wwPDB X-ray Structure Validation Summary Report (i)

Aug 6, 2023 – 04:22 AM EDT

PDB ID	:	1K9M
Title	:	Co-crystal structure of tylosin bound to the 50S ribosomal subunit of Haloarcula marismortui
Authors	:	Hansen, J.L.; Ippolito, J.A.; Ban, N.; Nissen, P.; Moore, P.B.; Steitz, T.A.
Deposited on	:	2001-10-29
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:

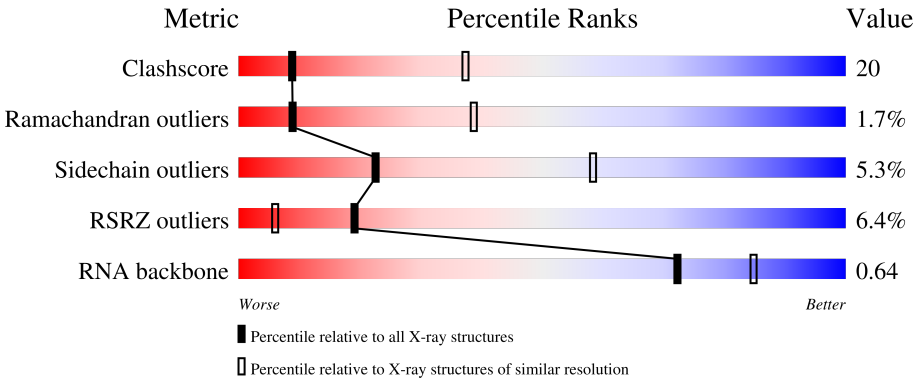
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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))
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)
RNA backbone	3102	1173 (3.30-2.70)

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	2922	2% 50% 36% 7% • 6%
2	B	122	4% 45% 39% 10% 6%
3	C	239	7% 54% 38% 7% •
4	D	337	50% 44% 6%
5	E	246	% 61% 34% 6%

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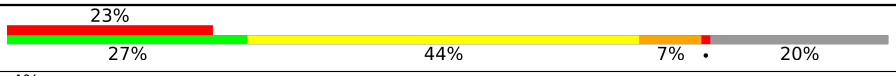
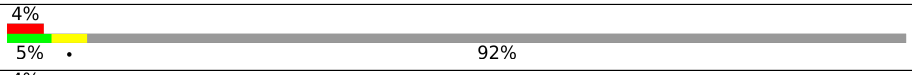
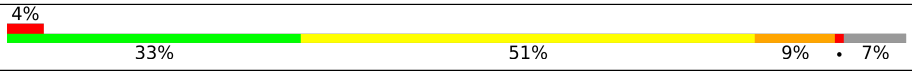
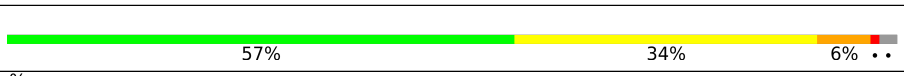
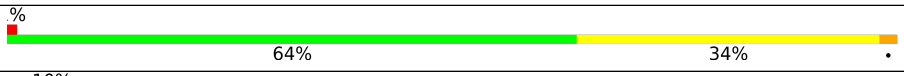
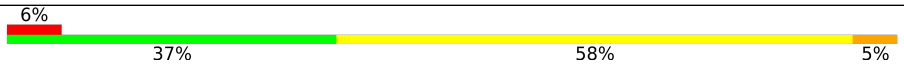
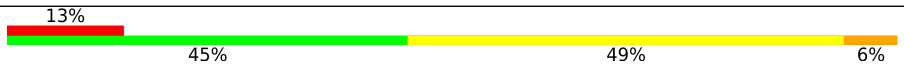
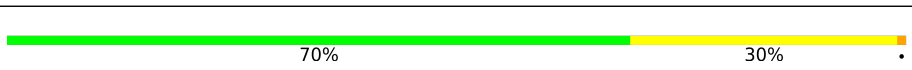
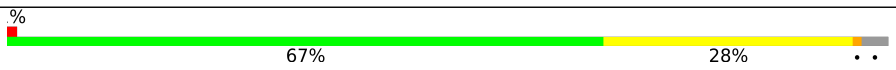
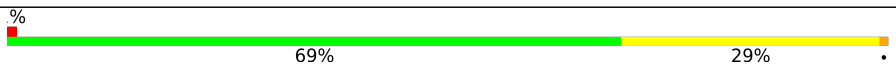
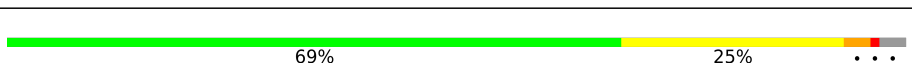
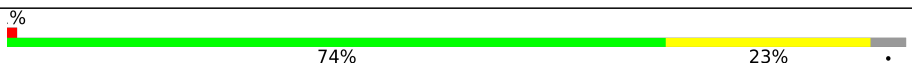
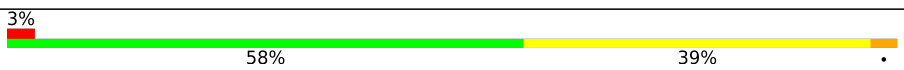
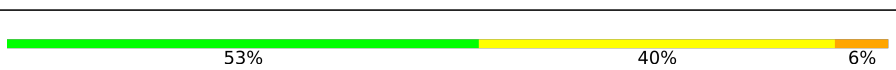
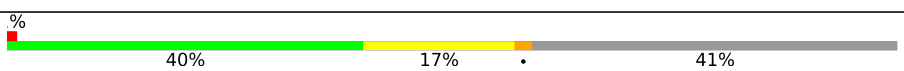
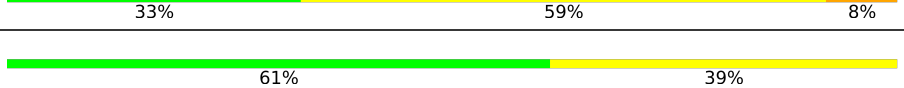
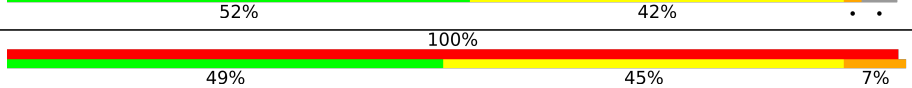
Mol	Chain	Length	Quality of chain
6	F	176	
7	G	177	
8	H	119	
9	I	348	
10	J	167	
11	K	145	
12	L	132	
13	M	164	
14	N	194	
15	O	186	
16	P	115	
17	Q	148	
18	R	95	
19	S	154	
20	T	84	
21	U	119	
22	V	66	
23	W	70	
24	X	154	
25	Y	91	
26	Z	240	
27	1	73	
28	2	56	
29	3	48	
30	4	92	

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
33	NA	A	8356	-	-	-	X
33	NA	A	8373	-	-	-	X
33	NA	A	8384	-	-	-	X
33	NA	J	8322	-	-	-	X
33	NA	S	8386	-	-	-	X
33	NA	T	8312	-	-	-	X
34	CL	4	8504	-	-	-	X
34	CL	A	8505	-	-	-	X
34	CL	O	8507	-	-	X	-
36	CD	4	8404	-	-	-	X
36	CD	V	8401	-	-	-	X

2 Entry composition (i)

There are 37 unique types of molecules in this entry. The entry contains 98593 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 RRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	A	2754	59017	26346	10878	19048	2745	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	560	C	U	conflict	? 3377779

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	B	122	2600	1160	472	847	121	0	0	0

- Molecule 3 is a protein called RIBOSOMAL PROTEIN L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	237	1754	1072	352	325	5	0	0	0

- Molecule 4 is a protein called RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	337	2624	1616	493	510	5	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	PRO	deletion	UNP P20279
D	310	ARG	PHE	conflict	UNP P20279

- Molecule 5 is a protein called RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	246	Total	C	N	O	S	0	0	0
			1858	1131	344	382	1			

- Molecule 6 is a protein called RIBOSOMAL PROTEIN L5.

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

- Molecule 7 is a protein called RIBOSOMAL PROTEIN L6.

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

- Molecule 8 is a protein called RIBOSOMAL PROTEIN L7AE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	119	Total	C	N	O	S	0	0	0
			885	552	141	191	1			

- Molecule 9 is a protein called RIBOSOMAL PROTEIN L10.

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

- Molecule 10 is a protein called RIBOSOMAL PROTEIN L10E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	156	Total	C	N	O	S	0	0	0
			1215	766	233	212	4			

- Molecule 11 is a protein called RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	142	Total	C	N	O	S	0	0	0
			1119	696	199	221	3			

- Molecule 12 is a protein called RIBOSOMAL PROTEIN L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	132	Total	C	N	O	S	0	0	0
			993	609	189	191	4			

- Molecule 13 is a protein called RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	M	145	Total	C	N	O	0	0	0
			1114	668	222	224			

- Molecule 14 is a protein called RIBOSOMAL PROTEIN L15E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	194	Total	C	N	O	S	0	0	0
			1605	988	346	266	5			

- Molecule 15 is a protein called RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	186	Total	C	N	O	S	0	0	0
			1444	895	262	285	2			

- Molecule 16 is a protein called RIBOSOMAL PROTEIN L18E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
16	P	115	Total	C	N	O	0	0	0
			864	529	161	174			

- Molecule 17 is a protein called RIBOSOMAL PROTEIN L19E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	Q	143	Total	C	N	O	0	0	0
			1133	680	230	223			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	71	LYS	TYR	conflict	UNP P14119

- Molecule 18 is a protein called RIBOSOMAL PROTEIN L21E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	R	95	Total	C	N	O	0	0	0
			734	450	141	143			

- Molecule 19 is a protein called RIBOSOMAL PROTEIN L22.

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

- Molecule 20 is a protein called RIBOSOMAL PROTEIN L23.

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

- Molecule 21 is a protein called RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	U	119	Total	C	N	O	0	0	0
			949	568	180	201			

- Molecule 22 is a protein called RIBOSOMAL PROTEIN L24E.

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

- Molecule 23 is a protein called RIBOSOMAL PROTEIN L29.

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

- Molecule 24 is a protein called RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	X	154	Total	C	N	O	S	0	0	0
			1195	737	209	243	6			

- Molecule 25 is a protein called RIBOSOMAL PROTEIN L31E.

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

- Molecule 26 is a protein called RIBOSOMAL PROTEIN L32E.

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

- Molecule 27 is a protein called RIBOSOMAL PROTEIN L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	1	73	Total	C	N	O	S	0	0	0
			563	359	111	86	7			

- Molecule 28 is a protein called RIBOSOMAL PROTEIN L37E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	2	56	Total	C	N	O	S	0	0	0
			430	258	86	82	4			

- Molecule 29 is a protein called RIBOSOMAL PROTEIN L39E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	3	46	Total	C	N	O	S	0	0	0
			393	238	86	68	1			

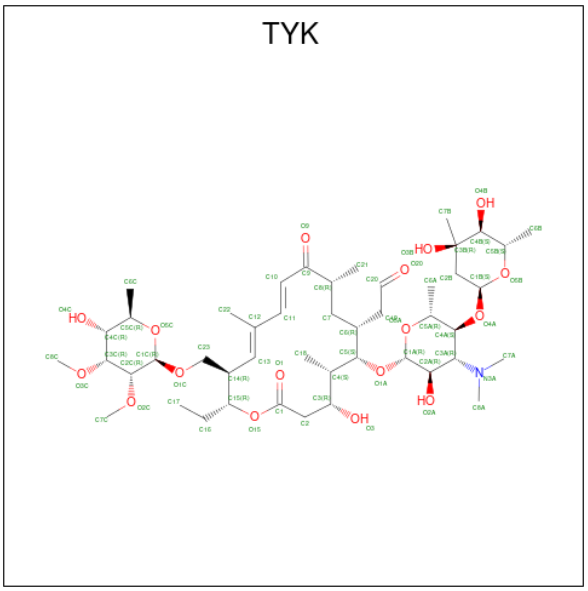
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	?	-	ARG	deletion	UNP P22452

- Molecule 30 is a protein called RIBOSOMAL PROTEIN L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	4	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 31 is TYLOSIN (three-letter code: TYK) (formula: $C_{46}H_{77}NO_{17}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	A	1	Total C N O 64 46 1 17	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	A	111	Total Mg 111 111	0	0
32	B	1	Total Mg 1 1	0	0
32	C	1	Total Mg 1 1	0	0
32	D	1	Total Mg 1 1	0	0
32	L	1	Total Mg 1 1	0	0
32	U	1	Total Mg 1 1	0	0
32	Z	1	Total Mg 1 1	0	0
32	1	1	Total Mg 1 1	0	0
32	4	1	Total Mg 1 1	0	0

