



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:04 AM UTC

PDB ID : 5BR8 / pdb_00005br8
Title : Ambient-temperature crystal structure of 30S ribosomal subunit from *Thermus thermophilus* in complex with paromomycin
Authors : Sierra, R.G.; Gati, C.; Laksmono, H.; Dao, E.H.; Gul, S.; Fuller, F.; Kern, J.; Chatterjee, R.; Ibrahim, M.; Brewster, A.; Young, I.D.; Michels-Clark, T.; Aquila, A.; Mengning, L.; Hunter, M.S.; Koglin, J.E.; Boutet, S.; Junco, E.A.; Hayes, B.; Bogan, M.J.; Hampton, C.Y.; Puglisi, E.V.; Sauter, N.K.; Stan, C.A.; Zouni, A.; Yano, J.; Yachandra, V.K.; Soltis, S.M.; Puglisi, J.D.; DeMirci, H.
Deposited on : 2015-05-29
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	: 4-5-2 with Phenix2.0
Mogul	: 2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	: 2.0
EDS	: 3.0
Buster-report	: wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	: 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	: 9.0.010 (Gargrove)

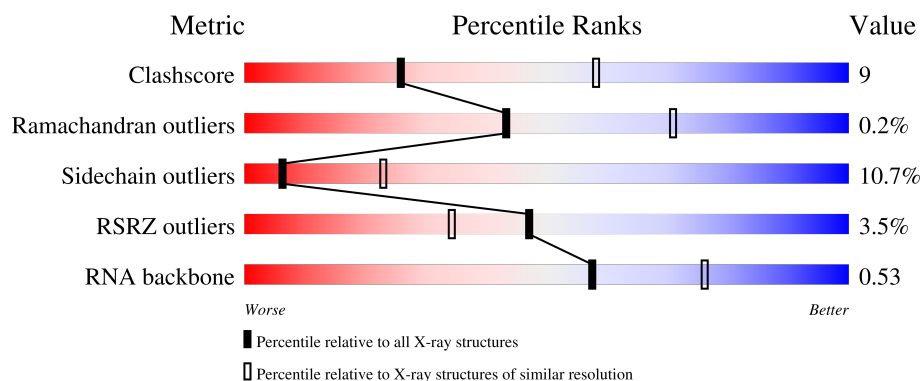
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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))
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)
RNA backbone	3983	1157 (3.80-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	1522	
2	B	256	

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Density-Fitness : 1.0.12
 Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
3	C	239	
4	D	209	
5	E	162	
6	F	101	
7	G	156	
8	H	138	
9	I	128	
10	J	105	
11	K	129	
12	L	135	
13	M	126	
14	N	61	
15	O	89	
16	P	88	
17	Q	105	
18	R	88	
19	S	93	
20	T	106	
21	U	27	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	MG	A	1626	-	-	-	X
23	MG	A	1837	-	-	-	X

2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 52496 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 ribosomal RNA.

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

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1534	C	-	expression tag	GB 55771382
A	1535	A	-	expression tag	GB 55771382
A	1536	C	-	expression tag	GB 55771382
A	1537	U	-	expression tag	GB 55771382
A	1538	C	-	expression tag	GB 55771382
A	1539	C	-	expression tag	GB 55771382
A	1540	PSU	-	expression tag	GB 55771382
A	1541	PSU	-	expression tag	GB 55771382
A	1542	U	-	expression tag	GB 55771382
A	1543	C	-	expression tag	GB 55771382
A	1544	U	-	expression tag	GB 55771382

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	236	Total	C	N	O	S	0	0	1
			1896	1211	337	343	5			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	1	MET	-	initiating methionine	UNP Q5SHN3
L	2	VAL	-	expression tag	UNP Q5SHN3
L	3	ALA	-	expression tag	UNP Q5SHN3
L	4	LEU	-	expression tag	UNP Q5SHN3

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	96	GLN	GLU	conflict	UNP Q5SHP7

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

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

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

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

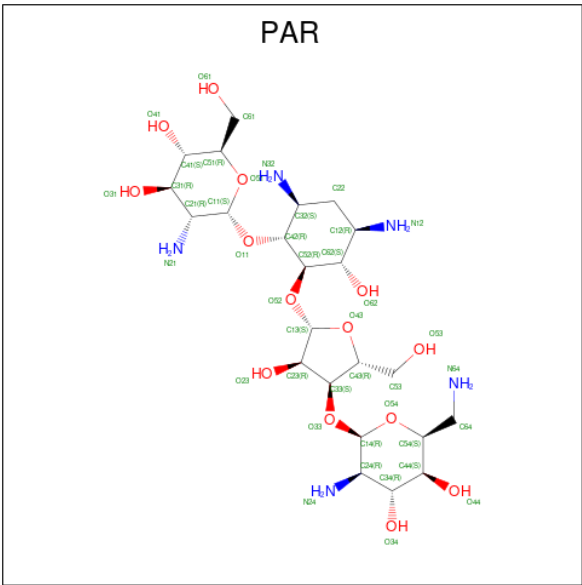
- Molecule 20 is a protein called 30S ribosomal protein S20.

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

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

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

- Molecule 22 is PAROMOMYCIN (CCD ID: PAR) (formula: C₂₃H₄₅N₅O₁₄).



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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	A	273	Total	Mg	0	0
			273	273		
23	B	1	Total	Mg	0	0
			1	1		
23	D	1	Total	Mg	0	0
			1	1		
23	E	1	Total	Mg	0	0
			1	1		
23	G	1	Total	Mg	0	0
			1	1		
23	H	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	I	1	Total 1	Mg 1	0	0
23	J	1	Total 1	Mg 1	0	0
23	L	1	Total 1	Mg 1	0	0
23	P	1	Total 1	Mg 1	0	0
23	Q	1	Total 1	Mg 1	0	0
23	S	3	Total 3	Mg 3	0	0
23	T	1	Total 1	Mg 1	0	0

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

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

- Molecule 25 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	A	293	Total 293	O 293	0	0
25	D	2	Total 2	O 2	0	0
25	E	5	Total 5	O 5	0	0
25	H	2	Total 2	O 2	0	0
25	K	1	Total 1	O 1	0	0
25	L	1	Total 1	O 1	0	0
25	N	1	Total 1	O 1	0	0
25	O	1	Total 1	O 1	0	0

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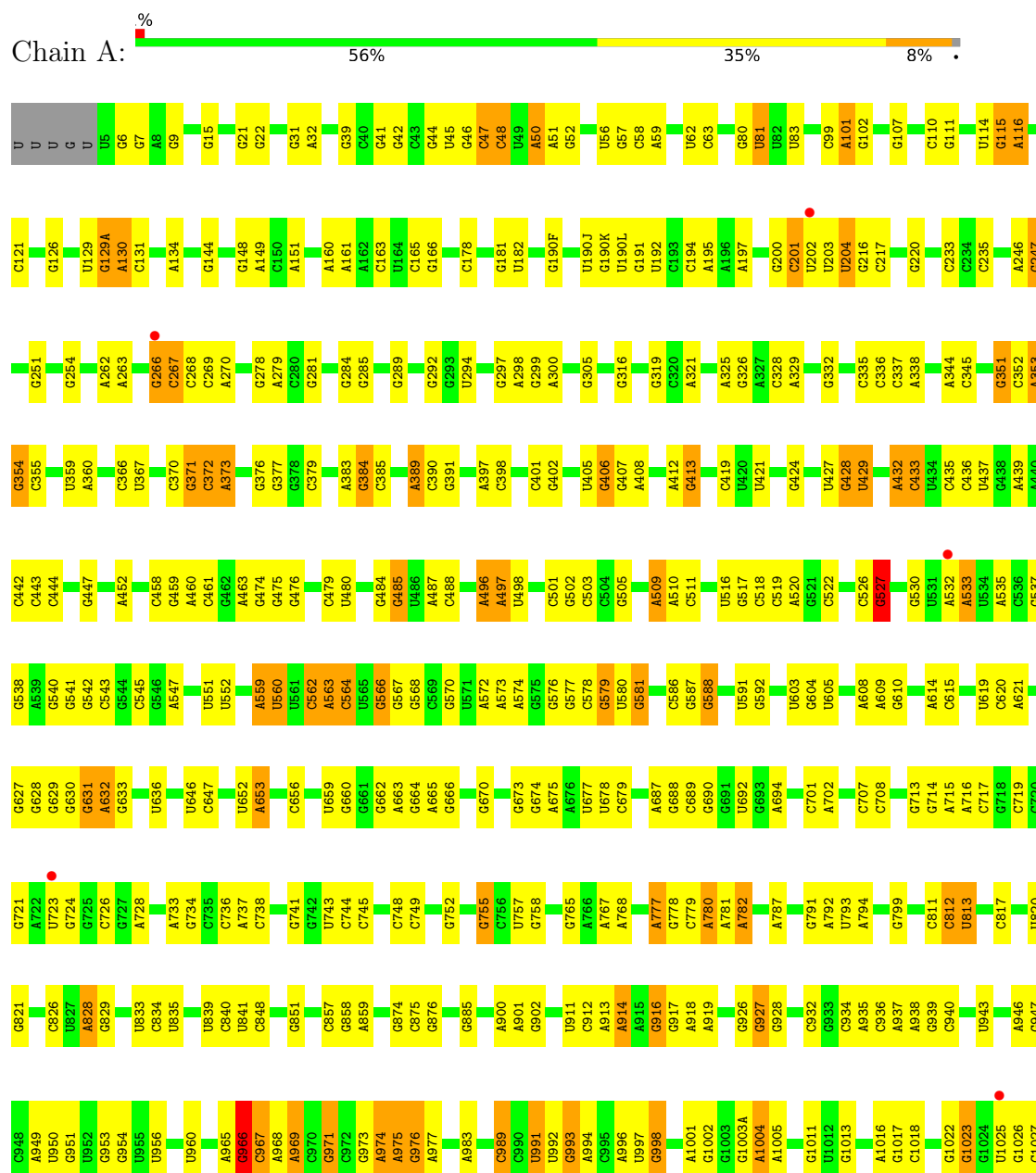
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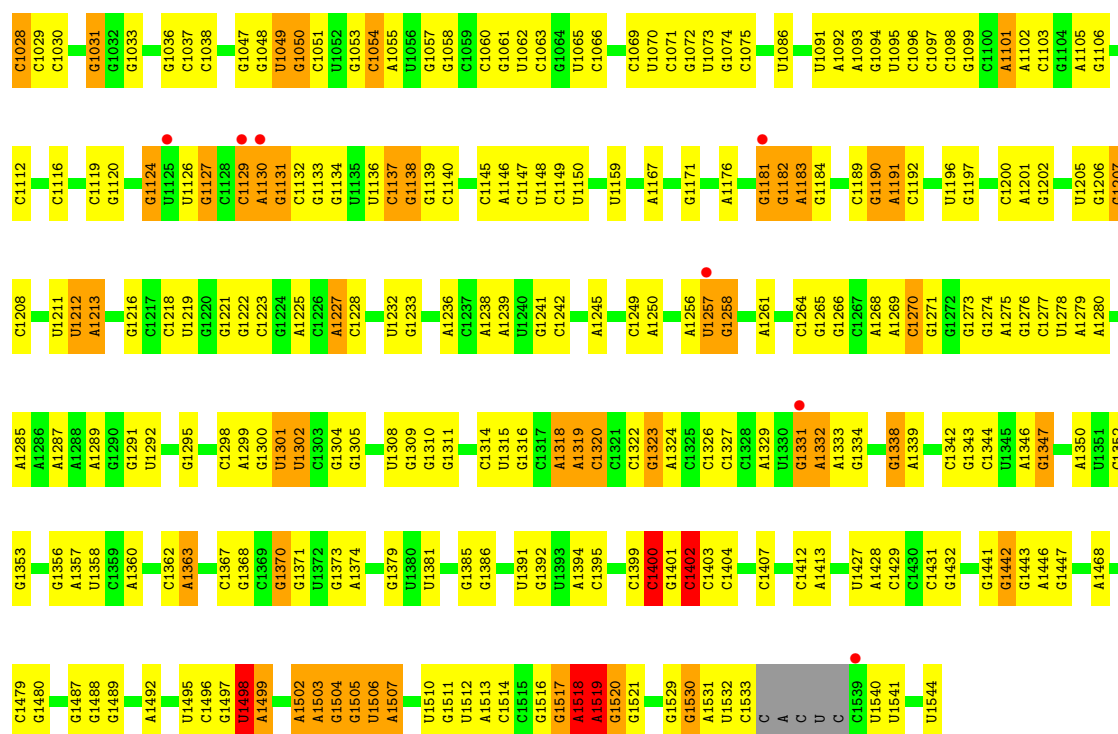
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	Q	1	Total	O	0	0
			1	1		
25	T	1	Total	O	0	0
			1	1		

3 Residue-property plots

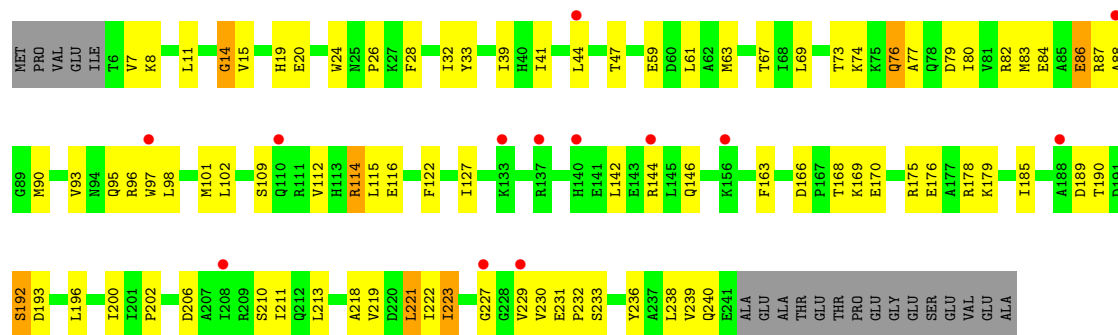
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 ribosomal RNA

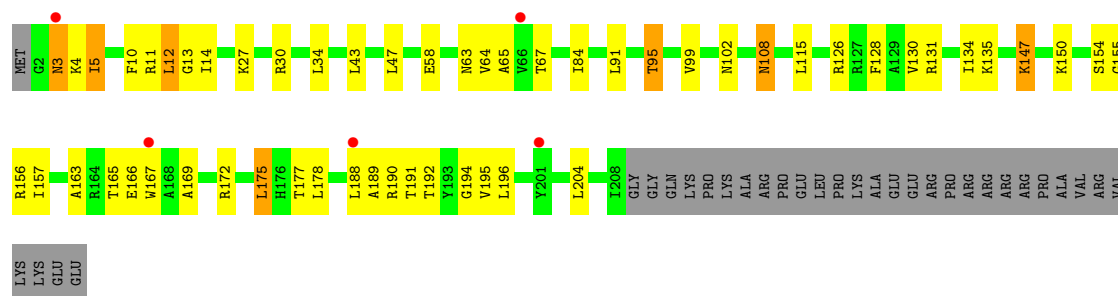




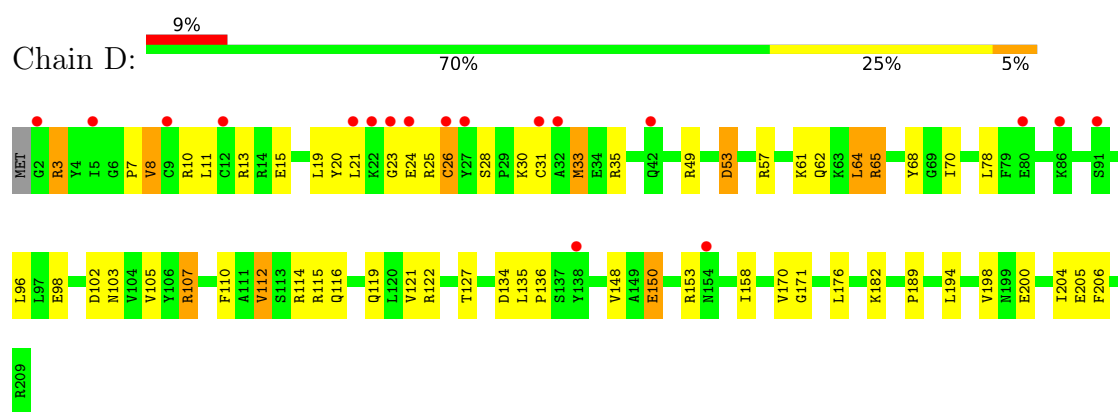
• Molecule 2: 30S ribosomal protein S2



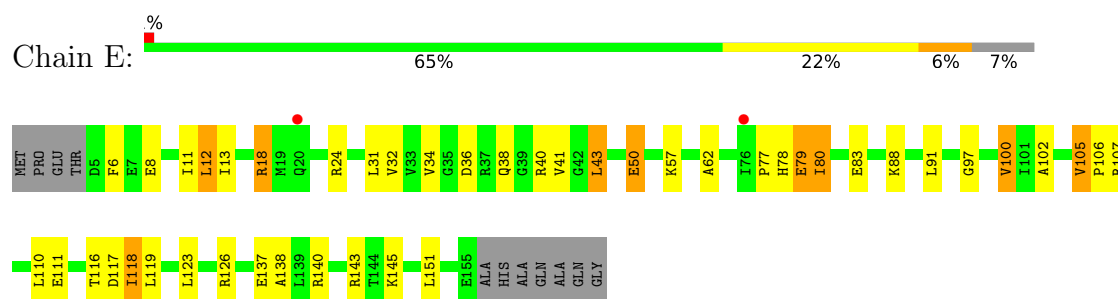
• Molecule 3: 30S ribosomal protein S3



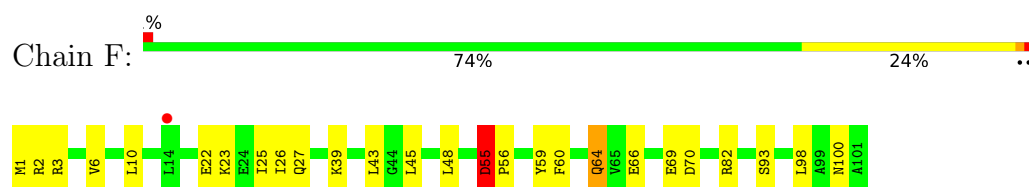
• Molecule 4: 30S ribosomal protein S4



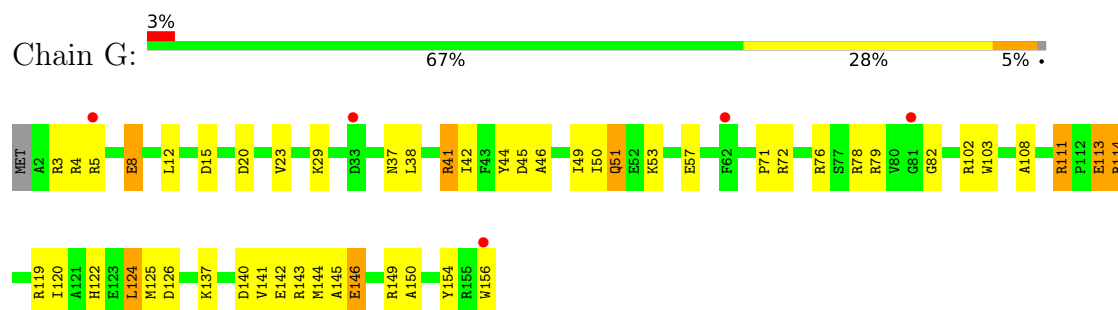
• Molecule 5: 30S ribosomal protein S5



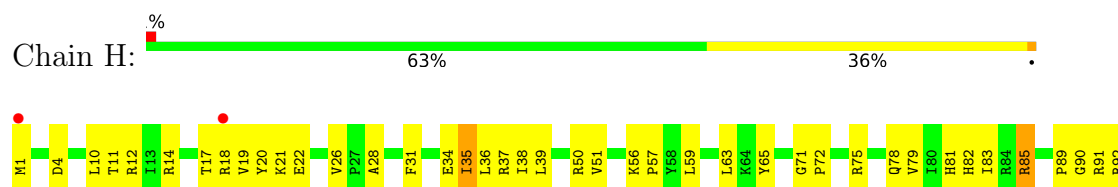
• Molecule 6: 30S ribosomal protein S6



• Molecule 7: 30S ribosomal protein S7

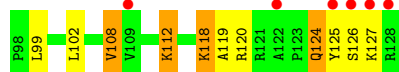


• Molecule 8: 30S ribosomal protein S8

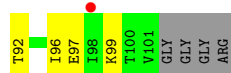
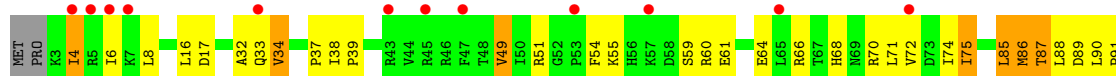




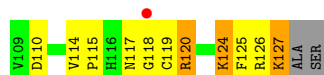
• Molecule 9: 30S ribosomal protein S9



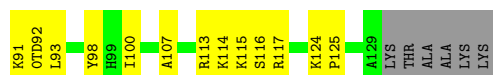
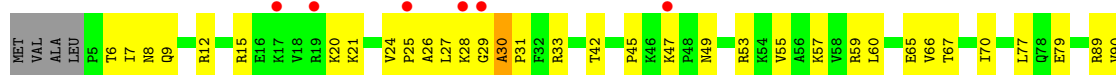
• Molecule 10: 30S ribosomal protein S10



• Molecule 11: 30S ribosomal protein S11

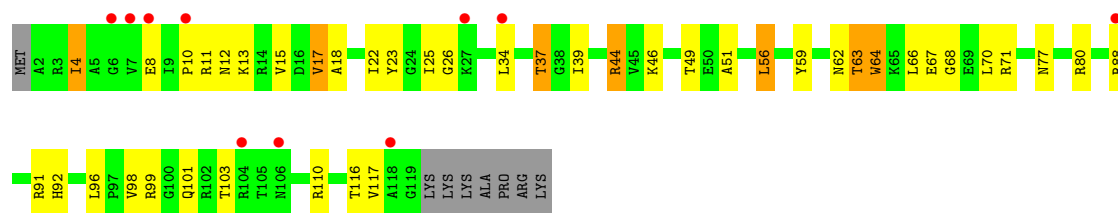


• Molecule 12: 30S ribosomal protein S12



• Molecule 13: 30S ribosomal protein S13





- Molecule 14: 30S ribosomal protein S14 type Z



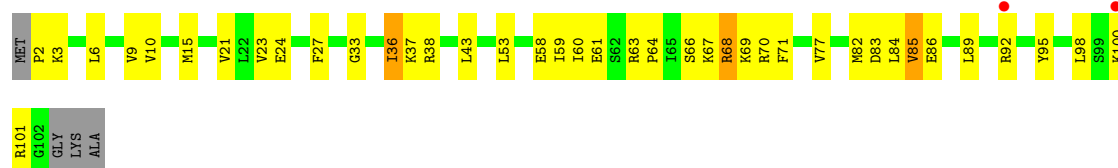
- Molecule 15: 30S ribosomal protein S15



- Molecule 16: 30S ribosomal protein S16



- Molecule 17: 30S ribosomal protein S17

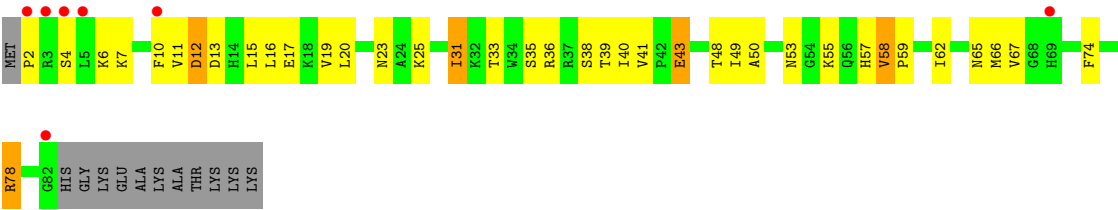


- Molecule 18: 30S ribosomal protein S18

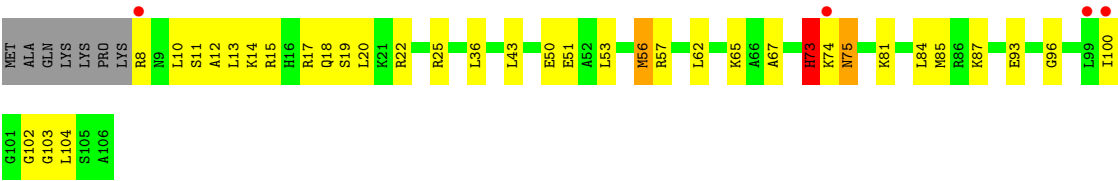


- Molecule 19: 30S ribosomal protein S19

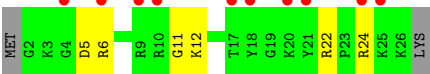




● Molecule 20: 30S ribosomal protein S20



● Molecule 21: 30S ribosomal protein Thx



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	401.30Å 401.30Å 176.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	52.84 – 3.40 52.84 – 3.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (52.84-3.40) 91.1 (52.84-3.40)	Depositor EDS
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 2.96Å)	Xtriage
Refinement program	PHENIX dev_1938	Depositor
R, R_{free}	0.193 , 0.234 0.194 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	56.6	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 154.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	52496	wwPDB-VP
Average B, all atoms (Å ²)	105.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.23% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 4OC, UR3, 5MC, PSU, MA6, 0TD, G7M, PAR, ZN, 2MG, M2G, MG

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	0.22	0/36037	0.40	0/56239
2	B	0.37	0/1931	0.83	5/2607 (0.2%)
3	C	0.42	0/1637	0.80	2/2207 (0.1%)
4	D	0.39	0/1733	0.84	5/2318 (0.2%)
5	E	0.49	0/1163	0.92	2/1566 (0.1%)
6	F	0.33	0/856	0.82	2/1154 (0.2%)
7	G	0.39	0/1276	0.82	2/1709 (0.1%)
8	H	0.43	0/1136	0.86	2/1527 (0.1%)
9	I	0.38	0/1029	0.85	1/1379 (0.1%)
10	J	0.42	0/806	0.83	0/1084
11	K	0.41	0/888	0.91	3/1198 (0.3%)
12	L	0.43	0/978	0.92	5/1308 (0.4%)
13	M	0.35	0/947	0.78	0/1270
14	N	0.37	0/500	0.84	1/663 (0.2%)
15	O	0.37	0/745	0.75	2/992 (0.2%)
16	P	0.39	0/717	0.77	1/965 (0.1%)
17	Q	0.41	0/851	0.84	1/1136 (0.1%)
18	R	0.38	0/604	0.76	0/801
19	S	0.33	0/662	0.83	0/892
20	T	0.44	0/765	0.94	2/1007 (0.2%)
21	U	0.33	0/213	0.74	0/279
All	All	0.29	0/55474	0.58	36/82301 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
8	H	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
10	J	0	1
All	All	0	3

There are no bond length outliers.

