	-2.59	119.93	122.79
23	b	34	70U	O4-C4-C5	-2.57	121.13	124.96
1	A	1540	PSU	O2-C2-N1	-2.49	120.05	122.79
1	A	516	PSU	C6-C5-C4	-2.47	116.47	118.20
1	A	527	7MG	C6-C5-C4	-2.45	117.58	122.62
23	b	37	12A	C4-C5-N7	-2.43	106.87	109.40
1	A	1407	5MC	N4-C4-N3	-2.39	114.11	118.48
1	A	527	7MG	C6-C5-N7	2.36	135.63	131.91
1	A	967	5MC	N4-C4-N3	-2.33	114.22	118.48
1	A	1400	5MC	N4-C4-N3	-2.28	114.33	118.48
1	A	516	PSU	O2-C2-N1	-2.20	120.36	122.79
1	A	1404	5MC	C5-C4-N3	2.19	124.03	121.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1400	5MC	C5-C4-N3	2.17	124.01	121.67
1	A	1402	4OC	C5-C4-N4	-2.14	118.25	122.61
1	A	1407	5MC	C5-C4-N3	2.13	123.97	121.67
1	A	1518	MA6	N1-C6-N6	-2.13	114.82	117.06
23	b	34	70U	C5M-C5-C4	2.08	120.86	118.27
23	b	37	12A	C2-N1-C6	2.07	120.90	117.19
12	L	92	0TD	CB-CA-N	-2.04	104.75	109.10
1	A	967	5MC	C5-C4-N3	2.02	123.86	121.67
12	L	92	0TD	OD2-CG-CB	2.02	117.51	113.15

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	966	M2G	C4'-C5'-O5'-P
1	A	967	5MC	O4'-C4'-C5'-O5'
1	A	1402	4OC	O4'-C4'-C5'-O5'
1	A	1519	MA6	C5-C6-N6-C9
23	b	37	12A	N1-C2-S2-C2M
23	b	37	12A	N3-C2-S2-C2M
23	b	37	12A	C-CA-CB-OG1
23	b	37	12A	C-CA-CB-CG2
23	b	34	70U	C5M-C8-O9-C9
1	A	527	7MG	C3'-C4'-C5'-O5'
1	A	967	5MC	C3'-C4'-C5'-O5'
1	A	1402	4OC	C3'-C4'-C5'-O5'
1	A	1519	MA6	C3'-C4'-C5'-O5'
1	A	527	7MG	O4'-C4'-C5'-O5'
1	A	1519	MA6	O4'-C4'-C5'-O5'
23	b	34	70U	O8-C8-O9-C9
1	A	966	M2G	O4'-C4'-C5'-O5'
1	A	1400	5MC	O4'-C4'-C5'-O5'
1	A	1518	MA6	O4'-C4'-C5'-O5'
1	A	1519	MA6	C5-C6-N6-C10
1	A	1518	MA6	C3'-C4'-C5'-O5'
1	A	1400	5MC	C3'-C4'-C5'-O5'
23	b	37	12A	CB-CA-N-CC
1	A	966	M2G	C3'-C4'-C5'-O5'
12	L	92	0TD	CG-CB-SB-CSB
12	L	92	0TD	SB-CB-CG-OD1
23	b	37	12A	N-CA-CB-CG2
23	b	34	70U	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
23	b	34	70U	O4'-C4'-C5'-O5'
23	b	37	12A	C5-C6-N6-CC
1	A	1541	PSU	O4'-C1'-C5-C4
1	A	1519	MA6	N1-C6-N6-C9
12	L	92	0TD	SB-CB-CG-OD2
23	b	34	70U	C5-C5M-C8-O9

There are no ring outliers.

7 monomers are involved in 13 short contacts:

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 355 ligands modelled in this entry, 349 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	1603	-	45,45,45	1.42	6 (13%)	64,67,67	1.67	13 (20%)
24	PAR	A	1602	-	45,45,45	1.34	7 (15%)	64,67,67	1.66	12 (18%)
24	PAR	A	1605	-	45,45,45	1.30	6 (13%)	64,67,67	1.64	11 (17%)
24	PAR	A	1604	-	45,45,45	1.31	7 (15%)	64,67,67	1.64	13 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
24	PAR	A	1601	-	45,45,45	1.25	5 (11%)	64,67,67	1.63	12 (18%)
24	PAR	A	1606	-	45,45,45	1.33	5 (11%)	64,67,67	1.65	12 (18%)

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	1603	-	-	5/18/94/94	1/4/4/4
24	PAR	A	1602	-	-	4/18/94/94	0/4/4/4
24	PAR	A	1605	-	-	4/18/94/94	1/4/4/4
24	PAR	A	1604	-	-	5/18/94/94	1/4/4/4
24	PAR	A	1601	-	-	7/18/94/94	0/4/4/4
24	PAR	A	1606	-	-	5/18/94/94	1/4/4/4

All (36) 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	3.87	1.60	1.52
24	A	1602	PAR	C13-C23	3.56	1.57	1.52
24	A	1606	PAR	C13-C23	3.54	1.57	1.52
24	A	1603	PAR	C52-C42	3.52	1.59	1.52
24	A	1604	PAR	C52-C42	3.19	1.58	1.52
24	A	1605	PAR	C13-C23	3.14	1.56	1.52
24	A	1606	PAR	C64-C54	2.89	1.56	1.52
24	A	1606	PAR	C31-C21	2.87	1.57	1.53
24	A	1605	PAR	C52-C42	2.86	1.58	1.52
24	A	1606	PAR	C52-C42	2.82	1.58	1.52
24	A	1605	PAR	C34-C24	2.79	1.57	1.53
24	A	1604	PAR	C64-C54	2.77	1.55	1.52
24	A	1602	PAR	C64-C54	2.74	1.55	1.52
24	A	1605	PAR	C64-C54	2.73	1.55	1.52
24	A	1604	PAR	C13-C23	2.67	1.56	1.52
24	A	1601	PAR	C64-C54	2.65	1.55	1.52
24	A	1603	PAR	C64-C54	2.65	1.55	1.52
24	A	1603	PAR	O43-C13	2.62	1.46	1.41
24	A	1604	PAR	C34-C24	2.56	1.56	1.53
24	A	1606	PAR	C34-C24	2.55	1.56	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1602	PAR	C31-C21	2.45	1.56	1.53
24	A	1602	PAR	C34-C24	2.45	1.56	1.53
24	A	1603	PAR	C34-C24	2.40	1.56	1.53
24	A	1604	PAR	C31-C21	2.39	1.56	1.53
24	A	1602	PAR	C52-C42	2.36	1.57	1.52
24	A	1603	PAR	C14-C24	2.34	1.56	1.52
24	A	1601	PAR	C62-C52	2.25	1.58	1.52
24	A	1602	PAR	C14-C24	2.24	1.56	1.52
24	A	1604	PAR	C33-C43	2.22	1.58	1.52
24	A	1601	PAR	C13-C23	2.21	1.55	1.52
24	A	1605	PAR	C14-C24	2.19	1.56	1.52
24	A	1604	PAR	C14-C24	2.15	1.56	1.52
24	A	1602	PAR	C11-C21	2.14	1.56	1.52
24	A	1605	PAR	C33-C43	2.13	1.58	1.52
24	A	1601	PAR	C33-C43	2.05	1.58	1.52