- Molecule 33 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	A	72	Total Na 72 72	0	0
33	B	2	Total Na 2 2	0	0
33	C	1	Total Na 1 1	0	0
33	E	1	Total Na 1 1	0	0
33	J	2	Total Na 2 2	0	0
33	K	1	Total Na 1 1	0	0
33	M	1	Total Na 1 1	0	0
33	N	1	Total Na 1 1	0	0
33	R	1	Total Na 1 1	0	0
33	S	2	Total Na 2 2	0	0
33	T	1	Total Na 1 1	0	0

- Molecule 34 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	A	8	Total Cl 8 8	0	0
34	C	1	Total Cl 1 1	0	0
34	D	1	Total Cl 1 1	0	0
34	K	4	Total Cl 4 4	0	0
34	M	1	Total Cl 1 1	0	0
34	N	1	Total Cl 1 1	0	0
34	O	1	Total Cl 1 1	0	0
34	P	1	Total Cl 1 1	0	0
34	R	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	S	1	Total Cl 1 1	0	0
34	Z	1	Total Cl 1 1	0	0
34	4	1	Total Cl 1 1	0	0

- Molecule 35 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	A	3	Total K 3 3	0	0

- Molecule 36 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	P	1	Total Cd 1 1	0	0
36	V	1	Total Cd 1 1	0	0
36	1	1	Total Cd 1 1	0	0
36	2	1	Total Cd 1 1	0	0
36	4	1	Total Cd 1 1	0	0

- Molecule 37 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	A	5921	Total O 5921 5921	0	0
37	B	142	Total O 142 142	0	0
37	C	126	Total O 126 126	0	0
37	D	146	Total O 146 146	0	0
37	E	174	Total O 174 174	0	0
37	F	51	Total O 51 51	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	G	42	Total O 42 42	0	0
37	H	26	Total O 26 26	0	0
37	I	22	Total O 22 22	0	0
37	J	79	Total O 79 79	0	0
37	K	54	Total O 54 54	0	0
37	L	60	Total O 60 60	0	0
37	M	84	Total O 84 84	0	0
37	N	127	Total O 127 127	0	0
37	O	64	Total O 64 64	0	0
37	P	42	Total O 42 42	0	0
37	Q	66	Total O 66 66	0	0
37	R	53	Total O 53 53	0	0
37	S	84	Total O 84 84	0	0
37	T	34	Total O 34 34	0	0
37	U	39	Total O 39 39	0	0
37	V	26	Total O 26 26	0	0
37	W	12	Total O 12 12	0	0
37	X	70	Total O 70 70	0	0
37	Y	29	Total O 29 29	0	0
37	Z	96	Total O 96 96	0	0
37	1	37	Total O 37 37	0	0

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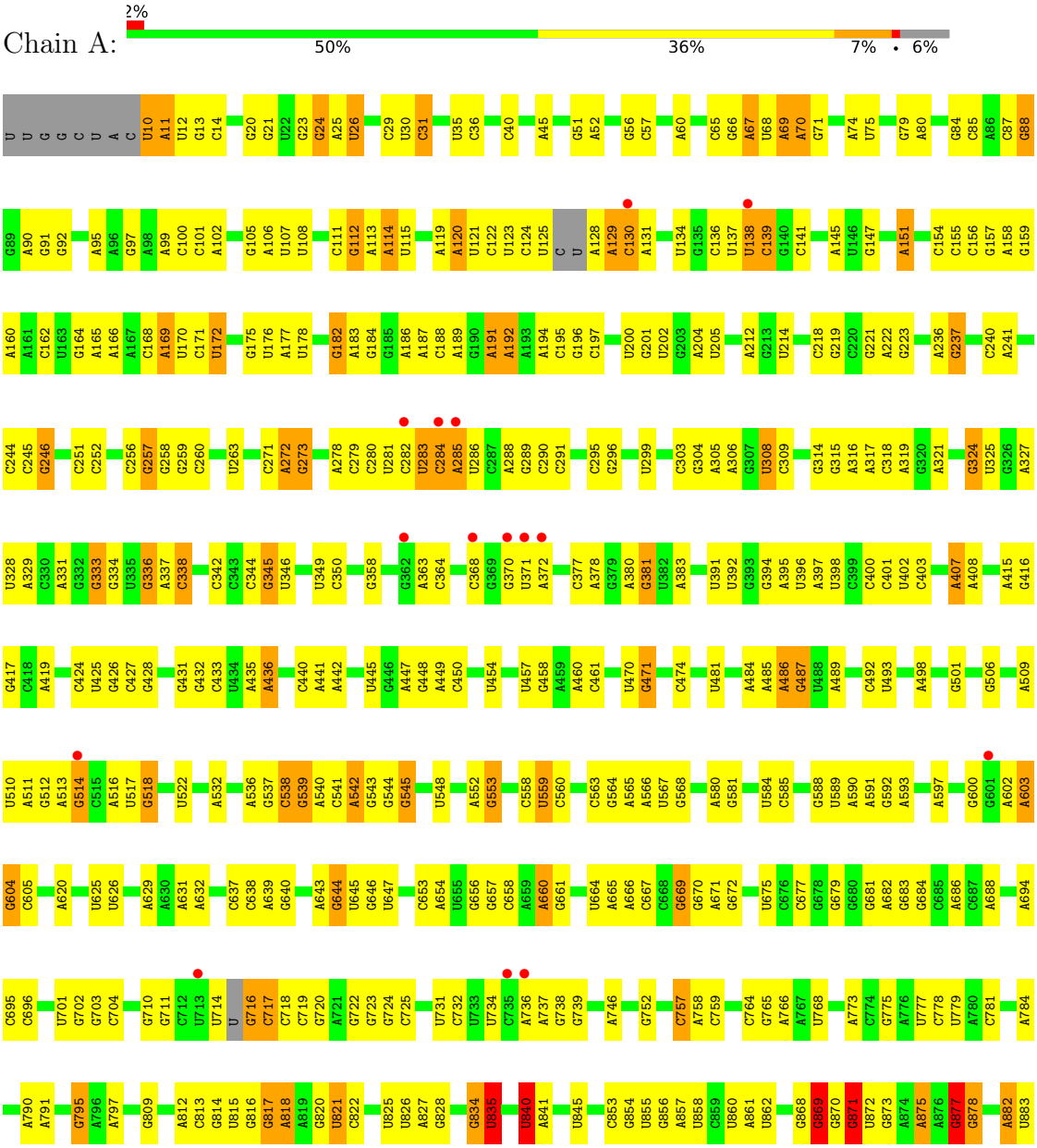
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	2	56	Total O 56 56	0	0
37	3	43	Total O 43 43	0	0
37	4	72	Total O 72 72	0	0

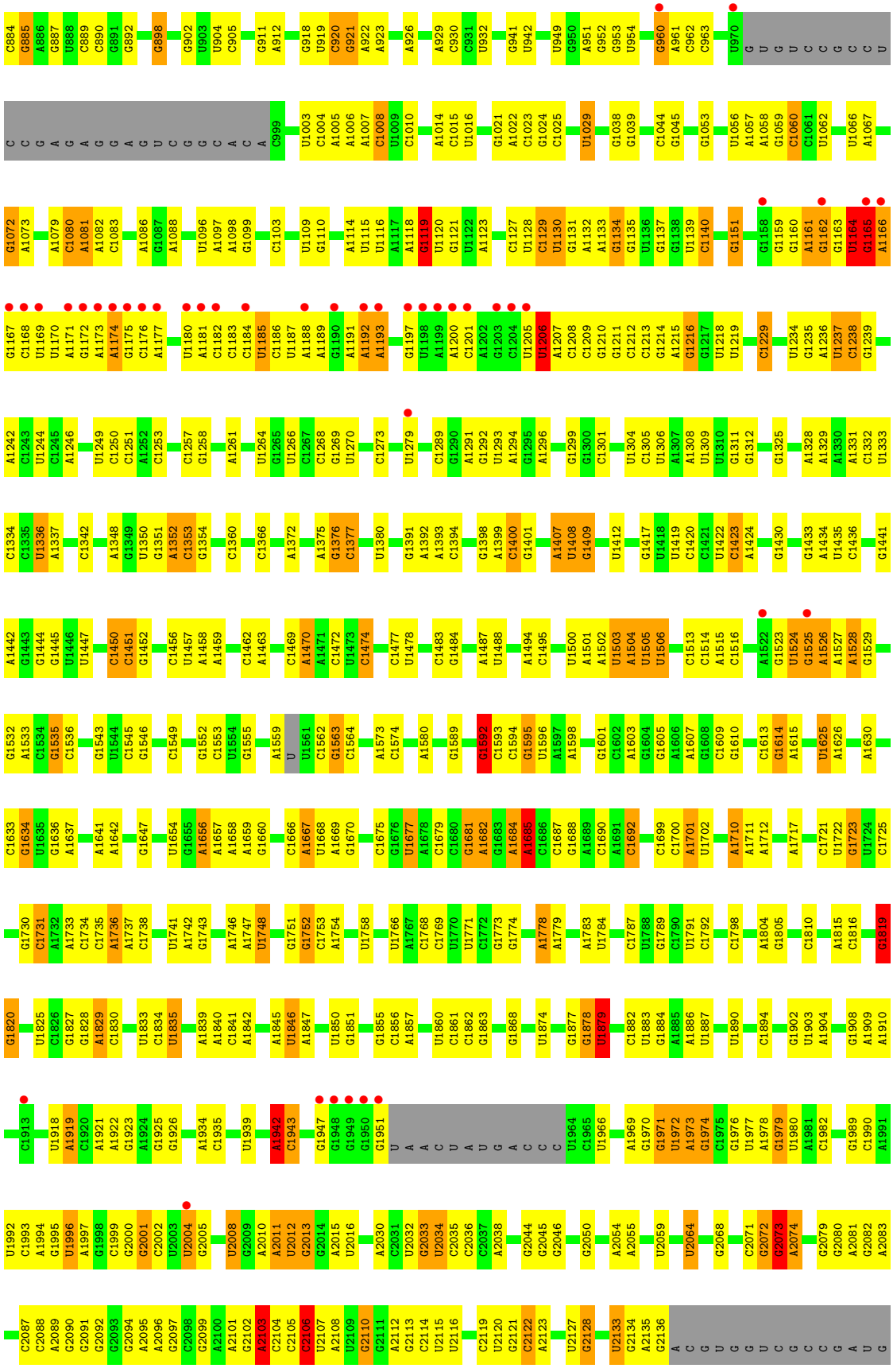
3 Residue-property plots (i)

