



wwPDB X-ray Structure Validation Summary Report ⓘ

May 25, 2020 – 06:02 am BST

PDB ID : 5BR8
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 following versions of software and data (see [references](#) ①) were used in the production of this report:

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

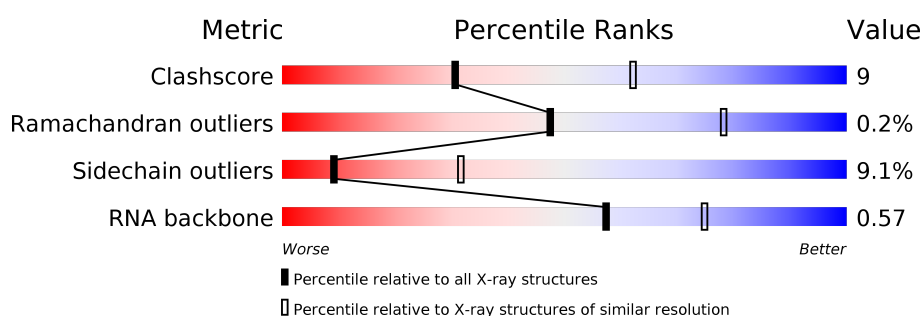
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RNA backbone	3102	1006 (3.84-2.96)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	1522	56% 35% 8% .
2	B	256	60% 29% . 8%
3	C	239	66% 19% . 13%
4	D	209	70% 26% .
5	E	162	67% 22% . . 7%
6	F	101	77% 21% .
7	G	156	68% 26% 6% .

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Mol	Chain	Length	Quality of chain
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	

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			

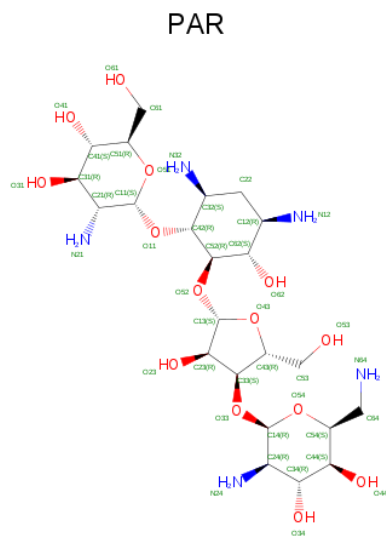
- Molecule 20 is a protein called 30S ribosomal protein S20.

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 (three-letter code: PAR) (formula: C₂₃H₄₅N₅O₁₄).

[illegible]

- Molecule 23 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	P	1	Total 1	Mg 1	0	0
23	G	1	Total 1	Mg 1	0	0
23	J	1	Total 1	Mg 1	0	0
23	Q	1	Total 1	Mg 1	0	0
23	D	1	Total 1	Mg 1	0	0
23	E	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	H	1	Total 1	Mg 1	0	0
23	B	1	Total 1	Mg 1	0	0
23	I	1	Total 1	Mg 1	0	0
23	A	273	Total 273	Mg 273	0	0
23	T	1	Total 1	Mg 1	0	0
23	L	1	Total 1	Mg 1	0	0
23	S	3	Total 3	Mg 3	0	0

- Molecule 24 is ZINC ION (three-letter code: 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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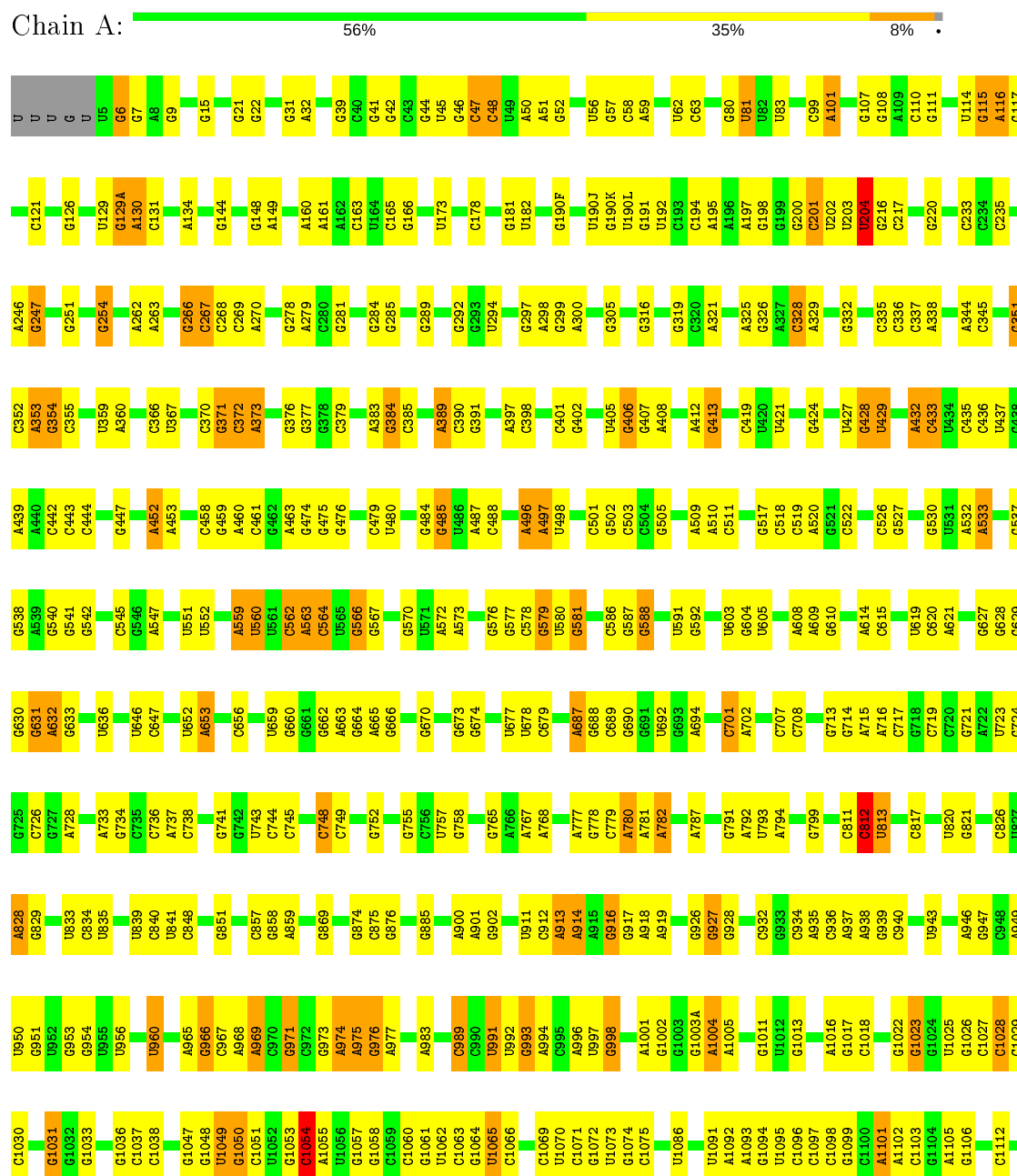
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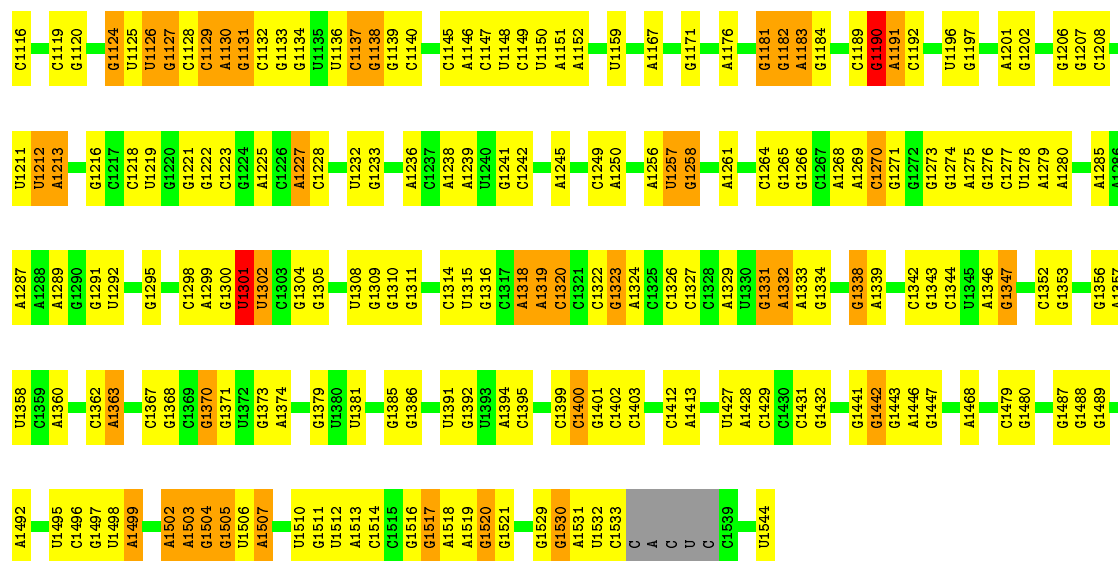
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	Q	1	Total	O	0	0
			1	1		
25	T	1	Total	O	0	0
			1	1		