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	1603	PAR	O33-C14-C24	6.15	118.80	108.22
24	A	1606	PAR	O33-C14-C24	6.11	118.73	108.22
24	A	1604	PAR	O33-C14-C24	6.10	118.72	108.22
24	A	1602	PAR	O33-C14-C24	6.09	118.70	108.22
24	A	1605	PAR	O33-C14-C24	6.06	118.66	108.22
24	A	1601	PAR	O33-C14-C24	6.04	118.61	108.22
24	A	1603	PAR	C13-C23-C33	3.87	106.75	102.10
24	A	1606	PAR	C13-C23-C33	3.65	106.49	102.10
24	A	1604	PAR	O52-C13-C23	3.56	115.34	107.96
24	A	1602	PAR	O52-C13-C23	3.52	115.26	107.96
24	A	1602	PAR	C13-C23-C33	3.49	106.30	102.10
24	A	1603	PAR	O52-C13-C23	3.39	114.98	107.96
24	A	1605	PAR	O52-C13-C23	3.37	114.95	107.96
24	A	1606	PAR	O52-C13-C23	3.33	114.85	107.96
24	A	1605	PAR	C13-C23-C33	3.22	105.97	102.10
24	A	1601	PAR	C34-C24-N24	-3.17	104.55	111.05
24	A	1603	PAR	C34-C24-N24	-3.13	104.63	111.05
24	A	1605	PAR	C34-C24-N24	-3.13	104.64	111.05
24	A	1601	PAR	O52-C13-C23	3.12	114.42	107.96
24	A	1606	PAR	C34-C24-N24	-3.08	104.75	111.05
24	A	1603	PAR	O34-C34-C44	-3.06	103.26	110.35
24	A	1601	PAR	O34-C34-C44	-3.05	103.30	110.35
24	A	1604	PAR	C34-C24-N24	-3.05	104.81	111.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	1602	PAR	C34-C24-N24	-3.05	104.81	111.05
24	A	1601	PAR	C13-C23-C33	3.01	105.72	102.10
24	A	1604	PAR	C13-C23-C33	3.01	105.72	102.10
24	A	1602	PAR	O34-C34-C44	-2.97	103.48	110.35
24	A	1604	PAR	O34-C34-C44	-2.96	103.50	110.35
24	A	1606	PAR	O34-C34-C44	-2.95	103.52	110.35
24	A	1602	PAR	O11-C11-O51	2.92	118.84	110.67
24	A	1605	PAR	O34-C34-C44	-2.91	103.63	110.35
24	A	1601	PAR	O11-C11-O51	2.90	118.76	110.67
24	A	1603	PAR	C14-O33-C33	-2.87	110.85	117.96
24	A	1606	PAR	O52-C13-O43	-2.87	108.33	111.43
24	A	1605	PAR	O11-C11-O51	2.80	118.49	110.67
24	A	1603	PAR	O11-C11-O51	2.76	118.37	110.67
24	A	1604	PAR	C13-O52-C52	-2.75	111.16	117.96
24	A	1606	PAR	C14-O33-C33	-2.73	111.21	117.96
24	A	1605	PAR	C14-O33-C33	-2.72	111.23	117.96
24	A	1604	PAR	C14-O33-C33	-2.71	111.26	117.96
24	A	1606	PAR	C13-O52-C52	-2.65	111.41	117.96
24	A	1604	PAR	O11-C11-O51	2.64	118.04	110.67
24	A	1602	PAR	C14-O33-C33	-2.63	111.45	117.96
24	A	1601	PAR	C14-O33-C33	-2.63	111.45	117.96
24	A	1601	PAR	O52-C13-O43	-2.62	108.59	111.43
24	A	1606	PAR	O11-C11-O51	2.59	117.90	110.67
24	A	1605	PAR	C13-O52-C52	-2.52	111.72	117.96
24	A	1603	PAR	C13-O52-C52	-2.49	111.80	117.96
24	A	1604	PAR	O52-C13-O43	-2.48	108.75	111.43
24	A	1602	PAR	C13-O52-C52	-2.47	111.85	117.96
24	A	1602	PAR	C22-C12-C62	2.44	113.72	110.04
24	A	1603	PAR	O52-C13-O43	-2.42	108.81	111.43
24	A	1605	PAR	O51-C51-C61	2.41	112.42	106.44
24	A	1605	PAR	O52-C13-O43	-2.40	108.83	111.43
24	A	1603	PAR	O51-C51-C61	2.39	112.37	106.44
24	A	1601	PAR	C11-O51-C51	2.36	118.31	113.69
24	A	1602	PAR	O51-C51-C61	2.29	112.13	106.44
24	A	1601	PAR	C13-O52-C52	-2.28	112.33	117.96
24	A	1602	PAR	C11-O51-C51	2.26	118.13	113.69
24	A	1606	PAR	O51-C51-C61	2.25	112.02	106.44
24	A	1604	PAR	O51-C51-C61	2.25	112.02	106.44
24	A	1602	PAR	O52-C13-O43	-2.24	109.00	111.43
24	A	1601	PAR	O51-C51-C61	2.18	111.87	106.44
24	A	1604	PAR	O54-C54-C44	2.17	113.64	109.69
24	A	1606	PAR	O54-C54-C44	2.16	113.62	109.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	1604	PAR	C22-C12-C62	2.12	113.25	110.04
24	A	1606	PAR	C22-C12-C62	2.12	113.23	110.04
24	A	1605	PAR	O54-C54-C44	2.07	113.45	109.69
24	A	1603	PAR	C11-O51-C51	2.06	117.74	113.69
24	A	1603	PAR	C22-C32-C42	2.04	114.68	109.53
24	A	1601	PAR	O54-C54-C44	2.03	113.38	109.69
24	A	1604	PAR	O52-C52-C42	2.01	112.59	107.48
24	A	1603	PAR	O52-C52-C42	2.00	112.57	107.48

There are no chirality outliers.

All (30) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
24	A	1604	PAR	C23-C33-O33-C14

All (4) ring outliers are listed below:

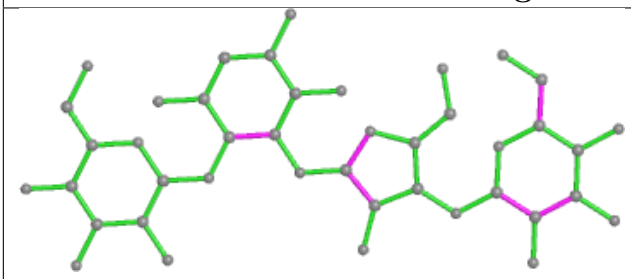
Mol	Chain	Res	Type	Atoms
24	A	1603	PAR	C12-C22-C32-C42-C52-C62
24	A	1605	PAR	C12-C22-C32-C42-C52-C62
24	A	1606	PAR	C12-C22-C32-C42-C52-C62
24	A	1604	PAR	C12-C22-C32-C42-C52-C62

5 monomers are involved in 13 short contacts:

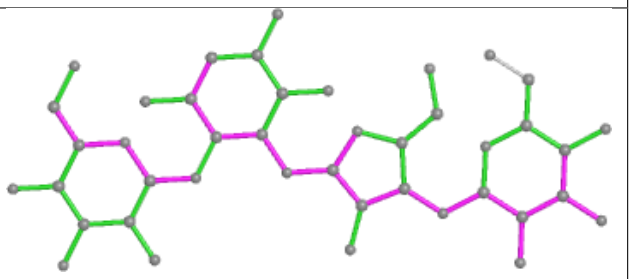
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A	1603	PAR	5	0
24	A	1602	PAR	2	0
24	A	1605	PAR	1	0
24	A	1604	PAR	3	0
24	A	1601	PAR	2	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

