wwPDB X-ray Structure Validation Summary Report (i)

Oct 12, 2021 – 11:58 AM EDT

PDB ID	:	1YIJ
Title	:	Crystal Structure Of Telithromycin Bound To The G2099A Mutant 50S Ribosomal Subunit Of Haloarcula Marismortui
Authors	:	Tu, D.; Blaha, G.; Moore, P.B.; Steitz, T.A.
Deposited on	:	2005-01-12
Resolution	:	2.60 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 following versions of software and data (see references (i)) were used in the production of this report:

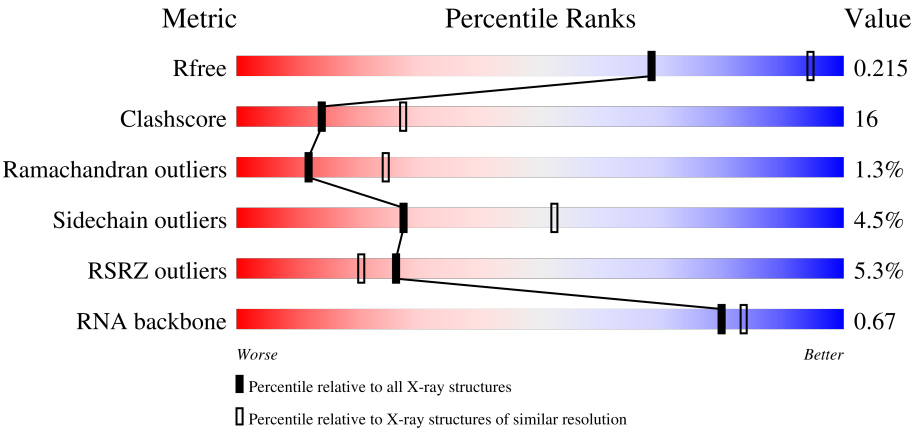
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)
RNA backbone	3102	1040 (2.90-2.30)

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	0	2922	2% 61% 27% 5% 6%
2	9	122	4% 53% 36% 9%
3	A	240	5% 60% 33% 5%
4	B	338	% 50% 45% 5%

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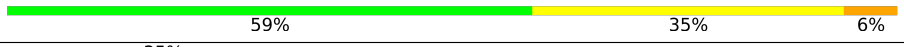
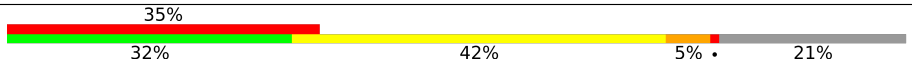
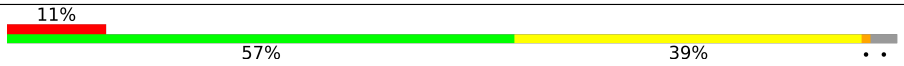
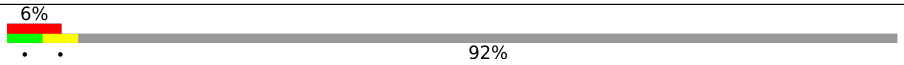
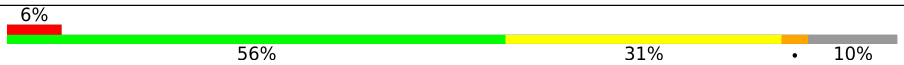
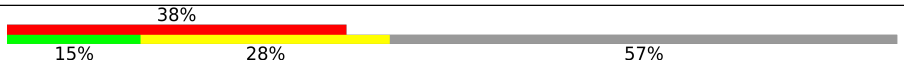
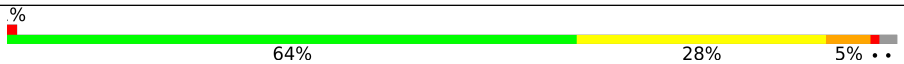
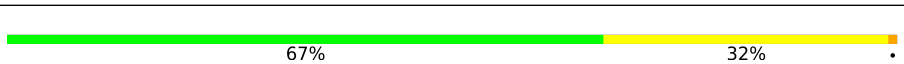
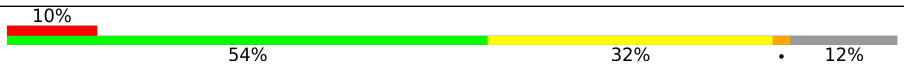
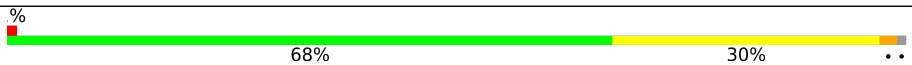
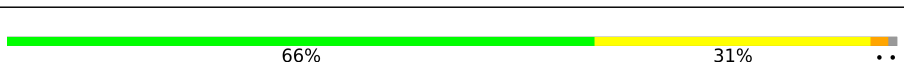
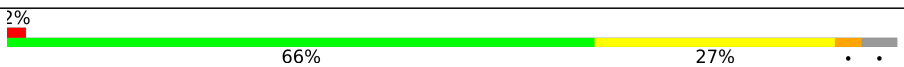
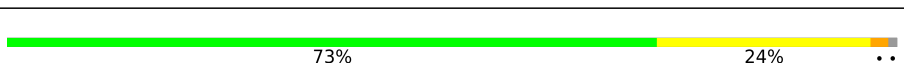
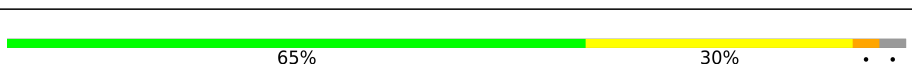
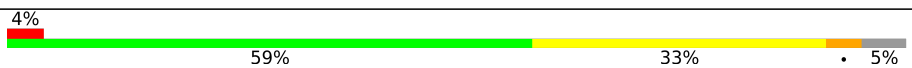
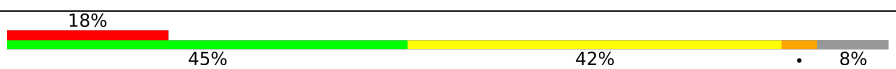
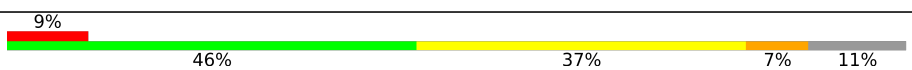
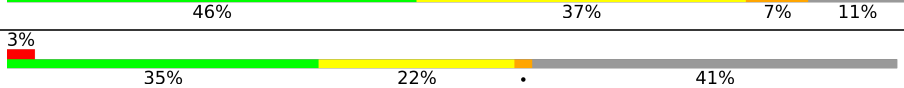
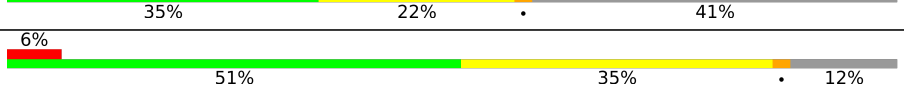
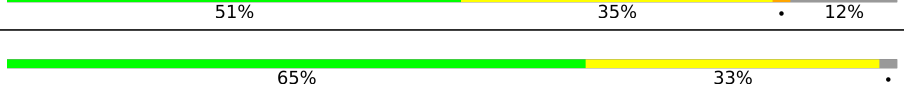
Mol	Chain	Length	Quality of chain
5	C	246	
6	D	177	
7	E	178	
8	F	120	
9	G	348	
10	H	177	
11	I	162	
12	J	145	
13	K	132	
14	L	165	
15	M	195	
16	N	187	
17	O	116	
18	P	149	
19	Q	96	
20	R	155	
21	S	85	
22	T	120	
23	U	66	
24	V	71	
25	W	154	
26	X	92	
27	Y	241	
28	Z	83	
29	1	57	

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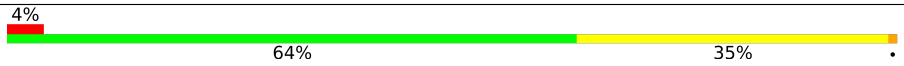
Mol	Chain	Length	Quality of chain
30	2	50	
31	3	92	

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
34	NA	0	8571	-	-	-	X
34	NA	R	8586	-	-	-	X

2 Entry composition (i)

There are 38 unique types of molecules in this entry. The entry contains 99097 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 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	0	2754	59020	26349	10873	19053	2745	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	628	1MA	A	modified residue	GB 55229667
0	2099	A	G	engineered mutation	GB 55229667
0	2587	OMU	U	modified residue	GB 55229667
0	2588	OMG	G	modified residue	GB 55229667
0	2619	UR3	U	modified residue	GB 55229667
0	2621	PSU	U	modified residue	GB 55229667

- Molecule 2 is a RNA chain called 5S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	9	122	2599	1160	471	847	121	0	0	0

- Molecule 3 is a protein called 50S ribosomal protein L2P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	237	1753	1072	352	324	5	0	0	0

- Molecule 4 is a protein called 50S ribosomal protein L3P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	B	337	2625	1616	493	511	5	0	0	0

- Molecule 5 is a protein called 50S ribosomal protein L4E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	246	Total	C	N	O	S	0	0	0
			1859	1131	344	383	1			

- Molecule 6 is a protein called 50S ribosomal protein L5P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	140	Total	C	N	O	S	0	0	0
			1094	685	195	210	4			

- Molecule 7 is a protein called 50S ribosomal protein L6P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	172	Total	C	N	O	S	0	0	0
			1357	840	224	289	4			

- Molecule 8 is a protein called 50S ribosomal protein L7AE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	119	Total	C	N	O	S	0	0	0
			890	551	141	197	1			

- Molecule 9 is a protein called ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	G	29	Total	C	N	O	S	0	0	0
			240	149	39	51	1			

- Molecule 10 is a protein called 50S RIBOSOMAL PROTEIN L10E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	H	160	Total	C	N	O	S	0	0	0
			1282	798	240	238	6			

- Molecule 11 is a protein called 50S RIBOSOMAL PROTEIN L11P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	I	70	Total	C	N	O	S	0	0	0
			519	323	81	114	1			

- Molecule 12 is a protein called 50S ribosomal protein L13P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	J	142	Total	C	N	O	S	0	0	0
			1120	696	199	222	3			

- Molecule 13 is a protein called 50S ribosomal protein L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	K	132	Total	C	N	O	S	0	0	0
			992	609	187	192	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	44	LEU	HIS	conflict	UNP P22450

- Molecule 14 is a protein called 50S ribosomal protein L15P.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	L	145	Total	C	N	O	0	0	0
			1118	670	222	226			

- Molecule 15 is a protein called 50S Ribosomal Protein L15E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	M	194	Total	C	N	O	S	0	0	0
			1558	942	332	283	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	13	GLU	LYS	conflict	GB 55231501

- Molecule 16 is a protein called 50S ribosomal protein L18P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	N	186	Total	C	N	O	S	0	0	0
			1445	895	262	286	2			

- Molecule 17 is a protein called 50S ribosomal protein L18e.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	O	115	Total	C	N	O	0	0	0
			865	529	161	175			

- Molecule 18 is a protein called 50S ribosomal protein L19E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	P	143	Total	C	N	O	0	0	0
			1136	683	229	224			

- Molecule 19 is a protein called 50S ribosomal protein L21e.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	Q	95	Total	C	N	O	0	0	0
			735	450	141	144			

- Molecule 20 is a protein called 50S ribosomal protein L22P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	150	Total	C	N	O	S	0	0	0
			1149	713	209	223	4			

- Molecule 21 is a protein called 50S ribosomal protein L23P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	S	81	Total	C	N	O	S	0	0	0
			641	389	111	138	3			

- Molecule 22 is a protein called 50S ribosomal protein L24P.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
22	T	119	Total	C	N	O	0	0	0
			950	568	180	202			

- Molecule 23 is a protein called 50S ribosomal protein L24E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	U	53	Total	C	N	O	S	0	0	0
			410	244	75	86	5			

- Molecule 24 is a protein called 50S ribosomal protein L29P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	V	65	Total	C	N	O	S	0	0	0
			499	304	94	100	1			

- Molecule 25 is a protein called 50S ribosomal protein L30P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	W	154	Total	C	N	O	S	0	0	0
			1196	737	209	244	6			

- Molecule 26 is a protein called 50S ribosomal protein L31e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	X	82	Total	C	N	O	S	0	0	0
			654	402	129	122	1			

- Molecule 27 is a protein called 50S ribosomal protein L32E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
27	Y	142	Total	C	N	O	0	0	0
			1130	686	228	216			

- Molecule 28 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	Z	73	Total	C	N	O	S	0	0	0
			578	346	116	111	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	10	ARG	SER	conflict	GB 55231162