3 Residue-property plots

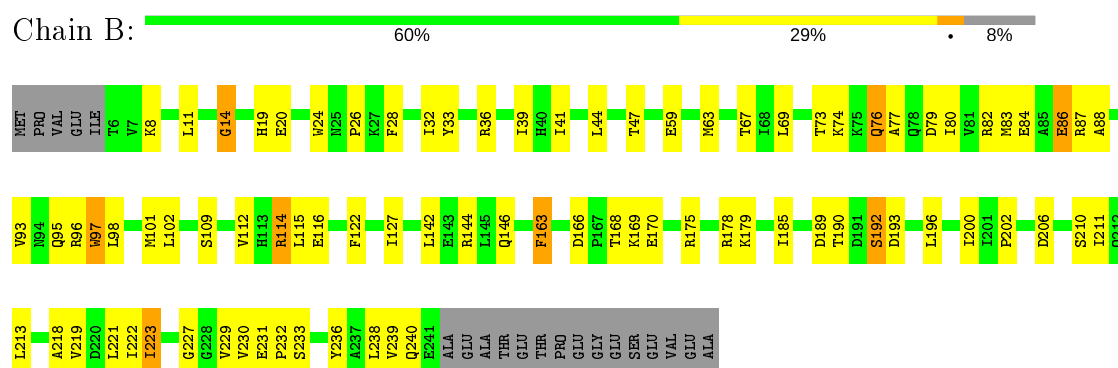
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