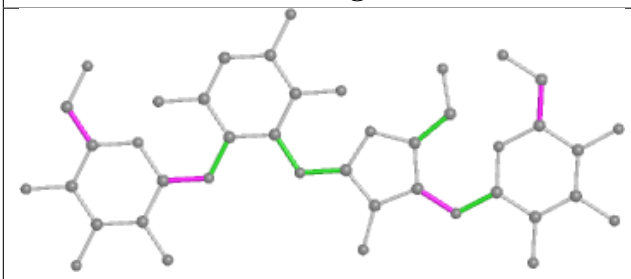
Ligand PAR A 1603



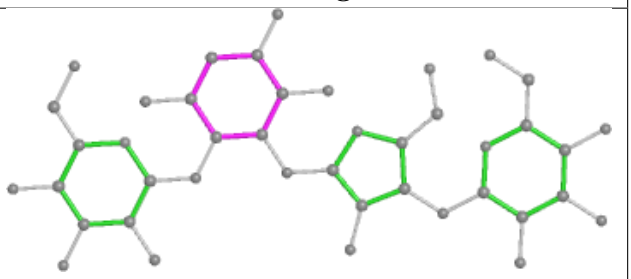
Bond lengths



Bond angles

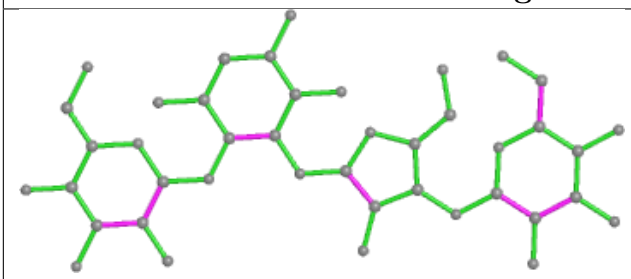


Torsions

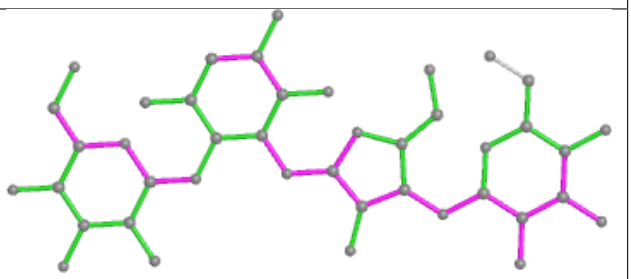


Rings

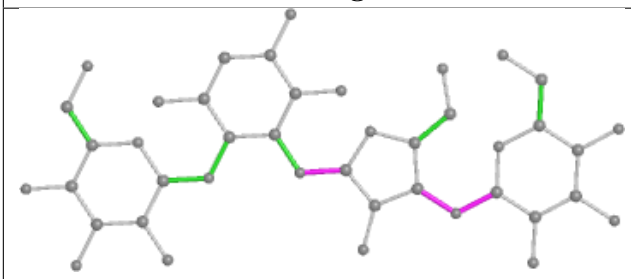
Ligand PAR A 1602



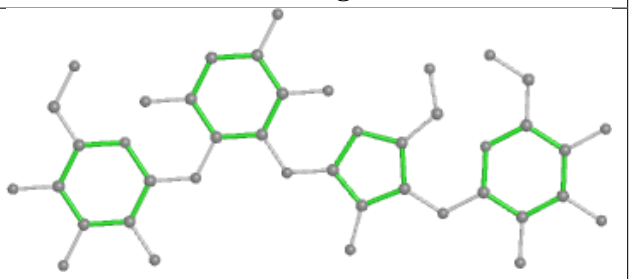
Bond lengths



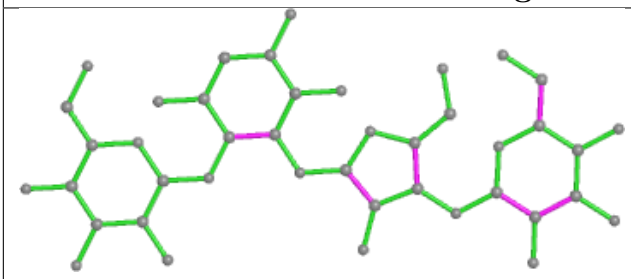
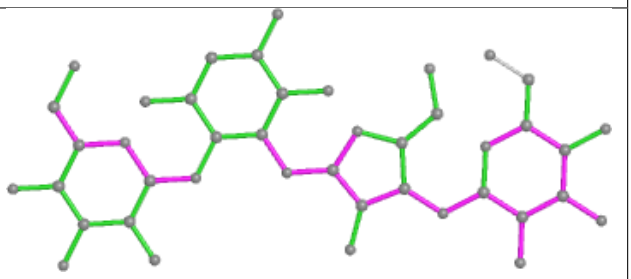
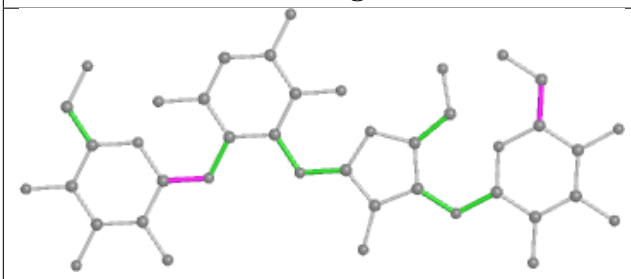
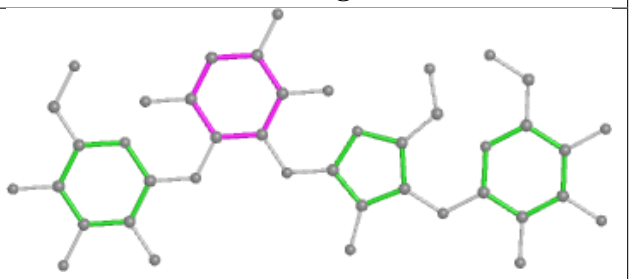
Bond angles

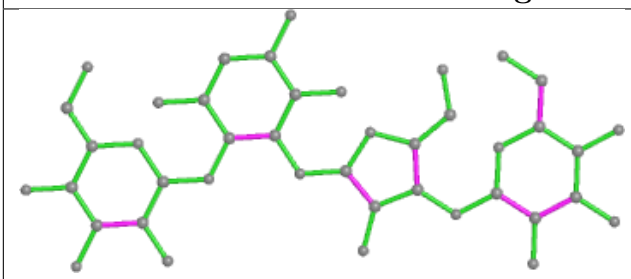
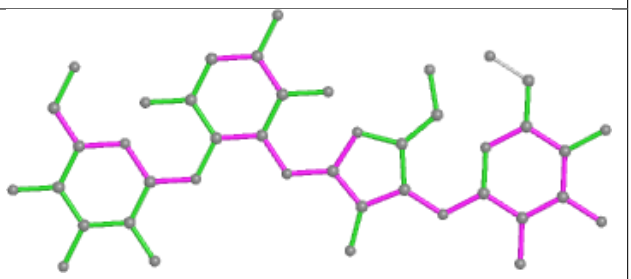
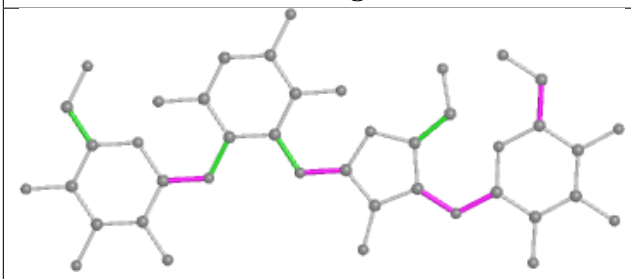
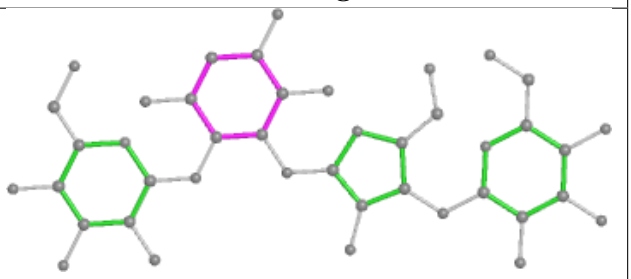


Torsions

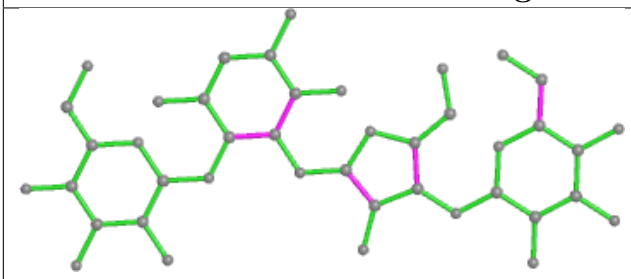


Rings

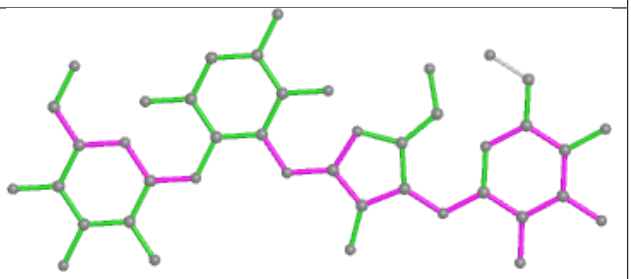
Ligand PAR A 1605	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PAR A 1604	
 Bond lengths	 Bond angles
 Torsions	 Rings

