wwPDB X-ray Structure Validation Summary Report (i)

Feb 19, 2016 – 09:00 PM GMT

PDB ID	:	4WF9
Title	:	The crystal structure of the large ribosomal subunit of Staphylococcus aureus in complex with telithromycin
Authors	:	Eyal, Z.; Matzov, D.; Krupkin, M.; Wekselman, I.; Zimmerman, E.; Rozenberg, H.; Bashan, A.; Yonath, A.E.
Deposited on	:	2014-09-14
Resolution	:	3.43 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

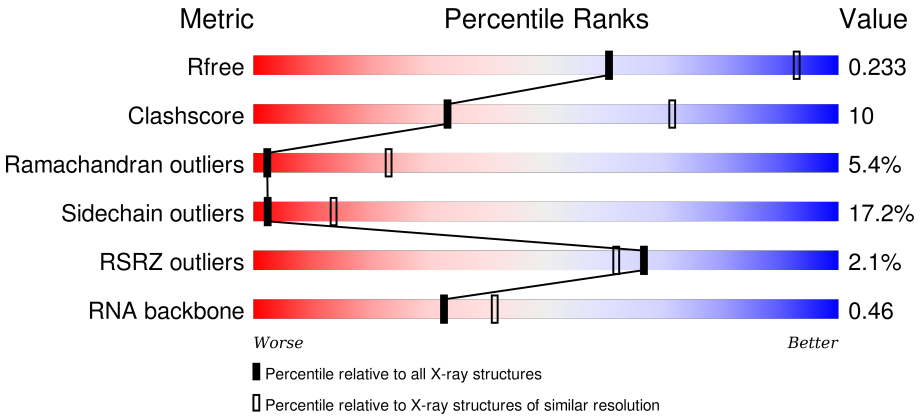
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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 3.43 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.



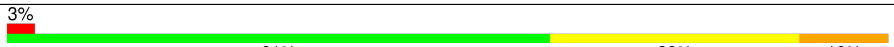
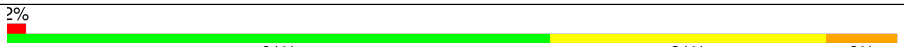
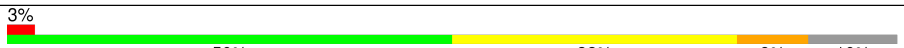
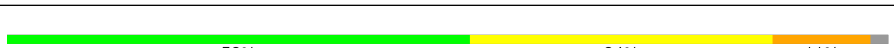
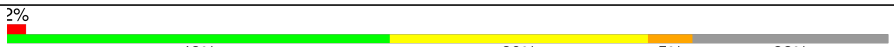
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1049 (3.52-3.32)
Clashscore	102246	1032 (3.50-3.34)
Ramachandran outliers	100387	1002 (3.50-3.34)
Sidechain outliers	100360	1003 (3.50-3.34)
RSRZ outliers	91569	1054 (3.52-3.32)
RNA backbone	2183	1042 (4.02-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	X	2923	51% 32% 9% • 7%
2	Y	114	49% 44% 5% •
3	A	277	5% 67% 26% • •
4	B	220	52% 36% 10% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	C	207	
6	D	179	
7	E	178	
8	G	145	
9	H	122	
10	I	146	
11	J	144	
12	K	122	
13	L	119	
14	M	116	
15	N	118	
16	O	102	
17	P	117	
18	Q	91	
19	R	105	
20	S	217	
21	T	94	
22	V	69	
23	W	59	
24	Z	58	
25	2	45	
26	3	66	

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
27	TEL	X	3001	-	-	-	X
28	MPD	X	3002	-	-	-	X
28	MPD	X	3003	-	-	-	X
28	MPD	X	3004	-	-	-	X
28	MPD	X	3005	-	-	X	X
28	MPD	X	3007	-	-	-	X
29	MG	A	301	-	-	-	X
29	MG	C	302	-	-	-	X
29	MG	X	3193	-	-	-	X
29	MG	X	3251	-	-	-	X
29	MG	X	3274	-	-	-	X
29	MG	X	3324	-	-	-	X
29	MG	X	3325	-	-	-	X
29	MG	X	3326	-	-	-	X
29	MG	X	3334	-	-	-	X
29	MG	X	3340	-	-	-	X
29	MG	X	3346	-	-	-	X
29	MG	X	3348	-	-	-	X
29	MG	Y	207	-	-	-	X
30	MN	X	3036	-	-	-	X
30	MN	X	3038	-	-	-	X
30	MN	X	3039	-	-	-	X
30	MN	X	3044	-	-	-	X
30	MN	X	3048	-	-	-	X
30	MN	X	3056	-	-	-	X
30	MN	X	3067	-	-	-	X
30	MN	X	3070	-	-	-	X
30	MN	X	3071	-	-	-	X
30	MN	X	3077	-	-	-	X
30	MN	X	3078	-	-	-	X
30	MN	X	3080	-	-	-	X
30	MN	X	3082	-	-	-	X
30	MN	X	3086	-	-	-	X
30	MN	X	3090	-	-	-	X
30	MN	X	3095	-	-	-	X
30	MN	X	3099	-	-	-	X
30	MN	X	3101	-	-	-	X
30	MN	X	3103	-	-	-	X
30	MN	X	3106	-	-	-	X
30	MN	X	3107	-	-	-	X
30	MN	X	3108	-	-	-	X
30	MN	X	3109	-	-	-	X
30	MN	X	3112	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	MN	X	3117	-	-	-	X
30	MN	X	3123	-	-	-	X
30	MN	X	3129	-	-	-	X
30	MN	X	3136	-	-	-	X
30	MN	X	3139	-	-	-	X
30	MN	X	3140	-	-	-	X
30	MN	X	3153	-	-	-	X
30	MN	X	3166	-	-	-	X
30	MN	X	3177	-	-	-	X
30	MN	X	3178	-	-	-	X
30	MN	X	3203	-	-	-	X
30	MN	X	3213	-	-	-	X
30	MN	X	3217	-	-	-	X
30	MN	X	3221	-	-	-	X
30	MN	X	3240	-	-	-	X
30	MN	X	3270	-	-	-	X
30	MN	X	3328	-	-	-	X
30	MN	X	3330	-	-	-	X
30	MN	X	3355	-	-	-	X
30	MN	X	3356	-	-	-	X
30	MN	X	3369	-	-	-	X
30	MN	X	3371	-	-	-	X
31	SPD	S	301	-	-	-	X
31	SPD	X	3362	-	-	-	X
31	SPD	X	3363	-	-	-	X
31	SPD	X	3364	-	-	-	X

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 81033 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	X	2712	58145	25958	10650	18825	2712	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	Y	114	2430	1086	436	794	114	0	0	0

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	269	1640	995	319	321	5	0	0	0

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	B	215	1566	980	291	290	5	0	0	0

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	C	200	1314	812	250	250	2	0	0	0

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	D	160	823	498	160	164	1	0	0	0

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	156	Total	C	N	O	S	0	0	0
			930	575	173	181	1			

- Molecule 8 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	G	145	Total	C	N	O	S	0	0	0
			1105	691	205	206	3			

- Molecule 9 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	H	122	Total	C	N	O	S	0	0	0
			877	542	166	165	4			

- Molecule 10 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	I	131	Total	C	N	O	S	0	0	0
			830	503	164	162	1			

- Molecule 11 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	141	Total	C	N	O	S	0	0	0
			1054	673	196	181	4			

- Molecule 12 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	119	Total	C	N	O	S	0	0	0
			900	554	174	171	1			

- Molecule 13 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	L	109	Total	C	N	O	0	0	0
			667	405	134	128			

- Molecule 14 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	M	110	Total	C	N	O	0	0	0
			834	526	167	141			

- Molecule 15 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	N	116	Total	C	N	O	S	0	0	0
			929	584	188	153	4			

- Molecule 16 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	O	102	Total	C	N	O	S	0	0	0
			756	481	138	136	1			

- Molecule 17 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	P	112	Total	C	N	O	S	0	0	0
			856	534	161	158	3			

- Molecule 18 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	Q	89	Total	C	N	O	S	0	0	0
			600	375	107	116	2			

- Molecule 19 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	R	101	Total	C	N	O	S	0	0	0
			609	373	111	124	1			

- Molecule 20 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	S	167	Total	C	N	O	S	0	0	0
			1082	680	192	208	2			

- Molecule 21 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	T	75	Total	C	N	O	0	0	0
			541	336	101	104			

- Molecule 22 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
22	V	63	Total	C	N	O	0	0	0
			416	256	75	85			

- Molecule 23 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	W	58	Total	C	N	O	S	0	0	0
			449	279	84	85	1			

- Molecule 24 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	Z	45	Total	C	N	O	S	0	0	0
			352	215	73	60	4			

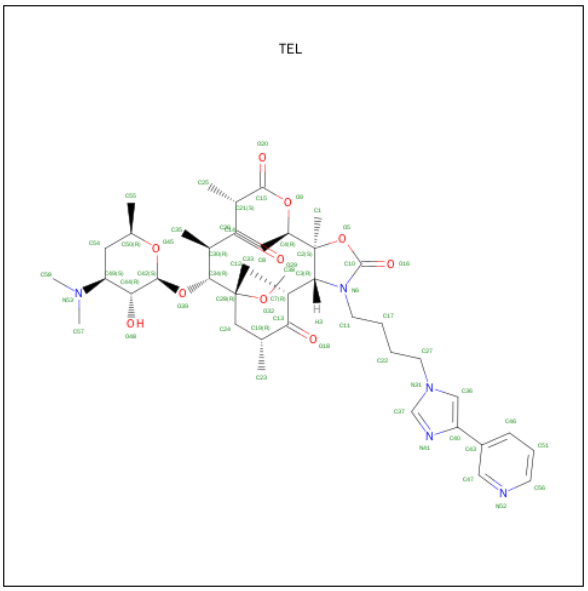
- Molecule 25 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	2	44	Total	C	N	O	S	0	0	0
			362	222	86	53	1			

- Molecule 26 is a protein called 50S ribosomal protein L35.

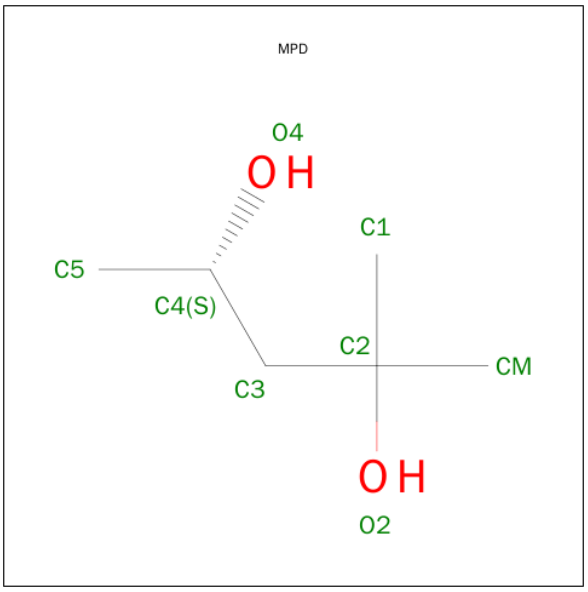
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	3	60	Total	C	N	O	S	0	0	0
			390	239	77	72	2			

- Molecule 27 is TELITHROMYCIN (three-letter code: TEL) (formula: $C_{43}H_{65}N_5O_{10}$).



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

- Molecule 28 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	X	1	Total	C	O	0	0
			8	6	2		
28	X	1	Total	C	O	0	0
			8	6	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	X	1	Total C O 8 6 2	0	0
28	X	1	Total C O 8 6 2	0	0
28	X	1	Total C O 8 6 2	0	0
28	X	1	Total C O 8 6 2	0	0
28	X	1	Total C O 8 6 2	0	0
28	X	1	Total C O 8 6 2	0	0

- Molecule 29 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	G	1	Total Mg 1 1	0	0
29	B	1	Total Mg 1 1	0	0
29	C	3	Total Mg 3 3	0	0
29	A	1	Total Mg 1 1	0	0
29	T	1	Total Mg 1 1	0	0
29	X	136	Total Mg 136 136	0	0
29	O	1	Total Mg 1 1	0	0
29	R	1	Total Mg 1 1	0	0
29	Y	4	Total Mg 4 4	0	0

- Molecule 30 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

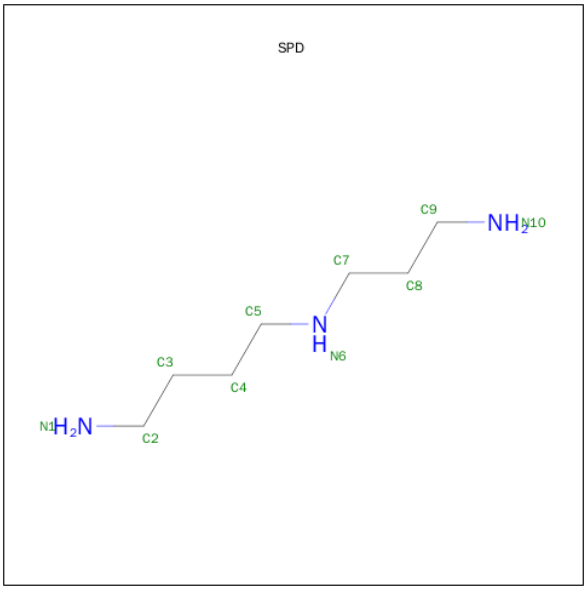
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	X	221	Total Mn 221 221	0	0
30	I	2	Total Mn 2 2	0	0

Continued on next page...

