



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 07:59 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 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 ⓘ 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)

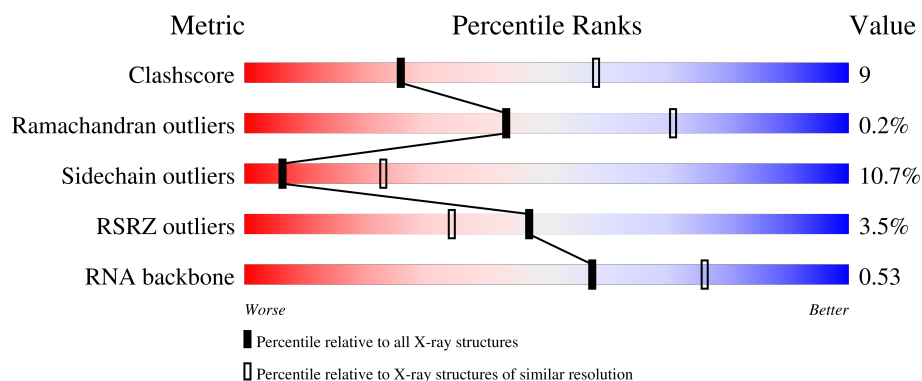
1 Overall quality at a glance

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	% 56% 35% 8%
2	B	256	5% 58% 31% 8%

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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			

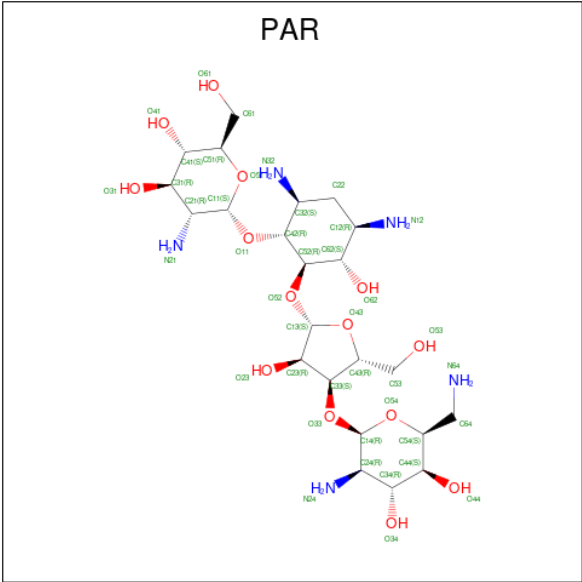
- Molecule 20 is a protein called 30S ribosomal protein S20.

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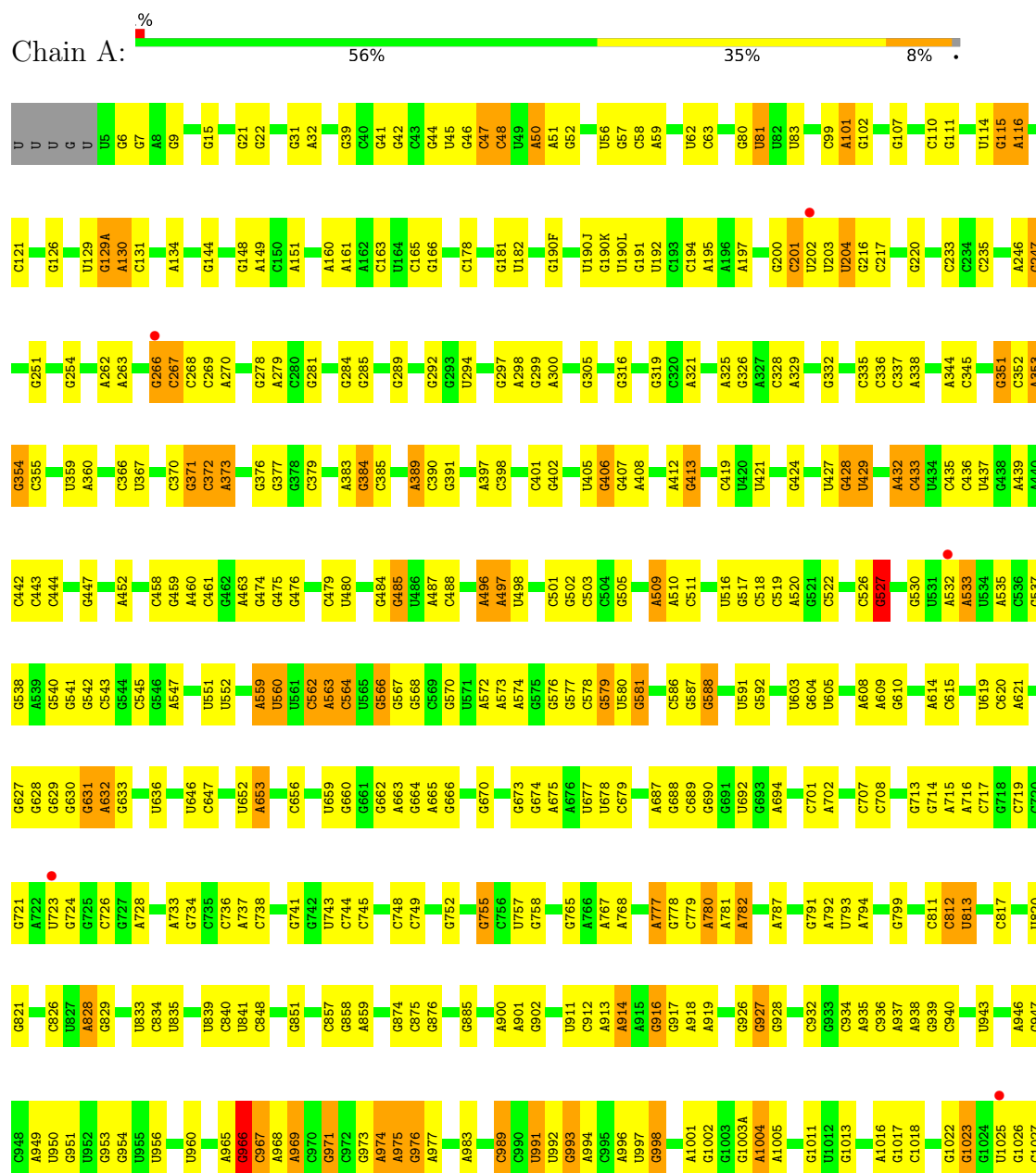
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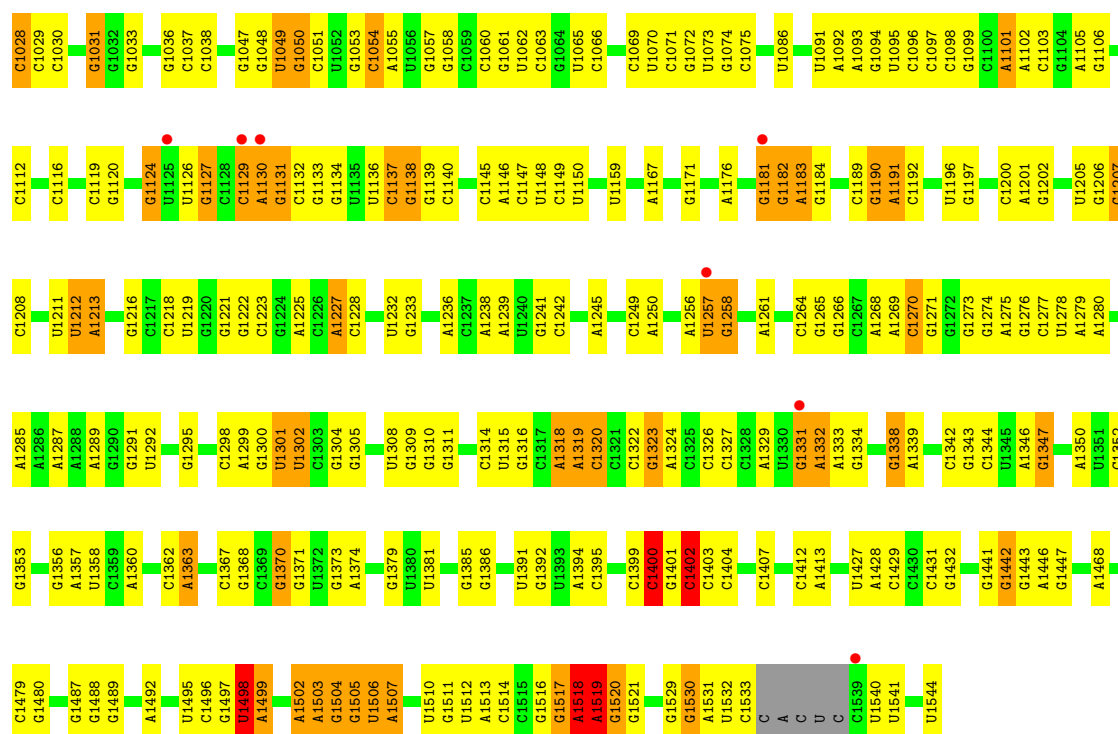
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	Q	1	Total	O	0	0
			1	1		
25	T	1	Total	O	0	0
			1	1		