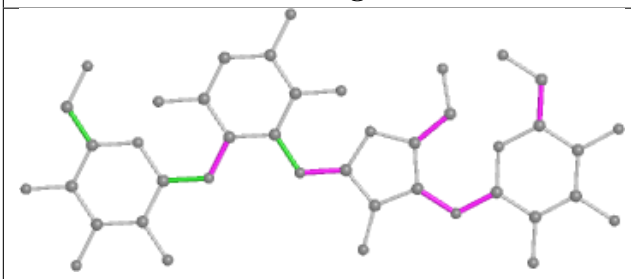
Ligand PAR A 1601



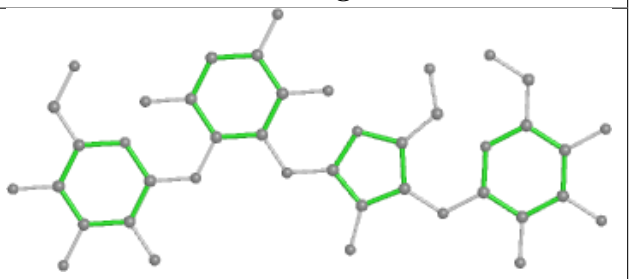
Bond lengths



Bond angles

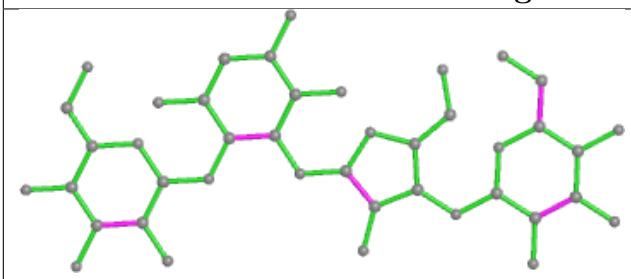


Torsions

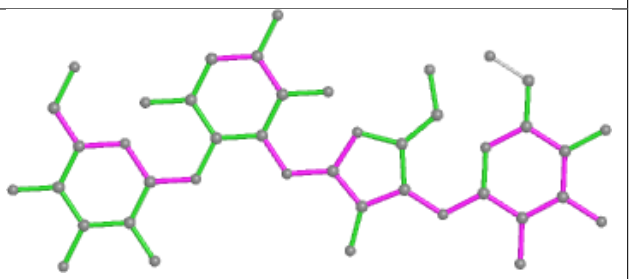


Rings

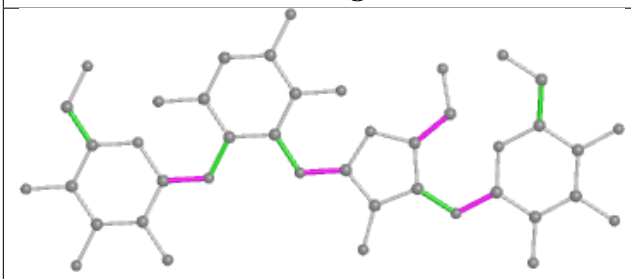
Ligand PAR A 1606



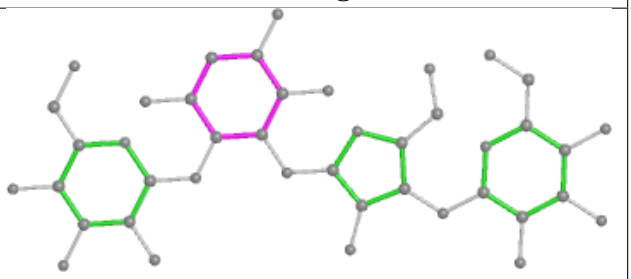
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (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%)	-0.22	5 (0%)	94	92	48, 77, 149, 270	0
2	B	236/236 (100%)	0.18	7 (2%)	50	48	71, 114, 202, 338	0
3	C	207/207 (100%)	-0.09	1 (0%)	91	89	42, 110, 165, 224	0
4	D	208/208 (100%)	-0.12	2 (0%)	82	79	59, 83, 129, 173	0
5	E	151/151 (100%)	-0.06	0	100	100	48, 73, 104, 190	0
6	F	101/101 (100%)	-0.11	1 (0%)	82	79	73, 110, 149, 183	0
7	G	155/155 (100%)	-0.17	1 (0%)	89	87	60, 92, 158, 228	0
8	H	138/138 (100%)	-0.09	0	100	100	50, 70, 95, 132	0
9	I	127/127 (100%)	0.37	4 (3%)	49	48	78, 111, 157, 196	0
10	J	99/99 (100%)	0.79	13 (13%)	3	5	64, 140, 237, 311	0
11	K	119/119 (100%)	0.21	3 (2%)	57	55	57, 76, 120, 171	0
12	L	124/125 (99%)	0.22	7 (5%)	24	25	44, 77, 115, 245	0
13	M	118/118 (100%)	0.44	5 (4%)	36	35	65, 96, 137, 217	0
14	N	60/60 (100%)	0.19	2 (3%)	46	45	80, 96, 154, 229	0
15	O	88/88 (100%)	0.11	2 (2%)	60	58	62, 86, 127, 184	0
16	P	84/84 (100%)	0.31	0	100	100	56, 69, 102, 156	0
17	Q	99/99 (100%)	0.18	0	100	100	53, 71, 119, 156	0
18	R	73/73 (100%)	0.09	2 (2%)	54	52	55, 89, 147, 202	0
19	S	81/81 (100%)	0.20	2 (2%)	57	55	39, 112, 196, 229	0
20	T	99/99 (100%)	0.24	2 (2%)	65	63	60, 74, 129, 193	0
21	U	25/25 (100%)	0.57	1 (4%)	38	37	48, 95, 133, 172	0
22	a	5/6 (83%)	0.96	0	100	100	89, 95, 127, 140	0
23	b	8/11 (72%)	0.08	0	100	100	91, 127, 166, 178	0
All	All	3903/3932 (99%)	-0.01	60 (1%)	73	71	39, 87, 159, 338	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	K	129	SER	7.5
11	K	128	ALA	6.2
15	O	89	GLY	5.8
2	B	131	PRO	5.5
14	N	12	ARG	4.9
10	J	34	VAL	4.4
15	O	88	ARG	4.4
2	B	134	GLU	4.0
2	B	130	ARG	3.9
10	J	5	ARG	3.8
9	I	128	ARG	3.6
13	M	7	VAL	3.4
9	I	15	ALA	3.3
14	N	13	THR	3.3
18	R	17	SER	3.2
2	B	132	LYS	3.1
13	M	2	ALA	3.1
10	J	6	ILE	3.1
20	T	100	ILE	3.1
11	K	127	LYS	3.1
4	D	179	GLU	2.9
2	B	127	ILE	2.8
1	A	1129	C	2.8
12	L	129	ALA	2.8
12	L	19	ARG	2.7
1	A	81	U	2.7
3	C	206	GLU	2.7
10	J	22	LYS	2.6
10	J	72	VAL	2.6
6	F	14	LEU	2.6
7	G	82	GLY	2.6
1	A	1533	C	2.6
13	M	119	GLY	2.6
10	J	74	ILE	2.5
12	L	28	LYS	2.5
2	B	135	GLN	2.5
10	J	7	LYS	2.4
12	L	128	ALA	2.4
18	R	16	PRO	2.4
12	L	127	GLU	2.3
10	J	25	GLU	2.3
20	T	9	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
19	S	28	LYS	2.2
1	A	723	U	2.2
13	M	15	VAL	2.2
10	J	90	LEU	2.2
10	J	70	ARG	2.2
19	S	27	GLU	2.2
10	J	73	ASP	2.1
4	D	23	GLY	2.1
12	L	20	LYS	2.1
2	B	36	ARG	2.1
21	U	18	TYR	2.1
9	I	8	GLY	2.1
10	J	10	GLY	2.1
9	I	67	GLY	2.0
10	J	8	LEU	2.0
12	L	62	SER	2.0
1	A	1531	A	2.0
13	M	8	GLU	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	0.84	0.30	165,171,179,181	0
12	0TD	L	92	10/11	0.88	0.35	70,79,96,100	0
1	PSU	A	1541	20/21	0.91	0.21	164,174,180,214	0
23	PSU	b	39	20/21	0.91	0.16	114,128,144,147	0
22	6MZ	a	3	23/24	0.92	0.24	86,98,109,113	0
23	70U	b	34	25/26	0.92	0.21	84,105,118,130	0
1	PSU	A	516	20/21	0.92	0.17	78,81,85,86	0
1	7MG	A	527	24/25	0.94	0.19	63,66,67,67	0
23	12A	b	37	34/35	0.94	0.20	82,96,119,122	0
1	M2G	A	966	25/26	0.94	0.20	67,68,87,95	0
1	2MG	A	1207	24/25	0.95	0.17	95,100,106,108	0
1	5MC	A	1400	21/22	0.95	0.21	64,65,69,74	0
1	4OC	A	1402	22/23	0.95	0.19	62,65,68,71	0
1	5MC	A	1407	21/22	0.95	0.17	68,69,71,72	0
1	MA6	A	1518	24/25	0.95	0.17	59,62,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	5MC	A	967	21/22	0.95	0.16	68,73,80,84	0
1	UR3	A	1498	21/22	0.96	0.20	57,59,62,63	0
1	MA6	A	1519	24/25	0.97	0.21	58,60,62,62	0
1	5MC	A	1404	21/22	0.97	0.18	62,63,64,65	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
25	MG	A	1796	1/1	0.31	0.38	71,71,71,71	0
26	K	A	1893	1/1	0.40	0.18	131,131,131,131	0
25	MG	H	202	1/1	0.42	0.36	84,84,84,84	0
25	MG	A	1820	1/1	0.42	0.84	74,74,74,74	0
25	MG	A	1775	1/1	0.43	0.65	99,99,99,99	0
25	MG	A	1748	1/1	0.44	0.66	85,85,85,85	0
25	MG	A	1667	1/1	0.54	0.50	52,52,52,52	0
25	MG	A	1772	1/1	0.55	0.57	62,62,62,62	0
26	K	A	1907	1/1	0.55	0.81	131,131,131,131	0
25	MG	A	1717	1/1	0.56	0.25	61,61,61,61	0
25	MG	Q	202	1/1	0.56	0.61	67,67,67,67	0
25	MG	A	1824	1/1	0.56	0.56	66,66,66,66	0
25	MG	C	301	1/1	0.56	0.40	82,82,82,82	0
25	MG	P	102	1/1	0.57	0.26	71,71,71,71	0
25	MG	A	1607	1/1	0.57	0.46	87,87,87,87	0
25	MG	H	201	1/1	0.58	0.44	61,61,61,61	0
26	K	A	1913	1/1	0.58	0.71	139,139,139,139	0
25	MG	A	1765	1/1	0.59	0.60	66,66,66,66	0
25	MG	L	201	1/1	0.60	0.49	64,64,64,64	0
25	MG	A	1852	1/1	0.60	0.49	73,73,73,73	0
25	MG	A	1753	1/1	0.60	0.50	84,84,84,84	0
25	MG	A	1868	1/1	0.61	0.32	71,71,71,71	0
25	MG	A	1855	1/1	0.61	0.54	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
25	MG	A	1819	1/1	0.62	0.49	74,74,74,74	0
25	MG	A	1866	1/1	0.62	0.48	46,46,46,46	0
26	K	A	1892	1/1	0.63	0.28	111,111,111,111	0
25	MG	A	1720	1/1	0.64	0.51	37,37,37,37	0
25	MG	A	1812	1/1	0.64	0.25	59,59,59,59	0
25	MG	A	1822	1/1	0.64	0.48	56,56,56,56	0
25	MG	A	1797	1/1	0.65	0.66	69,69,69,69	0
26	K	A	1912	1/1	0.65	0.41	116,116,116,116	0
25	MG	A	1827	1/1	0.65	0.31	65,65,65,65	0
26	K	A	1898	1/1	0.66	0.13	120,120,120,120	0
25	MG	A	1663	1/1	0.66	0.37	50,50,50,50	0
25	MG	A	1864	1/1	0.67	0.91	67,67,67,67	0
25	MG	A	1813	1/1	0.67	0.36	64,64,64,64	0
25	MG	A	1727	1/1	0.67	0.28	126,126,126,126	0
25	MG	A	1648	1/1	0.68	0.23	61,61,61,61	0
25	MG	G	201	1/1	0.69	0.54	52,52,52,52	0
25	MG	A	1830	1/1	0.70	0.99	95,95,95,95	0
26	K	A	1905	1/1	0.70	0.56	117,117,117,117	0
26	K	A	1891	1/1	0.70	0.88	142,142,142,142	0
25	MG	A	1782	1/1	0.70	0.42	63,63,63,63	0
25	MG	A	1881	1/1	0.70	0.39	79,79,79,79	0
26	K	A	1928	1/1	0.71	0.34	131,131,131,131	0
25	MG	A	1616	1/1	0.72	0.34	78,78,78,78	0
25	MG	A	1770	1/1	0.72	0.45	71,71,71,71	0
25	MG	A	1735	1/1	0.72	0.41	58,58,58,58	0
25	MG	A	1885	1/1	0.72	0.53	63,63,63,63	0
26	K	A	1889	1/1	0.73	0.36	124,124,124,124	0
26	K	A	1919	1/1	0.73	0.21	102,102,102,102	0
26	K	A	1923	1/1	0.73	0.26	113,113,113,113	0
25	MG	A	1844	1/1	0.73	0.26	65,65,65,65	0
25	MG	A	1843	1/1	0.74	0.18	70,70,70,70	0
25	MG	A	1865	1/1	0.74	0.17	67,67,67,67	0
25	MG	A	1876	1/1	0.74	0.25	80,80,80,80	0
26	K	A	1902	1/1	0.75	0.35	129,129,129,129	0
26	K	A	1888	1/1	0.75	0.55	113,113,113,113	0
25	MG	A	1709	1/1	0.75	0.49	162,162,162,162	0
25	MG	A	1848	1/1	0.75	0.48	61,61,61,61	0
26	K	A	1904	1/1	0.76	0.58	138,138,138,138	0
25	MG	A	1794	1/1	0.76	0.23	131,131,131,131	0
25	MG	A	1808	1/1	0.76	0.45	52,52,52,52	0
24	PAR	A	1602	42/42	0.76	0.45	120,192,236,255	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
25	MG	A	1762	1/1	0.77	0.34	67,67,67,67	0
25	MG	A	1860	1/1	0.77	0.23	56,56,56,56	0
25	MG	A	1732	1/1	0.77	0.27	66,66,66,66	0
25	MG	A	1847	1/1	0.77	0.61	51,51,51,51	0
25	MG	A	1778	1/1	0.77	0.29	82,82,82,82	0
26	K	A	1903	1/1	0.77	0.39	118,118,118,118	0
25	MG	A	1755	1/1	0.77	0.21	40,40,40,40	0
25	MG	A	1836	1/1	0.78	0.37	55,55,55,55	0
25	MG	A	1639	1/1	0.78	0.70	52,52,52,52	0
25	MG	A	1790	1/1	0.79	0.26	120,120,120,120	0
25	MG	A	1771	1/1	0.79	0.30	68,68,68,68	0
25	MG	A	1728	1/1	0.79	0.19	41,41,41,41	0
25	MG	A	1763	1/1	0.79	0.33	74,74,74,74	0
25	MG	A	1629	1/1	0.79	0.39	63,63,63,63	0
25	MG	A	1672	1/1	0.79	0.25	44,44,44,44	0
25	MG	Q	201	1/1	0.79	0.12	92,92,92,92	0
26	K	A	1926	1/1	0.79	0.32	119,119,119,119	0
25	MG	A	1788	1/1	0.79	0.41	68,68,68,68	0
25	MG	A	1773	1/1	0.80	0.30	30,30,30,30	0
25	MG	A	1795	1/1	0.80	0.37	75,75,75,75	0
25	MG	A	1837	1/1	0.80	0.40	70,70,70,70	0
25	MG	A	1724	1/1	0.80	0.38	60,60,60,60	0
25	MG	A	1871	1/1	0.80	0.14	58,58,58,58	0
25	MG	A	1857	1/1	0.80	0.20	45,45,45,45	0
26	K	A	1915	1/1	0.80	0.31	146,146,146,146	0
26	K	A	1894	1/1	0.80	0.41	100,100,100,100	0
26	K	A	1896	1/1	0.80	0.15	132,132,132,132	0
25	MG	A	1878	1/1	0.80	0.57	56,56,56,56	0
25	MG	A	1686	1/1	0.80	0.40	33,33,33,33	0
26	K	G	202	1/1	0.80	0.81	143,143,143,143	0
25	MG	A	1673	1/1	0.81	0.37	56,56,56,56	0
25	MG	A	1682	1/1	0.81	0.30	66,66,66,66	0
24	PAR	A	1603	42/42	0.81	0.38	92,128,169,179	0
26	K	A	1897	1/1	0.81	0.52	98,98,98,98	0
26	K	A	1886	1/1	0.81	0.21	107,107,107,107	0
25	MG	A	1816	1/1	0.81	0.47	50,50,50,50	0
25	MG	A	1817	1/1	0.81	0.23	52,52,52,52	0
26	K	A	1927	1/1	0.81	0.37	115,115,115,115	0
24	PAR	A	1605	42/42	0.81	0.35	149,168,179,187	0
25	MG	A	1623	1/1	0.81	0.28	46,46,46,46	0
25	MG	A	1783	1/1	0.82	0.28	54,54,54,54	0
25	MG	A	1745	1/1	0.82	0.27	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
25	MG	A	1633	1/1	0.82	0.54	50,50,50,50	0
25	MG	A	1751	1/1	0.82	0.13	54,54,54,54	0
26	K	A	1925	1/1	0.82	0.21	92,92,92,92	0
26	K	A	1895	1/1	0.82	0.21	81,81,81,81	0
26	K	A	1906	1/1	0.82	0.31	92,92,92,92	0
25	MG	A	1825	1/1	0.82	0.60	78,78,78,78	0
25	MG	A	1884	1/1	0.82	0.26	59,59,59,59	0