Continued from previous page...

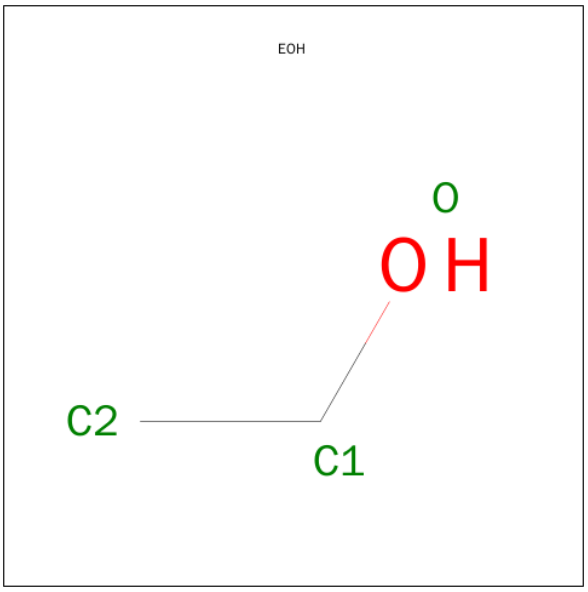
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	Y	6	Total Mn 6 6	0	0
30	J	1	Total Mn 1 1	0	0
30	M	1	Total Mn 1 1	0	0

- Molecule 31 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).



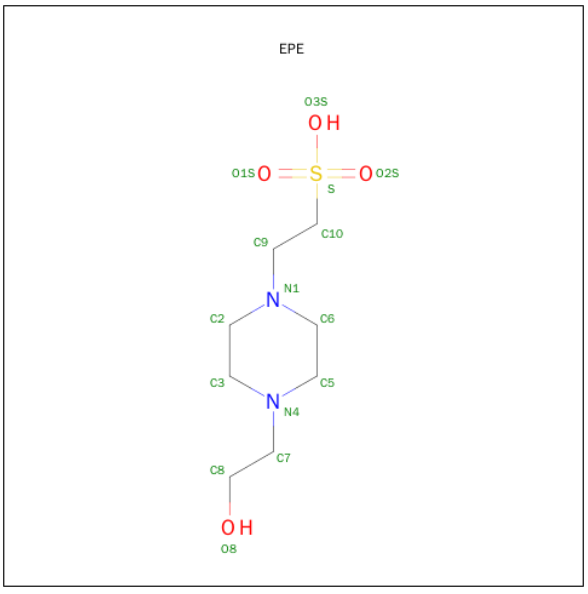
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	X	1	Total C N 10 7 3	0	0
31	X	1	Total C N 10 7 3	0	0
31	X	1	Total C N 10 7 3	0	0
31	X	1	Total C N 10 7 3	0	0
31	S	1	Total C N 10 7 3	0	0

- Molecule 32 is ETHANOL (three-letter code: EOH) (formula: C_2H_6O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	X	1	Total C O 3 2 1	0	0
32	X	1	Total C O 3 2 1	0	0
32	X	1	Total C O 3 2 1	0	0

- Molecule 33 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



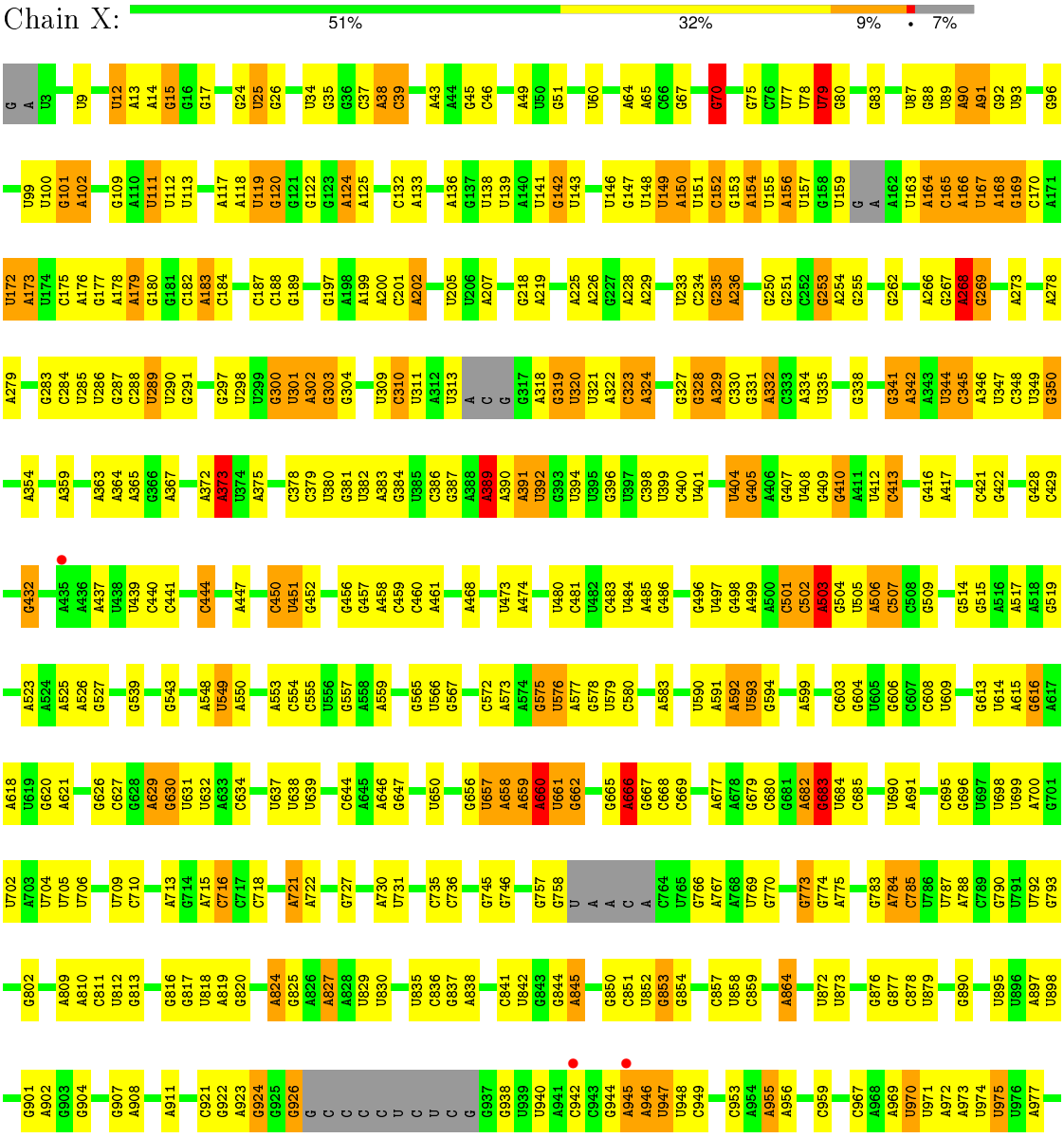
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
33	L	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

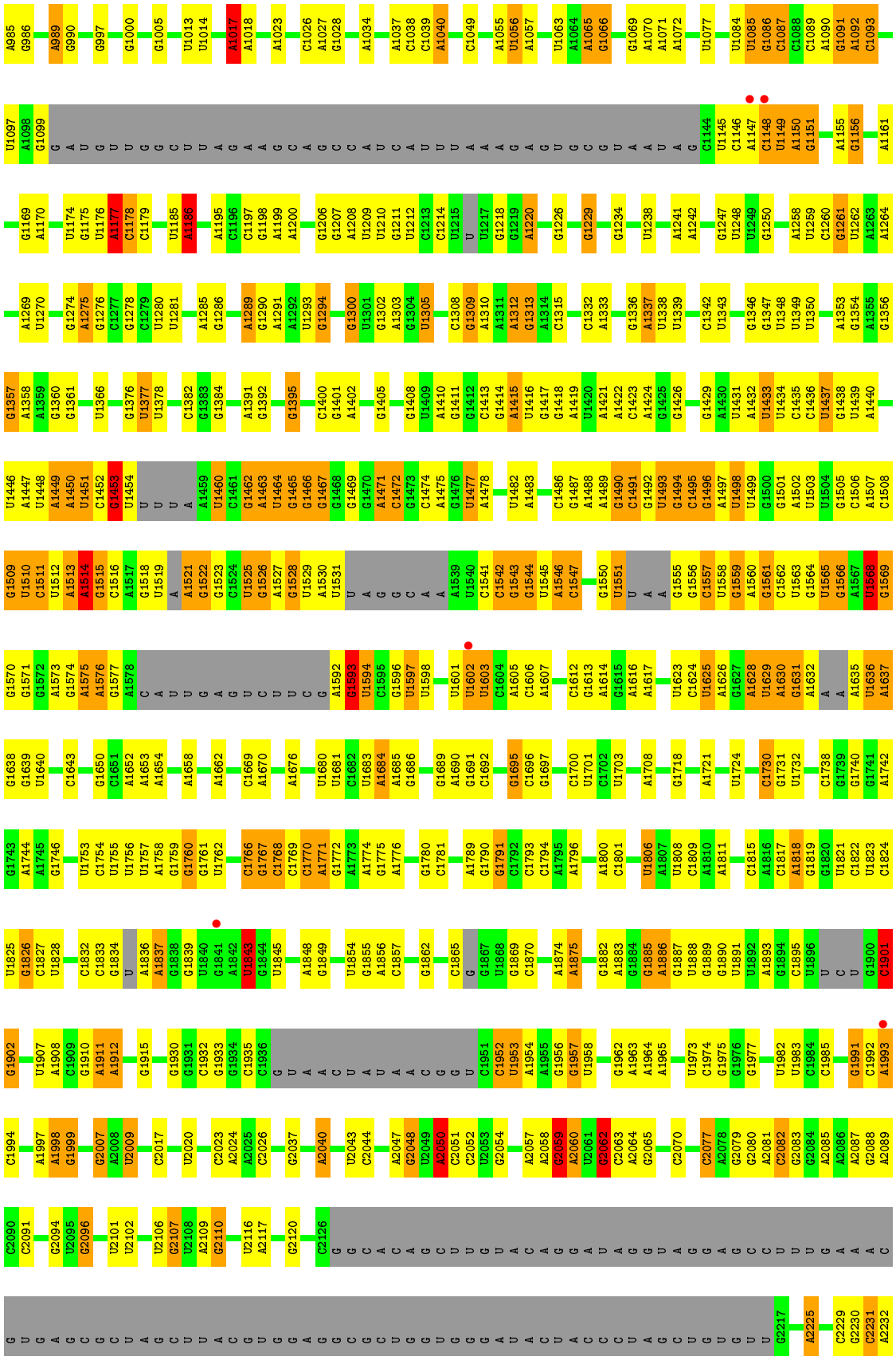
3 Residue-property plots (i)