- Molecule 29 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 30 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

- Molecule 31 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	0	106	Total	Mg	0	0
			106	106		
32	9	1	Total	Mg	0	0
			1	1		
32	A	2	Total	Mg	0	0
			2	2		
32	B	2	Total	Mg	0	0
			2	2		
32	K	1	Total	Mg	0	0
			1	1		
32	T	1	Total	Mg	0	0
			1	1		
32	Y	1	Total	Mg	0	0
			1	1		
32	2	1	Total	Mg	0	0
			1	1		
32	3	1	Total	Mg	0	0
			1	1		

- Molecule 33 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	2	Total	K	0	0
			2	2		

- Molecule 34 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	0	72	Total	Na	0	0
			72	72		
34	9	2	Total	Na	0	0
			2	2		
34	A	1	Total	Na	0	0
			1	1		
34	C	1	Total	Na	0	0
			1	1		

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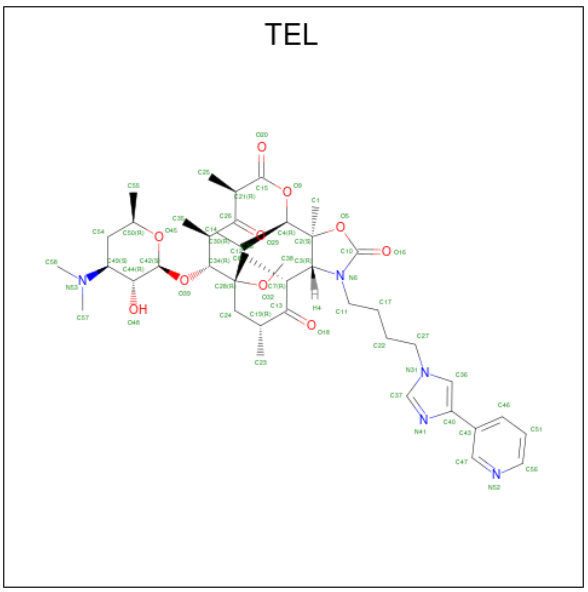
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	H	1	Total Na 1 1	0	0
34	J	1	Total Na 1 1	0	0
34	L	1	Total Na 1 1	0	0
34	M	1	Total Na 1 1	0	0
34	Q	1	Total Na 1 1	0	0
34	R	3	Total Na 3 3	0	0
34	S	1	Total Na 1 1	0	0
34	T	1	Total Na 1 1	0	0

- Molecule 35 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	0	9	Total Cl 9 9	0	0
35	A	1	Total Cl 1 1	0	0
35	B	1	Total Cl 1 1	0	0
35	J	3	Total Cl 3 3	0	0
35	L	1	Total Cl 1 1	0	0
35	M	1	Total Cl 1 1	0	0
35	N	1	Total Cl 1 1	0	0
35	O	1	Total Cl 1 1	0	0
35	R	1	Total Cl 1 1	0	0
35	Y	2	Total Cl 2 2	0	0
35	3	1	Total Cl 1 1	0	0

- Molecule 36 is TELITHROMYCIN (three-letter code: TEL) (formula: $C_{43}H_{65}N_5O_{10}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	0	1	Total C N O 58 43 5 10	0	0

- Molecule 37 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	O	1	Total Cd 1 1	0	0
37	U	1	Total Cd 1 1	0	0
37	Z	1	Total Cd 1 1	0	0
37	1	1	Total Cd 1 1	0	0
37	3	1	Total Cd 1 1	0	0

- Molecule 38 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	0	5881	Total O 5881 5881	0	0
38	9	140	Total O 140 140	0	0
38	A	120	Total O 120 120	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	B	153	Total O 153 153	0	0
38	C	174	Total O 174 174	0	0
38	D	46	Total O 46 46	0	0
38	E	41	Total O 41 41	0	0
38	F	27	Total O 27 27	0	0
38	G	18	Total O 18 18	0	0
38	H	71	Total O 71 71	0	0
38	I	9	Total O 9 9	0	0
38	J	54	Total O 54 54	0	0
38	K	65	Total O 65 65	0	0
38	L	83	Total O 83 83	0	0
38	M	130	Total O 130 130	0	0
38	N	62	Total O 62 62	0	0
38	O	41	Total O 41 41	0	0
38	P	62	Total O 62 62	0	0
38	Q	46	Total O 46 46	0	0
38	R	81	Total O 81 81	0	0
38	S	38	Total O 38 38	0	0
38	T	37	Total O 37 37	0	0
38	U	25	Total O 25 25	0	0
38	V	14	Total O 14 14	0	0

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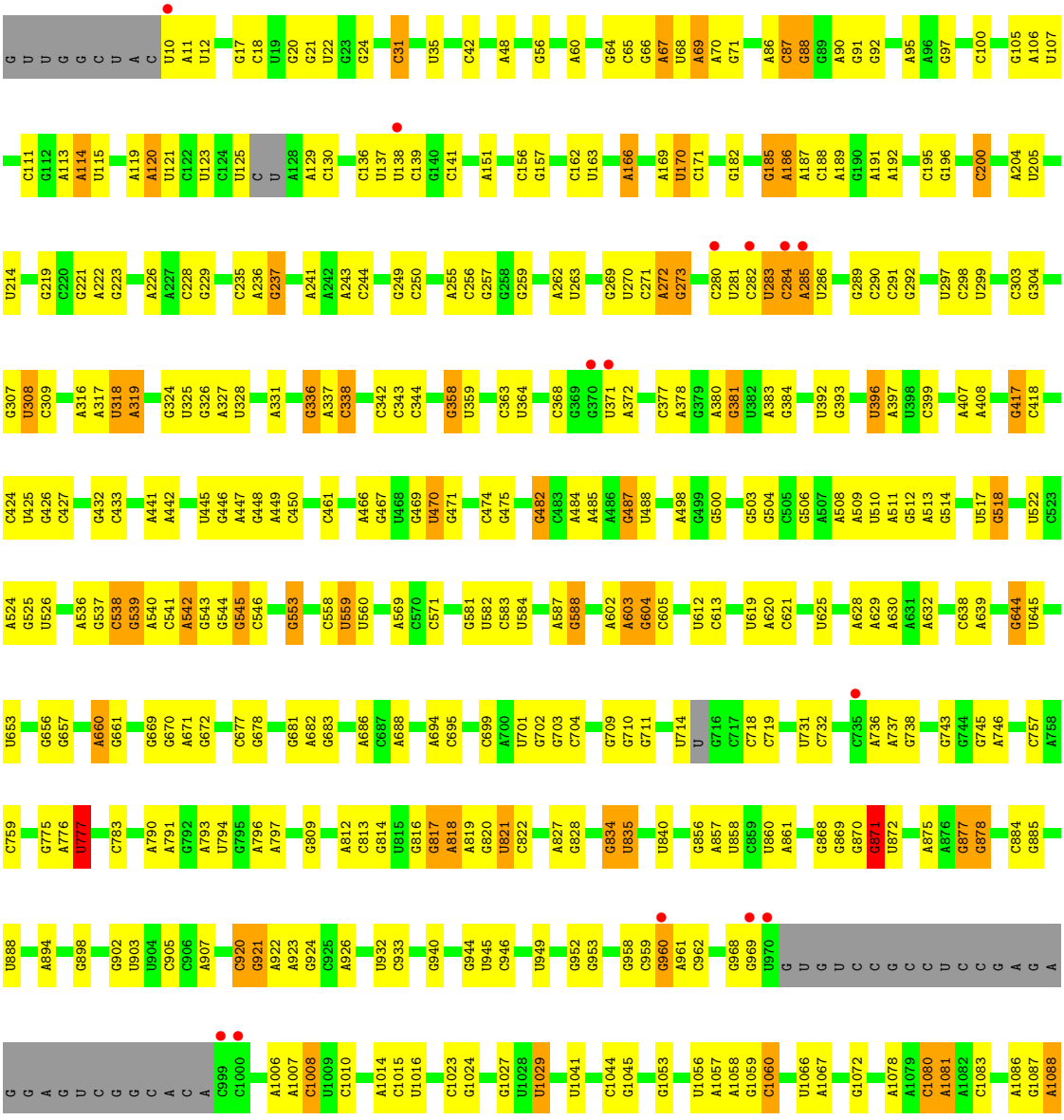
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	W	71	Total O 71 71	0	0
38	X	25	Total O 25 25	0	0
38	Y	96	Total O 96 96	0	0
38	Z	30	Total O 30 30	0	0
38	1	57	Total O 57 57	0	0
38	2	42	Total O 42 42	0	0
38	3	73	Total O 73 73	0	0

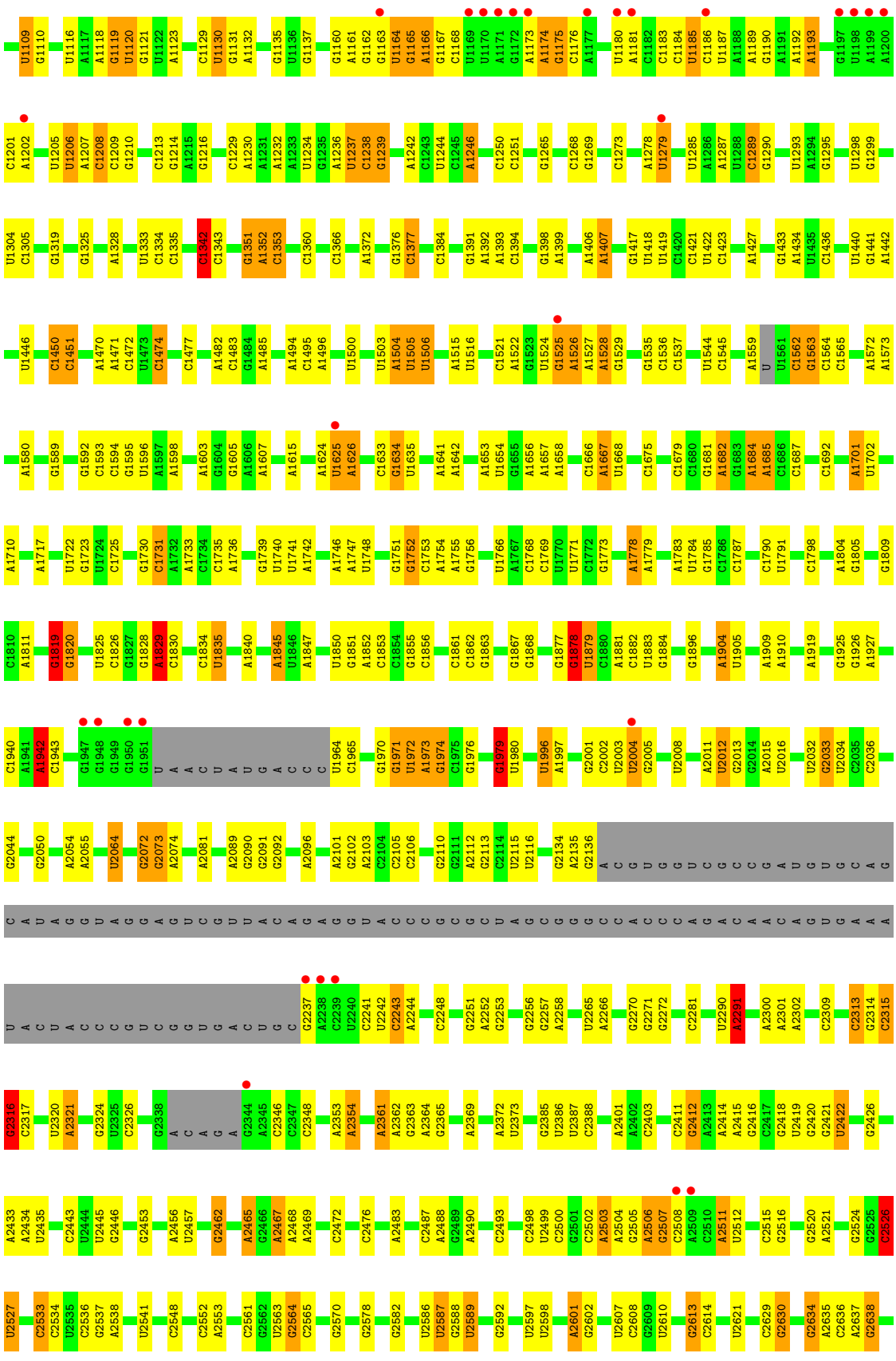
3 Residue-property plots (i)