26	K	A	1900	1/1	0.83	0.24	113,113,113,113	0
25	MG	A	1873	1/1	0.83	0.24	66,66,66,66	0
25	MG	A	1725	1/1	0.83	0.33	64,64,64,64	0
26	K	A	1922	1/1	0.83	0.32	99,99,99,99	0
25	MG	A	1877	1/1	0.83	0.35	69,69,69,69	0
25	MG	A	1736	1/1	0.83	0.45	55,55,55,55	0
25	MG	A	1870	1/1	0.83	0.60	58,58,58,58	0
25	MG	A	1832	1/1	0.83	0.24	57,57,57,57	0
26	K	A	1910	1/1	0.83	0.35	126,126,126,126	0
25	MG	P	101	1/1	0.83	0.36	38,38,38,38	0
25	MG	A	1883	1/1	0.84	0.36	59,59,59,59	0
25	MG	A	1801	1/1	0.84	0.27	70,70,70,70	0
25	MG	A	1804	1/1	0.84	0.27	61,61,61,61	0
25	MG	A	1692	1/1	0.84	0.14	89,89,89,89	0
25	MG	A	1766	1/1	0.84	0.89	56,56,56,56	0
25	MG	A	1679	1/1	0.84	0.37	78,78,78,78	0
26	K	A	1929	1/1	0.84	1.43	127,127,127,127	0
25	MG	A	1746	1/1	0.84	0.17	55,55,55,55	0
25	MG	A	1802	1/1	0.85	0.38	63,63,63,63	0
25	MG	A	1823	1/1	0.85	0.31	63,63,63,63	0
25	MG	A	1688	1/1	0.85	0.11	68,68,68,68	0
25	MG	A	1635	1/1	0.85	0.32	46,46,46,46	0
25	MG	A	1774	1/1	0.85	0.31	59,59,59,59	0
25	MG	A	1609	1/1	0.85	0.18	96,96,96,96	0
25	MG	A	1742	1/1	0.85	0.35	63,63,63,63	0
25	MG	A	1863	1/1	0.85	0.37	60,60,60,60	0
26	K	A	1887	1/1	0.85	0.29	104,104,104,104	0
25	MG	A	1730	1/1	0.85	0.21	59,59,59,59	0
25	MG	A	1798	1/1	0.85	0.34	46,46,46,46	0
25	MG	A	1841	1/1	0.85	0.26	103,103,103,103	0
25	MG	A	1759	1/1	0.85	0.23	47,47,47,47	0
25	MG	A	1625	1/1	0.86	0.28	61,61,61,61	0
25	MG	A	1650	1/1	0.86	0.25	41,41,41,41	0
25	MG	A	1767	1/1	0.86	0.26	55,55,55,55	0
26	K	A	1899	1/1	0.86	0.19	117,117,117,117	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
25	MG	A	1704	1/1	0.86	0.24	51,51,51,51	0
25	MG	A	1677	1/1	0.86	0.21	86,86,86,86	0
25	MG	A	1879	1/1	0.86	0.33	51,51,51,51	0
25	MG	A	1831	1/1	0.86	0.28	58,58,58,58	0
25	MG	A	1793	1/1	0.87	0.22	181,181,181,181	0
25	MG	A	1777	1/1	0.87	0.37	72,72,72,72	0
25	MG	A	1833	1/1	0.87	0.25	45,45,45,45	0
25	MG	A	1867	1/1	0.87	0.67	43,43,43,43	0
25	MG	A	1882	1/1	0.87	0.35	67,67,67,67	0
25	MG	A	1784	1/1	0.87	0.17	35,35,35,35	0
25	MG	A	1803	1/1	0.87	0.55	38,38,38,38	0
25	MG	A	1839	1/1	0.87	0.19	51,51,51,51	0
25	MG	A	1645	1/1	0.87	0.17	128,128,128,128	0
25	MG	A	1731	1/1	0.87	0.62	58,58,58,58	0
25	MG	A	1738	1/1	0.88	0.25	52,52,52,52	0
25	MG	A	1826	1/1	0.88	0.21	40,40,40,40	0
25	MG	a	101	1/1	0.88	0.56	50,50,50,50	0
25	MG	A	1726	1/1	0.88	0.67	58,58,58,58	0
25	MG	A	1743	1/1	0.88	0.22	81,81,81,81	0
25	MG	A	1815	1/1	0.88	0.17	29,29,29,29	0
25	MG	A	1641	1/1	0.88	0.16	66,66,66,66	0
25	MG	A	1733	1/1	0.88	0.48	53,53,53,53	0
25	MG	A	1834	1/1	0.88	0.17	44,44,44,44	0
26	K	A	1918	1/1	0.88	0.38	127,127,127,127	0
25	MG	A	1818	1/1	0.88	0.23	72,72,72,72	0
25	MG	A	1785	1/1	0.88	0.33	85,85,85,85	0
25	MG	D	302	1/1	0.88	0.13	72,72,72,72	0
25	MG	A	1787	1/1	0.88	0.41	43,43,43,43	0
25	MG	A	1691	1/1	0.88	0.23	50,50,50,50	0
25	MG	A	1842	1/1	0.88	0.22	57,57,57,57	0
24	PAR	A	1604	42/42	0.88	0.25	83,126,184,192	0
25	MG	A	1791	1/1	0.88	0.11	104,104,104,104	0
25	MG	A	1875	1/1	0.88	0.33	65,65,65,65	0
25	MG	A	1754	1/1	0.89	0.27	52,52,52,52	0
25	MG	A	1744	1/1	0.89	0.21	51,51,51,51	0
25	MG	S	102	1/1	0.89	0.11	43,43,43,43	0
25	MG	S	103	1/1	0.89	0.11	71,71,71,71	0
25	MG	A	1758	1/1	0.89	0.24	59,59,59,59	0
25	MG	A	1874	1/1	0.89	0.21	58,58,58,58	0
25	MG	A	1729	1/1	0.89	0.25	51,51,51,51	0
25	MG	A	1710	1/1	0.89	0.21	64,64,64,64	0
25	MG	A	1621	1/1	0.89	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	1846	1/1	0.89	0.23	41,41,41,41	0
25	MG	A	1689	1/1	0.89	0.23	135,135,135,135	0
25	MG	A	1681	1/1	0.89	0.40	198,198,198,198	0
25	MG	A	1851	1/1	0.89	0.16	60,60,60,60	0
26	K	A	1911	1/1	0.90	0.16	70,70,70,70	0
25	MG	A	1680	1/1	0.90	0.25	55,55,55,55	0
25	MG	A	1853	1/1	0.90	0.21	49,49,49,49	0
25	MG	A	1806	1/1	0.90	0.15	56,56,56,56	0
25	MG	A	1671	1/1	0.90	0.28	30,30,30,30	0
25	MG	A	1701	1/1	0.90	0.32	53,53,53,53	0
25	MG	E	201	1/1	0.90	0.14	80,80,80,80	0
25	MG	A	1644	1/1	0.90	0.15	60,60,60,60	0
25	MG	A	1640	1/1	0.90	0.27	128,128,128,128	0
25	MG	A	1835	1/1	0.90	0.28	55,55,55,55	0
24	PAR	A	1606	42/42	0.90	0.24	100,122,134,139	0
25	MG	A	1849	1/1	0.90	0.16	57,57,57,57	0
25	MG	A	1670	1/1	0.90	0.30	55,55,55,55	0
26	K	E	202	1/1	0.90	0.28	80,80,80,80	0
25	MG	P	103	1/1	0.90	0.37	65,65,65,65	0
25	MG	A	1757	1/1	0.91	0.20	34,34,34,34	0
25	MG	A	1828	1/1	0.91	0.59	72,72,72,72	0
25	MG	A	1845	1/1	0.91	0.16	32,32,32,32	0
25	MG	A	1613	1/1	0.91	0.20	49,49,49,49	0
25	MG	A	1723	1/1	0.91	0.41	31,31,31,31	0
25	MG	A	1760	1/1	0.91	0.14	35,35,35,35	0
25	MG	A	1658	1/1	0.91	0.21	40,40,40,40	0
26	K	A	1917	1/1	0.91	0.38	122,122,122,122	0
25	MG	A	1789	1/1	0.91	0.13	60,60,60,60	0
25	MG	A	1821	1/1	0.91	0.27	32,32,32,32	0
25	MG	A	1741	1/1	0.91	0.26	49,49,49,49	0
25	MG	A	1695	1/1	0.91	0.23	51,51,51,51	0
25	MG	A	1697	1/1	0.91	0.33	51,51,51,51	0
25	MG	A	1840	1/1	0.91	0.25	76,76,76,76	0
26	K	A	1901	1/1	0.91	0.24	112,112,112,112	0
25	MG	A	1861	1/1	0.91	0.38	73,73,73,73	0
25	MG	A	1862	1/1	0.91	0.24	53,53,53,53	0
25	MG	A	1781	1/1	0.91	0.25	58,58,58,58	0
25	MG	A	1700	1/1	0.91	0.34	35,35,35,35	0
25	MG	A	1810	1/1	0.92	0.08	195,195,195,195	0
25	MG	A	1811	1/1	0.92	0.19	41,41,41,41	0
26	K	A	1909	1/1	0.92	0.36	102,102,102,102	0
25	MG	A	1687	1/1	0.92	0.21	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	PAR	A	1601	42/42	0.92	0.24	50,61,121,159	0
25	MG	A	1814	1/1	0.92	0.25	56,56,56,56	0
25	MG	A	1737	1/1	0.92	0.15	62,62,62,62	0
25	MG	A	1869	1/1	0.92	0.26	58,58,58,58	0
25	MG	A	1611	1/1	0.92	0.18	37,37,37,37	0
25	MG	A	1637	1/1	0.92	0.41	52,52,52,52	0
25	MG	A	1715	1/1	0.92	0.55	102,102,102,102	0
26	K	A	1920	1/1	0.92	0.14	100,100,100,100	0
25	MG	A	1651	1/1	0.92	0.11	32,32,32,32	0
25	MG	A	1652	1/1	0.92	0.22	56,56,56,56	0
25	MG	A	1684	1/1	0.92	0.17	73,73,73,73	0
25	MG	A	1838	1/1	0.92	0.23	59,59,59,59	0
25	MG	A	1858	1/1	0.92	0.20	64,64,64,64	0
25	MG	A	1761	1/1	0.92	0.23	54,54,54,54	0
25	MG	A	1638	1/1	0.92	0.06	46,46,46,46	0
25	MG	A	1792	1/1	0.92	0.11	173,173,173,173	0
25	MG	b	101	1/1	0.92	0.13	46,46,46,46	0
25	MG	A	1636	1/1	0.93	0.20	44,44,44,44	0
25	MG	A	1780	1/1	0.93	0.16	42,42,42,42	0
25	MG	A	1872	1/1	0.93	0.20	49,49,49,49	0
25	MG	A	1659	1/1	0.93	0.20	92,92,92,92	0
25	MG	A	1718	1/1	0.93	0.26	32,32,32,32	0
26	K	A	1908	1/1	0.93	0.12	77,77,77,77	0
25	MG	A	1696	1/1	0.93	0.19	269,269,269,269	0
25	MG	A	1829	1/1	0.93	0.25	62,62,62,62	0
25	MG	A	1685	1/1	0.93	0.54	80,80,80,80	0
25	MG	A	1661	1/1	0.93	0.18	57,57,57,57	0
25	MG	A	1854	1/1	0.93	0.22	48,48,48,48	0
25	MG	A	1614	1/1	0.93	0.06	72,72,72,72	0
25	MG	A	1764	1/1	0.93	0.15	53,53,53,53	0
25	MG	A	1702	1/1	0.93	0.08	113,113,113,113	0
25	MG	A	1664	1/1	0.93	0.14	68,68,68,68	0
25	MG	A	1706	1/1	0.93	0.20	54,54,54,54	0
25	MG	A	1707	1/1	0.93	0.14	106,106,106,106	0
25	MG	A	1708	1/1	0.93	0.12	39,39,39,39	0
26	K	A	1924	1/1	0.93	0.17	113,113,113,113	0
25	MG	A	1752	1/1	0.93	0.10	38,38,38,38	0
25	MG	A	1631	1/1	0.93	0.19	75,75,75,75	0
25	MG	A	1653	1/1	0.93	0.19	105,105,105,105	0
25	MG	A	1714	1/1	0.93	0.12	159,159,159,159	0
25	MG	A	1756	1/1	0.93	0.21	61,61,61,61	0
25	MG	L	202	1/1	0.93	0.09	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
25	MG	A	1800	1/1	0.93	0.13	68,68,68,68	0
25	MG	A	1619	1/1	0.94	0.10	69,69,69,69	0
26	K	A	1916	1/1	0.94	0.27	108,108,108,108	0
25	MG	A	1722	1/1	0.94	0.24	31,31,31,31	0
25	MG	A	1665	1/1	0.94	0.24	86,86,86,86	0
25	MG	A	1666	1/1	0.94	0.19	75,75,75,75	0
25	MG	A	1850	1/1	0.94	0.21	30,30,30,30	0
25	MG	A	1734	1/1	0.94	0.25	45,45,45,45	0
26	K	A	1890	1/1	0.94	0.22	89,89,89,89	0
25	MG	A	1610	1/1	0.94	0.09	101,101,101,101	0
25	MG	A	1750	1/1	0.94	0.21	54,54,54,54	0
25	MG	A	1694	1/1	0.94	0.18	122,122,122,122	0
25	MG	P	104	1/1	0.94	0.57	72,72,72,72	0
25	MG	A	1776	1/1	0.94	0.16	47,47,47,47	0
25	MG	A	1716	1/1	0.94	0.42	79,79,79,79	0
25	MG	A	1668	1/1	0.94	0.38	30,30,30,30	0
25	MG	A	1647	1/1	0.94	0.20	78,78,78,78	0
25	MG	A	1711	1/1	0.95	0.18	61,61,61,61	0
25	MG	A	1712	1/1	0.95	0.13	20,20,20,20	0
25	MG	A	1675	1/1	0.95	0.16	80,80,80,80	0
25	MG	A	1676	1/1	0.95	0.17	49,49,49,49	0
25	MG	A	1693	1/1	0.95	0.19	67,67,67,67	0
25	MG	A	1649	1/1	0.95	0.10	35,35,35,35	0
25	MG	A	1678	1/1	0.95	0.17	69,69,69,69	0
25	MG	A	1634	1/1	0.95	0.12	103,103,103,103	0
25	MG	A	1721	1/1	0.95	0.40	204,204,204,204	0
25	MG	A	1786	1/1	0.95	0.15	49,49,49,49	0
25	MG	A	1646	1/1	0.95	0.18	38,38,38,38	0
25	MG	A	1930	1/1	0.95	0.07	57,57,57,57	0
25	MG	S	101	1/1	0.95	0.22	30,30,30,30	0
25	MG	A	1674	1/1	0.95	0.14	65,65,65,65	0
25	MG	A	1749	1/1	0.95	0.12	34,34,34,34	0
26	K	A	1914	1/1	0.95	0.11	124,124,124,124	0
27	ZN	N	101	1/1	0.95	0.11	77,77,77,77	0
25	MG	A	1642	1/1	0.96	0.14	75,75,75,75	0
25	MG	A	1719	1/1	0.96	0.06	43,43,43,43	0
25	MG	A	1769	1/1	0.96	0.13	70,70,70,70	0
25	MG	A	1779	1/1	0.96	0.38	26,26,26,26	0
25	MG	A	1713	1/1	0.96	0.18	242,242,242,242	0
25	MG	A	1655	1/1	0.96	0.23	52,52,52,52	0
25	MG	A	1880	1/1	0.96	0.22	48,48,48,48	0
25	MG	A	1690	1/1	0.96	0.12	84,84,84,84	0

