wwPDB X-ray Structure Validation Summary Report (i)

Oct 21, 2024 – 02:08 AM EDT

PDB ID	:	1N32
Title	:	Structure of the Thermus thermophilus 30S ribosomal subunit bound to codon and near-cognate transfer RNA anticodon stem-loop mismatched at the first codon position at the a site with paromomycin
Authors	:	Ogle, J.M.; Murphy IV, F.V.; Tarry, M.J.; Ramakrishnan, V.
Deposited on	:	2002-10-25
Resolution	:	3.00 Å(reported)

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

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

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

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

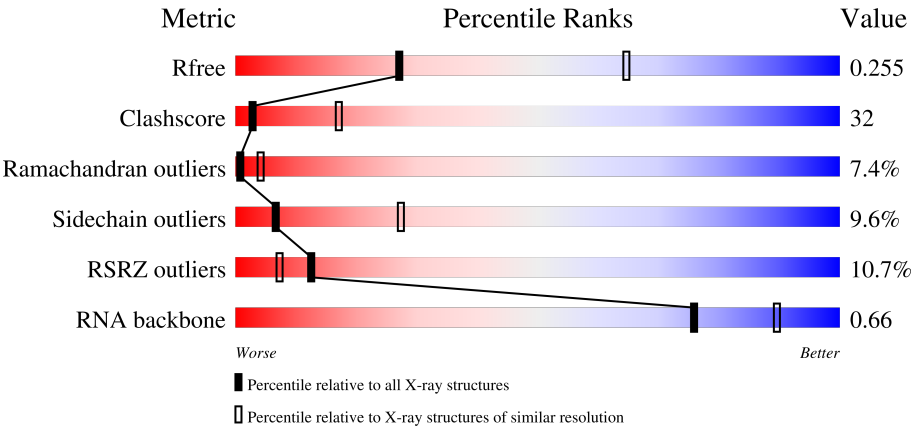
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	2511 (3.00-3.00)
Clashscore	180529	2866 (3.00-3.00)
Ramachandran outliers	177936	2778 (3.00-3.00)
Sidechain outliers	177891	2781 (3.00-3.00)
RSRZ outliers	164620	2523 (3.00-3.00)
RNA backbone	3690	1019 (3.20-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	1522	9% 34% 51% 11%
2	Y	17	29% 29% 47% 12% 12%
3	Z	6	33% 50% 17% 33%

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Mol	Chain	Length	Quality of chain
4	B	256	14% 24% 53% 13% 9%
5	C	239	16% 20% 51% 14% 14%
6	D	208	10% 41% 51% 7%
7	E	161	3% 35% 48% 9% 7%
8	F	101	6% 36% 53% 11%
9	G	155	8% 40% 55% 5%
10	H	138	2% 47% 46% 7%
11	I	128	17% 24% 63% 10%
12	J	104	34% 14% 60% 19% 6%
13	K	129	8% 40% 42% 11% 8%
14	L	135	10% 39% 44% 8% 8%
15	M	126	11% 27% 53% 13% 6%
16	N	60	23% 25% 57% 13% 5%
17	O	88	3% 52% 40% 8%
18	P	88	% 36% 49% 9% 6%
19	Q	104	9% 44% 46% 9%
20	R	88	3% 35% 42% 6% 17%
21	S	92	20% 27% 49% 10% 13%
22	T	106	8% 39% 44% 9% 7%
23	V	26	15% 46% 46% 8%

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
25	MG	A	1572	-	-	-	X
25	MG	A	1629	-	-	-	X
25	MG	A	1644	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	MG	A	1647	-	-	-	X
25	MG	A	1655	-	-	-	X
25	MG	A	1680	-	-	-	X
25	MG	A	441	-	-	-	X

2 Entry composition (i)

There are 26 unique types of molecules in this entry. The entry contains 52275 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
			Total	C	N	O	P			
1	A	1513	32508	14472	6016	10509	1511	0	0	0

- Molecule 2 is a RNA chain called ANTICODON STEM-LOOP OF LEU-2 TRANSFER RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	Y	15	318	143	56	105	14	0	0	0

- Molecule 3 is a RNA chain called A-SITE MESSENGER RNA FRAGMENT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	Z	4	77	36	8	30	3	0	0	0

- Molecule 4 is a protein called 30S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	B	234	1900	1213	341	341	5	0	0	0

- Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	C	206	1612	1016	314	281	1	0	0	0

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S4.

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

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	150	Total	C	N	O	S	0	0	0
			1146	724	217	201	4			

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S6.

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

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S7.

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

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S8.

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

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	25	ASP	GLU	conflict	UNP P24319
H	37	ARG	LYS	conflict	UNP P24319
H	52	ASP	GLU	conflict	UNP P24319
H	61	VAL	ILE	conflict	UNP P24319
H	62	TYR	HIS	conflict	UNP P24319
H	81	HIS	LYS	conflict	UNP P24319
H	88	LYS	ARG	conflict	UNP P24319
H	115	SER	PRO	conflict	UNP P24319

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	I	127	Total	C	N	O	0	0	0
			1011	639	198	174			

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	J	98	Total	C	N	O	S	0	0	0
			792	498	156	137	1			

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	K	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	L	124	Total	C	N	O	S	0	0	0
			970	611	195	163	1			

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S13.

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

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S14.

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

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S15.

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

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	P	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Q	104	Total	C	N	O	S	0	0	0
			857	547	161	147	2			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	50	LYS	ARG	conflict	UNP P24321
Q	53	LEU	VAL	conflict	UNP P24321
Q	62	SER	ALA	conflict	UNP P24321
Q	79	SER	GLU	conflict	UNP P24321
Q	82	MET	LEU	conflict	UNP P24321
Q	90	ILE	VAL	conflict	UNP P24321
Q	96	GLN	ALA	conflict	UNP P24321

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	R	73	Total	C	N	O	0	0	0
			597	380	118	99			

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	S	80	Total	C	N	O	S	0	0	0
			647	414	119	112	2			

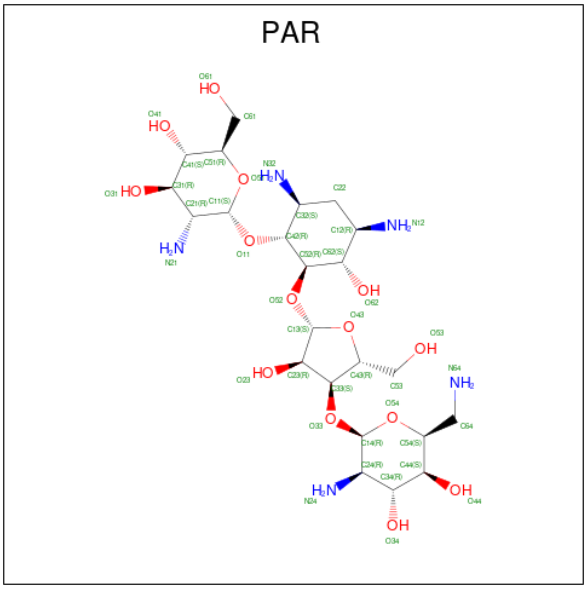
- Molecule 22 is a protein called 30S RIBOSOMAL PROTEIN S20.

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

- Molecule 23 is a protein called 30S RIBOSOMAL PROTEIN THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
23	V	24	Total	C	N	O	0	0	0
			208	128	50	30			

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



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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	A	153	Total	Mg	0	0
			153	153		
25	Y	1	Total	Mg	0	0
			1	1		
25	D	1	Total	Mg	0	0
			1	1		
25	E	1	Total	Mg	0	0
			1	1		
25	J	1	Total	Mg	0	0
			1	1		
25	M	1	Total	Mg	0	0
			1	1		

- Molecule 26 is ZINC ION (three-letter code: ZN) (formula: Zn).