3 Residue-property plots

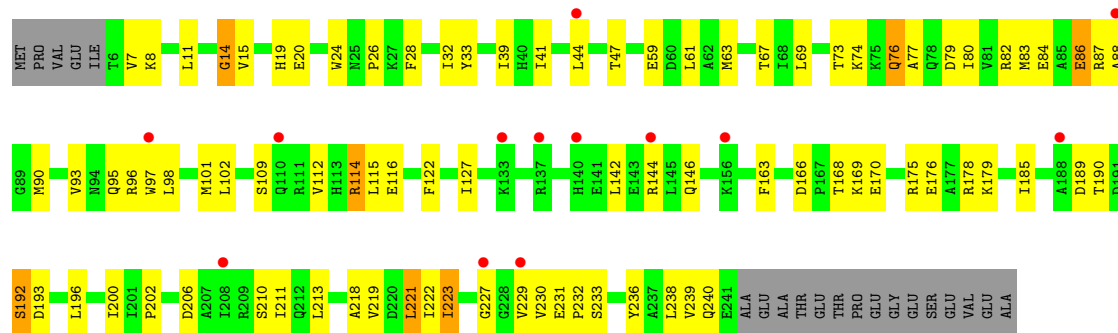
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

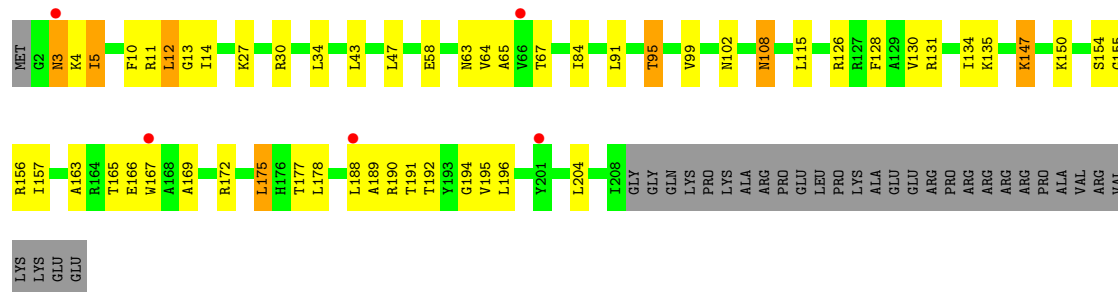




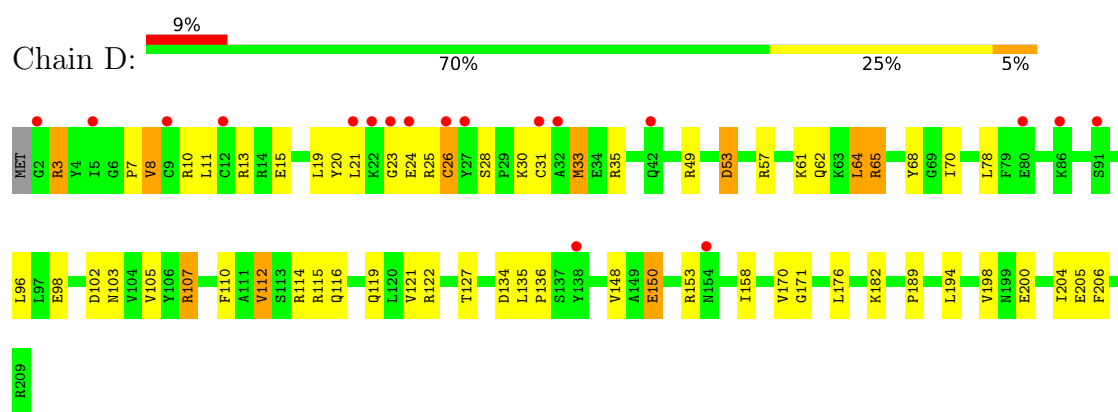
• Molecule 2: 30S ribosomal protein S2



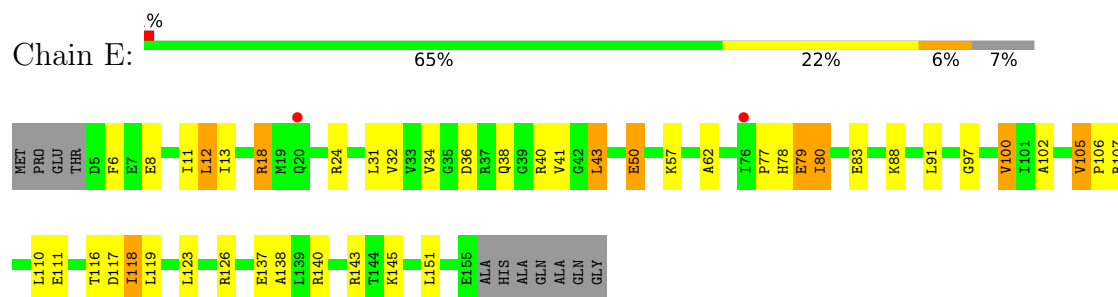
• Molecule 3: 30S ribosomal protein S3



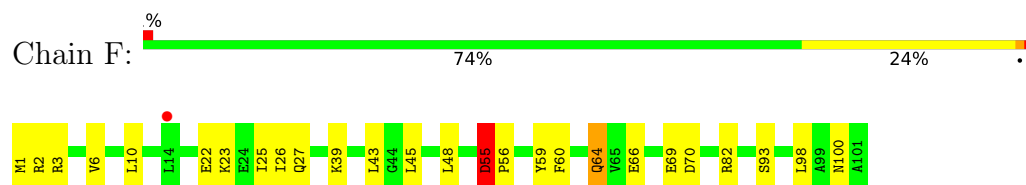
• Molecule 4: 30S ribosomal protein S4



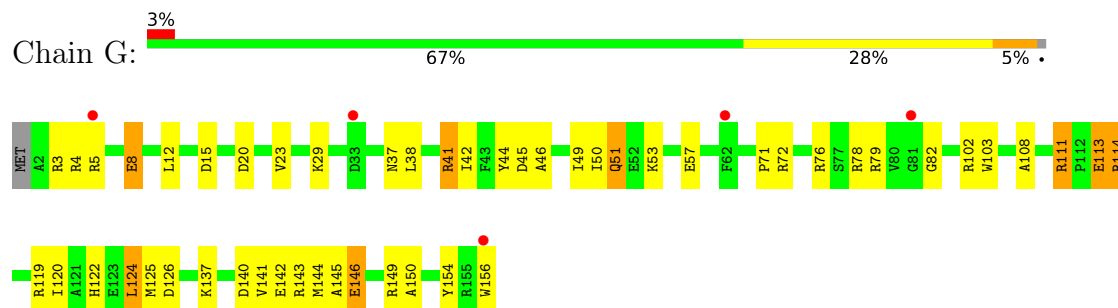
- Molecule 5: 30S ribosomal protein S5



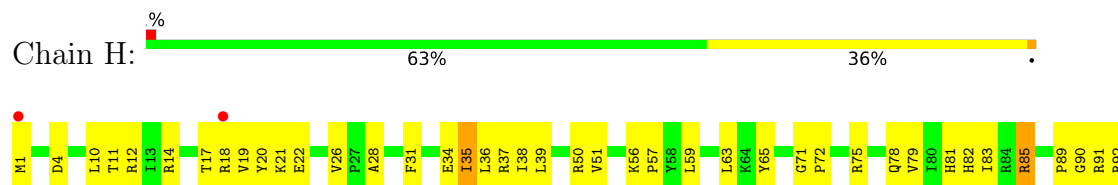
- Molecule 6: 30S ribosomal protein S6



- Molecule 7: 30S ribosomal protein S7

