wwPDB X-ray Structure Validation Summary Report (i)

Jun 24, 2024 – 04:33 PM EDT

PDB ID	:	6CAO
Title	:	Structure of the ribosomal decoding complex at ambient temperature
Authors	:	DeMirci, H.
Deposited on	:	2018-01-31
Resolution	:	3.45 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

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

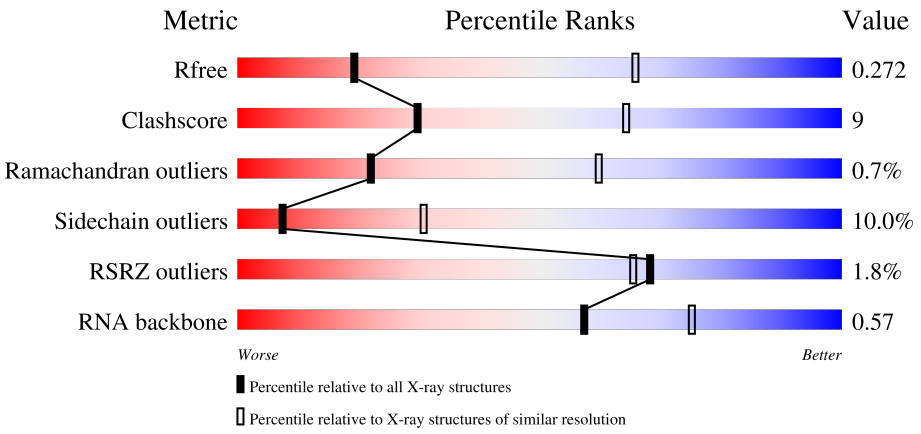
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh &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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.45 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1291 (3.52-3.40)
Clashscore	141614	1372 (3.52-3.40)
Ramachandran outliers	138981	1337 (3.52-3.40)
Sidechain outliers	138945	1338 (3.52-3.40)
RSRZ outliers	127900	1205 (3.52-3.40)
RNA backbone	3102	1036 (3.96-2.96)

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

Mol	Chain	Length	Quality of chain
1	A	1522	2% 58% 32% 9% ••
2	B	236	4% 67% 29% • •
3	C	207	69% 29% •
4	D	208	2% 68% 29% •

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Mol	Chain	Length	Quality of chain
5	E	151	66% 26% 7%
6	F	101	71% 27%
7	G	155	% 69% 28%
8	H	138	65% 28% 6%
9	I	127	% 65% 28% 8%
10	J	99	6% 56% 38% 6%
11	K	117	% 75% 21%
12	L	125	% 62% 30% 7%
13	M	118	% 57% 36% 7%
14	N	60	3% 70% 25% 5%
15	O	88	72% 25%
16	P	84	64% 35%
17	Q	99	67% 32%
18	R	73	3% 67% 27% 5%
19	S	81	2% 59% 33% 7%
20	T	99	2% 65% 28%
21	U	25	76% 24%
22	W	15	20% 67% 20% 13%
23	Y	6	17% 33% 67%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	PSU	A	1540	-	-	-	X
25	K	A	1619	-	-	-	X
25	K	A	1631	-	-	-	X
26	MG	A	1656	-	-	-	X
26	MG	A	1673	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	MG	A	1684	-	-	-	X
26	MG	A	1734	-	-	-	X
26	MG	A	1753	-	-	-	X
26	MG	A	1764	-	-	-	X
26	MG	A	1778	-	-	-	X
26	MG	A	1828	-	-	-	X
26	MG	A	1857	-	-	-	X
26	MG	A	1866	-	-	-	X
26	MG	A	1884	-	-	-	X
26	MG	A	1886	-	-	-	X
26	MG	A	1905	-	-	-	X
26	MG	C	301	-	-	-	X

2 Entry composition (i)

There are 28 unique types of molecules in this entry. The entry contains 52855 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 rRNA.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

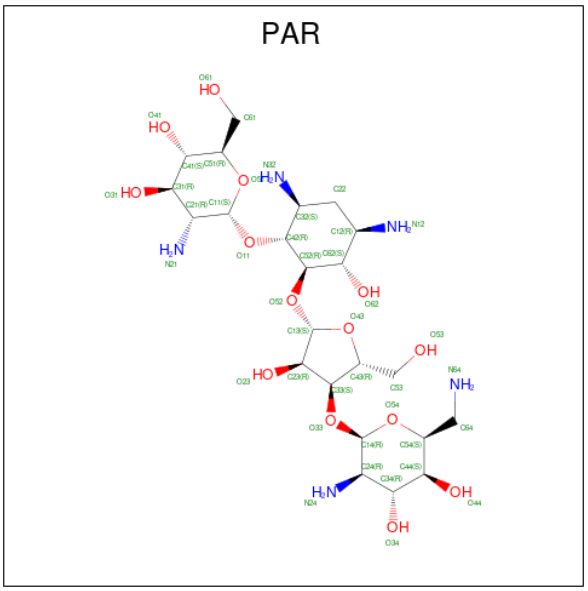
- Molecule 22 is a RNA chain called RNA (5'-R(*GP*GP*GP*AP*UP*UP*GP*AP*AP*AP *AP*UP*CP*CP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
22	W	15	319	144	60	101	14	0	0	0

- Molecule 23 is a RNA chain called RNA (5'-R(*UP*UP*UP*UP*UP*U)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
23	Y	6	117	54	12	46	5	0	0	0

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



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

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

- Molecule 25 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	K		
25	A	35	35	35	0	0
25	E	2	2	2	0	0

- Molecule 26 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
26	A	279	279	279	0	0
26	C	1	1	1	0	0
26	D	2	2	2	0	0
26	E	2	2	2	0	0
26	F	1	1	1	0	0
26	G	1	1	1	0	0
26	H	2	2	2	0	0
26	L	2	2	2	0	0
26	M	1	1	1	0	0
26	P	3	3	3	0	0
26	Q	4	4	4	0	0
26	S	3	3	3	0	0
26	T	1	1	1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
26	Y	1	1	1	0	0

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

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

- Molecule 28 is water.

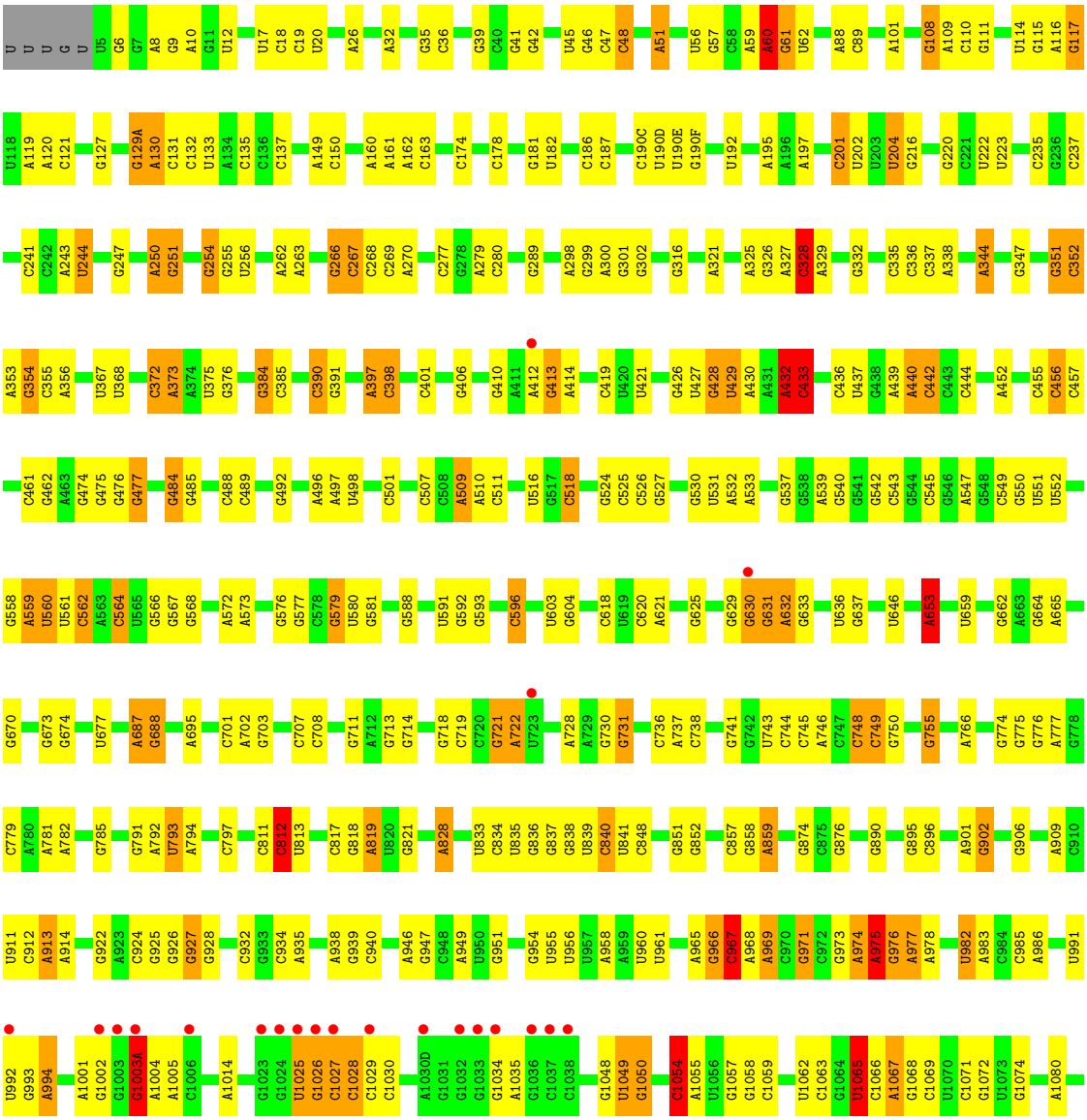
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
28	A	199	199	199	0	0
			Total	O		
28	D	2	2	2	0	0
			Total	O		
28	E	5	5	5	0	0
			Total	O		
28	I	1	1	1	0	0
			Total	O		
28	K	1	1	1	0	0
			Total	O		
28	L	2	2	2	0	0
			Total	O		
28	N	1	1	1	0	0
			Total	O		
28	O	2	2	2	0	0
			Total	O		
28	T	1	1	1	0	0

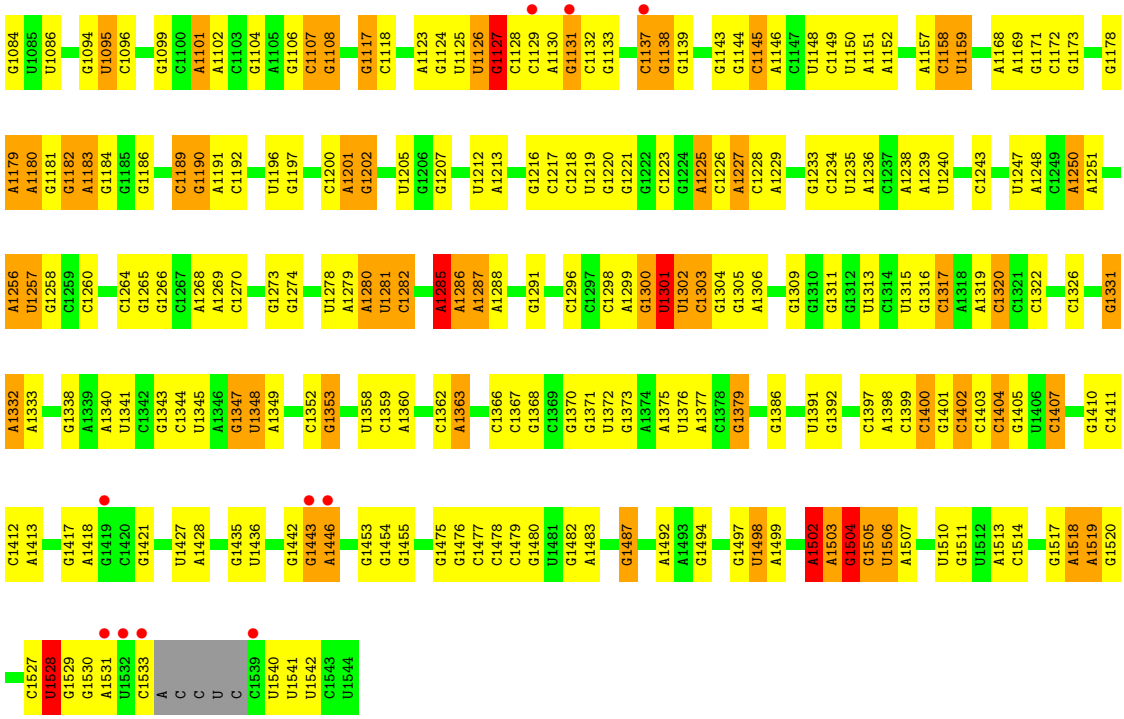
3 Residue-property plots (i)