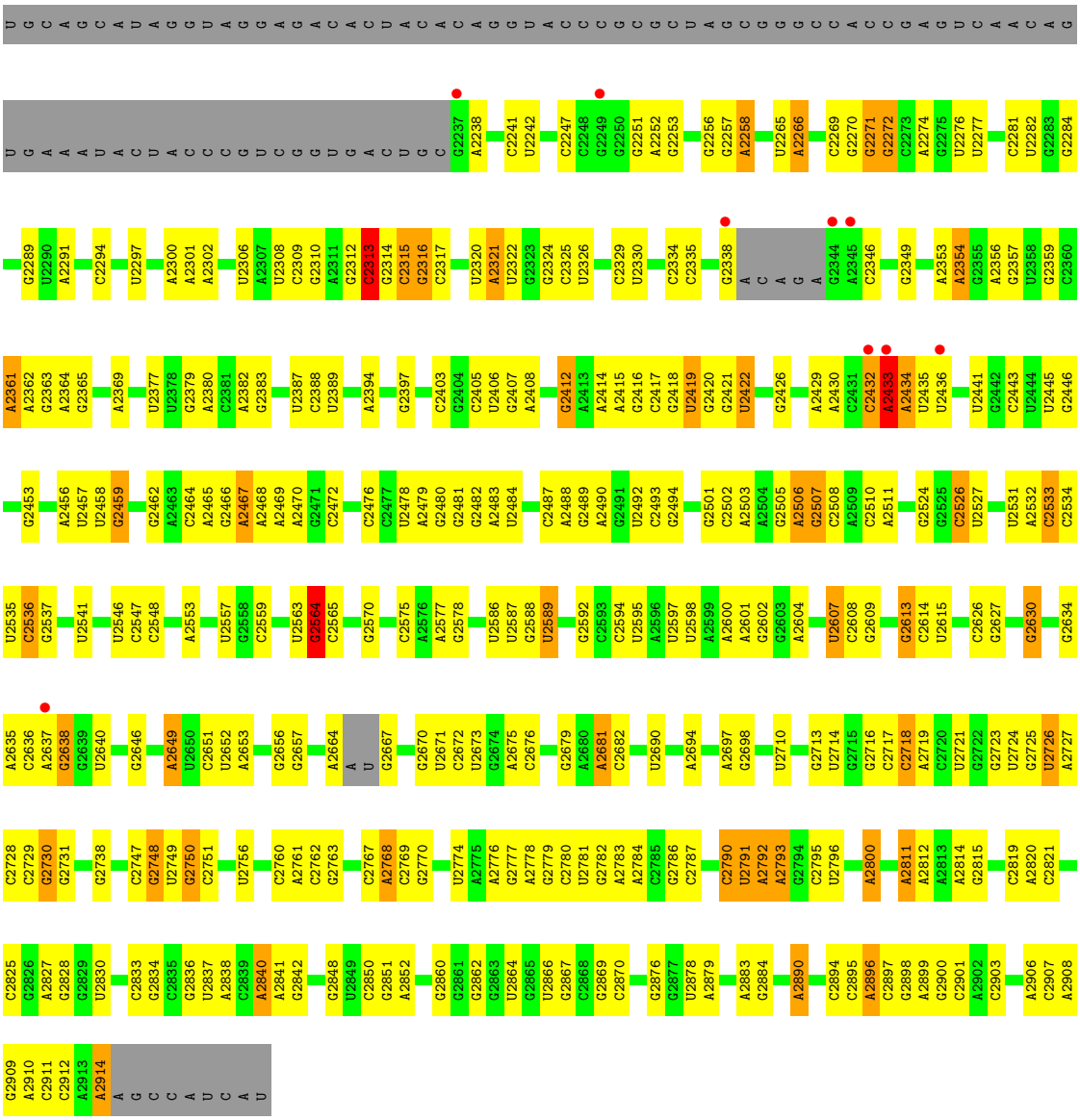
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

Chain A:

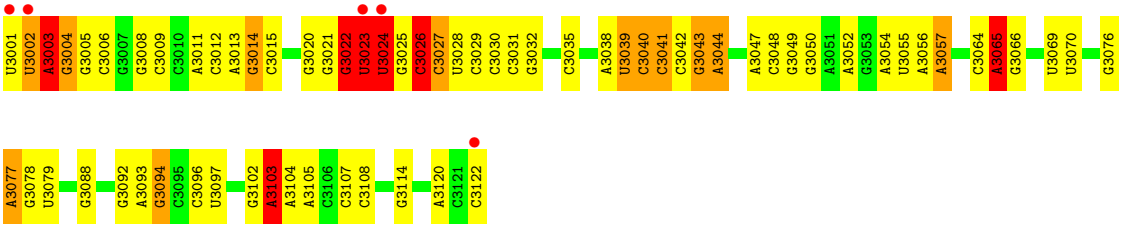






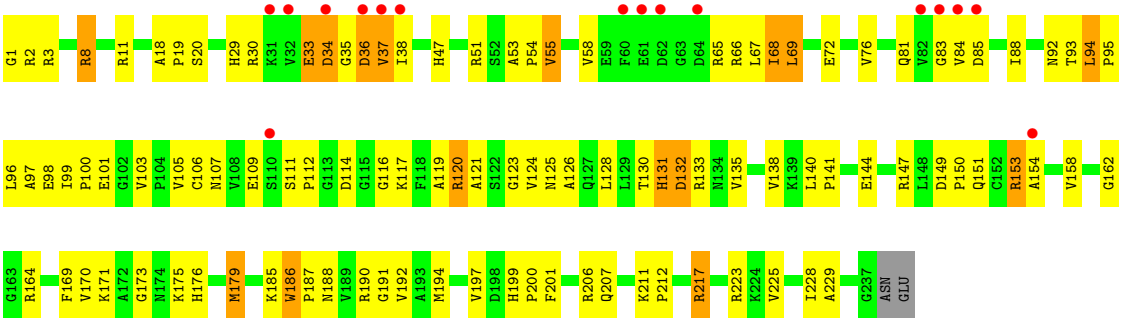
• Molecule 2: 5S RRNA

Chain B:



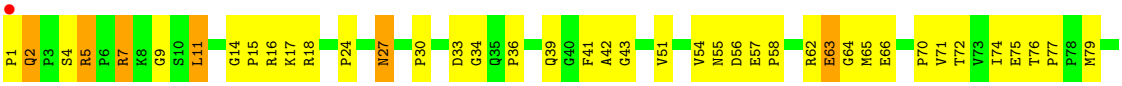
• Molecule 3: RIBOSOMAL PROTEIN L2

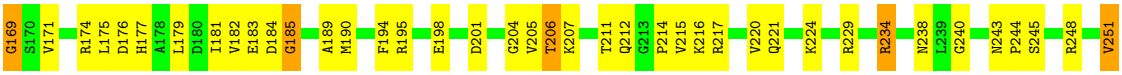
Chain C:

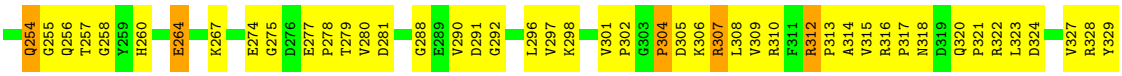


• Molecule 4: RIBOSOMAL PROTEIN L3

Chain D:

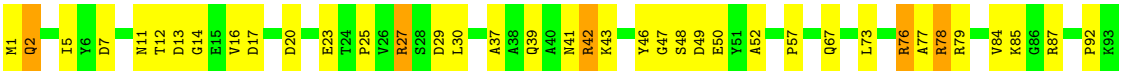


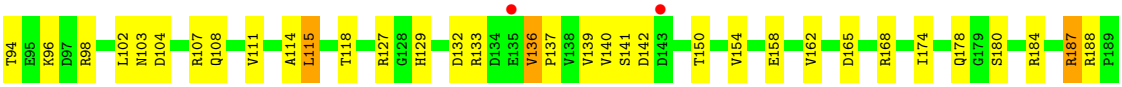


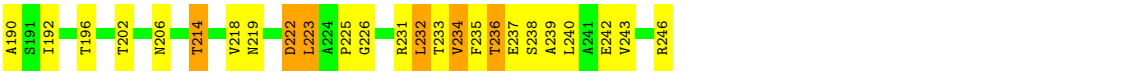


• Molecule 5: RIBOSOMAL PROTEIN L4

Chain E:

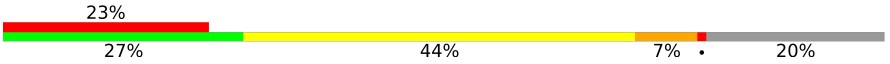


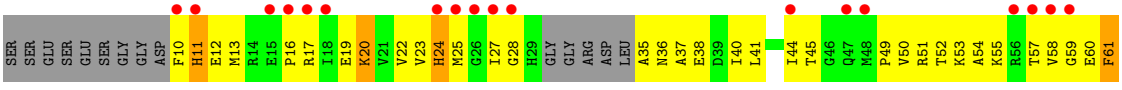


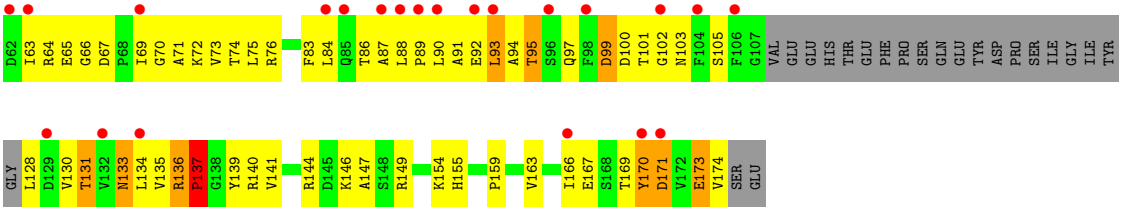


• Molecule 6: RIBOSOMAL PROTEIN L5

Chain F:

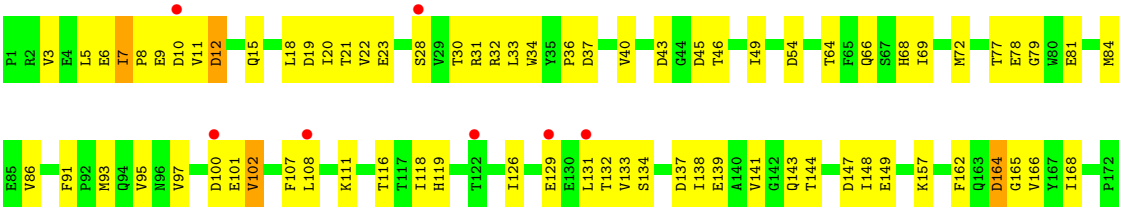






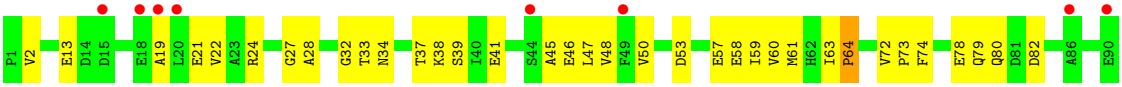
• Molecule 7: RIBOSOMAL PROTEIN L6

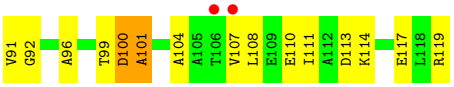
Chain G:



• Molecule 8: RIBOSOMAL PROTEIN L7AE

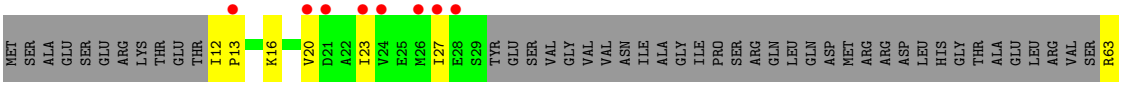
Chain H:

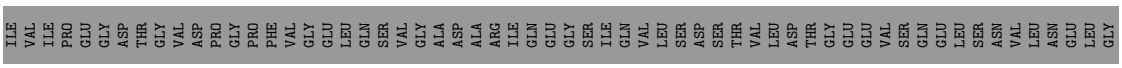


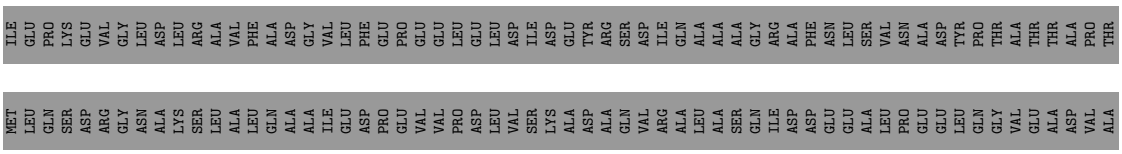


• Molecule 9: RIBOSOMAL PROTEIN L10

Chain I:

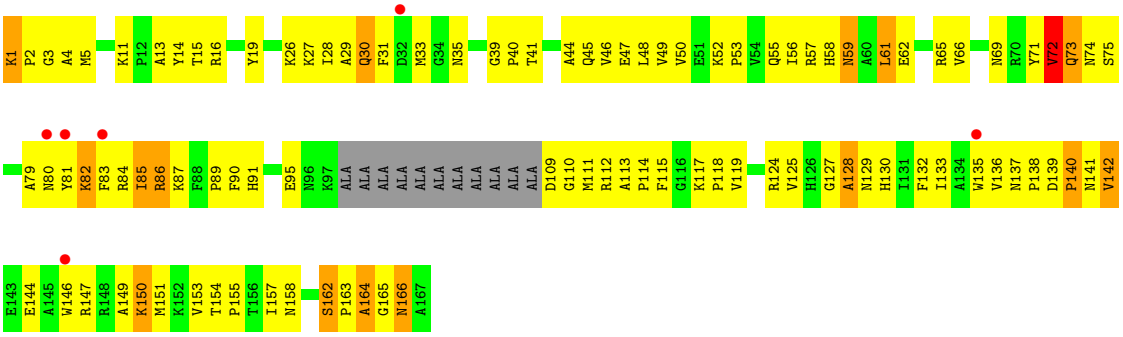






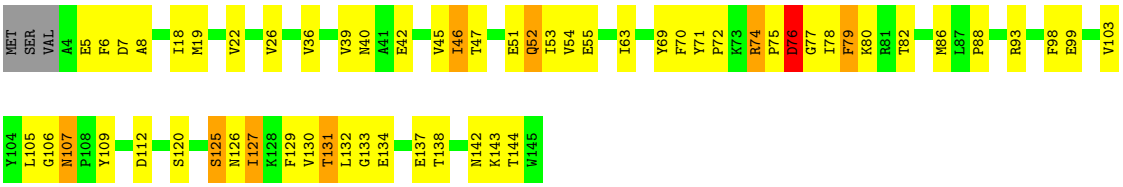
• Molecule 10: RIBOSOMAL PROTEIN L10E

Chain J:



• Molecule 11: RIBOSOMAL PROTEIN L13

Chain K:

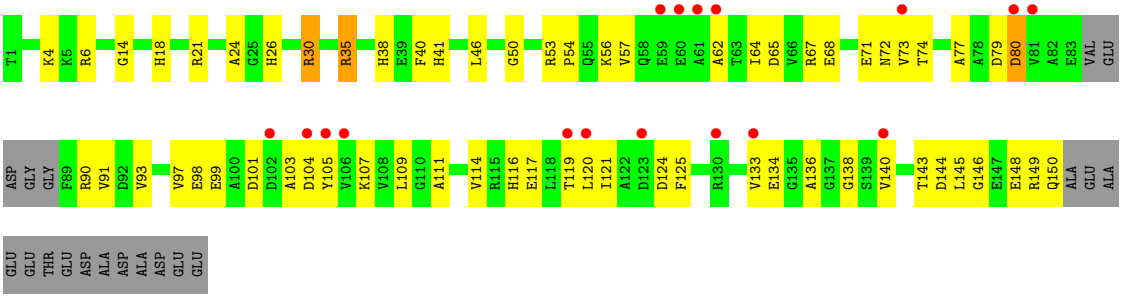


• Molecule 12: RIBOSOMAL PROTEIN L14

Chain L:

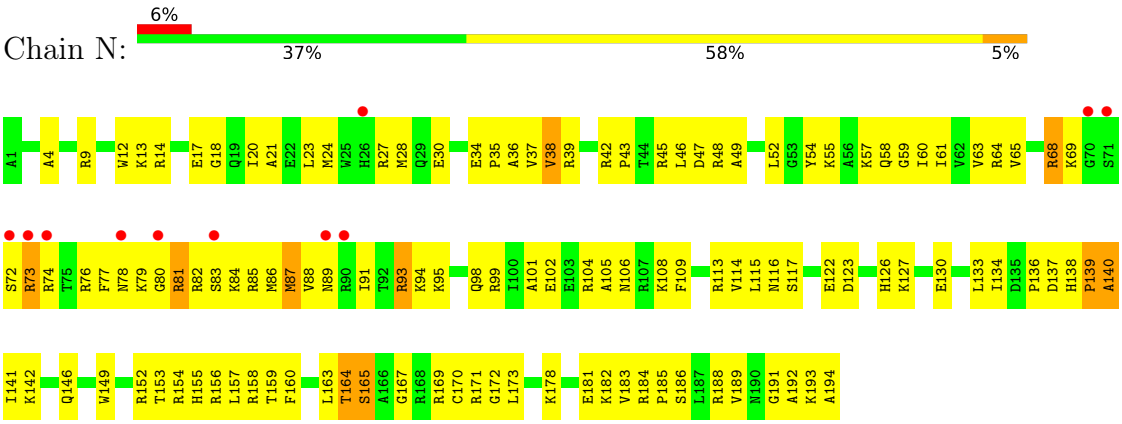
• Molecule 13: RIBOSOMAL PROTEIN L15

Chain M:



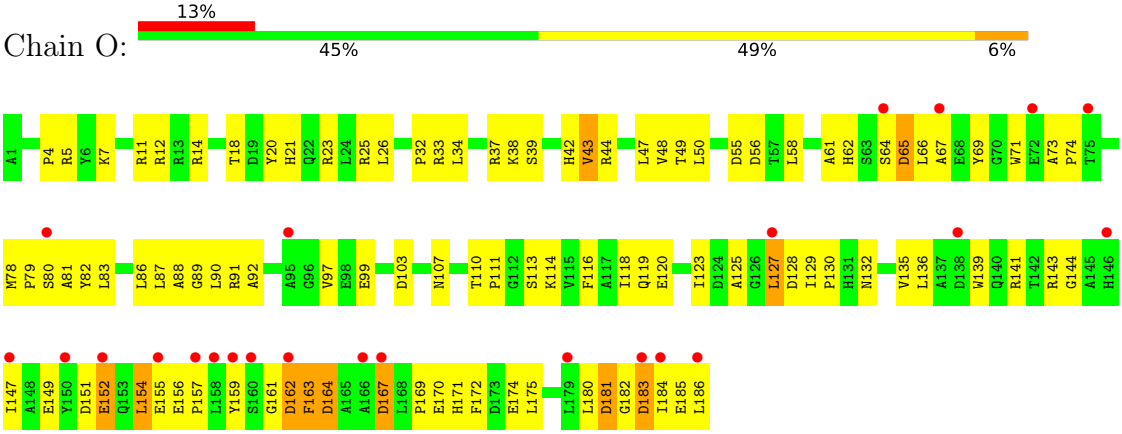
• Molecule 14: RIBOSOMAL PROTEIN L15E

Chain N:



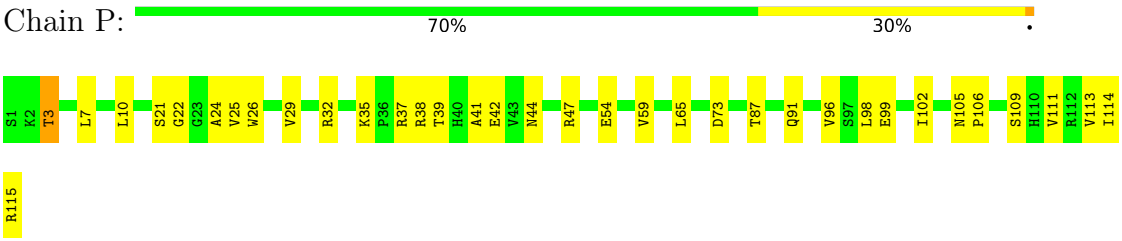
• Molecule 15: RIBOSOMAL PROTEIN L18

Chain O:



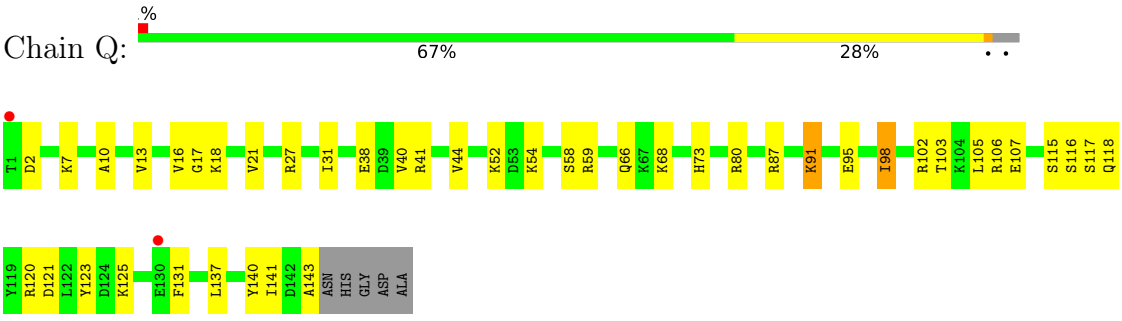
• Molecule 16: RIBOSOMAL PROTEIN L18E

Chain P:



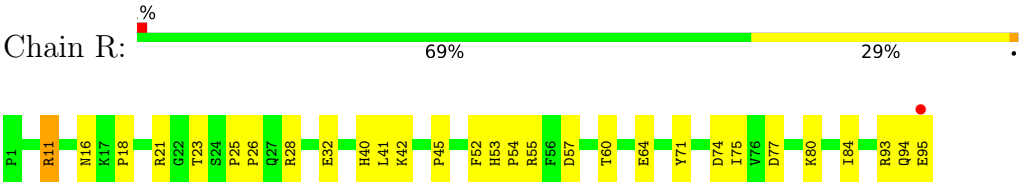
• Molecule 17: RIBOSOMAL PROTEIN L19E

Chain Q:



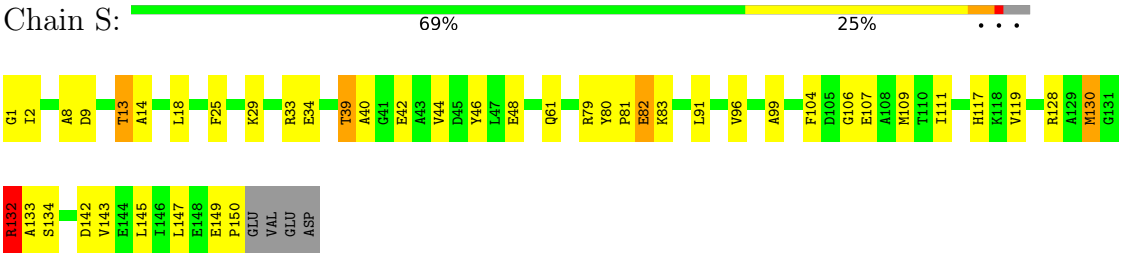
• Molecule 18: RIBOSOMAL PROTEIN L21E

Chain R:



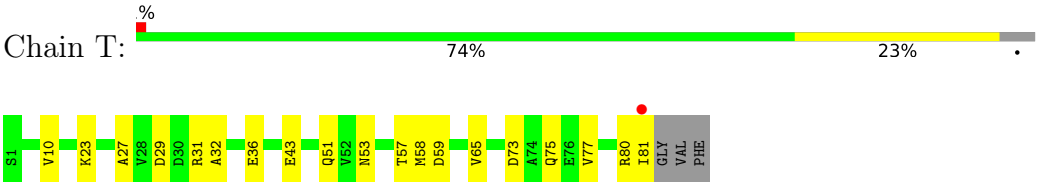
• Molecule 19: RIBOSOMAL PROTEIN L22

Chain S:



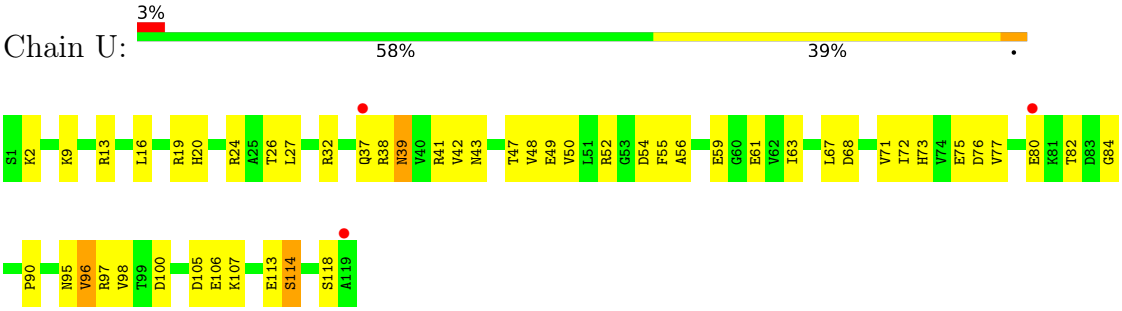
• Molecule 20: RIBOSOMAL PROTEIN L23

Chain T:



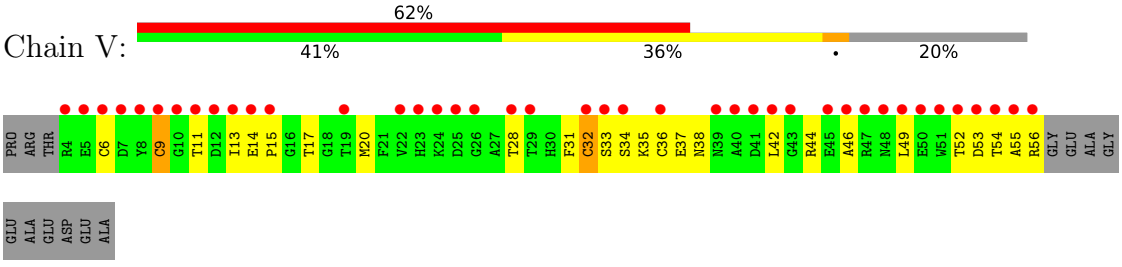
• Molecule 21: RIBOSOMAL PROTEIN L24

Chain U:



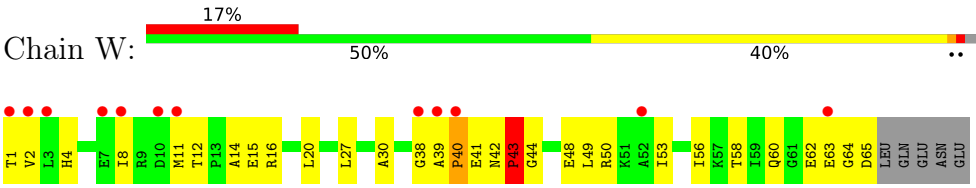
• Molecule 22: RIBOSOMAL PROTEIN L24E

Chain V:



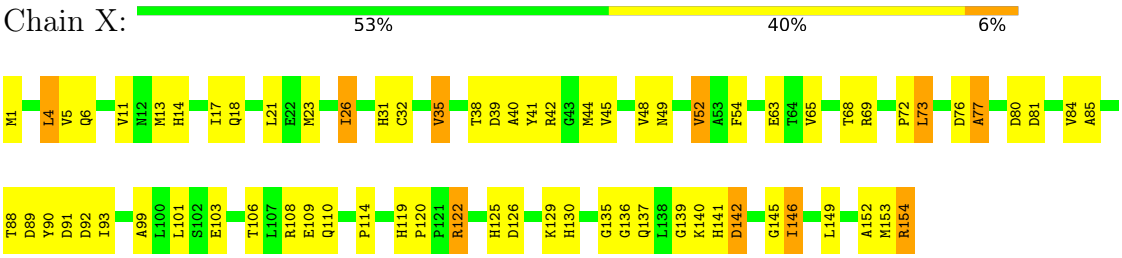
• Molecule 23: RIBOSOMAL PROTEIN L29

Chain W:



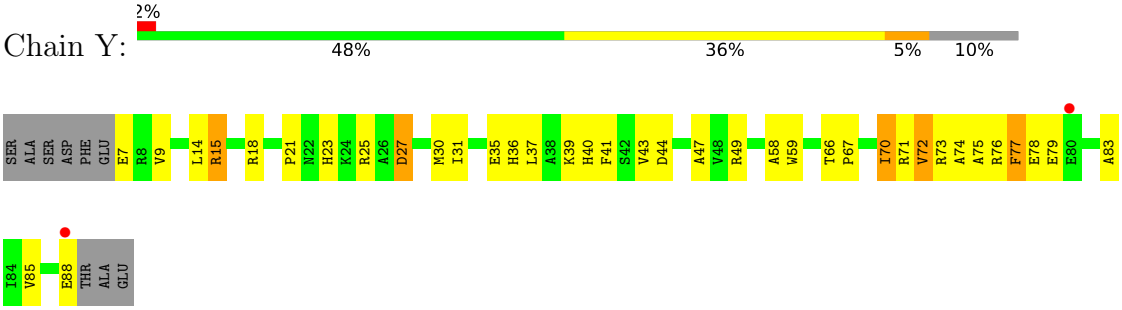
• Molecule 24: RIBOSOMAL PROTEIN L30

Chain X:



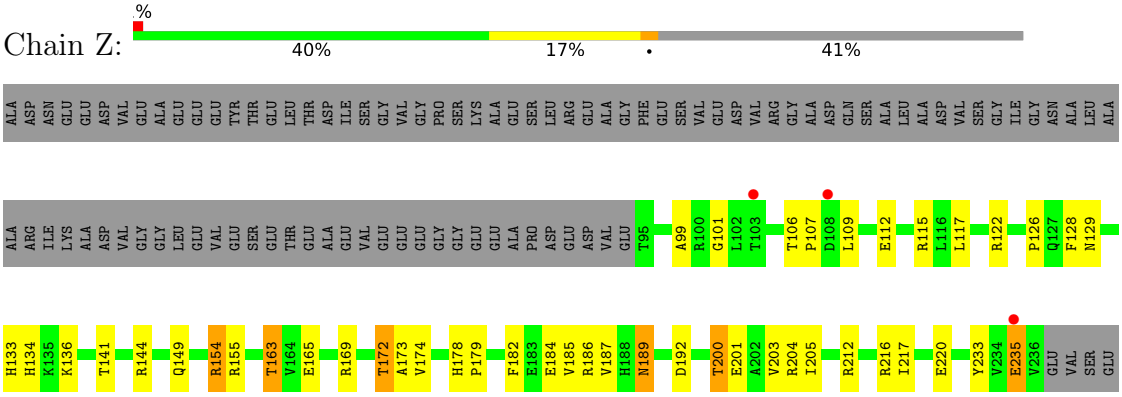
• Molecule 25: RIBOSOMAL PROTEIN L31E

Chain Y:



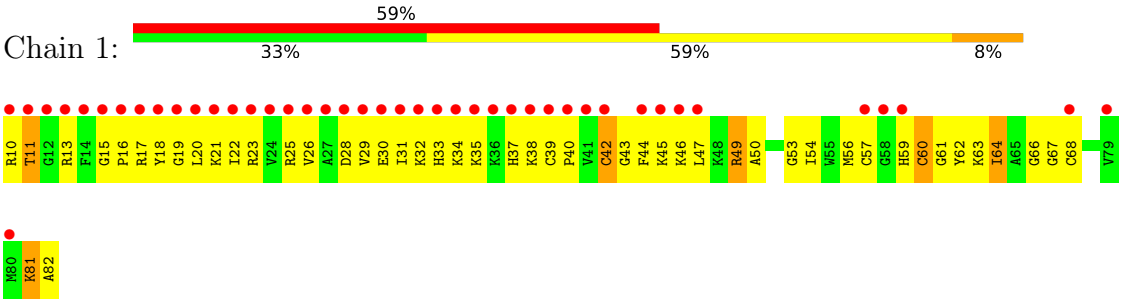
• Molecule 26: RIBOSOMAL PROTEIN L32E

Chain Z:



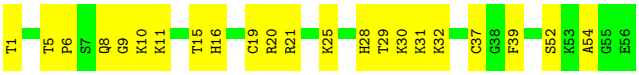
• Molecule 27: RIBOSOMAL PROTEIN L37Ae

Chain 1:



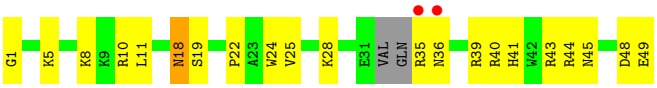
• Molecule 28: RIBOSOMAL PROTEIN L37E

Chain 2:



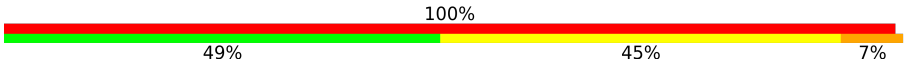
• Molecule 29: RIBOSOMAL PROTEIN L39E

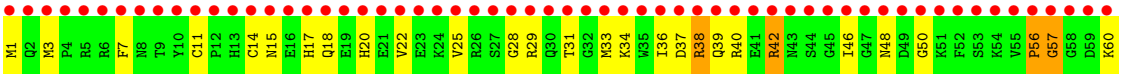
Chain 3:

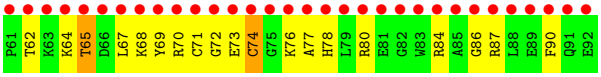


• Molecule 30: RIBOSOMAL PROTEIN L44E

Chain 4:







4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	212.90Å 300.47Å 575.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 3.00 49.92 – 2.99	Depositor EDS
% Data completeness (in resolution range)	92.9 (19.99-3.00) 92.3 (49.92-2.99)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.15	Depositor
$< I/\sigma(I) >$ [1]	2.65 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.219 , 0.262 0.220 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	46.7	Xtriage
Anisotropy	0.341	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 62.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	98593	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.47% 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, TYK, MG, K, NA, CL

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	0.59	13/66076 (0.0%)	0.77	38/103052 (0.0%)
2	B	0.89	17/2905 (0.6%)	0.91	16/4528 (0.4%)
3	C	0.57	3/1787 (0.2%)	0.78	1/2409 (0.0%)
4	D	0.48	0/2689	0.73	0/3652
5	E	0.51	0/1883	0.74	0/2551
6	F	0.41	0/1111	0.65	0/1498
7	G	0.44	0/1382	0.63	0/1880
8	H	0.43	0/896	0.65	0/1219
9	I	0.48	0/241	0.60	0/324
10	J	0.51	0/1246	0.80	2/1686 (0.1%)
11	K	0.49	0/1135	0.68	0/1530
12	L	0.48	0/1003	0.75	0/1351
13	M	0.46	0/1126	0.74	0/1504
14	N	0.59	0/1633	0.83	2/2180 (0.1%)
15	O	0.44	0/1473	0.74	0/1999
16	P	0.50	0/873	0.73	0/1181
17	Q	0.48	0/1143	0.64	0/1521
18	R	0.49	0/748	0.76	0/1005
19	S	0.63	1/1172 (0.1%)	0.82	2/1578 (0.1%)
20	T	0.46	0/648	0.68	1/875 (0.1%)
21	U	0.44	0/957	0.72	0/1289
22	V	0.70	0/417	0.81	1/562 (0.2%)
23	W	0.41	0/502	0.62	0/675
24	X	0.49	0/1218	0.73	0/1655
25	Y	0.48	0/664	0.68	0/895
26	Z	0.47	0/1146	0.72	0/1536
27	1	0.74	0/575	0.81	0/763
28	2	0.47	0/437	0.80	0/578
29	3	0.45	0/398	0.59	0/527
30	4	0.95	0/771	0.80	0/1024
All	All	0.58	34/98255 (0.0%)	0.76	63/147027 (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	1	150
2	B	0	4
All	All	1	154

The worst 5 of 34 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2104	C	O5'-C5'	-12.61	1.22	1.42
2	B	3023	U	C2'-O2'	12.28	1.57	1.41
1	A	2103	A	C6-N1	9.66	1.42	1.35
2	B	3025	G	O3'-P	9.21	1.72	1.61
1	A	2103	A	C5-C6	8.57	1.48	1.41

The worst 5 of 63 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1164	U	OP1-P-O3'	-19.07	63.25	105.20
1	A	1164	U	OP2-P-O3'	-17.80	66.05	105.20
1	A	1165	G	O5'-P-OP1	-13.80	93.28	105.70
1	A	2104	C	O5'-P-OP1	-13.33	93.70	105.70
1	A	2103	A	C5'-C4'-O4'	10.96	122.25	109.10

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1563	G	C3'