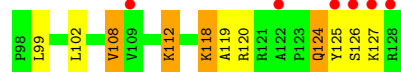


- Molecule 8: 30S ribosomal protein S8

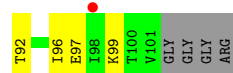
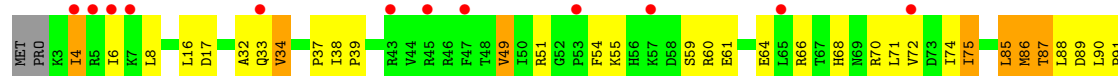




• Molecule 9: 30S ribosomal protein S9



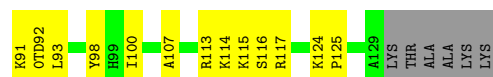
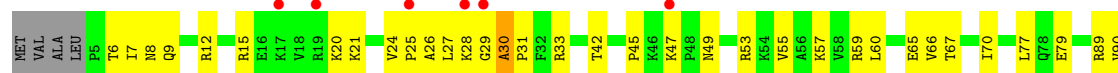
• Molecule 10: 30S ribosomal protein S10



• Molecule 11: 30S ribosomal protein S11

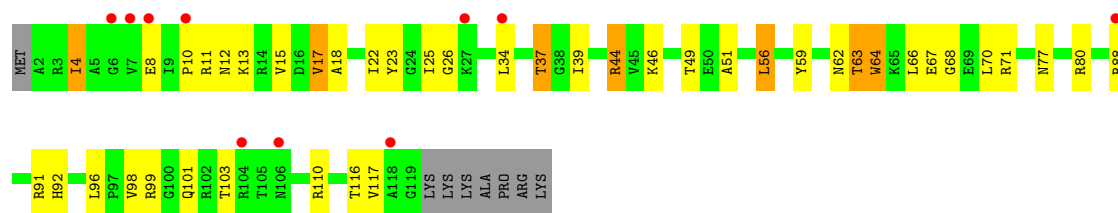


• Molecule 12: 30S ribosomal protein S12



• Molecule 13: 30S ribosomal protein S13





- Molecule 14: 30S ribosomal protein S14 type Z



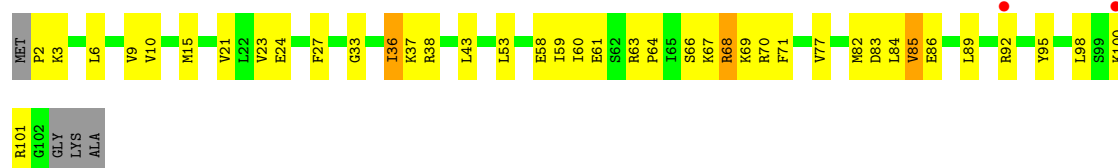
- Molecule 15: 30S ribosomal protein S15