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

- Molecule 1: 16S Ribosomal RNA rRNA

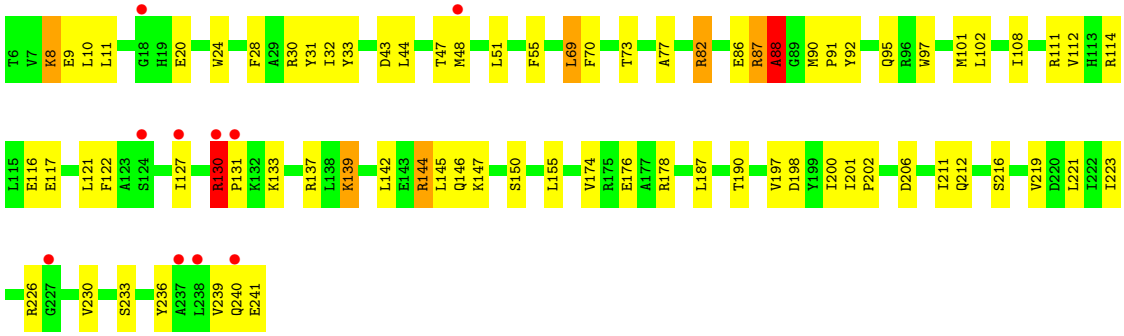
Chain A:





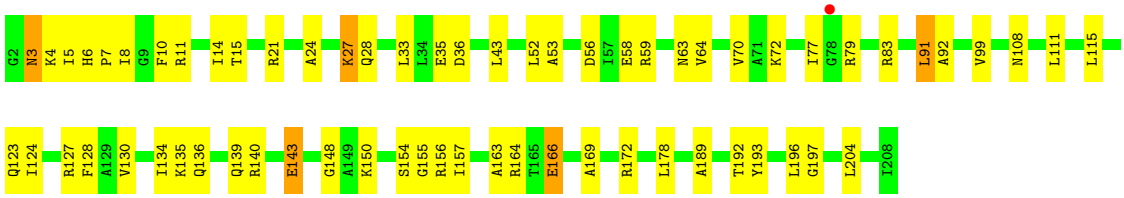
- Molecule 2: 30S ribosomal protein S2

Chain B:



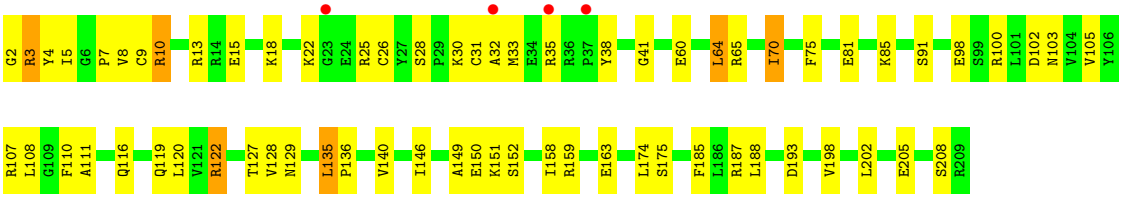
- Molecule 3: 30S ribosomal protein S3

Chain C:



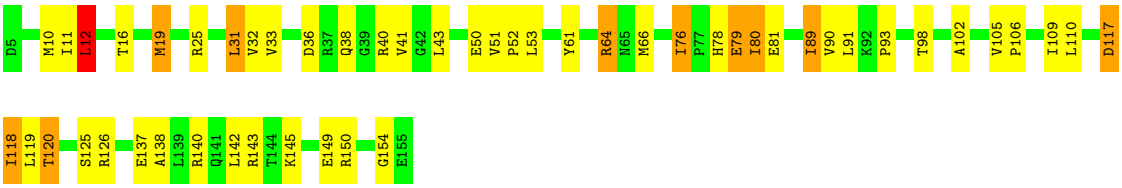
- Molecule 4: 30S ribosomal protein S4

Chain D:



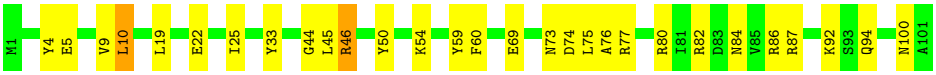
- Molecule 5: 30S ribosomal protein S5

Chain E:



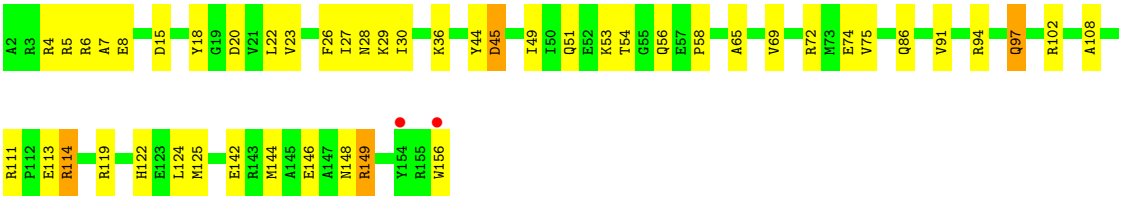
- Molecule 6: 30S ribosomal protein S6

Chain F:



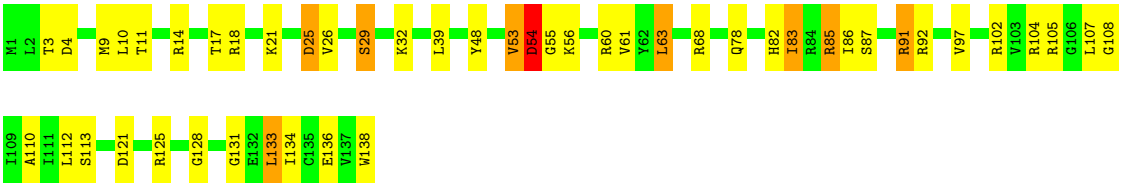
- Molecule 7: 30S ribosomal protein S7

Chain G:



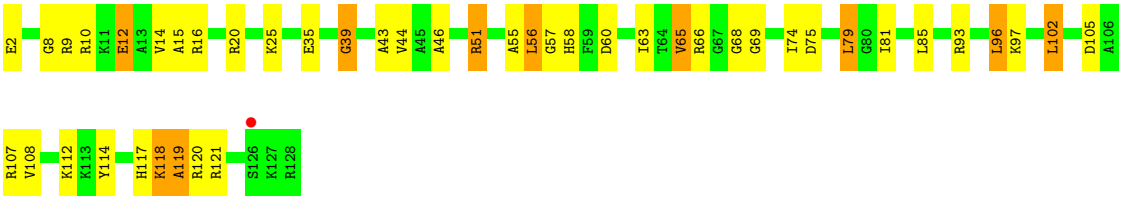
- Molecule 8: 30S ribosomal protein S8

Chain H:



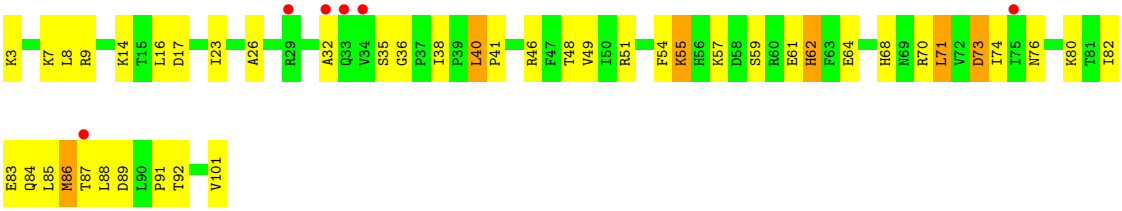
- Molecule 9: 30S ribosomal protein S9

Chain I:



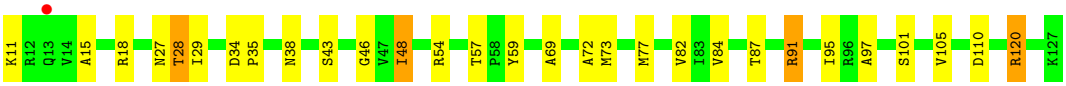
• Molecule 10: 30S ribosomal protein S10

Chain J:



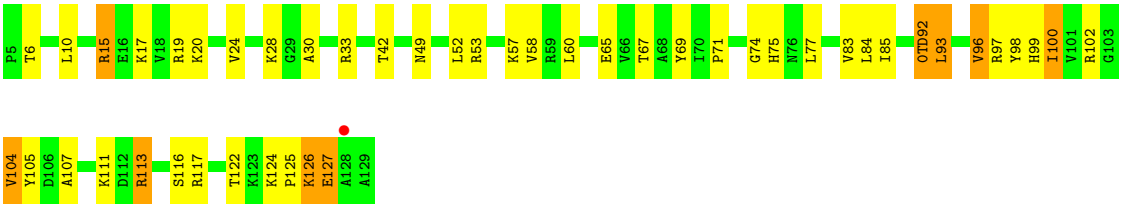
• Molecule 11: 30S ribosomal protein S11

Chain K:



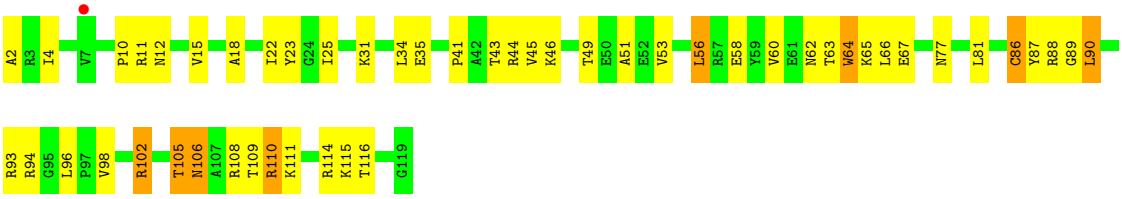
• Molecule 12: 30S ribosomal protein S12

Chain L:



• Molecule 13: 30S ribosomal protein S13

Chain M:

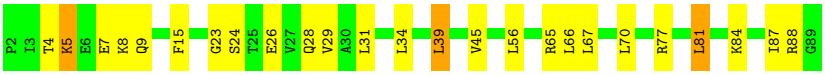


• Molecule 14: 30S ribosomal protein S14 type Z

Chain N:

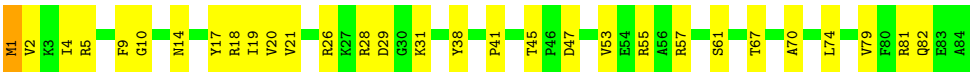
• Molecule 15: 30S ribosomal protein S15

Chain O:



• Molecule 16: 30S ribosomal protein S16

Chain P:



• Molecule 17: 30S ribosomal protein S17

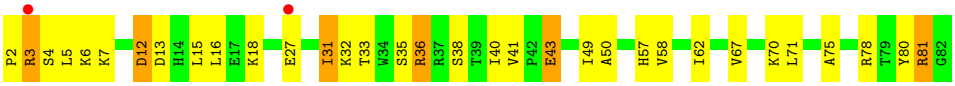
Chain Q:

• Molecule 18: 30S ribosomal protein S18

Chain R:

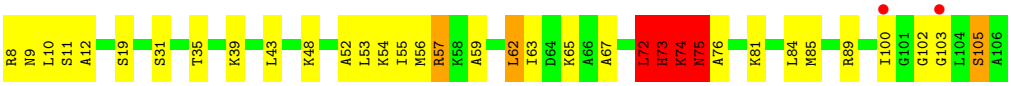
• Molecule 19: 30S ribosomal protein S19

Chain S:



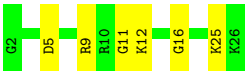
• Molecule 20: 30S ribosomal protein S20

Chain T:



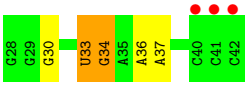
• Molecule 21: 30S ribosomal protein Thx

Chain U:



• Molecule 22: RNA (5'-R(*GP*GP*GP*AP*UP*UP*GP*AP*AP*AP*AP*UP*CP*CP*C)-3')

Chain W:



• Molecule 23: RNA (5'-R(*UP*UP*UP*UP*UP*U)-3')

Chain Y:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	402.30Å 402.30Å 176.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.22 – 3.45 39.22 – 3.45	Depositor EDS
% Data completeness (in resolution range)	100.0 (39.22-3.45) 100.0 (39.22-3.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.12 (at 3.48Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.219 , 0.272 0.219 , 0.272	Depositor DCC
R_{free} test set	1013 reflections (0.54%)	wwPDB-VP
Wilson B-factor (Å^2)	83.6	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 103.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.38$, $< L^2 > = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	52855	wwPDB-VP
Average B, all atoms (Å^2)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.39% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.43	0/36037	1.00	68/56239 (0.1%)
2	B	0.29	0/1909	0.48	0/2579
3	C	0.30	0/1637	0.50	0/2207
4	D	0.29	0/1733	0.46	0/2318
5	E	0.33	0/1163	0.54	1/1566 (0.1%)
6	F	0.27	0/856	0.46	0/1154
7	G	0.31	0/1276	0.46	0/1709
8	H	0.33	0/1136	0.53	0/1527
9	I	0.30	0/1029	0.54	1/1379 (0.1%)
10	J	0.28	0/806	0.60	0/1084
11	K	0.31	0/888	0.50	0/1198
12	L	0.32	0/978	0.56	0/1308
13	M	0.30	0/947	0.50	0/1270
14	N	0.33	0/501	0.49	0/664
15	O	0.28	0/745	0.48	0/992
16	P	0.31	0/717	0.50	0/965
17	Q	0.34	0/836	0.51	0/1117
18	R	0.31	0/604	0.51	0/801
19	S	0.27	0/662	0.51	0/892
20	T	0.29	0/765	0.52	0/1007
21	U	0.24	0/213	0.45	0/279
22	W	0.37	0/357	0.89	0/555
23	Y	0.48	0/128	1.39	1/196 (0.5%)
All	All	0.39	0/55923	0.87	71/83006 (0.1%)

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	4
8	H	0	1
10	J	0	1
12	L	0	2
13	M	0	1
16	P	0	1
20	T	0	1
All	All	0	11

There are no bond length outliers.

The worst 5 of 71 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	456	C	C6-N1-C2	-8.70	116.82	120.30
1	A	456	C	N3-C2-O2	-8.06	116.26	121.90
1	A	456	C	N1-C2-N3	7.85	124.70	119.20
1	A	477	G	N3-C4-N9	-7.82	121.31	126.00
1	A	328	C	C2-N1-C1'	7.48	127.03	118.80

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	130	ARG	Peptide
2	B	8	LYS	Peptide
2	B	87	ARG	Peptide
2	B	88	ALA	Peptide
8	H	53	VAL	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32504	0	16433	396	0
2	B	1874	0	1887	43	0
3	C	1613	0	1677	44	0
4	D	1703	0	1763	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	1147	0	1207	36	0
6	F	843	0	857	18	0
7	G	1257	0	1296	34	0
8	H	1116	0	1177	30	0
9	I	1010	0	1037	33	0
10	J	793	0	835	28	0
11	K	873	0	894	19	0
12	L	973	0	1058	30	0
13	M	937	0	995	40	0
14	N	492	0	529	13	0
15	O	734	0	771	13	0
16	P	701	0	720	17	0
17	Q	823	0	891	20	0
18	R	598	0	670	22	0
19	S	648	0	673	24	0
20	T	763	0	861	28	0
21	U	209	0	221	2	0
22	W	319	0	164	6	0
23	Y	117	0	61	1	0
24	A	252	0	269	14	0
25	A	35	0	0	0	0
25	E	2	0	0	0	0
26	A	279	0	0	0	0
26	C	1	0	0	0	0
26	D	2	0	0	0	0
26	E	2	0	0	0	0
26	F	1	0	0	0	0
26	G	1	0	0	0	0
26	H	2	0	0	0	0
26	L	2	0	0	0	0
26	M	1	0	0	0	0
26	P	3	0	0	0	0
26	Q	4	0	0	0	0
26	S	3	0	0	0	0
26	T	1	0	0	0	0
26	Y	1	0	0	0	0
27	D	1	0	0	0	0
27	N	1	0	0	0	0
28	A	199	0	0	4	0
28	D	2	0	0	0	0
28	E	5	0	0	0	0
28	I	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	K	1	0	0	0	0
28	L	2	0	0	0	0
28	N	1	0	0	0	0
28	O	2	0	0	0	0
28	T	1	0	0	0	0
All	All	52855	0	36946	830	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.

The worst 5 of 830 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:664:G:H22	1:A:741:G:H1	1.15	0.93
24:A:1606:PAR:HN21	24:A:1606:PAR:H322	1.17	0.93
19:S:33:THR:HG22	19:S:35:SER:H	1.33	0.93
1:A:298:A:N6	28:A:2001:HOH:O	2.03	0.90
1:A:954:G:H21	1:A:1227:A:H62	1.25	0.84

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	234/236 (99%)	209 (89%)	20 (8%)	5 (2%)	7 36
3	C	205/207 (99%)	181 (88%)	24 (12%)	0	100 100
4	D	206/208 (99%)	195 (95%)	11 (5%)	0	100 100
5	E	149/151 (99%)	143 (96%)	5 (3%)	1 (1%)	22 60
6	F	99/101 (98%)	98 (99%)	1 (1%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	G	153/155 (99%)	144 (94%)	9 (6%)	0	100	100
8	H	136/138 (99%)	128 (94%)	7 (5%)	1 (1%)	22	60
9	I	125/127 (98%)	111 (89%)	12 (10%)	2 (2%)	9	42
10	J	97/99 (98%)	76 (78%)	20 (21%)	1 (1%)	15	52
11	K	115/117 (98%)	105 (91%)	10 (9%)	0	100	100
12	L	122/125 (98%)	115 (94%)	5 (4%)	2 (2%)	9	42
13	M	116/118 (98%)	103 (89%)	13 (11%)	0	100	100
14	N	58/60 (97%)	53 (91%)	5 (9%)	0	100	100
15	O	86/88 (98%)	83 (96%)	3 (4%)	0	100	100
16	P	82/84 (98%)	81 (99%)	1 (1%)	0	100	100
17	Q	97/99 (98%)	91 (94%)	6 (6%)	0	100	100
18	R	71/73 (97%)	69 (97%)	2 (3%)	0	100	100
19	S	79/81 (98%)	70 (89%)	8 (10%)	1 (1%)	12	46
20	T	97/99 (98%)	87 (90%)	7 (7%)	3 (3%)	4	29
21	U	23/25 (92%)	22 (96%)	0	1 (4%)	2	21
All	All	2350/2391 (98%)	2164 (92%)	169 (7%)	17 (1%)	22	60

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	9	GLU
12	L	127	GLU
20	T	73	HIS
20	T	74	LYS
20	T	75	ASN

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	194/204 (95%)	181 (93%)	13 (7%)	16	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	160/161 (99%)	145 (91%)	15 (9%)	8	33
4	D	180/180 (100%)	169 (94%)	11 (6%)	18	51
5	E	115/116 (99%)	98 (85%)	17 (15%)	3	16
6	F	90/90 (100%)	83 (92%)	7 (8%)	12	41
7	G	126/126 (100%)	119 (94%)	7 (6%)	21	53
8	H	119/119 (100%)	105 (88%)	14 (12%)	5	23
9	I	98/98 (100%)	85 (87%)	13 (13%)	4	19
10	J	87/89 (98%)	74 (85%)	13 (15%)	3	16
11	K	89/89 (100%)	82 (92%)	7 (8%)	12	41
12	L	103/103 (100%)	91 (88%)	12 (12%)	5	24
13	M	94/94 (100%)	84 (89%)	10 (11%)	6	28
14	N	49/49 (100%)	43 (88%)	6 (12%)	5	22
15	O	79/79 (100%)	72 (91%)	7 (9%)	9	36
16	P	72/72 (100%)	67 (93%)	5 (7%)	15	47
17	Q	94/94 (100%)	85 (90%)	9 (10%)	8	32
18	R	64/64 (100%)	58 (91%)	6 (9%)	8	33
19	S	71/71 (100%)	60 (84%)	11 (16%)	2	14
20	T	76/76 (100%)	62 (82%)	14 (18%)	1	7
21	U	19/20 (95%)	18 (95%)	1 (5%)	22	54
All	All	1979/1994 (99%)	1781 (90%)	198 (10%)	7	31

5 of 198 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	K	91	ARG
14	N	22	THR
12	L	20	LYS
13	M	56	LEU
15	O	66	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
9	I	73	GLN

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Mol	Chain	Res	Type
10	J	84	GLN
16	P	82	GLN
13	M	106	ASN
7	G	148	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1507/1522 (99%)	226 (14%)	41 (2%)
22	W	14/15 (93%)	3 (21%)	0
23	Y	5/6 (83%)	2 (40%)	0
All	All	1526/1543 (98%)	231 (15%)	41 (2%)

5 of 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	47	C
1	A	48	C

5 of 41 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1182	G
1	A	1301	U
1	A	1201	A
1	A	1281	U
1	A	1347	G

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

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	PSU	A	1541	1	18,21,22	1.11	1 (5%)	22,30,33	1.73	4 (18%)
1	5MC	A	1404	1	18,22,23	1.20	2 (11%)	26,32,35	1.12	4 (15%)
1	G7M	A	527	1	20,26,27	1.37	2 (10%)	17,39,42	1.00	1 (5%)
1	M2G	A	966	1	20,27,28	1.31	4 (20%)	22,40,43	1.36	3 (13%)
1	5MC	A	1400	1	18,22,23	1.21	2 (11%)	26,32,35	1.13	2 (7%)
1	MA6	A	1519	1	18,26,27	1.18	2 (11%)	19,38,41	0.81	0
1	5MC	A	1407	1	18,22,23	1.10	1 (5%)	26,32,35	1.19	2 (7%)
1	PSU	A	1540	1	18,21,22	1.10	1 (5%)	22,30,33	1.77	4 (18%)
1	PSU	A	516	1,26	18,21,22	1.13	1 (5%)	22,30,33	1.61	3 (13%)
1	5MC	A	967	1	18,22,23	1.01	2 (11%)	26,32,35	0.95	2 (7%)
1	4OC	A	1402	1	20,23,24	1.05	2 (10%)	26,32,35	0.78	1 (3%)
12	0TD	L	92	12	7,9,10	1.21	0	6,11,13	1.71	1 (16%)
1	MA6	A	1518	1	18,26,27	0.90	1 (5%)	19,38,41	0.71	0
1	UR3	A	1498	1	19,22,23	0.69	0	26,32,35	1.04	1 (3%)
1	2MG	A	1207	1	18,26,27	1.54	4 (22%)	16,38,41	1.41	2 (12%)

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	PSU	A	1541	1	-	2/7/25/26	0/2/2/2
1	5MC	A	1404	1	-	2/7/25/26	0/2/2/2
1	G7M	A	527	1	-	1/3/25/26	0/3/3/3
1	M2G	A	966	1	-	3/7/29/30	0/3/3/3
1	5MC	A	1400	1	-	2/7/25/26	0/2/2/2
1	MA6	A	1519	1	-	2/7/29/30	0/3/3/3
1	5MC	A	1407	1	-	0/7/25/26	0/2/2/2
1	PSU	A	1540	1	-	2/7/25/26	0/2/2/2
1	PSU	A	516	1,26	-	0/7/25/26	0/2/2/2
1	5MC	A	967	1	-	2/7/25/26	0/2/2/2
1	4OC	A	1402	1	-	2/9/29/30	0/2/2/2
12	0TD	L	92	12	-	3/7/12/14	-
1	MA6	A	1518	1	-	2/7/29/30	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	UR3	A	1498	1	-	0/7/25/26	0/2/2/2
1	2MG	A	1207	1	-	0/5/27/28	0/3/3/3

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	527	G7M	C2-N2	4.51	1.44	1.34
1	A	516	PSU	C6-C5	3.78	1.39	1.35
1	A	1540	PSU	C6-C5	3.70	1.39	1.35
1	A	1541	PSU	C6-C5	3.67	1.39	1.35
1	A	1207	2MG	C6-N1	3.64	1.43	1.37

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1540	PSU	C4-N3-C2	-4.62	119.68	126.34
1	A	1541	PSU	C4-N3-C2	-4.60	119.70	126.34
1	A	1540	PSU	N1-C2-N3	4.41	120.13	115.13
1	A	1541	PSU	N1-C2-N3	4.33	120.03	115.13
1	A	516	PSU	N1-C2-N3	4.21	119.90	115.13

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	967	5MC	O4'-C4'-C5'-O5'
1	A	967	5MC	C3'-C4'-C5'-O5'
1	A	1519	MA6	C3'-C4'-C5'-O5'
1	A	1402	4OC	O4'-C4'-C5'-O5'
1	A	1519	MA6	O4'-C4'-C5'-O5'

There are no ring outliers.