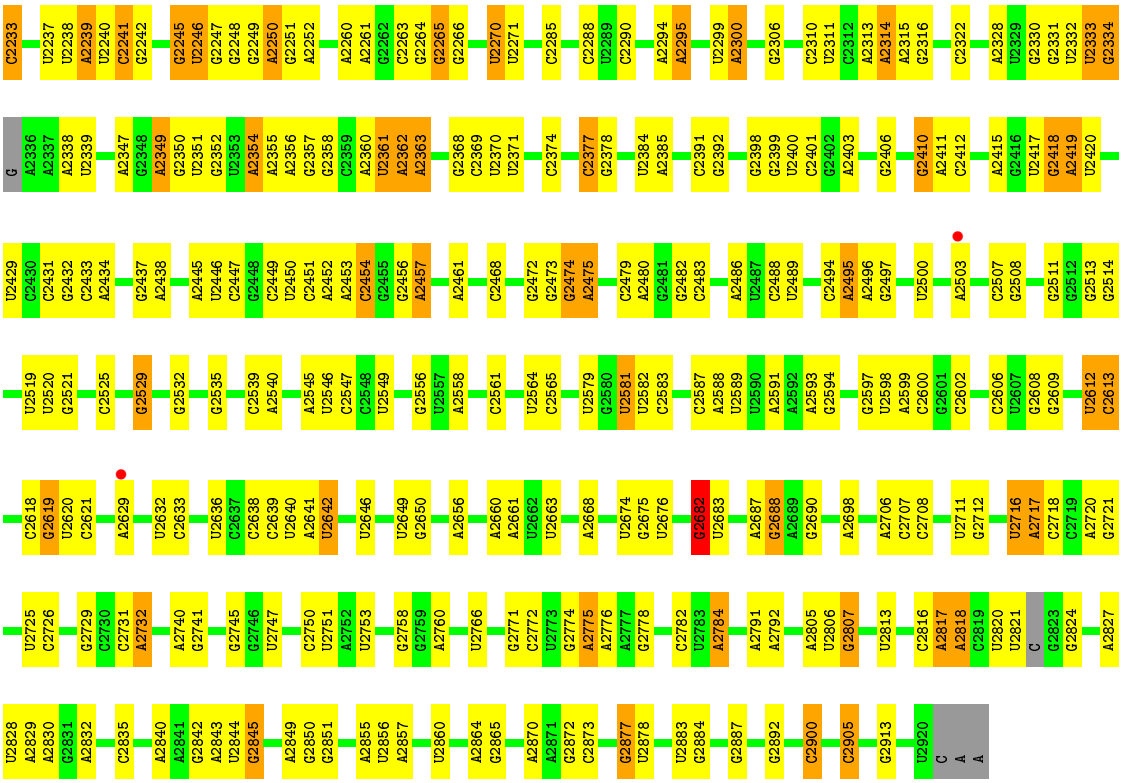
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

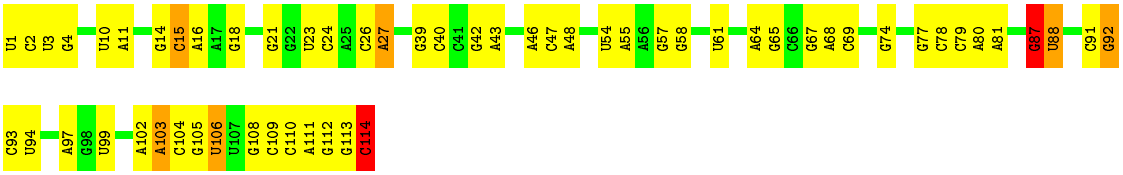






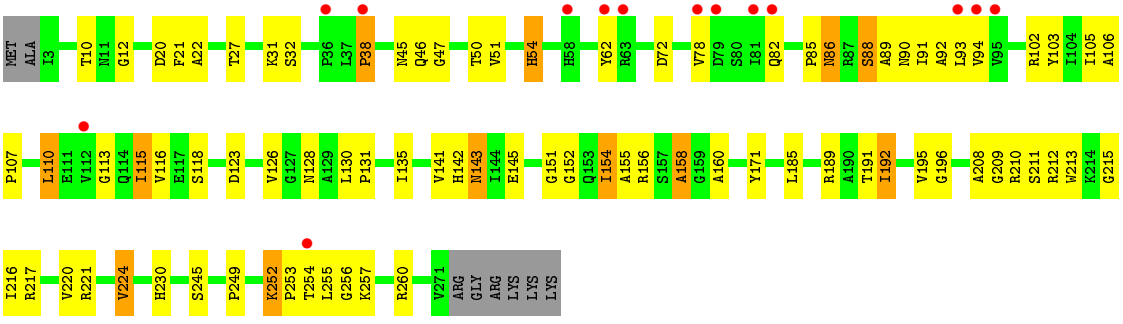
• Molecule 2: 5S ribosomal RNA

Chain Y:



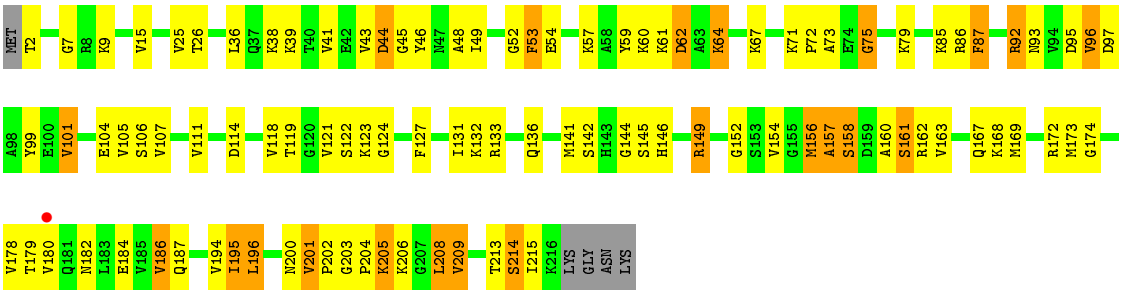
• Molecule 3: 50S ribosomal protein L2

Chain A:



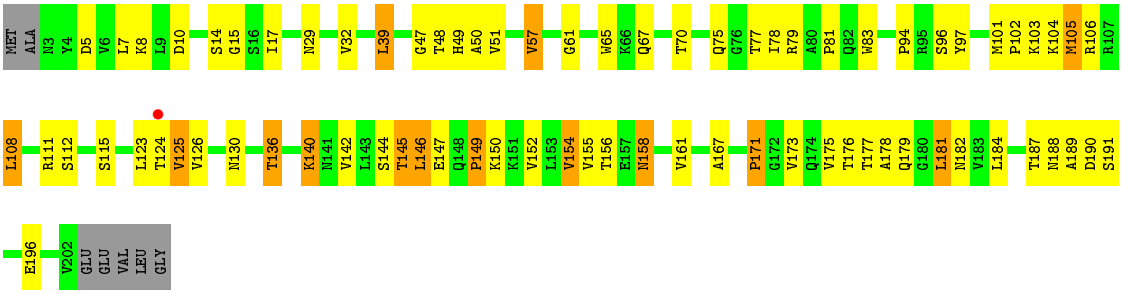
• Molecule 4: 50S ribosomal protein L3

Chain B:



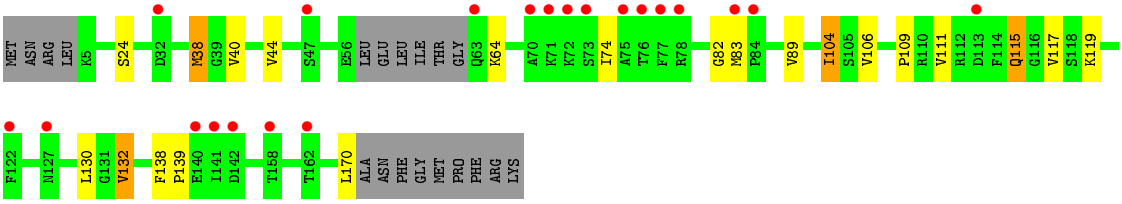
• Molecule 5: 50S ribosomal protein L4

Chain C:



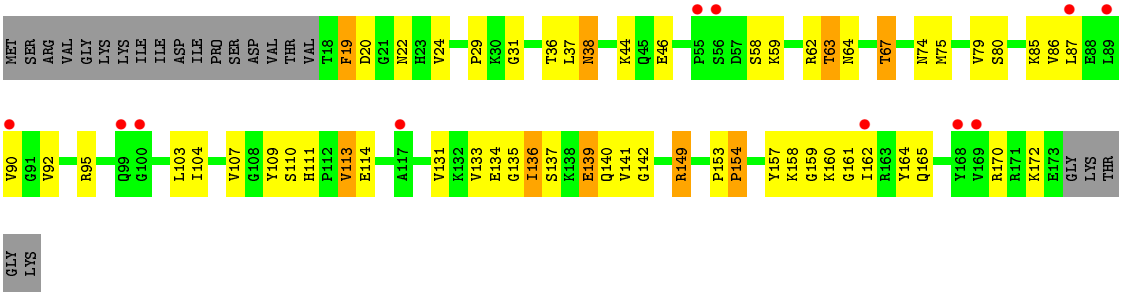
• Molecule 6: 50S ribosomal protein L5

Chain D:



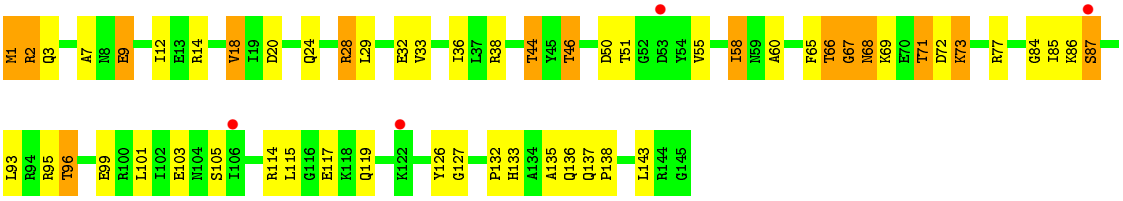
• Molecule 7: 50S ribosomal protein L6

Chain E:



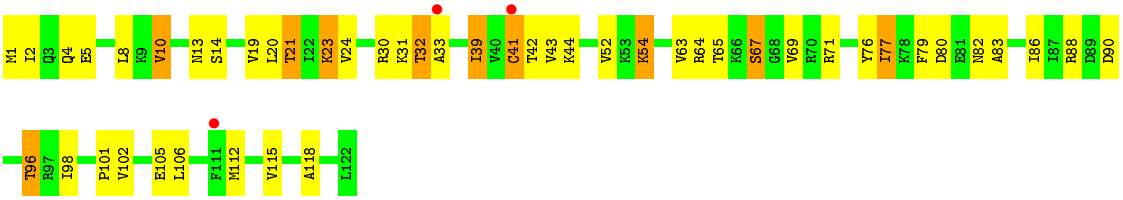
• Molecule 8: 50S ribosomal protein L13

Chain G:



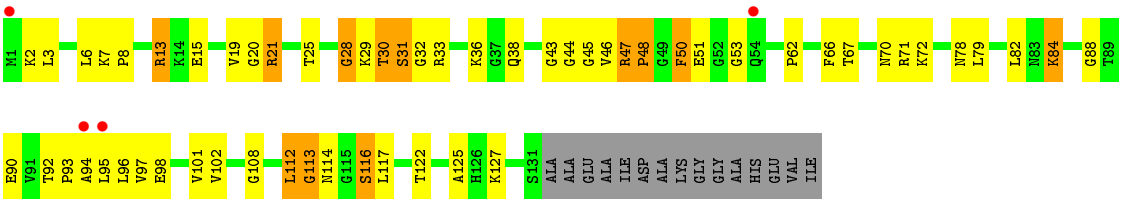
• Molecule 9: 50S ribosomal protein L14

Chain H:



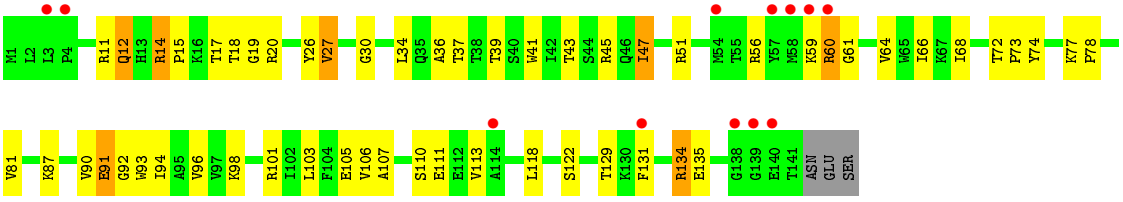
• Molecule 10: 50S ribosomal protein L15

Chain I:



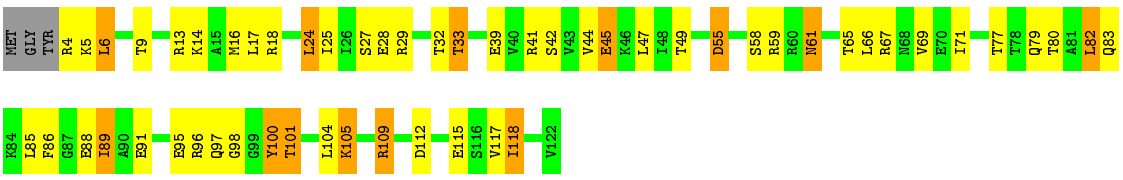
• Molecule 11: 50S ribosomal protein L16

Chain J:



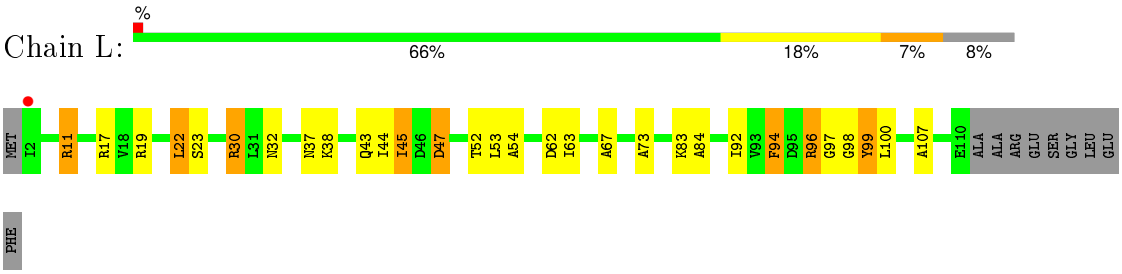
• Molecule 12: 50S ribosomal protein L17

Chain K:



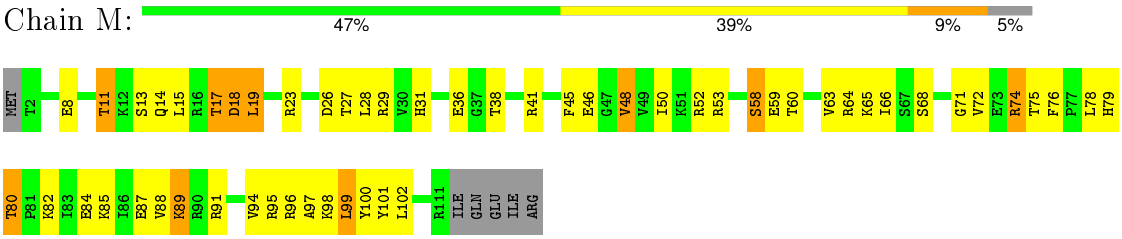
• Molecule 13: 50S ribosomal protein L18

Chain L:



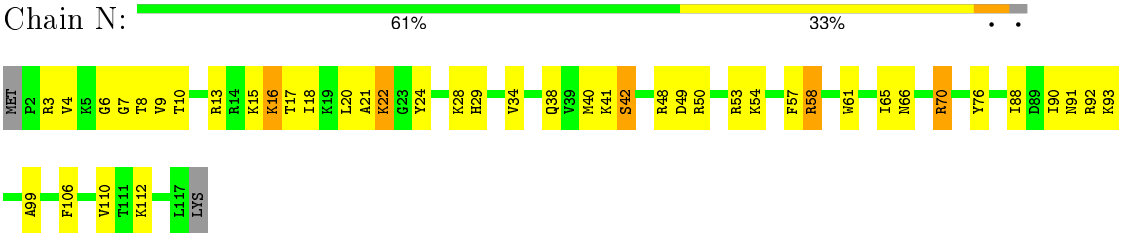
- Molecule 14: 50S ribosomal protein L19

Chain M:



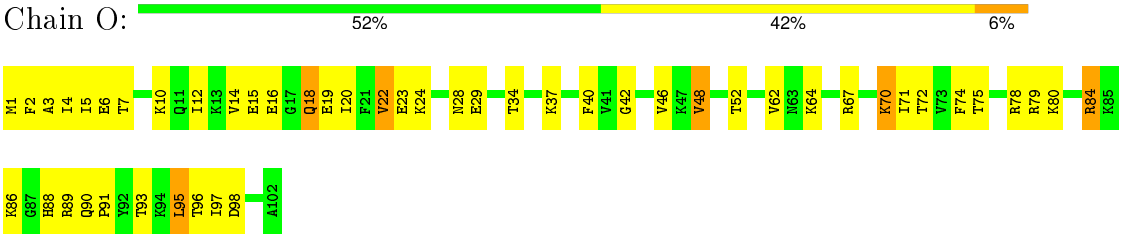
- Molecule 15: 50S ribosomal protein L20

Chain N:



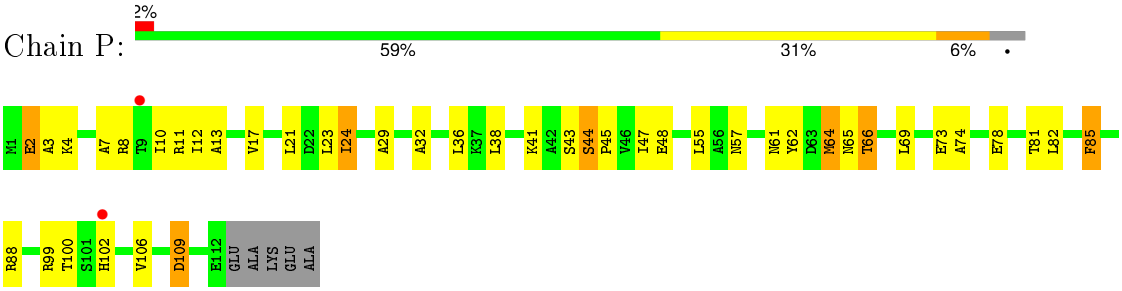
- Molecule 16: 50S ribosomal protein L21

Chain O:



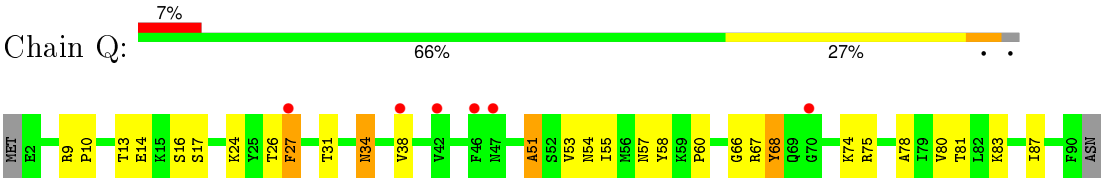
- Molecule 17: 50S ribosomal protein L22

Chain P:



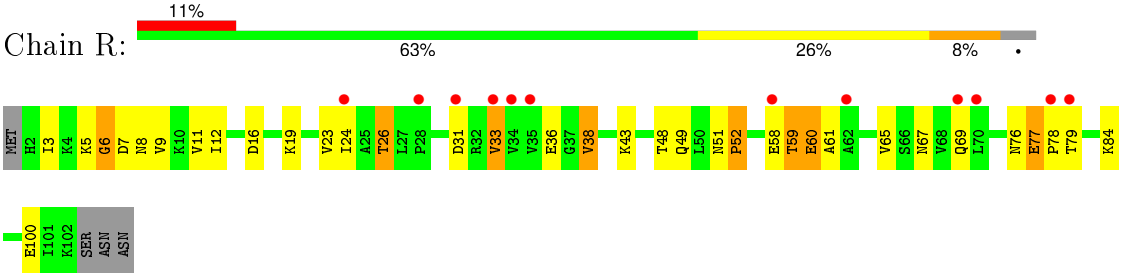
- Molecule 18: 50S ribosomal protein L23

Chain Q:



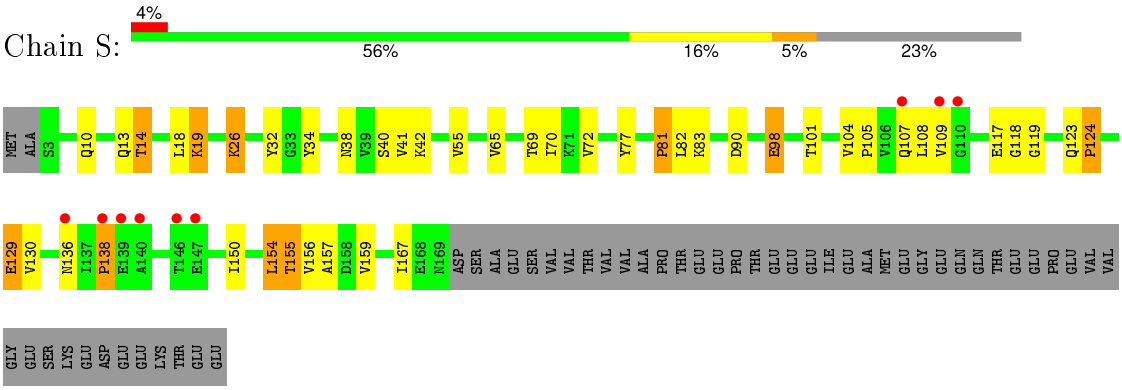
• Molecule 19: 50S ribosomal protein L24

Chain R:



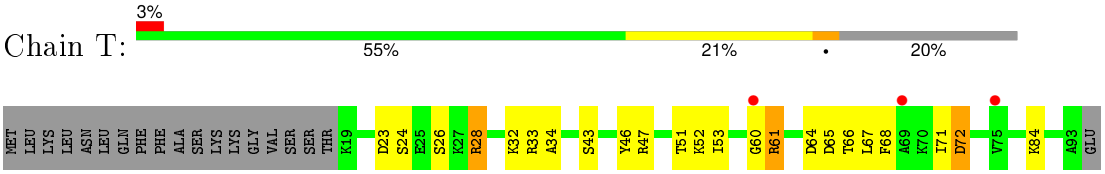
• Molecule 20: 50S ribosomal protein L25

Chain S:



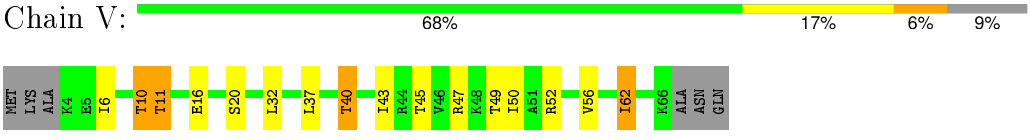
• Molecule 21: 50S ribosomal protein L27

Chain T:



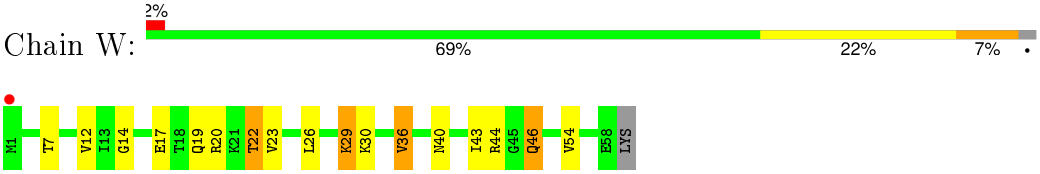
• Molecule 22: 50S ribosomal protein L29

Chain V:



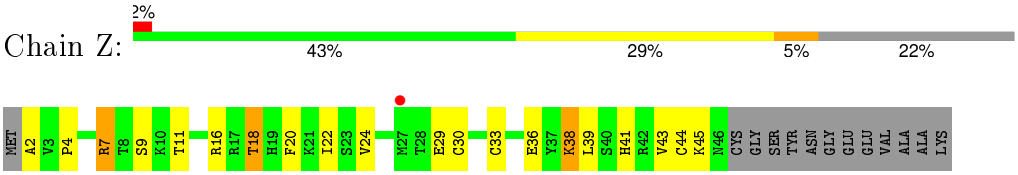
• Molecule 23: 50S ribosomal protein L30

Chain W:



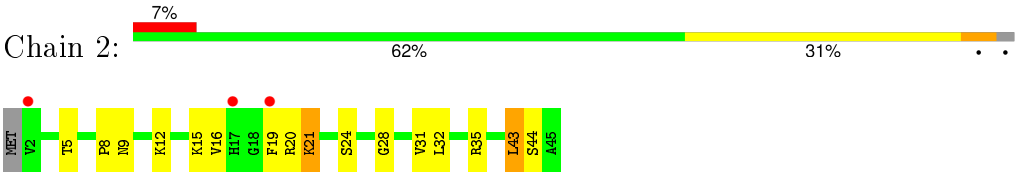
- Molecule 24: 50S ribosomal protein L32

Chain Z:



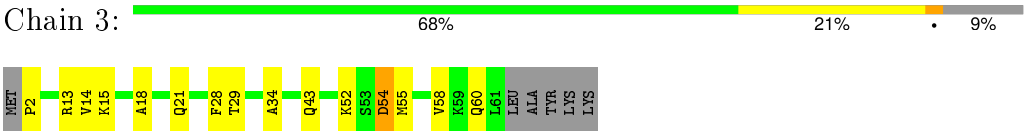
- Molecule 25: 50S ribosomal protein L34

Chain 2:



- Molecule 26: 50S ribosomal protein L35

Chain 3:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	282.66Å 282.66Å 877.08Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.19 – 3.43 50.19 – 3.43	Depositor EDS
% Data completeness (in resolution range)	97.4 (50.19-3.43) 97.4 (50.19-3.43)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.14 (at 3.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.192 , 0.232 0.195 , 0.233	Depositor DCC
R_{free} test set	13519 reflections (5.31%)	DCC
Wilson B-factor (Å^2)	114.5	Xtriage
Anisotropy	0.215	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.22 , 77.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 268009 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	81033	wwPDB-VP
Average B, all atoms (Å^2)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.30% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, MN, TEL, EOH, MPD, EPE, SPD

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	X	0.56	10/65105 (0.0%)	1.06	170/101500 (0.2%)
2	Y	0.52	1/2717 (0.0%)	1.06	14/4232 (0.3%)
3	A	0.35	0/1671	0.65	0/2304
4	B	0.51	0/1589	0.79	1/2139 (0.0%)
5	C	0.46	0/1332	0.72	0/1826
6	D	0.26	0/826	0.61	0/1147
7	E	0.51	0/941	0.79	0/1302
8	G	0.45	0/1127	0.68	0/1524
9	H	0.40	0/884	0.63	0/1195
10	I	0.56	0/838	0.91	1/1139 (0.1%)
11	J	0.43	0/1078	0.68	0/1457
12	K	0.44	0/903	0.71	0/1209
13	L	0.34	0/672	0.66	0/922
14	M	0.46	0/846	0.75	1/1139 (0.1%)
15	N	0.51	0/941	0.67	0/1248
16	O	0.46	0/766	0.68	0/1028
17	P	0.47	0/864	0.69	0/1164
18	Q	0.33	0/607	0.58	0/830
19	R	0.39	0/614	0.65	0/847
20	S	0.38	0/1094	0.64	1/1503 (0.1%)
21	T	0.44	0/547	0.63	0/733
22	V	0.36	0/417	0.53	0/571
23	W	0.47	0/451	0.66	0/607
24	Z	0.48	0/358	0.67	0/478
25	2	0.41	0/366	0.65	0/480
26	3	0.51	0/393	0.76	0/529
All	All	0.53	11/87947 (0.0%)	1.00	188/133053 (0.1%)

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
3	A	0	1
5	C	0	1
All	All	0	2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	2845	G	N9-C4	-7.38	1.32	1.38
1	X	2845	G	C2-N3	-5.96	1.27	1.32
1	X	350	G	N9-C4	5.89	1.42	1.38
1	X	2048	G	N9-C8	5.88	1.42	1.37
1	X	1065	A	N9-C4	-5.80	1.34	1.37

The worst 5 of 188 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	2845	G	N3-C4-N9	-15.55	116.67	126.00
1	X	2845	G	N3-C4-C5	13.97	135.58	128.60
1	X	2048	G	C5-N7-C8	-11.50	98.55	104.30
1	X	2048	G	N3-C4-C5	11.50	134.35	128.60
1	X	2048	G	C4-C5-N7	10.80	115.12	110.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	115	ILE	Peptide
5	C	140	LYS	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	X	58145	0	29245	725	1
2	Y	2430	0	1229	40	0
3	A	1640	0	1255	51	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1566	0	1559	68	0
5	C	1314	0	1146	44	0
6	D	823	0	433	7	0
7	E	930	0	688	32	0
8	G	1105	0	1064	34	0
9	H	877	0	882	33	0
10	I	830	0	703	32	0
11	J	1054	0	1040	30	0
12	K	900	0	924	38	0
13	L	667	0	507	20	0
14	M	834	0	850	33	0
15	N	929	0	988	34	0
16	O	756	0	754	32	0
17	P	856	0	909	33	0
18	Q	600	0	500	22	0
19	R	609	0	484	17	0
20	S	1082	0	919	17	0
21	T	541	0	518	12	0
22	V	416	0	348	5	0
23	W	449	0	490	8	0
24	Z	352	0	358	20	0
25	2	362	0	398	12	0
26	3	390	0	346	4	0
27	X	58	0	65	13	0
28	X	64	0	112	15	0
29	A	1	0	0	0	0
29	B	1	0	0	0	0
29	C	3	0	0	0	0
29	G	1	0	0	0	0
29	O	1	0	0	0	0
29	R	1	0	0	0	0
29	T	1	0	0	0	0
29	X	136	0	0	0	0
29	Y	4	0	0	0	0
30	I	2	0	0	0	0
30	J	1	0	0	0	0
30	M	1	0	0	0	0
30	X	221	0	0	0	0
30	Y	6	0	0	0	0
31	S	10	0	19	1	0
31	X	40	0	76	5	0
32	X	9	0	18	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	L	15	0	17	0	0
All	All	81033	0	48844	1274	1

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 10.

The worst 5 of 1274 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:X:2649:U:O2'	1:X:2845:G:N2	1.98	0.96
1:X:2231:C:HO2'	1:X:2232:A:H8	1.10	0.93
1:X:1886:A:N6	1:X:1910:G:O2'	2.06	0.89
1:X:721:A:H8	1:X:2096:G:H21	1.15	0.87
2:Y:18:G:H1	2:Y:61:U:H3	1.20	0.87

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:136:A:OP1	1:X:1453:G:N2[12_554]	2.19	0.01

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	267/277 (96%)	211 (79%)	34 (13%)	22 (8%)	1 12
4	B	213/220 (97%)	179 (84%)	18 (8%)	16 (8%)	1 14
5	C	198/207 (96%)	166 (84%)	20 (10%)	12 (6%)	2 19
6	D	156/179 (87%)	114 (73%)	30 (19%)	12 (8%)	1 14
7	E	154/178 (86%)	112 (73%)	29 (19%)	13 (8%)	1 12

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
8	G	143/145 (99%)	126 (88%)	13 (9%)	4 (3%)	6 42
9	H	120/122 (98%)	108 (90%)	12 (10%)	0	100 100
10	I	129/146 (88%)	89 (69%)	25 (19%)	15 (12%)	0 7
11	J	139/144 (96%)	119 (86%)	15 (11%)	5 (4%)	4 36
12	K	117/122 (96%)	99 (85%)	13 (11%)	5 (4%)	3 30
13	L	107/119 (90%)	88 (82%)	10 (9%)	9 (8%)	1 12
14	M	108/116 (93%)	94 (87%)	9 (8%)	5 (5%)	3 28
15	N	114/118 (97%)	107 (94%)	5 (4%)	2 (2%)	11 51
16	O	100/102 (98%)	90 (90%)	9 (9%)	1 (1%)	19 64
17	P	110/117 (94%)	104 (94%)	6 (6%)	0	100 100
18	Q	87/91 (96%)	76 (87%)	10 (12%)	1 (1%)	17 62
19	R	99/105 (94%)	72 (73%)	21 (21%)	6 (6%)	2 19
20	S	165/217 (76%)	129 (78%)	19 (12%)	17 (10%)	1 8
21	T	73/94 (78%)	66 (90%)	6 (8%)	1 (1%)	14 56
22	V	61/69 (88%)	57 (93%)	1 (2%)	3 (5%)	3 26
23	W	56/59 (95%)	51 (91%)	4 (7%)	1 (2%)	11 51
24	Z	43/58 (74%)	40 (93%)	3 (7%)	0	100 100
25	2	42/45 (93%)	39 (93%)	3 (7%)	0	100 100
26	3	58/66 (88%)	47 (81%)	6 (10%)	5 (9%)	1 12
All	All	2859/3116 (92%)	2383 (83%)	321 (11%)	155 (5%)	2 23

5 of 155 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	27	THR
3	A	51	VAL
3	A	126	VAL
3	A	141	VAL
3	A	154	ILE

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	109/224 (49%)	100 (92%)	9 (8%)	14 50
4	B	156/177 (88%)	125 (80%)	31 (20%)	1 8
5	C	103/169 (61%)	86 (84%)	17 (16%)	3 15
6	D	14/158 (9%)	12 (86%)	2 (14%)	4 22
7	E	56/155 (36%)	41 (73%)	15 (27%)	0 3
8	G	110/123 (89%)	88 (80%)	22 (20%)	1 7
9	H	89/100 (89%)	77 (86%)	12 (14%)	5 25
10	I	61/112 (54%)	45 (74%)	16 (26%)	0 3
11	J	99/119 (83%)	84 (85%)	15 (15%)	3 20
12	K	89/102 (87%)	72 (81%)	17 (19%)	2 9
13	L	36/95 (38%)	26 (72%)	10 (28%)	0 3
14	M	82/102 (80%)	63 (77%)	19 (23%)	1 4
15	N	92/98 (94%)	82 (89%)	10 (11%)	8 36
16	O	72/86 (84%)	58 (81%)	14 (19%)	2 8
17	P	90/94 (96%)	79 (88%)	11 (12%)	6 29
18	Q	46/82 (56%)	40 (87%)	6 (13%)	5 26
19	R	43/90 (48%)	30 (70%)	13 (30%)	0 3
20	S	84/190 (44%)	73 (87%)	11 (13%)	5 26
21	T	50/75 (67%)	40 (80%)	10 (20%)	1 7
22	V	33/62 (53%)	25 (76%)	8 (24%)	1 4
23	W	52/53 (98%)	44 (85%)	8 (15%)	3 19
24	Z	39/51 (76%)	34 (87%)	5 (13%)	5 27
25	2	37/40 (92%)	34 (92%)	3 (8%)	15 51
26	3	30/57 (53%)	26 (87%)	4 (13%)	5 25
All	All	1672/2614 (64%)	1384 (83%)	288 (17%)	2 14

5 of 288 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	J	41	TRP
13	L	52	THR
22	V	56	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	J	87	LYS
12	K	55	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	53	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	2693/2923 (92%)	619 (22%)	28 (1%)
2	Y	113/114 (99%)	16 (14%)	0
All	All	2806/3037 (92%)	635 (22%)	28 (0%)

5 of 635 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	X	9	U
1	X	14	A
1	X	15	G
1	X	25	U
1	X	34	U

5 of 28 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	X	1028	G
1	X	1510	U
1	X	2062	G
1	X	1091	G
1	X	1490	G

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 398 ligands modelled in this entry, 380 are monoatomic - leaving 18 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	$\#\|Z\| > 2$
33	EPE	L	201	-	15,15,15	0.73	1 (6%)	19,20,20	0.81	1 (5%)
31	SPD	S	301	-	9,9,9	0.21	0	8,8,8	0.40	0
27	TEL	X	3001	-	59,62,62	0.62	1 (1%)	71,92,92	1.46	7 (9%)
28	MPD	X	3002	-	6,7,7	0.39	0	6,10,10	0.43	0
28	MPD	X	3003	-	6,7,7	0.46	0	6,10,10	0.25	0
28	MPD	X	3004	-	6,7,7	0.42	0	6,10,10	0.09	0
28	MPD	X	3005	-	6,7,7	0.30	0	6,10,10	0.93	0
28	MPD	X	3006	-	6,7,7	0.52	0	6,10,10	0.28	0
28	MPD	X	3007	-	6,7,7	0.38	0	6,10,10	0.09	0
28	MPD	X	3008	-	6,7,7	0.48	0	6,10,10	0.20	0
28	MPD	X	3009	-	6,7,7	0.33	0	6,10,10	0.11	0
31	SPD	X	3362	-	9,9,9	0.17	0	8,8,8	0.28	0
31	SPD	X	3363	-	9,9,9	0.20	0	8,8,8	0.19	0
31	SPD	X	3364	-	9,9,9	0.26	0	8,8,8	0.33	0
31	SPD	X	3365	-	9,9,9	0.31	0	8,8,8	0.49	0
32	EOH	X	3366	-	2,2,2	0.57	0	1,1,1	0.61	0
32	EOH	X	3367	-	2,2,2	0.48	0	1,1,1	0.74	0
32	EOH	X	3368	-	2,2,2	0.53	0	1,1,1	0.65	0

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
33	EPE	L	201	-	-	0/9/19/19	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	SPD	S	301	-	-	0/7/7/7	0/0/0/0
27	TEL	X	3001	-	-	0/73/108/108	0/4/5/5
28	MPD	X	3002	-	-	0/5/5/5	0/0/0/0
28	MPD	X	3003	-	-	0/5/5/5	0/0/0/0
28	MPD	X	3004	-	-	0/5/5/5	0/0/0/0
28	MPD	X	3005	-	-	0/5/5/5	0/0/0/0
28	MPD	X	3006	-	-	0/5/5/5	0/0/0/0
28	MPD	X	3007	-	-	0/5/5/5	0/0/0/0
28	MPD	X	3008	-	-	0/5/5/5	0/0/0/0
28	MPD	X	3009	-	-	0/5/5/5	0/0/0/0
31	SPD	X	3362	-	-	0/7/7/7	0/0/0/0
31	SPD	X	3363	-	-	0/7/7/7	0/0/0/0
31	SPD	X	3364	-	-	0/7/7/7	0/0/0/0
31	SPD	X	3365	-	-	0/7/7/7	0/0/0/0
32	EOH	X	3366	-	-	0/0/0/0	0/0/0/0
32	EOH	X	3367	-	-	0/0/0/0	0/0/0/0
32	EOH	X	3368	-	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	L	201	EPE	C10-S	-2.59	1.73	1.77
27	X	3001	TEL	C21-C26	3.26	1.57	1.53