- Molecule 16: 30S ribosomal protein S16



- Molecule 17: 30S ribosomal protein S17

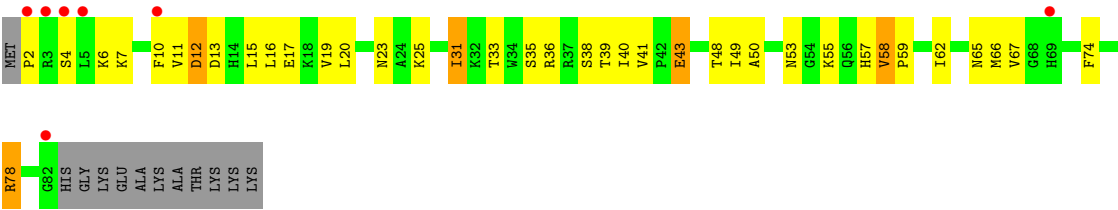


- Molecule 18: 30S ribosomal protein S18

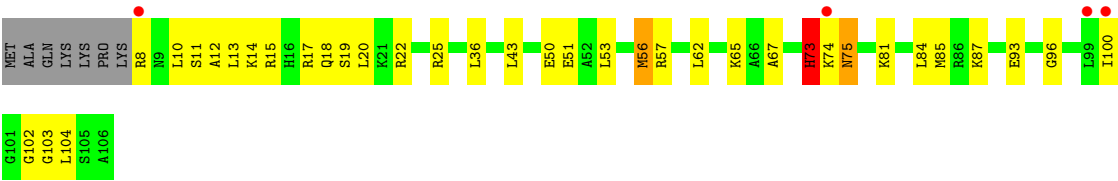


- Molecule 19: 30S ribosomal protein S19

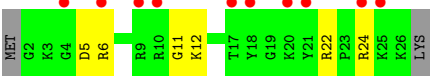




● Molecule 20: 30S ribosomal protein S20



● 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 i

5.1 Standard geometry i

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.

The worst 5 of 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

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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.

The worst 5 of 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

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	M	94/101 (93%)	83 (88%)	11 (12%)	5	20
14	N	48/50 (96%)	43 (90%)	5 (10%)	7	24
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

5 of 213 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	J	49	VAL
13	M	17	VAL
20	T	8	ARG
10	J	88	LEU
11	K	124	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
9	I	73	GLN
11	K	116	HIS
15	O	50	HIS
13	M	106	ASN
7	G	11	GLN

5.3.3 RNA ⓘ

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

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	44	G
1	A	47	C

5 of 29 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	701	C
1	A	1331	G
1	A	913	A
1	A	1212	U
1	A	812	C

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	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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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

The worst 5 of 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

The worst 5 of 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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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

There are no chirality outliers.

5 of 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

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

The worst 5 of 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

The worst 5 of 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

There are no chirality outliers.

5 of 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

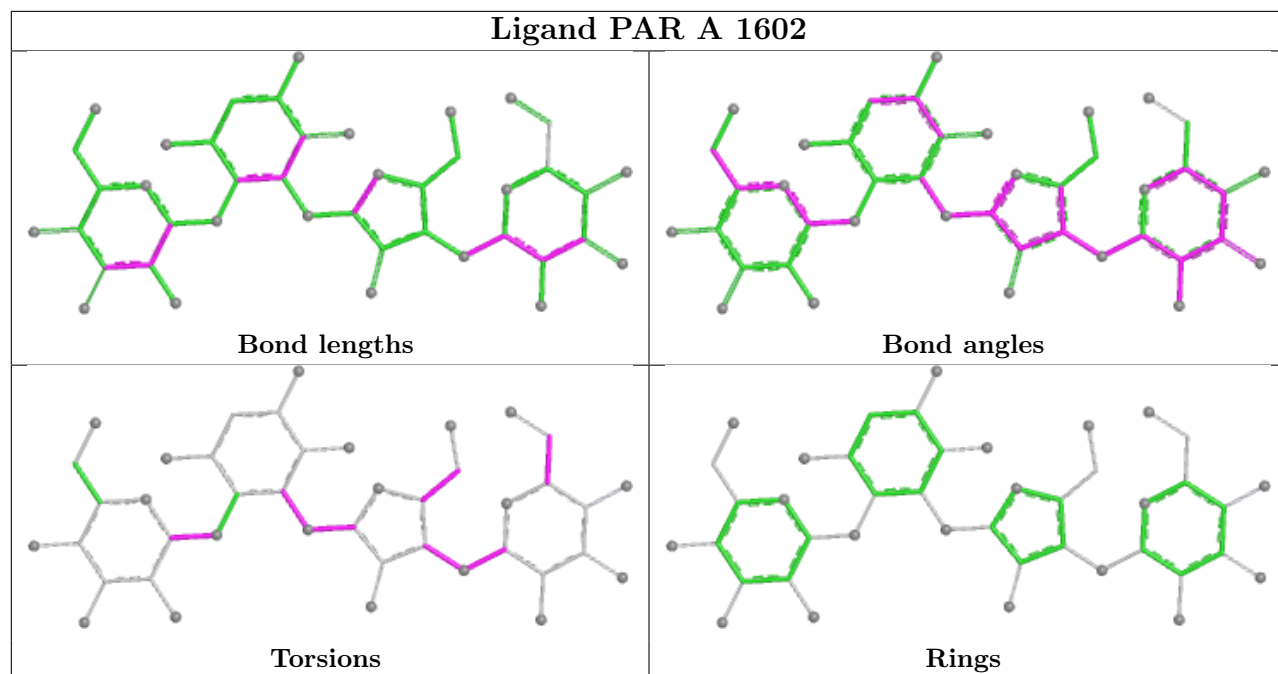
There are no ring outliers.