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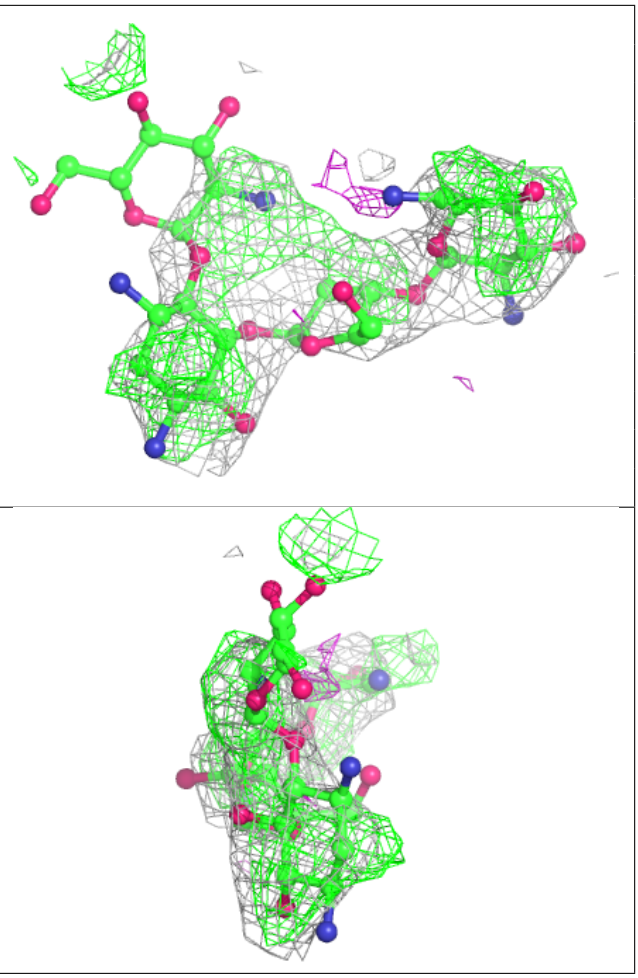
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
25	MG	A	1669	1/1	0.96	0.18	42,42,42,42	0
25	MG	A	1805	1/1	0.96	0.11	39,39,39,39	0
25	MG	A	1632	1/1	0.96	0.39	26,26,26,26	0
25	MG	A	1856	1/1	0.96	0.41	53,53,53,53	0
25	MG	A	1739	1/1	0.96	0.12	14,14,14,14	0
25	MG	A	1809	1/1	0.96	0.10	160,160,160,160	0
25	MG	A	1859	1/1	0.96	0.18	61,61,61,61	0
25	MG	T	201	1/1	0.96	0.12	38,38,38,38	0
25	MG	A	1624	1/1	0.97	0.12	51,51,51,51	0
25	MG	A	1612	1/1	0.97	0.08	56,56,56,56	0
26	K	A	1921	1/1	0.97	0.29	125,125,125,125	0
25	MG	A	1698	1/1	0.97	0.14	48,48,48,48	0
25	MG	A	1626	1/1	0.97	0.14	47,47,47,47	0
25	MG	A	1662	1/1	0.97	0.24	115,115,115,115	0
25	MG	A	1627	1/1	0.97	0.12	48,48,48,48	0
25	MG	A	1617	1/1	0.97	0.19	23,23,23,23	0
25	MG	A	1705	1/1	0.97	0.13	83,83,83,83	0
25	MG	A	1622	1/1	0.97	0.11	29,29,29,29	0
25	MG	A	1740	1/1	0.97	0.14	70,70,70,70	0
25	MG	A	1618	1/1	0.97	0.17	97,97,97,97	0
25	MG	A	1657	1/1	0.97	0.12	18,18,18,18	0
25	MG	A	1768	1/1	0.97	0.17	46,46,46,46	0
25	MG	F	201	1/1	0.98	0.08	52,52,52,52	0
25	MG	A	1683	1/1	0.98	0.09	68,68,68,68	0
25	MG	A	1807	1/1	0.98	0.15	42,42,42,42	0
25	MG	A	1608	1/1	0.98	0.15	67,67,67,67	0
25	MG	A	1747	1/1	0.98	0.08	59,59,59,59	0
25	MG	A	1656	1/1	0.98	0.08	85,85,85,85	0
25	MG	A	1799	1/1	0.98	0.11	73,73,73,73	0
25	MG	A	1703	1/1	0.98	0.12	65,65,65,65	0
25	MG	A	1628	1/1	0.98	0.19	42,42,42,42	0
25	MG	A	1615	1/1	0.98	0.09	34,34,34,34	0
25	MG	A	1630	1/1	0.98	0.28	10,10,10,10	0
25	MG	A	1660	1/1	0.98	0.11	18,18,18,18	0
27	ZN	D	301	1/1	0.98	0.26	46,46,46,46	0
25	MG	A	1643	1/1	0.98	0.49	92,92,92,92	0
25	MG	A	1654	1/1	0.99	0.11	57,57,57,57	0
25	MG	A	1699	1/1	0.99	0.26	21,21,21,21	0
25	MG	A	1620	1/1	0.99	0.08	66,66,66,66	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.