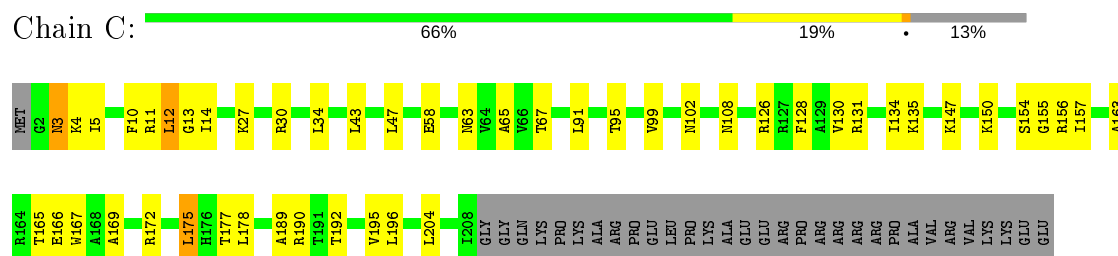




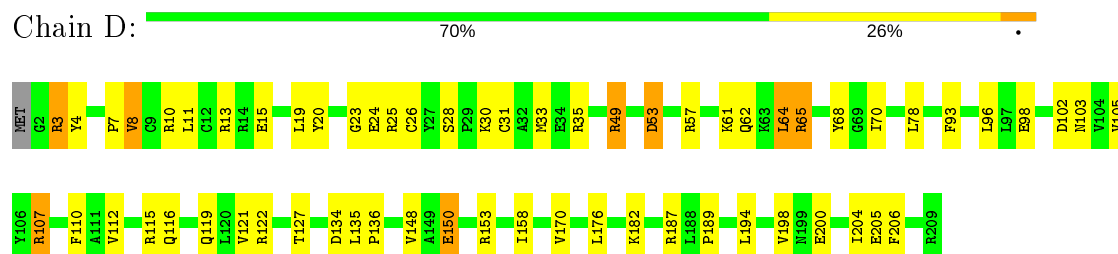
- Molecule 2: 30S ribosomal protein S2



- Molecule 3: 30S ribosomal protein S3

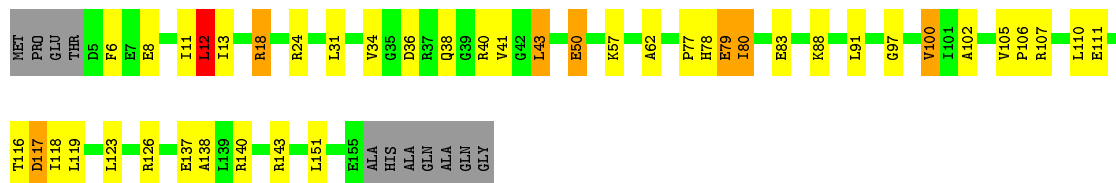


- Molecule 4: 30S ribosomal protein S4




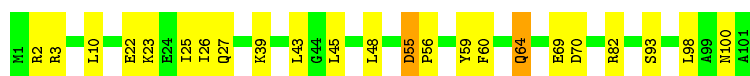
- Molecule 5: 30S ribosomal protein S5

Chain E:  67% 22% 7%



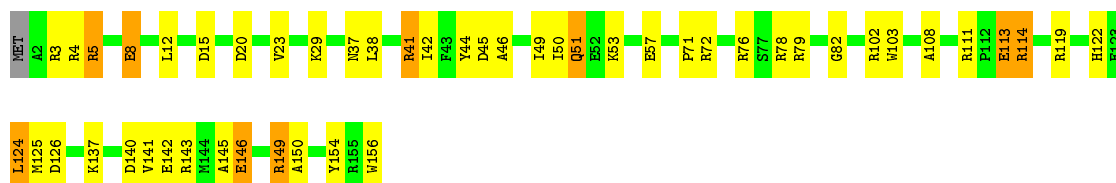
- Molecule 6: 30S ribosomal protein S6

Chain F:  77% 21% 2%

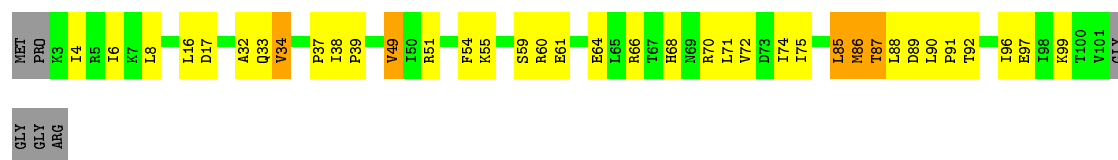


- Molecule 7: 30S ribosomal protein S7

Chain G:  68% 26% 6%

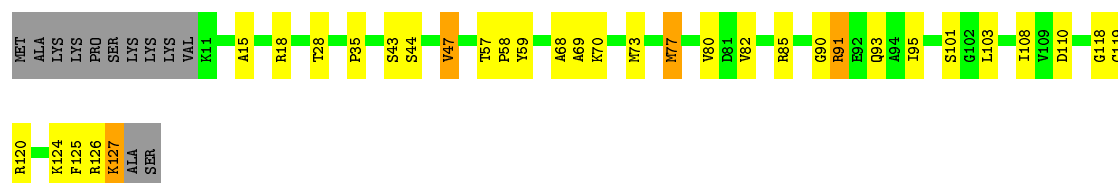


Chain J: 



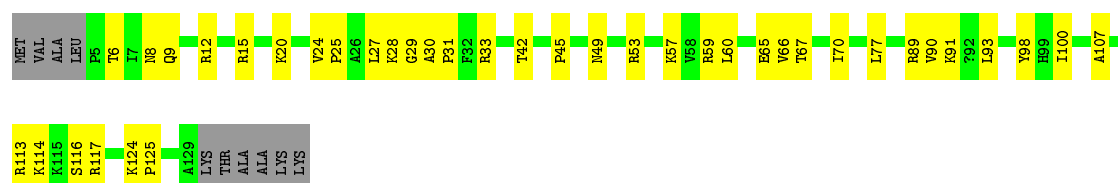
- Molecule 11: 30S ribosomal protein S11

Chain K: 



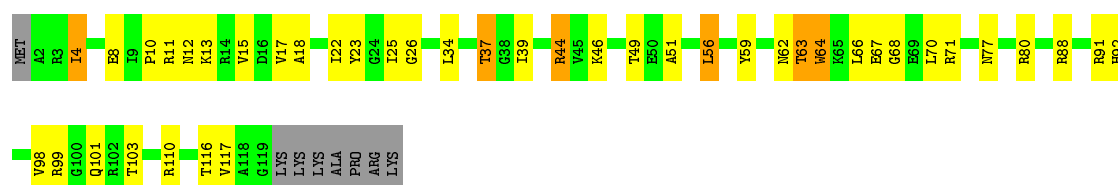
- Molecule 12: 30S ribosomal protein S12

Chain L: 



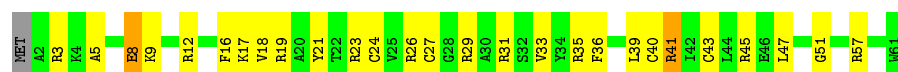
- Molecule 13: 30S ribosomal protein S13

Chain M: 



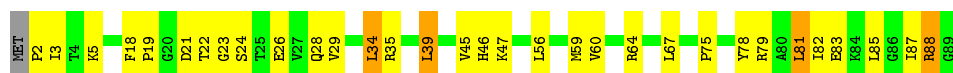
- Molecule 14: 30S ribosomal protein S14 type Z

Chain N: 



- Molecule 15: 30S ribosomal protein S15

Chain O: 



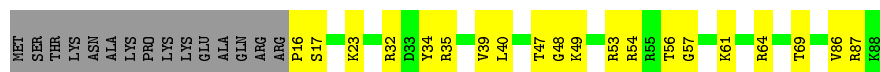
- Molecule 16: 30S ribosomal protein S16



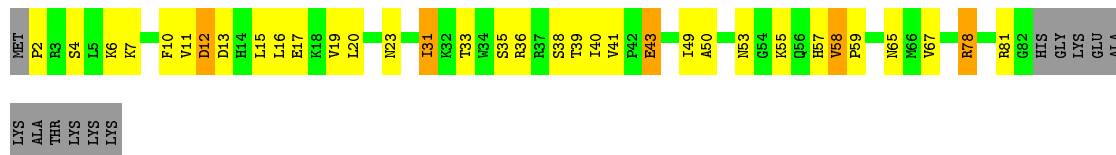
- Molecule 17: 30S ribosomal protein S17



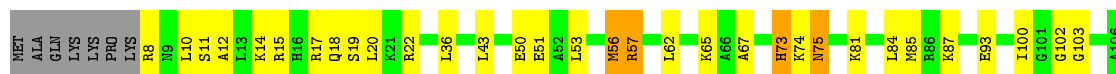
- Molecule 18: 30S ribosomal protein S18



- 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	401.30 Å 401.30 Å 176.40 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	52.84 – 3.40 52.83 – 2.97	Depositor EDS
% Data completeness (in resolution range)	100.0 (52.84-3.40) 78.1 (52.83-2.97)	Depositor EDS
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 2.96 Å)	Xtriage
Refinement program	PHENIX dev_1938	Depositor
R, R_{free}	0.193 , 0.234 0.193 , (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)	0.26 , 78.8	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	0.91	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: ZN, MA6, G7M, MG, 0TD, PAR, 2MG, 5MC, UR3, 4OC, M2G, PSU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.38	0/36037	0.87	28/56239 (0.0%)
2	B	0.28	0/1931	0.48	0/2607
3	C	0.29	0/1637	0.47	0/2207
4	D	0.30	0/1733	0.48	0/2318
5	E	0.35	0/1163	0.56	1/1566 (0.1%)
6	F	0.28	0/856	0.46	0/1154
7	G	0.30	0/1276	0.46	0/1709
8	H	0.32	0/1136	0.50	0/1527
9	I	0.30	0/1029	0.52	0/1379
10	J	0.30	0/806	0.52	0/1084
11	K	0.31	0/888	0.54	0/1198
12	L	0.33	0/978	0.54	0/1308
13	M	0.28	0/947	0.46	0/1270
14	N	0.31	0/500	0.48	0/663
15	O	0.30	0/745	0.47	0/992
16	P	0.32	0/717	0.51	0/965
17	Q	0.33	0/851	0.54	0/1136
18	R	0.30	0/604	0.46	0/801
19	S	0.26	0/662	0.53	0/892
20	T	0.32	0/765	0.55	0/1007
21	U	0.24	0/213	0.44	0/279
All	All	0.36	0/55474	0.77	29/82301 (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 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	204	U	C2-N1-C1'	8.33	127.70	117.70
1	A	328	C	C2-N1-C1'	6.69	126.16	118.80
1	A	204	U	N1-C2-O2	6.51	127.36	122.80
1	A	254	G	O5'-P-OP1	-6.43	99.91	105.70
1	A	204	U	N3-C2-O2	-6.37	117.74	122.20