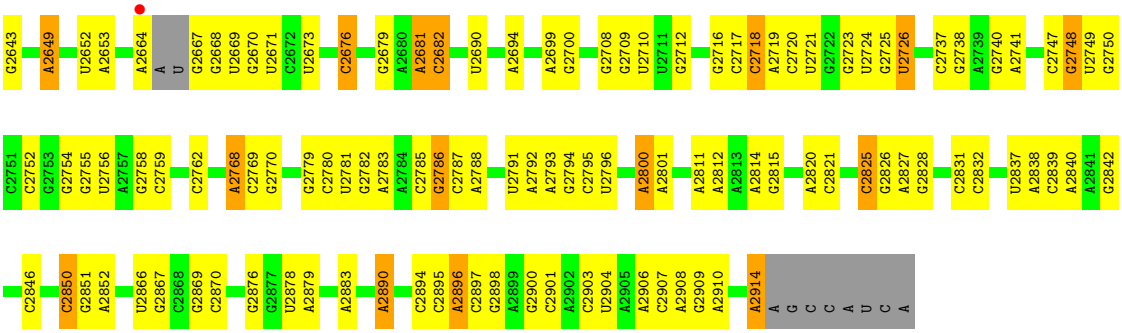
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 23S Ribosomal RNA

Chain 0:

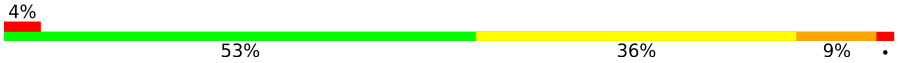


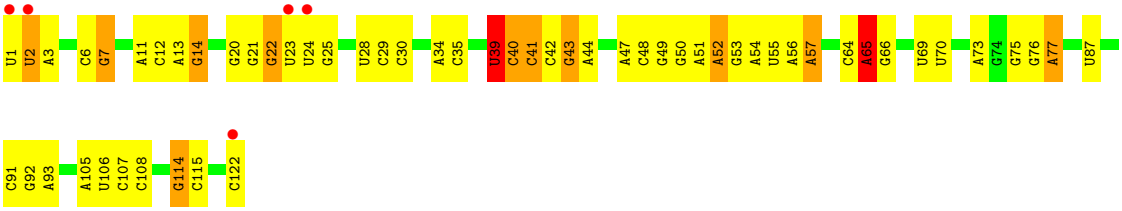




• Molecule 2: 5S Ribosomal RNA

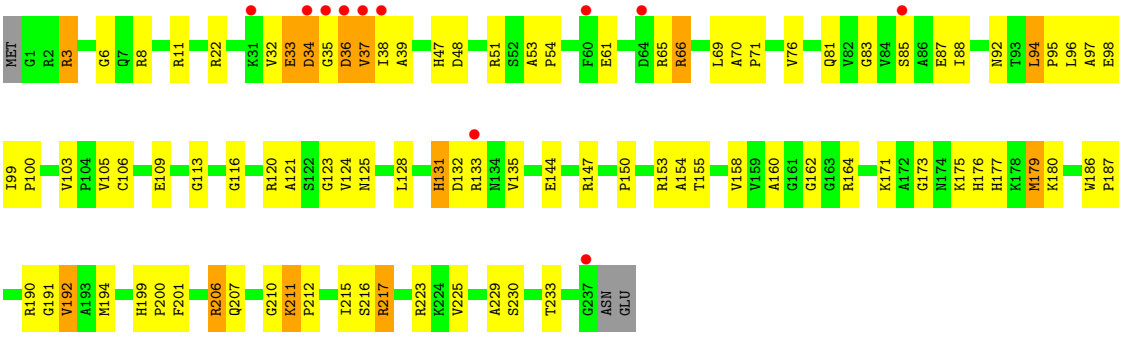
Chain 9:





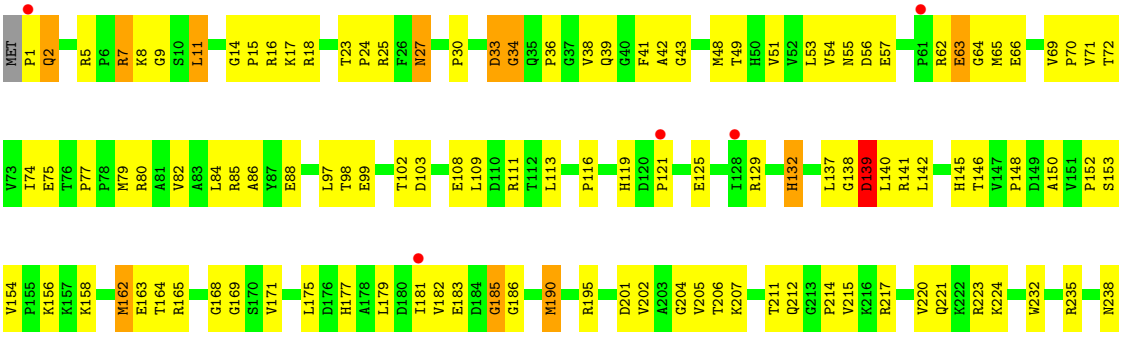
• Molecule 3: 50S ribosomal protein L2P

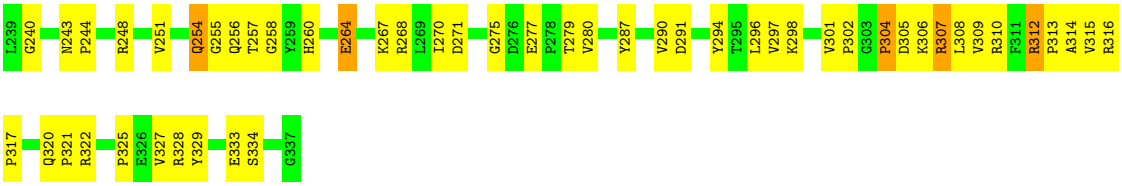
Chain A:



• Molecule 4: 50S ribosomal protein L3P

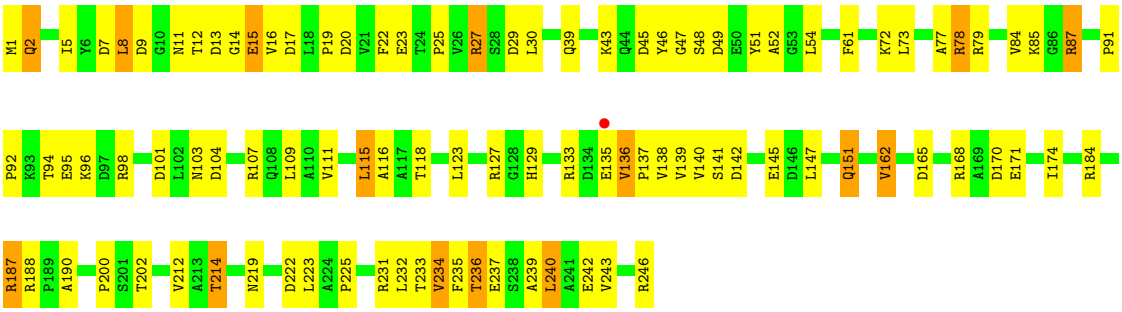
Chain B:





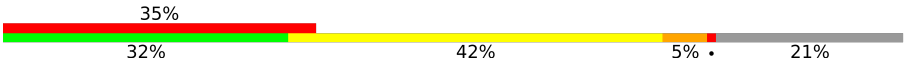
• Molecule 5: 50S ribosomal protein L4E

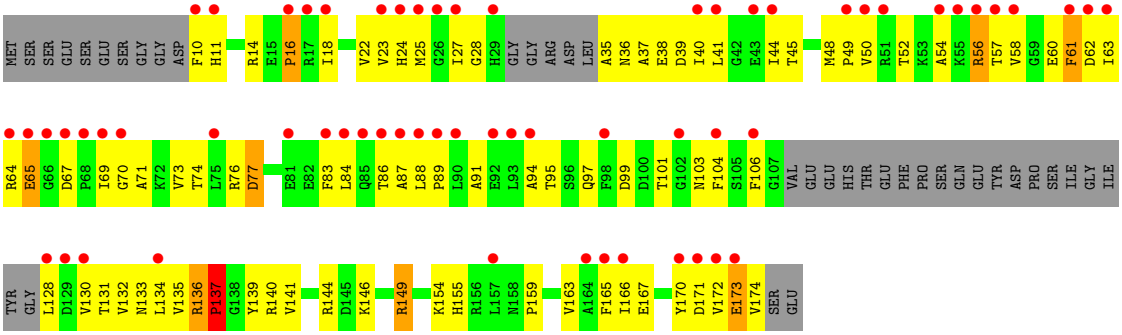
Chain C:



• Molecule 6: 50S ribosomal protein L5P

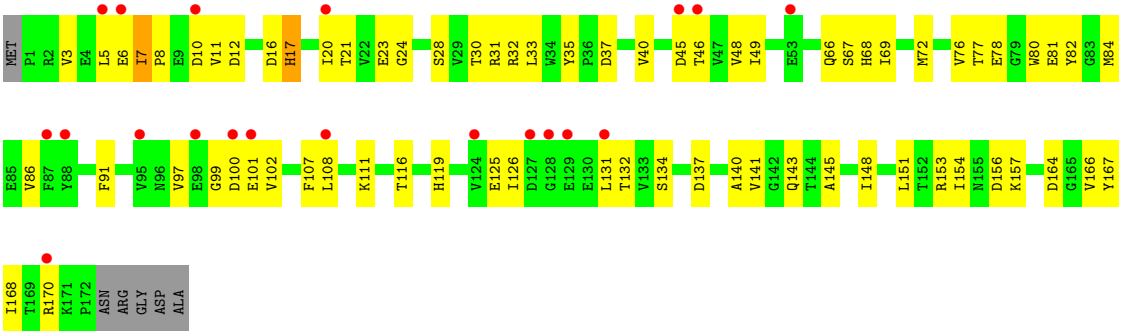
Chain D:





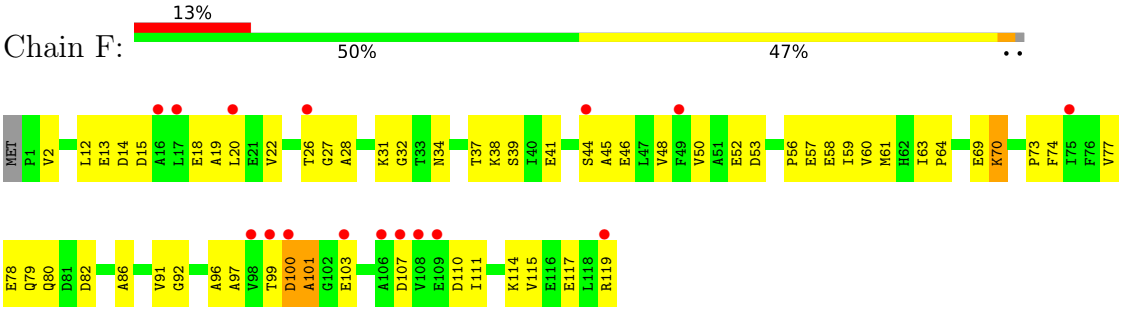
• Molecule 7: 50S ribosomal protein L6P

Chain E:



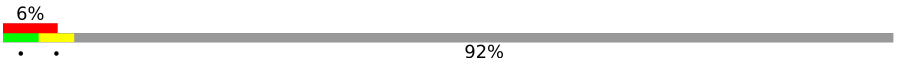
• Molecule 8: 50S ribosomal protein L7AE

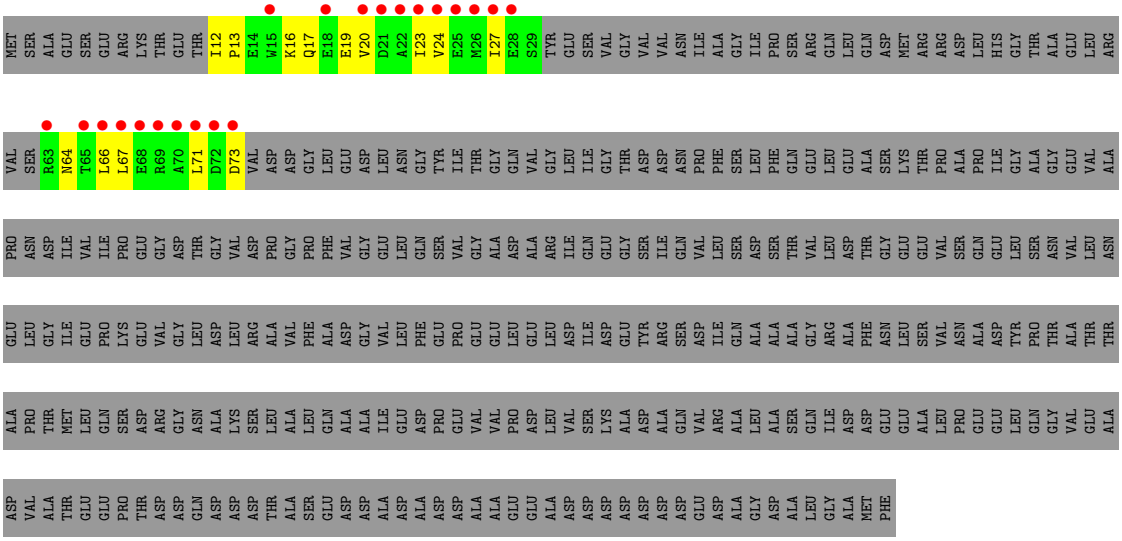
Chain F:



• Molecule 9: ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG

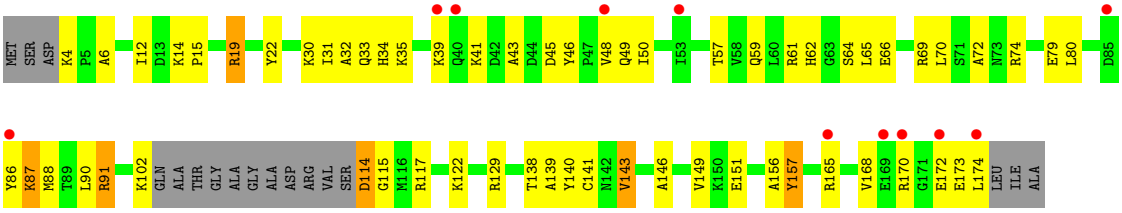
Chain G:





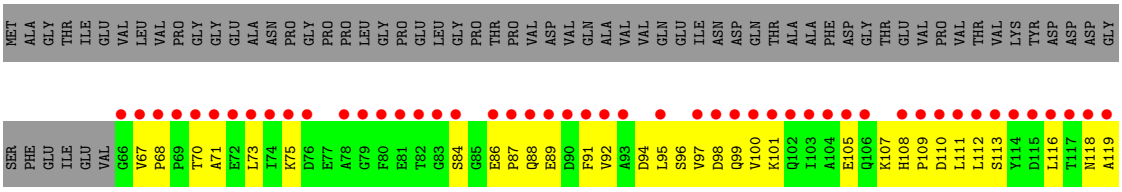
• Molecule 10: 50S RIBOSOMAL PROTEIN L10E

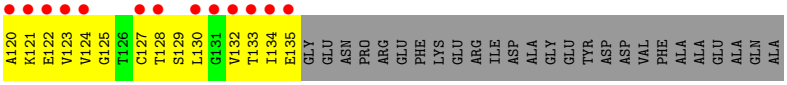
Chain H:



• Molecule 11: 50S RIBOSOMAL PROTEIN L11P

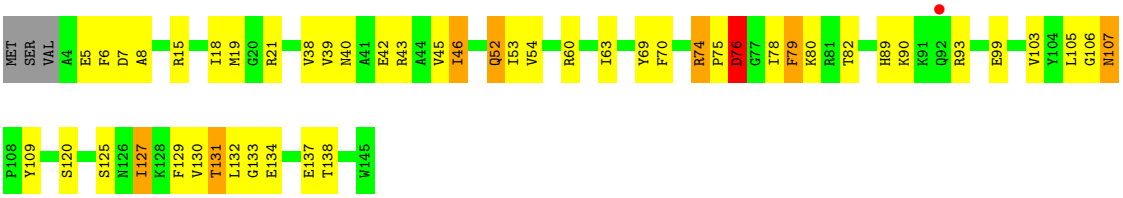
Chain I:





• Molecule 12: 50S ribosomal protein L13P

Chain J:

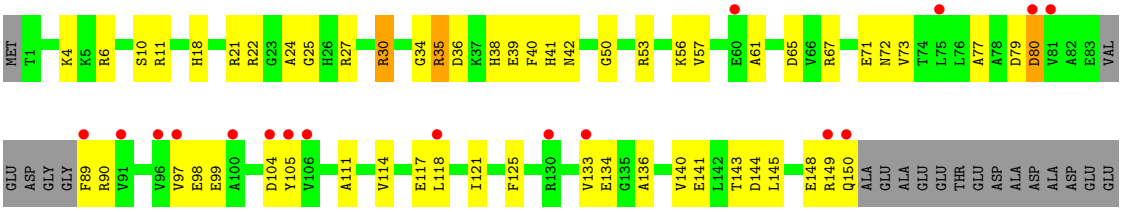


• Molecule 13: 50S ribosomal protein L14P

Chain K:

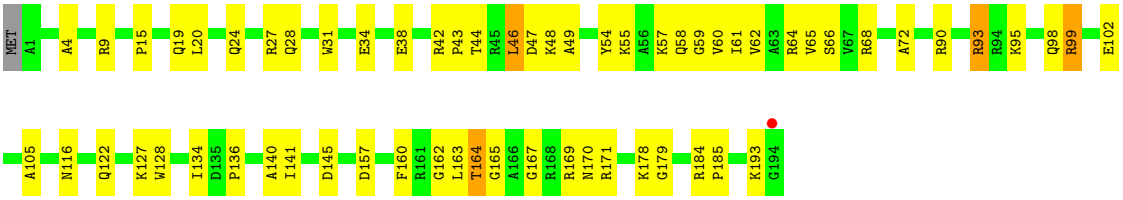
• Molecule 14: 50S ribosomal protein L15P

Chain L:



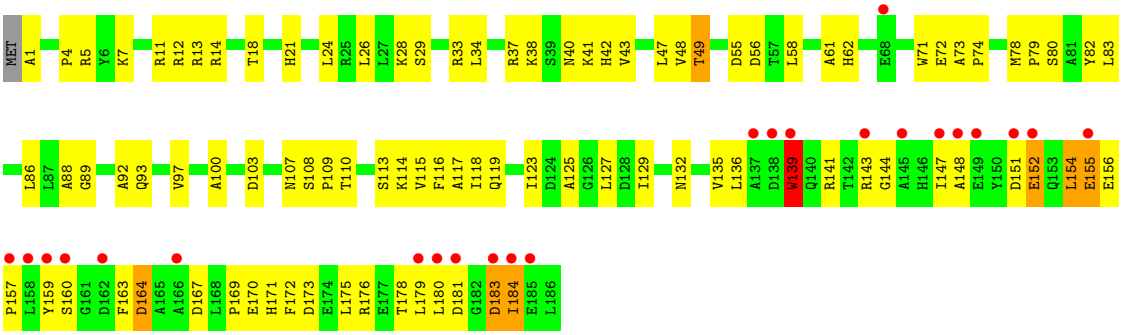
• Molecule 15: 50S Ribosomal Protein L15E

Chain M:



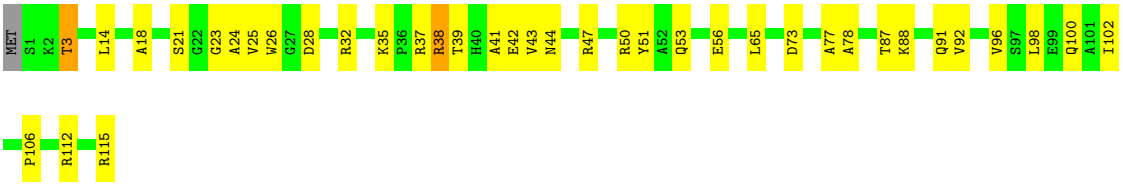
• Molecule 16: 50S ribosomal protein L18P

Chain N:



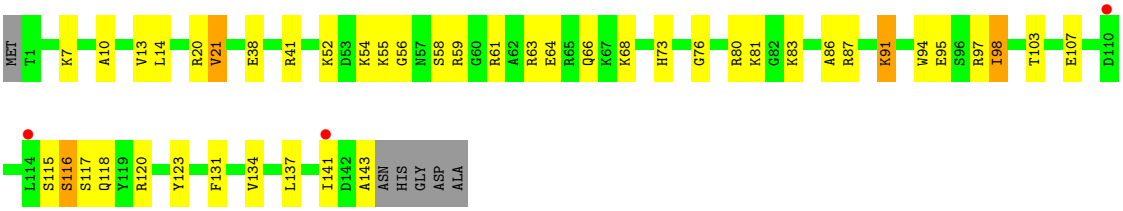
• Molecule 17: 50S ribosomal protein L18e

Chain O:



• Molecule 18: 50S ribosomal protein L19E

Chain P:

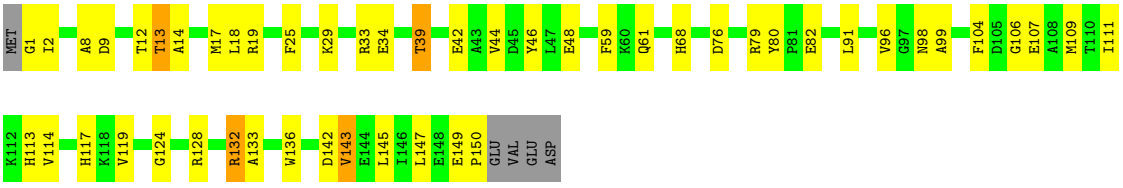


• Molecule 19: 50S ribosomal protein L21e

Chain Q:

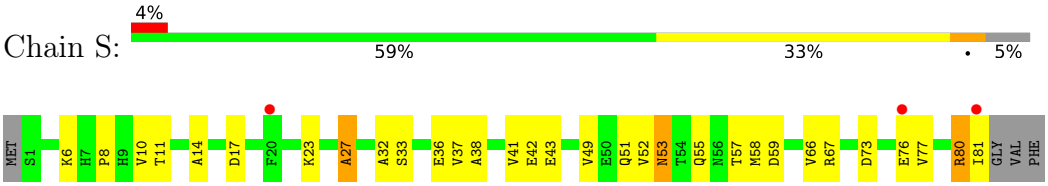
• Molecule 20: 50S ribosomal protein L22P

Chain R:



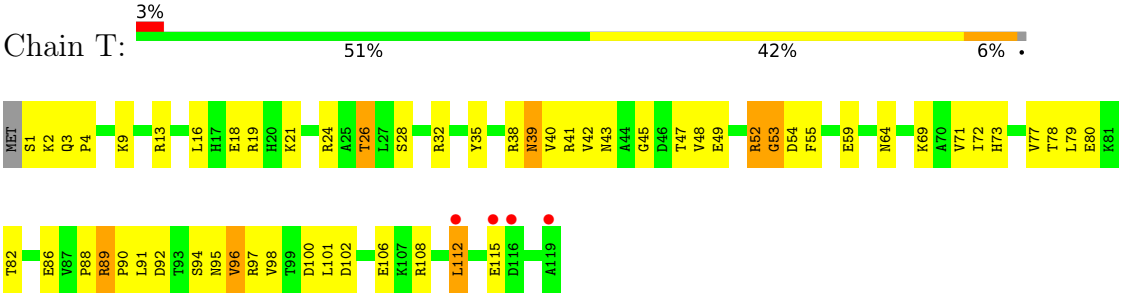
• Molecule 21: 50S ribosomal protein L23P

Chain S:



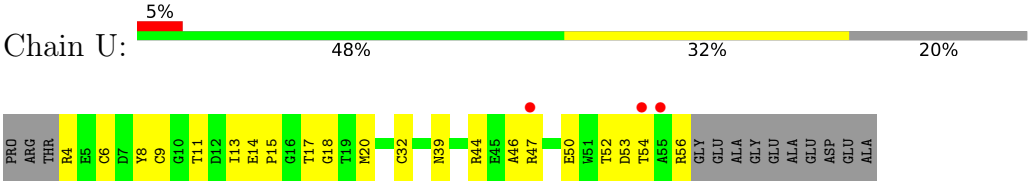
• Molecule 22: 50S ribosomal protein L24P

Chain T:



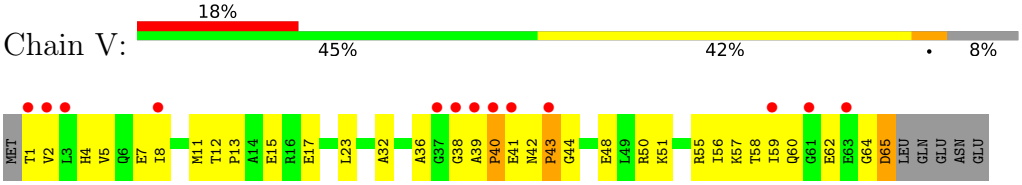
• Molecule 23: 50S ribosomal protein L24E

Chain U:



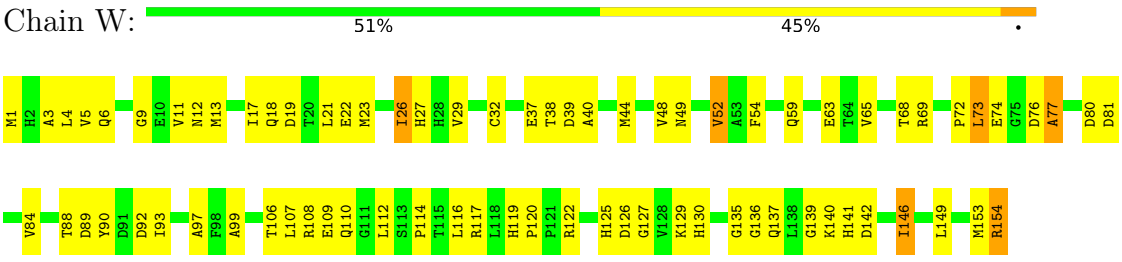
• Molecule 24: 50S ribosomal protein L29P

Chain V:



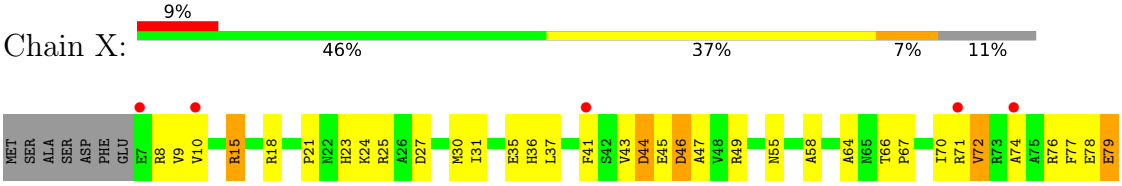
• Molecule 25: 50S ribosomal protein L30P

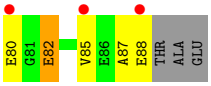
Chain W:



• Molecule 26: 50S ribosomal protein L31e

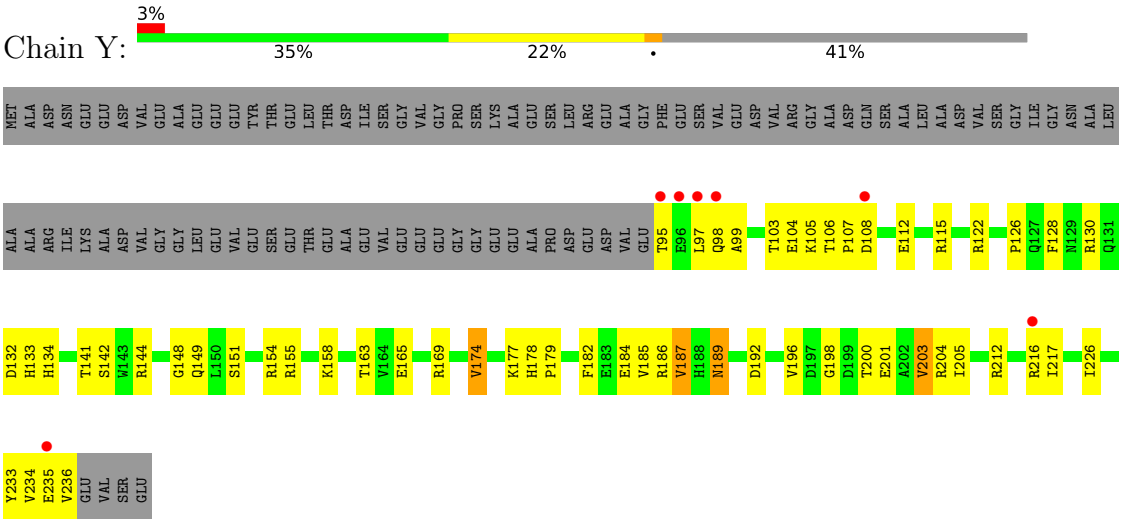
Chain X:





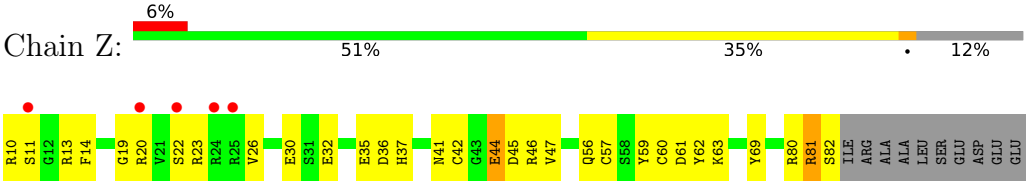
• Molecule 27: 50S ribosomal protein L32E

Chain Y:



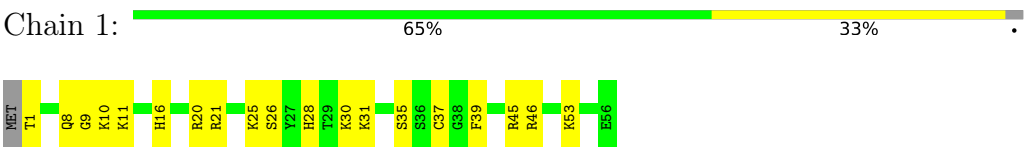
• Molecule 28: 50S ribosomal protein L37Ae

Chain Z:



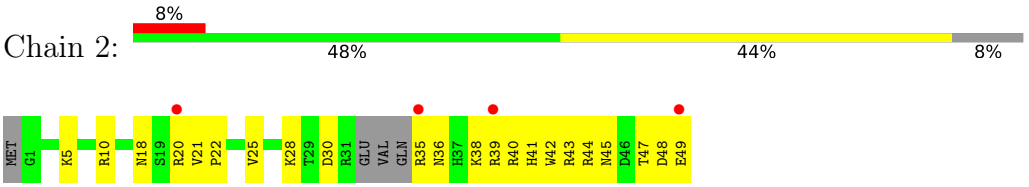
• Molecule 29: 50S ribosomal protein L37e

Chain 1:



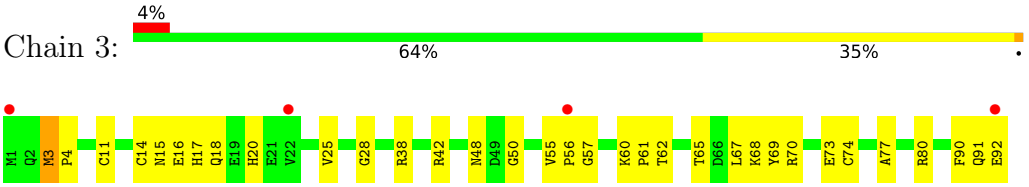
• Molecule 30: 50S ribosomal protein L39e

Chain 2:



• Molecule 31: 50S ribosomal protein L44E

Chain 3:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	212.22Å 300.19Å 574.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.96 – 2.60 49.84 – 2.60	Depositor EDS
% Data completeness (in resolution range)	93.6 (29.96-2.60) 93.7 (49.84-2.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.20 (at 2.61Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.182 , 0.220 0.177 , 0.215	Depositor DCC
R_{free} test set	5105 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å^2)	47.6	Xtriage
Anisotropy	0.245	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 55.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	99097	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.51% 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: CD, CL, 1MA, UR3, PSU, MG, K, OMG, TEL, OMU, NA

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	0	0.35	0/65957	0.69	18/102867 (0.0%)
2	9	0.33	0/2904	0.69	2/4526 (0.0%)
3	A	0.31	0/1786	0.64	0/2408
4	B	0.32	0/2690	0.64	0/3652
5	C	0.37	0/1884	0.64	0/2551
6	D	0.30	0/1111	0.53	0/1498
7	E	0.31	0/1382	0.56	0/1880
8	F	0.31	0/901	0.55	0/1224
9	G	0.27	0/241	0.46	0/324
10	H	0.33	0/1302	0.65	0/1743
11	I	0.30	0/526	0.53	0/716
12	J	0.35	0/1136	0.61	0/1530
13	K	0.34	0/1001	0.67	0/1347
14	L	0.32	0/1130	0.63	0/1509
15	M	0.34	0/1582	0.61	0/2117
16	N	0.29	0/1474	0.61	0/1999
17	O	0.32	0/874	0.57	0/1181
18	P	0.33	0/1147	0.53	0/1528
19	Q	0.35	0/749	0.69	0/1005
20	R	0.34	0/1172	0.64	0/1578
21	S	0.33	0/648	0.58	1/875 (0.1%)
22	T	0.30	0/958	0.62	1/1289 (0.1%)
23	U	0.32	0/417	0.55	0/562
24	V	0.28	0/502	0.54	0/675
25	W	0.34	0/1219	0.62	0/1655
26	X	0.34	0/664	0.57	0/895
27	Y	0.35	0/1146	0.63	0/1536
28	Z	0.32	0/589	0.62	0/787
29	1	0.39	0/438	0.63	0/578
30	2	0.33	0/401	0.53	0/529
31	3	0.36	0/771	0.57	0/1024
All	All	0.34	0/98702	0.67	22/147588 (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	0	0	46
2	9	0	3
All	All	0	49

There are no bond length outliers.

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	0	1563	G	C2'-C3'-O3'	9.32	130.00	109.50
1	0	1942	A	C5'-C4'-C3'	7.76	128.42	116.00
1	0	871	G	C5'-C4'-O4'	-7.10	100.58	109.10
2	9	39	U	N1-C1'-C2'	6.67	122.67	114.00
1	0	1504	A	C1'-O4'-C4'	-6.47	104.72	109.90

There are no chirality outliers.

5 of 49 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	22	U	Sidechain
1	0	221	G	Sidechain
1	0	270	U	Sidechain
1	0	396	U	Sidechain
1	0	48	A	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	0	59020	0	29810	819	0
2	9	2599	0	1325	62	0
3	A	1753	0	1766	126	0
4	B	2625	0	2533	173	0
5	C	1859	0	1816	118	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	1094	0	1085	81	0
7	E	1357	0	1266	63	0
8	F	890	0	843	53	0
9	G	240	0	231	15	0
10	H	1282	0	1292	71	0
11	I	519	0	500	60	0
12	J	1120	0	1098	62	0
13	K	992	0	1031	56	0
14	L	1118	0	1076	55	0
15	M	1558	0	1566	63	0
16	N	1445	0	1401	117	0
17	O	865	0	873	33	0
18	P	1136	0	1123	44	0
19	Q	735	0	729	25	0
20	R	1149	0	1122	59	0
21	S	641	0	605	26	0
22	T	950	0	923	60	0
23	U	410	0	364	22	0
24	V	499	0	511	38	0
25	W	1196	0	1137	93	0
26	X	654	0	653	44	0
27	Y	1130	0	1133	60	0
28	Z	578	0	540	25	0
29	1	431	0	426	29	0
30	2	396	0	413	29	0
31	3	755	0	728	29	0
32	0	106	0	0	0	0
32	2	1	0	0	0	0
32	3	1	0	0	0	0
32	9	1	0	0	0	0
32	A	2	0	0	0	0
32	B	2	0	0	0	0
32	K	1	0	0	0	0
32	T	1	0	0	0	0
32	Y	1	0	0	0	0
33	0	2	0	0	0	0
34	0	72	0	0	0	0
34	9	2	0	0	0	0
34	A	1	0	0	0	0
34	C	1	0	0	0	0
34	H	1	0	0	0	0
34	J	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	L	1	0	0	0	0
34	M	1	0	0	0	0
34	Q	1	0	0	0	0
34	R	3	0	0	0	0
34	S	1	0	0	0	0
34	T	1	0	0	0	0
35	0	9	0	0	0	0
35	3	1	0	0	0	0
35	A	1	0	0	0	0
35	B	1	0	0	0	0
35	J	3	0	0	1	0
35	L	1	0	0	0	0
35	M	1	0	0	0	0
35	N	1	0	0	0	0
35	O	1	0	0	0	0
35	R	1	0	0	0	0
35	Y	2	0	0	0	0
36	0	58	0	65	0	0
37	1	1	0	0	0	0
37	3	1	0	0	0	0
37	O	1	0	0	0	0
37	U	1	0	0	0	0
37	Z	1	0	0	0	0
38	0	5881	0	0	140	0
38	1	57	0	0	4	0
38	2	42	0	0	3	0
38	3	73	0	0	7	0
38	9	140	0	0	8	0
38	A	120	0	0	22	0
38	B	153	0	0	25	0
38	C	174	0	0	23	0
38	D	46	0	0	14	0
38	E	41	0	0	8	0
38	F	27	0	0	6	0
38	G	18	0	0	2	0
38	H	71	0	0	17	0
38	I	9	0	0	3	0
38	J	54	0	0	3	0
38	K	65	0	0	15	0
38	L	83	0	0	21	0
38	M	130	0	0	9	0
38	N	62	0	0	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	O	41	0	0	9	0
38	P	62	0	0	5	0
38	Q	46	0	0	5	0
38	R	81	0	0	9	0
38	S	38	0	0	4	0
38	T	37	0	0	7	0
38	U	25	0	0	2	0
38	V	14	0	0	3	0
38	W	71	0	0	9	0
38	X	25	0	0	7	0
38	Y	96	0	0	13	0
38	Z	30	0	0	1	0
All	All	99097	0	59984	2362	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 16.