9 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1404	5MC	1	0
1	A	1400	5MC	1	0
1	A	1519	MA6	2	0
1	A	1407	5MC	1	0
1	A	967	5MC	1	0
1	A	1402	4OC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	L	92	0TD	3	0
1	A	1518	MA6	1	0
1	A	1498	UR3	3	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 348 ligands modelled in this entry, 342 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
24	PAR	A	1606	-	45,45,45	1.40	6 (13%)	64,67,67	1.65	13 (20%)
24	PAR	A	1601	1	45,45,45	1.49	8 (17%)	64,67,67	1.63	11 (17%)
24	PAR	A	1602	-	45,45,45	1.45	9 (20%)	64,67,67	1.68	12 (18%)
24	PAR	A	1604	-	45,45,45	1.32	7 (15%)	64,67,67	1.67	13 (20%)
24	PAR	A	1605	-	45,45,45	1.39	8 (17%)	64,67,67	1.61	13 (20%)
24	PAR	A	1603	-	45,45,45	1.49	7 (15%)	64,67,67	1.66	13 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	PAR	A	1606	-	-	8/18/94/94	1/4/4/4
24	PAR	A	1601	1	-	1/18/94/94	0/4/4/4
24	PAR	A	1602	-	-	7/18/94/94	0/4/4/4
24	PAR	A	1604	-	-	4/18/94/94	1/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	PAR	A	1605	-	-	6/18/94/94	1/4/4/4
24	PAR	A	1603	-	-	7/18/94/94	0/4/4/4

The worst 5 of 45 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1603	PAR	C13-C23	4.77	1.59	1.52
24	A	1601	PAR	C34-C24	4.05	1.58	1.53
24	A	1601	PAR	C52-C42	3.79	1.60	1.52
24	A	1603	PAR	C52-C42	3.63	1.59	1.52
24	A	1606	PAR	C13-C23	3.44	1.57	1.52

The worst 5 of 75 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	1604	PAR	O33-C14-C24	6.30	119.07	108.22
24	A	1602	PAR	O33-C14-C24	6.27	119.02	108.22
24	A	1601	PAR	O33-C14-C24	6.21	118.91	108.22
24	A	1603	PAR	O33-C14-C24	6.19	118.88	108.22
24	A	1606	PAR	O33-C14-C24	6.05	118.64	108.22

There are no chirality outliers.

5 of 33 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	1601	PAR	O54-C54-C64-N64
24	A	1602	PAR	C23-C13-O52-C52
24	A	1602	PAR	O43-C13-O52-C52
24	A	1604	PAR	C21-C11-O11-C42
24	A	1605	PAR	C21-C11-O11-C42

All (3) ring outliers are listed below:

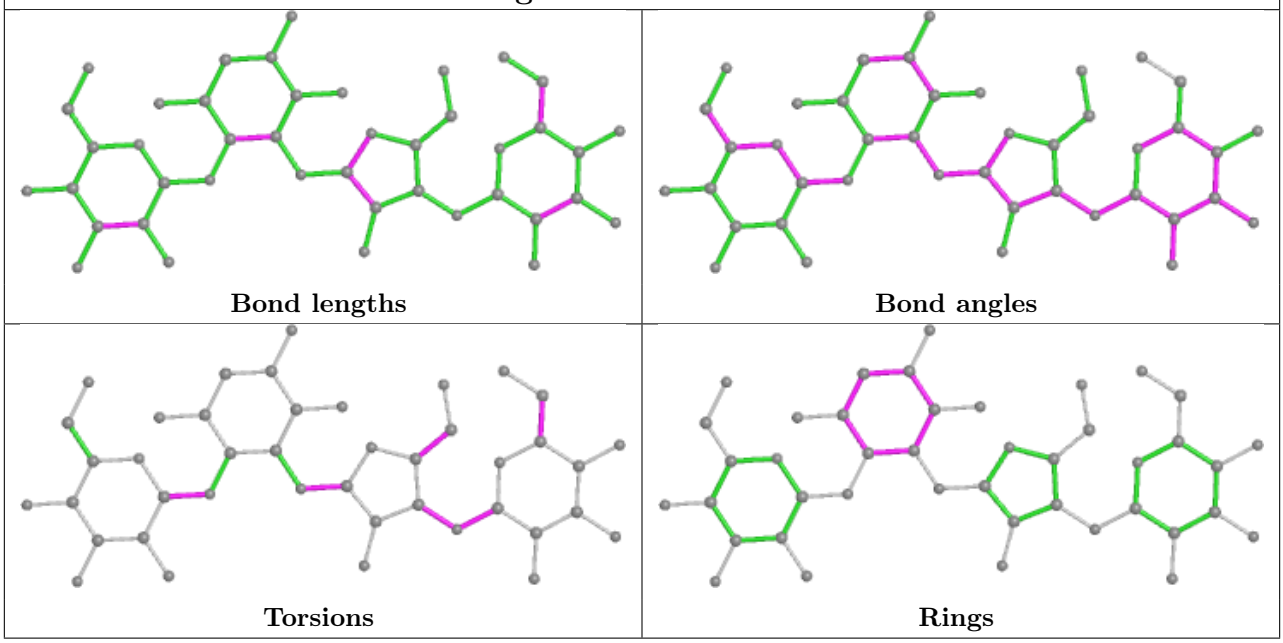
Mol	Chain	Res	Type	Atoms
24	A	1605	PAR	C12-C22-C32-C42-C52-C62
24	A	1606	PAR	C12-C22-C32-C42-C52-C62
24	A	1604	PAR	C12-C22-C32-C42-C52-C62

6 monomers are involved in 14 short contacts:

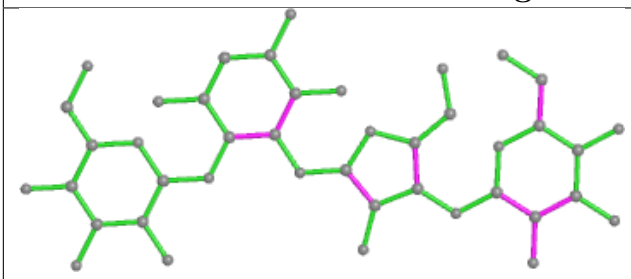
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A	1606	PAR	3	0
24	A	1601	PAR	2	0
24	A	1602	PAR	3	0
24	A	1604	PAR	2	0
24	A	1605	PAR	1	0
24	A	1603	PAR	3	0