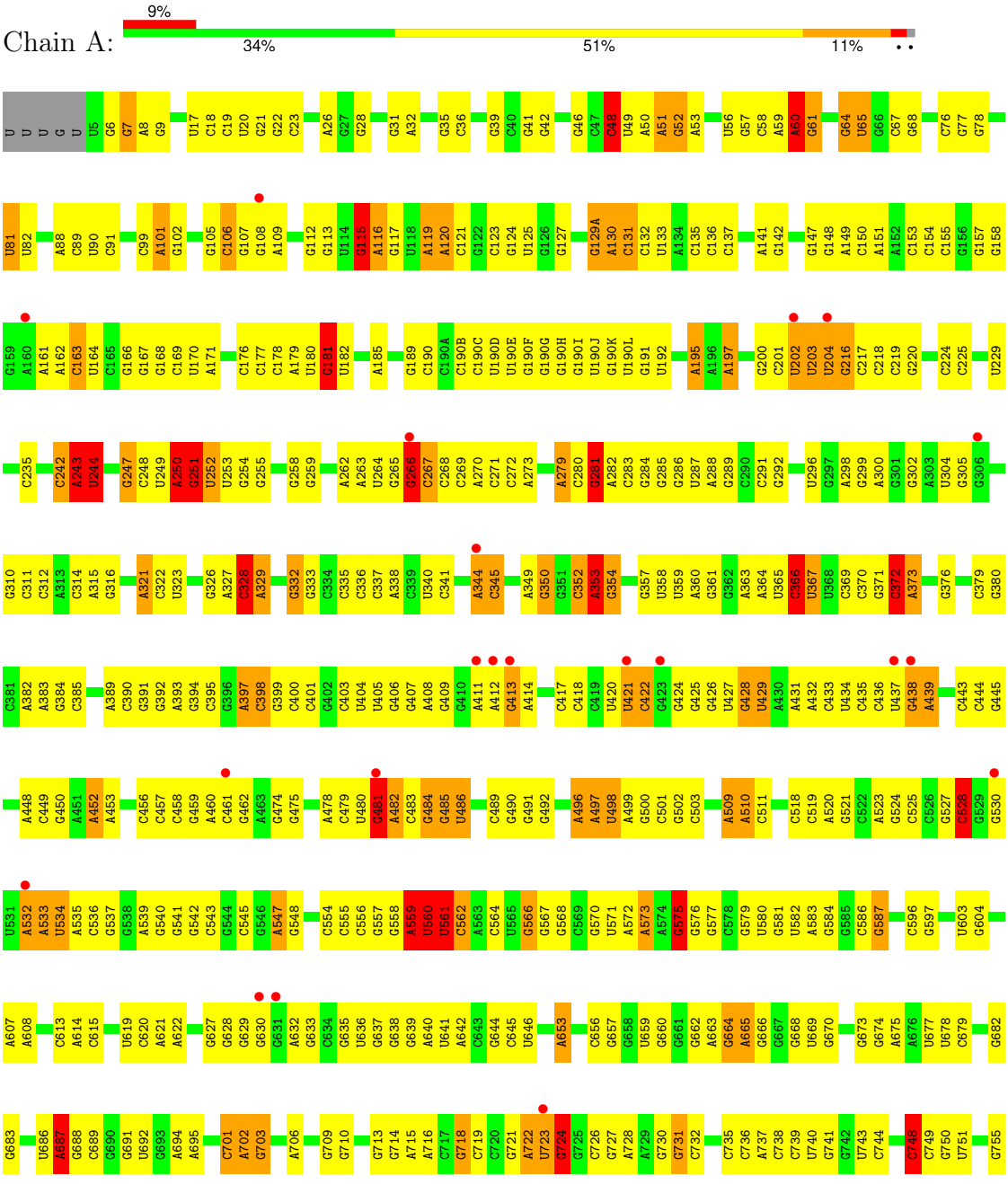
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	D	1	Total Zn 1 1	0	0
26	N	1	Total Zn 1 1	0	0

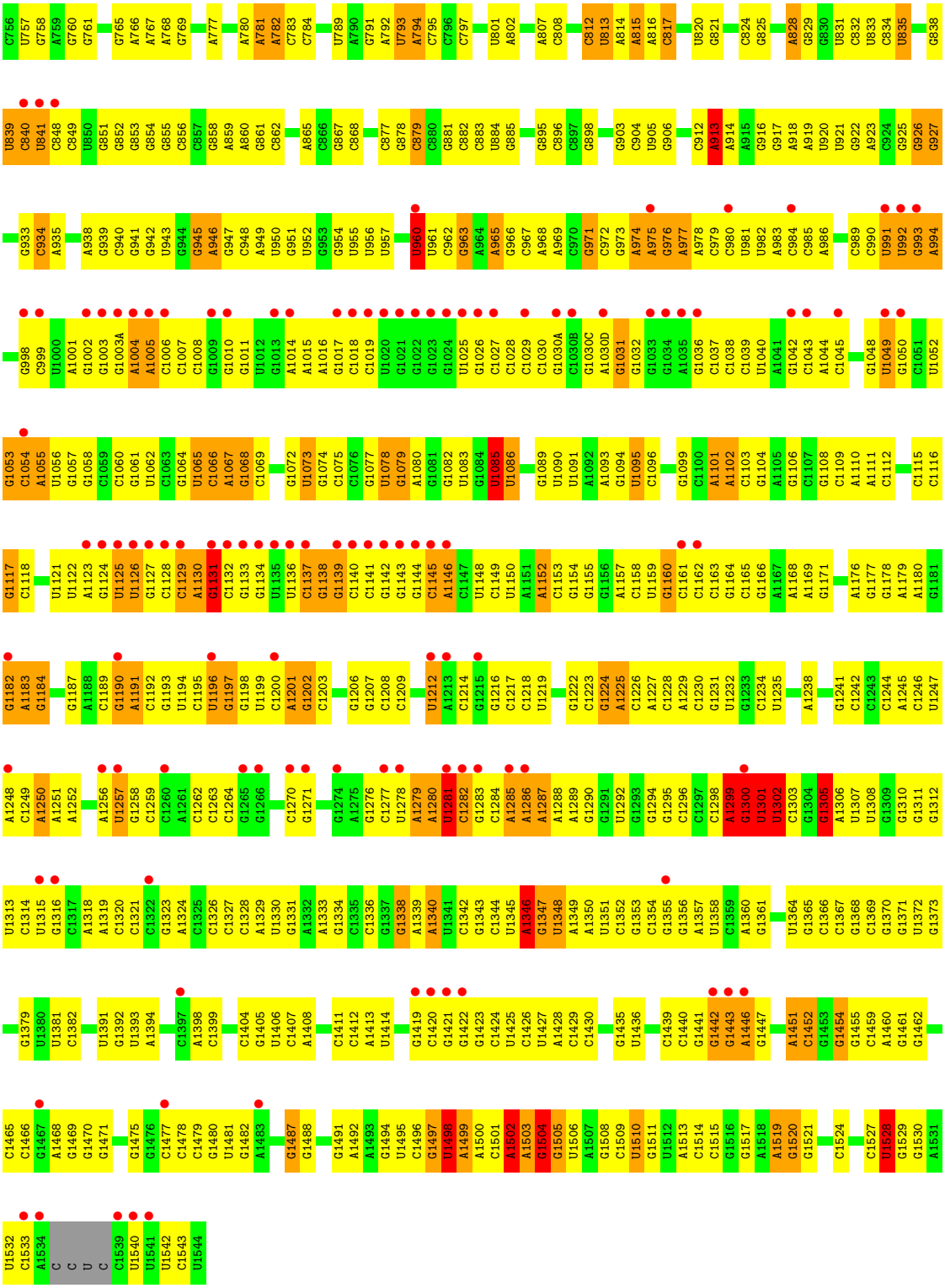
3 Residue-property plots (i)

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

- Molecule 1: 16S RIBOSOMAL RNA

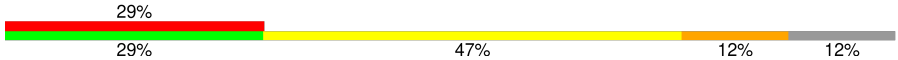
Chain A:

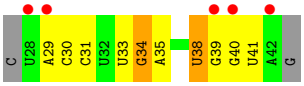




• Molecule 2: ANTICODON STEM-LOOP OF LEU-2 TRANSFER RNA

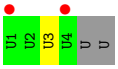
Chain Y:





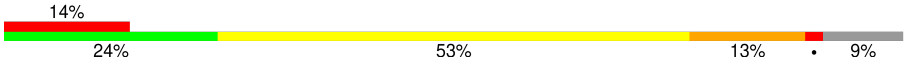
• Molecule 3: A-SITE MESSENGER RNA FRAGMENT

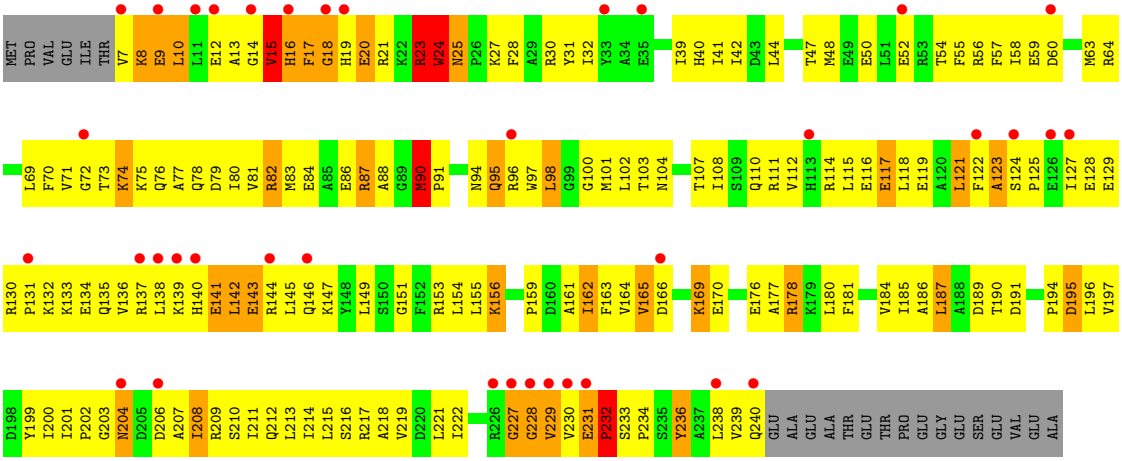
Chain Z:



• Molecule 4: 30S RIBOSOMAL PROTEIN S2

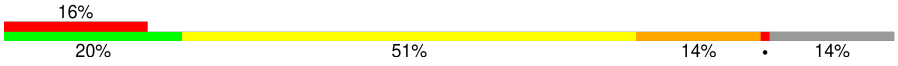
Chain B:

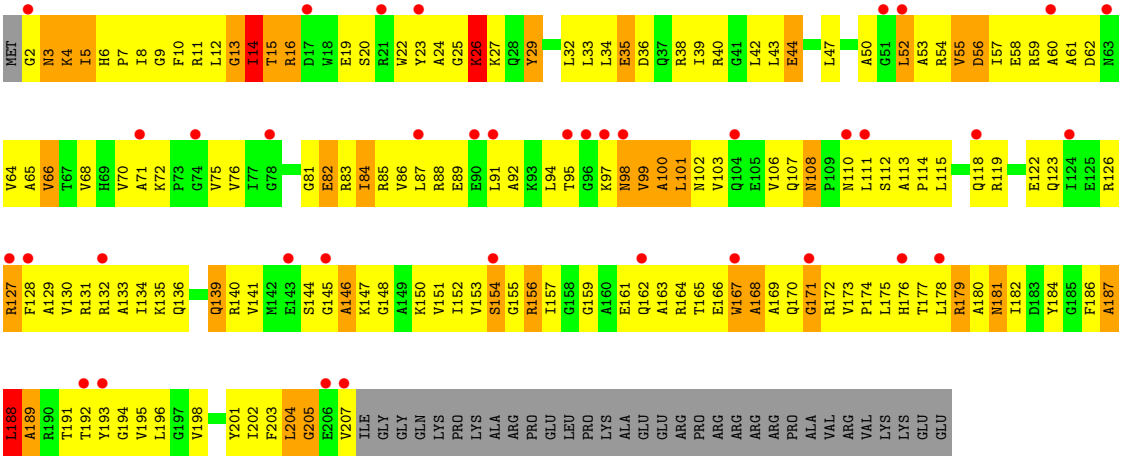




• Molecule 5: 30S RIBOSOMAL PROTEIN S3

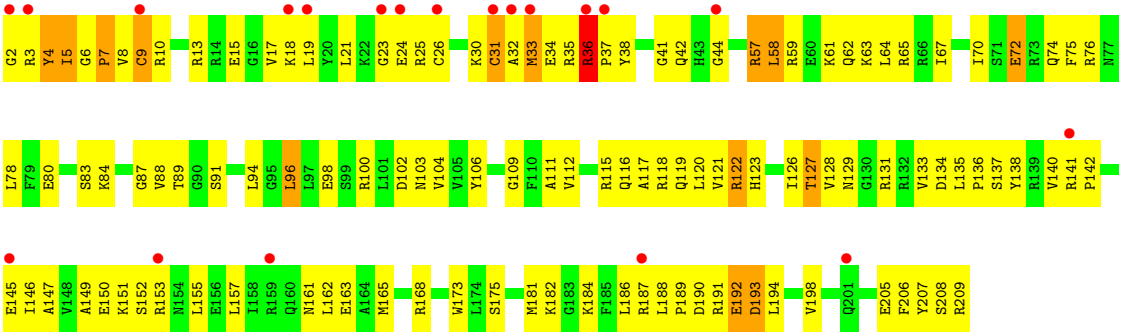
Chain C:



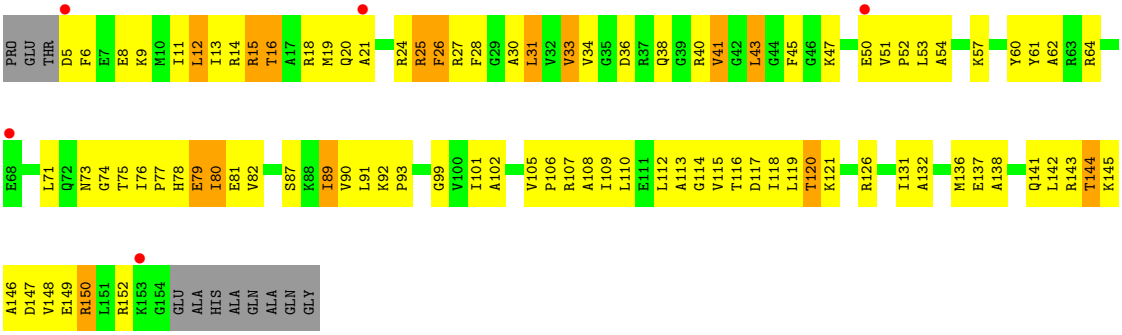


• Molecule 6: 30S RIBOSOMAL PROTEIN S4

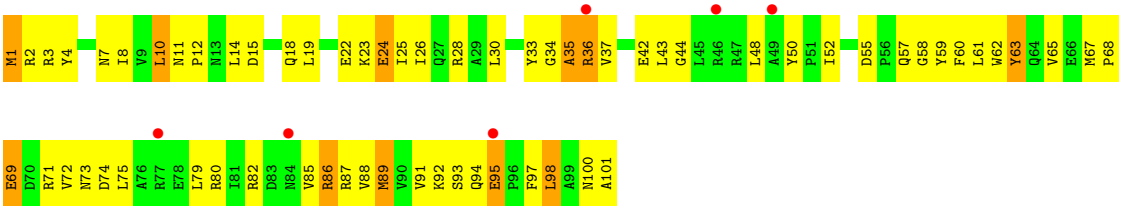
Chain D:



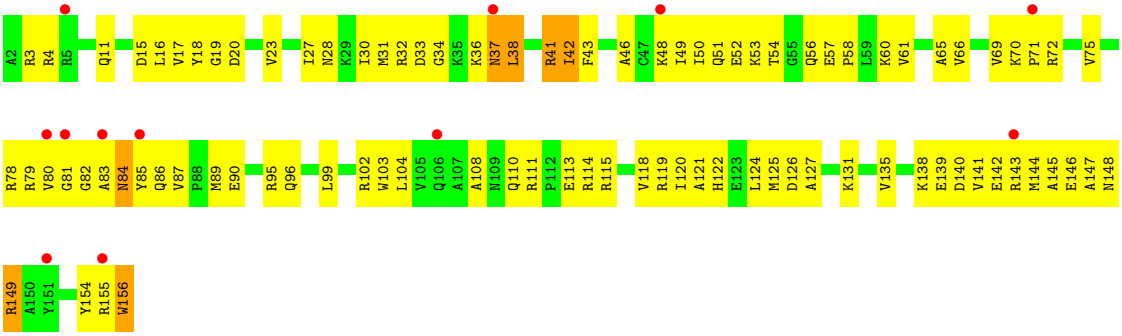
• Molecule 7: 30S RIBOSOMAL PROTEIN S5



• Molecule 8: 30S RIBOSOMAL PROTEIN S6

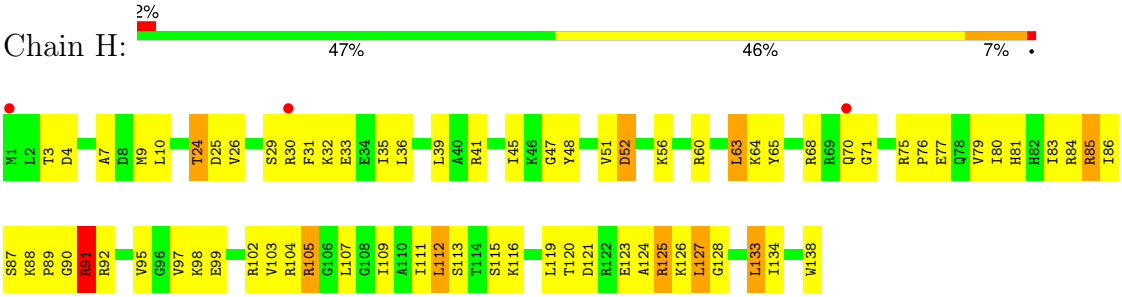


• Molecule 9: 30S RIBOSOMAL PROTEIN S7



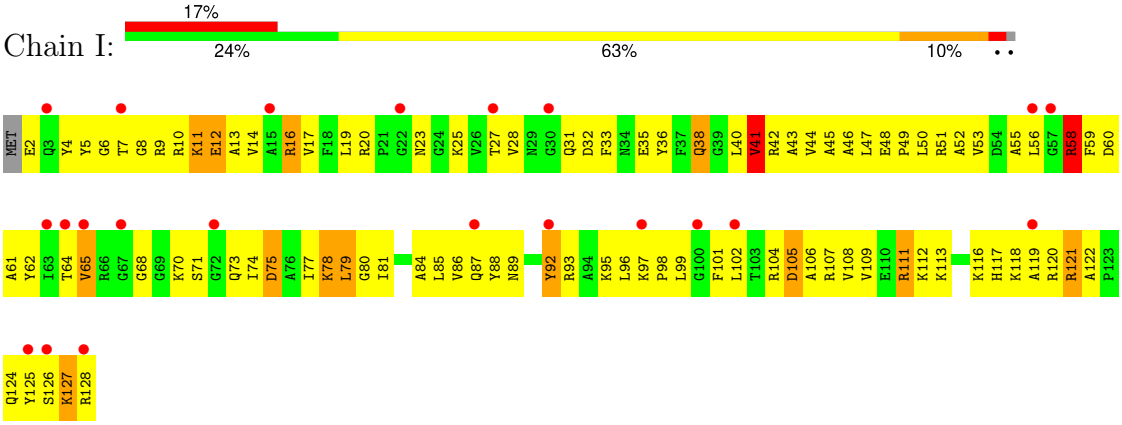
• Molecule 10: 30S RIBOSOMAL PROTEIN S8

Chain H:



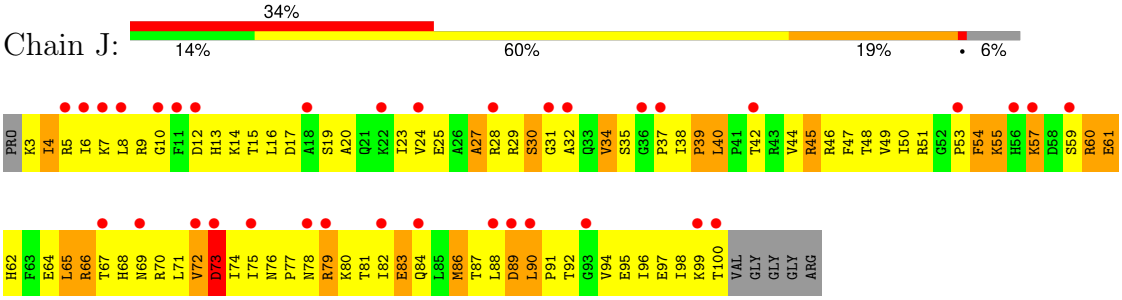
• Molecule 11: 30S RIBOSOMAL PROTEIN S9

Chain I:



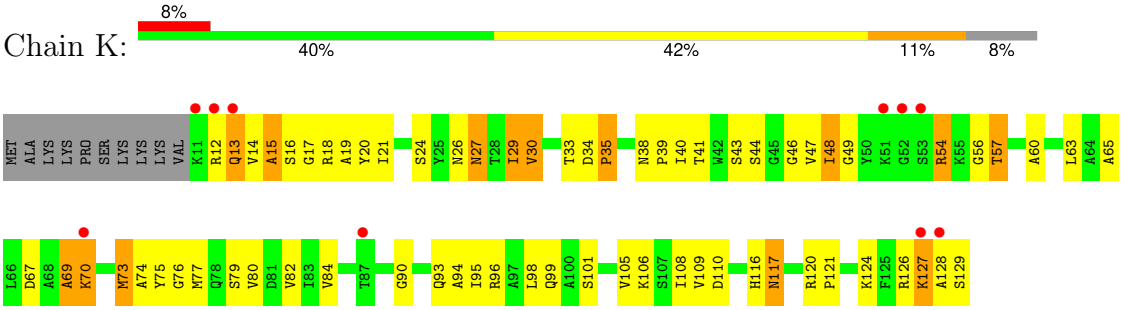
• Molecule 12: 30S RIBOSOMAL PROTEIN S10

Chain J:



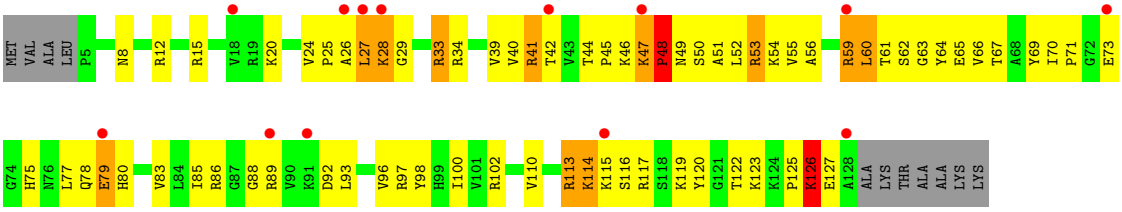
• Molecule 13: 30S RIBOSOMAL PROTEIN S11

Chain K:



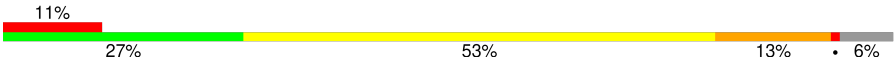
• Molecule 14: 30S RIBOSOMAL PROTEIN S12

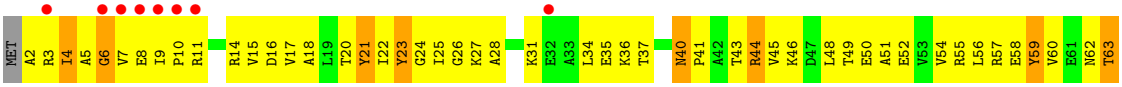
Chain L:

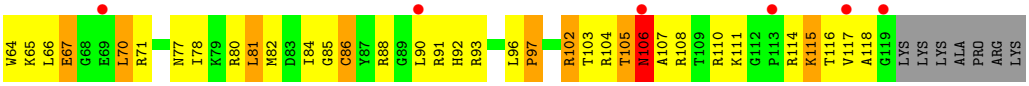


• Molecule 15: 30S RIBOSOMAL PROTEIN S13

Chain M:

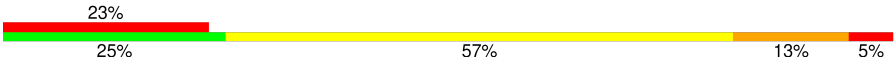


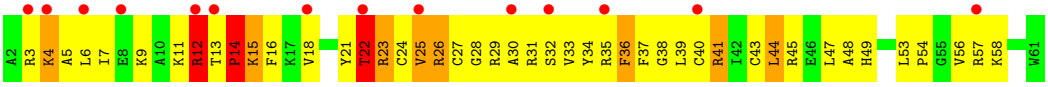




• Molecule 16: 30S RIBOSOMAL PROTEIN S14

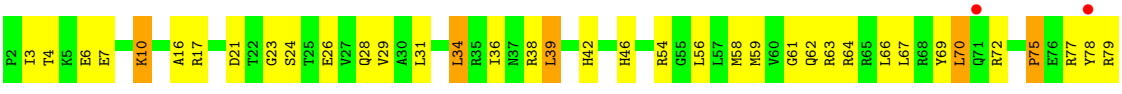
Chain N:

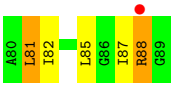




• Molecule 17: 30S RIBOSOMAL PROTEIN S15

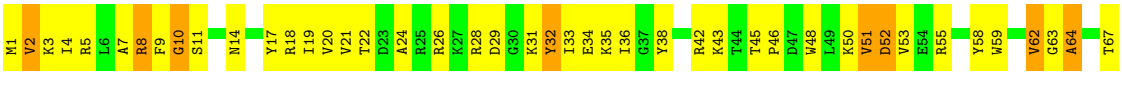
Chain O:

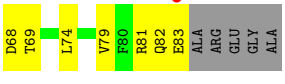




• Molecule 18: 30S RIBOSOMAL PROTEIN S16

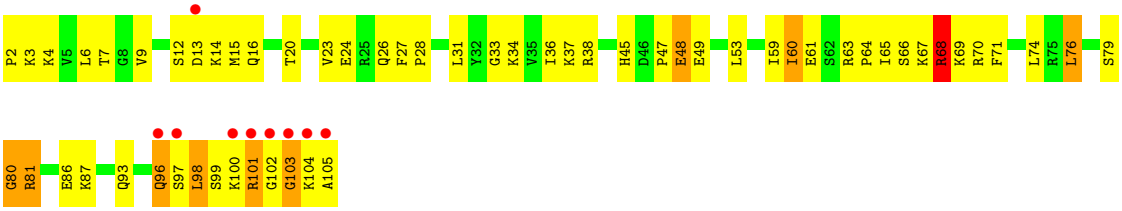
Chain P:



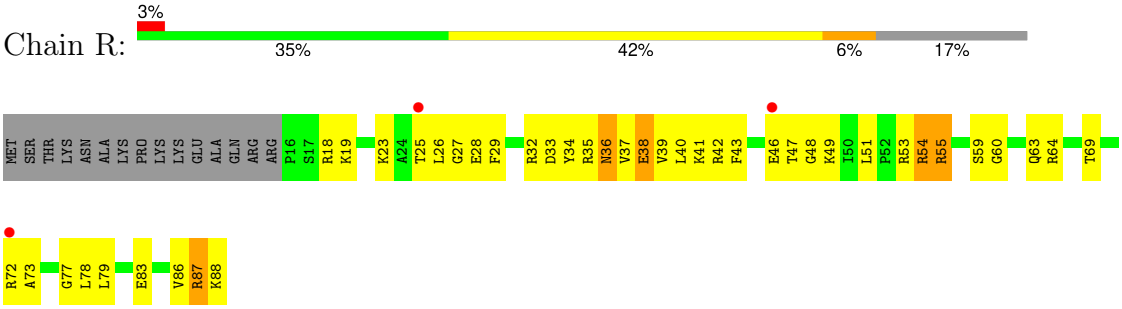


• Molecule 19: 30S RIBOSOMAL PROTEIN S17

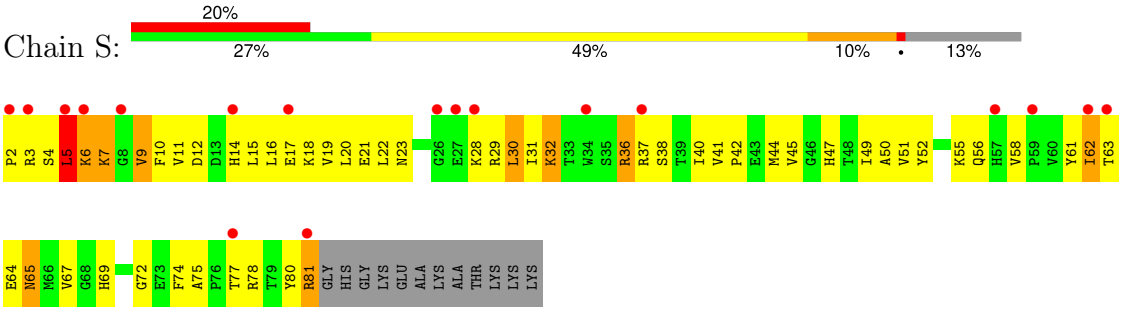
Chain Q:



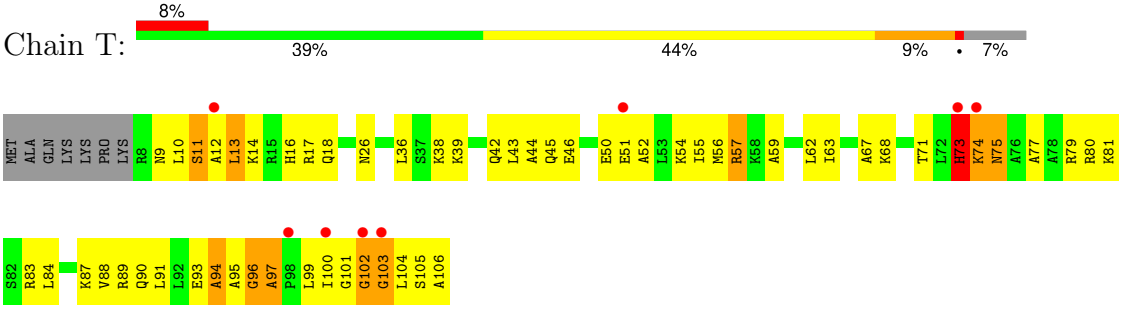
• Molecule 20: 30S RIBOSOMAL PROTEIN S18



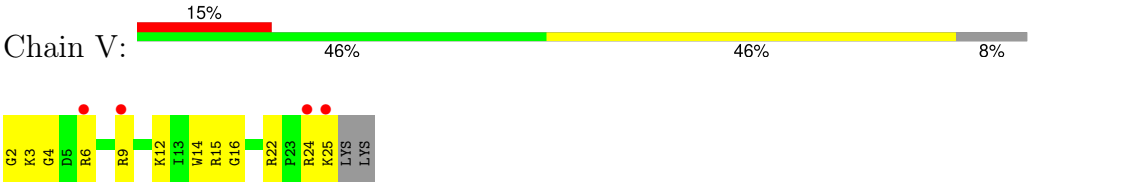
• Molecule 21: 30S RIBOSOMAL PROTEIN S19



• Molecule 22: 30S RIBOSOMAL PROTEIN S20



• Molecule 23: 30S RIBOSOMAL PROTEIN THX



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	400.30Å 400.30Å 175.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	141.42 – 3.00 141.42 – 3.00	Depositor EDS
% Data completeness (in resolution range)	91.9 (141.42-3.00) 91.9 (141.42-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	2.41 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.227 , 0.270 0.214 , 0.255	Depositor DCC
R_{free} test set	13154 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	67.3	Xtriage
Anisotropy	0.222	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 147.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	52275	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.45% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PSU, ZN, MG, PAR

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	0.46	0/36387	0.74	39/56789 (0.1%)
2	Y	0.41	0/333	0.71	0/518
3	Z	0.49	0/84	0.82	0/128
4	B	0.32	0/1935	0.64	0/2609
5	C	0.35	0/1636	0.62	0/2205
6	D	0.38	0/1733	0.67	0/2318
7	E	0.44	0/1162	0.71	0/1564
8	F	0.31	0/856	0.60	0/1154
9	G	0.36	0/1276	0.59	0/1709
10	H	0.44	0/1136	0.77	0/1527
11	I	0.35	0/1029	0.64	0/1378
12	J	0.36	0/805	0.64	0/1082
13	K	0.39	0/900	0.73	0/1213
14	L	0.43	0/986	0.77	0/1320
15	M	0.33	0/947	0.65	0/1270
16	N	0.41	0/501	0.68	0/664
17	O	0.36	0/745	0.58	0/992
18	P	0.45	0/716	0.73	0/963
19	Q	0.44	0/870	0.75	0/1159
20	R	0.33	0/603	0.62	0/799
21	S	0.32	0/661	0.64	0/890
22	T	0.39	0/765	0.71	0/1007
23	V	0.44	0/212	0.76	0/277
All	All	0.44	0/56278	0.72	39/83535 (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
1	A	4	35
18	P	0	1
All	All	4	36

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	48	C	C2'-C3'-O3'	11.02	133.74	109.50
1	A	1498	U	C2'-C3'-O3'	10.16	131.86	109.50
1	A	243	A	C2'-C3'-O3'	9.62	130.66	109.50
1	A	281	G	C2'-C3'-O3'	9.39	130.16	109.50
1	A	115	G	C2'-C3'-O3'	9.27	129.88	109.50

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	48	C	C3'
1	A	243	A	C3'
1	A	281	G	C3'
1	A	1528	U	C3'

5 of 36 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	106	C	Sidechain
1	A	229	U	Sidechain
1	A	242	C	Sidechain
1	A	250	A	Sidechain
1	A	251	G	Sidechain

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	32508	0	16413	1088	0
2	Y	318	0	162	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	Z	77	0	42	1	0
4	B	1900	0	1951	255	0
5	C	1612	0	1677	229	0
6	D	1703	0	1763	134	0
7	E	1146	0	1207	105	0
8	F	843	0	857	95	0
9	G	1257	0	1296	107	0
10	H	1116	0	1177	80	0
11	I	1011	0	1043	124	0
12	J	792	0	835	131	0
13	K	885	0	904	75	0
14	L	970	0	1057	101	0
15	M	937	0	995	110	0
16	N	492	0	530	71	0
17	O	734	0	771	41	0
18	P	700	0	720	56	0
19	Q	857	0	930	69	0
20	R	597	0	668	63	0
21	S	647	0	673	86	0
22	T	763	0	861	79	0
23	V	208	0	221	14	0
24	A	42	0	45	2	0
25	A	153	0	0	0	0
25	D	1	0	0	0	0
25	E	1	0	0	0	0
25	J	1	0	0	0	0
25	M	1	0	0	0	0
25	Y	1	0	0	0	0
26	D	1	0	0	0	0
26	N	1	0	0	0	0
All	All	52275	0	36798	2844	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 32.

The worst 5 of 2844 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)
6:D:36:ARG:H	6:D:37:PRO:HD3	1.02	1.18
15:M:10:PRO:HB2	15:M:18:ALA:HB1	1.29	1.14
7:E:15:ARG:HD3	7:E:26:PHE:HD2	1.13	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:975:A:H4'	1:A:976:G:H5"	1.31	1.11
1:A:1532:U:H2'	1:A:1533:C:H5"	1.19	1.09

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
4	B	232/256 (91%)	159 (68%)	49 (21%)	24 (10%)	0 2
5	C	204/239 (85%)	128 (63%)	44 (22%)	32 (16%)	0 0
6	D	206/208 (99%)	170 (82%)	25 (12%)	11 (5%)	1 9
7	E	148/161 (92%)	132 (89%)	15 (10%)	1 (1%)	19 54
8	F	99/101 (98%)	80 (81%)	16 (16%)	3 (3%)	3 20
9	G	153/155 (99%)	121 (79%)	28 (18%)	4 (3%)	4 23
10	H	136/138 (99%)	117 (86%)	17 (12%)	2 (2%)	8 36
11	I	125/128 (98%)	91 (73%)	24 (19%)	10 (8%)	1 3
12	J	96/104 (92%)	58 (60%)	21 (22%)	17 (18%)	0 0
13	K	117/129 (91%)	95 (81%)	13 (11%)	9 (8%)	1 4
14	L	122/135 (90%)	99 (81%)	16 (13%)	7 (6%)	1 8
15	M	116/126 (92%)	83 (72%)	21 (18%)	12 (10%)	0 2
16	N	58/60 (97%)	33 (57%)	15 (26%)	10 (17%)	0 0
17	O	86/88 (98%)	78 (91%)	6 (7%)	2 (2%)	5 26
18	P	81/88 (92%)	64 (79%)	13 (16%)	4 (5%)	2 10
19	Q	102/104 (98%)	85 (83%)	10 (10%)	7 (7%)	1 5
20	R	71/88 (81%)	62 (87%)	5 (7%)	4 (6%)	1 8
21	S	78/92 (85%)	57 (73%)	15 (19%)	6 (8%)	1 4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
22	T	97/106 (92%)	73 (75%)	15 (16%)	9 (9%)	0 2
23	V	22/26 (85%)	15 (68%)	6 (27%)	1 (4%)	2 12
All	All	2349/2532 (93%)	1800 (77%)	374 (16%)	175 (7%)	1 4