The worst 5 of 2362 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)
4:B:162:MET:HE1	4:B:308:LEU:HD21	1.31	1.06
5:C:236:THR:HG22	5:C:239:ALA:H	1.15	1.06
6:D:154:LYS:H	6:D:154:LYS:HD2	1.14	1.06
2:9:6:C:H5”	16:N:37:ARG:NH1	1.71	1.05
2:9:6:C:H5”	16:N:37:ARG:HH12	1.15	1.05

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
3	A	235/240 (98%)	205 (87%)	27 (12%)	3 (1%)	12 24
4	B	335/338 (99%)	302 (90%)	29 (9%)	4 (1%)	13 27
5	C	244/246 (99%)	225 (92%)	17 (7%)	2 (1%)	19 39
6	D	134/177 (76%)	103 (77%)	22 (16%)	9 (7%)	1 1
7	E	170/178 (96%)	159 (94%)	10 (6%)	1 (1%)	25 47
8	F	117/120 (98%)	103 (88%)	10 (8%)	4 (3%)	3 5
9	G	25/348 (7%)	23 (92%)	2 (8%)	0	100 100
10	H	156/177 (88%)	144 (92%)	10 (6%)	2 (1%)	12 24
11	I	68/162 (42%)	53 (78%)	15 (22%)	0	100 100
12	J	140/145 (97%)	128 (91%)	8 (6%)	4 (3%)	4 7
13	K	130/132 (98%)	119 (92%)	11 (8%)	0	100 100
14	L	141/165 (86%)	122 (86%)	18 (13%)	1 (1%)	22 43
15	M	192/195 (98%)	177 (92%)	15 (8%)	0	100 100
16	N	184/187 (98%)	169 (92%)	9 (5%)	6 (3%)	4 6
17	O	113/116 (97%)	109 (96%)	4 (4%)	0	100 100
18	P	141/149 (95%)	136 (96%)	4 (3%)	1 (1%)	22 43
19	Q	93/96 (97%)	87 (94%)	6 (6%)	0	100 100
20	R	148/155 (96%)	137 (93%)	11 (7%)	0	100 100
21	S	79/85 (93%)	72 (91%)	7 (9%)	0	100 100
22	T	117/120 (98%)	110 (94%)	6 (5%)	1 (1%)	17 35
23	U	51/66 (77%)	47 (92%)	4 (8%)	0	100 100
24	V	63/71 (89%)	57 (90%)	4 (6%)	2 (3%)	4 6
25	W	152/154 (99%)	148 (97%)	2 (1%)	2 (1%)	12 24
26	X	80/92 (87%)	70 (88%)	9 (11%)	1 (1%)	12 24
27	Y	140/241 (58%)	138 (99%)	2 (1%)	0	100 100
28	Z	71/83 (86%)	60 (84%)	8 (11%)	3 (4%)	3 3
29	1	54/57 (95%)	52 (96%)	2 (4%)	0	100 100
30	2	42/50 (84%)	39 (93%)	3 (7%)	0	100 100
31	3	90/92 (98%)	85 (94%)	4 (4%)	1 (1%)	14 30
All	All	3705/4437 (84%)	3379 (91%)	279 (8%)	47 (1%)	12 24

5 of 47 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	34	ASP
4	B	139	ASP
5	C	8	LEU
6	D	137	PRO
8	F	101	ALA

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	
3	A	179/182 (98%)	167 (93%)	12 (7%)	16	33
4	B	282/283 (100%)	264 (94%)	18 (6%)	17	35
5	C	193/193 (100%)	176 (91%)	17 (9%)	10	19
6	D	117/148 (79%)	111 (95%)	6 (5%)	24	46
7	E	152/156 (97%)	147 (97%)	5 (3%)	38	64
8	F	93/94 (99%)	92 (99%)	1 (1%)	73	88
9	G	27/283 (10%)	27 (100%)	0	100	100
10	H	134/145 (92%)	129 (96%)	5 (4%)	34	60
11	I	58/130 (45%)	58 (100%)	0	100	100
12	J	118/121 (98%)	109 (92%)	9 (8%)	13	26
13	K	106/106 (100%)	103 (97%)	3 (3%)	43	69
14	L	113/127 (89%)	109 (96%)	4 (4%)	36	62
15	M	158/159 (99%)	152 (96%)	6 (4%)	33	59
16	N	149/150 (99%)	145 (97%)	4 (3%)	44	71
17	O	93/94 (99%)	90 (97%)	3 (3%)	39	65
18	P	113/117 (97%)	108 (96%)	5 (4%)	28	53
19	Q	79/80 (99%)	76 (96%)	3 (4%)	33	59
20	R	117/122 (96%)	112 (96%)	5 (4%)	29	54
21	S	71/74 (96%)	69 (97%)	2 (3%)	43	69
22	T	105/106 (99%)	99 (94%)	6 (6%)	20	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
23	U	44/52 (85%)	44 (100%)	0	100 100
24	V	51/57 (90%)	50 (98%)	1 (2%)	55 78
25	W	130/130 (100%)	124 (95%)	6 (5%)	27 51
26	X	66/74 (89%)	58 (88%)	8 (12%)	5 9
27	Y	120/196 (61%)	115 (96%)	5 (4%)	30 55
28	Z	60/68 (88%)	59 (98%)	1 (2%)	60 81
29	1	46/47 (98%)	46 (100%)	0	100 100
30	2	42/46 (91%)	41 (98%)	1 (2%)	49 74
31	3	79/79 (100%)	77 (98%)	2 (2%)	47 73
All	All	3095/3619 (86%)	2957 (96%)	138 (4%)	27 52

5 of 138 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
25	W	26	ILE
25	W	146	ILE
27	Y	174	VAL
6	D	61	PHE
6	D	24	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 86 such sidechains are listed below:

Mol	Chain	Res	Type
23	U	39	ASN
27	Y	133	HIS
24	V	4	HIS
25	W	110	GLN
29	1	8	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2922 (93%)	236 (8%)	32 (1%)
2	9	121/122 (99%)	16 (13%)	1 (0%)
All	All	2866/3044 (94%)	252 (8%)	33 (1%)

5 of 252 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	31	C
1	0	60	A
1	0	67	A
1	0	69	A
1	0	70	A

5 of 33 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	2649	A
1	0	2718	C
2	9	65	A
1	0	1237	U
1	0	1232	A

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

5 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	UR3	0	2619	1	14,22,23	0.81	0	15,32,35	0.61	0
1	OMG	0	2588	1	18,26,27	1.09	2 (11%)	20,38,41	2.59	4 (20%)
1	1MA	0	628	1	15,25,26	0.71	0	15,37,40	1.41	1 (6%)
1	OMU	0	2587	1	14,22,23	0.99	1 (7%)	14,31,34	1.15	1 (7%)
1	PSU	0	2621	1	17,21,22	1.54	3 (17%)	20,30,33	5.48	4 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	UR3	0	2619	1	-	0/5/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	0	2588	1	-	0/5/27/28	0/3/3/3
1	1MA	0	628	1	-	0/3/25/26	0/3/3/3
1	OMU	0	2587	1	-	0/7/27/28	0/2/2/2
1	PSU	0	2621	1	-	0/7/25/26	0/2/2/2

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C5-C1'	-4.64	1.48	1.52
1	0	2588	OMG	C6-N1	3.53	1.39	1.33
1	0	2621	PSU	C4-N3	3.00	1.38	1.33
1	0	2621	PSU	C2-N1	2.64	1.43	1.38
1	0	2587	OMU	C4-N3	2.63	1.37	1.33

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	0	2621	PSU	N1-C2-N3	-17.47	114.54	128.43
1	0	2621	PSU	C4-N3-C2	14.45	127.34	115.14
1	0	2588	OMG	C5-C6-N1	-8.62	111.64	123.43
1	0	2621	PSU	C5-C4-N3	-8.19	114.80	125.36
1	0	2588	OMG	C6-N1-C2	5.80	125.15	115.93

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	0	2587	OMU	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 232 ligands modelled in this entry, 231 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	$\#\|Z\| > 2$
36	TEL	0	9000	-	59,62,62	1.68	14 (23%)	77,92,92	1.38	11 (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
36	TEL	0	9000	-	-	2/73/108/108	0/4/5/5

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	0	9000	TEL	C7-C3	4.57	1.60	1.54
36	0	9000	TEL	C47-C43	4.18	1.46	1.39
36	0	9000	TEL	C46-C43	3.90	1.47	1.39
36	0	9000	TEL	C7-C13	3.22	1.57	1.52
36	0	9000	TEL	C51-C46	3.02	1.45	1.38

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	0	9000	TEL	C17-C11-N6	-4.97	105.64	113.31
36	0	9000	TEL	C40-C36-N31	-4.16	103.56	107.91
36	0	9000	TEL	C2-O5-C10	3.14	111.77	109.29
36	0	9000	TEL	O9-C4-C2	2.81	111.82	105.48
36	0	9000	TEL	O16-C10-N6	2.58	131.41	128.01

There are no chirality outliers.

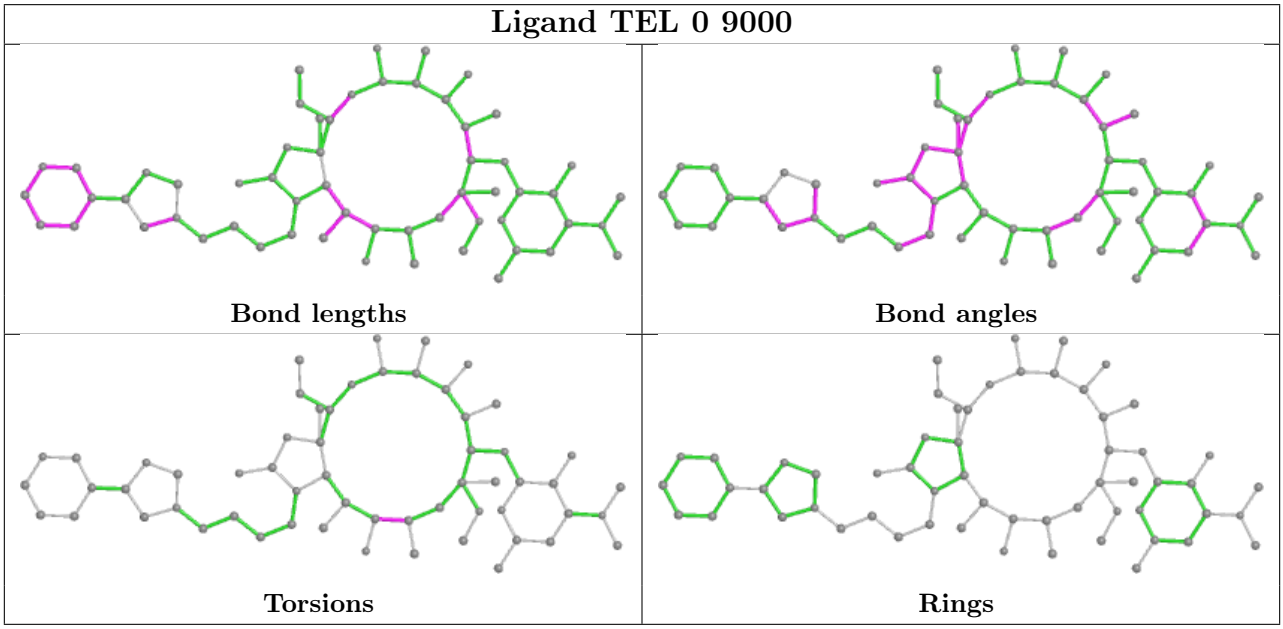
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
36	0	9000	TEL	O18-C13-C19-C23
36	0	9000	TEL	C7-C13-C19-C23

There are no ring outliers.

No monomer is involved in short contacts.

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.