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

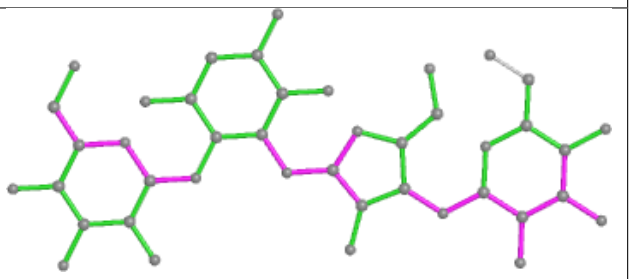
Ligand PAR A 1606



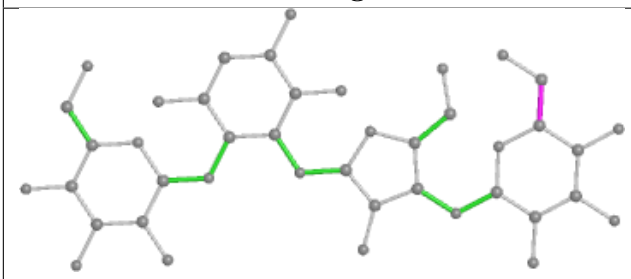
Ligand PAR A 1601



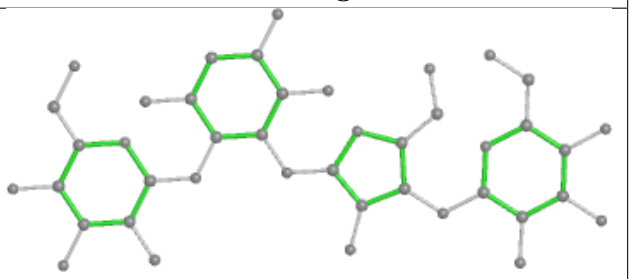
Bond lengths



Bond angles

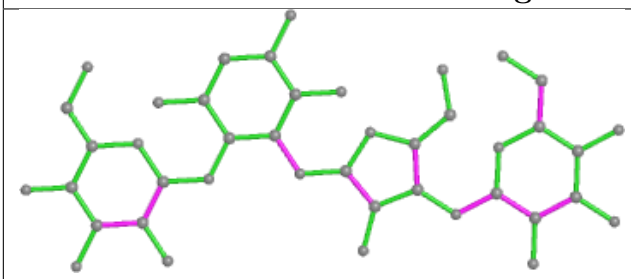


Torsions

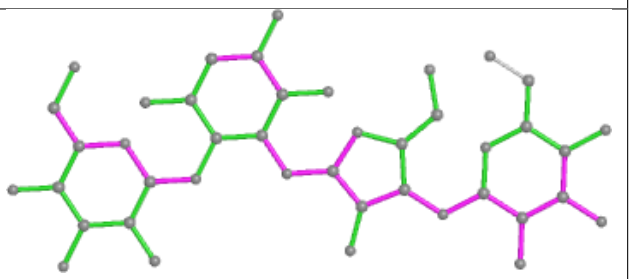


Rings

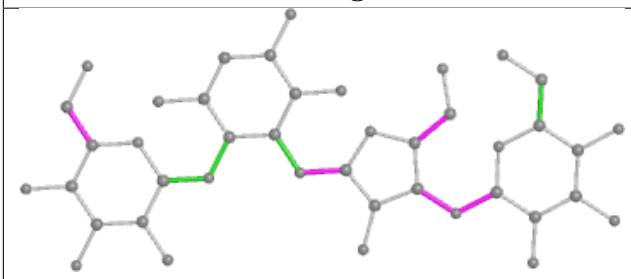
Ligand PAR A 1602



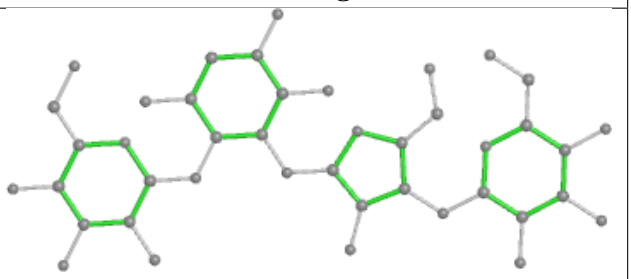
Bond lengths



Bond angles

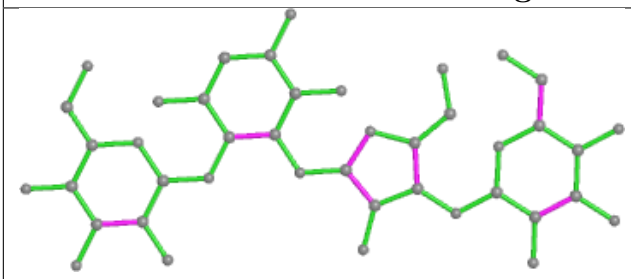


Torsions

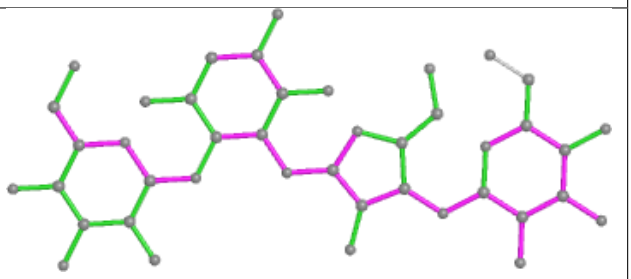


Rings

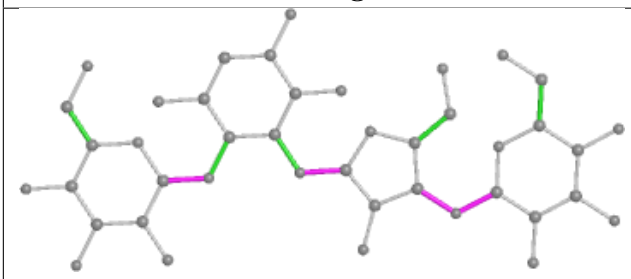
Ligand PAR A 1604



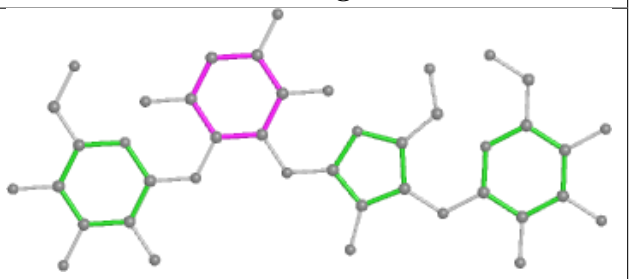
Bond lengths



Bond angles

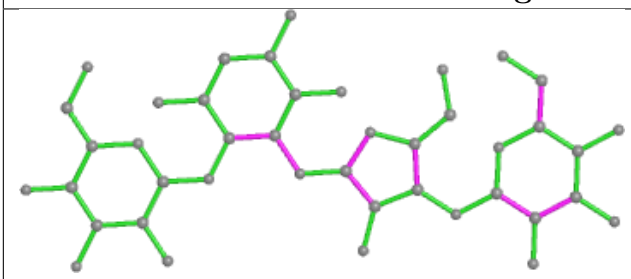


Torsions

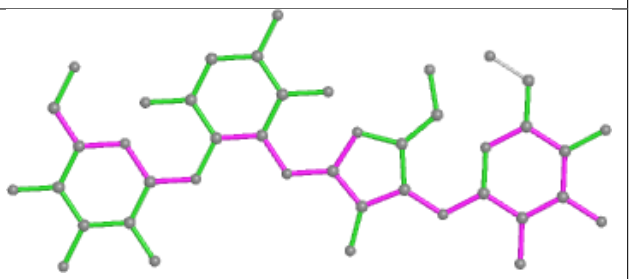


Rings

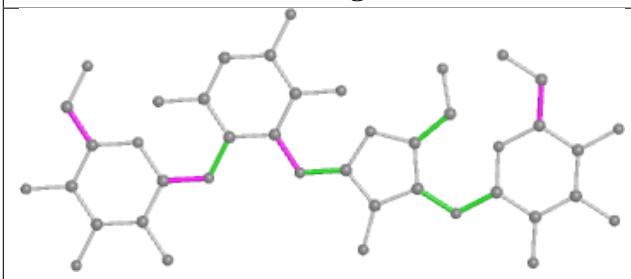
Ligand PAR A 1605



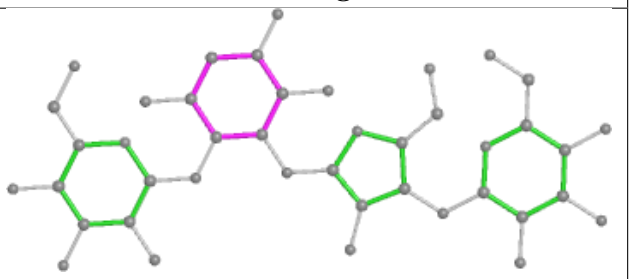
Bond lengths



Bond angles

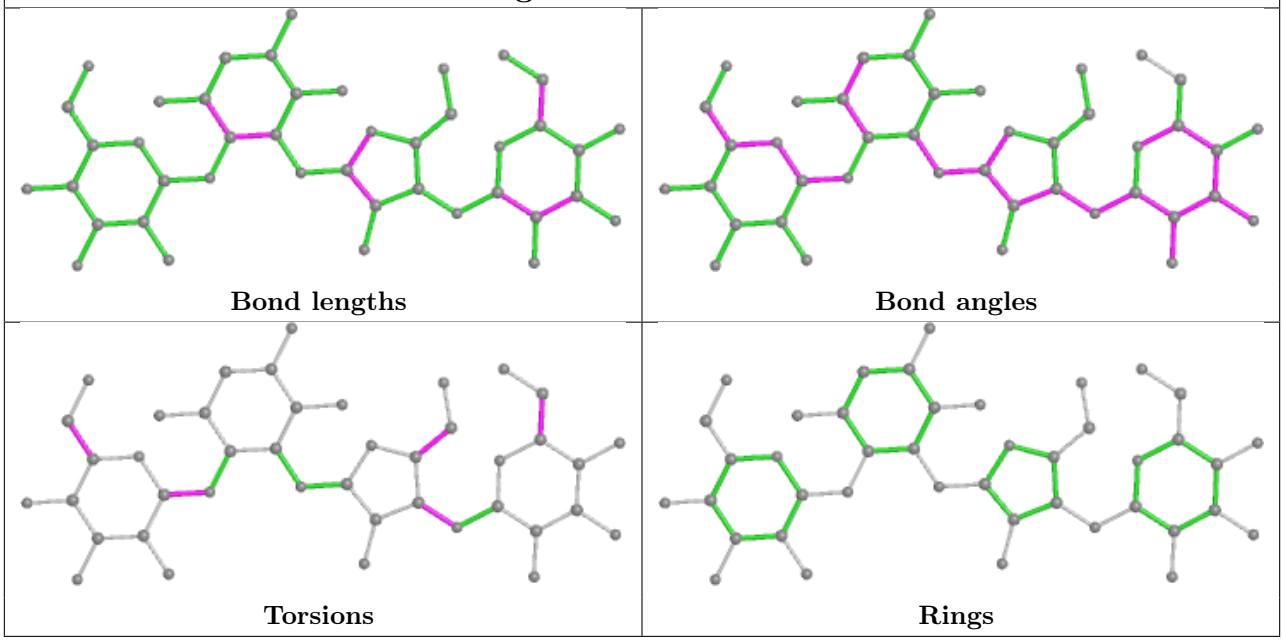


Torsions



Rings

Ligand PAR A 1603



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	1498/1522 (98%)	0.14	31 (2%)	63	61	43, 75, 152, 281	0
2	B	236/236 (100%)	-0.02	10 (4%)	36	35	50, 105, 192, 246	0
3	C	207/207 (100%)	-0.10	1 (0%)	91	89	17, 107, 144, 195	0
4	D	208/208 (100%)	-0.24	4 (1%)	66	64	47, 83, 143, 184	0
5	E	151/151 (100%)	-0.30	0	100	100	39, 64, 97, 161	0
6	F	101/101 (100%)	-0.18	0	100	100	58, 97, 135, 153	0
7	G	155/155 (100%)	-0.20	2 (1%)	77	73	57, 86, 177, 234	0
8	H	138/138 (100%)	-0.46	0	100	100	34, 59, 92, 120	0
9	I	127/127 (100%)	-0.09	1 (0%)	86	82	60, 101, 144, 163	0
10	J	99/99 (100%)	0.37	6 (6%)	21	22	38, 134, 197, 258	0
11	K	117/117 (100%)	-0.12	1 (0%)	84	81	45, 79, 113, 164	0
12	L	124/125 (99%)	-0.26	1 (0%)	86	82	36, 71, 111, 250	0
13	M	118/118 (100%)	-0.15	1 (0%)	86	82	66, 92, 136, 206	0
14	N	60/60 (100%)	-0.20	2 (3%)	46	44	63, 85, 150, 255	0
15	O	88/88 (100%)	-0.30	0	100	100	37, 74, 120, 150	0
16	P	84/84 (100%)	-0.42	0	100	100	40, 68, 97, 201	0
17	Q	99/99 (100%)	-0.31	0	100	100	34, 63, 104, 122	0
18	R	73/73 (100%)	-0.11	2 (2%)	54	52	53, 82, 145, 173	0
19	S	81/81 (100%)	0.20	2 (2%)	57	54	32, 113, 164, 209	0
20	T	99/99 (100%)	-0.27	2 (2%)	65	63	55, 71, 121, 157	0
21	U	25/25 (100%)	0.07	0	100	100	35, 105, 164, 172	0
22	W	15/15 (100%)	1.26	3 (20%)	1	1	80, 124, 197, 203	0
23	Y	6/6 (100%)	1.21	1 (16%)	1	2	92, 100, 173, 203	0
All	All	3909/3934 (99%)	-0.04	70 (1%)	68	65	17, 82, 152, 281	0

The worst 5 of 70 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1129	C	8.8
1	A	1533	C	5.1
18	R	17	SER	4.6
10	J	34	VAL	4.5
4	D	37	PRO	4.1