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 [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	420	0
2	B	1896	0	1936	47	0
3	C	1613	0	1677	36	0
4	D	1703	0	1763	45	0
5	E	1147	0	1207	31	0
6	F	843	0	857	13	0
7	G	1257	0	1296	36	0
8	H	1116	0	1177	26	0
9	I	1010	0	1037	28	0
10	J	793	0	835	24	0
11	K	873	0	894	20	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	27	0
14	N	491	0	524	21	0
15	O	734	0	771	23	0
16	P	701	0	720	12	0
17	Q	838	0	909	24	0
18	R	598	0	670	14	0
19	S	648	0	672	23	0
20	T	763	0	861	21	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	808	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 808 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
1:A:1502:A:H2	1:A:1505:G:H1	1.28	0.81
20:T:56:MET:HE1	20:T:85:MET:HA	1.63	0.79
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%)	34	67
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%)	19	51
10	J	97/105 (92%)	81 (84%)	15 (16%)	1 (1%)	15	46
11	K	115/129 (89%)	107 (93%)	8 (7%)	0	100	100
12	L	122/135 (90%)	113 (93%)	8 (7%)	1 (1%)	19	51
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%)	12	39
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%)	47	78

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%)	180 (90%)	21 (10%)	7	25
3	C	160/188 (85%)	146 (91%)	14 (9%)	10	33
4	D	180/181 (99%)	162 (90%)	18 (10%)	7	27
5	E	115/123 (94%)	104 (90%)	11 (10%)	8	29
6	F	90/90 (100%)	84 (93%)	6 (7%)	16	46
7	G	126/127 (99%)	113 (90%)	13 (10%)	7	26
8	H	119/119 (100%)	112 (94%)	7 (6%)	19	49
9	I	98/99 (99%)	88 (90%)	10 (10%)	7	26
10	J	87/92 (95%)	82 (94%)	5 (6%)	20	50
11	K	89/99 (90%)	81 (91%)	8 (9%)	9	32
12	L	103/110 (94%)	98 (95%)	5 (5%)	25	55

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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%)	42 (88%)	6 (12%)	4	17
15	O	79/80 (99%)	75 (95%)	4 (5%)	24	54
16	P	72/74 (97%)	64 (89%)	8 (11%)	6	22
17	Q	95/97 (98%)	86 (90%)	9 (10%)	8	29
18	R	64/77 (83%)	63 (98%)	1 (2%)	62	81
19	S	71/80 (89%)	60 (84%)	11 (16%)	2	11
20	T	76/82 (93%)	63 (83%)	13 (17%)	2	8
21	U	19/22 (86%)	19 (100%)	0	100	100
All	All	1986/2111 (94%)	1805 (91%)	181 (9%)	9	32

5 of 181 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	G	149	ARG
10	J	85	LEU
19	S	81	ARG
8	H	26	VAL
9	I	64	THR

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

Mol	Chain	Res	Type
9	I	3	GLN
9	I	73	GLN
13	M	106	ASN
15	O	46	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1507/1522 (99%)	226 (14%)	29 (1%)

5 of 226 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	9	G

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Mol	Chain	Res	Type
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	687	A
1	A	812	C
1	A	1301	U
1	A	701	C
1	A	913	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	5MC	A	1404	1	15,22,23	0.80	0	19,32,35	1.22	3 (15%)
1	5MC	A	1407	1	15,22,23	0.87	0	19,32,35	1.11	2 (10%)
1	G7M	A	527	1	20,26,27	1.78	3 (15%)	20,39,42	1.91	6 (30%)
1	4OC	A	1402	1	16,23,24	1.00	2 (12%)	17,32,35	0.82	0
1	MA6	A	1519	1	19,26,27	1.11	2 (10%)	18,38,41	0.77	0
1	UR3	A	1498	1,23	14,22,23	0.88	1 (7%)	15,32,35	1.16	1 (6%)
1	MA6	A	1518	1	19,26,27	1.14	1 (5%)	18,38,41	0.79	0
1	PSU	A	516	1,23	17,21,22	1.07	1 (5%)	20,30,33	3.33	5 (25%)
1	M2G	A	966	1	20,27,28	1.73	4 (20%)	22,40,43	2.54	4 (18%)
1	2MG	A	1207	1	19,26,27	2.25	4 (21%)	21,38,41	2.03	3 (14%)
1	5MC	A	967	1	15,22,23	0.89	0	19,32,35	1.06	1 (5%)
12	0TD	L	92	12	4,9,10	1.17	0	3,11,13	3.17	1 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	A	1540	1	17,21,22	1.00	1 (5%)	20,30,33	3.13	6 (30%)
1	PSU	A	1541	1,23	17,21,22	1.08	2 (11%)	20,30,33	3.21	6 (30%)
1	5MC	A	1400	1	15,22,23	0.91	0	19,32,35	0.99	1 (5%)

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

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

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1207	2MG	C2-N2	7.18	1.40	1.34
1	A	1207	2MG	C6-N1	5.58	1.42	1.33
1	A	966	M2G	C6-N1	5.08	1.41	1.33
1	A	527	G7M	C2-N2	4.99	1.43	1.33
1	A	527	G7M	C4-N3	3.86	1.41	1.35

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	516	PSU	N1-C2-N3	-11.54	119.26	128.43
1	A	1541	PSU	N1-C2-N3	-10.91	119.76	128.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1540	PSU	N1-C2-N3	-10.52	120.07	128.43
1	A	966	M2G	C5-C6-N1	-8.25	112.14	123.43
1	A	1207	2MG	C5-C6-N1	-7.44	113.26	123.43

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	527	G7M	O4'-C4'-C5'-O5'
1	A	527	G7M	C3'-C4'-C5'-O5'
1	A	1402	4OC	N3-C4-N4-CM4
1	A	1402	4OC	C5-C4-N4-CM4
1	A	966	M2G	N1-C2-N2-CM1

There are no ring outliers.

8 monomers are involved in 13 short contacts:

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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	-	45,45,45	1.49	9 (20%)	64,67,67	1.66	12 (18%)
22	PAR	A	1603	-	45,45,45	1.49	6 (13%)	64,67,67	1.65	12 (18%)
22	PAR	A	1604	-	45,45,45	1.39	6 (13%)	64,67,67	1.62	11 (17%)
22	PAR	A	1605	-	45,45,45	1.28	7 (15%)	64,67,67	1.62	12 (18%)
22	PAR	A	1601	-	45,45,45	1.18	7 (15%)	64,67,67	1.54	12 (18%)
22	PAR	A	1606	-	45,45,45	1.42	7 (15%)	64,67,67	1.63	12 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	PAR	A	1602	-	-	9/18/94/94	0/4/4/4
22	PAR	A	1603	-	-	7/18/94/94	0/4/4/4
22	PAR	A	1604	-	-	2/18/94/94	0/4/4/4
22	PAR	A	1605	-	-	6/18/94/94	0/4/4/4
22	PAR	A	1601	-	-	4/18/94/94	0/4/4/4
22	PAR	A	1606	-	-	11/18/94/94	0/4/4/4

The worst 5 of 42 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	1603	PAR	C52-C42	4.77	1.62	1.52
22	A	1604	PAR	C13-C23	4.04	1.58	1.52
22	A	1602	PAR	O43-C13	3.62	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 71 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1602	PAR	O33-C14-C24	6.87	120.05	108.22
22	A	1606	PAR	O33-C14-C24	6.22	118.93	108.22
22	A	1604	PAR	O33-C14-C24	6.15	118.82	108.22
22	A	1603	PAR	O33-C14-C24	5.96	118.48	108.22
22	A	1605	PAR	O33-C14-C24	5.69	118.02	108.22

There are no chirality outliers.