5 monomers are involved in 8 short contacts:

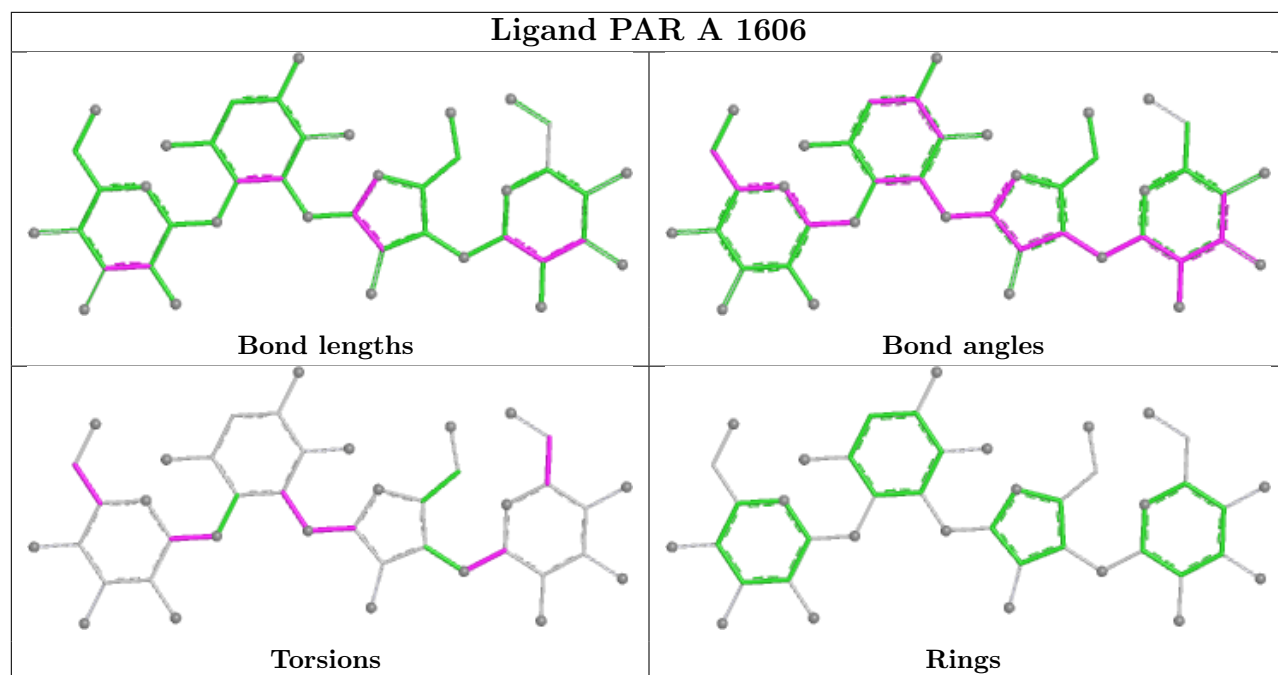
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	1602	PAR	1	0
22	A	1606	PAR	2	0
22	A	1603	PAR	3	0
22	A	1601	PAR	1	0
22	A	1604	PAR	1	0

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.