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	26	CYS	N-CA-C	-7.72	103.75	113.02
9	I	39	GLY	N-CA-C	-7.45	104.21	114.64
2	B	7	VAL	N-CA-C	7.21	117.30	110.30
12	L	26	ALA	N-CA-C	-7.05	104.56	113.02
6	F	55	ASP	CA-C-N	6.91	126.54	119.56
6	F	55	ASP	C-N-CA	6.91	126.54	119.56
20	T	96	GLY	N-CA-C	6.41	120.93	111.76
20	T	73	HIS	CB-CA-C	-6.30	108.29	115.79
14	N	7	ILE	N-CA-C	-6.28	105.58	112.80
5	E	105	VAL	CA-C-N	-6.15	113.35	119.56
5	E	105	VAL	C-N-CA	-6.15	113.35	119.56
7	G	111	ARG	CA-C-N	5.99	125.54	119.19
7	G	111	ARG	C-N-CA	5.99	125.54	119.19
4	D	21	LEU	N-CA-C	-5.99	106.02	113.38
16	P	5	ARG	N-CA-C	5.62	115.52	108.45
4	D	171	GLY	CA-C-N	5.59	125.69	119.32
4	D	171	GLY	C-N-CA	5.59	125.69	119.32
2	B	90	MET	CA-C-N	5.58	126.06	120.14
2	B	90	MET	C-N-CA	5.58	126.06	120.14
2	B	15	VAL	N-CA-C	5.52	115.61	110.42
15	O	18	PHE	CA-C-N	-5.49	114.14	119.90
15	O	18	PHE	C-N-CA	-5.49	114.14	119.90
12	L	30	ALA	CA-C-N	5.44	124.78	118.85
12	L	30	ALA	C-N-CA	5.44	124.78	118.85
2	B	90	MET	N-CA-C	5.39	118.12	110.24
4	D	33	MET	N-CA-C	-5.24	105.63	112.23
11	K	102	GLY	N-CA-C	-5.23	108.05	115.43
8	H	75	ARG	CA-C-N	5.13	125.41	119.92
8	H	75	ARG	C-N-CA	5.13	125.41	119.92
12	L	115	LYS	CA-C-N	-5.12	115.73	122.85
12	L	115	LYS	C-N-CA	-5.12	115.73	122.85
17	Q	33	GLY	N-CA-C	5.09	121.14	115.08
3	C	108	ASN	CA-C-N	5.06	124.72	119.56
3	C	108	ASN	C-N-CA	5.06	124.72	119.56
11	K	120	ARG	CA-C-N	5.01	124.99	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	120	ARG	C-N-CA	5.01	124.99	120.03

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	14	GLY	Peptide
8	H	90	GLY	Peptide
10	J	87	THR	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32504	0	16433	428	0
2	B	1896	0	1936	48	0
3	C	1613	0	1677	37	0
4	D	1703	0	1763	45	0
5	E	1147	0	1207	31	0
6	F	843	0	857	14	0
7	G	1257	0	1296	38	0
8	H	1116	0	1177	28	0
9	I	1010	0	1037	31	0
10	J	793	0	835	24	0
11	K	873	0	894	24	0
12	L	973	0	1058	22	0
13	M	937	0	995	28	0
14	N	491	0	524	21	0
15	O	734	0	771	21	0
16	P	701	0	720	12	0
17	Q	838	0	909	26	0
18	R	598	0	670	14	0
19	S	648	0	672	24	0
20	T	763	0	861	23	0
21	U	209	0	221	4	0
22	A	252	0	270	8	0
23	A	273	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	B	1	0	0	0	0
23	D	1	0	0	0	0
23	E	1	0	0	0	0
23	G	1	0	0	0	0
23	H	1	0	0	0	0
23	I	1	0	0	0	0
23	J	1	0	0	0	0
23	L	1	0	0	0	0
23	P	1	0	0	0	0
23	Q	1	0	0	0	0
23	S	3	0	0	0	0
23	T	1	0	0	0	0
24	D	1	0	0	0	0
24	N	1	0	0	0	0
25	A	293	0	0	1	0
25	D	2	0	0	0	0
25	E	5	0	0	0	0
25	H	2	0	0	0	0
25	K	1	0	0	0	0
25	L	1	0	0	0	0
25	N	1	0	0	0	0
25	O	1	0	0	0	0
25	Q	1	0	0	0	0
25	T	1	0	0	0	0
All	All	52496	0	36783	831	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 9.