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	0.79	0.45	248,254,267,267	0
1	PSU	A	1541	20/21	0.88	0.36	195,209,242,243	0
1	M2G	A	966	25/26	0.95	0.21	65,71,79,86	0
1	2MG	A	1207	24/25	0.95	0.16	88,93,104,109	0
1	5MC	A	1400	21/22	0.96	0.17	55,58,66,76	0
1	5MC	A	1404	21/22	0.96	0.16	53,54,56,58	0
1	5MC	A	1407	21/22	0.96	0.21	58,60,67,69	0
1	PSU	A	516	20/21	0.96	0.19	70,77,82,83	0
1	G7M	A	527	24/25	0.96	0.17	56,60,64,67	0
1	UR3	A	1498	21/22	0.97	0.22	55,57,58,65	0
1	MA6	A	1518	24/25	0.97	0.20	55,59,65,72	0
1	MA6	A	1519	24/25	0.97	0.23	53,56,63,69	0
1	5MC	A	967	21/22	0.97	0.16	62,71,77,80	0
1	4OC	A	1402	22/23	0.97	0.20	54,61,67,69	0
12	0TD	L	92	10/11	0.98	0.18	71,76,88,91	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
26	MG	A	1656	1/1	0.34	0.49	175,175,175,175	0
26	MG	A	1725	1/1	0.47	0.34	64,64,64,64	0
26	MG	A	1888	1/1	0.57	0.29	69,69,69,69	0
26	MG	A	1764	1/1	0.62	0.54	61,61,61,61	0
26	MG	A	1857	1/1	0.64	0.48	62,62,62,62	0
26	MG	A	1753	1/1	0.67	0.43	56,56,56,56	0
26	MG	A	1834	1/1	0.67	0.30	188,188,188,188	0
26	MG	A	1774	1/1	0.68	0.37	65,65,65,65	0
26	MG	A	1801	1/1	0.68	0.39	59,59,59,59	0
26	MG	A	1867	1/1	0.68	0.37	35,35,35,35	0
26	MG	A	1828	1/1	0.68	0.42	51,51,51,51	0
26	MG	A	1871	1/1	0.69	0.34	72,72,72,72	0
26	MG	A	1894	1/1	0.70	0.35	51,51,51,51	0
26	MG	A	1738	1/1	0.71	0.30	190,190,190,190	0
25	K	A	1631	1/1	0.71	0.58	102,102,102,102	0
26	MG	A	1910	1/1	0.71	0.27	38,38,38,38	0
26	MG	A	1778	1/1	0.72	0.41	66,66,66,66	0
26	MG	A	1718	1/1	0.72	0.36	62,62,62,62	0
26	MG	A	1846	1/1	0.72	0.34	56,56,56,56	0
26	MG	A	1773	1/1	0.73	0.26	55,55,55,55	0
26	MG	P	103	1/1	0.73	0.25	60,60,60,60	0
26	MG	A	1734	1/1	0.74	0.92	47,47,47,47	0
25	K	A	1619	1/1	0.75	0.43	121,121,121,121	0
26	MG	A	1868	1/1	0.75	0.38	75,75,75,75	0
26	MG	A	1862	1/1	0.75	0.37	49,49,49,49	0
26	MG	A	1884	1/1	0.75	0.40	82,82,82,82	0
26	MG	A	1905	1/1	0.76	0.49	65,65,65,65	0
26	MG	A	1684	1/1	0.76	0.54	365,365,365,365	0
26	MG	C	301	1/1	0.76	0.42	57,57,57,57	0
26	MG	A	1849	1/1	0.76	0.36	66,66,66,66	0
26	MG	A	1889	1/1	0.77	0.12	103,103,103,103	0
26	MG	A	1886	1/1	0.77	0.49	51,51,51,51	0
26	MG	A	1866	1/1	0.77	0.48	39,39,39,39	0
26	MG	A	1819	1/1	0.78	0.26	136,136,136,136	0
26	MG	A	1673	1/1	0.78	0.44	135,135,135,135	0
26	MG	P	102	1/1	0.78	0.26	53,53,53,53	0
26	MG	A	1830	1/1	0.78	0.17	50,50,50,50	0
26	MG	A	1757	1/1	0.79	0.27	74,74,74,74	0
26	MG	A	1903	1/1	0.80	0.22	83,83,83,83	0
26	MG	A	1704	1/1	0.80	0.72	54,54,54,54	0
26	MG	A	1759	1/1	0.80	0.23	61,61,61,61	0
26	MG	A	1686	1/1	0.81	0.36	111,111,111,111	0
26	MG	A	1908	1/1	0.81	0.32	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
26	MG	A	1746	1/1	0.82	0.55	238,238,238,238	0
26	MG	A	1762	1/1	0.82	0.22	41,41,41,41	0
26	MG	A	1735	1/1	0.82	0.24	106,106,106,106	0
26	MG	A	1878	1/1	0.82	0.27	38,38,38,38	0
26	MG	A	1902	1/1	0.82	0.44	52,52,52,52	0
26	MG	A	1652	1/1	0.82	0.41	377,377,377,377	0
26	MG	A	1795	1/1	0.83	0.50	51,51,51,51	0
26	MG	A	1766	1/1	0.83	0.16	29,29,29,29	0
26	MG	A	1712	1/1	0.83	0.27	44,44,44,44	0
26	MG	A	1823	1/1	0.83	0.50	50,50,50,50	0
26	MG	A	1913	1/1	0.83	0.21	55,55,55,55	0
26	MG	A	1790	1/1	0.83	0.27	39,39,39,39	0
26	MG	A	1874	1/1	0.83	0.50	53,53,53,53	0
26	MG	A	1877	1/1	0.83	0.30	48,48,48,48	0
26	MG	A	1724	1/1	0.84	0.26	64,64,64,64	0
26	MG	A	1760	1/1	0.84	0.27	28,28,28,28	0
26	MG	A	1786	1/1	0.84	0.24	57,57,57,57	0
25	K	A	1616	1/1	0.84	0.38	117,117,117,117	0
26	MG	A	1836	1/1	0.84	0.21	54,54,54,54	0
26	MG	A	1872	1/1	0.84	0.12	35,35,35,35	0
26	MG	A	1906	1/1	0.84	0.32	42,42,42,42	0
26	MG	A	1747	1/1	0.84	0.32	165,165,165,165	0
26	MG	A	1848	1/1	0.84	0.33	34,34,34,34	0
25	K	A	1618	1/1	0.84	0.23	109,109,109,109	0
26	MG	A	1881	1/1	0.84	0.43	48,48,48,48	0
26	MG	A	1850	1/1	0.84	0.42	59,59,59,59	0
24	PAR	A	1605	42/42	0.84	0.37	120,149,155,158	0
26	MG	A	1740	1/1	0.85	0.29	173,173,173,173	0
25	K	A	1610	1/1	0.85	0.29	110,110,110,110	0
26	MG	A	1798	1/1	0.85	0.23	44,44,44,44	0
26	MG	L	201	1/1	0.85	0.11	69,69,69,69	0
26	MG	A	1835	1/1	0.85	0.19	62,62,62,62	0
26	MG	A	1826	1/1	0.85	0.88	222,222,222,222	0
26	MG	A	1713	1/1	0.86	0.25	47,47,47,47	0
26	MG	A	1776	1/1	0.86	0.18	51,51,51,51	0
26	MG	A	1843	1/1	0.86	0.40	35,35,35,35	0
24	PAR	A	1602	42/42	0.86	0.31	60,95,137,138	0
26	MG	A	1887	1/1	0.86	0.20	47,47,47,47	0
26	MG	A	1912	1/1	0.86	0.19	37,37,37,37	0
26	MG	A	1737	1/1	0.86	0.25	59,59,59,59	0
26	MG	A	1705	1/1	0.86	0.14	49,49,49,49	0
26	MG	D	302	1/1	0.86	0.08	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
26	MG	G	201	1/1	0.86	0.18	41,41,41,41	0
26	MG	A	1772	1/1	0.86	0.31	43,43,43,43	0
26	MG	A	1900	1/1	0.86	0.20	41,41,41,41	0
25	K	A	1629	1/1	0.86	0.74	144,144,144,144	0
26	MG	A	1844	1/1	0.87	0.53	63,63,63,63	0
26	MG	A	1651	1/1	0.87	0.28	30,30,30,30	0
26	MG	A	1911	1/1	0.87	0.31	67,67,67,67	0
25	K	A	1609	1/1	0.87	0.66	99,99,99,99	0
26	MG	A	1714	1/1	0.87	0.47	206,206,206,206	0
26	MG	A	1915	1/1	0.87	0.23	66,66,66,66	0
26	MG	A	1897	1/1	0.87	0.13	38,38,38,38	0
26	MG	A	1775	1/1	0.87	0.29	70,70,70,70	0
26	MG	A	1800	1/1	0.87	0.19	41,41,41,41	0
25	K	A	1621	1/1	0.87	0.27	119,119,119,119	0
25	K	A	1632	1/1	0.87	0.52	121,121,121,121	0
26	MG	A	1821	1/1	0.87	0.28	39,39,39,39	0
26	MG	A	1909	1/1	0.88	0.47	60,60,60,60	0
26	MG	A	1706	1/1	0.88	0.27	48,48,48,48	0
26	MG	A	1813	1/1	0.88	0.17	35,35,35,35	0
26	MG	A	1758	1/1	0.88	0.49	59,59,59,59	0
26	MG	A	1672	1/1	0.88	0.68	48,48,48,48	0
26	MG	A	1899	1/1	0.88	0.24	29,29,29,29	0
26	MG	A	1861	1/1	0.88	0.27	42,42,42,42	0
26	MG	A	1880	1/1	0.88	0.45	59,59,59,59	0
26	MG	A	1841	1/1	0.88	0.21	26,26,26,26	0
26	MG	A	1700	1/1	0.88	0.57	57,57,57,57	0
25	K	A	1628	1/1	0.88	0.27	99,99,99,99	0
26	MG	A	1663	1/1	0.88	0.24	57,57,57,57	0
26	MG	A	1820	1/1	0.89	0.18	85,85,85,85	0
25	K	A	1641	1/1	0.89	0.49	108,108,108,108	0
26	MG	A	1822	1/1	0.89	0.45	71,71,71,71	0
26	MG	A	1771	1/1	0.89	0.37	44,44,44,44	0
26	MG	A	1678	1/1	0.89	0.30	120,120,120,120	0
26	MG	A	1914	1/1	0.89	0.19	60,60,60,60	0
26	MG	A	1827	1/1	0.89	0.31	77,77,77,77	0
25	K	A	1607	1/1	0.89	0.26	113,113,113,113	0
26	MG	A	1720	1/1	0.89	0.26	57,57,57,57	0
25	K	A	1633	1/1	0.89	0.10	102,102,102,102	0
26	MG	A	1689	1/1	0.89	0.30	97,97,97,97	0
26	MG	L	202	1/1	0.89	0.16	58,58,58,58	0
26	MG	A	1885	1/1	0.89	0.24	58,58,58,58	0
26	MG	A	1729	1/1	0.89	0.40	577,577,577,577	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
26	MG	S	103	1/1	0.89	0.30	97,97,97,97	0
26	MG	A	1832	1/1	0.90	0.42	49,49,49,49	0
26	MG	A	1816	1/1	0.90	0.18	64,64,64,64	0
26	MG	A	1670	1/1	0.90	0.27	54,54,54,54	0
26	MG	A	1863	1/1	0.90	0.22	43,43,43,43	0
26	MG	A	1784	1/1	0.90	0.30	45,45,45,45	0
26	MG	A	1767	1/1	0.90	0.15	17,17,17,17	0
25	K	A	1608	1/1	0.90	0.23	107,107,107,107	0
26	MG	A	1739	1/1	0.90	0.18	45,45,45,45	0
26	MG	A	1845	1/1	0.90	0.33	41,41,41,41	0
26	MG	A	1715	1/1	0.90	0.18	38,38,38,38	0
26	MG	A	1708	1/1	0.90	0.17	80,80,80,80	0
25	K	A	1611	1/1	0.90	0.16	101,101,101,101	0
26	MG	A	1879	1/1	0.90	0.22	49,49,49,49	0
26	MG	A	1750	1/1	0.90	0.19	61,61,61,61	0
26	MG	A	1855	1/1	0.90	0.27	54,54,54,54	0
26	MG	A	1646	1/1	0.91	0.35	27,27,27,27	0
26	MG	A	1883	1/1	0.91	0.24	36,36,36,36	0
26	MG	A	1761	1/1	0.91	0.20	31,31,31,31	0
26	MG	A	1642	1/1	0.91	0.18	50,50,50,50	0
26	MG	A	1658	1/1	0.91	0.15	51,51,51,51	0
26	MG	A	1662	1/1	0.91	0.29	92,92,92,92	0
26	MG	A	1805	1/1	0.91	0.53	52,52,52,52	0
26	MG	A	1730	1/1	0.91	0.25	61,61,61,61	0
26	MG	A	1873	1/1	0.91	0.25	38,38,38,38	0
26	MG	A	1920	1/1	0.91	0.19	56,56,56,56	0
26	MG	A	1895	1/1	0.91	0.20	65,65,65,65	0
26	MG	A	1896	1/1	0.91	0.24	56,56,56,56	0
26	MG	A	1815	1/1	0.91	0.31	35,35,35,35	0
26	MG	H	202	1/1	0.91	0.27	27,27,27,27	0
26	MG	A	1876	1/1	0.91	0.17	55,55,55,55	0
26	MG	A	1769	1/1	0.91	0.22	73,73,73,73	0
26	MG	A	1699	1/1	0.91	0.17	60,60,60,60	0
26	MG	A	1859	1/1	0.91	0.17	41,41,41,41	0
26	MG	Q	202	1/1	0.91	0.33	38,38,38,38	0
26	MG	S	102	1/1	0.91	0.13	61,61,61,61	0
26	MG	A	1787	1/1	0.91	0.45	51,51,51,51	0
26	MG	A	1882	1/1	0.92	0.56	46,46,46,46	0
26	MG	A	1645	1/1	0.92	0.14	90,90,90,90	0
25	K	A	1613	1/1	0.92	0.17	100,100,100,100	0
26	MG	A	1649	1/1	0.92	0.13	128,128,128,128	0
26	MG	A	1838	1/1	0.92	0.11	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
26	MG	A	1839	1/1	0.92	0.12	19,19,19,19	0
25	K	A	1639	1/1	0.92	0.27	89,89,89,89	0
26	MG	A	1842	1/1	0.92	0.30	28,28,28,28	0
26	MG	A	1741	1/1	0.92	0.13	45,45,45,45	0
25	K	A	1640	1/1	0.92	0.44	113,113,113,113	0
26	MG	A	1788	1/1	0.92	0.23	39,39,39,39	0
26	MG	A	1726	1/1	0.92	0.20	46,46,46,46	0
26	MG	A	1681	1/1	0.92	0.27	41,41,41,41	0
25	K	A	1622	1/1	0.92	0.16	97,97,97,97	0
26	MG	A	1755	1/1	0.92	0.26	36,36,36,36	0
24	PAR	A	1604	42/42	0.92	0.21	61,89,102,111	0
26	MG	A	1904	1/1	0.92	0.26	34,34,34,34	0
26	MG	A	1644	1/1	0.92	0.10	59,59,59,59	0
26	MG	A	1858	1/1	0.92	0.19	26,26,26,26	0
26	MG	A	1907	1/1	0.92	0.16	49,49,49,49	0
26	MG	A	1732	1/1	0.93	0.18	23,23,23,23	0
26	MG	A	1770	1/1	0.93	0.18	31,31,31,31	0
26	MG	A	1751	1/1	0.93	0.29	45,45,45,45	0
25	K	A	1623	1/1	0.93	0.23	85,85,85,85	0
26	MG	A	1806	1/1	0.93	0.18	62,62,62,62	0
24	PAR	A	1601	42/42	0.93	0.22	35,58,77,81	0
26	MG	A	1736	1/1	0.93	0.28	108,108,108,108	0
26	MG	A	1721	1/1	0.93	0.08	75,75,75,75	0
26	MG	A	1892	1/1	0.93	0.17	33,33,33,33	0
26	MG	A	1869	1/1	0.93	0.17	17,17,17,17	0
25	K	A	1617	1/1	0.93	0.63	112,112,112,112	0
26	MG	A	1696	1/1	0.93	0.21	61,61,61,61	0
26	MG	D	303	1/1	0.93	0.10	50,50,50,50	0
26	MG	A	1675	1/1	0.93	0.31	125,125,125,125	0
26	MG	A	1898	1/1	0.93	0.18	63,63,63,63	0
26	MG	A	1785	1/1	0.93	0.26	59,59,59,59	0
24	PAR	A	1606	42/42	0.93	0.29	87,95,101,105	0
26	MG	P	101	1/1	0.93	0.50	33,33,33,33	0
26	MG	A	1667	1/1	0.93	0.33	38,38,38,38	0
26	MG	A	1765	1/1	0.93	0.14	47,47,47,47	0
26	MG	A	1854	1/1	0.93	0.44	50,50,50,50	0
26	MG	A	1731	1/1	0.93	0.58	128,128,128,128	0
26	MG	A	1748	1/1	0.93	0.43	41,41,41,41	0
26	MG	A	1679	1/1	0.94	0.17	80,80,80,80	0
26	MG	A	1666	1/1	0.94	0.26	9,9,9,9	0
25	K	A	1612	1/1	0.94	0.21	96,96,96,96	0
26	MG	A	1860	1/1	0.94	0.80	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
26	MG	A	1669	1/1	0.94	0.20	22,22,22,22	0
25	K	A	1624	1/1	0.94	0.41	97,97,97,97	0
26	MG	A	1671	1/1	0.94	0.23	135,135,135,135	0
26	MG	A	1697	1/1	0.94	0.15	53,53,53,53	0
26	MG	A	1891	1/1	0.94	0.59	57,57,57,57	0
26	MG	A	1918	1/1	0.94	0.10	53,53,53,53	0
26	MG	A	1840	1/1	0.94	0.37	27,27,27,27	0
26	MG	A	1657	1/1	0.94	0.28	91,91,91,91	0
26	MG	A	1648	1/1	0.94	0.21	58,58,58,58	0
26	MG	A	1818	1/1	0.94	0.16	106,106,106,106	0
26	MG	E	204	1/1	0.94	0.14	47,47,47,47	0
26	MG	F	201	1/1	0.94	0.11	52,52,52,52	0
26	MG	A	1779	1/1	0.94	0.17	26,26,26,26	0
24	PAR	A	1603	42/42	0.94	0.24	34,78,97,101	0
26	MG	A	1745	1/1	0.94	0.26	18,18,18,18	0
26	MG	A	1677	1/1	0.94	0.20	28,28,28,28	0
26	MG	A	1901	1/1	0.94	0.19	32,32,32,32	0
25	K	A	1614	1/1	0.94	0.29	92,92,92,92	0
26	MG	A	1707	1/1	0.94	0.25	99,99,99,99	0
26	MG	A	1768	1/1	0.94	0.09	49,49,49,49	0
26	MG	A	1793	1/1	0.94	0.58	48,48,48,48	0
26	MG	A	1856	1/1	0.94	0.36	43,43,43,43	0
26	MG	A	1659	1/1	0.95	0.34	70,70,70,70	0
26	MG	A	1847	1/1	0.95	0.21	73,73,73,73	0
25	K	A	1637	1/1	0.95	0.17	123,123,123,123	0
26	MG	A	1692	1/1	0.95	0.25	120,120,120,120	0
26	MG	A	1789	1/1	0.95	0.13	24,24,24,24	0
26	MG	A	1824	1/1	0.95	0.13	72,72,72,72	0
26	MG	A	1694	1/1	0.95	0.12	35,35,35,35	0
26	MG	A	1791	1/1	0.95	0.07	43,43,43,43	0
26	MG	A	1695	1/1	0.95	0.32	107,107,107,107	0
26	MG	A	1829	1/1	0.95	0.36	41,41,41,41	0
25	K	A	1638	1/1	0.95	0.24	78,78,78,78	0
26	MG	A	1754	1/1	0.95	0.22	61,61,61,61	0
26	MG	A	1799	1/1	0.95	0.14	46,46,46,46	0
26	MG	A	1653	1/1	0.95	0.14	112,112,112,112	0
26	MG	A	1717	1/1	0.95	0.09	61,61,61,61	0
26	MG	E	203	1/1	0.95	0.17	96,96,96,96	0
26	MG	A	1864	1/1	0.95	0.19	26,26,26,26	0
26	MG	A	1865	1/1	0.95	0.41	27,27,27,27	0
26	MG	A	1837	1/1	0.95	0.13	31,31,31,31	0
26	MG	H	201	1/1	0.95	0.14	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
26	MG	A	1654	1/1	0.95	0.25	158,158,158,158	0
26	MG	A	1719	1/1	0.95	0.19	32,32,32,32	0
26	MG	A	1810	1/1	0.95	0.25	54,54,54,54	0
25	K	E	201	1/1	0.95	0.19	84,84,84,84	0
26	MG	A	1703	1/1	0.95	0.13	26,26,26,26	0
25	K	E	202	1/1	0.95	0.14	82,82,82,82	0
26	MG	A	1763	1/1	0.95	0.42	40,40,40,40	0
26	MG	A	1875	1/1	0.95	0.20	40,40,40,40	0
25	K	A	1635	1/1	0.95	0.29	67,67,67,67	0
26	MG	A	1796	1/1	0.96	0.41	27,27,27,27	0
26	MG	A	1674	1/1	0.96	0.10	9,9,9,9	0
26	MG	A	1728	1/1	0.96	0.27	23,23,23,23	0
26	MG	A	1742	1/1	0.96	0.29	172,172,172,172	0
26	MG	A	1701	1/1	0.96	0.52	18,18,18,18	0
26	MG	A	1802	1/1	0.96	0.14	26,26,26,26	0
26	MG	A	1916	1/1	0.96	0.22	52,52,52,52	0
26	MG	A	1804	1/1	0.96	0.39	23,23,23,23	0
25	K	A	1630	1/1	0.96	0.13	84,84,84,84	0
26	MG	A	1780	1/1	0.96	0.23	46,46,46,46	0
26	MG	A	1807	1/1	0.96	0.11	57,57,57,57	0
26	MG	A	1808	1/1	0.96	0.26	18,18,18,18	0
26	MG	A	1676	1/1	0.96	0.15	56,56,56,56	0
26	MG	A	1812	1/1	0.96	0.20	48,48,48,48	0
26	MG	A	1647	1/1	0.96	0.12	68,68,68,68	0
26	MG	A	1749	1/1	0.96	0.34	45,45,45,45	0
26	MG	A	1733	1/1	0.96	0.11	4,4,4,4	0
26	MG	A	1817	1/1	0.96	0.11	74,74,74,74	0
25	K	A	1636	1/1	0.96	0.12	101,101,101,101	0
25	K	A	1620	1/1	0.96	0.18	65,65,65,65	0
26	MG	A	1664	1/1	0.96	0.18	7,7,7,7	0
26	MG	A	1722	1/1	0.96	0.14	95,95,95,95	0
26	MG	A	1792	1/1	0.96	0.16	25,25,25,25	0
26	MG	A	1711	1/1	0.96	0.15	68,68,68,68	0
26	MG	A	1794	1/1	0.96	0.11	33,33,33,33	0
25	K	A	1634	1/1	0.96	0.25	108,108,108,108	0
26	MG	A	1727	1/1	0.97	0.29	105,105,105,105	0
25	K	A	1627	1/1	0.97	0.28	93,93,93,93	0
26	MG	A	1803	1/1	0.97	0.27	18,18,18,18	0
26	MG	A	1743	1/1	0.97	0.22	77,77,77,77	0
26	MG	A	1831	1/1	0.97	0.12	44,44,44,44	0
26	MG	A	1781	1/1	0.97	0.19	41,41,41,41	0
26	MG	A	1783	1/1	0.97	0.18	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
26	MG	A	1744	1/1	0.97	0.26	60,60,60,60	0
26	MG	A	1917	1/1	0.97	0.16	24,24,24,24	0
26	MG	A	1890	1/1	0.97	0.13	53,53,53,53	0
25	K	A	1615	1/1	0.97	0.13	77,77,77,77	0
26	MG	A	1643	1/1	0.97	0.19	50,50,50,50	0
26	MG	A	1893	1/1	0.97	0.31	33,33,33,33	0
26	MG	A	1811	1/1	0.97	0.70	40,40,40,40	0
26	MG	A	1655	1/1	0.97	0.13	55,55,55,55	0
26	MG	A	1702	1/1	0.97	0.27	74,74,74,74	0
26	MG	A	1687	1/1	0.97	0.25	76,76,76,76	0
26	MG	A	1665	1/1	0.97	0.13	53,53,53,53	0
26	MG	A	1691	1/1	0.97	0.12	27,27,27,27	0
26	MG	A	1752	1/1	0.97	0.15	57,57,57,57	0
25	K	A	1625	1/1	0.97	0.07	68,68,68,68	0
26	MG	A	1650	1/1	0.97	0.13	49,49,49,49	0
26	MG	A	1668	1/1	0.97	0.38	30,30,30,30	0
26	MG	A	1756	1/1	0.97	0.18	35,35,35,35	0
26	MG	A	1710	1/1	0.97	0.22	50,50,50,50	0
25	K	A	1626	1/1	0.97	0.14	90,90,90,90	0
26	MG	Q	203	1/1	0.97	0.06	44,44,44,44	0
26	MG	Q	204	1/1	0.97	0.09	46,46,46,46	0
26	MG	A	1825	1/1	0.97	0.20	40,40,40,40	0
26	MG	A	1777	1/1	0.97	0.15	64,64,64,64	0
27	ZN	N	101	1/1	0.97	0.14	101,101,101,101	0
26	MG	A	1680	1/1	0.98	0.15	37,37,37,37	0
26	MG	A	1833	1/1	0.98	0.18	146,146,146,146	0
26	MG	A	1685	1/1	0.98	0.42	53,53,53,53	0
26	MG	A	1693	1/1	0.98	0.13	14,14,14,14	0
26	MG	A	1661	1/1	0.98	0.15	54,54,54,54	0
26	MG	A	1814	1/1	0.98	0.22	11,11,11,11	0
26	MG	A	1682	1/1	0.98	0.15	43,43,43,43	0
26	MG	A	1851	1/1	0.98	0.16	46,46,46,46	0
26	MG	M	201	1/1	0.98	0.05	32,32,32,32	0
26	MG	A	1852	1/1	0.98	0.17	44,44,44,44	0
26	MG	A	1853	1/1	0.98	0.13	25,25,25,25	0
26	MG	A	1688	1/1	0.98	0.12	43,43,43,43	0
26	MG	Q	201	1/1	0.98	0.10	51,51,51,51	0
26	MG	A	1870	1/1	0.98	0.20	32,32,32,32	0
26	MG	A	1919	1/1	0.98	0.12	45,45,45,45	0
26	MG	A	1797	1/1	0.98	0.23	26,26,26,26	0
26	MG	A	1683	1/1	0.98	0.21	30,30,30,30	0
26	MG	A	1698	1/1	0.98	0.07	39,39,39,39	0