5 of 154 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	112	G	Sidechain
1	A	138	U	Sidechain
1	A	162	C	Sidechain
1	A	24	G	Sidechain
1	A	26	U	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	59017	0	29798	1175	0
2	B	2600	0	1326	79	0
3	C	1754	0	1763	134	0
4	D	2624	0	2533	189	0
5	E	1858	0	1816	121	0
6	F	1094	0	1085	137	0
7	G	1357	0	1266	76	0
8	H	885	0	854	62	0
9	I	240	0	231	20	0
10	J	1215	0	1215	160	0
11	K	1119	0	1098	67	0
12	L	993	0	1027	53	0
13	M	1114	0	1072	67	0
14	N	1605	0	1676	173	0
15	O	1444	0	1401	134	0
16	P	864	0	873	38	0
17	Q	1133	0	1127	51	0
18	R	734	0	728	24	0
19	S	1149	0	1122	57	0
20	T	641	0	605	22	0
21	U	949	0	923	56	0
22	V	410	0	368	37	0
23	W	499	0	511	31	0
24	X	1195	0	1137	98	0
25	Y	654	0	653	50	0
26	Z	1130	0	1133	62	0
27	1	563	0	601	76	0
28	2	430	0	426	26	0
29	3	393	0	406	26	0
30	4	755	0	732	59	0
31	A	64	0	76	2	0
32	1	1	0	0	0	0
32	4	1	0	0	0	0
32	A	111	0	0	0	0
32	B	1	0	0	0	0
32	C	1	0	0	0	0
32	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	L	1	0	0	0	0
32	U	1	0	0	0	0
32	Z	1	0	0	0	0
33	A	72	0	0	0	0
33	B	2	0	0	0	0
33	C	1	0	0	0	0
33	E	1	0	0	0	0
33	J	2	0	0	0	0
33	K	1	0	0	0	0
33	M	1	0	0	0	0
33	N	1	0	0	0	0
33	R	1	0	0	0	0
33	S	2	0	0	0	0
33	T	1	0	0	0	0
34	4	1	0	0	0	0
34	A	8	0	0	1	0
34	C	1	0	0	0	0
34	D	1	0	0	0	0
34	K	4	0	0	2	0
34	M	1	0	0	0	0
34	N	1	0	0	1	0
34	O	1	0	0	2	0
34	P	1	0	0	0	0
34	R	1	0	0	0	0
34	S	1	0	0	0	0
34	Z	1	0	0	0	0
35	A	3	0	0	0	0
36	1	1	0	0	0	0
36	2	1	0	0	0	0
36	4	1	0	0	0	0
36	P	1	0	0	0	0
36	V	1	0	0	0	0
37	1	37	0	0	10	0
37	2	56	0	0	4	0
37	3	43	0	0	4	0
37	4	72	0	0	4	0
37	A	5921	0	0	271	0
37	B	142	0	0	14	0
37	C	126	0	0	20	0
37	D	146	0	0	27	0
37	E	174	0	0	34	0
37	F	51	0	0	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	G	42	0	0	9	0
37	H	26	0	0	11	0
37	I	22	0	0	5	0
37	J	79	0	0	19	0
37	K	54	0	0	5	0
37	L	60	0	0	11	0
37	M	84	0	0	18	0
37	N	127	0	0	29	0
37	O	64	0	0	18	0
37	P	42	0	0	12	0
37	Q	66	0	0	5	0
37	R	53	0	0	3	0
37	S	84	0	0	7	0
37	T	34	0	0	4	0
37	U	39	0	0	4	0
37	V	26	0	0	5	0
37	W	12	0	0	1	0
37	X	70	0	0	10	0
37	Y	29	0	0	12	0
37	Z	96	0	0	17	0
All	All	98593	0	59582	3067	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 20.

The worst 5 of 3067 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1160:G:H5'	1:A:1161:A:H5'	1.25	1.15
23:W:12:THR:HG22	23:W:15:GLU:HG3	1.30	1.13
10:J:86:ARG:NH1	10:J:133:ILE:HG13	1.64	1.13
14:N:87:MET:HG2	30:4:46:ILE:HG21	1.14	1.10
14:N:87:MET:CG	30:4:46:ILE:HG21	1.84	1.08

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	C	235/239 (98%)	207 (88%)	24 (10%)	4 (2%)	9 39
4	D	335/337 (99%)	304 (91%)	22 (7%)	9 (3%)	5 26
5	E	244/246 (99%)	220 (90%)	23 (9%)	1 (0%)	34 72
6	F	134/176 (76%)	93 (69%)	30 (22%)	11 (8%)	1 4
7	G	170/177 (96%)	159 (94%)	11 (6%)	0	100 100
8	H	117/119 (98%)	102 (87%)	13 (11%)	2 (2%)	9 39
9	I	25/348 (7%)	24 (96%)	1 (4%)	0	100 100
10	J	152/167 (91%)	131 (86%)	14 (9%)	7 (5%)	2 14
11	K	140/145 (97%)	128 (91%)	8 (6%)	4 (3%)	4 24
12	L	130/132 (98%)	119 (92%)	9 (7%)	2 (2%)	10 42
13	M	141/164 (86%)	120 (85%)	20 (14%)	1 (1%)	22 60
14	N	192/194 (99%)	173 (90%)	17 (9%)	2 (1%)	15 53
15	O	184/186 (99%)	166 (90%)	11 (6%)	7 (4%)	3 18
16	P	113/115 (98%)	106 (94%)	7 (6%)	0	100 100
17	Q	141/148 (95%)	137 (97%)	3 (2%)	1 (1%)	22 60
18	R	93/95 (98%)	87 (94%)	5 (5%)	1 (1%)	14 50
19	S	148/154 (96%)	139 (94%)	9 (6%)	0	100 100
20	T	79/84 (94%)	73 (92%)	6 (8%)	0	100 100
21	U	117/119 (98%)	110 (94%)	6 (5%)	1 (1%)	17 55
22	V	51/66 (77%)	48 (94%)	3 (6%)	0	100 100
23	W	63/70 (90%)	57 (90%)	4 (6%)	2 (3%)	4 22
24	X	152/154 (99%)	145 (95%)	5 (3%)	2 (1%)	12 45
25	Y	80/91 (88%)	72 (90%)	6 (8%)	2 (2%)	5 28
26	Z	140/240 (58%)	139 (99%)	1 (1%)	0	100 100
27	1	71/73 (97%)	63 (89%)	7 (10%)	1 (1%)	11 43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
28	2	54/56 (96%)	50 (93%)	4 (7%)	0	100 100
29	3	42/48 (88%)	42 (100%)	0	0	100 100
30	4	90/92 (98%)	86 (96%)	2 (2%)	2 (2%)	6 31
All	All	3633/4235 (86%)	3300 (91%)	271 (8%)	62 (2%)	9 39

5 of 62 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	139	ASP
6	F	93	LEU
6	F	95	THR
6	F	173	GLU
8	H	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	C	179/181 (99%)	166 (93%)	13 (7%)	14 44
4	D	282/282 (100%)	265 (94%)	17 (6%)	19 53
5	E	193/193 (100%)	176 (91%)	17 (9%)	10 36
6	F	117/147 (80%)	108 (92%)	9 (8%)	13 42
7	G	152/155 (98%)	147 (97%)	5 (3%)	38 73
8	H	92/92 (100%)	91 (99%)	1 (1%)	73 90
9	I	27/283 (10%)	27 (100%)	0	100 100
10	J	122/122 (100%)	110 (90%)	12 (10%)	8 30
11	K	118/121 (98%)	107 (91%)	11 (9%)	9 33
12	L	106/106 (100%)	103 (97%)	3 (3%)	43 77
13	M	112/126 (89%)	108 (96%)	4 (4%)	35 70
14	N	166/166 (100%)	158 (95%)	8 (5%)	25 62
15	O	149/149 (100%)	143 (96%)	6 (4%)	31 68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
16	P	93/93 (100%)	92 (99%)	1 (1%)	73 90
17	Q	113/116 (97%)	110 (97%)	3 (3%)	44 77
18	R	79/79 (100%)	75 (95%)	4 (5%)	24 60
19	S	117/121 (97%)	112 (96%)	5 (4%)	29 66
20	T	71/73 (97%)	70 (99%)	1 (1%)	67 88
21	U	105/105 (100%)	102 (97%)	3 (3%)	42 76
22	V	44/52 (85%)	42 (96%)	2 (4%)	27 64
23	W	51/56 (91%)	50 (98%)	1 (2%)	55 83
24	X	130/130 (100%)	121 (93%)	9 (7%)	15 48
25	Y	66/73 (90%)	62 (94%)	4 (6%)	18 53
26	Z	120/195 (62%)	113 (94%)	7 (6%)	20 55
27	1	56/56 (100%)	50 (89%)	6 (11%)	6 26
28	2	46/46 (100%)	46 (100%)	0	100 100
29	3	42/44 (96%)	41 (98%)	1 (2%)	49 79
30	4	79/79 (100%)	73 (92%)	6 (8%)	13 43
All	All	3027/3441 (88%)	2868 (95%)	159 (5%)	22 58

5 of 159 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
19	S	39	THR
26	Z	200	THR
20	T	10	VAL
24	X	73	LEU
27	1	60	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 91 such sidechains are listed below:

Mol	Chain	Res	Type
18	R	40	HIS
24	X	28	HIS
19	S	94	ASN
20	T	53	ASN
24	X	125	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2747/2922 (94%)	244 (8%)	33 (1%)
2	B	121/122 (99%)	16 (13%)	6 (4%)
All	All	2868/3044 (94%)	260 (9%)	39 (1%)

5 of 260 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	11	A
1	A	31	C
1	A	60	A
1	A	67	A
1	A	69	A

5 of 39 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	2526	C
2	B	3026	C
1	A	2536	C
1	A	2791	U
2	B	3065	A

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 235 ligands modelled in this entry, 234 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	$\#\|Z\| > 2$
31	TYK	A	9000	1	67,67,67	3.43	31 (46%)	83,97,97	2.34	23 (27%)

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
31	TYK	A	9000	1	-	9/67/126/126	0/3/4/4

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	9000	TYK	O1C-C1C	12.47	1.61	1.40
31	A	9000	TYK	O9-C9	9.87	1.37	1.22
31	A	9000	TYK	C22-C12	8.42	1.68	1.50
31	A	9000	TYK	C8-C9	6.67	1.62	1.51
31	A	9000	TYK	C4-C3	-6.43	1.41	1.54

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	A	9000	TYK	O20-C20-C19	-11.11	93.06	125.43
31	A	9000	TYK	O15-C15-C16	-6.77	96.12	106.92
31	A	9000	TYK	C6C-C5C-C4C	-6.10	101.81	113.07
31	A	9000	TYK	O1A-C5-C4	4.69	113.87	108.22
31	A	9000	TYK	C10-C11-C12	-4.46	119.50	126.23

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

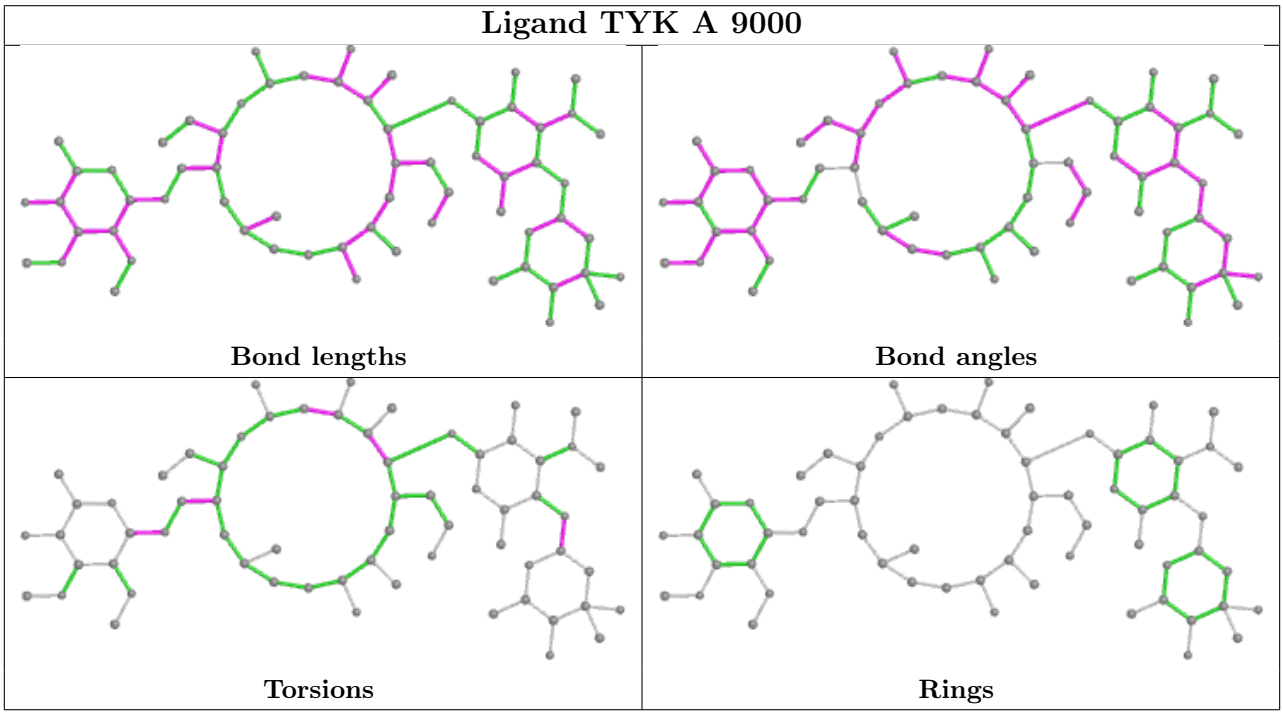
Mol	Chain	Res	Type	Atoms
31	A	9000	TYK	C2B-C1B-O4A-C4A
31	A	9000	TYK	O5C-C1C-O1C-C23
31	A	9000	TYK	C2C-C1C-O1C-C23
31	A	9000	TYK	O5B-C1B-O4A-C4A
31	A	9000	TYK	C1-C2-C3-C4

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	A	9000	TYK	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.