5 of 175 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	B	15	VAL
4	B	17	PHE
4	B	21	ARG
4	B	23	ARG
4	B	24	TRP

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	B	202/220 (92%)	175 (87%)	27 (13%)	3 15
5	C	160/188 (85%)	144 (90%)	16 (10%)	6 25
6	D	180/180 (100%)	167 (93%)	13 (7%)	12 39
7	E	115/122 (94%)	99 (86%)	16 (14%)	3 14
8	F	90/90 (100%)	80 (89%)	10 (11%)	5 21
9	G	126/126 (100%)	120 (95%)	6 (5%)	21 55
10	H	119/119 (100%)	106 (89%)	13 (11%)	5 22
11	I	98/99 (99%)	87 (89%)	11 (11%)	5 21
12	J	87/91 (96%)	79 (91%)	8 (9%)	7 29
13	K	90/99 (91%)	83 (92%)	7 (8%)	10 36
14	L	104/111 (94%)	94 (90%)	10 (10%)	7 27
15	M	94/101 (93%)	83 (88%)	11 (12%)	4 19
16	N	49/49 (100%)	43 (88%)	6 (12%)	4 18
17	O	79/79 (100%)	73 (92%)	6 (8%)	11 37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
18	P	72/74 (97%)	68 (94%)	4 (6%)	17 49
19	Q	96/96 (100%)	87 (91%)	9 (9%)	7 28
20	R	64/77 (83%)	61 (95%)	3 (5%)	22 56
21	S	71/79 (90%)	62 (87%)	9 (13%)	3 17
22	T	76/82 (93%)	70 (92%)	6 (8%)	10 35
23	V	19/21 (90%)	19 (100%)	0	100 100
All	All	1991/2103 (95%)	1800 (90%)	191 (10%)	7 27

5 of 191 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	J	60	ARG
15	M	102	ARG
12	J	89	ASP
14	L	53	ARG
16	N	22	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 57 such sidechains are listed below:

Mol	Chain	Res	Type
8	F	94	GLN
21	S	47	HIS
9	G	96	GLN
21	S	23	ASN
17	O	46	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1511/1522 (99%)	211 (13%)	69 (4%)
2	Y	14/17 (82%)	1 (7%)	0
3	Z	3/6 (50%)	0	0
All	All	1528/1545 (98%)	212 (13%)	69 (4%)

5 of 212 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	8	A

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Mol	Chain	Res	Type
1	A	9	G
1	A	32	A
1	A	39	G
1	A	48	C

5 of 69 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1281	U
1	A	1300	G
1	A	1498	U
1	A	421	U
1	A	372	C

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

1 non-standard protein/DNA/RNA residue is 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	$\#\|Z\| > 2$
2	PSU	Y	38	2	18,21,22	1.86	2 (11%)	21,30,33	1.52	3 (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
2	PSU	Y	38	2	-	0/7/25/26	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Y	38	PSU	C2-N1	6.29	1.44	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Y	38	PSU	C6-N1	3.20	1.41	1.36

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Y	38	PSU	C6-C5-C4	3.91	120.81	118.17
2	Y	38	PSU	O2-C2-N1	3.76	126.66	122.79
2	Y	38	PSU	O4'-C1'-C2'	2.14	108.11	105.15

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Y	38	PSU	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 161 ligands modelled in this entry, 160 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
24	PAR	A	1545	-	44,45,45	1.53	11 (25%)	63,67,67	1.06	4 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	PAR	A	1545	-	-	4/18/94/94	0/4/4/4

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1545	PAR	O54-C14	3.96	1.52	1.41
24	A	1545	PAR	O33-C14	2.73	1.49	1.41
24	A	1545	PAR	C31-C21	2.47	1.56	1.53
24	A	1545	PAR	C11-C21	2.40	1.57	1.52
24	A	1545	PAR	C41-C51	2.25	1.57	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	1545	PAR	O54-C54-C64	3.33	112.47	106.07
24	A	1545	PAR	C14-O54-C54	2.87	119.32	113.72
24	A	1545	PAR	O11-C11-C21	2.36	111.93	108.08
24	A	1545	PAR	C22-C32-C42	2.09	114.63	109.50

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	1545	PAR	C24-C14-O33-C33
24	A	1545	PAR	C33-C43-C53-O53
24	A	1545	PAR	O54-C54-C64-N64
24	A	1545	PAR	C23-C33-O33-C14

There are no ring outliers.

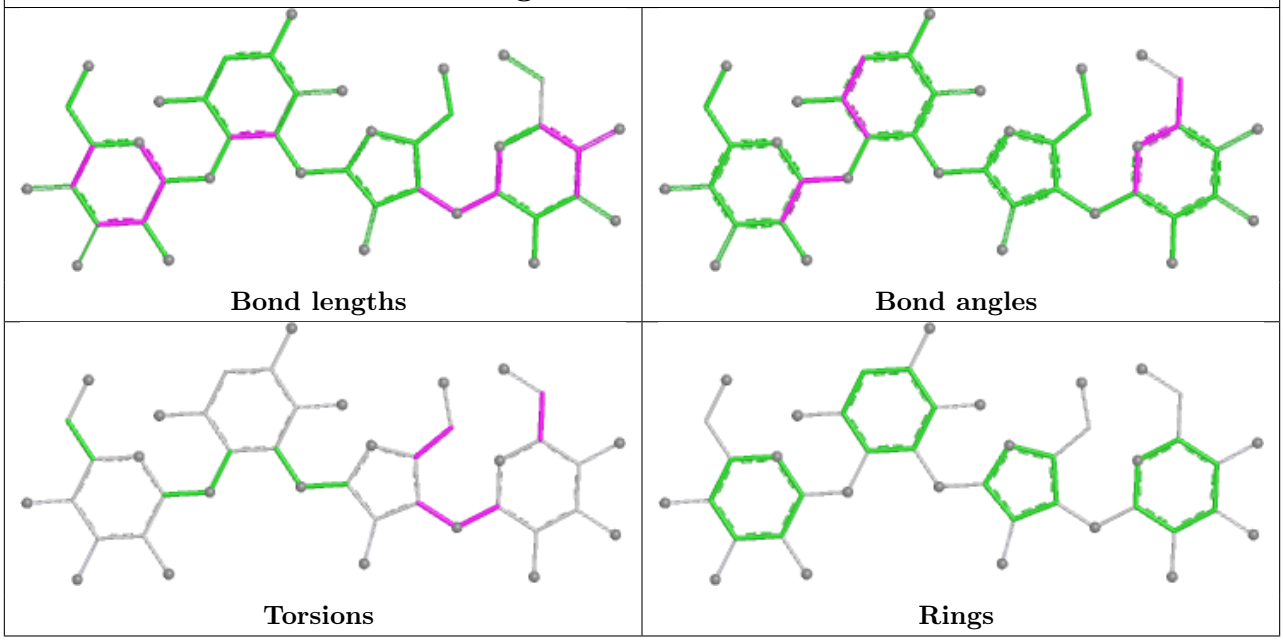
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A	1545	PAR	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand PAR A 1545