5 of 39 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A	1605	PAR	O43-C43-C53-O53
22	A	1603	PAR	C23-C13-O52-C52
22	A	1603	PAR	C44-C54-C64-N64
22	A	1606	PAR	C23-C13-O52-C52
22	A	1606	PAR	O54-C14-O33-C33

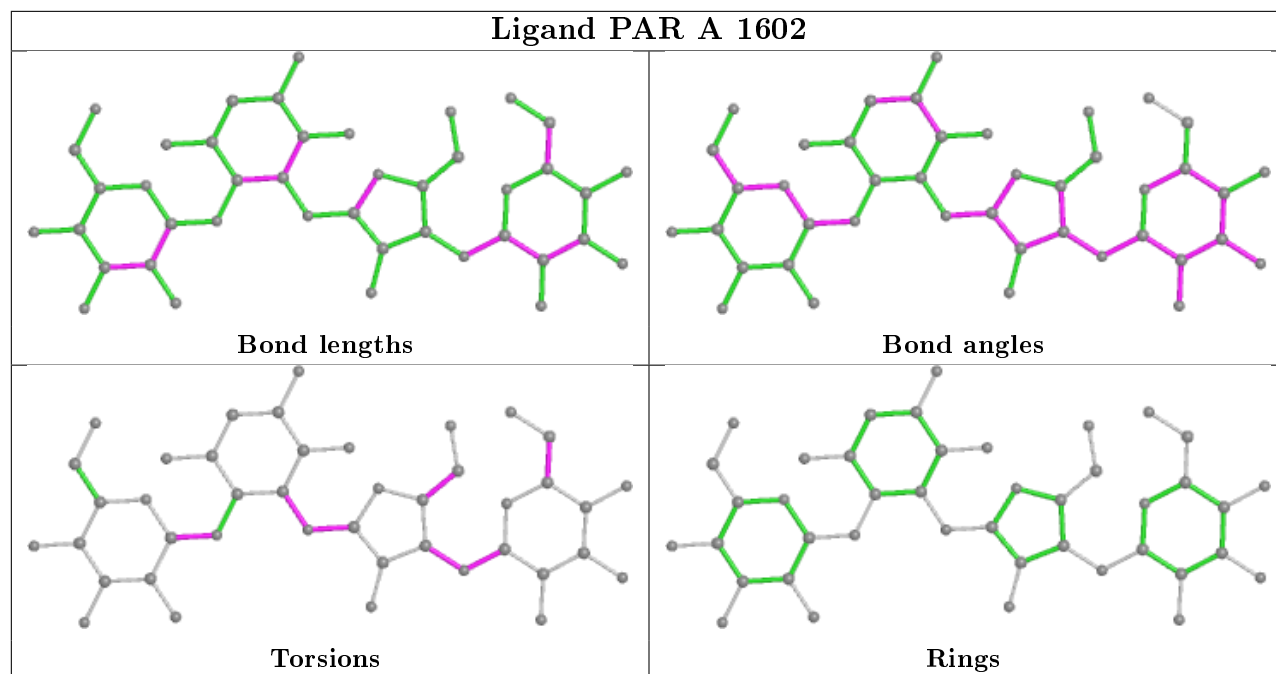
There are no ring outliers.

5 monomers are involved in 8 short contacts:

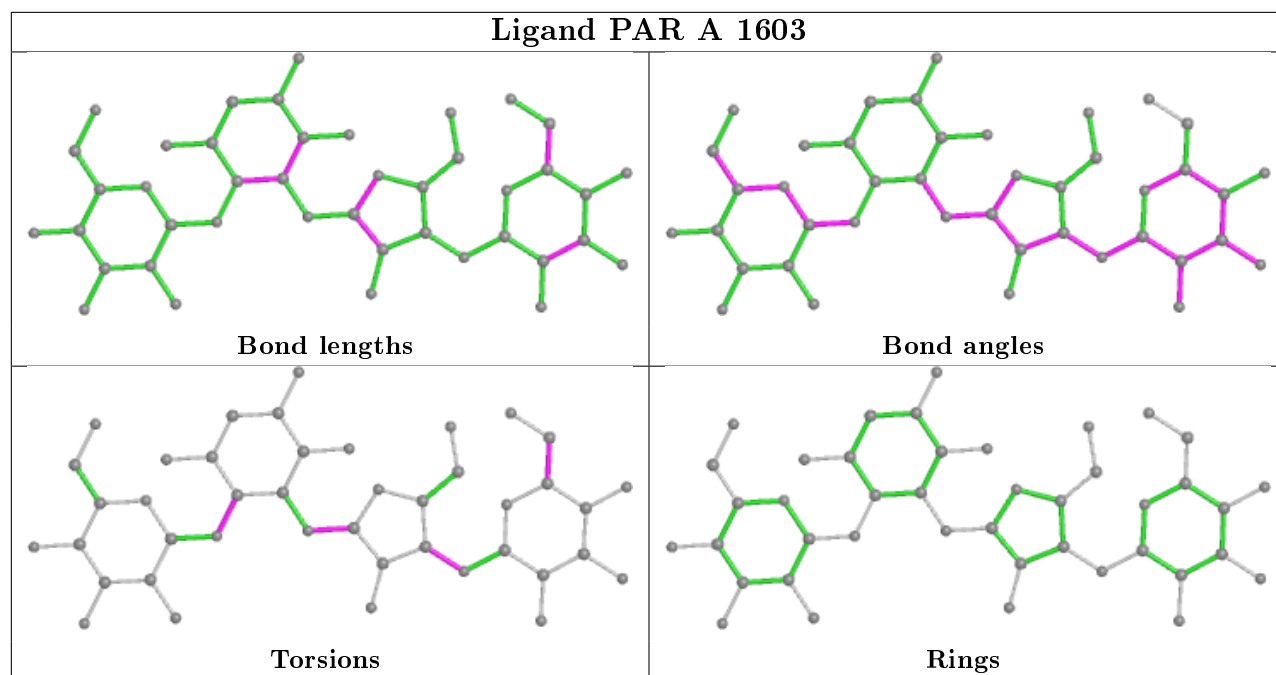
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	1602	PAR	1	0
22	A	1603	PAR	3	0
22	A	1604	PAR	1	0
22	A	1601	PAR	1	0
22	A	1606	PAR	2	0