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	0	2749/2922 (94%)	-0.49	44 (1%) 72 68	21, 45, 89, 149	0
2	9	122/122 (100%)	-0.39	5 (4%) 37 30	37, 61, 87, 150	0
3	A	237/240 (98%)	0.22	11 (4%) 32 26	27, 50, 86, 107	0
4	B	337/338 (99%)	0.03	5 (1%) 73 70	26, 54, 78, 90	0
5	C	246/246 (100%)	-0.17	1 (0%) 92 91	22, 43, 68, 78	0
6	D	140/177 (79%)	2.05	62 (44%) 0 0	52, 98, 120, 129	0
7	E	172/178 (96%)	0.74	20 (11%) 4 3	42, 67, 86, 90	0
8	F	119/120 (99%)	0.78	16 (13%) 3 2	46, 71, 93, 108	0
9	G	29/348 (8%)	2.53	21 (72%) 0 0	71, 88, 98, 99	0
10	H	160/177 (90%)	0.42	11 (6%) 16 12	40, 59, 92, 96	0
11	I	70/162 (43%)	4.49	62 (88%) 0 0	106, 119, 137, 138	0
12	J	142/145 (97%)	-0.06	1 (0%) 87 86	32, 48, 69, 89	0
13	K	132/132 (100%)	-0.11	0 100 100	31, 51, 71, 82	0
14	L	145/165 (87%)	0.55	17 (11%) 4 3	23, 63, 106, 119	0
15	M	194/195 (99%)	-0.19	1 (0%) 91 89	30, 40, 57, 64	0
16	N	186/187 (99%)	0.60	24 (12%) 3 2	36, 62, 106, 114	0
17	O	115/116 (99%)	-0.06	0 100 100	35, 52, 70, 73	0
18	P	143/149 (95%)	0.10	3 (2%) 63 58	35, 53, 69, 78	0
19	Q	95/96 (98%)	-0.09	0 100 100	35, 41, 59, 72	0
20	R	150/155 (96%)	-0.25	0 100 100	29, 42, 63, 72	0
21	S	81/85 (95%)	0.08	3 (3%) 41 34	40, 58, 77, 85	0
22	T	119/120 (99%)	0.32	4 (3%) 45 38	35, 55, 79, 96	0
23	U	53/66 (80%)	0.24	3 (5%) 23 18	40, 55, 73, 82	0
24	V	65/71 (91%)	1.45	13 (20%) 1 0	52, 72, 111, 114	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
25	W	154/154 (100%)	-0.27	0 100 100	34, 44, 61, 74	0
26	X	82/92 (89%)	0.40	8 (9%) 7 5	42, 57, 79, 96	0
27	Y	142/241 (58%)	-0.03	7 (4%) 29 23	24, 43, 66, 84	0
28	Z	73/83 (87%)	0.30	5 (6%) 17 12	49, 65, 81, 94	0
29	1	56/57 (98%)	-0.53	0 100 100	24, 31, 36, 44	0
30	2	46/50 (92%)	0.18	4 (8%) 10 7	29, 54, 82, 98	0
31	3	92/92 (100%)	0.23	4 (4%) 35 28	33, 53, 67, 80	0
All	All	6646/7481 (88%)	-0.02	355 (5%) 26 20	21, 50, 96, 150	0

The worst 5 of 355 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	D	63	ILE	11.5
11	I	128	THR	11.5
11	I	66	GLY	9.8
24	V	1	THR	9.3
11	I	104	ALA	9.2

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	OMU	0	2587	21/22	0.98	0.13	30,32,34,37	0
1	OMG	0	2588	24/25	0.98	0.13	30,33,34,35	0
1	UR3	0	2619	21/22	0.98	0.13	29,35,39,43	0
1	PSU	0	2621	20/21	0.98	0.14	24,27,32,32	0
1	1MA	0	628	23/24	0.99	0.16	25,28,29,29	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
34	NA	0	8571	1/1	0.49	0.45	62,62,62,62	0
34	NA	0	8582	1/1	0.65	0.29	88,88,88,88	0
34	NA	R	8586	1/1	0.66	0.80	90,90,90,90	0
34	NA	0	8529	1/1	0.70	0.21	66,66,66,66	0
32	MG	0	8031	1/1	0.71	0.19	35,35,35,35	0
32	MG	0	8087	1/1	0.72	0.19	61,61,61,61	0
34	NA	0	8563	1/1	0.76	0.35	58,58,58,58	0
32	MG	0	8090	1/1	0.78	0.24	61,61,61,61	0
34	NA	0	8569	1/1	0.81	0.42	59,59,59,59	0
34	NA	0	8526	1/1	0.81	0.32	51,51,51,51	0
34	NA	9	8551	1/1	0.82	0.25	36,36,36,36	0
34	NA	0	8566	1/1	0.82	0.27	59,59,59,59	0
34	NA	0	8577	1/1	0.83	0.42	64,64,64,64	0
32	MG	0	8041	1/1	0.83	0.18	52,52,52,52	0
34	NA	0	8581	1/1	0.84	0.32	59,59,59,59	0
34	NA	0	8584	1/1	0.85	0.10	53,53,53,53	0
34	NA	0	8524	1/1	0.85	0.19	56,56,56,56	0
32	MG	0	8050	1/1	0.85	0.09	72,72,72,72	0
32	MG	2	8076	1/1	0.86	0.09	56,56,56,56	0
34	NA	0	8541	1/1	0.86	0.17	46,46,46,46	0
34	NA	0	8550	1/1	0.87	0.36	48,48,48,48	0
34	NA	0	8507	1/1	0.88	0.31	51,51,51,51	0
32	MG	0	8049	1/1	0.88	0.29	68,68,68,68	0
34	NA	0	8585	1/1	0.88	0.44	46,46,46,46	0
34	NA	0	8532	1/1	0.88	0.17	40,40,40,40	0
34	NA	0	8533	1/1	0.88	0.12	28,28,28,28	0
34	NA	0	8511	1/1	0.89	0.10	53,53,53,53	0
34	NA	0	8568	1/1	0.89	0.14	61,61,61,61	0
34	NA	0	8542	1/1	0.89	0.25	49,49,49,49	0
32	MG	0	8092	1/1	0.89	0.48	93,93,93,93	0
34	NA	0	8573	1/1	0.89	0.27	54,54,54,54	0
34	NA	R	8537	1/1	0.89	0.08	40,40,40,40	0
32	MG	0	8105	1/1	0.89	0.27	55,55,55,55	0
34	NA	0	8540	1/1	0.90	0.35	46,46,46,46	0
32	MG	K	8069	1/1	0.90	0.08	47,47,47,47	0
34	NA	0	8567	1/1	0.90	0.11	46,46,46,46	0
32	MG	0	8103	1/1	0.90	0.19	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	MG	0	8070	1/1	0.90	0.07	41,41,41,41	0
34	NA	0	8570	1/1	0.90	0.30	52,52,52,52	0
34	NA	0	8552	1/1	0.90	0.38	54,54,54,54	0
34	NA	0	8557	1/1	0.90	0.07	53,53,53,53	0
35	CL	J	8802	1/1	0.90	0.11	61,61,61,61	0
34	NA	0	8508	1/1	0.91	0.25	56,56,56,56	0
34	NA	0	8555	1/1	0.91	0.49	72,72,72,72	0
34	NA	C	8504	1/1	0.91	0.12	34,34,34,34	0
32	MG	0	8112	1/1	0.91	0.12	44,44,44,44	0
34	NA	0	8514	1/1	0.91	0.20	44,44,44,44	0
32	MG	0	8081	1/1	0.91	0.10	56,56,56,56	0
34	NA	0	8561	1/1	0.92	0.23	50,50,50,50	0
34	NA	9	8583	1/1	0.92	0.35	61,61,61,61	0
32	MG	0	8100	1/1	0.92	0.18	68,68,68,68	0
34	NA	0	8564	1/1	0.92	0.23	42,42,42,42	0
32	MG	0	8099	1/1	0.92	0.16	44,44,44,44	0
35	CL	A	8809	1/1	0.92	0.16	61,61,61,61	0
34	NA	0	8517	1/1	0.92	0.12	44,44,44,44	0
36	TEL	0	9000	58/58	0.92	0.21	53,63,75,76	0
34	NA	0	8527	1/1	0.93	0.17	39,39,39,39	0
32	MG	0	8053	1/1	0.93	0.10	48,48,48,48	0
32	MG	T	8073	1/1	0.93	0.06	60,60,60,60	0
32	MG	0	8045	1/1	0.93	0.09	62,62,62,62	0
34	NA	0	8535	1/1	0.93	0.29	44,44,44,44	0
34	NA	J	8546	1/1	0.93	0.10	49,49,49,49	0
34	NA	0	8572	1/1	0.93	0.30	67,67,67,67	0
34	NA	0	8562	1/1	0.93	0.23	63,63,63,63	0
32	MG	0	8047	1/1	0.93	0.11	72,72,72,72	0
34	NA	0	8525	1/1	0.93	0.23	54,54,54,54	0
32	MG	0	8085	1/1	0.93	0.09	38,38,38,38	0
32	MG	0	8097	1/1	0.94	0.08	34,34,34,34	0
34	NA	0	8510	1/1	0.94	0.19	40,40,40,40	0
32	MG	A	8066	1/1	0.94	0.05	63,63,63,63	0
34	NA	0	8513	1/1	0.94	0.10	62,62,62,62	0
34	NA	A	8545	1/1	0.94	0.14	53,53,53,53	0
34	NA	0	8559	1/1	0.94	0.20	57,57,57,57	0
32	MG	0	8057	1/1	0.94	0.16	48,48,48,48	0
34	NA	L	8580	1/1	0.94	0.36	48,48,48,48	0
34	NA	Q	8548	1/1	0.94	0.20	45,45,45,45	0
34	NA	0	8515	1/1	0.94	0.21	45,45,45,45	0
32	MG	0	8091	1/1	0.94	0.05	49,49,49,49	0
35	CL	0	8822	1/1	0.94	0.21	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
34	NA	0	8579	1/1	0.94	0.14	61,61,61,61	0
32	MG	0	8068	1/1	0.94	0.12	68,68,68,68	0
35	CL	N	8807	1/1	0.94	0.17	58,58,58,58	0
32	MG	0	8093	1/1	0.94	0.08	51,51,51,51	0
32	MG	0	8113	1/1	0.95	0.12	45,45,45,45	0
34	NA	0	8565	1/1	0.95	0.27	37,37,37,37	0
32	MG	0	8114	1/1	0.95	0.07	46,46,46,46	0
32	MG	9	8095	1/1	0.95	0.08	68,68,68,68	0
32	MG	0	8048	1/1	0.95	0.13	58,58,58,58	0
32	MG	0	8101	1/1	0.95	0.09	61,61,61,61	0
34	NA	0	8516	1/1	0.95	0.15	41,41,41,41	0
32	MG	0	8088	1/1	0.95	0.06	31,31,31,31	0
32	MG	0	8104	1/1	0.95	0.17	49,49,49,49	0
34	NA	R	8538	1/1	0.95	0.08	54,54,54,54	0
34	NA	0	8556	1/1	0.95	0.43	44,44,44,44	0
33	K	0	8401	1/1	0.95	0.17	72,72,72,72	0
34	NA	0	8502	1/1	0.95	0.15	50,50,50,50	0
35	CL	J	8801	1/1	0.95	0.11	64,64,64,64	0
34	NA	0	8505	1/1	0.95	0.14	33,33,33,33	0
32	MG	0	8062	1/1	0.95	0.10	56,56,56,56	0
35	CL	Y	8820	1/1	0.95	0.09	42,42,42,42	0
32	MG	0	8014	1/1	0.95	0.06	33,33,33,33	0
34	NA	0	8534	1/1	0.96	0.07	37,37,37,37	0
32	MG	0	8027	1/1	0.96	0.08	44,44,44,44	0
32	MG	0	8028	1/1	0.96	0.09	31,31,31,31	0
32	MG	0	8046	1/1	0.96	0.07	42,42,42,42	0
34	NA	S	8512	1/1	0.96	0.23	16,16,16,16	0
34	NA	T	8543	1/1	0.96	0.09	38,38,38,38	0
35	CL	0	8805	1/1	0.96	0.09	56,56,56,56	0
34	NA	0	8560	1/1	0.96	0.41	45,45,45,45	0
32	MG	0	8107	1/1	0.96	0.12	77,77,77,77	0
34	NA	0	8544	1/1	0.96	0.06	28,28,28,28	0
34	NA	0	8549	1/1	0.96	0.10	36,36,36,36	0
34	NA	0	8519	1/1	0.96	0.08	35,35,35,35	0
32	MG	0	8007	1/1	0.96	0.08	23,23,23,23	0
35	CL	3	8804	1/1	0.96	0.11	65,65,65,65	0
34	NA	M	8547	1/1	0.96	0.14	29,29,29,29	0
34	NA	0	8531	1/1	0.97	0.12	38,38,38,38	0
34	NA	0	8574	1/1	0.97	0.68	68,68,68,68	0
34	NA	0	8575	1/1	0.97	0.20	45,45,45,45	0
34	NA	0	8576	1/1	0.97	0.19	51,51,51,51	0
32	MG	B	8055	1/1	0.97	0.07	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
34	NA	0	8578	1/1	0.97	0.21	42,42,42,42	0
32	MG	0	8051	1/1	0.97	0.07	52,52,52,52	0
32	MG	0	8040	1/1	0.97	0.10	46,46,46,46	0
32	MG	0	8022	1/1	0.97	0.10	36,36,36,36	0
32	MG	3	8078	1/1	0.97	0.12	41,41,41,41	0
32	MG	0	8061	1/1	0.97	0.08	37,37,37,37	0
32	MG	0	8094	1/1	0.97	0.06	70,70,70,70	0
32	MG	0	8042	1/1	0.97	0.10	37,37,37,37	0
34	NA	0	8506	1/1	0.97	0.47	39,39,39,39	0
32	MG	0	8064	1/1	0.97	0.08	28,28,28,28	0
34	NA	H	8522	1/1	0.97	0.17	61,61,61,61	0
32	MG	0	8067	1/1	0.97	0.12	37,37,37,37	0
34	NA	0	8509	1/1	0.97	0.08	37,37,37,37	0
32	MG	0	8023	1/1	0.97	0.08	33,33,33,33	0
32	MG	0	8013	1/1	0.97	0.15	34,34,34,34	0
32	MG	0	8072	1/1	0.97	0.10	53,53,53,53	0
32	MG	0	8080	1/1	0.97	0.08	45,45,45,45	0
32	MG	0	8006	1/1	0.97	0.04	33,33,33,33	0
32	MG	0	8110	1/1	0.97	0.08	40,40,40,40	0
32	MG	0	8111	1/1	0.97	0.07	35,35,35,35	0
35	CL	0	8803	1/1	0.97	0.14	52,52,52,52	0
34	NA	0	8518	1/1	0.97	0.11	31,31,31,31	0
35	CL	0	8815	1/1	0.97	0.28	77,77,77,77	0
32	MG	0	8082	1/1	0.97	0.12	50,50,50,50	0
34	NA	0	8521	1/1	0.97	0.32	57,57,57,57	0
32	MG	0	8083	1/1	0.97	0.05	35,35,35,35	0
32	MG	0	8016	1/1	0.97	0.16	33,33,33,33	0
35	CL	J	8821	1/1	0.97	0.14	52,52,52,52	0
35	CL	L	8810	1/1	0.97	0.17	60,60,60,60	0
32	MG	0	8116	1/1	0.97	0.09	36,36,36,36	0
35	CL	R	8806	1/1	0.97	0.09	40,40,40,40	0
32	MG	0	8033	1/1	0.97	0.10	32,32,32,32	0
32	MG	0	8036	1/1	0.97	0.06	33,33,33,33	0
34	NA	0	8530	1/1	0.97	0.13	41,41,41,41	0
32	MG	0	8003	1/1	0.98	0.14	33,33,33,33	0
34	NA	0	8553	1/1	0.98	0.13	27,27,27,27	0
34	NA	0	8554	1/1	0.98	0.16	31,31,31,31	0
32	MG	0	8012	1/1	0.98	0.09	26,26,26,26	0
32	MG	0	8115	1/1	0.98	0.07	47,47,47,47	0
32	MG	0	8035	1/1	0.98	0.03	36,36,36,36	0
34	NA	0	8558	1/1	0.98	0.46	86,86,86,86	0
32	MG	0	8004	1/1	0.98	0.05	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	MG	0	8038	1/1	0.98	0.10	28,28,28,28	0
34	NA	0	8520	1/1	0.98	0.11	34,34,34,34	0
32	MG	0	8096	1/1	0.98	0.08	40,40,40,40	0
34	NA	0	8523	1/1	0.98	0.12	33,33,33,33	0
32	MG	0	8071	1/1	0.98	0.07	49,49,49,49	0
32	MG	0	8098	1/1	0.98	0.08	37,37,37,37	0
32	MG	Y	8108	1/1	0.98	0.08	31,31,31,31	0
32	MG	0	8025	1/1	0.98	0.08	36,36,36,36	0
32	MG	0	8077	1/1	0.98	0.10	23,23,23,23	0
32	MG	0	8002	1/1	0.98	0.05	31,31,31,31	0
35	CL	0	8812	1/1	0.98	0.10	48,48,48,48	0
35	CL	0	8814	1/1	0.98	0.07	44,44,44,44	0
33	K	0	8402	1/1	0.98	0.12	59,59,59,59	0
34	NA	0	8501	1/1	0.98	0.21	23,23,23,23	0
32	MG	0	8102	1/1	0.98	0.13	56,56,56,56	0
32	MG	0	8052	1/1	0.98	0.07	44,44,44,44	0
32	MG	0	8015	1/1	0.98	0.08	29,29,29,29	0
34	NA	0	8539	1/1	0.98	0.11	32,32,32,32	0
32	MG	0	8043	1/1	0.98	0.08	40,40,40,40	0
35	CL	M	8818	1/1	0.98	0.18	43,43,43,43	0
32	MG	0	8084	1/1	0.98	0.07	49,49,49,49	0
35	CL	O	8808	1/1	0.98	0.16	66,66,66,66	0
32	MG	0	8109	1/1	0.98	0.12	16,16,16,16	0
32	MG	0	8059	1/1	0.98	0.05	27,27,27,27	0
32	MG	0	8060	1/1	0.98	0.14	40,40,40,40	0
32	MG	0	8044	1/1	0.98	0.09	39,39,39,39	0
37	CD	O	8705	1/1	0.98	0.09	65,65,65,65	0
32	MG	0	8020	1/1	0.99	0.08	25,25,25,25	0
32	MG	0	8054	1/1	0.99	0.08	26,26,26,26	0
32	MG	0	8086	1/1	0.99	0.14	45,45,45,45	0
32	MG	0	8037	1/1	0.99	0.05	43,43,43,43	0
32	MG	0	8058	1/1	0.99	0.08	36,36,36,36	0
32	MG	0	8089	1/1	0.99	0.10	59,59,59,59	0
32	MG	A	8065	1/1	0.99	0.07	32,32,32,32	0
32	MG	0	8005	1/1	0.99	0.12	24,24,24,24	0
32	MG	0	8039	1/1	0.99	0.04	41,41,41,41	0
32	MG	B	8056	1/1	0.99	0.09	51,51,51,51	0
32	MG	0	8008	1/1	0.99	0.07	27,27,27,27	0
32	MG	0	8024	1/1	0.99	0.14	23,23,23,23	0
34	NA	0	8528	1/1	0.99	0.33	39,39,39,39	0
32	MG	0	8063	1/1	0.99	0.12	68,68,68,68	0
35	CL	0	8811	1/1	0.99	0.10	48,48,48,48	0