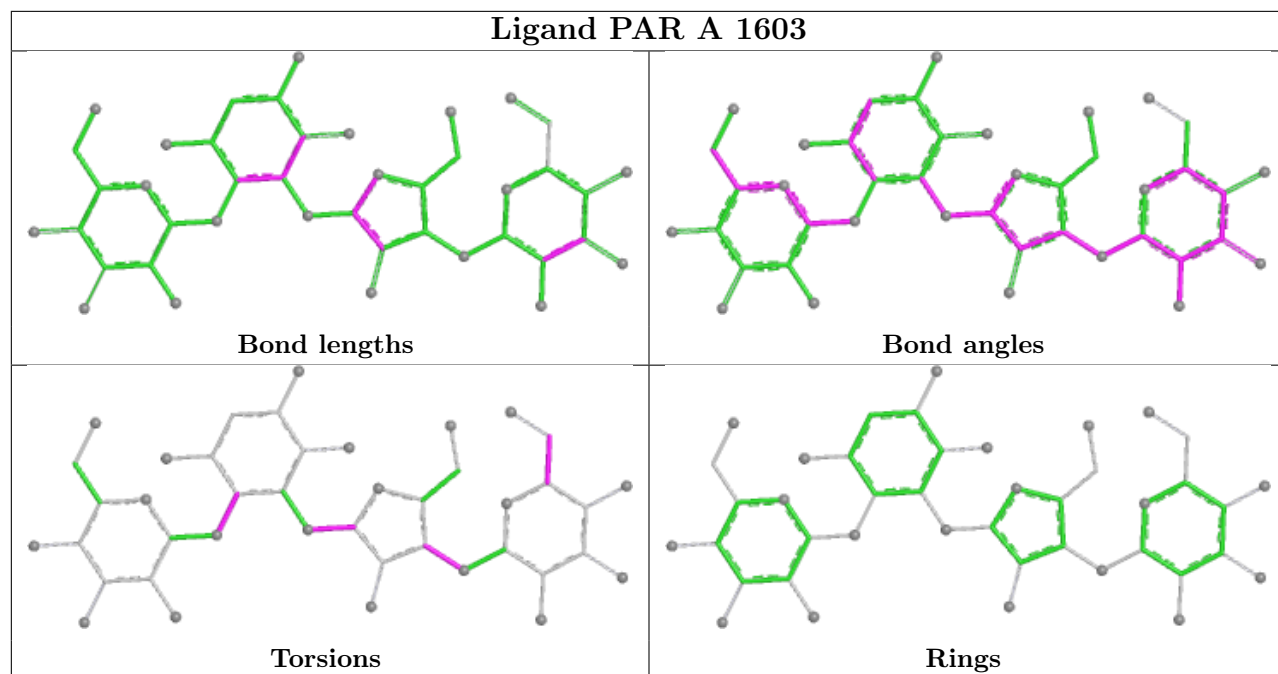
Ligand PAR A 1602



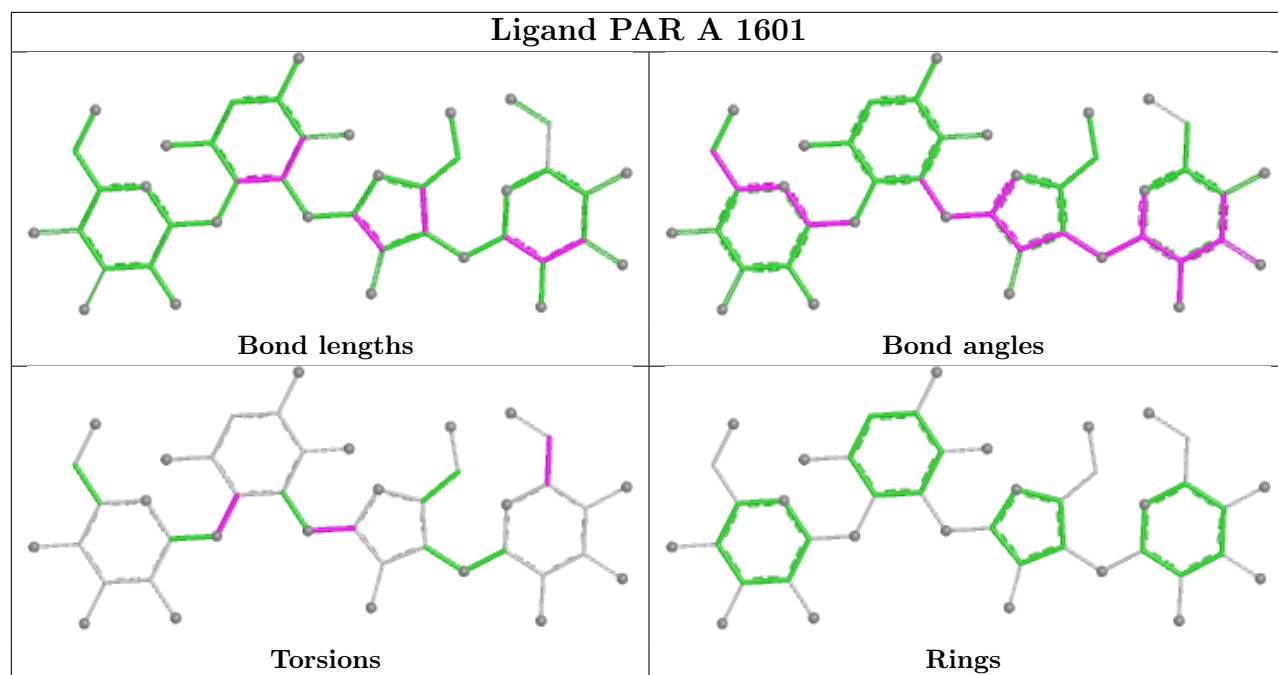
Ligand PAR A 1606

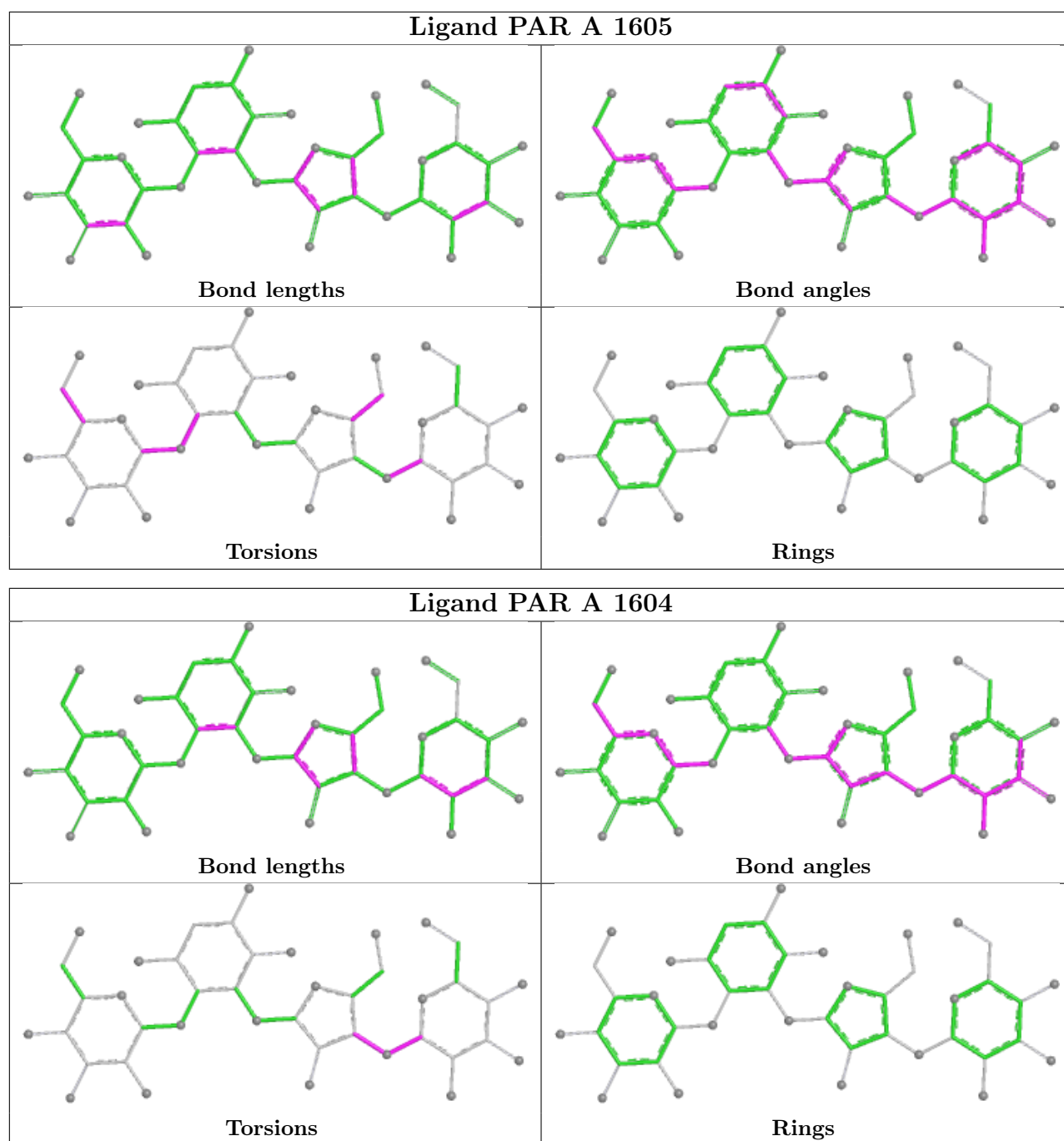


Ligand PAR A 1603



Ligand PAR A 1601





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%)	0.10	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

The worst 5 of 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

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 [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($\text{\AA}^2$)	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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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
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