All (831) 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:559:A:OP1	5:E:126:ARG:NH2	2.08	0.86
19:S:33:THR:HG22	19:S:35:SER:H	1.39	0.86
7:G:122:HIS:HA	7:G:125:MET:HE2	1.60	0.83
1:A:1502:A:H2	1:A:1505:G:H1	1.28	0.81
11:K:58:PRO:HB3	11:K:93:GLN:HG3	1.66	0.78
1:A:975:A:H4'	1:A:976:G:H5''	1.65	0.78
13:M:10:PRO:HB2	13:M:18:ALA:HB1	1.67	0.77
1:A:542:G:OP1	4:D:10:ARG:NH2	2.19	0.76
1:A:427:U:OP1	4:D:13:ARG:NH2	2.17	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:16:ARG:HG3	9:I:64:THR:HG22	1.68	0.76
1:A:266:G:H5'	1:A:268:C:H41	1.51	0.75
1:A:1176:A:N6	1:A:1181:G:O6	2.19	0.75
1:A:1086:U:H3	1:A:1099:G:H22	1.33	0.75
11:K:91:ARG:NH2	11:K:110:ASP:OD2	2.20	0.74
11:K:15:ALA:HA	11:K:77:MET:HA	1.68	0.74
7:G:146:GLU:HA	7:G:149:ARG:HG2	1.70	0.74
19:S:50:ALA:HB1	19:S:57:HIS:HB3	1.68	0.74
14:N:24:CYS:HB3	14:N:29:ARG:H	1.54	0.73
1:A:1316:G:H4'	14:N:18:VAL:HG11	1.70	0.73
2:B:77:ALA:HB2	2:B:211:ILE:HD13	1.70	0.73
1:A:279:A:OP2	17:Q:95:TYR:OH	2.06	0.73
15:O:64:ARG:HH11	15:O:88:ARG:HH22	1.35	0.73
1:A:413:G:N2	1:A:429:U:OP2	2.19	0.72
6:F:39:LYS:HB3	6:F:64:GLN:HB3	1.72	0.72
16:P:57:ARG:NH1	16:P:79:VAL:O	2.23	0.72
1:A:201:C:H42	1:A:216:G:H1	1.36	0.71
1:A:677:U:H3	1:A:713:G:H22	1.39	0.71
16:P:15:PRO:HD2	16:P:42:ARG:HD2	1.72	0.71
1:A:522:C:H41	12:L:53:ARG:HH22	1.38	0.71
8:H:113:SER:HB2	8:H:134:ILE:HD11	1.73	0.70
17:Q:66:SER:O	17:Q:70:ARG:NH1	2.24	0.70
2:B:74:LYS:HD2	2:B:166:ASP:HB2	1.72	0.70
20:T:56:MET:HE1	20:T:85:MET:HA	1.73	0.70
1:A:537:G:OP1	12:L:113:ARG:NH2	2.25	0.70
11:K:90:GLY:HA2	11:K:93:GLN:HB2	1.74	0.70
10:J:6:ILE:HB	10:J:72:VAL:HB	1.73	0.69
2:B:19:HIS:NE2	2:B:206:ASP:OD2	2.23	0.69
2:B:14:GLY:HA3	2:B:210:SER:HB2	1.73	0.69
1:A:1182:G:O2'	1:A:1183:A:OP2	2.08	0.69
1:A:1057:G:H5''	3:C:154:SER:HB2	1.75	0.68
1:A:1310:G:OP2	13:M:88:ARG:NH2	2.22	0.68
2:B:8:LYS:HA	2:B:11:LEU:HD13	1.75	0.68
3:C:150:LYS:HG3	3:C:169:ALA:HB2	1.76	0.68
1:A:235:C:H5'	17:Q:70:ARG:HG2	1.76	0.68
1:A:1003(A):G:H2'	1:A:1004:A:H4'	1.77	0.67
2:B:223:ILE:HD13	2:B:230:VAL:H	1.59	0.67
5:E:8:GLU:HG2	5:E:34:VAL:HG22	1.77	0.66
2:B:179:LYS:HA	8:H:72:PRO:HD3	1.77	0.66
12:L:77:LEU:HD21	12:L:107:ALA:HB2	1.79	0.66
13:M:11:ARG:HG3	13:M:12:ASN:HB2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:538:G:H5''	12:L:114:LYS:HB2	1.78	0.65
4:D:49:ARG:H	4:D:49:ARG:HD2	1.62	0.65
1:A:975:A:H5'	1:A:975:A:H8	1.60	0.65
6:F:25:ILE:HG21	6:F:82:ARG:HD2	1.78	0.65
1:A:1030:C:N3	1:A:1031:G:N2	2.42	0.65
9:I:10:ARG:NH1	9:I:75:ASP:OD2	2.30	0.64
1:A:15:G:O2'	5:E:24:ARG:NH1	2.31	0.64
1:A:1391:U:H2'	1:A:1392:G:C8	2.32	0.64
1:A:835:U:OP1	18:R:64:ARG:NH2	2.31	0.64
1:A:1189:C:OP1	10:J:51:ARG:NH2	2.28	0.64
1:A:603:U:H2'	1:A:604:G:H8	1.62	0.64
4:D:64:LEU:HG	4:D:198:VAL:HG11	1.77	0.64
1:A:1510:U:H2'	1:A:1511:G:C8	2.33	0.64
9:I:32:ASP:HB3	9:I:35:GLU:HB2	1.80	0.64
1:A:664:G:H22	1:A:741:G:H1	1.46	0.63
1:A:976:G:H5'	1:A:1358:U:O2'	1.97	0.63
1:A:1206:G:OP1	3:C:190:ARG:NH2	2.31	0.63
1:A:1256:A:H5'	1:A:1258:G:H1'	1.80	0.63
1:A:578:C:O2'	1:A:728:A:N3	2.28	0.63
1:A:653:A:OP1	8:H:56:LYS:NZ	2.31	0.63
1:A:1360:A:OP2	14:N:35:ARG:NH2	2.32	0.63
19:S:31:ILE:HG22	19:S:49:ILE:HA	1.80	0.63
1:A:501:C:H2'	1:A:502:G:H8	1.62	0.63
1:A:1132:C:H2'	1:A:1133:G:H8	1.64	0.63
10:J:85:LEU:HD13	10:J:86:MET:H	1.64	0.63
7:G:15:ASP:OD1	7:G:44:TYR:OH	2.16	0.62
1:A:246:A:N1	1:A:278:G:O2'	2.32	0.62
1:A:974:A:OP2	14:N:29:ARG:NH2	2.33	0.62
1:A:1003(A):G:N2	1:A:1038:C:O2	2.32	0.62
1:A:1127:G:H1	1:A:1145:C:N4	1.97	0.62
17:Q:63:ARG:HG2	17:Q:64:PRO:HD2	1.81	0.62
5:E:110:LEU:HD13	5:E:118:ILE:HG21	1.81	0.62
9:I:46:ALA:HB2	9:I:74:ILE:HG23	1.81	0.62
4:D:20:TYR:HD1	4:D:26:CYS:HB3	1.65	0.62
20:T:75:ASN:OD1	20:T:75:ASN:N	2.31	0.62
1:A:501:C:H2'	1:A:502:G:C8	2.34	0.62
1:A:670:G:OP2	22:A:1606:PAR:N24	2.33	0.62
1:A:765:G:N2	1:A:813:U:OP2	2.32	0.61
1:A:603:U:H2'	1:A:604:G:C8	2.35	0.61
19:S:13:ASP:HA	19:S:16:LEU:HB3	1.82	0.61
16:P:18:ARG:HD3	16:P:35:LYS:HD2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:22:GLU:OE1	6:F:82:ARG:NH1	2.34	0.61
1:A:939:G:H5''	7:G:102:ARG:NH2	2.16	0.61
7:G:51:GLN:C	7:G:53:LYS:H	2.09	0.61
6:F:100:ASN:ND2	18:R:23:LYS:O	2.34	0.60
14:N:12:ARG:H	14:N:12:ARG:HD2	1.66	0.60
4:D:102:ASP:OD1	4:D:103:ASN:N	2.34	0.60
22:A:1601:PAR:H532	22:A:1601:PAR:HN61	1.65	0.60
1:A:1327:C:H5	21:U:6:ARG:HH12	1.48	0.60
1:A:372:C:H4'	1:A:373:A:O5'	2.02	0.60
9:I:49:PRO:HD3	9:I:78:LYS:HG3	1.84	0.60
1:A:946:A:H2'	1:A:947:G:C8	2.37	0.60
1:A:652:U:O4	1:A:752:G:O2'	2.14	0.60
1:A:1352:C:N4	25:A:1901:HOH:O	2.34	0.60
3:C:91:LEU:HG	3:C:99:VAL:HG21	1.84	0.60
1:A:716:A:H1'	11:K:118:GLY:HA2	1.83	0.59
1:A:1124:G:H2'	1:A:1145:C:H5	1.66	0.59
1:A:1049:U:H4'	1:A:1050:G:O5'	2.02	0.59
13:M:77:ASN:OD1	13:M:80:ARG:NH2	2.35	0.59
4:D:23:GLY:HA3	4:D:112:VAL:HG22	1.83	0.59
1:A:630:G:H5'	1:A:631:G:OP2	2.03	0.59
2:B:79:ASP:HB3	2:B:238:LEU:HD13	1.84	0.59
9:I:51:ARG:HA	9:I:56:LEU:HD11	1.85	0.59
11:K:18:ARG:NH1	11:K:35:PRO:O	2.35	0.59
4:D:98:GLU:HG2	4:D:189:PRO:HG2	1.84	0.58
14:N:27:CYS:SG	14:N:29:ARG:HB2	2.42	0.58
1:A:6:G:H4'	1:A:298:A:H4'	1.85	0.58
14:N:26:ARG:HD3	14:N:43:CYS:HB3	1.85	0.58
8:H:108:GLY:HA3	8:H:138:TRP:HB3	1.86	0.58
3:C:155:GLY:HA3	3:C:163:ALA:HB1	1.85	0.58
4:D:24:GLU:HG2	4:D:25:ARG:H	1.68	0.58
5:E:140:ARG:O	5:E:143:ARG:NH2	2.37	0.58
7:G:113:GLU:HG2	7:G:119:ARG:HG3	1.85	0.58
9:I:118:LYS:O	9:I:120:ARG:N	2.30	0.58
18:R:17:SER:OG	18:R:54:ARG:O	2.17	0.58
1:A:1367:C:H5'	10:J:60:ARG:NH1	2.18	0.58
12:L:27:LEU:O	12:L:29:GLY:N	2.37	0.58
1:A:1270:C:H2'	1:A:1271:G:C8	2.39	0.57
19:S:33:THR:HG22	19:S:35:SER:N	2.15	0.57
1:A:673:G:H2'	1:A:674:G:C8	2.39	0.57
7:G:111:ARG:NH2	7:G:126:ASP:OD2	2.37	0.57
1:A:1148:U:H2'	1:A:1149:C:O4'	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:46:ALA:O	7:G:50:ILE:HG12	2.05	0.57
1:A:1028:C:H42	1:A:1033:G:H1	1.53	0.57
9:I:56:LEU:HD12	9:I:56:LEU:H	1.70	0.57
1:A:570:G:H1'	1:A:820:U:C4	2.39	0.57
10:J:97:GLU:OE1	10:J:99:LYS:NZ	2.36	0.57
18:R:47:THR:HG22	18:R:48:GLY:H	1.69	0.57
1:A:1011:G:N2	1:A:1018:C:O2	2.37	0.57
1:A:1266:G:N2	1:A:1269:A:OP2	2.30	0.57
1:A:1001:A:H2'	1:A:1002:G:C8	2.39	0.57
2:B:97:TRP:HZ2	2:B:102:LEU:HD13	1.70	0.57
1:A:269:C:H2'	1:A:270:A:C8	2.40	0.56
2:B:84:GLU:OE2	2:B:233:SER:OG	2.19	0.56
7:G:140:ASP:OD1	7:G:143:ARG:NH2	2.38	0.56
1:A:1499:A:H1'	1:A:1520:G:H5'	1.88	0.56
2:B:122:PHE:HD1	2:B:127:ILE:HG12	1.70	0.56
1:A:509:A:N3	1:A:543:C:O2'	2.31	0.56
1:A:619:U:N3	4:D:134:ASP:OD1	2.24	0.56
19:S:41:VAL:HG23	19:S:43:GLU:HG2	1.88	0.56
13:M:64:TRP:HE3	13:M:66:LEU:HD21	1.70	0.56
1:A:299:G:H2'	1:A:300:A:C8	2.41	0.56
1:A:407:G:OP1	4:D:115:ARG:NH2	2.38	0.56
7:G:72:ARG:NH2	7:G:142:GLU:OE2	2.34	0.56
8:H:89:PRO:HA	8:H:92:ARG:NH1	2.21	0.56
10:J:49:VAL:HG23	14:N:41:ARG:HB2	1.87	0.56
1:A:316:G:OP2	1:A:351:G:O2'	2.23	0.56
1:A:1001:A:H2'	1:A:1002:G:H8	1.71	0.56
4:D:31:CYS:C	4:D:33:MET:H	2.11	0.56
4:D:68:TYR:OH	4:D:98:GLU:OE1	2.18	0.56
10:J:33:GLN:HB2	10:J:75:ILE:HD11	1.88	0.56
1:A:517:G:N1	1:A:533:A:OP2	2.25	0.55
7:G:15:ASP:HB3	7:G:20:ASP:H	1.70	0.55
8:H:83:ILE:HG13	8:H:137:VAL:HG22	1.89	0.55
20:T:67:ALA:O	20:T:73:HIS:ND1	2.33	0.55
1:A:1192:C:OP2	3:C:4:LYS:NZ	2.40	0.55
7:G:15:ASP:N	7:G:20:ASP:O	2.38	0.55
9:I:8:GLY:HA2	9:I:79:LEU:HD13	1.87	0.55
1:A:1371:G:O3'	9:I:69:GLY:HA3	2.07	0.55
4:D:24:GLU:C	4:D:26:CYS:H	2.15	0.55
1:A:821:G:N7	22:A:1602:PAR:H641	2.22	0.54
1:A:1057:G:H5''	3:C:154:SER:CB	2.36	0.54
4:D:62:GLN:OE1	4:D:65:ARG:NH1	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:141:VAL:HA	7:G:144:MET:HE2	1.89	0.54
1:A:782:A:OP1	1:A:1521:G:N2	2.38	0.54
1:A:1305:G:N2	1:A:1331:G:H1'	2.22	0.54
10:J:8:LEU:HB2	10:J:70:ARG:HB2	1.89	0.54
1:A:736:C:H2'	1:A:737:A:C8	2.42	0.54
1:A:1291:G:OP1	7:G:37:ASN:ND2	2.41	0.54
15:O:39:LEU:HD13	15:O:56:LEU:HB2	1.88	0.54
13:M:101:GLN:OE1	13:M:101:GLN:N	2.38	0.54
1:A:447:G:O6	1:A:485:G:O2'	2.24	0.54
1:A:1502:A:H2	1:A:1505:G:N1	2.01	0.54
5:E:80:ILE:HD13	5:E:91:LEU:HB2	1.89	0.54
5:E:102:ALA:HB1	5:E:106:PRO:HG2	1.90	0.54
17:Q:6:LEU:HD13	17:Q:23:VAL:HG11	1.90	0.54
1:A:1022:G:H2'	1:A:1023:G:H8	1.72	0.54
4:D:150:GLU:HA	4:D:153:ARG:HG3	1.90	0.54
1:A:1103:C:OP1	2:B:96:ARG:NH1	2.40	0.54
8:H:97:VAL:HG21	8:H:128:GLY:HA2	1.90	0.54
8:H:19:VAL:HG23	8:H:21:LYS:HD3	1.90	0.54
13:M:92:HIS:CD2	13:M:98:VAL:HG11	2.43	0.54
1:A:355:C:H5'	1:A:389:A:OP2	2.07	0.54
1:A:1013:G:N2	1:A:1016:A:OP2	2.39	0.54
1:A:689:C:H2'	1:A:690:G:O4'	2.08	0.53
1:A:1074:G:O2'	1:A:1101:A:N1	2.41	0.53
3:C:130:VAL:HG12	3:C:134:ILE:HD11	1.90	0.53
6:F:43:LEU:HD12	6:F:60:PHE:HB3	1.90	0.53
13:M:91:ARG:HB2	13:M:98:VAL:HG12	1.89	0.53
1:A:1342:C:O2'	9:I:124:GLN:HB2	2.08	0.53
2:B:193:ASP:HB3	2:B:196:LEU:HD12	1.90	0.53
1:A:1343:G:H2'	1:A:1344:C:C6	2.43	0.53
7:G:108:ALA:O	7:G:119:ARG:HG2	2.07	0.53
1:A:928:G:O2'	1:A:1533:C:OP1	2.25	0.53
1:A:971:G:N2	1:A:1363:A:OP2	2.38	0.53
1:A:1030:C:H42	1:A:1031:G:H1	1.56	0.53
1:A:1292:U:OP2	7:G:41:ARG:NH2	2.42	0.53
5:E:79:GLU:O	8:H:104:ARG:NH1	2.41	0.53
6:F:23:LYS:O	6:F:27:GLN:HG2	2.09	0.53
18:R:32:ARG:HA	18:R:69:THR:HG21	1.91	0.53
1:A:779:C:H2'	1:A:780:A:O4'	2.09	0.53
4:D:28:SER:O	4:D:30:LYS:N	2.38	0.53
3:C:3:ASN:OD1	3:C:3:ASN:N	2.42	0.53
12:L:57:LYS:HG2	12:L:67:THR:HG22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1129:C:N4	1:A:1134:G:N7	2.56	0.53
6:F:10:LEU:HB2	6:F:59:TYR:HB3	1.90	0.53
13:M:63:THR:HG23	13:M:64:TRP:H	1.73	0.53
1:A:1124:G:H2'	1:A:1145:C:C5	2.44	0.52
20:T:67:ALA:HA	20:T:73:HIS:H	1.73	0.52
1:A:401:C:H2'	1:A:402:G:C8	2.45	0.52
1:A:1256:A:H4'	1:A:1257:U:O5'	2.08	0.52
1:A:1427:U:H2'	1:A:1428:A:C8	2.44	0.52
1:A:383:A:C5	1:A:384:G:H1'	2.45	0.52
1:A:1399:C:H4'	1:A:1400:5MC:H5''	1.90	0.52
4:D:148:VAL:HG11	4:D:158:ILE:HG21	1.92	0.52
17:Q:43:LEU:HD12	17:Q:68:ARG:HG2	1.91	0.52
1:A:81:U:H2'	1:A:83:U:OP2	2.09	0.52
1:A:911:U:H2'	1:A:912:C:C6	2.45	0.52
2:B:73:THR:HG23	2:B:95:GLN:O	2.10	0.52
5:E:97:GLY:N	5:E:117:ASP:OD2	2.43	0.52
7:G:5:ARG:HH22	7:G:8:GLU:CD	2.16	0.52
1:A:279:A:H5''	1:A:281:G:O4'	2.09	0.52
1:A:359:U:H2'	1:A:360:A:C8	2.44	0.52
5:E:36:ASP:OD2	5:E:38:GLN:HB2	2.10	0.52
7:G:79:ARG:HD3	7:G:82:GLY:H	1.74	0.52
1:A:406:G:H21	4:D:119:GLN:HE22	1.57	0.52
1:A:580:U:H2'	1:A:581:G:O4'	2.10	0.52
1:A:857:C:H2'	1:A:858:G:O4'	2.10	0.52
1:A:939:G:H2'	1:A:940:C:C6	2.45	0.52
3:C:189:ALA:HB3	3:C:196:LEU:HB2	1.90	0.52
1:A:7:G:H5'	1:A:298:A:O4'	2.10	0.51
3:C:5:ILE:HD13	3:C:10:PHE:HB2	1.90	0.51
1:A:1347:G:N2	1:A:1374:A:OP2	2.39	0.51
11:K:77:MET:HE1	11:K:80:VAL:HG12	1.91	0.51
14:N:21:TYR:HE2	14:N:23:ARG:HH21	1.57	0.51
1:A:614:A:H2'	1:A:615:C:C6	2.46	0.51
1:A:1516:G:N2	1:A:1519:MA6:OP2	2.36	0.51
5:E:151:LEU:HB3	8:H:79:VAL:HG22	1.91	0.51
1:A:216:G:O2'	1:A:217:C:O4'	2.28	0.51
1:A:262:A:C6	1:A:263:A:C6	2.98	0.51
1:A:662:G:H2'	1:A:663:A:C8	2.46	0.51
16:P:42:ARG:HB2	16:P:44:THR:HG23	1.92	0.51
1:A:591:U:H2'	1:A:592:G:C8	2.46	0.51
1:A:1112:C:C2	3:C:178:LEU:HB2	2.45	0.51
2:B:93:VAL:HG11	2:B:97:TRP:CD1	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:81:LYS:O	20:T:85:MET:HG3	2.10	0.51
1:A:435:C:H2'	1:A:436:C:C6	2.46	0.51
2:B:88:ALA:HB2	2:B:219:VAL:HG13	1.93	0.51
8:H:97:VAL:HG13	8:H:98:LYS:HD2	1.93	0.51
12:L:25:PRO:C	12:L:27:LEU:H	2.19	0.51
1:A:47:C:OP1	22:A:1603:PAR:N32	2.43	0.51
1:A:148:G:H2'	1:A:149:A:C8	2.46	0.51
9:I:37:PHE:O	9:I:38:GLN:HG3	2.11	0.51
14:N:16:PHE:HD2	14:N:19:ARG:HD2	1.76	0.51
1:A:191:G:N2	20:T:103:GLY:O	2.30	0.51
4:D:121:VAL:HG11	4:D:136:PRO:HA	1.93	0.51
11:K:43:SER:HB3	11:K:68:ALA:HB2	1.93	0.51
1:A:371:G:O2'	1:A:372:C:H5'	2.11	0.51
1:A:517:G:N2	1:A:530:G:OP1	2.42	0.51
8:H:10:LEU:HD22	8:H:83:ILE:HD11	1.93	0.51
13:M:49:THR:HG22	13:M:51:ALA:H	1.76	0.51
17:Q:58:GLU:HG3	17:Q:77:VAL:HG22	1.93	0.51
3:C:157:ILE:HD13	3:C:166:GLU:HG2	1.93	0.50
1:A:99:C:H2'	1:A:101:A:C8	2.46	0.50
1:A:192:U:H4'	20:T:57:ARG:HD2	1.92	0.50
1:A:401:C:H2'	1:A:402:G:H8	1.76	0.50
1:A:501:C:OP1	12:L:117:ARG:NH2	2.44	0.50
2:B:28:PHE:CD2	2:B:190:THR:HA	2.46	0.50
4:D:57:ARG:HB3	4:D:206:PHE:HB2	1.93	0.50
11:K:57:THR:HG22	11:K:59:TYR:H	1.76	0.50
1:A:487:A:H2'	1:A:488:C:O4'	2.12	0.50
1:A:1218:C:H2'	1:A:1219:U:C6	2.46	0.50
16:P:22:THR:HA	16:P:33:ILE:HG13	1.94	0.50
2:B:93:VAL:HG11	2:B:97:TRP:HD1	1.74	0.50
16:P:34:GLU:OE1	16:P:55:ARG:NH1	2.43	0.50
1:A:966:M2G:HM22	1:A:967:5MC:H1'	1.91	0.50
11:K:91:ARG:O	11:K:95:ILE:HG13	2.12	0.50
1:A:129:U:O3'	1:A:129(A):G:H3'	2.12	0.50
1:A:1101:A:H4'	1:A:1102:A:O5'	2.11	0.50
1:A:1412:C:H2'	1:A:1413:A:C8	2.47	0.50
1:A:201:C:N4	1:A:216:G:H1	2.08	0.50
1:A:627:G:H2'	1:A:628:G:C8	2.47	0.50
1:A:1329:A:H5''	13:M:26:GLY:H	1.76	0.50
1:A:1333:A:H2'	1:A:1334:G:O4'	2.12	0.50
1:A:1338:G:H2'	1:A:1339:A:C8	2.47	0.50
1:A:1356:G:H2'	1:A:1357:A:C8	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:107:ARG:O	5:E:111:GLU:HB2	2.11	0.50
1:A:560:U:H5'	1:A:566:G:C2	2.46	0.50
1:A:1070:U:OP1	5:E:18:ARG:NH2	2.45	0.50
1:A:1207:2MG:HM23	1:A:1208:C:H1'	1.94	0.50
2:B:24:TRP:HB2	2:B:190:THR:HG22	1.93	0.50
11:K:73:MET:HG2	11:K:103:LEU:HD21	1.94	0.50
12:L:89:ARG:NH2	12:L:91:LYS:HD2	2.27	0.50
5:E:43:LEU:O	5:E:62:ALA:HA	2.12	0.49
1:A:45:U:H2'	1:A:46:G:C8	2.47	0.49
1:A:107:G:N7	20:T:15:ARG:NH2	2.55	0.49
1:A:1239:A:C4	1:A:1298:C:N4	2.80	0.49
1:A:1402:4OC:H2'	1:A:1403:C:O4'	2.12	0.49
1:A:1402:4OC:HM22	1:A:1403:C:H5'	1.94	0.49
3:C:126:ARG:CZ	3:C:128:PHE:HB2	2.42	0.49
1:A:148:G:H2'	1:A:149:A:H8	1.76	0.49
5:E:11:ILE:HG22	5:E:12:LEU:HB3	1.94	0.49
1:A:266:G:H5''	1:A:267:C:H5	1.77	0.49
1:A:943:U:H1'	9:I:124:GLN:HE22	1.77	0.49
5:E:80:ILE:HD11	5:E:138:ALA:HB1	1.94	0.49
1:A:1097:C:H2'	1:A:1098:C:C6	2.47	0.49
2:B:33:TYR:HB3	2:B:41:ILE:HG22	1.95	0.49
4:D:103:ASN:O	4:D:107:ARG:HB2	2.12	0.49
6:F:1:MET:HE2	6:F:66:GLU:HG2	1.94	0.49
3:C:156:ARG:H	3:C:163:ALA:HA	1.76	0.49
10:J:51:ARG:HD2	10:J:59:SER:HB2	1.95	0.49
17:Q:15:MET:HE1	17:Q:43:LEU:HD22	1.94	0.49
17:Q:53:LEU:HD23	17:Q:82:MET:HE1	1.93	0.49
19:S:11:VAL:HG22	19:S:39:THR:HB	1.95	0.49
1:A:975:A:H5'	1:A:975:A:C8	2.43	0.49
1:A:1200:C:O2'	1:A:1205:U:O4	2.30	0.49
1:A:1301:U:O2'	1:A:1302:U:O5'	2.29	0.49
1:A:932:C:H5''	7:G:3:ARG:HG2	1.94	0.49
1:A:738:C:H5''	6:F:69:GLU:HB3	1.94	0.49
1:A:52:G:O6	22:A:1603:PAR:O44	2.22	0.48
1:A:646:U:H2'	1:A:647:C:C6	2.48	0.48
1:A:743:U:H2'	1:A:744:C:C6	2.48	0.48
10:J:17:ASP:OD1	10:J:70:ARG:NH1	2.45	0.48
12:L:24:VAL:HG13	12:L:98:TYR:HE1	1.78	0.48
1:A:1029:C:N3	1:A:1033:G:N2	2.60	0.48
1:A:1261:A:OP1	21:U:24:ARG:NH2	2.46	0.48
8:H:34:GLU:OE2	8:H:37:ARG:NH1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:45:ALA:O	9:I:78:LYS:HD3	2.13	0.48
1:A:80:G:H2'	1:A:81:U:H5'	1.95	0.48
1:A:413:G:N2	1:A:428:G:H1'	2.27	0.48
1:A:587:G:O2'	1:A:588:G:OP2	2.24	0.48
1:A:1347:G:H22	1:A:1374:A:P	2.35	0.48
1:A:1236:A:H4'	1:A:1304:G:H4'	1.95	0.48
5:E:12:LEU:HD22	5:E:13:ILE:N	2.28	0.48
7:G:145:ALA:O	7:G:146:GLU:HB3	2.13	0.48
10:J:54:PHE:HD1	10:J:55:LYS:HG2	1.78	0.48
20:T:50:GLU:HG3	20:T:100:ILE:HB	1.94	0.48
1:A:376:G:H2'	1:A:377:G:H8	1.77	0.48
1:A:563:A:H2'	1:A:567:G:C8	2.49	0.48
1:A:997:U:H2'	1:A:998:G:O4'	2.14	0.48
1:A:1132:C:H2'	1:A:1133:G:C8	2.46	0.48
19:S:20:LEU:HA	19:S:23:ASN:HB2	1.96	0.48
1:A:994:A:N1	1:A:1047:G:H4'	2.29	0.48
4:D:64:LEU:HD23	4:D:198:VAL:HG21	1.96	0.48
11:K:77:MET:HE3	11:K:77:MET:HB3	1.65	0.48
1:A:21:G:H2'	1:A:22:G:C8	2.49	0.48
1:A:62:U:O2'	1:A:379:C:O2	2.26	0.48
1:A:436:C:H2'	1:A:437:U:C6	2.49	0.48
1:A:900:A:H2'	1:A:901:A:C8	2.48	0.48
1:A:335:C:H2'	1:A:336:C:C6	2.49	0.48
1:A:1136:U:H5''	1:A:1137:C:OP2	2.13	0.48
8:H:36:LEU:HD12	8:H:59:LEU:HD13	1.96	0.48
13:M:4:ILE:HD11	13:M:56:LEU:HB3	1.95	0.48
15:O:26:GLU:HA	15:O:81:LEU:HD11	1.96	0.48
1:A:738:C:OP1	6:F:2:ARG:NH1	2.47	0.48
1:A:1249:C:O2'	9:I:73:GLN:NE2	2.46	0.48
2:B:74:LYS:C	2:B:76:GLN:H	2.21	0.48
1:A:325:A:H2'	1:A:326:G:O4'	2.13	0.47
1:A:967:5MC:H2'	1:A:968:A:N7	2.29	0.47
20:T:10:LEU:HG	20:T:12:ALA:H	1.79	0.47
1:A:1241:G:H2'	1:A:1242:C:C6	2.49	0.47
13:M:22:ILE:HB	13:M:25:ILE:HB	1.96	0.47
7:G:150:ALA:HB1	11:K:57:THR:HG21	1.97	0.47
12:L:24:VAL:HG13	12:L:98:TYR:CE1	2.49	0.47
1:A:591:U:H2'	1:A:592:G:H8	1.79	0.47
1:A:1392:G:N2	1:A:1502:A:H8	2.12	0.47
2:B:47:THR:HA	2:B:202:PRO:HG2	1.96	0.47
7:G:15:ASP:HB2	7:G:23:VAL:HB	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:5:ALA:O	14:N:8:GLU:HB3	2.14	0.47
1:A:204:U:H5'	1:A:216:G:C4	2.50	0.47
1:A:551:U:H2'	1:A:552:U:C6	2.50	0.47
3:C:130:VAL:HG21	3:C:157:ILE:HG23	1.96	0.47
1:A:1060:C:H2'	1:A:1061:G:H8	1.79	0.47
1:A:1315:U:H2'	1:A:1316:G:O4'	2.15	0.47
1:A:130:A:C8	17:Q:63:ARG:HG3	2.49	0.47
1:A:144:G:H1	1:A:178:C:H42	1.63	0.47
1:A:165:C:H2'	1:A:166:G:C8	2.50	0.47
1:A:527:G7M:O2'	1:A:535:A:N1	2.40	0.47
1:A:1069:C:O2'	1:A:1192:C:H1'	2.15	0.47
1:A:1505:G:O2'	1:A:1506:U:OP2	2.31	0.47
22:A:1604:PAR:N21	22:A:1604:PAR:O53	2.48	0.47
3:C:12:LEU:HD23	3:C:12:LEU:HA	1.74	0.47
3:C:12:LEU:HD11	14:N:51:GLY:HA2	1.96	0.47
3:C:43:LEU:HD12	3:C:47:LEU:HD22	1.96	0.47
5:E:137:GLU:OE2	5:E:140:ARG:HD2	2.15	0.47
1:A:192:U:H1'	20:T:103:GLY:HA2	1.96	0.47
1:A:660:G:OP2	15:O:5:LYS:HE2	2.15	0.47
1:A:755:G:H1'	8:H:1:MET:HE3	1.96	0.47
1:A:918:A:H2'	1:A:919:A:C8	2.49	0.47
1:A:1479:C:H2'	1:A:1480:G:H8	1.80	0.47
22:A:1603:PAR:H11	22:A:1603:PAR:O52	2.15	0.47
2:B:98:LEU:HB2	2:B:101:MET:HG3	1.96	0.47
2:B:189:ASP:O	2:B:192:SER:OG	2.31	0.47
1:A:130:A:H1'	1:A:263:A:O2'	2.14	0.47
10:J:90:LEU:N	10:J:91:PRO:HD2	2.30	0.47
13:M:91:ARG:HH22	13:M:103:THR:HG21	1.80	0.47
1:A:826:C:H4'	8:H:12:ARG:HG2	1.97	0.46
3:C:191:THR:OG1	3:C:194:GLY:O	2.31	0.46
4:D:112:VAL:HG12	4:D:116:GLN:OE1	2.15	0.46
15:O:3:ILE:HD13	15:O:34:LEU:HD13	1.97	0.46
1:A:954:G:H21	1:A:1227:A:H62	1.63	0.46
1:A:1167:A:H8	1:A:1167:A:OP1	1.98	0.46
3:C:58:GLU:HB3	10:J:92:THR:HG21	1.97	0.46
15:O:29:VAL:HG11	15:O:67:LEU:HD21	1.96	0.46
1:A:1268:A:N3	1:A:1326:C:O2'	2.45	0.46
1:A:1314:C:C5	19:S:6:LYS:HE2	2.50	0.46
2:B:223:ILE:H	2:B:223:ILE:HG13	1.54	0.46
15:O:78:TYR:CZ	15:O:82:ILE:HD11	2.51	0.46
20:T:18:GLN:O	20:T:22:ARG:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1347:G:N1	1:A:1374:A:OP2	2.45	0.46
1:A:1432:G:O2'	1:A:1468:A:N6	2.48	0.46
2:B:115:LEU:HD11	2:B:146:GLN:HG3	1.96	0.46
4:D:98:GLU:OE2	4:D:103:ASN:ND2	2.32	0.46
1:A:1277:C:O2'	1:A:1279:A:H8	1.99	0.46
1:A:1385:G:H2'	1:A:1386:G:O4'	2.15	0.46
1:A:130:A:N1	1:A:233:C:O2'	2.43	0.46
1:A:1028:C:N4	1:A:1033:G:H1	2.12	0.46
12:L:90:VAL:HB	12:L:93:LEU:HB2	1.96	0.46
13:M:67:GLU:HB3	13:M:68:GLY:H	1.47	0.46
7:G:111:ARG:HB2	7:G:119:ARG:HG2	1.98	0.46
8:H:28:ALA:HB3	8:H:57:PRO:HB2	1.97	0.46
12:L:70:ILE:HG12	12:L:100:ILE:HD12	1.98	0.46
1:A:560:U:H5'	1:A:566:G:N2	2.31	0.46
15:O:56:LEU:O	15:O:60:VAL:HG23	2.14	0.46
19:S:11:VAL:HG13	19:S:38:SER:HB3	1.97	0.46
1:A:405:U:OP2	4:D:3:ARG:HD3	2.16	0.46
1:A:631:G:O3'	1:A:632:A:H8	1.98	0.46
1:A:811:C:H4'	1:A:900:A:N6	2.31	0.46
1:A:949:A:OP1	13:M:101:GLN:HB3	2.15	0.46
1:A:757:U:H2'	1:A:758:G:O4'	2.16	0.46
1:A:833:U:H2'	1:A:834:C:C6	2.50	0.46
1:A:875:C:O2'	8:H:14:ARG:NH1	2.46	0.46
2:B:87:ARG:CZ	2:B:233:SER:HB2	2.46	0.46
3:C:67:THR:HA	3:C:102:ASN:HB2	1.97	0.46
7:G:71:PRO:HG3	7:G:103:TRP:CH2	2.51	0.46
7:G:113:GLU:O	7:G:119:ARG:HD3	2.16	0.46
1:A:337:C:H2'	1:A:338:A:C8	2.51	0.45
1:A:636:U:H5'	17:Q:2:PRO:HG3	1.97	0.45
19:S:36:ARG:HH21	19:S:53:ASN:HA	1.81	0.45
19:S:43:GLU:CD	19:S:43:GLU:H	2.24	0.45
20:T:56:MET:HE3	20:T:56:MET:HB2	1.84	0.45
1:A:134:A:H1'	1:A:325:A:C5	2.51	0.45
1:A:820:U:H4'	1:A:821:G:OP2	2.17	0.45
1:A:1232:U:H2'	1:A:1233:G:O4'	2.15	0.45
1:A:1399:C:C2	1:A:1502:A:N6	2.84	0.45
1:A:1518:MA6:O5'	1:A:1518:MA6:H8	2.15	0.45
1:A:562:C:H1'	12:L:15:ARG:HB3	1.98	0.45
4:D:30:LYS:HA	4:D:35:ARG:HH11	1.82	0.45
1:A:916:G:H2'	1:A:917:G:H8	1.81	0.45
1:A:996:A:H2'	1:A:997:U:C6	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1495:U:H2'	1:A:1496:C:C6	2.52	0.45
2:B:223:ILE:O	2:B:227:GLY:N	2.49	0.45
8:H:11:THR:HG23	8:H:14:ARG:HH12	1.82	0.45
20:T:43:LEU:HD13	20:T:51:GLU:HG3	1.98	0.45
1:A:110:C:H2'	1:A:111:G:O4'	2.17	0.45
1:A:294:U:OP1	1:A:610:G:O2'	2.28	0.45
1:A:496:A:H4'	1:A:497:A:OP1	2.16	0.45
1:A:767:A:H2'	1:A:768:A:O4'	2.17	0.45
1:A:989:C:H42	1:A:1216:G:H1	1.62	0.45
1:A:991:U:O4	1:A:1212:U:H1'	2.16	0.45
2:B:239:VAL:O	2:B:240:GLN:HB3	2.17	0.45
6:F:55:ASP:HA	6:F:56:PRO:HD3	1.68	0.45
7:G:5:ARG:NH2	7:G:8:GLU:OE2	2.37	0.45
8:H:20:TYR:HD1	8:H:65:TYR:CE1	2.33	0.45
12:L:8:ASN:O	12:L:12:ARG:HG3	2.16	0.45
1:A:46:G:H2'	1:A:366:C:C5	2.51	0.45
1:A:627:G:H2'	1:A:628:G:H8	1.80	0.45
10:J:64:GLU:CD	10:J:66:ARG:HH21	2.24	0.45
12:L:124:LYS:HA	12:L:125:PRO:HD2	1.85	0.45
1:A:300:A:O2'	1:A:564:C:N3	2.45	0.45
1:A:1149:C:H2'	1:A:1150:U:C6	2.51	0.45
2:B:114:ARG:O	2:B:114:ARG:HD3	2.17	0.45
17:Q:59:ILE:CG2	17:Q:71:PHE:HB3	2.46	0.45
1:A:56:U:H2'	1:A:57:G:C8	2.51	0.45
1:A:458:C:H2'	1:A:459:G:O4'	2.17	0.45
1:A:620:C:C2	4:D:135:LEU:HD13	2.51	0.45
1:A:620:C:N1	4:D:135:LEU:HD13	2.31	0.45
1:A:1308:U:OP2	13:M:99:ARG:HG3	2.17	0.45
2:B:80:ILE:HG21	2:B:211:ILE:HG22	1.98	0.45
5:E:80:ILE:HD11	5:E:91:LEU:HD12	1.99	0.45
10:J:38:ILE:HB	10:J:71:LEU:HB2	1.98	0.45
11:K:82:VAL:HB	11:K:108:ILE:HG12	1.98	0.45
1:A:297:G:N2	1:A:300:A:OP2	2.47	0.45
1:A:1127:G:H21	1:A:1147:C:H41	1.65	0.45
3:C:30:ARG:HB3	14:N:36:PHE:O	2.17	0.45
19:S:50:ALA:HA	19:S:58:VAL:O	2.17	0.45
1:A:57:G:H2'	1:A:58:C:C6	2.53	0.45
1:A:107:G:O6	20:T:15:ARG:NE	2.50	0.45
1:A:568:G:O2'	1:A:574:A:N1	2.47	0.45
2:B:32:ILE:HD11	2:B:190:THR:HG23	1.98	0.45
1:A:713:G:H2'	1:A:714:G:C8	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1371:G:OP2	9:I:11:LYS:HE2	2.17	0.44
4:D:7:PRO:HB2	4:D:10:ARG:HD2	2.00	0.44
13:M:37:THR:HB	13:M:39:ILE:HG13	2.00	0.44
1:A:629:G:H2'	1:A:630:G:O4'	2.18	0.44
1:A:666:G:H5'	1:A:726:C:H1'	1.99	0.44
1:A:885:G:O2'	1:A:914:A:N1	2.46	0.44
5:E:77:PRO:HB2	5:E:78:HIS:HD2	1.82	0.44
10:J:16:LEU:HD12	10:J:68:HIS:HB2	1.99	0.44
14:N:26:ARG:NH1	14:N:47:LEU:HD21	2.32	0.44
17:Q:66:SER:OG	17:Q:69:LYS:HB2	2.16	0.44
1:A:663:A:H5''	18:R:61:LYS:HE3	1.98	0.44
1:A:1075:C:H4'	2:B:175:ARG:HH22	1.81	0.44
5:E:77:PRO:HB2	5:E:78:HIS:CD2	2.52	0.44
1:A:1119:C:H2'	1:A:1120:G:H8	1.82	0.44
7:G:45:ASP:O	7:G:49:ILE:HG13	2.18	0.44
11:K:44:SER:H	11:K:47:VAL:HB	1.80	0.44
16:P:7:ALA:O	16:P:17:TYR:HA	2.18	0.44
1:A:284:G:H2'	1:A:285:G:H8	1.83	0.44
1:A:292:G:OP2	1:A:305:G:N2	2.38	0.44
1:A:620:C:H2'	1:A:621:A:C8	2.53	0.44
1:A:660:G:H1	1:A:745:C:H42	1.65	0.44
2:B:74:LYS:HE2	2:B:74:LYS:HB3	1.84	0.44
5:E:117:ASP:OD1	5:E:117:ASP:N	2.49	0.44
10:J:39:PRO:HA	10:J:70:ARG:HE	1.82	0.44
10:J:89:ASP:HB2	10:J:91:PRO:HD2	2.00	0.44
18:R:53:ARG:O	18:R:57:GLY:N	2.38	0.44
3:C:11:ARG:NH1	3:C:177:THR:O	2.51	0.44
5:E:88:LYS:HB3	5:E:123:LEU:HB2	1.99	0.44
10:J:32:ALA:O	10:J:34:VAL:HG23	2.18	0.44
17:Q:59:ILE:HG22	17:Q:71:PHE:HD2	1.83	0.44
17:Q:85:VAL:O	17:Q:89:LEU:HG	2.18	0.44
20:T:53:LEU:HB3	20:T:102:GLY:HA3	1.99	0.44
1:A:59:A:H1'	1:A:354:G:N2	2.32	0.44
1:A:1022:G:H2'	1:A:1023:G:C8	2.52	0.44
1:A:1191:A:H5''	3:C:4:LYS:HE3	2.00	0.44
2:B:223:ILE:HD13	2:B:230:VAL:N	2.30	0.44
20:T:85:MET:HE2	20:T:104:LEU:HD23	1.99	0.44
1:A:41:G:H2'	1:A:42:G:C8	2.53	0.44
1:A:102:G:O2'	1:A:151:A:N3	2.45	0.44
1:A:266:G:H5''	1:A:267:C:C5	2.52	0.44
1:A:479:C:H2'	1:A:480:U:O4'	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1298:C:H4'	1:A:1299:A:O4'	2.18	0.44
12:L:30:ALA:HA	12:L:31:PRO:HD3	1.84	0.44
19:S:16:LEU:HA	19:S:19:VAL:HG12	1.99	0.44
1:A:408:A:H4'	4:D:112:VAL:HG11	2.00	0.43
1:A:463:A:H2'	1:A:474:G:O4'	2.18	0.43
1:A:973:G:H3'	1:A:974:A:H5''	2.00	0.43
1:A:1062:U:H2'	1:A:1063:C:C6	2.53	0.43
1:A:1301:U:HO2'	1:A:1302:U:P	2.41	0.43
3:C:58:GLU:HB2	3:C:65:ALA:HB3	2.00	0.43
9:I:69:GLY:O	9:I:73:GLN:HG3	2.17	0.43
13:M:96:LEU:C	13:M:110:ARG:HG2	2.43	0.43
1:A:463:A:OP1	16:P:75:ARG:NH1	2.49	0.43
1:A:659:U:H2'	1:A:660:G:C8	2.53	0.43
1:A:707:C:H2'	1:A:708:C:H6	1.83	0.43
1:A:719:C:O2'	18:R:49:LYS:HB3	2.17	0.43
1:A:1105:A:H2'	1:A:1106:G:C8	2.52	0.43
1:A:1189:C:H5''	3:C:5:ILE:HG12	2.00	0.43
7:G:51:GLN:C	7:G:53:LYS:N	2.76	0.43
9:I:22:GLY:HA3	9:I:60:ASP:CG	2.42	0.43
10:J:4:ILE:HD11	10:J:74:ILE:HB	1.99	0.43
17:Q:66:SER:OG	17:Q:69:LYS:HD3	2.18	0.43
1:A:1129:C:H4'	1:A:1130:A:OP2	2.16	0.43
1:A:1137:C:H5'	1:A:1138:G:C4	2.52	0.43
1:A:1223:C:OP1	19:S:78:ARG:NH1	2.39	0.43
9:I:118:LYS:C	9:I:120:ARG:H	2.22	0.43
12:L:59:ARG:NH1	12:L:65:GLU:OE2	2.52	0.43
17:Q:27:PHE:CZ	17:Q:36:ILE:HD11	2.54	0.43
17:Q:83:ASP:OD1	17:Q:84:LEU:N	2.51	0.43
1:A:165:C:H2'	1:A:166:G:H8	1.82	0.43
1:A:190(J):U:H2'	1:A:190(K):G:C8	2.54	0.43
1:A:1182:G:H4'	1:A:1183:A:O5'	2.18	0.43
1:A:1428:A:H2'	1:A:1429:C:C6	2.53	0.43
1:A:1431:C:H2'	1:A:1432:G:O4'	2.19	0.43
4:D:135:LEU:HA	4:D:136:PRO:HD3	1.89	0.43
9:I:126:SER:O	9:I:127:LYS:HB3	2.19	0.43
15:O:18:PHE:HB2	15:O:19:PRO:HD2	2.00	0.43
1:A:359:U:H2'	1:A:360:A:H8	1.83	0.43
1:A:372:C:H1'	1:A:373:A:OP2	2.19	0.43
1:A:927:G:OP2	1:A:1503:A:H2'	2.18	0.43
1:A:1016:A:H2'	1:A:1017:G:O4'	2.18	0.43
1:A:1057:G:H2'	1:A:1058:G:O4'	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:17:VAL:HG13	9:I:63:ILE:HG12	2.01	0.43
17:Q:3:LYS:HB3	17:Q:61:GLU:HB3	2.01	0.43
1:A:1513:A:H2'	1:A:1514:C:C6	2.53	0.43
2:B:219:VAL:O	2:B:223:ILE:HG13	2.18	0.43
13:M:15:VAL:HB	13:M:34:LEU:HD11	2.00	0.43
1:A:405:U:H5''	1:A:496:A:H2	1.83	0.43
1:A:406:G:H2'	1:A:407:G:C8	2.53	0.43
1:A:983:A:N1	1:A:1222:G:N2	2.66	0.43
4:D:105:VAL:HG13	4:D:110:PHE:HB2	2.01	0.43
5:E:11:ILE:HD13	5:E:105:VAL:HG13	2.00	0.43
13:M:44:ARG:HD2	13:M:44:ARG:N	2.34	0.43
20:T:53:LEU:HB2	20:T:100:ILE:HG22	2.01	0.43
1:A:376:G:H2'	1:A:377:G:C8	2.54	0.43
1:A:828:A:H2'	1:A:829:G:O4'	2.19	0.43
2:B:73:THR:N	2:B:170:GLU:OE1	2.40	0.43
7:G:124:LEU:HD12	7:G:124:LEU:HA	1.84	0.43
12:L:6:THR:OG1	12:L:9:GLN:HG3	2.17	0.43
1:A:406:G:H2'	1:A:407:G:H8	1.83	0.43
1:A:938:A:N6	1:A:939:G:C6	2.86	0.43
1:A:1342:C:H2'	1:A:1343:G:C8	2.53	0.43
1:A:1511:G:H2'	1:A:1512:U:O4'	2.18	0.43
1:A:1532:U:H2'	1:A:1533:C:H3'	1.99	0.43
4:D:150:GLU:OE2	4:D:150:GLU:N	2.51	0.43
1:A:1401:G:C2	1:A:1402:4OC:H1'	2.53	0.43
9:I:45:ALA:HA	9:I:48:GLU:HG2	2.01	0.43
1:A:692:U:H2'	1:A:694:A:OP2	2.19	0.42
1:A:1048:G:O3'	1:A:1049:U:H3'	2.19	0.42
1:A:1060:C:H2'	1:A:1061:G:C8	2.54	0.42
1:A:1318:A:H5''	1:A:1319:A:OP2	2.19	0.42
1:A:1392:G:N2	1:A:1502:A:C8	2.86	0.42
1:A:1517:G:H2'	1:A:1518:MA6:H8	2.01	0.42
2:B:97:TRP:HH2	2:B:176:GLU:CD	2.27	0.42
3:C:58:GLU:HB2	3:C:65:ALA:CB	2.49	0.42
4:D:176:LEU:HD12	4:D:182:LYS:O	2.19	0.42
15:O:21:ASP:OD2	15:O:24:SER:OG	2.26	0.42
18:R:34:TYR:CE1	18:R:35:ARG:HG3	2.54	0.42
20:T:36:LEU:HD23	20:T:36:LEU:HA	1.81	0.42
1:A:115:G:H1'	1:A:116:A:N7	2.35	0.42
1:A:192:U:C1'	20:T:103:GLY:HA2	2.49	0.42
1:A:586:C:O2'	1:A:587:G:H5'	2.19	0.42
1:A:812:C:H6	1:A:812:C:H2'	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1427:U:H2'	1:A:1428:A:H8	1.84	0.42
1:A:1479:C:H2'	1:A:1480:G:C8	2.55	0.42
1:A:1488:G:H2'	1:A:1489:G:H8	1.85	0.42
2:B:112:VAL:O	2:B:116:GLU:HG2	2.20	0.42
4:D:78:LEU:HD22	4:D:96:LEU:HB3	2.01	0.42
21:U:5:ASP:O	21:U:11:GLY:HA3	2.18	0.42
1:A:160:A:H2'	1:A:161:A:O4'	2.19	0.42
1:A:950:U:H2'	1:A:951:G:C8	2.55	0.42
1:A:1275:A:H2'	1:A:1276:G:O4'	2.20	0.42
1:A:1298:C:C4	7:G:114:ARG:HG2	2.54	0.42
4:D:53:ASP:O	4:D:57:ARG:HG2	2.20	0.42
19:S:58:VAL:HA	19:S:59:PRO:HD3	1.69	0.42
1:A:126:G:OP1	1:A:605:U:O2'	2.31	0.42
1:A:384:G:H2'	1:A:385:C:C6	2.54	0.42
1:A:540:G:H2'	1:A:541:G:O4'	2.20	0.42
1:A:1495:U:H2'	1:A:1496:C:H6	1.83	0.42
3:C:135:LYS:NZ	5:E:50:GLU:OE1	2.51	0.42
5:E:6:PHE:CE1	5:E:36:ASP:HB3	2.55	0.42
5:E:118:ILE:HG12	5:E:119:LEU:N	2.34	0.42
18:R:16:PRO:HB2	18:R:17:SER:H	1.64	0.42
1:A:31:G:N2	1:A:48:C:OP1	2.48	0.42
1:A:115:G:H4'	1:A:116:A:O5'	2.19	0.42
1:A:269:C:H2'	1:A:270:A:H8	1.84	0.42
1:A:432:A:O2'	1:A:433:C:OP1	2.31	0.42
1:A:694:A:N1	1:A:787:A:O2'	2.52	0.42
1:A:1073:U:OP1	5:E:57:LYS:HE2	2.19	0.42
1:A:1264:C:H2'	1:A:1265:G:C8	2.54	0.42
1:A:1305:G:N2	1:A:1332:A:OP2	2.52	0.42
11:K:108:ILE:HB	18:R:87:ARG:O	2.18	0.42
1:A:656:C:O2'	15:O:28:GLN:OE1	2.34	0.42
1:A:983:A:O2'	1:A:1050:G:OP2	2.37	0.42
1:A:1137:C:H4'	1:A:1138:G:C2	2.54	0.42
1:A:1323:G:H2'	1:A:1324:A:C8	2.55	0.42
8:H:18:ARG:NH2	8:H:81:HIS:O	2.50	0.42
11:K:69:ALA:O	11:K:73:MET:HG3	2.19	0.42
17:Q:10:VAL:HG22	17:Q:21:VAL:HG22	2.01	0.42
17:Q:59:ILE:HG22	17:Q:71:PHE:CD2	2.54	0.42
1:A:63:C:OP1	1:A:383:A:N6	2.50	0.42
1:A:407:G:H5''	4:D:115:ARG:HB3	2.01	0.42
1:A:413:G:H1'	1:A:428:G:H21	1.84	0.42
1:A:932:C:H4'	7:G:4:ARG:NH2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1131:G:H2'	1:A:1132:C:C6	2.54	0.42
2:B:218:ALA:O	2:B:222:ILE:HG13	2.20	0.42
8:H:4:ASP:OD1	8:H:85:ARG:NH1	2.53	0.42
11:K:115:PRO:C	11:K:117:ASN:H	2.28	0.42
18:R:39:VAL:HG12	18:R:40:LEU:HD23	2.00	0.42
1:A:1320:C:O2	19:S:36:ARG:NH1	2.53	0.42
8:H:4:ASP:CG	8:H:85:ARG:HH11	2.27	0.42
10:J:61:GLU:OE1	14:N:45:ARG:NH1	2.45	0.42
19:S:66:MET:HE3	19:S:74:PHE:CZ	2.54	0.42
1:A:1092:A:N3	1:A:1183:A:N6	2.67	0.42
2:B:87:ARG:NH2	2:B:233:SER:HB2	2.34	0.42
7:G:51:GLN:O	7:G:53:LYS:N	2.53	0.42
7:G:137:LYS:O	7:G:141:VAL:HG23	2.20	0.42
8:H:34:GLU:O	8:H:38:ILE:HG12	2.20	0.42
11:K:124:LYS:HE2	11:K:125:PHE:CE2	2.54	0.42
12:L:53:ARG:HB3	12:L:93:LEU:HD11	2.02	0.42
14:N:33:VAL:HA	14:N:40:CYS:HA	2.02	0.42
20:T:14:LYS:HA	20:T:17:ARG:CZ	2.49	0.42
1:A:204:U:H2'	1:A:204:U:O2	2.19	0.42
1:A:370:C:H2'	1:A:371:G:O4'	2.20	0.42
1:A:707:C:H2'	1:A:708:C:C6	2.55	0.42
1:A:1053:G:C3'	1:A:1054:C:H5'	2.50	0.42
1:A:1216:G:H5''	14:N:5:ALA:CB	2.50	0.42
1:A:1225:A:H4'	19:S:78:ARG:HD3	2.02	0.42
1:A:1347:G:N2	1:A:1373:G:H2'	2.34	0.42
1:A:1504:G:OP1	1:A:1507:A:H4'	2.20	0.42
10:J:37:PRO:HA	10:J:71:LEU:O	2.19	0.42
13:M:34:LEU:HD22	13:M:39:ILE:HB	2.01	0.42
15:O:87:ILE:HG22	15:O:88:ARG:H	1.85	0.42
19:S:40:ILE:HG22	19:S:67:VAL:HA	2.01	0.42
1:A:114:U:H2'	1:A:115:G:C8	2.55	0.41
1:A:1497:G:C2'	1:A:1498:UR3:H5'	2.50	0.41
2:B:59:GLU:HB2	2:B:221:LEU:HD11	2.02	0.41
7:G:78:ARG:NH1	7:G:154:TYR:O	2.53	0.41
8:H:31:PHE:O	8:H:35:ILE:HD12	2.20	0.41
11:K:70:LYS:HA	11:K:73:MET:HE2	2.02	0.41
17:Q:63:ARG:HG2	17:Q:64:PRO:CD	2.48	0.41
1:A:247:G:OP2	17:Q:100:LYS:HG3	2.20	0.41
1:A:608:A:H2'	1:A:609:A:O4'	2.20	0.41
1:A:936:C:H2'	1:A:937:A:O4'	2.20	0.41
1:A:956:U:C2	1:A:1225:A:C2	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1105:A:H2'	1:A:1106:G:H8	1.83	0.41
2:B:24:TRP:CZ3	2:B:26:PRO:HA	2.55	0.41
4:D:205:GLU:OE1	5:E:100:VAL:HG23	2.20	0.41
15:O:64:ARG:HD3	15:O:88:ARG:NH2	2.35	0.41
20:T:50:GLU:HA	20:T:100:ILE:HB	2.01	0.41
1:A:50:A:N1	1:A:360:A:O2'	2.46	0.41
1:A:190(K):G:H2'	1:A:190(L):U:C6	2.55	0.41
1:A:254:G:OP1	17:Q:67:LYS:O	2.38	0.41
1:A:1092:A:H5''	7:G:4:ARG:NH1	2.36	0.41
1:A:1145:C:H6	1:A:1145:C:H2'	1.71	0.41
1:A:1228:C:O2'	13:M:117:VAL:HG22	2.20	0.41
1:A:1311:G:N7	19:S:2:PRO:HA	2.34	0.41
1:A:1320:C:N3	19:S:36:ARG:HD3	2.36	0.41
6:F:3:ARG:HG2	6:F:93:SER:OG	2.20	0.41
8:H:82:HIS:HE1	8:H:136:GLU:OE2	2.02	0.41
13:M:13:LYS:HD3	13:M:17:VAL:HG12	2.02	0.41
14:N:39:LEU:HD11	14:N:47:LEU:HD12	2.02	0.41
15:O:79:ARG:NH1	15:O:83:GLU:HB2	2.35	0.41
16:P:9:PHE:N	16:P:16:HIS:O	2.51	0.41
1:A:545:C:OP1	4:D:61:LYS:NZ	2.52	0.41
1:A:724:G:O6	1:A:733:A:N6	2.53	0.41
1:A:1071:C:H2'	1:A:1072:G:C8	2.56	0.41
1:A:1291:G:H4'	9:I:39:GLY:HA3	2.01	0.41
1:A:1368:G:H5''	9:I:112:LYS:HB3	2.02	0.41
3:C:95:THR:O	3:C:95:THR:OG1	2.35	0.41
4:D:8:VAL:O	4:D:11:LEU:N	2.40	0.41
4:D:200:GLU:O	4:D:204:ILE:HG13	2.20	0.41
7:G:29:LYS:HD2	7:G:29:LYS:HA	1.86	0.41
1:A:953:G:C2	1:A:954:G:H1'	2.55	0.41
1:A:1190:G:OP1	3:C:4:LYS:HA	2.20	0.41
1:A:1304:G:C6	1:A:1305:G:N1	2.88	0.41
3:C:175:LEU:HD22	3:C:175:LEU:HA	1.90	0.41
4:D:24:GLU:HG2	4:D:25:ARG:N	2.35	0.41
13:M:67:GLU:O	13:M:71:ARG:HG3	2.19	0.41
14:N:8:GLU:O	14:N:8:GLU:HG2	2.20	0.41
1:A:200:G:H2'	1:A:201:C:O4'	2.19	0.41
1:A:389:A:C6	1:A:390:C:H1'	2.55	0.41
1:A:391:G:O3'	16:P:8:ARG:NH2	2.53	0.41
1:A:502:G:H2'	1:A:503:C:O4'	2.20	0.41
1:A:578:C:H2'	1:A:579:G:O4'	2.21	0.41
1:A:677:U:O2	1:A:777:A:O2'	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:967:5MC:H2'	1:A:968:A:C8	2.55	0.41
1:A:1036:G:H3'	1:A:1037:C:C6	2.56	0.41
1:A:1116:C:O2'	9:I:108:VAL:HG21	2.21	0.41
1:A:1211:U:O2'	1:A:1213:A:N1	2.53	0.41
1:A:1318:A:H4'	19:S:10:PHE:CE2	2.56	0.41
2:B:163:PHE:HA	2:B:185:ILE:O	2.20	0.41
16:P:4:ILE:HG13	16:P:64:ALA:HB1	2.01	0.41
1:A:235:C:H5'	17:Q:70:ARG:CG	2.48	0.41
1:A:284:G:H2'	1:A:285:G:C8	2.56	0.41
1:A:791:G:C6	1:A:792:A:N7	2.88	0.41
1:A:993:G:O2'	1:A:994:A:N7	2.53	0.41
1:A:1221:G:C4	1:A:1222:G:C8	3.09	0.41
1:A:1242:C:H42	1:A:1295:G:H1	1.69	0.41
1:A:1370:G:H5'	9:I:12:GLU:OE1	2.21	0.41
10:J:86:MET:HB3	10:J:87:THR:H	1.73	0.41
13:M:23:TYR:HB3	13:M:67:GLU:HA	2.02	0.41
15:O:47:LYS:H	15:O:47:LYS:HG3	1.61	0.41
15:O:75:PRO:O	15:O:78:TYR:HB3	2.20	0.41
18:R:87:ARG:HD2	18:R:87:ARG:HA	1.93	0.41
1:A:194:C:H5''	20:T:65:LYS:HG3	2.02	0.41
1:A:475:G:H2'	1:A:476:G:C8	2.56	0.41
1:A:505:G:H1	1:A:526:C:H42	1.66	0.41
1:A:714:G:H2'	1:A:715:A:O4'	2.20	0.41
1:A:1265:G:C2	1:A:1271:G:C2	3.09	0.41
3:C:147:LYS:HE2	3:C:147:LYS:HB3	1.83	0.41
13:M:59:TYR:O	13:M:63:THR:HG22	2.21	0.41
15:O:85:LEU:HD23	15:O:85:LEU:HA	1.90	0.41
1:A:267:C:H2'	1:A:268:C:C6	2.56	0.41
1:A:353:A:H5'	1:A:353:A:H8	1.86	0.41
1:A:675:A:O2'	11:K:114:VAL:O	2.37	0.41
1:A:717:C:N4	22:A:1606:PAR:O31	2.53	0.41
1:A:1441:G:H4'	1:A:1442:G:C6	2.56	0.41
2:B:178:ARG:O	8:H:71:GLY:HA2	2.20	0.41
3:C:43:LEU:O	3:C:47:LEU:HB2	2.21	0.41
4:D:64:LEU:HD23	4:D:64:LEU:HA	1.97	0.41
5:E:83:GLU:HG2	5:E:88:LYS:HG3	2.03	0.41
7:G:38:LEU:O	7:G:42:ILE:HG13	2.20	0.41
7:G:79:ARG:HD2	7:G:79:ARG:C	2.46	0.41
8:H:17:THR:O	8:H:78:GLN:NE2	2.46	0.41
12:L:45:PRO:HG2	12:L:49:ASN:O	2.20	0.41
15:O:5:LYS:HD3	15:O:5:LYS:HA	1.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:24:GLU:OE2	17:Q:37:LYS:HD3	2.21	0.41
1:A:519:C:H2'	1:A:520:A:C8	2.55	0.41
1:A:1350:A:OP2	9:I:118:LYS:NZ	2.42	0.41
2:B:20:GLU:HA	2:B:39:ILE:HG13	2.02	0.41
4:D:78:LEU:HA	4:D:78:LEU:HD23	1.85	0.41
6:F:2:ARG:NE	6:F:69:GLU:HG2	2.36	0.41
6:F:22:GLU:O	6:F:26:ILE:HG12	2.21	0.41
13:M:8:GLU:OE1	13:M:22:ILE:HA	2.21	0.41
1:A:432:A:H2'	1:A:433:C:O4'	2.21	0.40
1:A:632:A:H2'	1:A:633:G:O4'	2.22	0.40
1:A:708:C:OP1	11:K:85:ARG:NH2	2.54	0.40
3:C:13:GLY:HA3	14:N:57:ARG:NH2	2.36	0.40
9:I:43:ALA:HA	9:I:74:ILE:HD13	2.03	0.40
1:A:778:G:H8	1:A:778:G:O5'	2.04	0.40
1:A:791:G:C5	1:A:792:A:N7	2.89	0.40
1:A:965:A:C2	1:A:969:A:C2	3.09	0.40
1:A:966:M2G:O2'	9:I:127:LYS:HG3	2.21	0.40
1:A:1091:U:O2	1:A:1093:A:C8	2.75	0.40
1:A:1245:A:N6	1:A:1291:G:O6	2.54	0.40
1:A:1273:G:H2'	1:A:1274:G:O4'	2.22	0.40
1:A:1530:G:H2'	1:A:1531:A:C8	2.56	0.40
2:B:231:GLU:HA	2:B:232:PRO:HD3	1.97	0.40
16:P:2:VAL:O	16:P:64:ALA:HA	2.21	0.40
21:U:12:LYS:CB	21:U:22:ARG:HB2	2.51	0.40
3:C:196:LEU:HD13	3:C:196:LEU:HA	1.95	0.40
15:O:2:PRO:HB2	15:O:3:ILE:H	1.73	0.40
1:A:678:U:H2'	1:A:679:C:C6	2.56	0.40
1:A:1308:U:H2'	1:A:1309:G:C8	2.57	0.40
2:B:82:ARG:O	2:B:86:GLU:HB2	2.21	0.40
3:C:131:ARG:HA	3:C:134:ILE:HD12	2.04	0.40
12:L:113:ARG:NH1	12:L:116:SER:H	2.19	0.40
18:R:53:ARG:HA	18:R:56:THR:OG1	2.21	0.40
1:A:778:G:O2'	11:K:120:ARG:O	2.37	0.40
1:A:953:G:H2'	1:A:954:G:O4'	2.22	0.40
1:A:1315:U:O2'	1:A:1360:A:N3	2.55	0.40
5:E:12:LEU:HD12	5:E:31:LEU:HB2	2.04	0.40
9:I:32:ASP:OD1	9:I:33:PHE:N	2.55	0.40
9:I:50:LEU:HD22	9:I:55:ALA:HB3	2.03	0.40
10:J:49:VAL:CG2	14:N:41:ARG:HB2	2.52	0.40
11:K:126:ARG:O	11:K:127:LYS:HB2	2.21	0.40
15:O:45:VAL:HG12	15:O:46:HIS:H	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:88:ARG:HD2	15:O:88:ARG:HA	1.93	0.40
19:S:12:ASP:HB2	19:S:38:SER:OG	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	234/256 (91%)	217 (93%)	16 (7%)	1 (0%)	30	59
3	C	205/239 (86%)	189 (92%)	16 (8%)	0	100	100
4	D	206/209 (99%)	201 (98%)	5 (2%)	0	100	100
5	E	149/162 (92%)	145 (97%)	4 (3%)	0	100	100
6	F	99/101 (98%)	96 (97%)	3 (3%)	0	100	100
7	G	153/156 (98%)	146 (95%)	7 (5%)	0	100	100
8	H	136/138 (99%)	133 (98%)	3 (2%)	0	100	100
9	I	125/128 (98%)	117 (94%)	7 (6%)	1 (1%)	16	44
10	J	97/105 (92%)	81 (84%)	15 (16%)	1 (1%)	12	40
11	K	115/129 (89%)	107 (93%)	8 (7%)	0	100	100
12	L	122/135 (90%)	113 (93%)	8 (7%)	1 (1%)	16	44
13	M	116/126 (92%)	109 (94%)	7 (6%)	0	100	100
14	N	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
15	O	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
16	P	82/88 (93%)	78 (95%)	4 (5%)	0	100	100
17	Q	99/105 (94%)	91 (92%)	8 (8%)	0	100	100
18	R	71/88 (81%)	64 (90%)	7 (10%)	0	100	100
19	S	79/93 (85%)	70 (89%)	8 (10%)	1 (1%)	9	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	T	97/106 (92%)	89 (92%)	8 (8%)	0	100	100
21	U	23/27 (85%)	22 (96%)	1 (4%)	0	100	100
All	All	2352/2541 (93%)	2206 (94%)	141 (6%)	5 (0%)	43	71