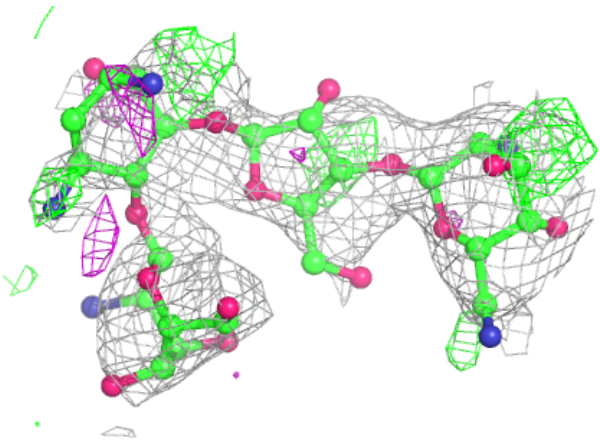
Electron density around PAR A 1602:

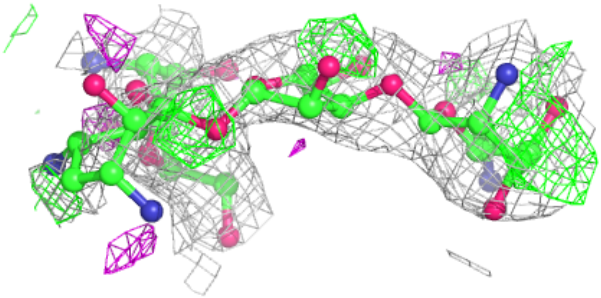
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

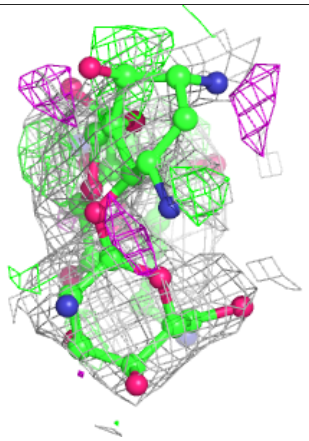


Electron density around PAR A 1603:

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

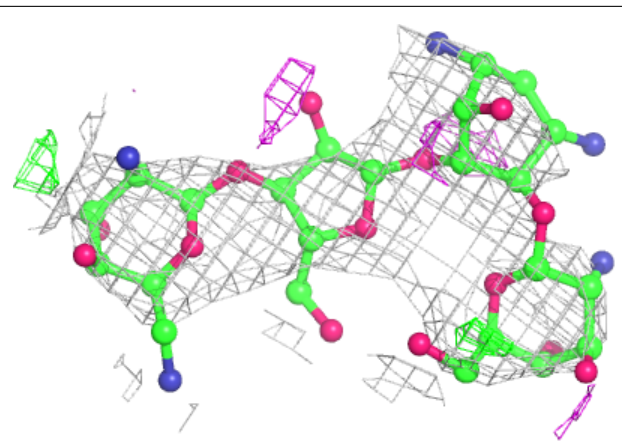


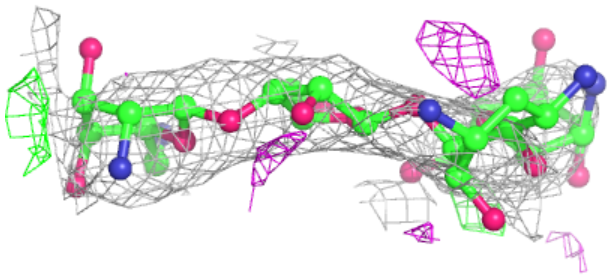


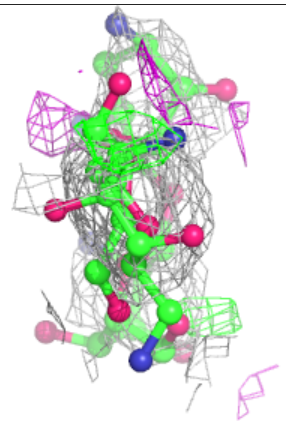


Electron density around PAR A 1605:

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

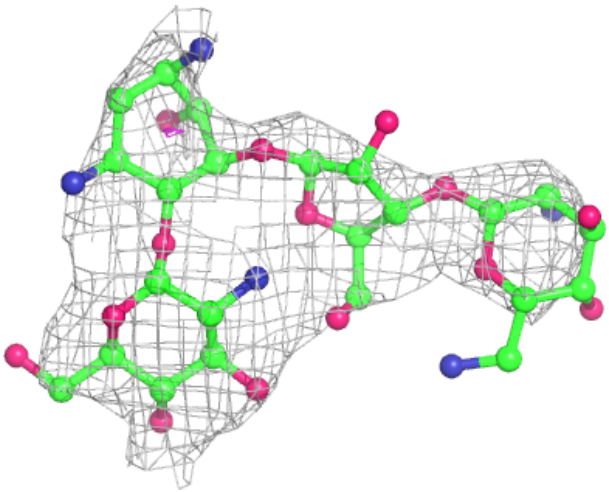


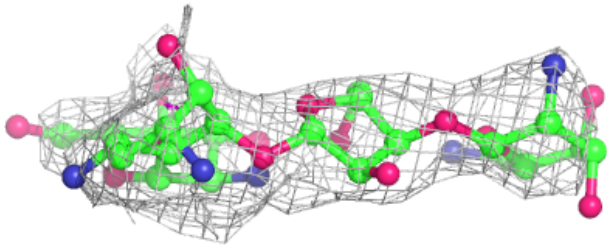


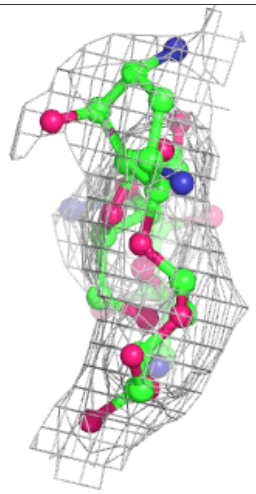


Electron density around PAR A 1604:

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

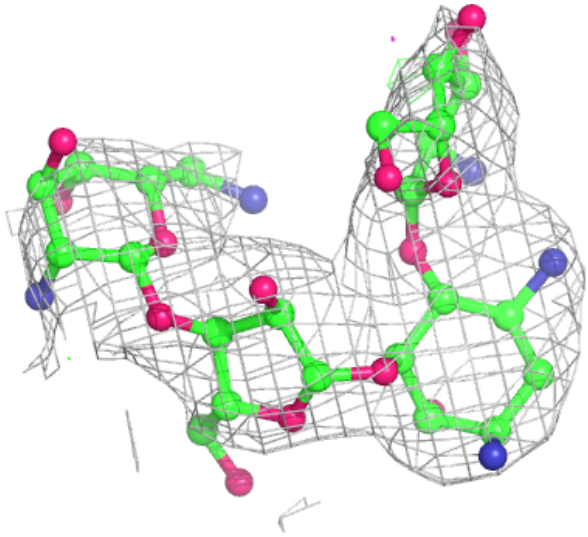


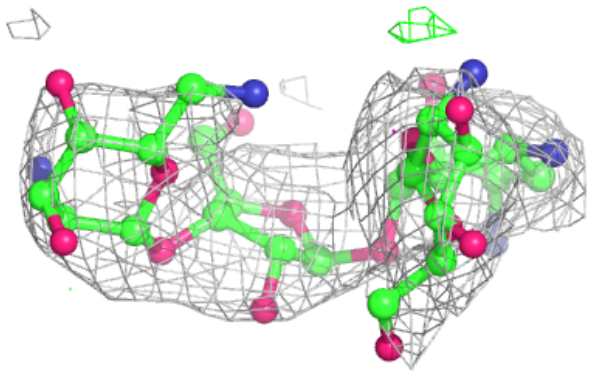


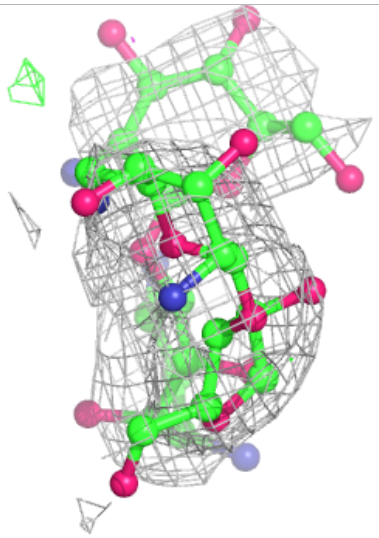


Electron density around PAR A 1606:

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

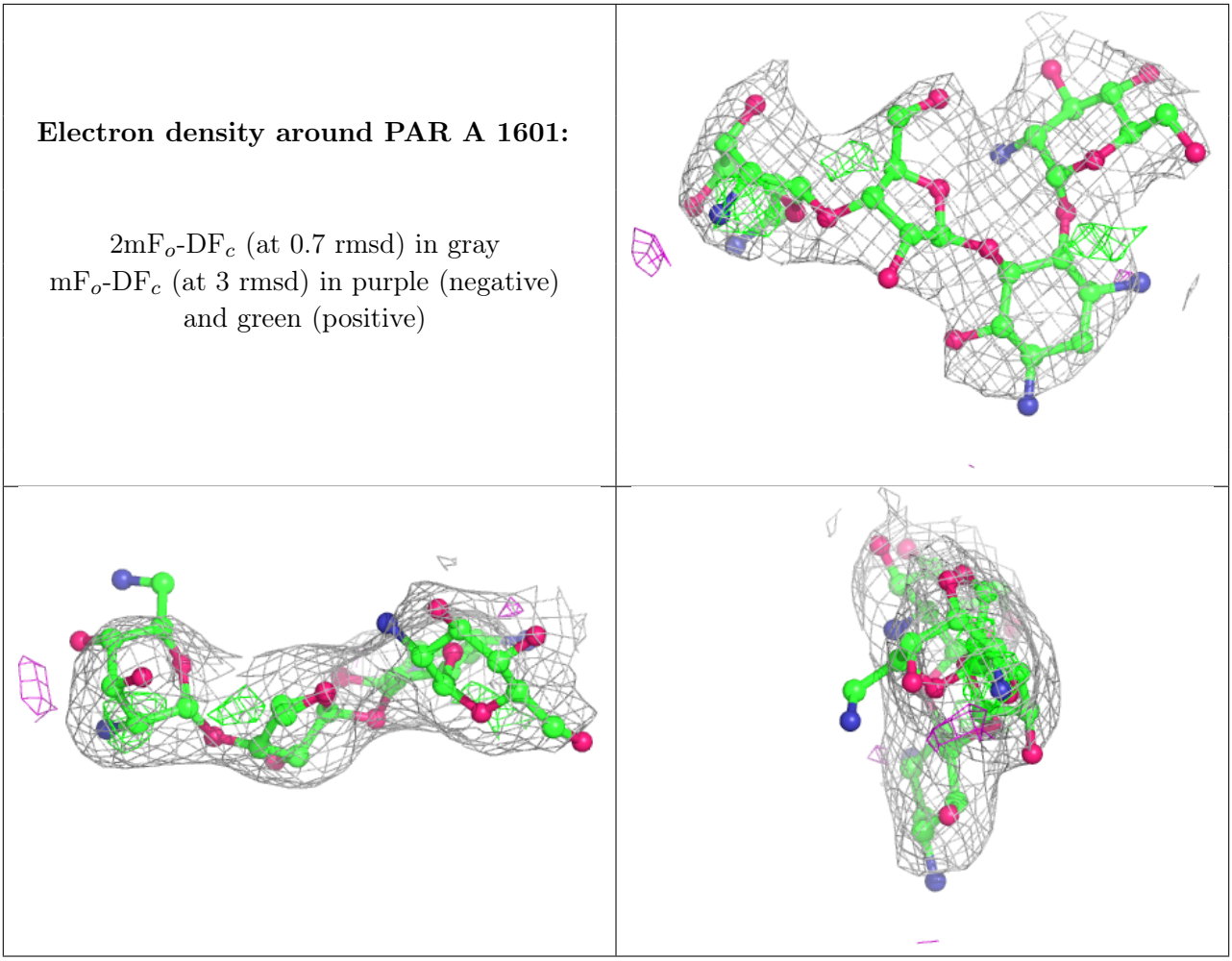






Electron density around PAR A 1601:

$2mF_o$-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 (i)

There are no such residues in this entry.