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	X	3001	TEL	O5-C2-C4	-6.48	90.45	105.61
27	X	3001	TEL	C2-O5-C10	-4.34	105.67	109.28
33	L	201	EPE	O1S-S-C10	-2.96	104.78	106.87
27	X	3001	TEL	O29-C26-C30	-2.25	117.08	120.55
27	X	3001	TEL	O32-C28-C33	-2.11	102.79	110.76

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	S	301	SPD	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	X	3001	TEL	13	0
28	X	3002	MPD	1	0
28	X	3003	MPD	3	0
28	X	3005	MPD	6	0
28	X	3006	MPD	1	0
28	X	3007	MPD	2	0
28	X	3008	MPD	1	0
28	X	3009	MPD	1	0
31	X	3364	SPD	1	0
31	X	3365	SPD	4	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	X	2712/2923 (92%)	-0.40	10 (0%) 93 91	27, 74, 174, 288	0
2	Y	114/114 (100%)	-0.53	0 100 100	48, 98, 151, 203	0
3	A	269/277 (97%)	-0.04	14 (5%) 31 27	56, 101, 146, 177	0
4	B	215/220 (97%)	-0.18	1 (0%) 91 89	34, 49, 101, 155	0
5	C	200/207 (96%)	-0.29	1 (0%) 91 89	40, 65, 112, 165	0
6	D	160/179 (89%)	0.28	21 (13%) 5 5	88, 155, 209, 263	0
7	E	156/178 (87%)	-0.19	11 (7%) 19 18	71, 131, 190, 205	0
8	G	145/145 (100%)	0.15	4 (2%) 56 51	36, 51, 83, 115	0
9	H	122/122 (100%)	-0.14	3 (2%) 61 55	57, 75, 116, 154	0
10	I	131/146 (89%)	-0.12	4 (3%) 52 47	22, 78, 139, 210	0
11	J	141/144 (97%)	0.55	12 (8%) 13 13	43, 73, 162, 258	0
12	K	119/122 (97%)	-0.26	0 100 100	31, 57, 129, 169	0
13	L	109/119 (91%)	-0.55	1 (0%) 85 80	55, 96, 149, 205	0
14	M	110/116 (94%)	-0.26	0 100 100	46, 69, 127, 189	0
15	N	116/118 (98%)	-0.37	0 100 100	18, 45, 80, 106	0
16	O	102/102 (100%)	-0.46	0 100 100	23, 60, 93, 179	0
17	P	112/117 (95%)	0.20	2 (1%) 71 65	37, 50, 116, 177	0
18	Q	89/91 (97%)	0.27	6 (6%) 21 19	63, 93, 138, 173	0
19	R	101/105 (96%)	0.32	12 (11%) 6 7	54, 98, 196, 218	0
20	S	167/217 (76%)	-0.29	9 (5%) 29 26	48, 83, 170, 292	0
21	T	75/94 (79%)	0.45	3 (4%) 42 37	44, 65, 106, 134	0
22	V	63/69 (91%)	-0.10	0 100 100	82, 107, 145, 185	0
23	W	58/59 (98%)	0.17	1 (1%) 73 67	26, 52, 98, 195	0
24	Z	45/58 (77%)	-0.18	1 (2%) 65 60	29, 60, 157, 181	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
25	2	44/45 (97%)	0.42	3 (6%) 20 19	59, 67, 97, 140	0
26	3	60/66 (90%)	-0.08	0 100 100	35, 57, 91, 96	0
All	All	5735/6153 (93%)	-0.23	119 (2%) 67 62	18, 75, 168, 292	0

The worst 5 of 119 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
23	W	1	MET	5.8
6	D	83	MET	5.8
11	J	139	GLY	5.7
20	S	146	THR	5.7
3	A	94	VAL	5.6