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	2754/2922 (94%)	-0.04	66 (2%) 59 30	20, 47, 93, 139	0
2	B	122/122 (100%)	0.22	5 (4%) 37 14	31, 65, 95, 145	0
3	C	237/239 (99%)	0.22	16 (6%) 17 5	27, 61, 90, 109	0
4	D	337/337 (100%)	-0.07	1 (0%) 94 84	20, 54, 81, 90	0
5	E	246/246 (100%)	-0.15	2 (0%) 86 65	19, 49, 72, 81	0
6	F	140/176 (79%)	1.49	40 (28%) 0 0	54, 101, 118, 126	0
7	G	172/177 (97%)	0.60	7 (4%) 37 14	39, 65, 88, 94	0
8	H	119/119 (100%)	0.79	10 (8%) 11 3	56, 78, 99, 103	0
9	I	29/348 (8%)	2.05	14 (48%) 0 0	68, 91, 100, 101	0
10	J	156/167 (93%)	0.23	6 (3%) 40 16	32, 55, 79, 88	0
11	K	142/145 (97%)	-0.10	0 100 100	32, 47, 71, 82	0
12	L	132/132 (100%)	-0.00	1 (0%) 86 65	30, 53, 76, 82	0
13	M	145/164 (88%)	0.58	17 (11%) 4 1	23, 72, 105, 115	0
14	N	194/194 (100%)	0.09	11 (5%) 23 8	34, 53, 83, 88	0
15	O	186/186 (100%)	0.70	24 (12%) 3 1	41, 69, 107, 119	0
16	P	115/115 (100%)	-0.06	0 100 100	38, 57, 76, 80	0
17	Q	143/148 (96%)	0.05	2 (1%) 75 49	33, 58, 73, 81	0
18	R	95/95 (100%)	-0.21	1 (1%) 80 56	33, 48, 59, 73	0
19	S	150/154 (97%)	-0.12	0 100 100	27, 42, 66, 74	0
20	T	81/84 (96%)	0.13	1 (1%) 79 54	47, 62, 80, 84	0
21	U	119/119 (100%)	0.37	3 (2%) 57 29	37, 58, 81, 91	0
22	V	53/66 (80%)	3.14	41 (77%) 0 0	81, 91, 97, 105	0
23	W	65/70 (92%)	1.17	12 (18%) 1 0	52, 77, 106, 113	0
24	X	154/154 (100%)	-0.31	0 100 100	31, 46, 66, 74	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
25	Y	82/91 (90%)	0.30	2 (2%) 59 30	39, 55, 81, 93	0
26	Z	142/240 (59%)	-0.01	3 (2%) 63 34	25, 45, 69, 85	0
27	1	73/73 (100%)	2.99	43 (58%) 0 0	79, 92, 98, 99	0
28	2	56/56 (100%)	-0.50	0 100 100	26, 34, 41, 47	0
29	3	46/48 (95%)	0.11	2 (4%) 35 13	33, 59, 85, 97	0
30	4	92/92 (100%)	6.13	92 (100%) 0 0	90, 101, 105, 107	0
All	All	6577/7279 (90%)	0.25	422 (6%) 19 6	19, 54, 99, 145	0

The worst 5 of 422 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
30	4	37	ASP	14.5
30	4	62	THR	13.3
30	4	82	GLY	12.7
30	4	83	TRP	11.3
30	4	38	ARG	11.2

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
33	NA	A	8384	1/1	0.27	1.11	106,106,106,106	0
33	NA	S	8337	1/1	0.47	0.33	34,34,34,34	0
34	CL	4	8504	1/1	0.48	1.29	112,112,112,112	0
33	NA	E	8304	1/1	0.62	0.16	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
33	NA	J	8322	1/1	0.63	0.46	56,56,56,56	0
33	NA	S	8386	1/1	0.64	0.54	75,75,75,75	0
36	CD	V	8401	1/1	0.68	0.41	142,142,142,142	0
33	NA	T	8312	1/1	0.70	0.79	69,69,69,69	0
36	CD	P	8405	1/1	0.72	0.20	154,154,154,154	0
32	MG	A	8112	1/1	0.73	0.19	58,58,58,58	0
36	CD	4	8404	1/1	0.74	0.52	148,148,148,148	0
32	MG	A	8104	1/1	0.75	0.38	51,51,51,51	0
33	NA	A	8373	1/1	0.77	0.49	37,37,37,37	0
33	NA	A	8357	1/1	0.77	0.10	53,53,53,53	0
33	NA	B	8351	1/1	0.77	0.18	58,58,58,58	0
33	NA	A	8356	1/1	0.78	0.73	57,57,57,57	0
34	CL	A	8505	1/1	0.78	0.53	83,83,83,83	0
33	NA	A	8332	1/1	0.79	0.18	34,34,34,34	0
32	MG	A	8050	1/1	0.80	0.21	77,77,77,77	0
33	NA	A	8382	1/1	0.81	0.30	41,41,41,41	0
33	NA	B	8383	1/1	0.81	0.19	54,54,54,54	0
33	NA	A	8326	1/1	0.81	0.25	56,56,56,56	0
32	MG	A	8071	1/1	0.82	0.11	84,84,84,84	0
32	MG	A	8001	1/1	0.82	0.11	38,38,38,38	0
32	MG	A	8070	1/1	0.83	0.80	70,70,70,70	0
32	MG	D	8055	1/1	0.84	0.17	84,84,84,84	0
33	NA	A	8377	1/1	0.84	0.32	77,77,77,77	0
33	NA	A	8310	1/1	0.84	0.20	31,31,31,31	0
32	MG	A	8118	1/1	0.84	0.33	31,31,31,31	0
33	NA	A	8362	1/1	0.85	0.32	63,63,63,63	0
33	NA	A	8369	1/1	0.85	0.23	53,53,53,53	0
34	CL	M	8510	1/1	0.85	0.33	75,75,75,75	0
33	NA	A	8303	1/1	0.85	0.26	53,53,53,53	0
33	NA	A	8354	1/1	0.85	0.20	40,40,40,40	0
32	MG	A	8081	1/1	0.85	0.18	64,64,64,64	0
32	MG	A	8101	1/1	0.85	0.16	38,38,38,38	0
32	MG	A	8023	1/1	0.86	0.10	42,42,42,42	0
34	CL	A	8503	1/1	0.86	0.26	55,55,55,55	0
33	NA	A	8321	1/1	0.87	0.29	45,45,45,45	0
33	NA	A	8301	1/1	0.87	0.17	20,20,20,20	0
33	NA	A	8364	1/1	0.87	0.23	39,39,39,39	0
32	MG	A	8090	1/1	0.87	0.21	11,11,11,11	0
33	NA	A	8370	1/1	0.87	0.37	55,55,55,55	0
33	NA	A	8371	1/1	0.87	0.21	31,31,31,31	0
32	MG	A	8087	1/1	0.87	0.18	52,52,52,52	0
33	NA	A	8311	1/1	0.87	0.22	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	MG	A	8116	1/1	0.88	0.21	80,80,80,80	0
32	MG	A	8024	1/1	0.88	0.55	99,99,99,99	0
34	CL	A	8522	1/1	0.88	0.74	80,80,80,80	0
33	NA	A	8323	1/1	0.88	0.29	38,38,38,38	0
33	NA	A	8372	1/1	0.89	0.48	53,53,53,53	0
34	CL	A	8513	1/1	0.89	0.19	64,64,64,64	0
32	MG	A	8082	1/1	0.89	0.23	59,59,59,59	0
33	NA	A	8376	1/1	0.89	0.33	80,80,80,80	0
33	NA	A	8366	1/1	0.89	0.28	43,43,43,43	0
35	K	A	8602	1/1	0.89	0.13	56,56,56,56	0
32	MG	A	8046	1/1	0.89	0.07	62,62,62,62	0
32	MG	B	8095	1/1	0.89	0.06	68,68,68,68	0
33	NA	A	8341	1/1	0.89	0.10	17,17,17,17	0
32	MG	A	8059	1/1	0.90	0.09	33,33,33,33	0
32	MG	A	8066	1/1	0.90	0.07	70,70,70,70	0
32	MG	A	8100	1/1	0.90	0.15	48,48,48,48	0
34	CL	K	8502	1/1	0.90	0.12	56,56,56,56	0
33	NA	A	8374	1/1	0.90	0.30	41,41,41,41	0
33	NA	A	8307	1/1	0.91	0.10	20,20,20,20	0
33	NA	A	8330	1/1	0.91	0.18	46,46,46,46	0
33	NA	A	8365	1/1	0.91	0.33	41,41,41,41	0
34	CL	A	8515	1/1	0.91	0.49	97,97,97,97	0
33	NA	A	8331	1/1	0.91	0.18	46,46,46,46	0
33	NA	A	8368	1/1	0.91	0.16	43,43,43,43	0
33	NA	A	8308	1/1	0.91	0.12	50,50,50,50	0
34	CL	Z	8520	1/1	0.91	0.14	30,30,30,30	0
32	MG	A	8041	1/1	0.91	0.34	62,62,62,62	0
32	MG	A	8115	1/1	0.91	0.10	46,46,46,46	0
35	K	A	8603	1/1	0.91	0.44	76,76,76,76	0
33	NA	A	8355	1/1	0.91	0.68	55,55,55,55	0
32	MG	A	8061	1/1	0.91	0.06	35,35,35,35	0
32	MG	A	8045	1/1	0.91	0.11	61,61,61,61	0
32	MG	A	8064	1/1	0.92	0.15	18,18,18,18	0
33	NA	A	8302	1/1	0.92	0.16	24,24,24,24	0
33	NA	A	8324	1/1	0.92	0.12	42,42,42,42	0
33	NA	A	8359	1/1	0.92	0.44	52,52,52,52	0
33	NA	A	8378	1/1	0.92	0.30	30,30,30,30	0
32	MG	A	8027	1/1	0.92	0.06	51,51,51,51	0
33	NA	A	8305	1/1	0.92	0.13	33,33,33,33	0
34	CL	R	8511	1/1	0.92	0.13	57,57,57,57	0
32	MG	A	8092	1/1	0.92	0.16	83,83,83,83	0
32	MG	A	8053	1/1	0.92	0.10	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
33	NA	A	8333	1/1	0.92	0.16	26,26,26,26	0
33	NA	A	8336	1/1	0.92	0.16	46,46,46,46	0
32	MG	Z	8109	1/1	0.92	0.14	39,39,39,39	0
33	NA	A	8342	1/1	0.92	0.17	39,39,39,39	0
32	MG	4	8078	1/1	0.92	0.42	91,91,91,91	0
33	NA	A	8350	1/1	0.93	0.21	24,24,24,24	0
34	CL	A	8517	1/1	0.93	0.24	49,49,49,49	0
32	MG	A	8040	1/1	0.93	0.10	84,84,84,84	0
32	MG	A	8106	1/1	0.93	0.13	62,62,62,62	0
34	CL	K	8516	1/1	0.93	0.19	40,40,40,40	0
32	MG	A	8108	1/1	0.93	0.11	73,73,73,73	0
32	MG	A	8088	1/1	0.93	0.07	28,28,28,28	0
33	NA	M	8380	1/1	0.93	0.25	49,49,49,49	0
32	MG	A	8114	1/1	0.93	0.23	82,82,82,82	0
33	NA	A	8338	1/1	0.93	0.12	59,59,59,59	0
33	NA	A	8363	1/1	0.93	0.19	49,49,49,49	0
33	NA	A	8340	1/1	0.93	0.37	31,31,31,31	0
32	MG	A	8103	1/1	0.93	0.20	69,69,69,69	0
36	CD	1	8403	1/1	0.93	0.21	139,139,139,139	0
33	NA	A	8327	1/1	0.93	0.15	28,28,28,28	0
33	NA	A	8343	1/1	0.94	0.08	11,11,11,11	0
32	MG	U	8073	1/1	0.94	0.12	38,38,38,38	0
34	CL	A	8512	1/1	0.94	0.15	32,32,32,32	0
33	NA	A	8352	1/1	0.94	0.47	37,37,37,37	0
32	MG	A	8067	1/1	0.94	0.26	49,49,49,49	0
33	NA	A	8375	1/1	0.94	0.25	53,53,53,53	0
32	MG	A	8022	1/1	0.94	0.18	39,39,39,39	0
32	MG	A	8111	1/1	0.94	0.06	54,54,54,54	0
32	MG	A	8089	1/1	0.94	0.11	64,64,64,64	0
32	MG	A	8113	1/1	0.94	0.13	40,40,40,40	0
34	CL	N	8518	1/1	0.94	0.17	38,38,38,38	0
32	MG	A	8062	1/1	0.94	0.11	46,46,46,46	0
32	MG	A	8075	1/1	0.94	0.11	38,38,38,38	0
33	NA	A	8334	1/1	0.94	0.06	26,26,26,26	0
35	K	A	8601	1/1	0.94	0.12	62,62,62,62	0
31	TYK	A	9000	64/64	0.94	0.21	33,43,48,51	0
32	MG	A	8049	1/1	0.94	0.16	62,62,62,62	0
33	NA	A	8367	1/1	0.94	0.15	37,37,37,37	0
32	MG	A	8084	1/1	0.94	0.09	40,40,40,40	0
33	NA	A	8319	1/1	0.94	0.14	39,39,39,39	0
32	MG	A	8085	1/1	0.94	0.11	79,79,79,79	0
33	NA	N	8347	1/1	0.95	0.11	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
34	CL	K	8521	1/1	0.95	0.21	50,50,50,50	0
32	MG	A	8044	1/1	0.95	0.17	44,44,44,44	0
33	NA	A	8320	1/1	0.95	0.11	32,32,32,32	0
34	CL	O	8507	1/1	0.95	0.14	54,54,54,54	0
32	MG	A	8093	1/1	0.95	0.12	38,38,38,38	0
32	MG	A	8096	1/1	0.95	0.10	54,54,54,54	0
32	MG	A	8110	1/1	0.95	0.11	23,23,23,23	0
33	NA	A	8385	1/1	0.95	0.25	28,28,28,28	0
33	NA	A	8325	1/1	0.95	0.15	47,47,47,47	0
32	MG	A	8048	1/1	0.95	0.15	47,47,47,47	0
32	MG	A	8057	1/1	0.95	0.18	34,34,34,34	0
32	MG	A	8102	1/1	0.95	0.86	82,82,82,82	0
34	CL	D	8519	1/1	0.95	0.49	59,59,59,59	0
32	MG	A	8018	1/1	0.95	0.08	32,32,32,32	0
32	MG	A	8006	1/1	0.96	0.06	48,48,48,48	0
32	MG	A	8042	1/1	0.96	0.13	31,31,31,31	0
33	NA	A	8344	1/1	0.96	0.07	16,16,16,16	0
34	CL	A	8514	1/1	0.96	0.12	51,51,51,51	0
32	MG	1	8105	1/1	0.96	0.18	42,42,42,42	0
32	MG	A	8097	1/1	0.96	0.23	37,37,37,37	0
32	MG	A	8052	1/1	0.96	0.05	36,36,36,36	0
32	MG	A	8007	1/1	0.96	0.06	24,24,24,24	0
32	MG	A	8002	1/1	0.96	0.12	42,42,42,42	0
33	NA	A	8379	1/1	0.96	0.15	32,32,32,32	0
32	MG	A	8031	1/1	0.96	0.04	14,14,14,14	0
33	NA	A	8328	1/1	0.96	0.13	24,24,24,24	0
33	NA	A	8360	1/1	0.96	0.54	38,38,38,38	0
33	NA	A	8361	1/1	0.96	0.13	48,48,48,48	0
34	CL	P	8508	1/1	0.96	0.24	83,83,83,83	0
33	NA	A	8306	1/1	0.96	0.37	36,36,36,36	0
32	MG	A	8072	1/1	0.96	0.15	88,88,88,88	0
32	MG	A	8119	1/1	0.96	0.10	30,30,30,30	0
33	NA	K	8346	1/1	0.96	0.12	17,17,17,17	0
32	MG	A	8003	1/1	0.96	0.12	19,19,19,19	0
32	MG	A	8079	1/1	0.96	0.09	24,24,24,24	0
33	NA	A	8314	1/1	0.96	0.14	45,45,45,45	0
33	NA	A	8316	1/1	0.96	0.12	31,31,31,31	0
33	NA	A	8317	1/1	0.96	0.11	9,9,9,9	0
33	NA	A	8318	1/1	0.96	0.14	37,37,37,37	0
32	MG	A	8051	1/1	0.97	0.07	66,66,66,66	0
32	MG	A	8016	1/1	0.97	0.08	43,43,43,43	0
33	NA	A	8339	1/1	0.97	0.16	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
33	NA	A	8313	1/1	0.97	0.17	64,64,64,64	0
32	MG	A	8094	1/1	0.97	0.05	60,60,60,60	0
32	MG	A	8004	1/1	0.97	0.11	35,35,35,35	0
32	MG	A	8054	1/1	0.97	0.08	50,50,50,50	0
34	CL	C	8509	1/1	0.97	0.33	74,74,74,74	0
32	MG	A	8099	1/1	0.97	0.09	46,46,46,46	0
33	NA	A	8349	1/1	0.97	0.29	33,33,33,33	0
32	MG	C	8065	1/1	0.97	0.07	52,52,52,52	0
32	MG	A	8076	1/1	0.97	0.13	61,61,61,61	0
32	MG	L	8069	1/1	0.97	0.10	72,72,72,72	0
32	MG	A	8077	1/1	0.97	0.09	28,28,28,28	0
32	MG	A	8025	1/1	0.97	0.09	54,54,54,54	0
32	MG	A	8021	1/1	0.97	0.08	27,27,27,27	0
32	MG	A	8060	1/1	0.97	0.10	48,48,48,48	0
34	CL	S	8506	1/1	0.97	0.14	42,42,42,42	0
32	MG	A	8028	1/1	0.97	0.07	43,43,43,43	0
32	MG	A	8107	1/1	0.97	0.06	51,51,51,51	0
33	NA	A	8329	1/1	0.97	0.09	33,33,33,33	0
32	MG	A	8011	1/1	0.97	0.07	25,25,25,25	0
32	MG	A	8032	1/1	0.97	0.10	29,29,29,29	0
32	MG	A	8033	1/1	0.97	0.09	22,22,22,22	0
32	MG	A	8039	1/1	0.97	0.09	54,54,54,54	0
32	MG	A	8068	1/1	0.97	0.12	40,40,40,40	0
33	NA	A	8335	1/1	0.97	0.18	45,45,45,45	0
32	MG	A	8029	1/1	0.98	0.12	51,51,51,51	0
33	NA	A	8381	1/1	0.98	0.09	33,33,33,33	0
32	MG	A	8008	1/1	0.98	0.08	41,41,41,41	0
32	MG	A	8074	1/1	0.98	0.07	12,12,12,12	0
32	MG	A	8056	1/1	0.98	0.07	41,41,41,41	0
34	CL	K	8501	1/1	0.98	0.21	58,58,58,58	0
32	MG	A	8043	1/1	0.98	0.06	58,58,58,58	0
32	MG	A	8058	1/1	0.98	0.11	34,34,34,34	0
33	NA	C	8345	1/1	0.98	0.10	34,34,34,34	0
32	MG	A	8017	1/1	0.98	0.05	28,28,28,28	0
33	NA	J	8309	1/1	0.98	0.13	25,25,25,25	0
32	MG	A	8005	1/1	0.98	0.14	47,47,47,47	0
32	MG	A	8034	1/1	0.98	0.05	32,32,32,32	0
32	MG	A	8083	1/1	0.98	0.07	47,47,47,47	0
32	MG	A	8047	1/1	0.98	0.14	45,45,45,45	0
33	NA	R	8348	1/1	0.98	0.06	15,15,15,15	0
32	MG	A	8063	1/1	0.98	0.09	73,73,73,73	0
32	MG	A	8086	1/1	0.98	0.11	40,40,40,40	0