All (5) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	201/220 (91%)	181 (90%)	20 (10%)	7	26
3	C	160/188 (85%)	139 (87%)	21 (13%)	4	16
4	D	180/181 (99%)	164 (91%)	16 (9%)	9	31
5	E	115/123 (94%)	102 (89%)	13 (11%)	5	21
6	F	90/90 (100%)	83 (92%)	7 (8%)	11	37
7	G	126/127 (99%)	114 (90%)	12 (10%)	8	29
8	H	119/119 (100%)	110 (92%)	9 (8%)	12	38
9	I	98/99 (99%)	82 (84%)	16 (16%)	2	10
10	J	87/92 (95%)	80 (92%)	7 (8%)	11	36
11	K	89/99 (90%)	78 (88%)	11 (12%)	4	18
12	L	103/110 (94%)	93 (90%)	10 (10%)	8	28
13	M	94/101 (93%)	83 (88%)	11 (12%)	5	20
14	N	48/50 (96%)	43 (90%)	5 (10%)	7	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	O	79/80 (99%)	72 (91%)	7 (9%)	9	31
16	P	72/74 (97%)	65 (90%)	7 (10%)	8	28
17	Q	95/97 (98%)	85 (90%)	10 (10%)	6	23
18	R	64/77 (83%)	60 (94%)	4 (6%)	16	42
19	S	71/80 (89%)	58 (82%)	13 (18%)	2	7
20	T	76/82 (93%)	62 (82%)	14 (18%)	1	7
21	U	19/22 (86%)	19 (100%)	0	100	100
All	All	1986/2111 (94%)	1773 (89%)	213 (11%)	6	23