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	1513/1522 (99%)	0.49	136 (8%) 17 9	25, 57, 134, 201	0
2	Y	14/17 (82%)	1.78	5 (35%) 1 1	60, 113, 163, 179	0
3	Z	4/6 (66%)	1.82	2 (50%) 0 0	65, 69, 85, 179	0
4	B	234/256 (91%)	1.02	37 (15%) 6 4	38, 96, 154, 190	0
5	C	206/239 (86%)	1.12	38 (18%) 4 3	44, 83, 144, 182	0
6	D	208/208 (100%)	0.55	20 (9%) 15 8	39, 64, 115, 166	0
7	E	150/161 (93%)	0.12	5 (3%) 49 29	27, 50, 86, 155	0
8	F	101/101 (100%)	0.67	6 (5%) 29 16	51, 87, 132, 156	0
9	G	155/155 (100%)	0.61	12 (7%) 21 12	38, 70, 130, 175	0
10	H	138/138 (100%)	-0.03	3 (2%) 62 40	25, 46, 90, 127	0
11	I	127/128 (99%)	1.10	22 (17%) 5 3	39, 86, 135, 161	0
12	J	98/104 (94%)	1.78	35 (35%) 1 1	42, 110, 178, 201	0
13	K	119/129 (92%)	0.45	10 (8%) 18 10	27, 61, 104, 180	0
14	L	124/135 (91%)	0.60	13 (10%) 13 7	22, 61, 114, 166	0
15	M	118/126 (93%)	0.74	14 (11%) 10 6	41, 73, 119, 146	0
16	N	60/60 (100%)	1.31	14 (23%) 2 2	49, 80, 123, 174	0
17	O	88/88 (100%)	0.27	3 (3%) 48 28	34, 60, 109, 178	0
18	P	83/88 (94%)	0.03	1 (1%) 76 56	28, 48, 70, 146	0
19	Q	104/104 (100%)	0.23	9 (8%) 17 10	28, 48, 149, 201	0
20	R	73/88 (82%)	0.37	3 (4%) 42 24	41, 70, 152, 186	0
21	S	80/92 (86%)	1.42	18 (22%) 3 2	53, 101, 164, 180	0
22	T	99/106 (93%)	0.46	8 (8%) 19 11	30, 55, 105, 159	0
23	V	24/26 (92%)	0.95	4 (16%) 5 3	42, 64, 114, 151	0
All	All	3920/4077 (96%)	0.61	418 (10%) 12 7	22, 65, 141, 201	0

The worst 5 of 418 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
21	S	2	PRO	7.0
1	A	1539	C	7.0
6	D	23	GLY	6.3
6	D	31	CYS	6.2
1	A	1129	C	6.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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
2	PSU	Y	38	20/21	0.91	0.19	24,24,24,24	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
25	MG	A	441	1/1	0.39	0.50	24,24,24,24	1
25	MG	A	1655	1/1	0.52	0.47	24,24,24,24	1
25	MG	A	1645	1/1	0.59	0.39	24,24,24,24	1
25	MG	A	1644	1/1	0.66	0.45	24,24,24,24	1
25	MG	A	1615	1/1	0.69	0.18	24,24,24,24	1
25	MG	A	1629	1/1	0.75	0.49	24,24,24,24	1
25	MG	A	1680	1/1	0.75	0.44	24,24,24,24	1
25	MG	A	1635	1/1	0.76	0.38	24,24,24,24	1
25	MG	A	1617	1/1	0.76	0.29	24,24,24,24	1
25	MG	E	468	1/1	0.76	0.18	24,24,24,24	1
25	MG	A	1647	1/1	0.77	0.59	24,24,24,24	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
25	MG	A	1625	1/1	0.79	0.21	24,24,24,24	1
25	MG	A	1675	1/1	0.79	0.27	24,24,24,24	1
25	MG	A	1643	1/1	0.79	0.22	24,24,24,24	1
25	MG	A	1572	1/1	0.79	0.67	24,24,24,24	1
25	MG	A	1567	1/1	0.80	0.32	24,24,24,24	1
25	MG	A	1633	1/1	0.80	0.27	24,24,24,24	1
25	MG	A	71	1/1	0.80	0.39	24,24,24,24	1
25	MG	A	1605	1/1	0.80	0.16	24,24,24,24	1
25	MG	A	1618	1/1	0.81	0.57	24,24,24,24	1
25	MG	A	1678	1/1	0.81	0.30	24,24,24,24	1
25	MG	A	1623	1/1	0.81	0.11	24,24,24,24	1
25	MG	A	1641	1/1	0.81	0.23	24,24,24,24	1
25	MG	A	1619	1/1	0.82	0.40	24,24,24,24	1
25	MG	A	493	1/1	0.82	0.43	24,24,24,24	1
25	MG	A	1620	1/1	0.82	0.37	24,24,24,24	1
25	MG	A	1631	1/1	0.83	0.31	24,24,24,24	1
25	MG	A	1632	1/1	0.83	0.25	24,24,24,24	1
25	MG	A	1669	1/1	0.83	0.14	24,24,24,24	1
25	MG	A	1547	1/1	0.83	0.25	24,24,24,24	0
25	MG	Y	500	1/1	0.84	0.43	24,24,24,24	1
25	MG	A	1603	1/1	0.84	0.29	24,24,24,24	1
25	MG	A	1646	1/1	0.85	0.16	24,24,24,24	0
25	MG	A	1673	1/1	0.85	0.60	24,24,24,24	1
25	MG	A	1676	1/1	0.86	0.18	24,24,24,24	1
25	MG	A	1662	1/1	0.86	0.14	24,24,24,24	1
25	MG	A	1663	1/1	0.86	0.27	24,24,24,24	1
25	MG	A	1597	1/1	0.86	0.30	24,24,24,24	0
25	MG	A	1650	1/1	0.86	0.43	24,24,24,24	1
25	MG	A	1602	1/1	0.86	0.41	24,24,24,24	1
25	MG	A	1664	1/1	0.87	0.27	24,24,24,24	1
25	MG	A	1592	1/1	0.87	0.23	24,24,24,24	1
25	MG	A	1555	1/1	0.87	0.22	24,24,24,24	0
25	MG	A	1624	1/1	0.87	0.51	24,24,24,24	1
25	MG	A	1583	1/1	0.87	0.32	24,24,24,24	1
25	MG	A	1630	1/1	0.88	0.27	24,24,24,24	1
25	MG	A	1649	1/1	0.88	0.19	24,24,24,24	1
25	MG	A	1674	1/1	0.88	0.36	24,24,24,24	1
25	MG	A	210	1/1	0.88	0.14	24,24,24,24	1
24	PAR	A	1545	42/42	0.88	0.12	24,24,24,24	0
25	MG	A	1599	1/1	0.88	0.19	24,24,24,24	0
25	MG	A	1621	1/1	0.88	0.36	24,24,24,24	1
25	MG	A	473	1/1	0.88	0.23	24,24,24,24	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
25	MG	A	1636	1/1	0.88	0.34	24,24,24,24	1
25	MG	D	215	1/1	0.88	0.07	24,24,24,24	1
25	MG	A	1666	1/1	0.88	0.13	24,24,24,24	1
25	MG	A	469	1/1	0.89	0.23	24,24,24,24	1
25	MG	A	1609	1/1	0.89	0.20	24,24,24,24	1
25	MG	A	1613	1/1	0.89	0.36	24,24,24,24	1
25	MG	A	1654	1/1	0.89	0.32	24,24,24,24	1
25	MG	A	1573	1/1	0.89	0.31	24,24,24,24	1
25	MG	A	1672	1/1	0.89	0.15	24,24,24,24	1
25	MG	A	87	1/1	0.89	0.35	24,24,24,24	1
25	MG	A	1563	1/1	0.89	0.27	24,24,24,24	0
25	MG	A	1628	1/1	0.90	0.17	24,24,24,24	0
25	MG	A	1679	1/1	0.90	0.36	24,24,24,24	1
25	MG	A	465	1/1	0.90	0.12	24,24,24,24	1
25	MG	A	1551	1/1	0.90	0.19	24,24,24,24	1
25	MG	A	1610	1/1	0.90	0.09	24,24,24,24	0
25	MG	A	1571	1/1	0.90	0.14	24,24,24,24	1
25	MG	A	1552	1/1	0.90	0.36	24,24,24,24	0
25	MG	J	449	1/1	0.90	0.12	24,24,24,24	1
25	MG	A	213	1/1	0.91	0.17	24,24,24,24	1
25	MG	A	467	1/1	0.91	0.10	24,24,24,24	1
25	MG	A	1575	1/1	0.91	0.10	24,24,24,24	1
25	MG	A	1660	1/1	0.91	0.16	24,24,24,24	0
25	MG	A	1639	1/1	0.91	0.08	24,24,24,24	0
25	MG	A	1653	1/1	0.91	0.34	24,24,24,24	1
25	MG	A	1668	1/1	0.91	0.20	24,24,24,24	1
25	MG	A	471	1/1	0.92	0.38	24,24,24,24	1
25	MG	A	1591	1/1	0.92	0.20	24,24,24,24	1
25	MG	A	1659	1/1	0.92	0.32	24,24,24,24	1
25	MG	A	1556	1/1	0.92	0.23	24,24,24,24	0
25	MG	A	1640	1/1	0.92	0.12	24,24,24,24	0
25	MG	A	1681	1/1	0.92	0.48	24,24,24,24	1
25	MG	A	1604	1/1	0.92	0.12	24,24,24,24	1
25	MG	A	1671	1/1	0.92	0.38	24,24,24,24	1
25	MG	A	1585	1/1	0.92	0.46	24,24,24,24	1
25	MG	A	1607	1/1	0.92	0.30	24,24,24,24	1
25	MG	A	214	1/1	0.92	0.40	24,24,24,24	1
25	MG	A	1656	1/1	0.93	0.14	24,24,24,24	0
25	MG	A	1658	1/1	0.93	0.26	24,24,24,24	1
25	MG	A	1642	1/1	0.93	0.19	24,24,24,24	1
25	MG	A	1582	1/1	0.93	0.13	24,24,24,24	0
25	MG	A	1558	1/1	0.93	0.18	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
25	MG	A	1565	1/1	0.93	0.13	24,24,24,24	0
25	MG	A	464	1/1	0.93	0.10	24,24,24,24	1
25	MG	A	1588	1/1	0.93	0.21	24,24,24,24	0
25	MG	A	466	1/1	0.93	0.47	24,24,24,24	1
25	MG	A	1566	1/1	0.93	0.25	24,24,24,24	0
25	MG	A	1546	1/1	0.93	0.18	24,24,24,24	0
25	MG	A	1594	1/1	0.93	0.22	24,24,24,24	0
25	MG	A	1637	1/1	0.93	0.10	24,24,24,24	0
25	MG	A	1568	1/1	0.93	0.21	24,24,24,24	0
25	MG	A	1577	1/1	0.93	0.18	24,24,24,24	0
25	MG	A	1580	1/1	0.93	0.18	24,24,24,24	1
25	MG	A	1579	1/1	0.94	0.49	24,24,24,24	1
25	MG	A	1677	1/1	0.94	0.41	24,24,24,24	1
25	MG	A	1665	1/1	0.94	0.08	24,24,24,24	1
25	MG	A	1589	1/1	0.94	0.24	24,24,24,24	0
25	MG	A	1561	1/1	0.94	0.18	24,24,24,24	0
25	MG	A	1570	1/1	0.94	0.34	24,24,24,24	1
25	MG	A	1638	1/1	0.94	0.32	24,24,24,24	1
25	MG	A	1553	1/1	0.94	0.18	24,24,24,24	0
25	MG	A	1612	1/1	0.94	0.25	24,24,24,24	1
25	MG	A	1549	1/1	0.94	0.29	24,24,24,24	1
25	MG	A	1661	1/1	0.94	0.25	24,24,24,24	1
25	MG	A	1611	1/1	0.95	0.44	24,24,24,24	1
25	MG	A	1562	1/1	0.95	0.10	24,24,24,24	1
25	MG	A	1590	1/1	0.95	0.42	24,24,24,24	1
25	MG	A	1614	1/1	0.95	0.16	24,24,24,24	1
25	MG	A	1601	1/1	0.95	0.20	24,24,24,24	0
25	MG	A	1616	1/1	0.95	0.49	24,24,24,24	1
25	MG	A	1648	1/1	0.95	0.31	24,24,24,24	1
25	MG	A	1581	1/1	0.95	0.14	24,24,24,24	0
25	MG	A	1557	1/1	0.95	0.24	24,24,24,24	0
25	MG	A	1593	1/1	0.95	0.15	24,24,24,24	0
25	MG	A	1550	1/1	0.95	0.26	24,24,24,24	0
25	MG	A	1606	1/1	0.95	0.09	24,24,24,24	0
25	MG	A	1559	1/1	0.95	0.20	24,24,24,24	0
25	MG	A	1657	1/1	0.95	0.12	24,24,24,24	1
25	MG	A	1587	1/1	0.95	0.22	24,24,24,24	0
25	MG	A	1548	1/1	0.95	0.10	24,24,24,24	0
25	MG	A	1598	1/1	0.96	0.12	24,24,24,24	1
25	MG	A	1578	1/1	0.96	0.17	24,24,24,24	0
25	MG	A	1574	1/1	0.96	0.11	24,24,24,24	0
25	MG	A	1569	1/1	0.96	0.35	24,24,24,24	1