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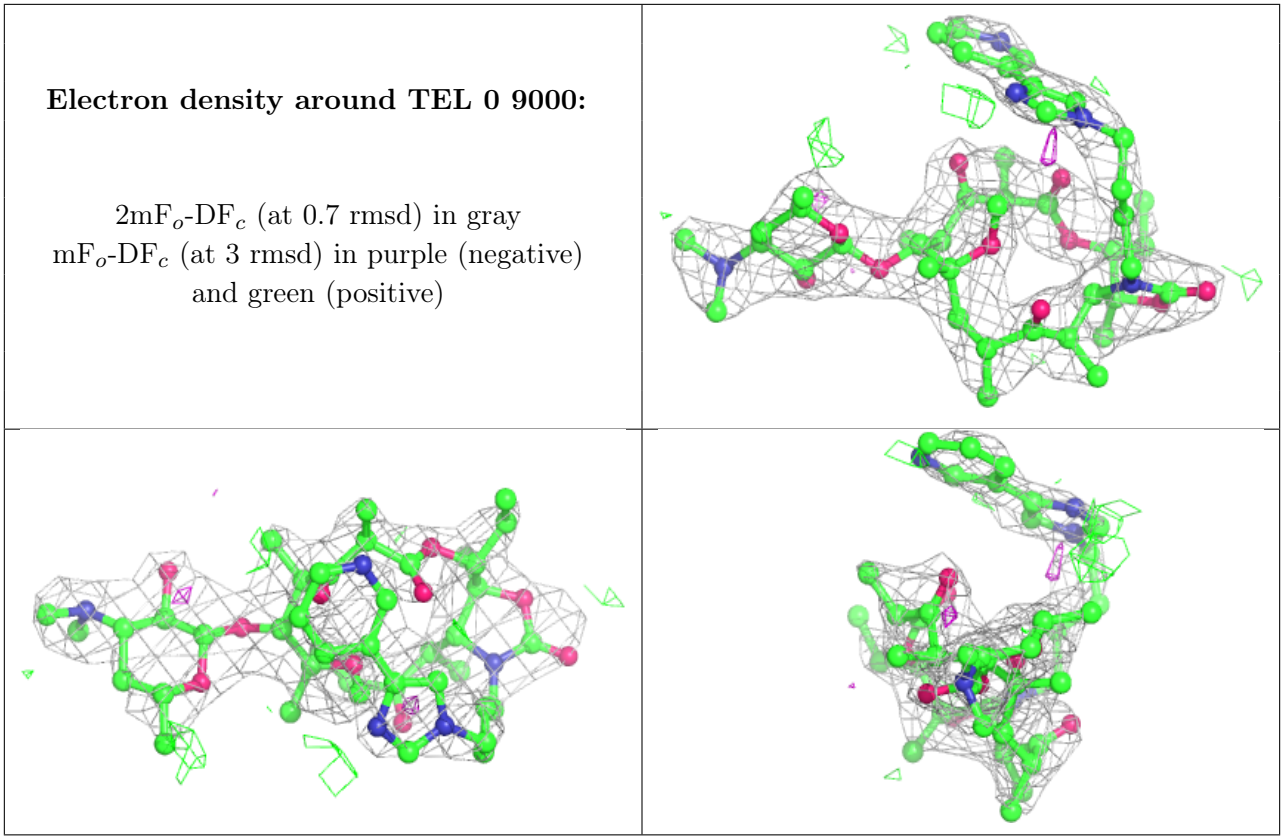
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	MG	0	8009	1/1	0.99	0.06	30,30,30,30	0
35	CL	0	8813	1/1	0.99	0.15	49,49,49,49	0
32	MG	0	8026	1/1	0.99	0.09	25,25,25,25	0
32	MG	0	8010	1/1	0.99	0.08	31,31,31,31	0
35	CL	0	8816	1/1	0.99	0.12	54,54,54,54	0
32	MG	0	8011	1/1	0.99	0.10	22,22,22,22	0
32	MG	0	8029	1/1	0.99	0.10	37,37,37,37	0
35	CL	B	8819	1/1	0.99	0.10	45,45,45,45	0
32	MG	0	8030	1/1	0.99	0.09	24,24,24,24	0
34	NA	0	8536	1/1	0.99	0.07	48,48,48,48	0
34	NA	0	8503	1/1	0.99	0.12	34,34,34,34	0
32	MG	0	8074	1/1	0.99	0.06	35,35,35,35	0
32	MG	0	8075	1/1	0.99	0.07	33,33,33,33	0
32	MG	0	8017	1/1	0.99	0.05	23,23,23,23	0
32	MG	0	8079	1/1	0.99	0.12	26,26,26,26	0
32	MG	0	8106	1/1	0.99	0.06	34,34,34,34	0
35	CL	Y	8817	1/1	0.99	0.14	58,58,58,58	0
32	MG	0	8032	1/1	0.99	0.08	32,32,32,32	0
32	MG	0	8018	1/1	0.99	0.10	38,38,38,38	0
32	MG	0	8034	1/1	0.99	0.06	28,28,28,28	0
32	MG	0	8019	1/1	0.99	0.05	31,31,31,31	0
37	CD	U	8701	1/1	0.99	0.10	61,61,61,61	0
37	CD	Z	8703	1/1	0.99	0.09	67,67,67,67	0
37	CD	3	8704	1/1	0.99	0.06	61,61,61,61	0
32	MG	0	8001	1/1	1.00	0.06	31,31,31,31	0
37	CD	1	8702	1/1	1.00	0.04	51,51,51,51	0
32	MG	0	8021	1/1	1.00	0.10	28,28,28,28	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 TEL 0 9000:

$2mF_o$-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.