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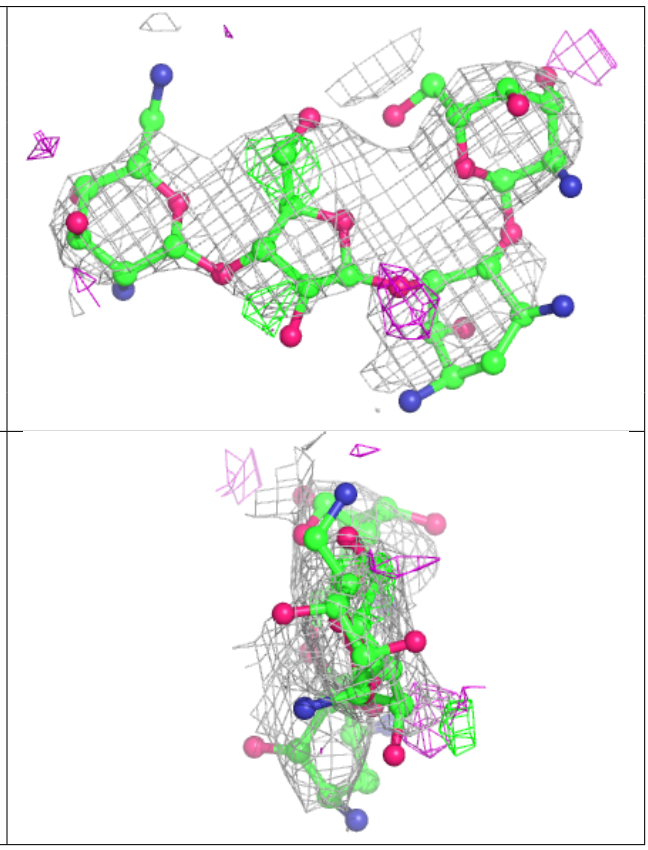
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
26	MG	T	201	1/1	0.98	0.18	33,33,33,33	0
26	MG	Y	101	1/1	0.98	0.20	74,74,74,74	0
26	MG	A	1809	1/1	0.98	0.11	28,28,28,28	0
26	MG	A	1690	1/1	0.99	0.07	0,0,0,0	0
26	MG	S	101	1/1	0.99	0.14	15,15,15,15	0
26	MG	A	1723	1/1	0.99	0.25	49,49,49,49	0
26	MG	A	1709	1/1	0.99	0.13	28,28,28,28	0
26	MG	A	1716	1/1	0.99	0.14	64,64,64,64	0
26	MG	A	1660	1/1	0.99	0.09	38,38,38,38	0
27	ZN	D	301	1/1	0.99	0.19	69,69,69,69	0
26	MG	A	1782	1/1	0.99	0.12	23,23,23,23	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.