All (213) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	44	LEU
2	B	61	LEU
2	B	63	MET
2	B	67	THR
2	B	69	LEU
2	B	76	GLN
2	B	83	MET
2	B	86	GLU
2	B	109	SER
2	B	114	ARG
2	B	142	LEU
2	B	144	ARG
2	B	168	THR
2	B	169	LYS
2	B	192	SER
2	B	200	ILE
2	B	213	LEU
2	B	221	LEU
2	B	223	ILE
2	B	236	TYR
3	C	3	ASN
3	C	5	ILE
3	C	12	LEU
3	C	14	ILE
3	C	27	LYS
3	C	34	LEU
3	C	63	ASN
3	C	64	VAL

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Mol	Chain	Res	Type
3	C	84	ILE
3	C	95	THR
3	C	108	ASN
3	C	115	LEU
3	C	147	LYS
3	C	165	THR
3	C	167	TRP
3	C	172	ARG
3	C	175	LEU
3	C	188	LEU
3	C	192	THR
3	C	195	VAL
3	C	204	LEU
4	D	3	ARG
4	D	8	VAL
4	D	15	GLU
4	D	19	LEU
4	D	53	ASP
4	D	64	LEU
4	D	65	ARG
4	D	70	ILE
4	D	107	ARG
4	D	112	VAL
4	D	114	ARG
4	D	122	ARG
4	D	127	THR
4	D	150	GLU
4	D	170	VAL
4	D	194	LEU
5	E	12	LEU
5	E	18	ARG
5	E	32	VAL
5	E	40	ARG
5	E	41	VAL
5	E	43	LEU
5	E	50	GLU
5	E	79	GLU
5	E	80	ILE
5	E	100	VAL
5	E	116	THR
5	E	118	ILE
5	E	145	LYS

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Mol	Chain	Res	Type
6	F	6	VAL
6	F	45	LEU
6	F	48	LEU
6	F	55	ASP
6	F	64	GLN
6	F	70	ASP
6	F	98	LEU
7	G	8	GLU
7	G	12	LEU
7	G	41	ARG
7	G	51	GLN
7	G	57	GLU
7	G	76	ARG
7	G	113	GLU
7	G	114	ARG
7	G	120	ILE
7	G	124	LEU
7	G	146	GLU
7	G	156	TRP
8	H	22	GLU
8	H	26	VAL
8	H	35	ILE
8	H	39	LEU
8	H	50	ARG
8	H	51	VAL
8	H	63	LEU
8	H	85	ARG
8	H	91	ARG
9	I	16	ARG
9	I	34	ASN
9	I	42	ARG
9	I	50	LEU
9	I	64	THR
9	I	79	LEU
9	I	85	LEU
9	I	96	LEU
9	I	97	LYS
9	I	99	LEU
9	I	102	LEU
9	I	108	VAL
9	I	112	LYS
9	I	118	LYS

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Mol	Chain	Res	Type
9	I	124	GLN
9	I	125	TYR
10	J	4	ILE
10	J	49	VAL
10	J	75	ILE
10	J	85	LEU
10	J	86	MET
10	J	88	LEU
10	J	96	ILE
11	K	18	ARG
11	K	28	THR
11	K	40	ILE
11	K	47	VAL
11	K	77	MET
11	K	80	VAL
11	K	91	ARG
11	K	101	SER
11	K	119	CYS
11	K	124	LYS
11	K	127	LYS
12	L	7	ILE
12	L	20	LYS
12	L	21	LYS
12	L	33	ARG
12	L	42	THR
12	L	47	LYS
12	L	55	VAL
12	L	60	LEU
12	L	66	VAL
12	L	79	GLU
13	M	4	ILE
13	M	17	VAL
13	M	37	THR
13	M	44	ARG
13	M	46	LYS
13	M	56	LEU
13	M	62	ASN
13	M	63	THR
13	M	64	TRP
13	M	70	LEU
13	M	116	THR
14	N	3	ARG

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Mol	Chain	Res	Type
14	N	8	GLU
14	N	9	LYS
14	N	11	LYS
14	N	17	LYS
15	O	32	LEU
15	O	34	LEU
15	O	36	ILE
15	O	39	LEU
15	O	45	VAL
15	O	48	LYS
15	O	81	LEU
16	P	1	MET
16	P	2	VAL
16	P	3	LYS
16	P	8	ARG
16	P	21	VAL
16	P	28	ARG
16	P	67	THR
17	Q	9	VAL
17	Q	36	ILE
17	Q	38	ARG
17	Q	60	ILE
17	Q	68	ARG
17	Q	85	VAL
17	Q	86	GLU
17	Q	92	ARG
17	Q	98	LEU
17	Q	101	ARG
18	R	38	GLU
18	R	75	ILE
18	R	76	LEU
18	R	86	VAL
19	S	4	SER
19	S	7	LYS
19	S	12	ASP
19	S	15	LEU
19	S	17	GLU
19	S	25	LYS
19	S	43	GLU
19	S	48	THR
19	S	55	LYS
19	S	58	VAL

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Mol	Chain	Res	Type
19	S	62	ILE
19	S	65	ASN
19	S	78	ARG
20	T	8	ARG
20	T	11	SER
20	T	13	LEU
20	T	19	SER
20	T	20	LEU
20	T	25	ARG
20	T	56	MET
20	T	62	LEU
20	T	73	HIS
20	T	74	LYS
20	T	75	ASN
20	T	84	LEU
20	T	87	LYS
20	T	93	GLU

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

Mol	Chain	Res	Type
2	B	95	GLN
3	C	63	ASN
3	C	110	ASN
3	C	118	GLN
7	G	11	GLN
8	H	82	HIS
9	I	3	GLN
9	I	73	GLN
11	K	116	HIS
13	M	106	ASN
15	O	50	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1510/1522 (99%)	231 (15%)	29 (1%)

All (231) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	9	G
1	A	32	A
1	A	39	G
1	A	44	G
1	A	47	C
1	A	48	C
1	A	50	A
1	A	51	A
1	A	81	U
1	A	101	A
1	A	115	G
1	A	116	A
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(F)	G
1	A	195	A
1	A	197	A
1	A	201	C
1	A	202	U
1	A	204	U
1	A	220	G
1	A	247	G
1	A	251	G
1	A	267	C
1	A	289	G
1	A	319	G
1	A	321	A
1	A	328	C
1	A	329	A
1	A	332	G
1	A	344	A
1	A	345	C
1	A	351	G
1	A	352	C
1	A	353	A
1	A	354	G
1	A	367	U
1	A	371	G
1	A	373	A

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Mol	Chain	Res	Type
1	A	384	G
1	A	389	A
1	A	397	A
1	A	398	C
1	A	406	G
1	A	412	A
1	A	413	G
1	A	419	C
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	443	C
1	A	444	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	527	G7M
1	A	532	A
1	A	533	A
1	A	547	A
1	A	559	A
1	A	560	U
1	A	562	C
1	A	563	A
1	A	564	C
1	A	566	G
1	A	572	A
1	A	573	A
1	A	576	G
1	A	577	G
1	A	579	G
1	A	581	G

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Mol	Chain	Res	Type
1	A	588	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	721	G
1	A	723	U
1	A	734	G
1	A	749	C
1	A	755	G
1	A	777	A
1	A	780	A
1	A	781	A
1	A	782	A
1	A	793	U
1	A	794	A
1	A	799	G
1	A	813	U
1	A	817	C
1	A	828	A
1	A	839	U
1	A	840	C
1	A	841	U
1	A	848	C
1	A	851	G
1	A	859	A
1	A	874	G
1	A	876	G
1	A	902	G
1	A	914	A
1	A	916	G
1	A	926	G
1	A	927	G
1	A	934	C
1	A	935	A
1	A	960	U
1	A	966	M2G
1	A	969	A
1	A	971	G

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Mol	Chain	Res	Type
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	998	G
1	A	1004	A
1	A	1005	A
1	A	1023	G
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	1051	C
1	A	1054	C
1	A	1055	A
1	A	1065	U
1	A	1066	C
1	A	1094	G
1	A	1095	U
1	A	1096	C
1	A	1101	A
1	A	1124	G
1	A	1126	U
1	A	1127	G
1	A	1129	C
1	A	1130	A
1	A	1131	G
1	A	1137	C
1	A	1138	G
1	A	1139	G
1	A	1140	C
1	A	1146	A
1	A	1159	U
1	A	1171	G
1	A	1181	G
1	A	1183	A

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Mol	Chain	Res	Type
1	A	1184	G
1	A	1191	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	1227	A
1	A	1238	A
1	A	1250	A
1	A	1257	U
1	A	1258	G
1	A	1270	C
1	A	1278	U
1	A	1280	A
1	A	1285	A
1	A	1287	A
1	A	1289	A
1	A	1300	G
1	A	1301	U
1	A	1302	U
1	A	1318	A
1	A	1319	A
1	A	1320	C
1	A	1322	C
1	A	1323	G
1	A	1332	A
1	A	1338	G
1	A	1346	A
1	A	1347	G
1	A	1353	G
1	A	1362	C
1	A	1363	A
1	A	1370	G
1	A	1379	G
1	A	1381	U
1	A	1394	A
1	A	1395	C
1	A	1400	5MC
1	A	1402	4OC
1	A	1442	G

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Mol	Chain	Res	Type
1	A	1443	G
1	A	1446	A
1	A	1447	G
1	A	1487	G
1	A	1492	A
1	A	1498	UR3
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	1507	A
1	A	1517	G
1	A	1518	MA6
1	A	1519	MA6
1	A	1520	G
1	A	1529	G
1	A	1530	G
1	A	1544	U

All (29) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	115	G
1	A	129(A)	G
1	A	181	G
1	A	203	U
1	A	266	G
1	A	328	C
1	A	372	C
1	A	428	G
1	A	432	A
1	A	484	G
1	A	496	A
1	A	509	A
1	A	559	A
1	A	687	A
1	A	701	C
1	A	748	C
1	A	812	C
1	A	913	A

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Mol	Chain	Res	Type
1	A	1049	U
1	A	1065	U
1	A	1129	C
1	A	1182	G
1	A	1190	G
1	A	1201	A
1	A	1212	U
1	A	1300	G
1	A	1301	U
1	A	1331	G
1	A	1505	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	MA6	A	1518	1	23,26,27	1.15	2 (8%)	33,38,41	0.92	1 (3%)
1	PSU	A	1541	23,1	18,21,22	1.09	1 (5%)	21,30,33	1.84	4 (19%)
1	5MC	A	1404	1	19,22,23	1.31	3 (15%)	26,32,35	0.91	1 (3%)
1	5MC	A	967	1	19,22,23	1.04	2 (10%)	26,32,35	1.02	2 (7%)
1	5MC	A	1407	1	19,22,23	0.99	1 (5%)	26,32,35	1.04	2 (7%)
1	5MC	A	1400	1	19,22,23	1.04	2 (10%)	26,32,35	1.01	2 (7%)
12	0TD	L	92	12	8,9,10	2.14	1 (12%)	6,11,13	2.66	3 (50%)
1	4OC	A	1402	1	20,23,24	1.11	2 (10%)	25,32,35	0.80	0
1	PSU	A	1540	1	18,21,22	1.15	1 (5%)	21,30,33	1.90	5 (23%)
1	UR3	A	1498	23,1	19,22,23	0.90	1 (5%)	26,32,35	1.02	0
1	G7M	A	527	1	23,26,27	1.35	3 (13%)	34,39,42	1.77	7 (20%)
1	M2G	A	966	1	24,27,28	1.14	2 (8%)	33,40,43	0.99	2 (6%)
1	MA6	A	1519	1	23,26,27	1.21	3 (13%)	33,38,41	0.95	1 (3%)
1	2MG	A	1207	1	23,26,27	1.37	5 (21%)	33,38,41	1.18	5 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	A	516	23,1	18,21,22	1.25	1 (5%)	21,30,33	1.61	4 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MA6	A	1518	1	-	2/11/29/30	0/3/3/3
1	PSU	A	1541	23,1	-	1/7/25/26	0/2/2/2
1	5MC	A	1404	1	-	0/7/25/26	0/2/2/2
1	5MC	A	967	1	-	0/7/25/26	0/2/2/2
1	5MC	A	1407	1	-	0/7/25/26	0/2/2/2
1	5MC	A	1400	1	-	2/7/25/26	0/2/2/2
12	0TD	L	92	12	-	3/7/12/14	-
1	4OC	A	1402	1	-	2/9/29/30	0/2/2/2
1	PSU	A	1540	1	-	1/7/25/26	0/2/2/2
1	UR3	A	1498	23,1	-	0/7/25/26	0/2/2/2
1	G7M	A	527	1	-	2/7/25/26	0/3/3/3
1	M2G	A	966	1	-	7/11/29/30	0/3/3/3
1	MA6	A	1519	1	-	1/11/29/30	0/3/3/3
1	2MG	A	1207	1	-	0/9/27/28	0/3/3/3
1	PSU	A	516	23,1	-	0/7/25/26	0/2/2/2

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	L	92	0TD	CB-CA	-5.12	1.53	1.54
1	A	516	PSU	C6-C5	4.39	1.40	1.35
1	A	527	G7M	C2-N2	4.14	1.43	1.34
1	A	1540	PSU	C6-C5	3.90	1.39	1.35
1	A	1404	5MC	C5-C4	-3.71	1.41	1.44
1	A	1541	PSU	C6-C5	3.46	1.39	1.35
1	A	527	G7M	C4-N3	3.26	1.41	1.34
1	A	1207	2MG	C2-N2	3.25	1.40	1.33
1	A	966	M2G	C2-N2	3.13	1.40	1.35
1	A	1498	UR3	C2-N1	2.99	1.42	1.38
1	A	1400	5MC	C2-N1	2.98	1.46	1.40
1	A	1519	MA6	C5-C4	2.81	1.44	1.39
1	A	967	5MC	C2-N1	2.69	1.45	1.40
1	A	1207	2MG	C2-N1	2.67	1.40	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1402	4OC	C2-N3	2.63	1.41	1.36
1	A	1518	MA6	C5-C4	2.61	1.43	1.39
1	A	527	G7M	CN7-N7	-2.45	1.42	1.46
1	A	966	M2G	C4-N3	2.45	1.39	1.34
1	A	1207	2MG	C8-N9	2.41	1.42	1.37
1	A	1404	5MC	C2-N3	2.35	1.41	1.36
1	A	1519	MA6	C2-N1	2.34	1.38	1.33
1	A	1400	5MC	C2-N3	2.24	1.40	1.36
1	A	1402	4OC	C4-N4	2.20	1.40	1.36
1	A	967	5MC	C2-N3	2.19	1.40	1.36
1	A	1407	5MC	C2-N1	2.13	1.44	1.40
1	A	1207	2MG	C4-N3	2.09	1.39	1.34
1	A	1207	2MG	C6-N1	2.09	1.42	1.38
1	A	1518	MA6	C8-N9	2.05	1.41	1.37
1	A	1404	5MC	C6-C5	2.03	1.37	1.34
1	A	1519	MA6	C8-N9	2.03	1.41	1.37

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	92	0TD	CB-CA-N	-5.12	98.72	109.10
1	A	1540	PSU	C4-N3-C2	-4.86	119.68	126.37
1	A	527	G7M	C2-N3-C4	4.78	120.54	112.30
1	A	1541	PSU	C4-N3-C2	-4.72	119.86	126.37
1	A	1540	PSU	N1-C2-N3	4.65	120.07	115.17
1	A	1541	PSU	N1-C2-N3	4.35	119.76	115.17
1	A	527	G7M	C5-C4-N3	-4.30	120.02	128.15
1	A	516	PSU	C4-N3-C2	-3.94	120.94	126.37
1	A	516	PSU	N1-C2-N3	3.88	119.26	115.17
1	A	527	G7M	C5-C6-N1	3.76	119.62	111.84
1	A	527	G7M	N9-C4-N3	3.33	132.62	125.95
1	A	527	G7M	O6-C6-C5	-3.29	120.66	128.01
1	A	1207	2MG	C5-C4-N3	-2.82	123.91	128.39
1	A	1541	PSU	O2-C2-N1	-2.74	119.96	122.79
1	A	527	G7M	C6-C5-N7	2.74	135.60	132.17
1	A	516	PSU	C6-N1-C2	-2.64	120.24	122.69
1	A	527	G7M	C2-N1-C6	-2.64	120.33	125.11
1	A	966	M2G	C5-C4-N3	-2.61	124.24	128.39
1	A	1207	2MG	N9-C4-N3	2.57	131.10	125.95
1	A	1540	PSU	O2-C2-N1	-2.54	120.17	122.79
1	A	516	PSU	O2-C2-N1	-2.49	120.22	122.79
1	A	1407	5MC	N4-C4-N3	-2.48	114.01	118.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1407	5MC	C5-C4-N3	2.42	124.23	121.75
12	L	92	0TD	CSB-SB-CB	-2.42	98.02	102.36
1	A	1400	5MC	N4-C4-N3	-2.38	114.20	118.51
1	A	967	5MC	N4-C4-N3	-2.36	114.23	118.51
1	A	1207	2MG	O6-C6-N1	-2.29	115.80	120.11
1	A	1207	2MG	C2-N1-C6	-2.22	121.86	124.55
1	A	1540	PSU	C6-N1-C2	-2.19	120.66	122.69
1	A	1400	5MC	C5-C4-N3	2.17	123.98	121.75
1	A	1519	MA6	C2-N1-C6	2.16	117.11	111.83
1	A	1207	2MG	C6-C5-N7	-2.09	126.48	130.29
1	A	1404	5MC	N4-C4-N3	-2.08	114.74	118.51
1	A	967	5MC	C5-C4-N3	2.07	123.88	121.75
1	A	1540	PSU	O4'-C1'-C2'	2.05	107.99	105.15
1	A	1518	MA6	C2-N1-C6	2.04	116.82	111.83
1	A	966	M2G	C6-C5-C4	2.04	121.89	118.83
1	A	1541	PSU	C6-N1-C2	-2.03	120.81	122.69
12	L	92	0TD	OD1-CG-CB	-2.02	118.20	122.44

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	527	G7M	O4'-C4'-C5'-O5'
1	A	966	M2G	N1-C2-N2-CM1
1	A	966	M2G	N3-C2-N2-CM1
1	A	966	M2G	N3-C2-N2-CM2
12	L	92	0TD	CG-CB-SB-CSB
1	A	527	G7M	C3'-C4'-C5'-O5'
1	A	966	M2G	O4'-C4'-C5'-O5'
1	A	1400	5MC	O4'-C4'-C5'-O5'
1	A	1402	4OC	O4'-C4'-C5'-O5'
1	A	1518	MA6	O4'-C4'-C5'-O5'
1	A	1519	MA6	C4'-C5'-O5'-P
1	A	966	M2G	C3'-C4'-C5'-O5'
1	A	1400	5MC	C3'-C4'-C5'-O5'
1	A	1518	MA6	C3'-C4'-C5'-O5'
1	A	1402	4OC	C3'-C4'-C5'-O5'
1	A	966	M2G	C4'-C5'-O5'-P
1	A	966	M2G	N1-C2-N2-CM2
12	L	92	0TD	SB-CB-CG-OD1
1	A	1540	PSU	O4'-C1'-C5-C4
1	A	1541	PSU	O4'-C1'-C5-C4

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Mol	Chain	Res	Type	Atoms
12	L	92	0TD	SB-CB-CG-OD2

There are no ring outliers.