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
29	MG	X	3274	1/1	0.81	0.94	54.22	44,44,44,44	0
29	MG	A	301	1/1	0.90	0.74	28.05	45,45,45,45	0
30	MN	X	3328	1/1	0.96	0.39	24.58	88,88,88,88	0
28	MPD	X	3002	8/8	0.90	0.20	20.30	44,44,44,44	0
29	MG	X	3326	1/1	0.95	0.57	19.85	71,71,71,71	0
30	MN	X	3221	1/1	0.97	0.47	18.22	51,51,51,51	0
30	MN	X	3070	1/1	0.96	0.43	17.05	74,74,74,74	0
30	MN	X	3099	1/1	0.95	0.57	16.86	88,88,88,88	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
29	MG	X	3348	1/1	0.85	0.56	14.79	46,46,46,46	0
30	MN	X	3270	1/1	0.97	0.41	14.65	120,120,120,120	0
29	MG	Y	207	1/1	0.71	0.41	13.83	51,51,51,51	0
30	MN	X	3103	1/1	0.99	0.48	13.69	41,41,41,41	0
30	MN	X	3106	1/1	0.98	0.36	12.81	42,42,42,42	0
29	MG	X	3251	1/1	0.93	0.24	12.51	59,59,59,59	0
30	MN	X	3355	1/1	0.98	0.35	12.02	68,68,68,68	0
28	MPD	X	3003	8/8	0.90	0.41	11.60	64,64,64,64	0
30	MN	X	3044	1/1	0.97	0.35	11.05	34,34,34,34	0
29	MG	X	3334	1/1	0.92	0.20	11.00	64,64,64,64	0
30	MN	X	3240	1/1	0.98	0.58	10.88	52,52,52,52	0
30	MN	X	3108	1/1	0.96	0.29	10.86	70,70,70,70	0
30	MN	X	3107	1/1	0.93	0.42	10.71	62,62,62,62	0
29	MG	X	3193	1/1	0.97	0.23	10.25	27,27,27,27	0
29	MG	X	3325	1/1	0.69	0.34	10.18	49,49,49,49	0
30	MN	X	3153	1/1	0.95	0.37	8.92	41,41,41,41	0
29	MG	X	3340	1/1	0.68	0.43	8.85	55,55,55,55	0
30	MN	X	3356	1/1	0.97	0.41	8.60	41,41,41,41	0
30	MN	X	3036	1/1	0.58	0.34	8.49	96,96,96,96	0
30	MN	X	3067	1/1	0.98	0.48	8.32	83,83,83,83	0
27	TEL	X	3001	58/58	0.90	0.39	7.68	30,40,52,52	0
30	MN	X	3077	1/1	0.95	0.21	7.14	62,62,62,62	0
29	MG	X	3346	1/1	0.96	0.24	6.86	31,31,31,31	0
30	MN	X	3166	1/1	0.90	0.33	6.49	72,72,72,72	0
30	MN	X	3177	1/1	0.95	0.31	6.10	89,89,89,89	0
30	MN	X	3117	1/1	0.86	0.28	5.97	67,67,67,67	0
30	MN	X	3038	1/1	0.89	0.28	5.91	151,151,151,151	0
30	MN	X	3095	1/1	0.95	0.51	5.87	87,87,87,87	0
30	MN	X	3071	1/1	0.95	0.36	5.84	77,77,77,77	0
30	MN	X	3048	1/1	0.99	0.28	5.52	90,90,90,90	0
28	MPD	X	3005	8/8	0.94	0.28	5.01	20,20,20,20	0
29	MG	X	3324	1/1	0.88	0.26	4.92	55,55,55,55	0
30	MN	X	3090	1/1	0.99	0.27	4.90	54,54,54,54	0
30	MN	X	3082	1/1	0.94	0.33	4.85	71,71,71,71	0
31	SPD	X	3364	10/10	0.74	0.26	4.82	80,80,80,80	0
30	MN	X	3101	1/1	0.84	0.26	4.67	83,83,83,83	0
28	MPD	X	3004	8/8	0.88	0.26	4.54	86,86,86,86	0
28	MPD	X	3007	8/8	0.92	0.46	4.31	70,70,70,70	0
31	SPD	X	3363	10/10	0.83	0.33	4.29	75,75,75,75	0
30	MN	X	3203	1/1	0.97	0.31	4.26	78,78,78,78	0
30	MN	X	3109	1/1	0.95	0.22	4.04	62,62,62,62	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
30	MN	X	3139	1/1	0.93	0.28	4.02	121,121,121,121	0
30	MN	X	3217	1/1	0.93	0.28	3.98	116,116,116,116	0
30	MN	X	3330	1/1	0.99	0.25	3.86	83,83,83,83	0
30	MN	X	3136	1/1	0.97	0.25	3.85	59,59,59,59	0
30	MN	X	3086	1/1	0.95	0.21	3.65	74,74,74,74	0
30	MN	X	3178	1/1	0.92	0.25	3.53	98,98,98,98	0
30	MN	X	3056	1/1	0.92	0.22	3.47	135,135,135,135	0
30	MN	X	3039	1/1	0.93	0.41	3.45	107,107,107,107	0
30	MN	X	3369	1/1	0.95	0.41	3.44	70,70,70,70	0
29	MG	C	302	1/1	0.95	0.44	3.38	44,44,44,44	0
31	SPD	S	301	10/10	0.63	0.39	3.34	67,67,67,67	0
30	MN	X	3371	1/1	0.98	0.25	3.23	34,34,34,34	0
30	MN	X	3129	1/1	0.98	0.23	2.79	61,61,61,61	0
30	MN	X	3123	1/1	0.97	0.22	2.74	38,38,38,38	0
30	MN	X	3213	1/1	0.99	0.24	2.55	63,63,63,63	0
30	MN	X	3078	1/1	0.99	0.28	2.51	54,54,54,54	0
30	MN	X	3112	1/1	0.87	0.35	2.49	77,77,77,77	0
30	MN	X	3140	1/1	0.88	0.28	2.25	127,127,127,127	0
30	MN	X	3080	1/1	0.93	0.24	2.10	55,55,55,55	0
31	SPD	X	3362	10/10	0.93	0.24	2.03	16,16,16,16	0
30	MN	X	3168	1/1	0.99	0.21	1.94	40,40,40,40	0
30	MN	X	3219	1/1	0.94	0.22	1.89	90,90,90,90	0
30	MN	X	3248	1/1	0.91	0.12	1.82	115,115,115,115	0
29	MG	X	3232	1/1	0.91	0.21	1.72	42,42,42,42	0
30	MN	X	3053	1/1	0.96	0.22	1.52	63,63,63,63	0
28	MPD	X	3009	8/8	0.90	0.28	1.49	99,99,99,99	0
31	SPD	X	3365	10/10	0.94	0.20	1.44	54,54,54,54	0
30	MN	X	3052	1/1	0.99	0.23	1.39	57,57,57,57	0
30	MN	X	3373	1/1	0.95	0.27	1.34	44,44,44,44	0
30	MN	X	3215	1/1	0.95	0.24	1.11	95,95,95,95	0
30	MN	X	3049	1/1	0.99	0.17	1.02	81,81,81,81	0
29	MG	X	3317	1/1	0.96	0.17	1.02	49,49,49,49	0
29	MG	X	3309	1/1	0.99	0.19	0.77	30,30,30,30	0
30	MN	X	3174	1/1	0.97	0.21	0.53	77,77,77,77	0
29	MG	X	3019	1/1	0.94	0.23	0.34	32,32,32,32	0
33	EPE	L	201	15/15	0.89	0.13	0.11	125,125,125,125	0
30	MN	X	3084	1/1	0.86	0.21	0.02	72,72,72,72	0
30	MN	X	3076	1/1	0.91	0.17	-0.09	85,85,85,85	0
30	MN	X	3143	1/1	0.97	0.13	-0.52	85,85,85,85	0
30	MN	X	3164	1/1	0.86	0.12	-0.64	103,103,103,103	0
29	MG	X	3316	1/1	0.61	0.12	-0.86	38,38,38,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
29	MG	X	3345	1/1	0.95	0.13	-0.90	56,56,56,56	0
30	MN	J	201	1/1	0.82	0.10	-1.25	103,103,103,103	0
30	MN	X	3089	1/1	0.98	0.14	-1.27	89,89,89,89	0
29	MG	X	3311	1/1	0.95	0.15	-1.39	39,39,39,39	0
30	MN	X	3060	1/1	0.97	0.12	-1.96	67,67,67,67	0
29	MG	X	3337	1/1	0.93	0.28	-	69,69,69,69	0
29	MG	X	3010	1/1	0.47	0.52	-	84,84,84,84	0
30	MN	X	3199	1/1	0.88	0.47	-	132,132,132,132	0
30	MN	X	3110	1/1	0.96	0.31	-	51,51,51,51	0
29	MG	X	3339	1/1	0.83	0.37	-	66,66,66,66	0
29	MG	X	3295	1/1	0.91	0.48	-	57,57,57,57	0
30	MN	X	3271	1/1	0.86	0.21	-	140,140,140,140	0
30	MN	X	3172	1/1	0.94	0.58	-	113,113,113,113	0
30	MN	X	3085	1/1	0.89	0.35	-	77,77,77,77	0
30	MN	X	3244	1/1	0.91	0.18	-	96,96,96,96	0
30	MN	X	3198	1/1	0.87	1.23	-	162,162,162,162	0
30	MN	X	3167	1/1	0.95	0.59	-	110,110,110,110	0
29	MG	X	3358	1/1	0.72	0.56	-	59,59,59,59	0
29	MG	X	3259	1/1	0.84	0.98	-	63,63,63,63	0
29	MG	X	3352	1/1	0.90	0.39	-	66,66,66,66	0
30	MN	X	3127	1/1	0.99	0.23	-	48,48,48,48	0
30	MN	X	3165	1/1	0.88	0.38	-	83,83,83,83	0
30	MN	X	3092	1/1	0.81	0.56	-	103,103,103,103	0
30	MN	X	3265	1/1	0.86	0.36	-	148,148,148,148	0
29	MG	X	3335	1/1	0.60	0.28	-	81,81,81,81	0
29	MG	X	3016	1/1	0.76	1.25	-	12,12,12,12	1
29	MG	X	3011	1/1	0.76	0.76	-	50,50,50,50	0
30	MN	X	3200	1/1	0.54	0.63	-	161,161,161,161	0
29	MG	X	3194	1/1	0.98	0.46	-	34,34,34,34	0
29	MG	X	3303	1/1	0.53	0.74	-	63,63,63,63	0
30	MN	X	3091	1/1	0.83	0.27	-	78,78,78,78	0
30	MN	X	3237	1/1	0.86	0.50	-	87,87,87,87	0
29	MG	X	3021	1/1	0.88	0.27	-	56,56,56,56	0
29	MG	X	3299	1/1	0.91	1.21	-	52,52,52,52	0
30	MN	X	3162	1/1	0.94	0.22	-	114,114,114,114	0
29	MG	X	3286	1/1	0.94	0.12	-	30,30,30,30	0
29	MG	X	3197	1/1	0.95	0.15	-	58,58,58,58	0
29	MG	X	3024	1/1	0.85	0.42	-	31,31,31,31	1
30	MN	X	3142	1/1	0.89	0.17	-	117,117,117,117	0
30	MN	X	3059	1/1	0.96	0.40	-	111,111,111,111	0
30	MN	X	3133	1/1	0.98	0.17	-	81,81,81,81	0
29	MG	X	3344	1/1	0.89	0.09	-	67,67,67,67	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
29	MG	X	3014	1/1	0.76	0.40	-	26,26,26,26	1
29	MG	X	3026	1/1	0.95	0.30	-	41,41,41,41	0
29	MG	Y	203	1/1	0.98	0.38	-	19,19,19,19	0
29	MG	X	3300	1/1	0.94	0.67	-	59,59,59,59	0
30	MN	X	3118	1/1	0.99	0.20	-	32,32,32,32	0
30	MN	X	3137	1/1	0.95	0.29	-	103,103,103,103	0
30	MN	X	3254	1/1	0.94	0.27	-	105,105,105,105	0
30	MN	M	201	1/1	0.77	0.20	-	105,105,105,105	0
29	MG	X	3298	1/1	0.92	0.47	-	41,41,41,41	0
30	MN	X	3034	1/1	0.98	0.18	-	81,81,81,81	0
30	MN	X	3075	1/1	0.93	0.20	-	33,33,33,33	0
30	MN	X	3227	1/1	0.95	0.47	-	116,116,116,116	0
30	MN	X	3073	1/1	0.89	0.23	-	65,65,65,65	0
30	MN	X	3079	1/1	0.98	0.19	-	52,52,52,52	0
30	MN	X	3185	1/1	0.84	0.32	-	112,112,112,112	0
29	MG	X	3283	1/1	0.97	0.28	-	36,36,36,36	0
29	MG	X	3191	1/1	0.84	0.83	-	79,79,79,79	0
30	MN	X	3236	1/1	0.94	0.31	-	105,105,105,105	0
30	MN	X	3120	1/1	0.90	0.21	-	98,98,98,98	0
29	MG	X	3349	1/1	0.74	0.73	-	74,74,74,74	0
29	MG	X	3351	1/1	0.92	0.07	-	57,57,57,57	0
30	MN	X	3170	1/1	0.83	0.39	-	70,70,70,70	0
29	MG	X	3289	1/1	0.98	0.15	-	61,61,61,61	0
29	MG	X	3336	1/1	0.94	0.61	-	40,40,40,40	0
30	MN	X	3040	1/1	0.56	0.55	-	100,100,100,100	0
30	MN	X	3180	1/1	0.52	0.23	-	121,121,121,121	0
30	MN	Y	202	1/1	0.96	0.16	-	126,126,126,126	0
30	MN	X	3097	1/1	0.98	0.23	-	64,64,64,64	0
30	MN	X	3272	1/1	0.58	0.52	-	156,156,156,156	0
30	MN	X	3065	1/1	0.87	0.40	-	76,76,76,76	0
30	MN	X	3158	1/1	0.98	0.37	-	91,91,91,91	0
30	MN	X	3211	1/1	1.00	0.12	-	64,64,64,64	0
30	MN	X	3179	1/1	0.97	0.18	-	69,69,69,69	0
29	MG	X	3276	1/1	0.78	0.65	-	51,51,51,51	0
30	MN	X	3043	1/1	0.94	0.28	-	67,67,67,67	0
30	MN	X	3332	1/1	0.72	0.14	-	122,122,122,122	0
29	MG	X	3013	1/1	0.97	0.98	-	41,41,41,41	0
30	MN	I	201	1/1	0.95	0.28	-	71,71,71,71	0
29	MG	G	201	1/1	0.88	0.29	-	31,31,31,31	0
30	MN	X	3125	1/1	0.99	0.21	-	60,60,60,60	0
30	MN	X	3032	1/1	0.76	0.44	-	122,122,122,122	0
29	MG	X	3224	1/1	0.87	1.04	-	70,70,70,70	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
30	MN	X	3216	1/1	0.98	0.24	-	78,78,78,78	0
30	MN	X	3132	1/1	0.94	0.70	-	116,116,116,116	0
29	MG	X	3282	1/1	0.82	0.41	-	43,43,43,43	0
29	MG	X	3255	1/1	0.81	0.42	-	59,59,59,59	0
29	MG	X	3030	1/1	0.83	0.38	-	48,48,48,48	0
30	MN	X	3176	1/1	0.93	0.28	-	78,78,78,78	0
30	MN	X	3181	1/1	0.76	0.51	-	121,121,121,121	0
30	MN	X	3266	1/1	0.88	0.36	-	147,147,147,147	0
29	MG	X	3338	1/1	0.96	0.33	-	64,64,64,64	0
29	MG	X	3279	1/1	0.95	0.29	-	66,66,66,66	0
30	MN	X	3041	1/1	0.80	0.36	-	127,127,127,127	0
29	MG	X	3333	1/1	0.88	0.21	-	45,45,45,45	0
29	MG	X	3273	1/1	0.80	0.26	-	78,78,78,78	0
30	MN	X	3159	1/1	0.91	0.20	-	81,81,81,81	0
30	MN	X	3066	1/1	0.97	0.38	-	49,49,49,49	0
30	MN	X	3262	1/1	0.93	0.09	-	130,130,130,130	0
30	MN	X	3269	1/1	0.92	0.37	-	134,134,134,134	0
30	MN	X	3149	1/1	0.97	0.33	-	112,112,112,112	0
29	MG	X	3235	1/1	0.82	0.62	-	62,62,62,62	0
30	MN	X	3114	1/1	0.96	0.17	-	59,59,59,59	0
30	MN	X	3046	1/1	0.78	0.37	-	97,97,97,97	0