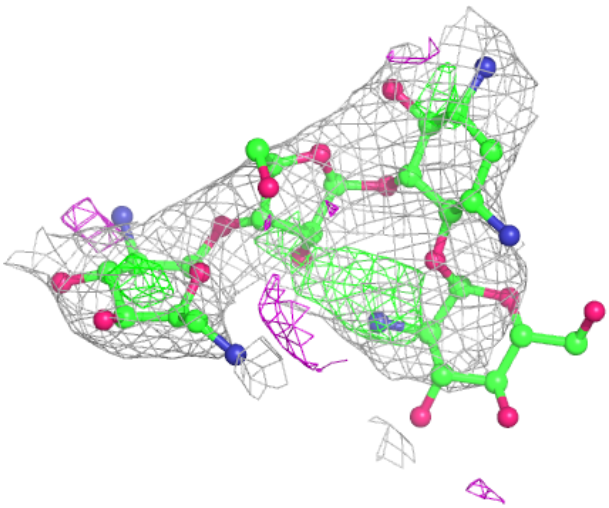
Electron density around PAR A 1605:

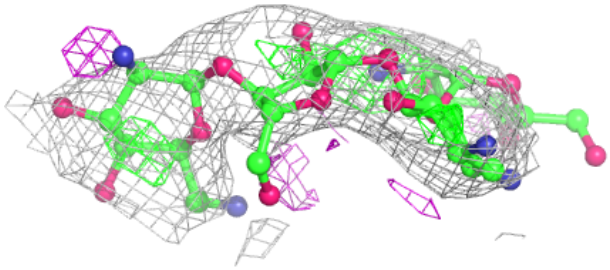
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

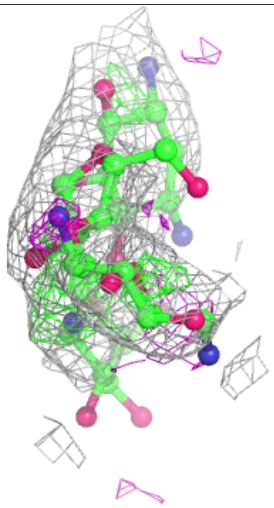


Electron density around PAR A 1602:

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

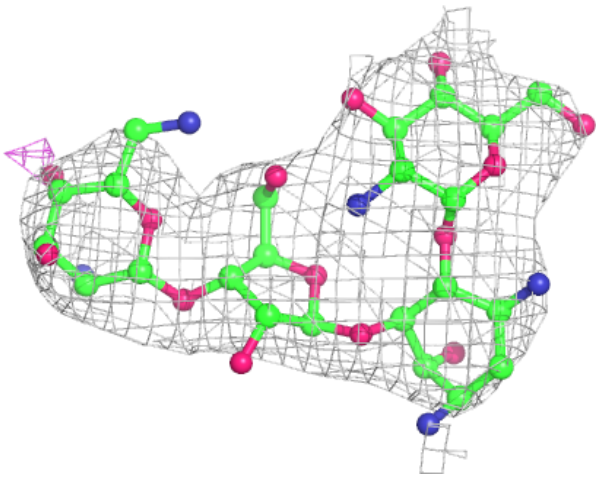


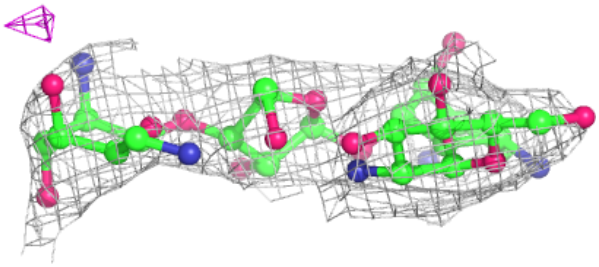


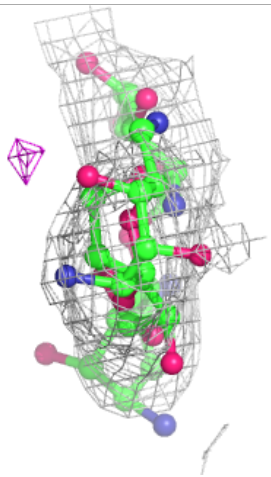


Electron density around PAR A 1604:

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

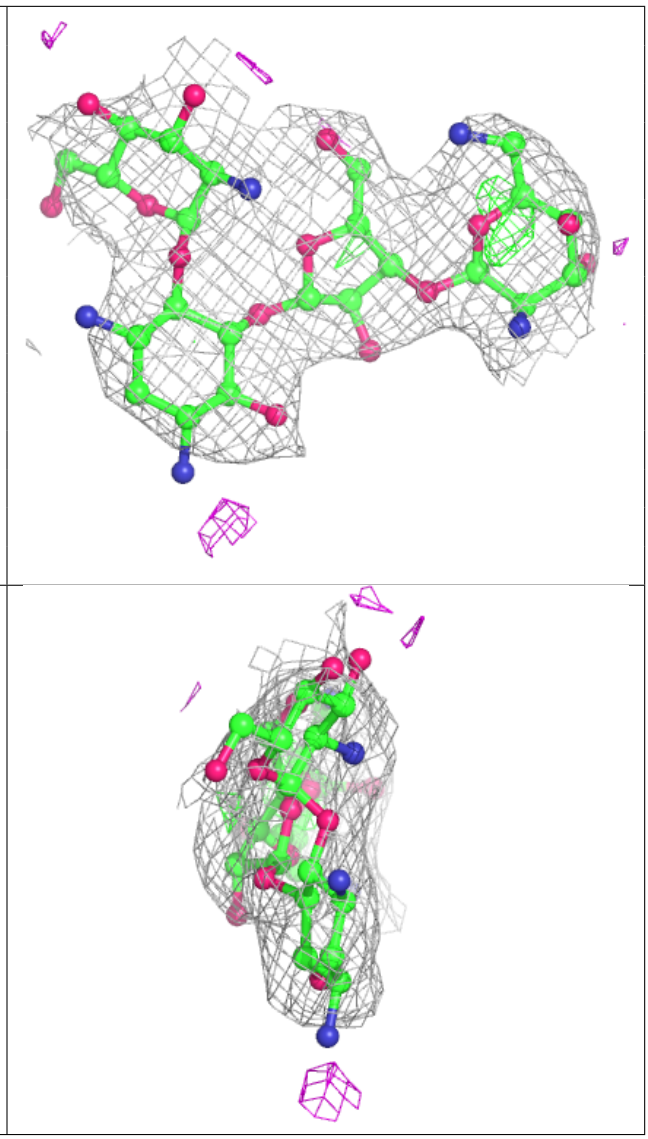






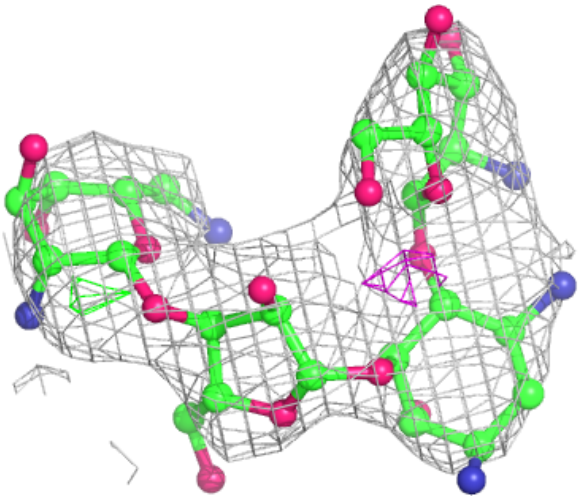
Electron density around PAR A 1601:

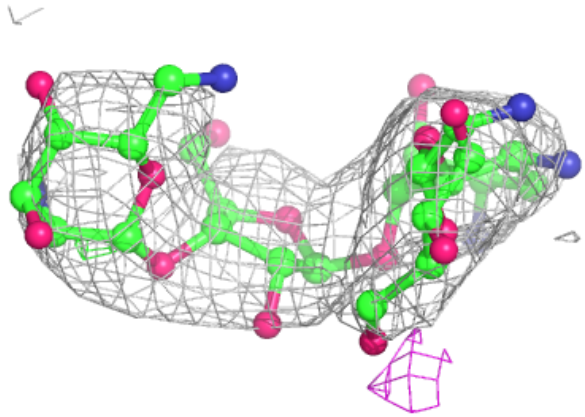
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

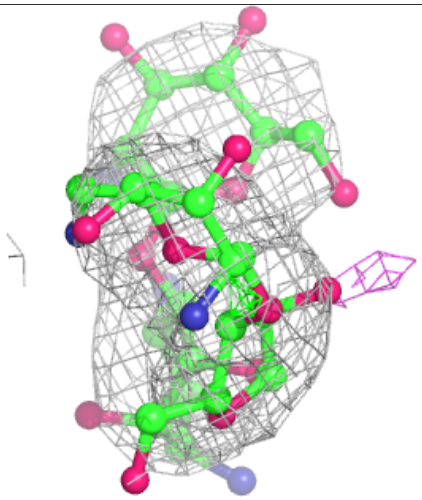


Electron density around PAR A 1606:

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

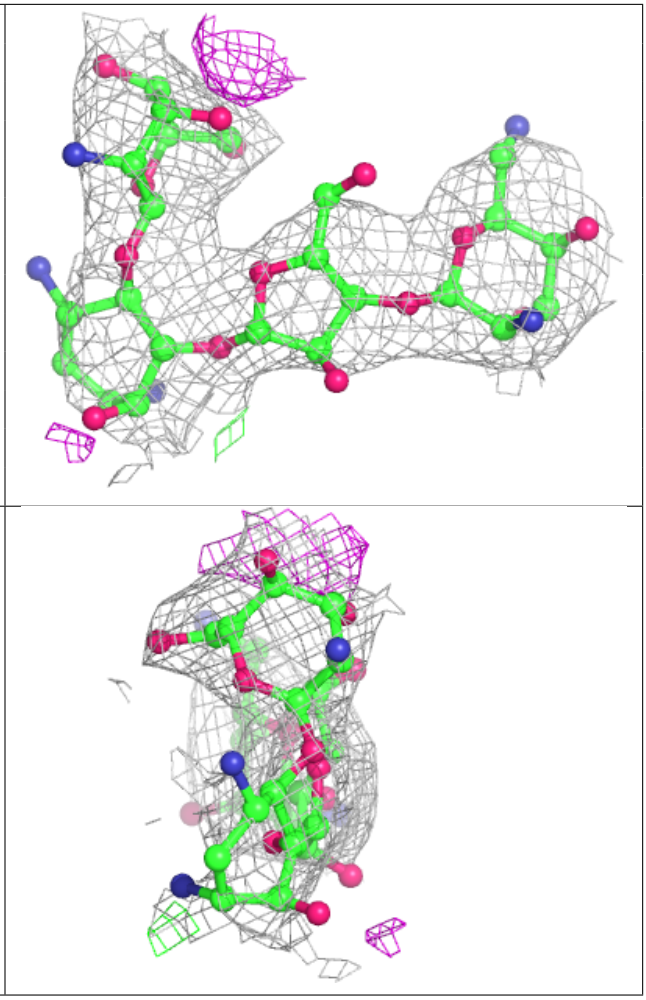






Electron density around PAR A 1603:

$2mF_o$-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.