9 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1518	MA6	2	0
1	A	967	5MC	3	0
1	A	1400	5MC	1	0
1	A	1402	4OC	3	0
1	A	1498	UR3	1	0
1	A	527	G7M	1	0
1	A	966	M2G	2	0
1	A	1519	MA6	1	0
1	A	1207	2MG	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 295 ligands modelled in this entry, 289 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	$\# Z > 2$
22	PAR	A	1602	-	44,45,45	1.45	8 (18%)	63,67,67	1.69	12 (19%)
22	PAR	A	1606	-	44,45,45	1.37	6 (13%)	63,67,67	1.64	11 (17%)
22	PAR	A	1603	-	44,45,45	1.46	5 (11%)	63,67,67	1.65	12 (19%)
22	PAR	A	1601	-	44,45,45	1.13	6 (13%)	63,67,67	1.54	11 (17%)
22	PAR	A	1605	-	44,45,45	1.22	6 (13%)	63,67,67	1.60	12 (19%)
22	PAR	A	1604	-	44,45,45	1.35	6 (13%)	63,67,67	1.62	9 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	PAR	A	1602	-	-	10/18/94/94	0/4/4/4
22	PAR	A	1606	-	-	11/18/94/94	0/4/4/4
22	PAR	A	1603	-	-	7/18/94/94	0/4/4/4
22	PAR	A	1601	-	-	4/18/94/94	0/4/4/4
22	PAR	A	1605	-	-	7/18/94/94	0/4/4/4
22	PAR	A	1604	-	-	2/18/94/94	0/4/4/4

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	1603	PAR	C52-C42	4.81	1.62	1.52
22	A	1604	PAR	C13-C23	4.04	1.58	1.52
22	A	1602	PAR	O43-C13	3.67	1.48	1.41
22	A	1602	PAR	C31-C21	3.53	1.58	1.53
22	A	1606	PAR	C34-C24	3.47	1.57	1.53
22	A	1603	PAR	C13-C23	3.28	1.57	1.52
22	A	1602	PAR	C52-C42	3.24	1.58	1.52
22	A	1605	PAR	C52-C42	3.08	1.58	1.52
22	A	1601	PAR	C52-C42	3.00	1.58	1.52
22	A	1606	PAR	O43-C13	2.99	1.47	1.41
22	A	1603	PAR	O43-C13	2.98	1.46	1.41
22	A	1604	PAR	C52-C42	2.98	1.58	1.52
22	A	1606	PAR	C31-C21	2.93	1.57	1.53
22	A	1606	PAR	C13-C23	2.82	1.56	1.52
22	A	1603	PAR	C34-C24	2.79	1.57	1.53
22	A	1602	PAR	C34-C24	2.74	1.57	1.53
22	A	1602	PAR	C11-C21	2.63	1.57	1.52
22	A	1606	PAR	C14-C24	2.61	1.57	1.52
22	A	1604	PAR	C14-C24	2.59	1.57	1.52
22	A	1605	PAR	C31-C21	2.51	1.56	1.53
22	A	1602	PAR	C14-C24	2.47	1.57	1.52
22	A	1604	PAR	C34-C24	2.47	1.56	1.53
22	A	1606	PAR	C52-C42	2.46	1.57	1.52
22	A	1605	PAR	C33-C43	2.45	1.59	1.52
22	A	1605	PAR	O43-C13	2.39	1.45	1.41
22	A	1601	PAR	C33-C43	2.33	1.59	1.52
22	A	1601	PAR	C34-C24	2.31	1.56	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	1605	PAR	C34-C24	2.24	1.56	1.53
22	A	1605	PAR	C13-C23	2.16	1.55	1.52
22	A	1602	PAR	O33-C14	2.13	1.47	1.41
22	A	1601	PAR	C14-C24	2.10	1.56	1.52
22	A	1602	PAR	C62-C52	2.08	1.57	1.52
22	A	1603	PAR	C62-C52	2.06	1.57	1.52
22	A	1601	PAR	C13-C23	2.06	1.55	1.52
22	A	1604	PAR	O43-C13	2.04	1.45	1.41
22	A	1604	PAR	C33-C43	2.01	1.58	1.52
22	A	1601	PAR	C62-C52	2.00	1.57	1.52

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1602	PAR	O33-C14-C24	7.31	120.05	108.08
22	A	1606	PAR	O33-C14-C24	6.63	118.93	108.08
22	A	1604	PAR	O33-C14-C24	6.56	118.82	108.08
22	A	1603	PAR	O33-C14-C24	6.36	118.48	108.08
22	A	1605	PAR	O33-C14-C24	6.08	118.02	108.08
22	A	1601	PAR	O33-C14-C24	5.81	117.59	108.08
22	A	1604	PAR	C13-C23-C33	3.59	106.42	102.10
22	A	1603	PAR	C13-C23-C33	3.37	106.16	102.10
22	A	1602	PAR	C14-O33-C33	-3.27	110.23	117.98
22	A	1605	PAR	O11-C11-O51	3.18	119.07	110.69
22	A	1603	PAR	O11-C11-O51	3.16	119.02	110.69
22	A	1605	PAR	C34-C24-N24	-3.13	104.63	111.05
22	A	1601	PAR	C34-C24-N24	-3.01	104.89	111.05
22	A	1606	PAR	C34-C24-N24	-2.99	104.93	111.05
22	A	1605	PAR	C13-O52-C52	-2.98	110.91	117.98
22	A	1604	PAR	C34-C24-N24	-2.98	104.95	111.05
22	A	1602	PAR	O52-C13-O43	-2.97	108.33	111.37
22	A	1604	PAR	C14-O33-C33	-2.94	111.00	117.98
22	A	1602	PAR	O34-C34-C44	-2.92	103.49	110.38
22	A	1602	PAR	O11-C11-O51	2.91	118.36	110.69
22	A	1603	PAR	O34-C34-C44	-2.91	103.51	110.38
22	A	1606	PAR	O34-C34-C44	-2.90	103.53	110.38
22	A	1602	PAR	C34-C24-N24	-2.89	105.14	111.05
22	A	1603	PAR	C34-C24-N24	-2.88	105.15	111.05
22	A	1606	PAR	O52-C13-O43	-2.86	108.44	111.37
22	A	1605	PAR	O34-C34-C44	-2.85	103.65	110.38
22	A	1601	PAR	O34-C34-C44	-2.84	103.69	110.38
22	A	1604	PAR	O34-C34-C44	-2.84	103.69	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1602	PAR	O54-C54-C44	2.83	114.80	109.70
22	A	1606	PAR	O11-C11-O51	2.81	118.09	110.69
22	A	1601	PAR	O11-C11-O51	2.80	118.07	110.69
22	A	1603	PAR	C14-O33-C33	-2.78	111.39	117.98
22	A	1606	PAR	C14-O33-C33	-2.78	111.40	117.98
22	A	1604	PAR	O11-C11-O51	2.76	117.96	110.69
22	A	1606	PAR	C13-C23-C33	2.76	105.42	102.10
22	A	1601	PAR	C14-O33-C33	-2.71	111.56	117.98
22	A	1604	PAR	C13-O52-C52	-2.67	111.64	117.98
22	A	1603	PAR	O52-C13-O43	-2.63	108.68	111.37
22	A	1601	PAR	C13-O52-C52	-2.54	111.97	117.98
22	A	1605	PAR	C14-O33-C33	-2.53	111.99	117.98
22	A	1603	PAR	O54-C54-C44	2.45	114.12	109.70
22	A	1603	PAR	C13-O52-C52	-2.44	112.20	117.98
22	A	1606	PAR	C22-C12-C62	2.41	113.69	110.08
22	A	1603	PAR	C11-O51-C51	2.40	118.41	113.72
22	A	1601	PAR	C13-C23-C33	2.39	104.98	102.10
22	A	1601	PAR	O52-C13-O43	-2.37	108.94	111.37
22	A	1605	PAR	O52-C13-O43	-2.36	108.96	111.37
22	A	1602	PAR	O51-C51-C61	2.34	112.24	106.44
22	A	1606	PAR	O51-C51-C61	2.34	112.24	106.44
22	A	1606	PAR	C13-O52-C52	-2.33	112.46	117.98
22	A	1604	PAR	O51-C51-C61	2.29	112.10	106.44
22	A	1604	PAR	O52-C13-O43	-2.27	109.05	111.37
22	A	1601	PAR	O51-C51-C61	2.25	112.03	106.44
22	A	1605	PAR	C11-O51-C51	2.24	118.10	113.72
22	A	1605	PAR	O54-C54-C44	2.23	113.72	109.70
22	A	1603	PAR	O51-C51-C61	2.22	111.94	106.44
22	A	1601	PAR	O33-C14-O54	-2.22	104.85	110.69
22	A	1605	PAR	O51-C51-C61	2.21	111.91	106.44
22	A	1602	PAR	C22-C12-C62	2.20	113.37	110.08
22	A	1602	PAR	C23-C33-C43	-2.16	99.45	103.24
22	A	1602	PAR	O43-C13-C23	-2.15	102.25	104.98
22	A	1605	PAR	C22-C12-C62	2.14	113.29	110.08
22	A	1606	PAR	O52-C52-C42	2.10	112.76	107.42
22	A	1602	PAR	C13-O52-C52	-2.07	113.08	117.98
22	A	1603	PAR	C22-C32-C42	2.05	114.52	109.50
22	A	1601	PAR	O43-C13-C23	-2.03	102.40	104.98
22	A	1605	PAR	O43-C13-C23	-2.00	102.43	104.98

There are no chirality outliers.

All (41) torsion outliers are listed below:

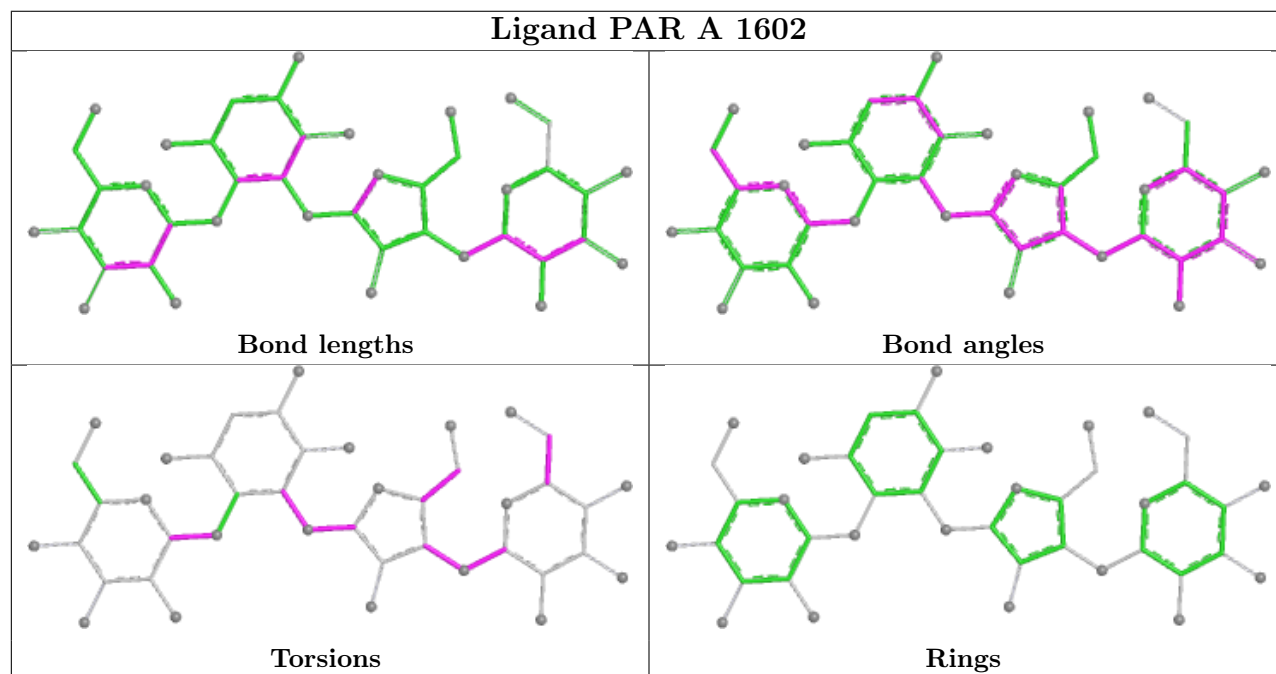
Mol	Chain	Res	Type	Atoms
22	A	1602	PAR	C23-C13-O52-C52
22	A	1602	PAR	O43-C13-O52-C52
22	A	1602	PAR	C24-C14-O33-C33
22	A	1602	PAR	O54-C54-C64-N64
22	A	1603	PAR	C23-C13-O52-C52
22	A	1603	PAR	C44-C54-C64-N64
22	A	1605	PAR	O43-C43-C53-O53
22	A	1606	PAR	C23-C13-O52-C52
22	A	1606	PAR	O54-C14-O33-C33
22	A	1606	PAR	C44-C54-C64-N64
22	A	1606	PAR	O54-C54-C64-N64
22	A	1606	PAR	O51-C11-O11-C42
22	A	1604	PAR	O54-C14-O33-C33
22	A	1605	PAR	C33-C43-C53-O53
22	A	1605	PAR	C41-C51-C61-O61
22	A	1605	PAR	O51-C51-C61-O61
22	A	1602	PAR	O43-C43-C53-O53
22	A	1603	PAR	C52-C42-O11-C11
22	A	1602	PAR	C33-C43-C53-O53
22	A	1606	PAR	C62-C52-O52-C13
22	A	1605	PAR	O54-C14-O33-C33
22	A	1606	PAR	C42-C52-O52-C13
22	A	1606	PAR	C41-C51-C61-O61
22	A	1601	PAR	O43-C13-O52-C52
22	A	1603	PAR	O43-C13-O52-C52
22	A	1606	PAR	O43-C13-O52-C52
22	A	1601	PAR	C23-C13-O52-C52
22	A	1603	PAR	C32-C42-O11-C11
22	A	1601	PAR	O54-C54-C64-N64
22	A	1603	PAR	O54-C54-C64-N64
22	A	1606	PAR	C24-C14-O33-C33
22	A	1602	PAR	O51-C11-O11-C42
22	A	1604	PAR	C43-C33-O33-C14
22	A	1605	PAR	C52-C42-O11-C11
22	A	1602	PAR	C62-C52-O52-C13
22	A	1606	PAR	O51-C51-C61-O61
22	A	1601	PAR	C52-C42-O11-C11
22	A	1602	PAR	C42-C52-O52-C13
22	A	1602	PAR	C43-C33-O33-C14
22	A	1603	PAR	C23-C33-O33-C14
22	A	1605	PAR	O51-C11-O11-C42

There are no ring outliers.

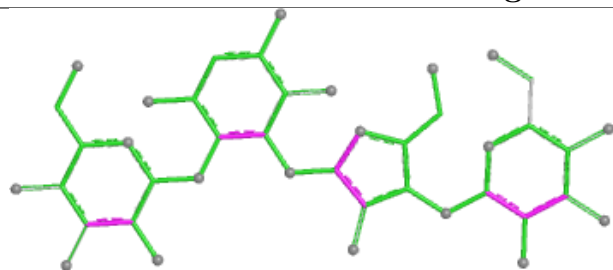
5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	1602	PAR	1	0
22	A	1606	PAR	2	0
22	A	1603	PAR	3	0
22	A	1601	PAR	1	0
22	A	1604	PAR	1	0

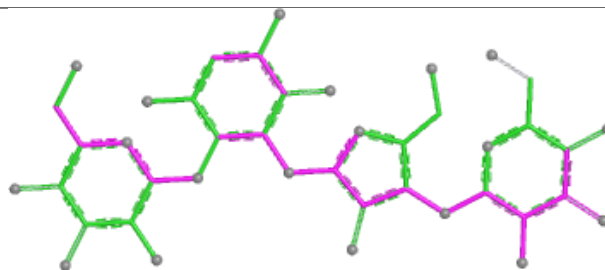
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