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

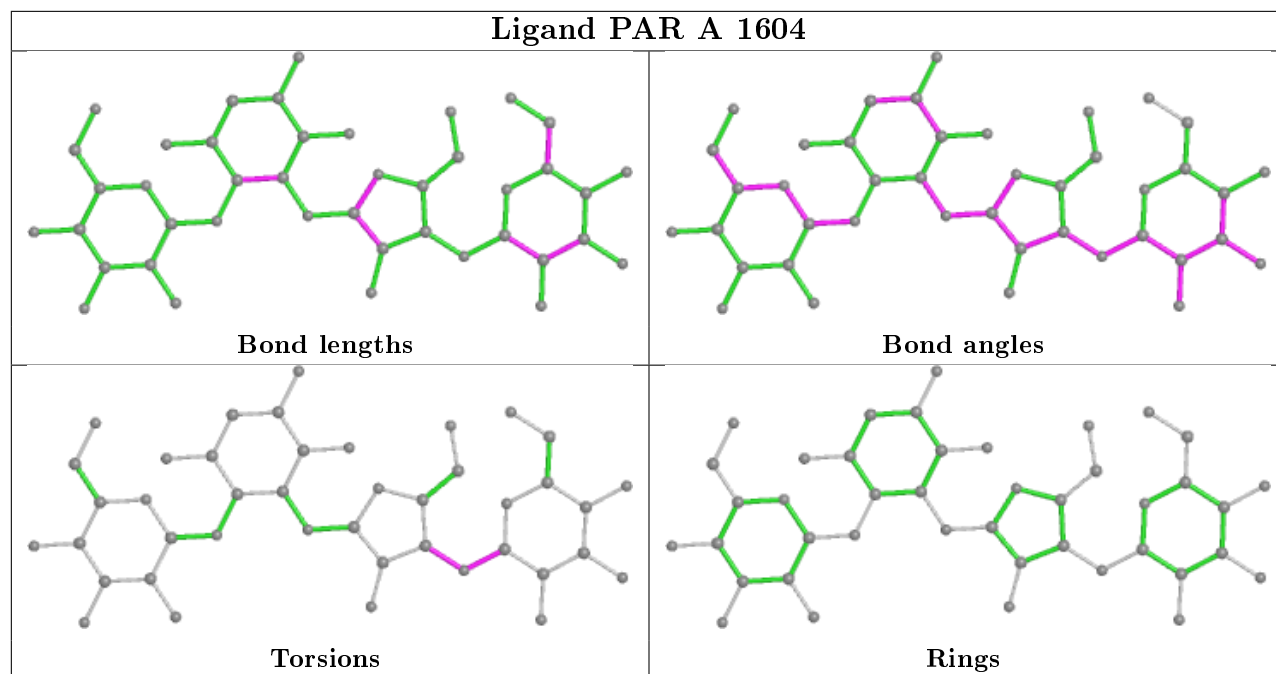
Ligand PAR A 1602



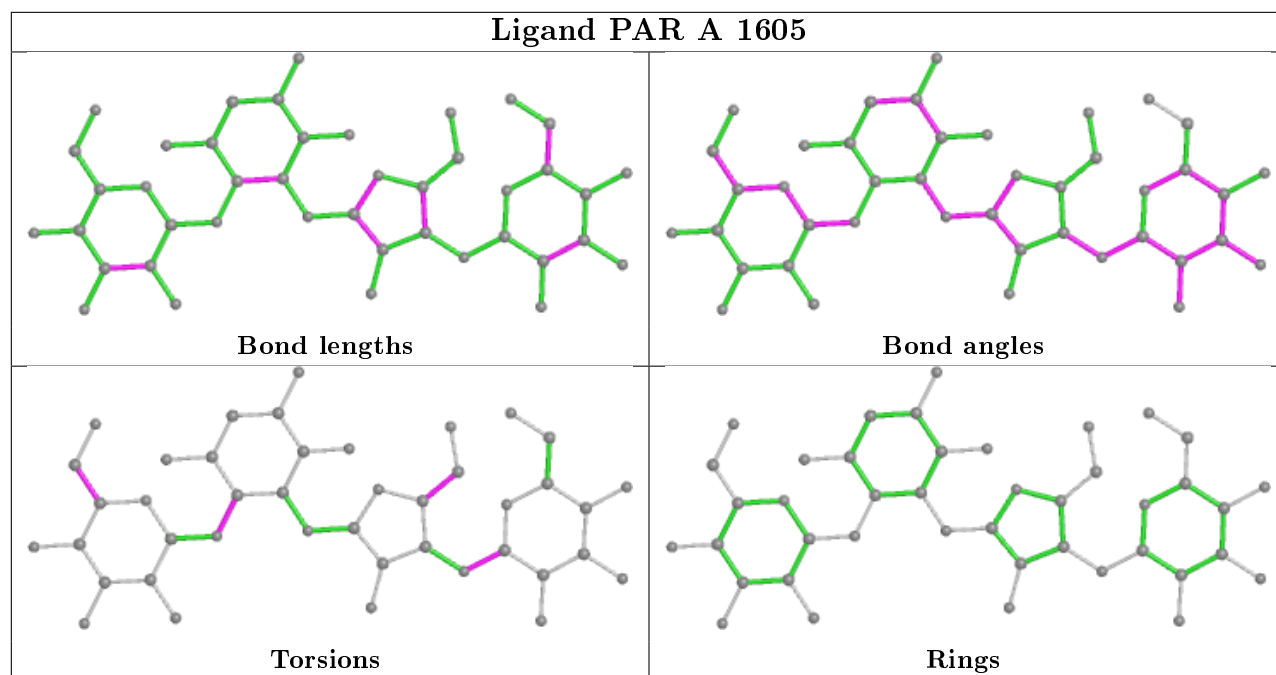
Ligand PAR A 1603

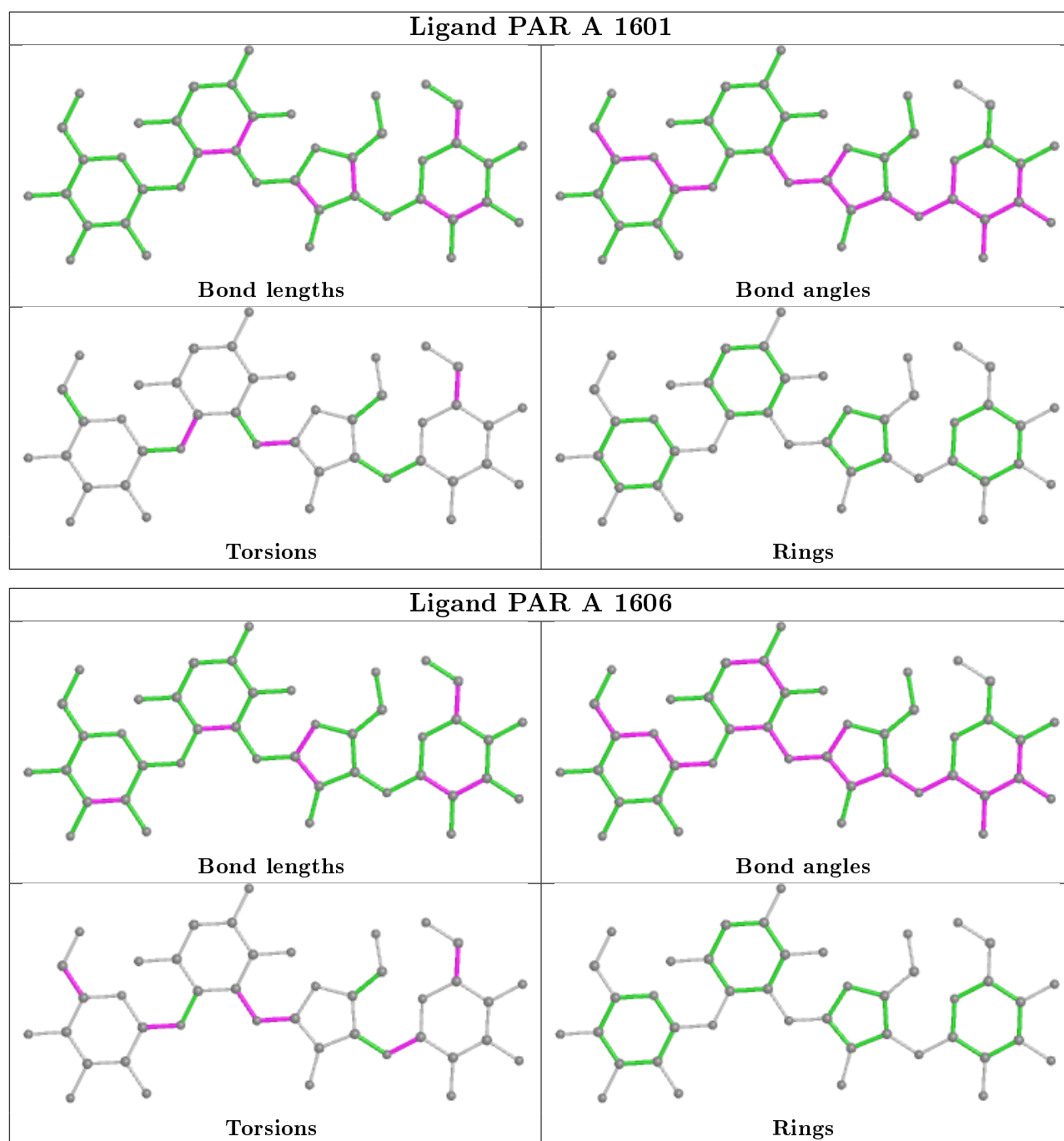


Ligand PAR A 1604



Ligand PAR A 1605





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

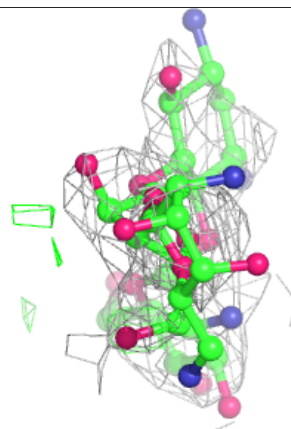
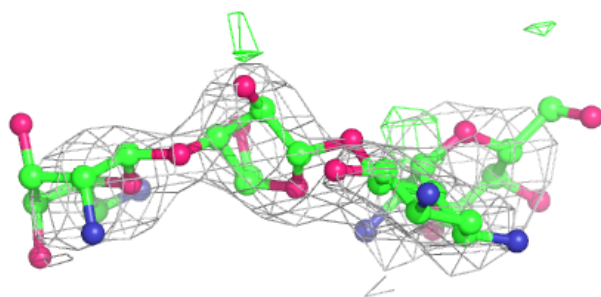
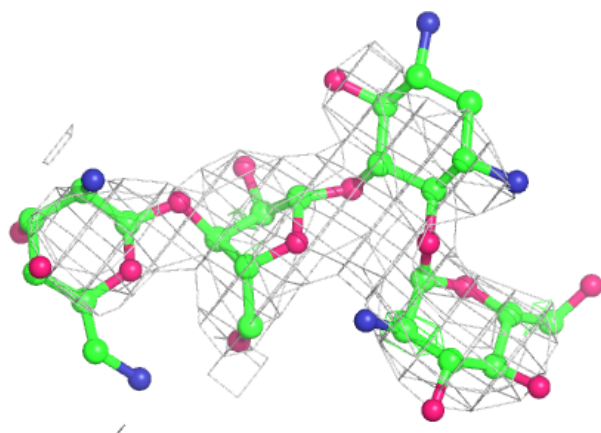