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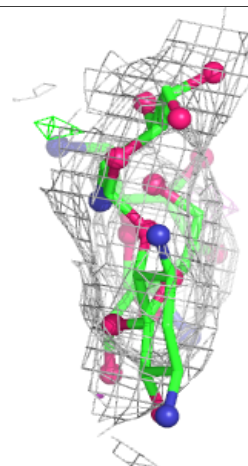
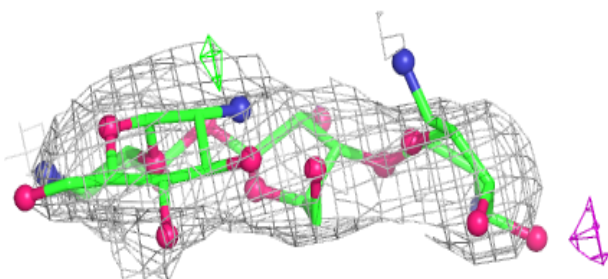
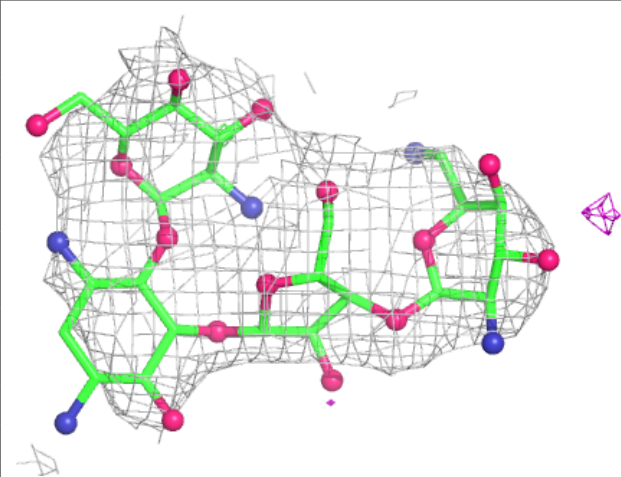
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	MG	A	1716	1/1	0.96	0.19	112,112,112,112	0
23	MG	A	1610	1/1	0.96	0.26	143,143,143,143	0
23	MG	A	1744	1/1	0.96	0.09	91,91,91,91	0
23	MG	A	1617	1/1	0.96	0.08	108,108,108,108	0
23	MG	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
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.

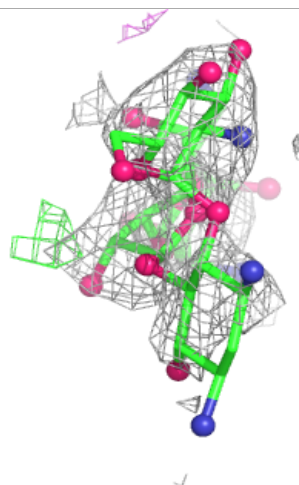
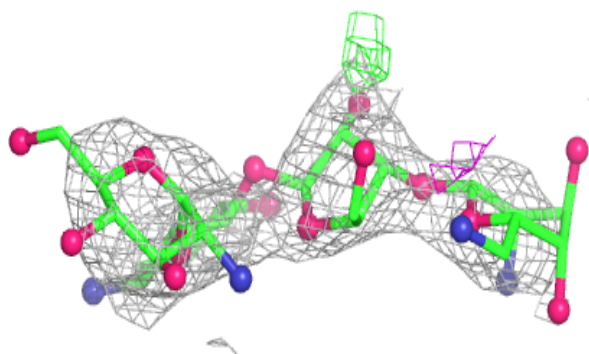
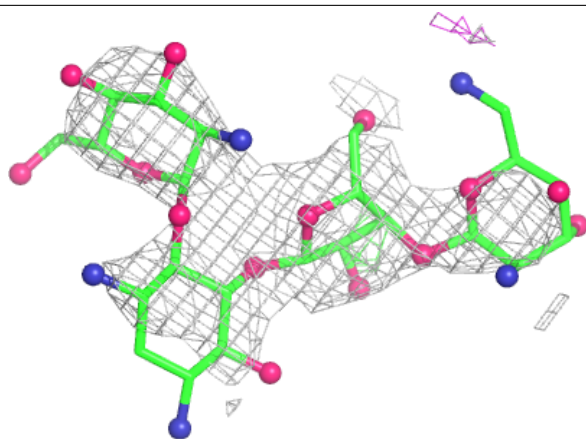
Electron density around PAR A 1604:

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



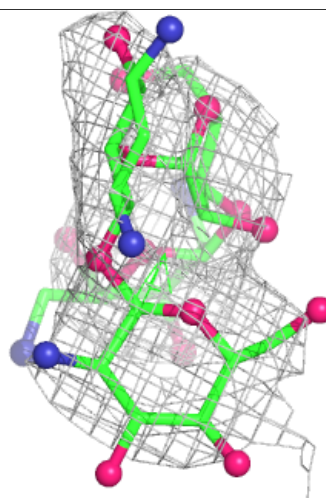
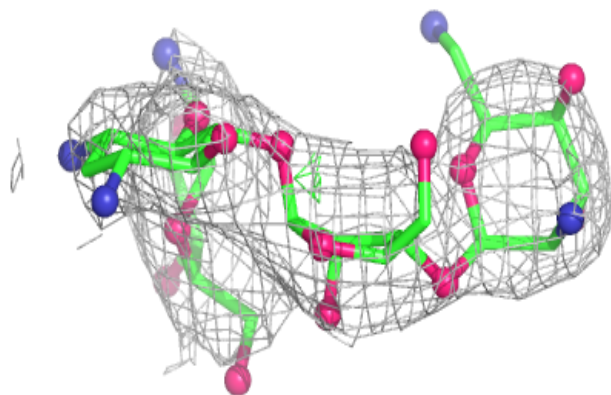
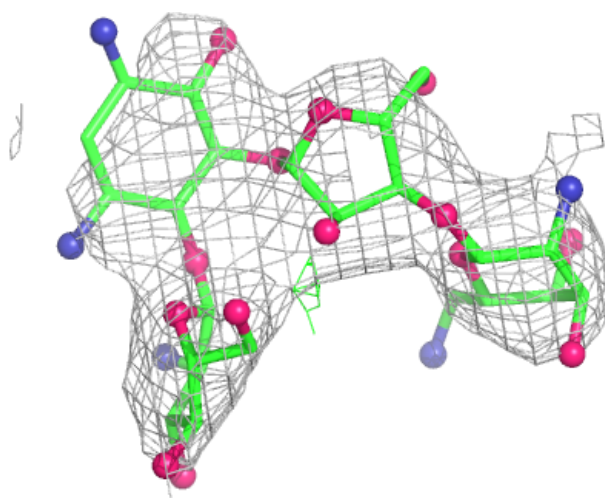
Electron density around PAR A 1605:

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



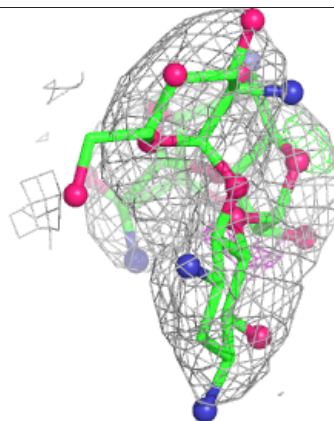
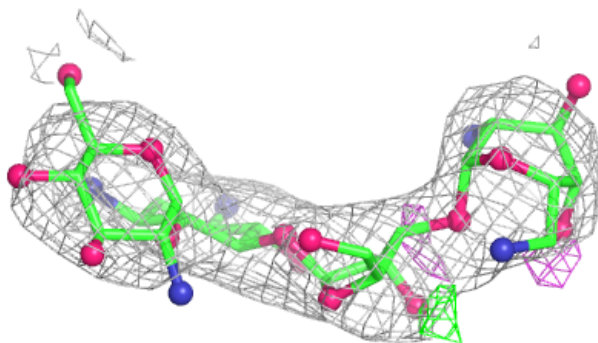
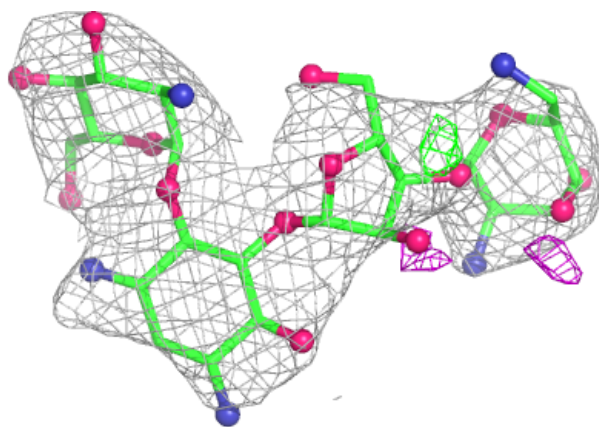
Electron density around PAR A 1606:

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



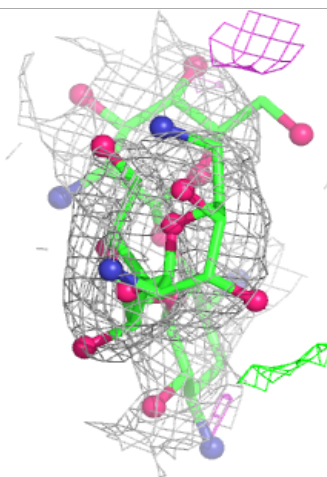
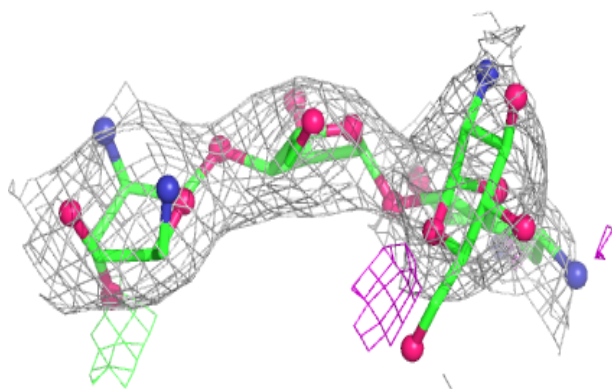
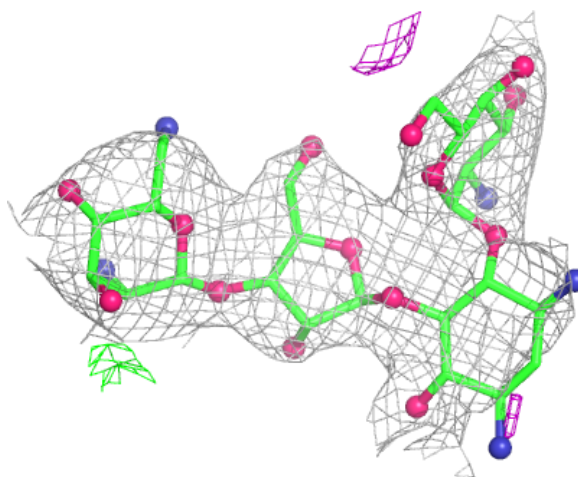
Electron density around PAR A 1602:

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



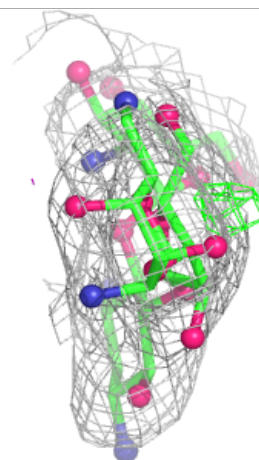
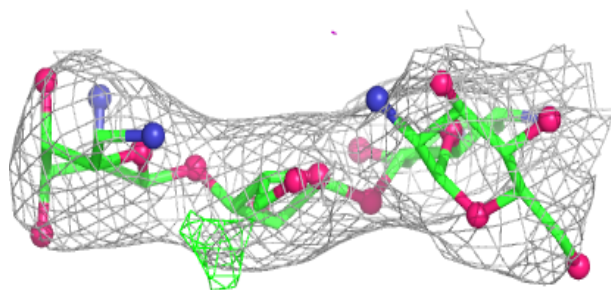
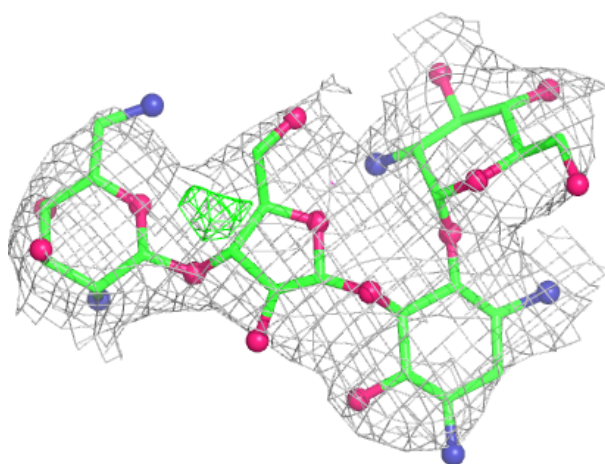
Electron density around PAR A 1603:

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



Electron density around PAR A 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.