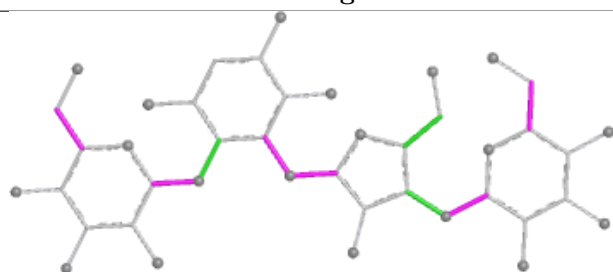
Ligand PAR A 1606



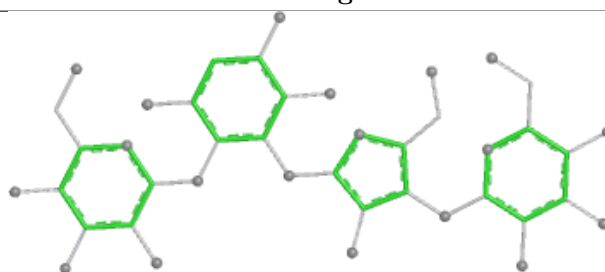
Bond lengths



Bond angles

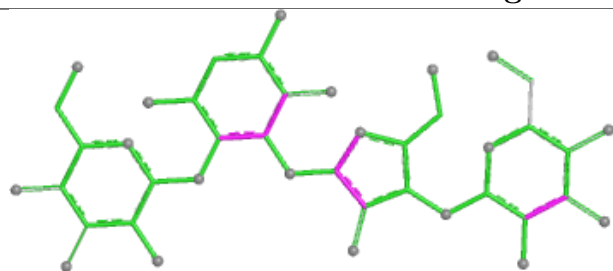


Torsions

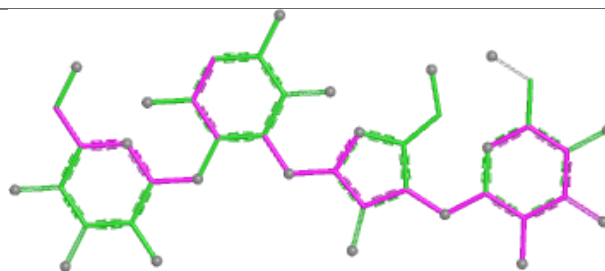


Rings

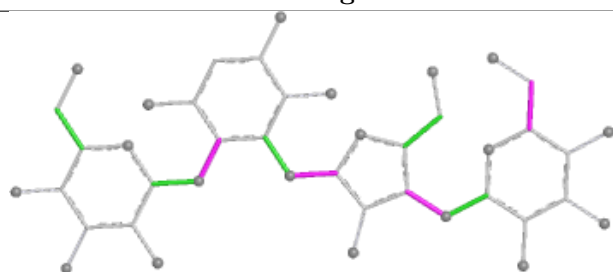
Ligand PAR A 1603



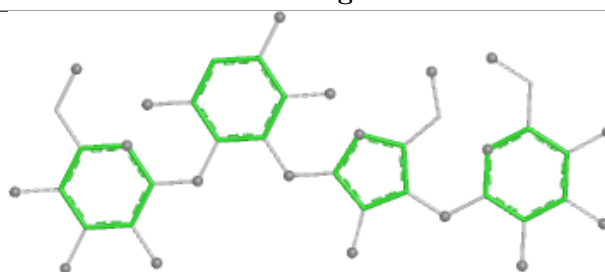
Bond lengths



Bond angles

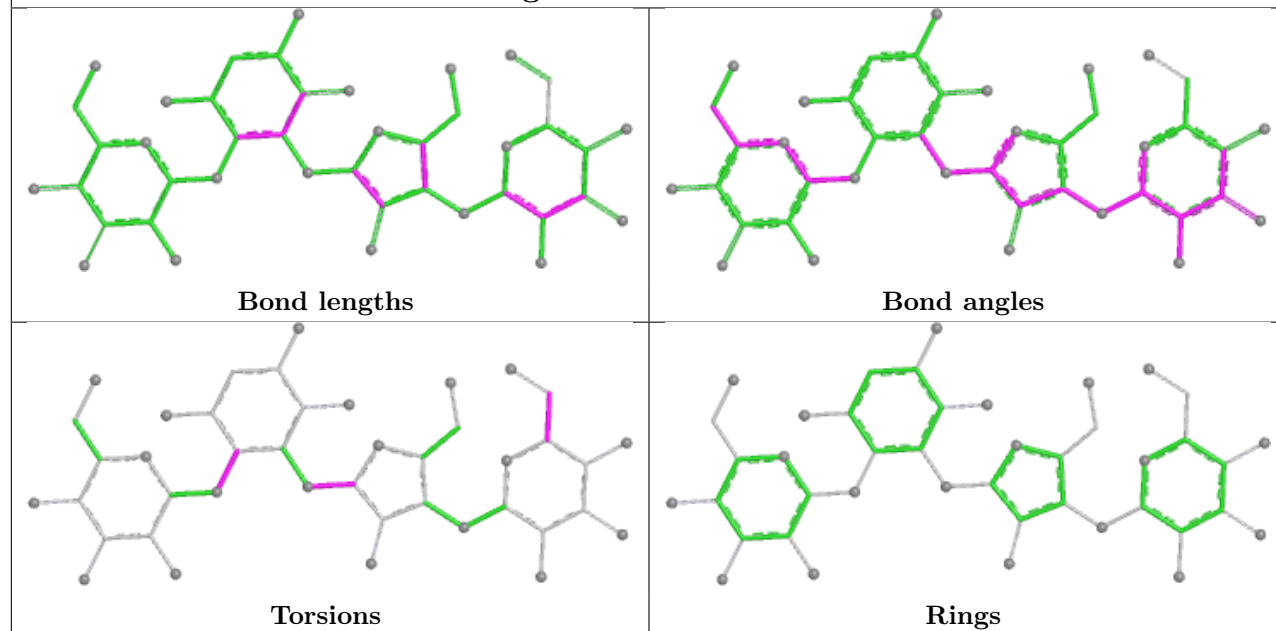


Torsions

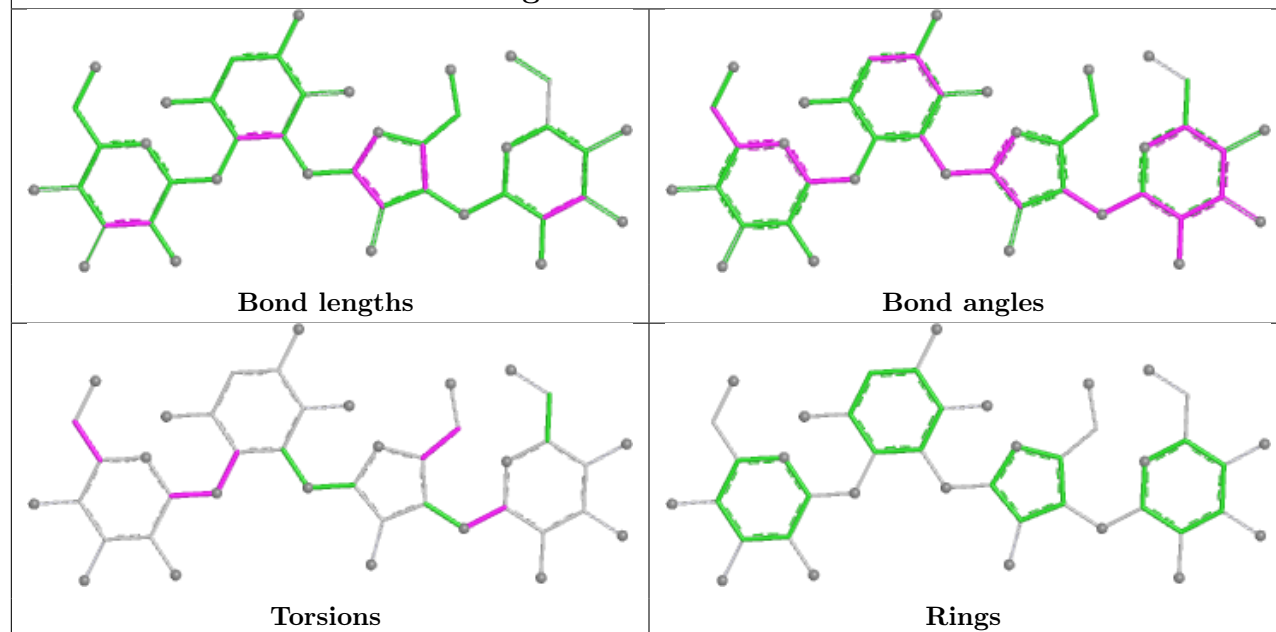


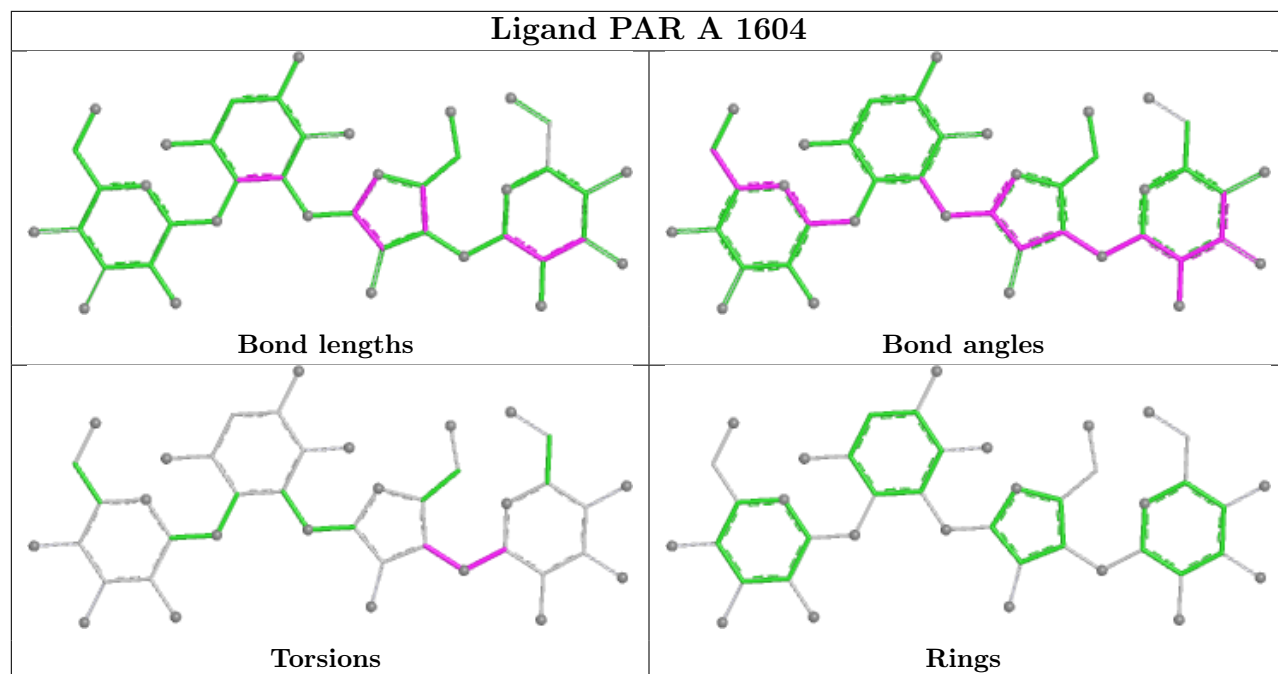
Rings

Ligand PAR A 1601



Ligand PAR A 1605





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1498/1522 (98%)	0.10	12 (0%) 82 71	63, 92, 172, 311	0
2	B	236/256 (92%)	0.51	13 (5%) 30 23	47, 118, 206, 258	0
3	C	207/239 (86%)	0.42	5 (2%) 59 45	39, 115, 163, 196	0
4	D	208/209 (99%)	0.66	18 (8%) 16 14	65, 97, 141, 190	0
5	E	151/162 (93%)	0.18	2 (1%) 75 61	57, 81, 112, 199	0
6	F	101/101 (100%)	0.34	1 (0%) 79 66	84, 116, 147, 164	0
7	G	155/156 (99%)	0.42	5 (3%) 50 37	78, 105, 167, 213	0
8	H	138/138 (100%)	0.17	2 (1%) 73 59	59, 79, 106, 140	0
9	I	127/128 (99%)	0.78	12 (9%) 14 14	79, 117, 159, 187	0
10	J	99/105 (94%)	1.02	13 (13%) 7 8	80, 142, 221, 310	0
11	K	117/129 (90%)	0.41	3 (2%) 57 42	66, 92, 132, 160	0
12	L	124/135 (91%)	0.52	6 (4%) 35 26	58, 93, 129, 225	0
13	M	118/126 (93%)	0.71	10 (8%) 16 15	82, 113, 160, 275	0
14	N	60/61 (98%)	0.93	7 (11%) 9 10	79, 109, 158, 228	0
15	O	88/89 (98%)	0.43	2 (2%) 61 46	63, 97, 139, 202	0
16	P	84/88 (95%)	0.33	0 100 100	74, 89, 116, 219	0
17	Q	101/105 (96%)	0.45	2 (1%) 65 49	62, 88, 130, 157	0
18	R	73/88 (82%)	0.39	2 (2%) 56 42	76, 100, 158, 215	0
19	S	81/93 (87%)	0.94	7 (8%) 16 15	54, 129, 170, 258	0
20	T	99/106 (93%)	0.55	4 (4%) 42 30	71, 94, 130, 199	0
21	U	25/27 (92%)	2.04	10 (40%) 1 1	70, 153, 188, 223	0
All	All	3890/4063 (95%)	0.37	136 (3%) 47 34	39, 99, 169, 311	0

All (136) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
19	S	3	ARG	13.9
1	A	1129	C	8.3
21	U	6	ARG	7.0
4	D	23	GLY	5.7
14	N	13	THR	5.6
9	I	126	SER	5.4
4	D	31	CYS	4.9
20	T	100	ILE	4.5
8	H	1	MET	4.5
21	U	25	LYS	4.5
12	L	47	LYS	4.2
13	M	27	LYS	4.2
19	S	2	PRO	4.1
11	K	51	LYS	4.0
19	S	69	HIS	4.0
7	G	5	ARG	3.9
9	I	128	ARG	3.9
12	L	28	LYS	3.8
13	M	104	ARG	3.8
3	C	188	LEU	3.8
4	D	9	CYS	3.7
9	I	127	LYS	3.7
2	B	156	LYS	3.6
4	D	26	CYS	3.6
1	A	1539	C	3.5
13	M	118	ALA	3.5
10	J	53	PRO	3.4
1	A	1125	U	3.3
1	A	532	A	3.3
10	J	6	ILE	3.2
4	D	22	LYS	3.2
4	D	42	GLN	3.1
21	U	18	TYR	3.1
10	J	5	ARG	3.0
21	U	24	ARG	3.0
12	L	19	ARG	3.0
1	A	202	U	3.0
7	G	81	GLY	3.0
19	S	82	GLY	2.9
14	N	10	ALA	2.9
2	B	227	GLY	2.9
4	D	2	GLY	2.8
14	N	2	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
21	U	4	GLY	2.8
2	B	88	ALA	2.8
12	L	29	GLY	2.8
19	S	4	SER	2.8
2	B	137	ARG	2.7
21	U	9	ARG	2.7
2	B	133	LYS	2.7
21	U	21	TYR	2.7
14	N	6	LEU	2.7
9	I	70	LYS	2.7
1	A	1181	G	2.7
9	I	122	ALA	2.7
3	C	201	TYR	2.6
10	J	57	LYS	2.6
10	J	98	ILE	2.6
10	J	33	GLN	2.6
2	B	44	LEU	2.6
6	F	14	LEU	2.6
15	O	50	HIS	2.5
4	D	21	LEU	2.5
19	S	5	LEU	2.5
4	D	24	GLU	2.5
18	R	17	SER	2.5
10	J	45	ARG	2.5
7	G	33	ASP	2.5
9	I	12	GLU	2.5
9	I	125	TYR	2.5
21	U	17	THR	2.5
10	J	7	LYS	2.5
3	C	66	VAL	2.5
9	I	15	ALA	2.4
14	N	12	ARG	2.4
18	R	68	LYS	2.4
21	U	10	ARG	2.4
4	D	27	TYR	2.4
2	B	110	GLN	2.4
14	N	4	LYS	2.4
21	U	20	LYS	2.4
1	A	723	U	2.4
1	A	1025	U	2.4
5	E	76	ILE	2.4
19	S	10	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
4	D	5	ILE	2.4
9	I	40	LEU	2.4
4	D	91	SER	2.4
2	B	140	HIS	2.4
4	D	32	ALA	2.3
4	D	138	TYR	2.3
9	I	109	VAL	2.3
10	J	43	ARG	2.3
10	J	72	VAL	2.3
20	T	74	LYS	2.3
3	C	167	TRP	2.3
13	M	106	ASN	2.3
2	B	97	TRP	2.3
13	M	6	GLY	2.2
1	A	1257	U	2.2
2	B	229	VAL	2.2
10	J	4	ILE	2.2
9	I	8	GLY	2.2
12	L	25	PRO	2.2
13	M	10	PRO	2.2
20	T	99	LEU	2.2
5	E	20	GLN	2.2
3	C	3	ASN	2.2
13	M	88	ARG	2.2
7	G	62	PHE	2.2
1	A	1130	A	2.2
12	L	17	LYS	2.1
7	G	156	TRP	2.1
17	Q	100	LYS	2.1
1	A	266	G	2.1
1	A	1331	G	2.1
4	D	154	ASN	2.1
4	D	86	LYS	2.1
15	O	57	LEU	2.1
8	H	18	ARG	2.1
20	T	8	ARG	2.1
4	D	80	GLU	2.1
13	M	8	GLU	2.1
10	J	47	PHE	2.1
13	M	7	VAL	2.1
2	B	208	ILE	2.1
4	D	12	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	144	ARG	2.1
11	K	118	GLY	2.1
9	I	66	ARG	2.1
10	J	65	LEU	2.1
13	M	34	LEU	2.0
17	Q	92	ARG	2.0
2	B	188	ALA	2.0
14	N	35	ARG	2.0
11	K	56	GLY	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	0.85	0.26	208,247,264,265	0
1	PSU	A	1541	20/21	0.90	0.21	202,223,242,268	0
1	PSU	A	516	20/21	0.91	0.11	85,108,115,120	0
1	2MG	A	1207	24/25	0.94	0.11	93,112,121,126	0
12	0TD	L	92	10/11	0.94	0.13	76,85,100,101	0
1	5MC	A	967	21/22	0.95	0.11	70,95,105,112	0
1	MA6	A	1518	24/25	0.96	0.12	72,77,82,83	0
1	MA6	A	1519	24/25	0.96	0.14	69,74,82,89	0
1	G7M	A	527	24/25	0.96	0.11	67,76,82,90	0
1	M2G	A	966	25/26	0.96	0.10	72,89,105,110	0
1	5MC	A	1400	21/22	0.96	0.09	64,76,101,107	0
1	UR3	A	1498	21/22	0.97	0.10	70,74,81,83	0
1	5MC	A	1404	21/22	0.97	0.11	70,72,83,86	0
1	5MC	A	1407	21/22	0.97	0.10	80,86,100,102	0
1	4OC	A	1402	22/23	0.98	0.10	72,77,89,97	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
23	MG	A	1845	1/1	0.43	0.17	115,115,115,115	0
23	MG	A	1837	1/1	0.57	0.49	101,101,101,101	0
23	MG	A	1689	1/1	0.59	0.18	84,84,84,84	0
23	MG	A	1755	1/1	0.61	0.27	118,118,118,118	0
23	MG	A	1705	1/1	0.62	0.17	135,135,135,135	0
23	MG	A	1811	1/1	0.66	0.29	72,72,72,72	0
23	MG	A	1712	1/1	0.66	0.17	68,68,68,68	0
23	MG	A	1626	1/1	0.66	0.53	89,89,89,89	0
23	MG	A	1877	1/1	0.66	0.30	142,142,142,142	0
23	MG	A	1739	1/1	0.67	0.16	158,158,158,158	0
23	MG	A	1612	1/1	0.72	0.19	130,130,130,130	0
23	MG	A	1869	1/1	0.72	0.14	68,68,68,68	0
23	MG	A	1732	1/1	0.72	0.17	177,177,177,177	0
23	MG	A	1724	1/1	0.73	0.14	145,145,145,145	0
23	MG	A	1679	1/1	0.73	0.15	94,94,94,94	0
23	MG	A	1713	1/1	0.73	0.21	187,187,187,187	0
23	MG	A	1674	1/1	0.74	0.31	122,122,122,122	0
23	MG	A	1829	1/1	0.74	0.11	88,88,88,88	0
23	MG	A	1760	1/1	0.74	0.29	87,87,87,87	0
23	MG	B	301	1/1	0.74	0.18	75,75,75,75	0
23	MG	A	1856	1/1	0.75	0.23	81,81,81,81	0
23	MG	A	1878	1/1	0.75	0.13	66,66,66,66	0
23	MG	A	1709	1/1	0.75	0.22	157,157,157,157	0
23	MG	E	201	1/1	0.75	0.12	154,154,154,154	0
23	MG	A	1824	1/1	0.76	0.09	87,87,87,87	0
23	MG	A	1853	1/1	0.76	0.31	101,101,101,101	0
23	MG	A	1720	1/1	0.76	0.21	147,147,147,147	0
23	MG	A	1817	1/1	0.76	0.14	56,56,56,56	0
23	MG	A	1843	1/1	0.77	0.24	97,97,97,97	0
23	MG	A	1790	1/1	0.77	0.21	88,88,88,88	0
23	MG	A	1715	1/1	0.77	0.25	91,91,91,91	0
23	MG	A	1746	1/1	0.77	0.36	204,204,204,204	0
23	MG	A	1860	1/1	0.77	0.20	69,69,69,69	0
23	MG	A	1865	1/1	0.78	0.23	92,92,92,92	0
23	MG	A	1782	1/1	0.78	0.17	74,74,74,74	0
23	MG	A	1772	1/1	0.78	0.14	83,83,83,83	0
23	MG	A	1812	1/1	0.79	0.23	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	MG	A	1826	1/1	0.79	0.31	87,87,87,87	0
23	MG	A	1685	1/1	0.79	0.18	82,82,82,82	0
23	MG	A	1851	1/1	0.79	0.12	82,82,82,82	0
23	MG	A	1867	1/1	0.79	0.15	95,95,95,95	0
23	MG	A	1836	1/1	0.80	0.23	75,75,75,75	0
23	MG	A	1730	1/1	0.80	0.30	142,142,142,142	0
23	MG	A	1875	1/1	0.80	0.11	114,114,114,114	0
23	MG	A	1838	1/1	0.80	0.27	99,99,99,99	0
23	MG	A	1798	1/1	0.80	0.24	85,85,85,85	0
23	MG	A	1864	1/1	0.80	0.20	72,72,72,72	0
23	MG	A	1832	1/1	0.80	0.14	74,74,74,74	0
23	MG	S	103	1/1	0.80	0.12	90,90,90,90	0
23	MG	A	1850	1/1	0.81	0.12	90,90,90,90	0
23	MG	A	1695	1/1	0.81	0.14	94,94,94,94	0
23	MG	A	1870	1/1	0.81	0.23	95,95,95,95	0
23	MG	A	1813	1/1	0.81	0.11	86,86,86,86	0
23	MG	A	1766	1/1	0.81	0.35	81,81,81,81	0
23	MG	A	1797	1/1	0.81	0.20	109,109,109,109	0
23	MG	A	1862	1/1	0.81	0.18	59,59,59,59	0
23	MG	A	1700	1/1	0.81	0.27	83,83,83,83	0
23	MG	A	1774	1/1	0.81	0.25	80,80,80,80	0
23	MG	A	1651	1/1	0.82	0.19	183,183,183,183	0
23	MG	A	1710	1/1	0.82	0.11	196,196,196,196	0
23	MG	A	1639	1/1	0.83	0.19	80,80,80,80	0
23	MG	A	1609	1/1	0.83	0.25	200,200,200,200	0
23	MG	A	1654	1/1	0.83	0.41	107,107,107,107	0
23	MG	A	1757	1/1	0.83	0.11	84,84,84,84	0
23	MG	A	1719	1/1	0.83	0.28	108,108,108,108	0
23	MG	A	1736	1/1	0.83	0.10	83,83,83,83	0
23	MG	A	1773	1/1	0.84	0.10	48,48,48,48	0
23	MG	A	1840	1/1	0.84	0.11	104,104,104,104	0
23	MG	A	1765	1/1	0.84	0.19	58,58,58,58	0
23	MG	A	1684	1/1	0.84	0.21	80,80,80,80	0
23	MG	A	1771	1/1	0.84	0.13	90,90,90,90	0
23	MG	A	1660	1/1	0.84	0.17	114,114,114,114	0
23	MG	A	1819	1/1	0.84	0.21	82,82,82,82	0
23	MG	A	1698	1/1	0.85	0.25	241,241,241,241	0
23	MG	A	1692	1/1	0.85	0.29	167,167,167,167	0
23	MG	A	1816	1/1	0.85	0.29	72,72,72,72	0
23	MG	A	1662	1/1	0.85	0.22	184,184,184,184	0
23	MG	A	1726	1/1	0.85	0.18	113,113,113,113	0
23	MG	A	1767	1/1	0.85	0.12	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	MG	A	1749	1/1	0.85	0.15	81,81,81,81	0
23	MG	Q	201	1/1	0.85	0.08	70,70,70,70	0
23	MG	A	1696	1/1	0.85	0.30	118,118,118,118	0
23	MG	A	1791	1/1	0.86	0.18	58,58,58,58	0
23	MG	A	1655	1/1	0.86	0.15	107,107,107,107	0
23	MG	A	1833	1/1	0.86	0.11	80,80,80,80	0
23	MG	A	1687	1/1	0.86	0.33	156,156,156,156	0
23	MG	A	1799	1/1	0.86	0.19	80,80,80,80	0
23	MG	A	1857	1/1	0.86	0.23	69,69,69,69	0
23	MG	A	1823	1/1	0.86	0.13	76,76,76,76	0
23	MG	A	1785	1/1	0.86	0.18	84,84,84,84	0
23	MG	A	1841	1/1	0.86	0.24	60,60,60,60	0
23	MG	A	1754	1/1	0.86	0.21	106,106,106,106	0
23	MG	A	1628	1/1	0.87	0.15	83,83,83,83	0
23	MG	A	1693	1/1	0.87	0.22	145,145,145,145	0
23	MG	A	1733	1/1	0.87	0.33	121,121,121,121	0
23	MG	A	1807	1/1	0.87	0.14	88,88,88,88	0
23	MG	A	1711	1/1	0.87	0.27	113,113,113,113	0
23	MG	A	1645	1/1	0.87	0.11	81,81,81,81	0
23	MG	A	1839	1/1	0.87	0.10	64,64,64,64	0
23	MG	A	1675	1/1	0.87	0.17	77,77,77,77	0
23	MG	A	1686	1/1	0.87	0.26	116,116,116,116	0
23	MG	A	1677	1/1	0.87	0.15	118,118,118,118	0
23	MG	A	1783	1/1	0.87	0.08	67,67,67,67	0
23	MG	A	1703	1/1	0.87	0.11	98,98,98,98	0
23	MG	A	1678	1/1	0.87	0.42	183,183,183,183	0
23	MG	A	1825	1/1	0.87	0.11	82,82,82,82	0
23	MG	A	1707	1/1	0.87	0.17	149,149,149,149	0
23	MG	A	1763	1/1	0.88	0.12	84,84,84,84	0
23	MG	A	1778	1/1	0.88	0.14	85,85,85,85	0
23	MG	A	1690	1/1	0.88	0.22	64,64,64,64	0
23	MG	A	1866	1/1	0.88	0.25	55,55,55,55	0
23	MG	A	1808	1/1	0.88	0.23	65,65,65,65	0
23	MG	A	1827	1/1	0.88	0.14	89,89,89,89	0
23	MG	A	1847	1/1	0.88	0.27	72,72,72,72	0
23	MG	A	1608	1/1	0.88	0.15	94,94,94,94	0
23	MG	A	1734	1/1	0.88	0.14	72,72,72,72	0
23	MG	A	1852	1/1	0.88	0.22	68,68,68,68	0
23	MG	A	1728	1/1	0.88	0.21	169,169,169,169	0
23	MG	A	1666	1/1	0.88	0.09	71,71,71,71	0
23	MG	A	1793	1/1	0.88	0.25	69,69,69,69	0
23	MG	A	1745	1/1	0.88	0.23	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	MG	A	1743	1/1	0.89	0.18	126,126,126,126	0
23	MG	A	1861	1/1	0.89	0.12	54,54,54,54	0
23	MG	A	1665	1/1	0.89	0.29	94,94,94,94	0
23	MG	A	1784	1/1	0.89	0.17	78,78,78,78	0
23	MG	A	1625	1/1	0.89	0.14	69,69,69,69	0
23	MG	A	1786	1/1	0.89	0.13	110,110,110,110	0
23	MG	A	1789	1/1	0.89	0.06	87,87,87,87	0
23	MG	A	1717	1/1	0.89	0.29	175,175,175,175	0
23	MG	A	1770	1/1	0.89	0.14	70,70,70,70	0
23	MG	A	1874	1/1	0.89	0.07	59,59,59,59	0
23	MG	A	1751	1/1	0.89	0.09	44,44,44,44	0
23	MG	A	1635	1/1	0.89	0.22	103,103,103,103	0
23	MG	A	1680	1/1	0.89	0.13	296,296,296,296	0
23	MG	A	1681	1/1	0.89	0.27	97,97,97,97	0
22	PAR	A	1604	42/42	0.89	0.15	76,123,134,148	0
23	MG	H	201	1/1	0.89	0.10	68,68,68,68	0
23	MG	A	1779	1/1	0.89	0.46	76,76,76,76	0
23	MG	S	101	1/1	0.89	0.08	83,83,83,83	0
23	MG	A	1835	1/1	0.89	0.19	81,81,81,81	0
23	MG	A	1611	1/1	0.90	0.13	127,127,127,127	0
23	MG	A	1615	1/1	0.90	0.16	51,51,51,51	0
23	MG	A	1794	1/1	0.90	0.24	111,111,111,111	0
23	MG	A	1795	1/1	0.90	0.31	74,74,74,74	0
23	MG	A	1619	1/1	0.90	0.15	79,79,79,79	0
23	MG	A	1697	1/1	0.90	0.12	56,56,56,56	0
23	MG	A	1859	1/1	0.90	0.19	71,71,71,71	0
23	MG	A	1630	1/1	0.90	0.17	74,74,74,74	0
23	MG	A	1623	1/1	0.90	0.46	55,55,55,55	0
23	MG	A	1742	1/1	0.90	0.10	87,87,87,87	0
23	MG	A	1759	1/1	0.90	0.34	80,80,80,80	0
23	MG	A	1657	1/1	0.90	0.12	57,57,57,57	0
23	MG	A	1849	1/1	0.90	0.18	70,70,70,70	0
23	MG	A	1777	1/1	0.91	0.09	46,46,46,46	0
23	MG	A	1618	1/1	0.91	0.24	147,147,147,147	0
23	MG	A	1830	1/1	0.91	0.15	75,75,75,75	0
23	MG	A	1722	1/1	0.91	0.30	191,191,191,191	0
23	MG	A	1780	1/1	0.91	0.18	101,101,101,101	0
23	MG	A	1806	1/1	0.91	0.15	67,67,67,67	0
23	MG	A	1863	1/1	0.91	0.29	73,73,73,73	0
23	MG	A	1629	1/1	0.91	0.15	119,119,119,119	0
22	PAR	A	1605	42/42	0.91	0.22	81,104,114,116	42
23	MG	A	1664	1/1	0.91	0.15	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	MG	A	1699	1/1	0.91	0.12	87,87,87,87	0
23	MG	A	1621	1/1	0.91	0.20	93,93,93,93	0
23	MG	A	1788	1/1	0.91	0.09	72,72,72,72	0
23	MG	A	1753	1/1	0.91	0.19	128,128,128,128	0
23	MG	A	1637	1/1	0.91	0.16	166,166,166,166	0
23	MG	A	1846	1/1	0.91	0.13	78,78,78,78	0
23	MG	A	1820	1/1	0.91	0.23	73,73,73,73	0
23	MG	A	1821	1/1	0.91	0.13	74,74,74,74	0
23	MG	A	1656	1/1	0.91	0.15	97,97,97,97	0
23	MG	A	1792	1/1	0.91	0.43	72,72,72,72	0
23	MG	A	1706	1/1	0.91	0.10	131,131,131,131	0
23	MG	A	1775	1/1	0.91	0.35	82,82,82,82	0
23	MG	A	1854	1/1	0.91	0.07	53,53,53,53	0
23	MG	A	1834	1/1	0.92	0.11	62,62,62,62	0
22	PAR	A	1606	42/42	0.92	0.15	102,118,130,135	0
23	MG	A	1644	1/1	0.92	0.17	120,120,120,120	0
23	MG	A	1801	1/1	0.92	0.11	75,75,75,75	0
23	MG	A	1872	1/1	0.92	0.23	79,79,79,79	0
22	PAR	A	1602	42/42	0.92	0.15	71,102,116,125	0
23	MG	A	1752	1/1	0.92	0.23	246,246,246,246	0
23	MG	A	1627	1/1	0.92	0.10	60,60,60,60	0
23	MG	A	1809	1/1	0.92	0.16	75,75,75,75	0
23	MG	A	1768	1/1	0.92	0.15	83,83,83,83	0
23	MG	D	302	1/1	0.92	0.11	72,72,72,72	0
23	MG	A	1740	1/1	0.92	0.21	118,118,118,118	0
23	MG	A	1653	1/1	0.92	0.11	66,66,66,66	0
23	MG	A	1663	1/1	0.92	0.16	86,86,86,86	0
23	MG	A	1848	1/1	0.92	0.10	70,70,70,70	0
23	MG	A	1624	1/1	0.92	0.18	99,99,99,99	0
23	MG	A	1868	1/1	0.93	0.41	82,82,82,82	0
23	MG	A	1632	1/1	0.93	0.08	73,73,73,73	0
23	MG	A	1667	1/1	0.93	0.13	66,66,66,66	0
23	MG	A	1741	1/1	0.93	0.23	117,117,117,117	0
23	MG	A	1769	1/1	0.93	0.12	95,95,95,95	0
23	MG	A	1810	1/1	0.93	0.24	85,85,85,85	0
23	MG	A	1781	1/1	0.93	0.18	88,88,88,88	0
23	MG	A	1844	1/1	0.93	0.10	61,61,61,61	0
23	MG	A	1879	1/1	0.93	0.10	77,77,77,77	0
23	MG	A	1638	1/1	0.93	0.18	74,74,74,74	0
23	MG	A	1647	1/1	0.93	0.23	94,94,94,94	0
23	MG	A	1650	1/1	0.93	0.13	96,96,96,96	0
23	MG	A	1614	1/1	0.93	0.11	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	MG	A	1818	1/1	0.93	0.13	61,61,61,61	0
23	MG	A	1704	1/1	0.93	0.08	88,88,88,88	0
23	MG	A	1738	1/1	0.93	0.12	160,160,160,160	0
23	MG	A	1787	1/1	0.94	0.15	89,89,89,89	0
23	MG	A	1702	1/1	0.94	0.09	110,110,110,110	0
23	MG	A	1761	1/1	0.94	0.12	64,64,64,64	0
23	MG	A	1776	1/1	0.94	0.10	84,84,84,84	0
23	MG	A	1669	1/1	0.94	0.14	36,36,36,36	0
23	MG	A	1735	1/1	0.94	0.16	103,103,103,103	0
23	MG	A	1642	1/1	0.94	0.19	159,159,159,159	0
23	MG	A	1814	1/1	0.94	0.14	80,80,80,80	0
23	MG	A	1815	1/1	0.94	0.28	27,27,27,27	0
23	MG	A	1876	1/1	0.94	0.09	59,59,59,59	1
22	PAR	A	1603	42/42	0.94	0.13	65,83,95,103	0
23	MG	A	1616	1/1	0.94	0.08	109,109,109,109	0
23	MG	A	1714	1/1	0.94	0.26	134,134,134,134	0
23	MG	A	1858	1/1	0.94	0.16	54,54,54,54	0
23	MG	A	1729	1/1	0.94	0.12	114,114,114,114	0
23	MG	A	1688	1/1	0.94	0.11	56,56,56,56	0
23	MG	A	1758	1/1	0.94	0.30	84,84,84,84	0
23	MG	L	201	1/1	0.94	0.07	93,93,93,93	0
23	MG	A	1842	1/1	0.94	0.07	92,92,92,92	0
23	MG	A	1803	1/1	0.94	0.16	61,61,61,61	0
23	MG	A	1708	1/1	0.94	0.09	148,148,148,148	0
23	MG	A	1805	1/1	0.95	0.09	55,55,55,55	0
23	MG	A	1659	1/1	0.95	0.12	80,80,80,80	0
23	MG	A	1756	1/1	0.95	0.09	66,66,66,66	0
23	MG	A	1855	1/1	0.95	0.13	63,63,63,63	0
23	MG	A	1822	1/1	0.95	0.10	68,68,68,68	0
23	MG	A	1668	1/1	0.95	0.08	74,74,74,74	0
22	PAR	A	1601	42/42	0.95	0.11	58,77,91,94	0
23	MG	A	1723	1/1	0.95	0.12	62,62,62,62	0
23	MG	A	1747	1/1	0.95	0.17	111,111,111,111	0
23	MG	A	1796	1/1	0.95	0.08	85,85,85,85	0
23	MG	A	1670	1/1	0.95	0.08	60,60,60,60	0
23	MG	A	1673	1/1	0.95	0.08	85,85,85,85	0
23	MG	G	201	1/1	0.95	0.05	52,52,52,52	0
23	MG	A	1831	1/1	0.95	0.10	67,67,67,67	0
23	MG	A	1661	1/1	0.95	0.32	106,106,106,106	0
23	MG	P	101	1/1	0.95	0.12	52,52,52,52	0
23	MG	A	1607	1/1	0.95	0.11	109,109,109,109	0
23	MG	A	1802	1/1	0.95	0.17	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	MG	A	1718	1/1	0.95	0.19	149,149,149,149	0
23	MG	A	1873	1/1	0.96	0.11	65,65,65,65	0
23	MG	A	1643	1/1	0.96	0.09	118,118,118,118	0
23	MG	A	1828	1/1	0.96	0.12	52,52,52,52	0
23	MG	A	1671	1/1	0.96	0.09	96,96,96,96	0
23	MG	A	1636	1/1	0.96	0.10	91,91,91,91	0
23	MG	A	1716	1/1	0.96	0.19	112,112,112,112	0
23	MG	A	1610	1/1	0.96	0.26	143,143,143,143	0
23	MG	A	1744	1/1	0.96	0.09	91,91,91,91	0
23	MG	A	1617	1/1	0.96	0.08	108,108,108,108	0
23	MG	A	1658	1/1	0.96	0.22	117,117,117,117	0
23	MG	A	1633	1/1	0.96	0.11	126,126,126,126	0
23	MG	A	1764	1/1	0.96	0.13	77,77,77,77	0
23	MG	I	201	1/1	0.96	0.11	84,84,84,84	0
23	MG	J	201	1/1	0.96	0.09	75,75,75,75	0
23	MG	A	1721	1/1	0.96	0.15	88,88,88,88	0
23	MG	A	1640	1/1	0.96	0.14	116,116,116,116	0
23	MG	A	1737	1/1	0.96	0.15	129,129,129,129	0
23	MG	A	1871	1/1	0.96	0.28	88,88,88,88	0
23	MG	A	1613	1/1	0.96	0.14	97,97,97,97	0
24	ZN	D	301	1/1	0.96	0.27	83,83,83,83	0
23	MG	A	1676	1/1	0.97	0.07	102,102,102,102	0
23	MG	A	1694	1/1	0.97	0.12	102,102,102,102	0
23	MG	A	1727	1/1	0.97	0.08	118,118,118,118	0
23	MG	A	1648	1/1	0.97	0.13	87,87,87,87	0
23	MG	A	1634	1/1	0.97	0.09	91,91,91,91	0
23	MG	A	1622	1/1	0.97	0.09	80,80,80,80	0
23	MG	A	1731	1/1	0.97	0.10	74,74,74,74	0
23	MG	A	1646	1/1	0.97	0.06	70,70,70,70	0
23	MG	A	1631	1/1	0.97	0.09	71,71,71,71	0
23	MG	A	1682	1/1	0.97	0.10	98,98,98,98	0
23	MG	A	1691	1/1	0.97	0.16	86,86,86,86	0
23	MG	A	1762	1/1	0.97	0.20	84,84,84,84	0
23	MG	A	1683	1/1	0.97	0.07	62,62,62,62	0
23	MG	T	201	1/1	0.97	0.18	74,74,74,74	0
23	MG	A	1750	1/1	0.97	0.11	68,68,68,68	0
23	MG	A	1641	1/1	0.98	0.07	57,57,57,57	0
23	MG	A	1804	1/1	0.98	0.07	48,48,48,48	0
23	MG	A	1748	1/1	0.98	0.15	150,150,150,150	0
23	MG	A	1672	1/1	0.98	0.11	74,74,74,74	0
23	MG	S	102	1/1	0.98	0.15	58,58,58,58	0
23	MG	A	1800	1/1	0.98	0.05	63,63,63,63	0