6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

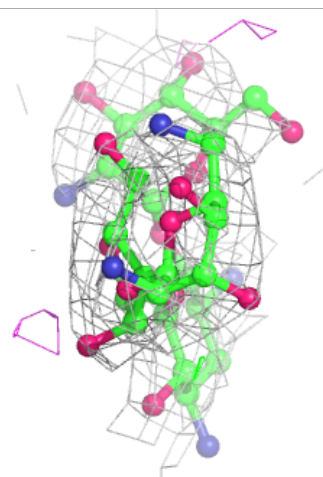
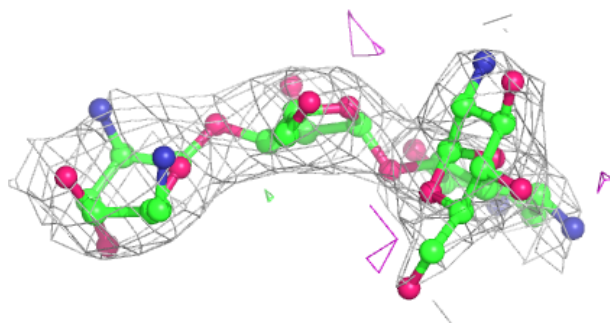
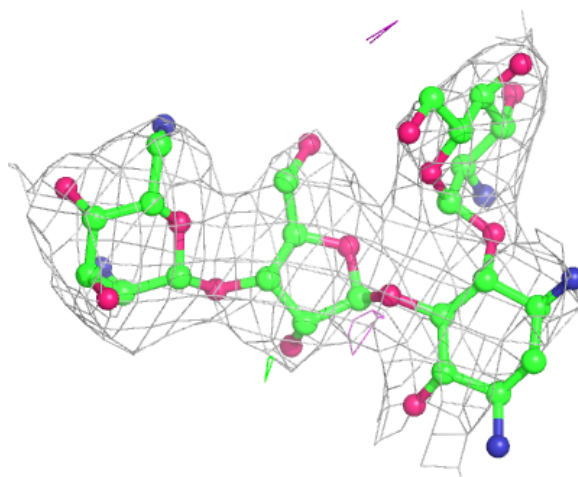
Electron density around PAR A 1605:

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



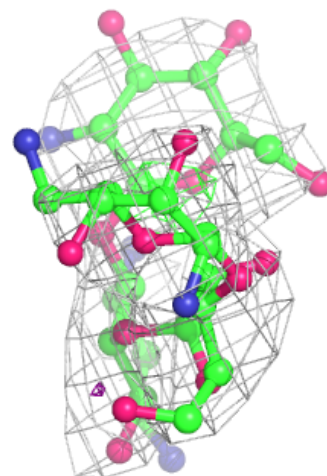
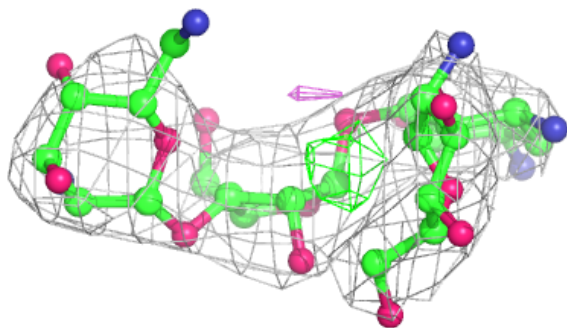
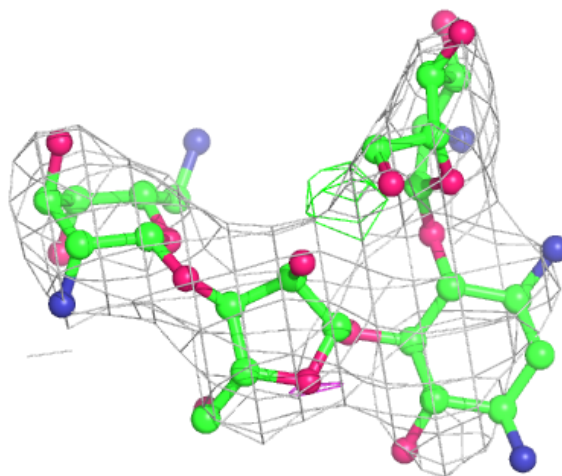
Electron density around PAR A 1603:

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



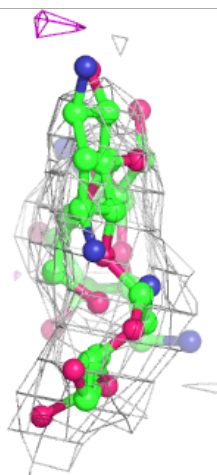
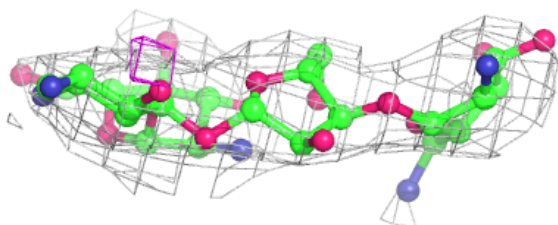
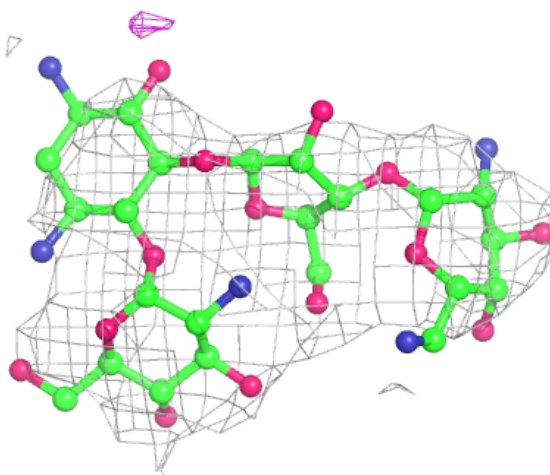
Electron density around PAR A 1606:

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



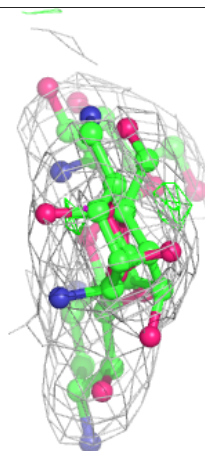
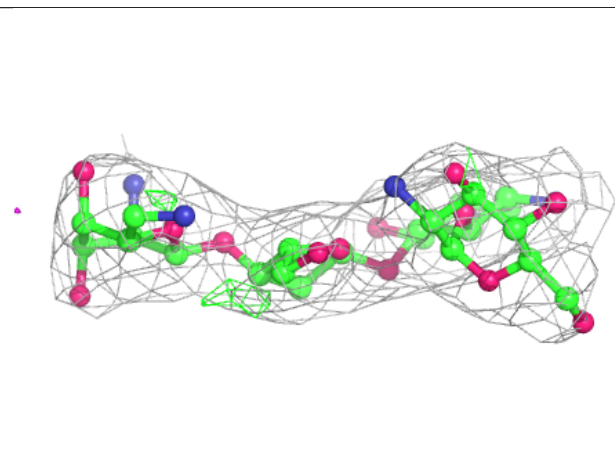
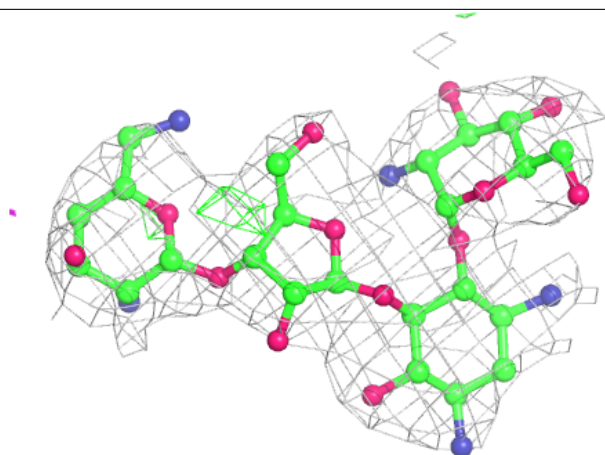
Electron density around PAR A 1604:

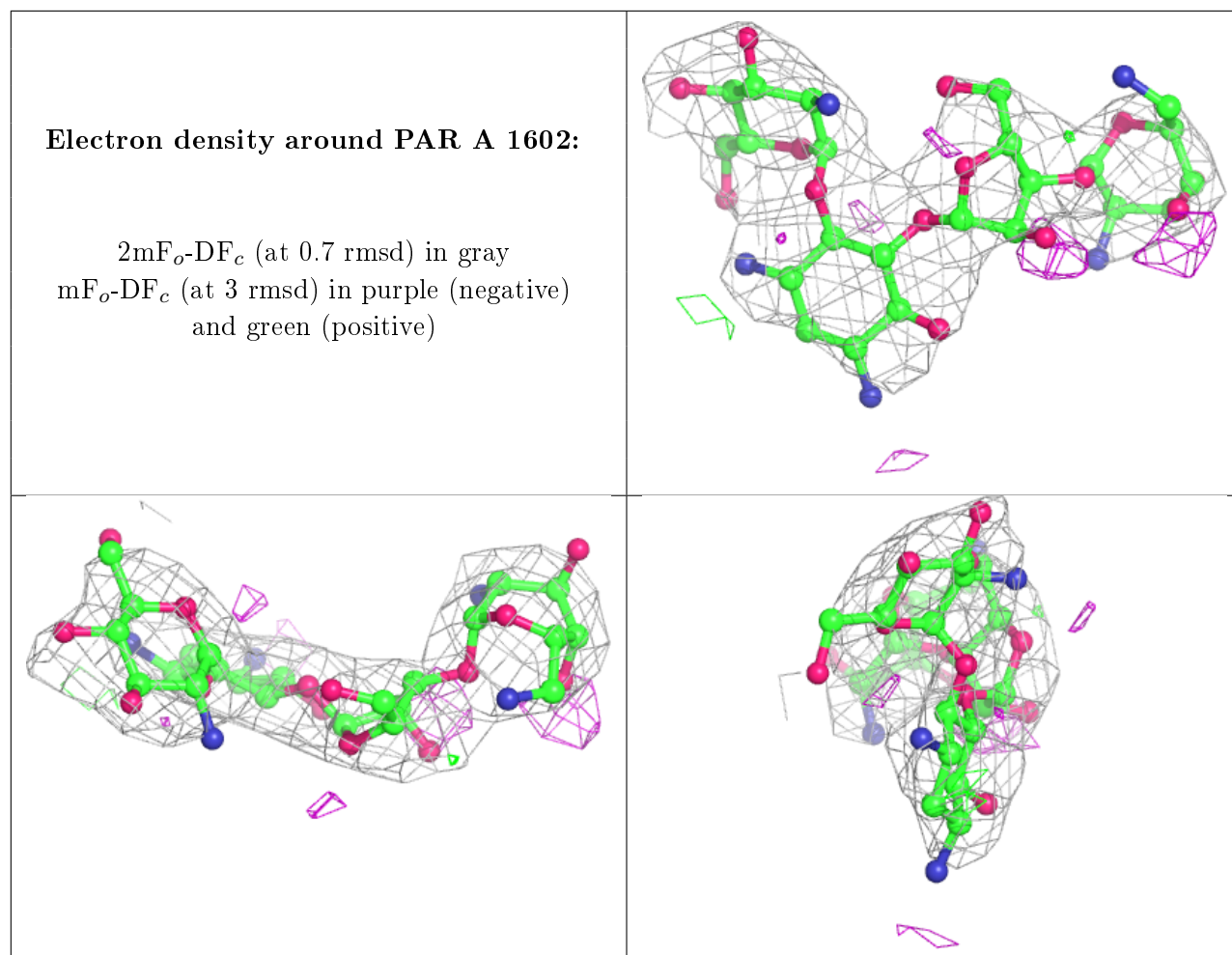
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.