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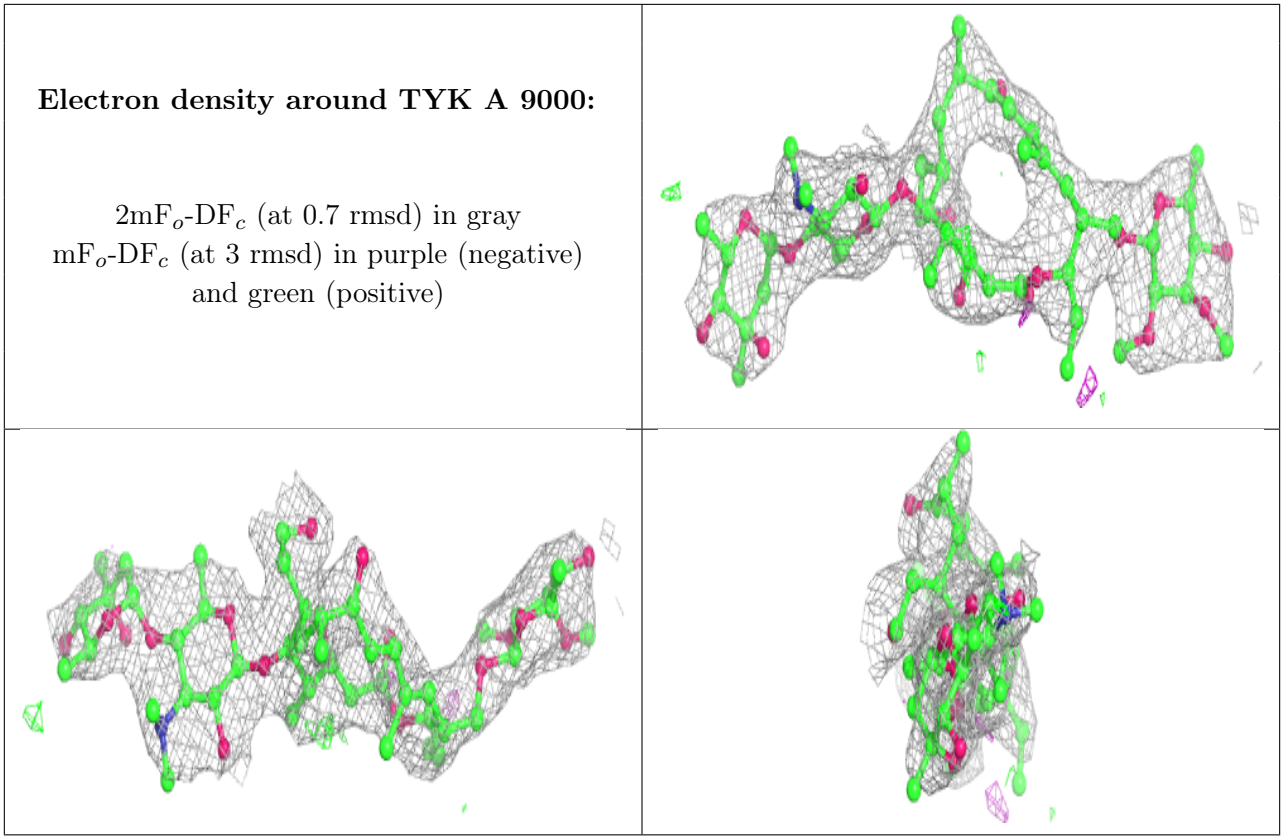
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	MG	A	8035	1/1	0.98	0.06	48,48,48,48	0
32	MG	A	8037	1/1	0.98	0.12	45,45,45,45	0
32	MG	A	8038	1/1	0.98	0.05	14,14,14,14	0
32	MG	A	8014	1/1	0.98	0.05	13,13,13,13	0
32	MG	A	8091	1/1	0.98	0.07	45,45,45,45	0
36	CD	2	8402	1/1	0.98	0.08	52,52,52,52	0
32	MG	A	8015	1/1	0.98	0.08	46,46,46,46	0
32	MG	A	8010	1/1	0.99	0.07	29,29,29,29	0
32	MG	A	8020	1/1	0.99	0.05	34,34,34,34	0
32	MG	A	8026	1/1	0.99	0.05	15,15,15,15	0
32	MG	A	8098	1/1	0.99	0.20	43,43,43,43	0
32	MG	A	8009	1/1	0.99	0.04	19,19,19,19	0
33	NA	A	8353	1/1	0.99	0.08	16,16,16,16	0
32	MG	A	8080	1/1	0.99	0.06	35,35,35,35	0
32	MG	A	8012	1/1	0.99	0.11	34,34,34,34	0
32	MG	A	8036	1/1	0.99	0.06	41,41,41,41	0
32	MG	A	8013	1/1	0.99	0.18	42,42,42,42	0
32	MG	A	8030	1/1	0.99	0.09	29,29,29,29	0
33	NA	A	8315	1/1	0.99	0.12	27,27,27,27	0
32	MG	A	8117	1/1	0.99	0.15	19,19,19,19	0
32	MG	A	8019	1/1	1.00	0.05	27,27,27,27	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 TYK A 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.