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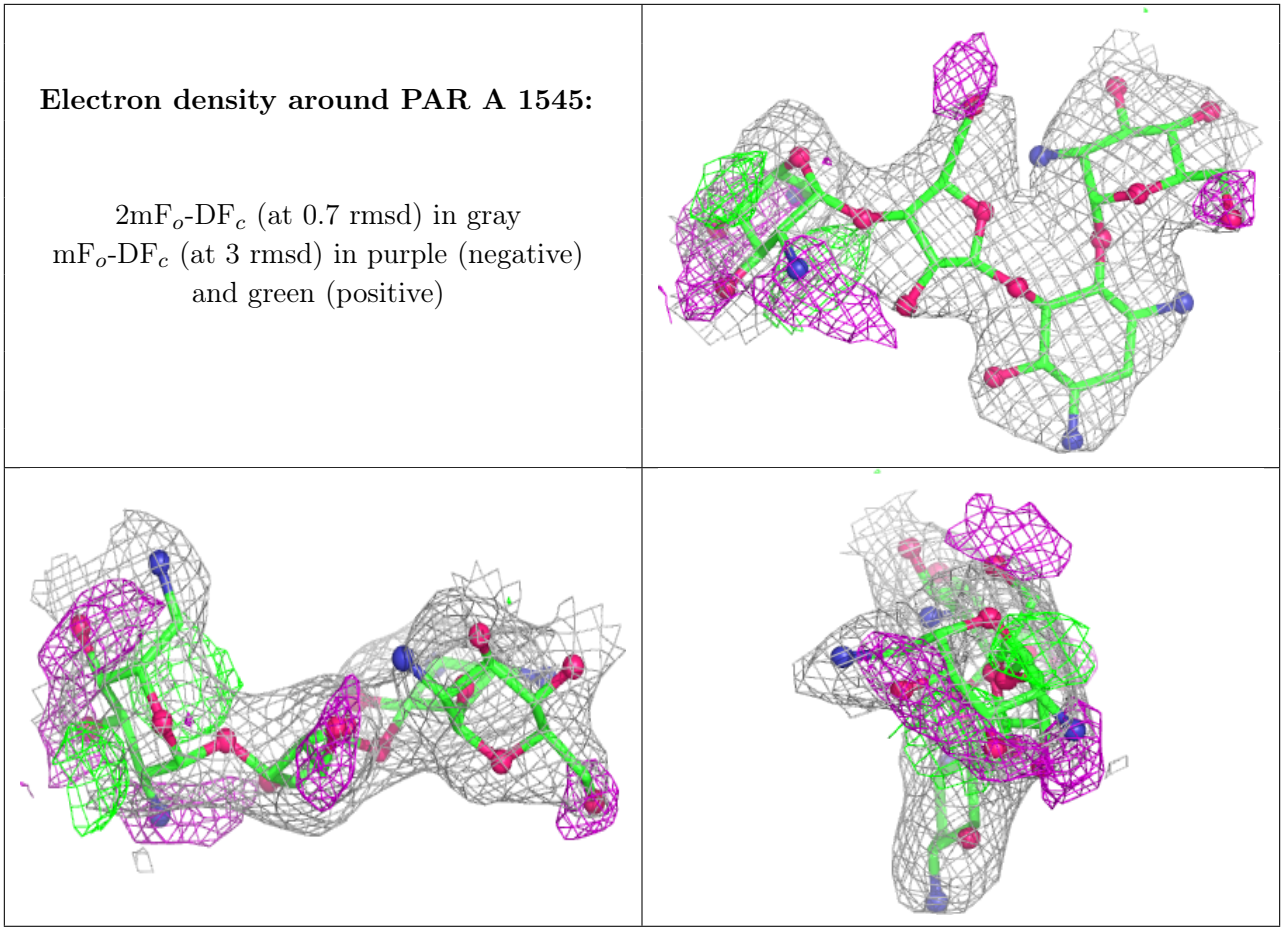
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
25	MG	A	1651	1/1	0.96	0.29	24,24,24,24	1
25	MG	A	1667	1/1	0.96	0.09	24,24,24,24	1
25	MG	A	1652	1/1	0.96	0.09	24,24,24,24	0
25	MG	A	1634	1/1	0.96	0.15	24,24,24,24	1
25	MG	A	1626	1/1	0.96	0.08	24,24,24,24	0
25	MG	A	1627	1/1	0.96	0.23	24,24,24,24	1
25	MG	A	1596	1/1	0.96	0.28	24,24,24,24	0
25	MG	A	1560	1/1	0.96	0.17	24,24,24,24	0
25	MG	M	475	1/1	0.96	0.15	24,24,24,24	1
25	MG	A	1600	1/1	0.97	0.18	24,24,24,24	0
25	MG	A	1586	1/1	0.97	0.07	24,24,24,24	0
25	MG	A	1564	1/1	0.97	0.24	24,24,24,24	1
25	MG	A	86	1/1	0.97	0.17	24,24,24,24	0
25	MG	A	470	1/1	0.97	0.31	24,24,24,24	1
25	MG	A	1622	1/1	0.97	0.32	24,24,24,24	1
25	MG	A	1670	1/1	0.97	0.14	24,24,24,24	1
25	MG	A	1595	1/1	0.97	0.08	24,24,24,24	0
25	MG	A	1584	1/1	0.98	0.29	24,24,24,24	1
25	MG	A	1608	1/1	0.98	0.18	24,24,24,24	1
25	MG	A	1576	1/1	0.98	0.13	24,24,24,24	1
25	MG	A	1554	1/1	0.98	0.26	24,24,24,24	0
25	MG	A	211	1/1	0.98	0.18	24,24,24,24	0
26	ZN	D	306	1/1	0.98	0.17	24,24,24,24	1
26	ZN	N	307	1/1	1.00	0.03	24,24,24,24	1

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 1545:

$2mF_o$-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.