29	MG	X	3302	1/1	0.93	0.11	-	61,61,61,61	0
30	MN	X	3246	1/1	0.83	0.21	-	104,104,104,104	0
30	MN	X	3212	1/1	0.91	0.18	-	94,94,94,94	0
29	MG	X	3315	1/1	0.86	0.38	-	60,60,60,60	0
29	MG	X	3284	1/1	0.99	0.22	-	12,12,12,12	0
29	MG	X	3253	1/1	0.79	0.19	-	65,65,65,65	0
30	MN	X	3239	1/1	0.88	0.17	-	154,154,154,154	0
29	MG	X	3228	1/1	0.96	0.41	-	62,62,62,62	0
30	MN	X	3126	1/1	0.95	0.24	-	62,62,62,62	0
29	MG	X	3308	1/1	0.82	0.49	-	44,44,44,44	0
29	MG	X	3310	1/1	0.96	0.44	-	36,36,36,36	0
30	MN	X	3096	1/1	0.98	0.22	-	46,46,46,46	0
30	MN	X	3130	1/1	0.99	0.19	-	63,63,63,63	0
30	MN	X	3150	1/1	0.90	0.52	-	123,123,123,123	0
30	MN	X	3051	1/1	0.74	0.60	-	120,120,120,120	0
29	MG	X	3312	1/1	0.94	0.50	-	36,36,36,36	0
29	MG	X	3319	1/1	0.91	0.62	-	53,53,53,53	0
29	MG	X	3234	1/1	0.92	0.20	-	34,34,34,34	0
30	MN	X	3035	1/1	0.98	0.53	-	149,149,149,149	0
32	EOH	X	3366	3/3	0.88	0.27	-	32,32,32,32	0
30	MN	X	3033	1/1	0.83	0.28	-	106,106,106,106	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
30	MN	X	3145	1/1	0.94	0.39	-	122,122,122,122	0
30	MN	X	3205	1/1	0.81	0.10	-	141,141,141,141	0
30	MN	X	3256	1/1	0.99	0.08	-	79,79,79,79	0
29	MG	C	303	1/1	0.96	0.15	-	38,38,38,38	0
29	MG	X	3278	1/1	0.94	0.56	-	63,63,63,63	0
30	MN	X	3098	1/1	0.94	0.26	-	94,94,94,94	0
30	MN	X	3169	1/1	0.96	0.13	-	85,85,85,85	0
30	MN	X	3146	1/1	0.80	0.30	-	124,124,124,124	0
29	MG	X	3305	1/1	0.93	0.46	-	60,60,60,60	0
30	MN	X	3115	1/1	0.89	0.38	-	65,65,65,65	0
29	MG	O	201	1/1	0.87	0.25	-	0,0,0,0	1
29	MG	X	3342	1/1	0.89	0.17	-	53,53,53,53	0
30	MN	X	3135	1/1	0.87	0.15	-	99,99,99,99	0
30	MN	X	3163	1/1	0.95	0.35	-	118,118,118,118	0
30	MN	X	3144	1/1	0.86	0.40	-	127,127,127,127	0
28	MPD	X	3008	8/8	0.87	0.35	-	61,61,61,61	0
30	MN	Y	210	1/1	0.91	1.00	-	176,176,176,176	0
30	MN	X	3083	1/1	0.99	0.19	-	59,59,59,59	0
30	MN	X	3264	1/1	0.98	0.32	-	103,103,103,103	0
30	MN	X	3190	1/1	0.99	0.21	-	77,77,77,77	0
30	MN	X	3094	1/1	0.85	0.57	-	94,94,94,94	0
30	MN	X	3209	1/1	0.70	0.26	-	122,122,122,122	0
30	MN	X	3058	1/1	0.81	0.49	-	113,113,113,113	0
30	MN	X	3152	1/1	0.81	0.37	-	104,104,104,104	0
30	MN	X	3121	1/1	0.95	0.33	-	71,71,71,71	0
30	MN	X	3268	1/1	0.89	0.41	-	81,81,81,81	0
30	MN	X	3210	1/1	0.91	0.14	-	128,128,128,128	0
30	MN	X	3329	1/1	0.96	0.05	-	95,95,95,95	0
30	MN	X	3238	1/1	0.98	0.36	-	126,126,126,126	0
30	MN	Y	201	1/1	0.96	0.13	-	84,84,84,84	0
30	MN	X	3074	1/1	0.97	0.44	-	68,68,68,68	0
29	MG	X	3275	1/1	0.85	0.64	-	29,29,29,29	0
29	MG	X	3257	1/1	0.95	0.08	-	48,48,48,48	0
30	MN	X	3183	1/1	0.87	0.29	-	128,128,128,128	0
32	EOH	X	3368	3/3	0.82	0.70	-	55,55,55,55	0
30	MN	X	3124	1/1	0.95	0.21	-	67,67,67,67	0
30	MN	X	3050	1/1	0.97	0.22	-	87,87,87,87	0
30	MN	X	3087	1/1	0.99	0.30	-	85,85,85,85	0
30	MN	X	3161	1/1	0.90	0.24	-	93,93,93,93	0
30	MN	X	3064	1/1	0.96	0.36	-	94,94,94,94	0
29	MG	X	3280	1/1	0.94	0.28	-	51,51,51,51	0
30	MN	X	3081	1/1	0.98	0.32	-	49,49,49,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
30	MN	X	3261	1/1	0.94	0.21	-	89,89,89,89	0
29	MG	X	3320	1/1	0.96	0.23	-	53,53,53,53	0
30	MN	X	3331	1/1	0.89	0.71	-	119,119,119,119	0
29	MG	X	3327	1/1	0.79	0.38	-	48,48,48,48	0
30	MN	X	3218	1/1	0.59	0.22	-	128,128,128,128	0
29	MG	X	3196	1/1	0.95	1.05	-	41,41,41,41	0
29	MG	X	3314	1/1	0.91	0.44	-	55,55,55,55	0
29	MG	X	3297	1/1	0.84	0.74	-	44,44,44,44	0
30	MN	X	3088	1/1	0.98	0.24	-	97,97,97,97	0
30	MN	X	3042	1/1	0.68	0.18	-	161,161,161,161	0
30	MN	X	3063	1/1	0.99	0.27	-	42,42,42,42	0
30	MN	X	3247	1/1	0.81	0.18	-	104,104,104,104	0
29	MG	X	3012	1/1	0.92	0.46	-	16,16,16,16	1
30	MN	X	3062	1/1	0.97	0.32	-	72,72,72,72	0
28	MPD	X	3006	8/8	0.92	0.25	-	74,74,74,74	0
29	MG	X	3372	1/1	0.90	1.48	-	56,56,56,56	0
29	MG	Y	209	1/1	0.95	0.35	-	59,59,59,59	0
29	MG	X	3285	1/1	0.97	0.28	-	56,56,56,56	0
30	MN	X	3208	1/1	0.96	0.40	-	109,109,109,109	0
29	MG	X	3307	1/1	0.89	0.18	-	49,49,49,49	0
30	MN	X	3201	1/1	0.94	0.37	-	106,106,106,106	0
29	MG	X	3020	1/1	0.81	0.97	-	40,40,40,40	0
29	MG	B	301	1/1	0.82	0.35	-	46,46,46,46	0
30	MN	X	3263	1/1	0.93	0.21	-	114,114,114,114	0
30	MN	X	3202	1/1	0.93	0.17	-	124,124,124,124	0
29	MG	X	3287	1/1	0.91	0.55	-	36,36,36,36	0
30	MN	X	3105	1/1	0.94	0.49	-	48,48,48,48	0
29	MG	X	3304	1/1	0.92	0.65	-	40,40,40,40	0
30	MN	X	3134	1/1	0.97	0.28	-	90,90,90,90	0
30	MN	X	3186	1/1	0.97	0.13	-	142,142,142,142	0
29	MG	X	3350	1/1	0.93	0.29	-	71,71,71,71	0
30	MN	X	3148	1/1	0.88	0.35	-	112,112,112,112	0
29	MG	X	3023	1/1	0.90	0.28	-	26,26,26,26	1
30	MN	Y	208	1/1	0.85	0.58	-	173,173,173,173	0
29	MG	X	3341	1/1	0.92	0.14	-	92,92,92,92	0
30	MN	X	3206	1/1	0.85	0.51	-	133,133,133,133	0
29	MG	X	3359	1/1	0.91	0.46	-	60,60,60,60	0
30	MN	X	3061	1/1	0.97	0.34	-	69,69,69,69	0
29	MG	X	3288	1/1	0.94	1.06	-	39,39,39,39	0
29	MG	X	3157	1/1	0.90	0.53	-	61,61,61,61	0
29	MG	X	3301	1/1	0.87	0.15	-	30,30,30,30	0
29	MG	Y	206	1/1	0.87	0.49	-	45,45,45,45	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
30	MN	X	3267	1/1	0.73	0.56	-	140,140,140,140	0
29	MG	X	3306	1/1	0.90	0.64	-	66,66,66,66	0
30	MN	X	3361	1/1	0.80	0.23	-	158,158,158,158	0
30	MN	X	3204	1/1	0.88	0.37	-	141,141,141,141	0
29	MG	X	3343	1/1	0.85	1.29	-	53,53,53,53	0
30	MN	X	3116	1/1	0.98	0.47	-	70,70,70,70	0
29	MG	X	3353	1/1	0.83	0.39	-	39,39,39,39	0
30	MN	X	3222	1/1	0.90	0.26	-	101,101,101,101	0
29	MG	X	3156	1/1	0.98	0.44	-	14,14,14,14	0
29	MG	X	3225	1/1	0.87	0.54	-	56,56,56,56	0
30	MN	X	3072	1/1	0.96	0.25	-	74,74,74,74	0
30	MN	X	3147	1/1	0.89	0.40	-	89,89,89,89	0
29	MG	X	3277	1/1	0.94	0.30	-	51,51,51,51	0
29	MG	X	3025	1/1	0.71	0.47	-	16,16,16,16	1
29	MG	X	3347	1/1	0.85	0.40	-	37,37,37,37	0
29	MG	X	3360	1/1	0.76	1.34	-	78,78,78,78	0
29	MG	R	201	1/1	0.91	0.20	-	24,24,24,24	0
29	MG	X	3015	1/1	0.95	0.42	-	48,48,48,48	0
29	MG	X	3231	1/1	0.85	0.68	-	64,64,64,64	0
29	MG	X	3229	1/1	0.86	1.14	-	62,62,62,62	0
29	MG	X	3292	1/1	0.95	0.32	-	30,30,30,30	0
29	MG	X	3293	1/1	0.92	0.35	-	32,32,32,32	0
30	MN	X	3138	1/1	0.95	0.12	-	91,91,91,91	0
30	MN	X	3173	1/1	0.98	0.39	-	72,72,72,72	0
30	MN	X	3141	1/1	0.98	0.24	-	99,99,99,99	0
29	MG	X	3323	1/1	0.88	0.12	-	48,48,48,48	0
30	MN	X	3189	1/1	0.98	0.26	-	43,43,43,43	0
29	MG	X	3031	1/1	0.78	0.20	-	45,45,45,45	0
30	MN	X	3151	1/1	0.36	0.57	-	135,135,135,135	0
30	MN	X	3102	1/1	0.98	0.47	-	100,100,100,100	0
29	MG	X	3018	1/1	0.81	1.03	-	42,42,42,42	0
30	MN	X	3037	1/1	0.81	0.59	-	131,131,131,131	0
29	MG	X	3290	1/1	0.92	0.56	-	45,45,45,45	0
30	MN	X	3055	1/1	0.91	0.62	-	121,121,121,121	0
29	MG	X	3322	1/1	0.91	0.10	-	67,67,67,67	0
30	MN	X	3207	1/1	0.90	0.34	-	130,130,130,130	0
29	MG	T	101	1/1	0.55	0.35	-	44,44,44,44	0
30	MN	X	3220	1/1	0.84	0.91	-	153,153,153,153	0
30	MN	X	3171	1/1	0.69	0.19	-	82,82,82,82	0
30	MN	X	3122	1/1	0.88	0.22	-	71,71,71,71	0
29	MG	X	3027	1/1	0.93	0.32	-	38,38,38,38	0
30	MN	X	3128	1/1	0.95	0.19	-	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
29	MG	X	3230	1/1	0.86	0.28	-	71,71,71,71	0
30	MN	X	3188	1/1	0.98	0.27	-	54,54,54,54	0
30	MN	X	3160	1/1	0.97	0.24	-	101,101,101,101	0
29	MG	X	3252	1/1	0.54	0.52	-	45,45,45,45	0
30	MN	X	3068	1/1	0.93	0.25	-	102,102,102,102	0
29	MG	X	3354	1/1	0.52	0.49	-	59,59,59,59	0
29	MG	C	301	1/1	0.83	0.13	-	31,31,31,31	0
30	MN	X	3054	1/1	0.97	0.19	-	76,76,76,76	0
29	MG	X	3195	1/1	0.93	0.80	-	28,28,28,28	0
29	MG	X	3017	1/1	0.92	0.93	-	46,46,46,46	0
29	MG	X	3155	1/1	0.94	0.68	-	21,21,21,21	0
29	MG	X	3313	1/1	0.93	0.27	-	67,67,67,67	0
29	MG	X	3294	1/1	0.95	0.43	-	32,32,32,32	0
29	MG	X	3028	1/1	0.69	1.51	-	66,66,66,66	0
29	MG	X	3291	1/1	0.98	0.27	-	26,26,26,26	0
30	MN	X	3241	1/1	0.96	0.23	-	66,66,66,66	0
29	MG	X	3250	1/1	0.96	0.60	-	25,25,25,25	0
30	MN	X	3069	1/1	0.96	0.54	-	76,76,76,76	0
30	MN	X	3243	1/1	0.94	0.58	-	107,107,107,107	0
29	MG	X	3029	1/1	0.95	0.13	-	51,51,51,51	0
29	MG	X	3022	1/1	0.65	1.10	-	62,62,62,62	0
30	MN	X	3111	1/1	0.99	0.56	-	71,71,71,71	0
29	MG	X	3281	1/1	0.92	0.43	-	21,21,21,21	0
29	MG	X	3258	1/1	0.68	0.65	-	73,73,73,73	0
30	MN	X	3113	1/1	0.98	0.35	-	62,62,62,62	0
30	MN	X	3045	1/1	0.94	0.09	-	82,82,82,82	0
30	MN	I	202	1/1	0.92	0.33	-	100,100,100,100	0
30	MN	X	3057	1/1	0.99	0.35	-	28,28,28,28	0
32	EOH	X	3367	3/3	0.66	0.70	-	77,77,77,77	0
30	MN	X	3370	1/1	0.99	0.31	-	98,98,98,98	0
30	MN	X	3175	1/1	0.81	0.07	-	111,111,111,111	0
30	MN	Y	205	1/1	0.76	0.24	-	132,132,132,132	0
29	MG	X	3226	1/1	0.60	0.45	-	64,64,64,64	0
29	MG	X	3321	1/1	0.94	0.48	-	74,74,74,74	0
30	MN	Y	204	1/1	0.96	0.40	-	146,146,146,146	0
30	MN	X	3047	1/1	0.93	0.32	-	94,94,94,94	0
29	MG	X	3357	1/1	0.76	0.41	-	51,51,51,51	0
30	MN	X	3100	1/1	0.94	0.23	-	57,57,57,57	0
30	MN	X	3242	1/1	0.99	0.19	-	68,68,68,68	0
29	MG	X	3318	1/1	0.90	0.30	-	47,47,47,47	0
29	MG	X	3296	1/1	0.97	0.37	-	56,56,56,56	0
30	MN	X	3245	1/1	0.93	0.47	-	98,98,98,98	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
30	MN	X	3184	1/1	0.97	0.17	-	99,99,99,99	0
29	MG	X	3233	1/1	0.89	0.95	-	57,57,57,57	0
30	MN	X	3214	1/1	0.88	0.18	-	78,78,78,78	0
30	MN	X	3154	1/1	0.97	0.47	-	47,47,47,47	0
29	MG	X	3260	1/1	0.55	0.54	-	64,64,64,64	0
29	MG	X	3192	1/1	0.89	0.66	-	45,45,45,45	0
30	MN	X	3187	1/1	0.98	0.21	-	45,45,45,45	0
30	MN	X	3104	1/1	0.96	0.47	-	53,53,53,53	0
29	MG	X	3223	1/1	0.98	0.10	-	42,42,42,42	0
30	MN	X	3131	1/1	0.89	0.57	-	109,109,109,109	0
30	MN	X	3182	1/1	0.75	0.24	-	117,117,117,117	0
29	MG	X	3249	1/1	0.83	0.28	-	59,59,59,59	0
30	MN	X	3119	1/1	0.97	0.32	-	87,87,87,87	0
30	MN	X	3093	1/1	0.89	0.40	-	83,83,83,83	0

6.5 Other polymers (i)

There are no such residues in this entry.