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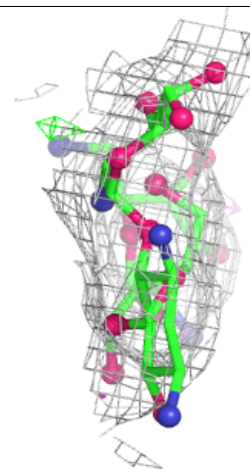
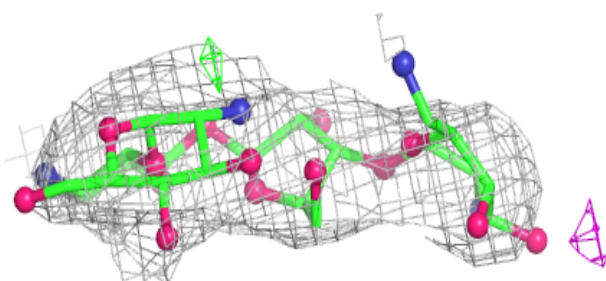
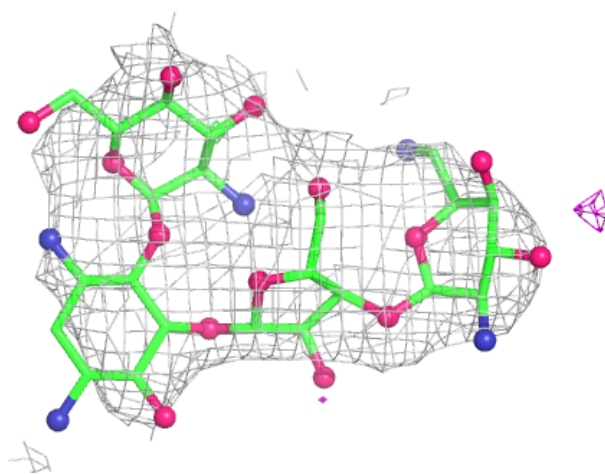
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	MG	A	1725	1/1	0.98	0.06	73,73,73,73	0
23	MG	A	1649	1/1	0.98	0.18	54,54,54,54	0
24	ZN	N	101	1/1	0.98	0.13	120,120,120,120	0
23	MG	A	1701	1/1	0.99	0.03	84,84,84,84	0
23	MG	A	1620	1/1	0.99	0.06	60,60,60,60	0
23	MG	A	1652	1/1	0.99	0.05	78,78,78,78	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.

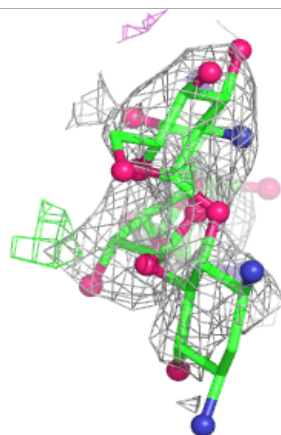
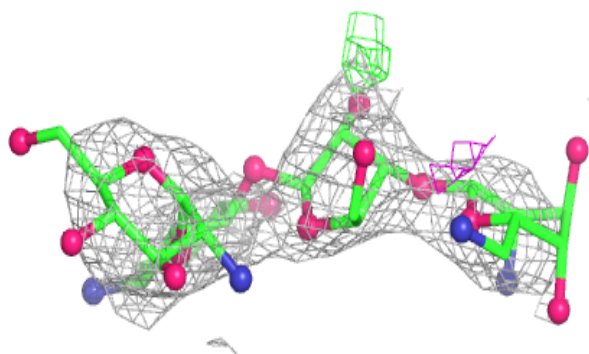
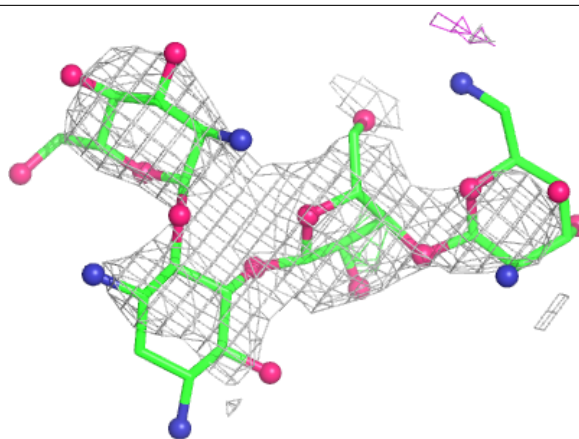
Electron density around PAR A 1604:

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



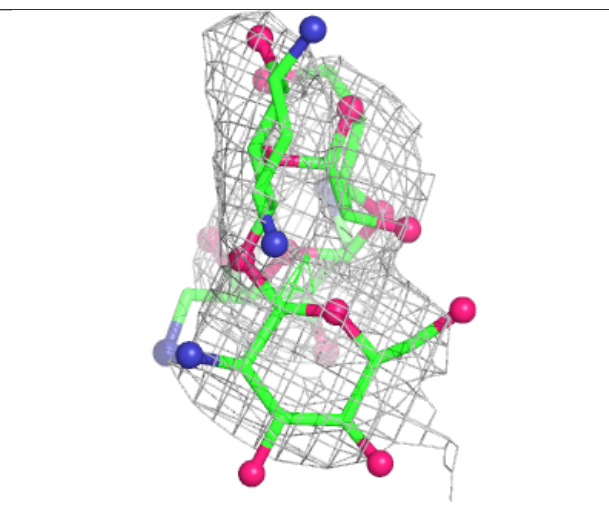
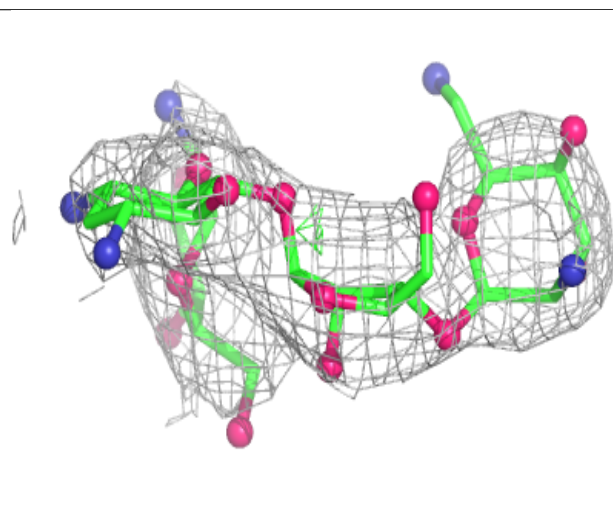
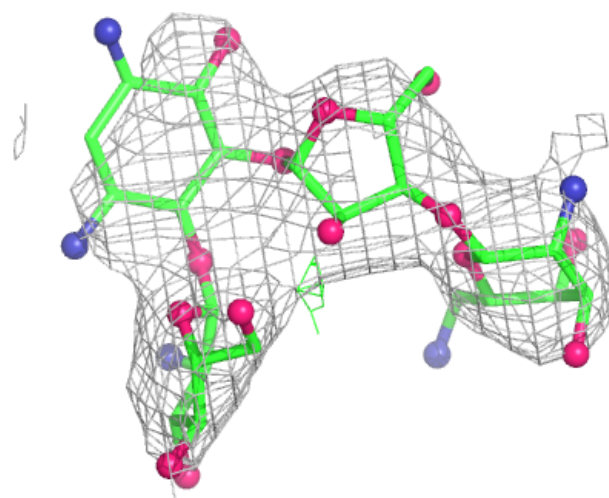
Electron density around PAR A 1605:

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



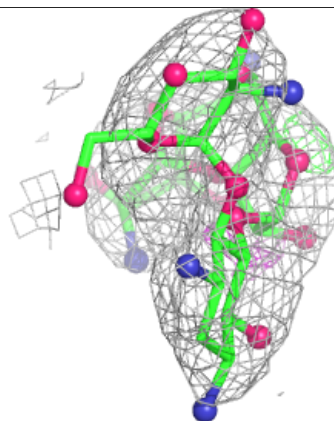
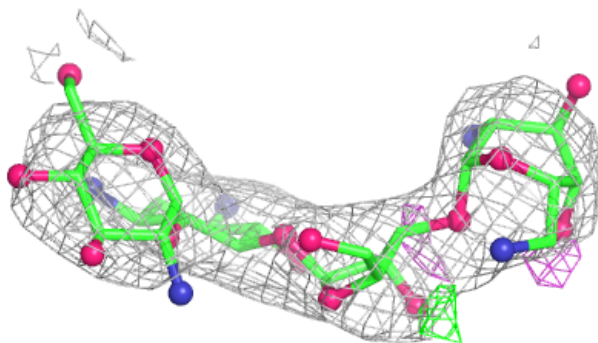
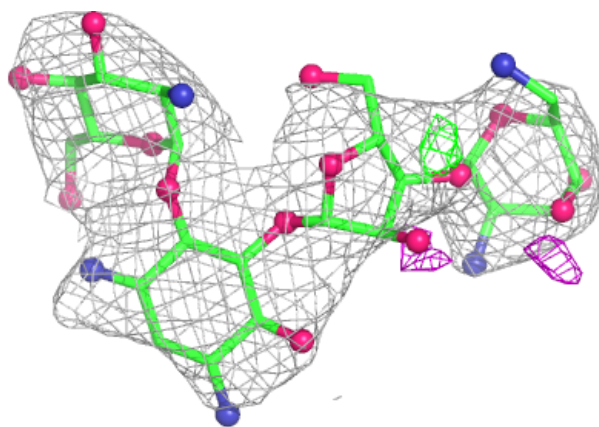
Electron density around PAR A 1606:

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



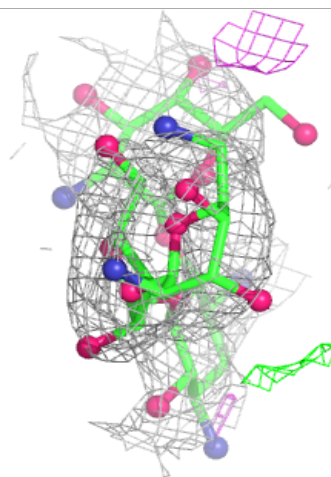
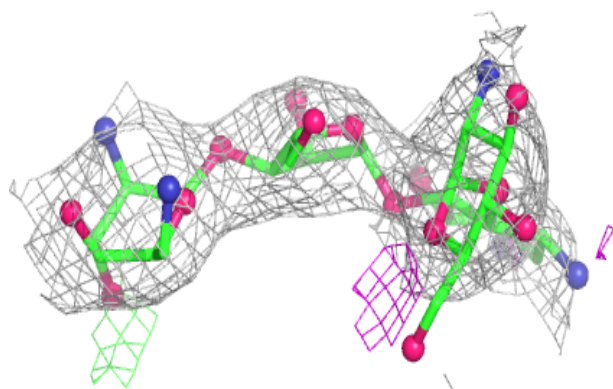
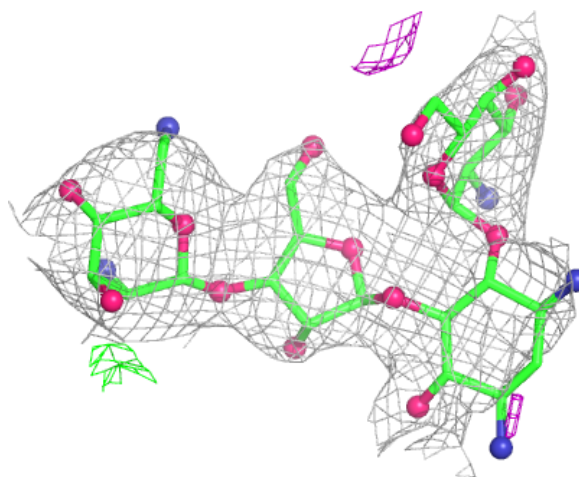
Electron density around PAR A 1602:

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



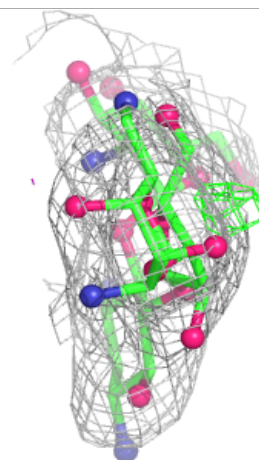
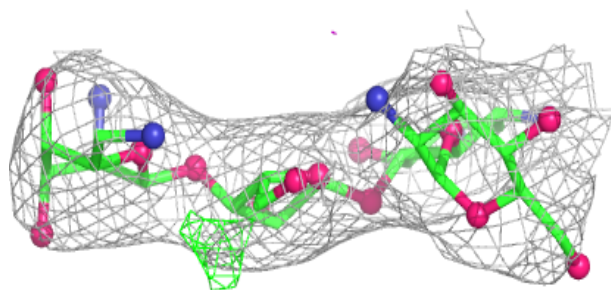
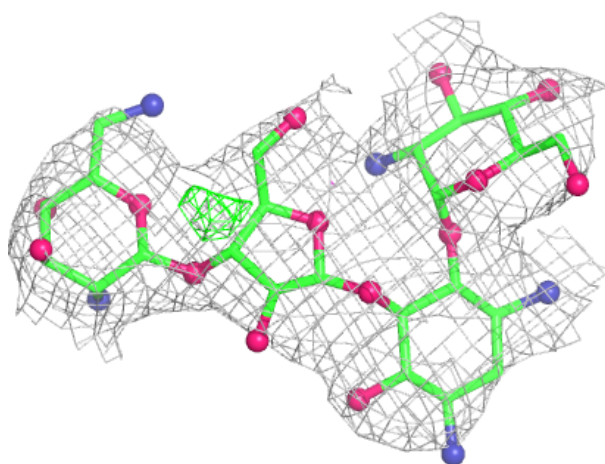
Electron density around PAR A 1603:

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



Electron density around PAR A 1601:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.