wwPDB X-ray Structure Validation Summary Report (i)

Aug 27, 2023 – 03:44 AM EDT

PDB ID	:	3G71
Title	:	Co-crystal structure of Bruceantin bound to the large ribosomal subunit
Authors	:	Gurel, G.; Blaha, G.; Moore, P.B.; Steitz, T.A.
Deposited on	:	2009-02-09
Resolution	:	2.85 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:

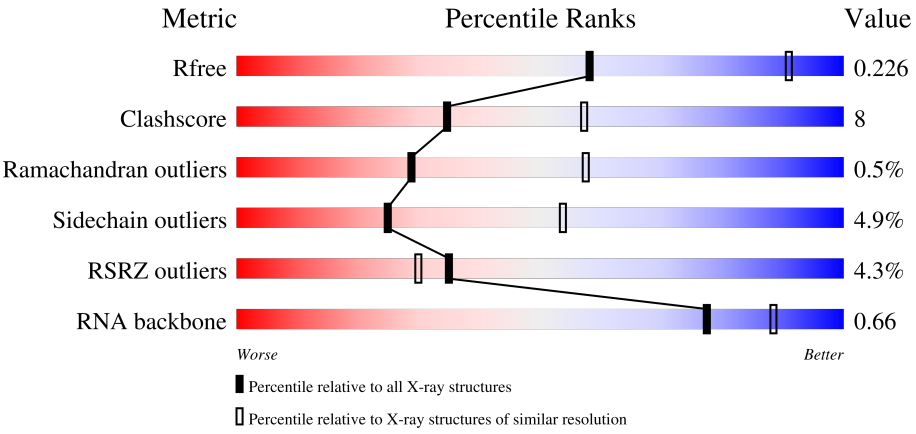
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.85 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)
RNA backbone	3102	1088 (3.12-2.60)

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

Mol	Chain	Length	Quality of chain
1	0	2923	54% 34% 5% 6%
2	A	237	6% 84% 14% ·
3	B	337	85% 14% ·
4	C	246	84% 13% ·

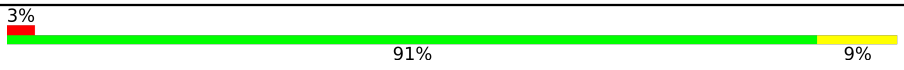
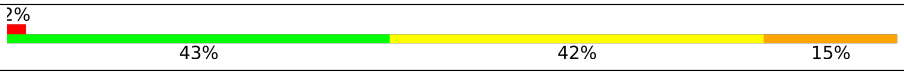
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	D	177	26% 63% 15% 21%
6	E	172	% 88% 12%
7	F	119	9% 93% 7%
8	G	348	% 8% 92%
9	H	177	11% 78% 11% 10%
10	I	70	77% 96%
11	J	142	% 86% 12%
12	K	132	2% 86% 13%
13	L	165	9% 82% 6% 12%
14	M	194	87% 12%
15	N	186	11% 86% 14%
16	O	115	90% 9%
17	P	143	% 87% 13%
18	Q	95	87% 12%
19	R	150	89% 9%
20	S	81	2% 88% 12%
21	T	119	3% 84% 14%
22	U	53	91% 9%
23	V	65	25% 88% 12%
24	W	154	% 81% 18%
25	X	82	6% 79% 20%
26	Y	142	% 89% 10%
27	Z	73	71% 90% 10%
28	1	56	80% 20%
29	2	50	6% 74% 18% 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
30	3	92	
31	9	122	

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
32	MG	0	8090	-	-	-	X
33	K	0	8401	-	-	-	X
34	NA	0	8524	-	-	-	X
34	NA	0	8527	-	-	-	X
34	NA	0	8542	-	-	-	X
34	NA	0	8549	-	-	-	X
34	NA	0	8554	-	-	-	X
34	NA	0	8556	-	-	-	X
34	NA	0	8560	-	-	-	X
34	NA	0	8566	-	-	-	X
34	NA	9	8572	-	-	-	X
34	NA	H	8518	-	-	-	X
36	SR	0	8913	-	-	-	X
36	SR	0	8982	-	-	-	X
36	SR	0	8996	-	-	-	X
36	SR	0	9006	-	-	-	X
36	SR	B	8987	-	-	-	X

2 Entry composition (i)

There are 39 unique types of molecules in this entry. The entry contains 99174 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	0	2754	59021	26349	10873	19054	2745	0	0	0

- Molecule 2 is a protein called 50S ribosomal protein L2P.

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

- Molecule 3 is a protein called 50S ribosomal protein L3P.

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

- Molecule 4 is a protein called 50S ribosomal protein L4P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	C	246	1860	1130	345	384	1	0	0	0

- Molecule 5 is a protein called 50S ribosomal protein L5P.

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

- Molecule 6 is a protein called 50S ribosomal protein L6P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	E	172	1358	840	224	290	4	0	0	0

- Molecule 7 is a protein called 50S ribosomal protein L7Ae.

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

- Molecule 8 is a protein called 50S ribosomal protein L10E.

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

- Molecule 9 is a protein called 50S ribosomal protein L10e.

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

- Molecule 10 is a protein called 50S ribosomal protein L11P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	I	70	Total	C	N	O	S	0	0	0
			520	323	81	115	1			

- Molecule 11 is a protein called 50S ribosomal protein L13P.

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

- Molecule 12 is a protein called 50S ribosomal protein L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	132	Total	C	N	O	S	0	0	0
			994	609	189	192	4			

- Molecule 13 is a protein called 50S ribosomal protein L15P.

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

- Molecule 14 is a protein called 50S ribosomal protein L15e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	M	194	Total	C	N	O	S	0	0	0
			1559	943	333	282	1			

- Molecule 15 is a protein called 50S ribosomal protein L18P.

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

- Molecule 16 is a protein called 50S ribosomal protein L18e.

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

- Molecule 17 is a protein called 50S ribosomal protein L19e.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	P	143	Total	C	N	O	0	0	0
			1137	683	229	225			

- Molecule 18 is a protein called 50S ribosomal protein L21e.

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

- Molecule 19 is a protein called 50S ribosomal protein L22P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	R	150	Total	C	N	O	S	0	0	0
			1150	713	209	224	4			

- Molecule 20 is a protein called 50S ribosomal protein L23P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	S	81	Total	C	N	O	S	0	0	0
			642	389	111	139	3			

- Molecule 21 is a protein called 50S ribosomal protein L24P.

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

- Molecule 22 is a protein called 50S ribosomal protein L24e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	U	53	Total	C	N	O	S	0	0	0
			411	244	75	87	5			

- Molecule 23 is a protein called 50S ribosomal protein L29P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	V	65	Total	C	N	O	S	0	0	0
			500	304	94	101	1			

- Molecule 24 is a protein called 50S ribosomal protein L30P.

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

- Molecule 25 is a protein called 50S ribosomal protein L31e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	X	82	Total	C	N	O	S	0	0	0
			655	402	129	123	1			

- Molecule 26 is a protein called 50S ribosomal protein L32e.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
26	Y	142	Total	C	N	O	0	0	0
			1131	686	228	217			

- Molecule 27 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	Z	73	Total	C	N	O	S	0	0	0
			574	343	113	113	5			

- Molecule 28 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 29 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

- Molecule 30 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 31 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	9	122	Total	C	N	O	P	0	0	0
			2599	1160	471	847	121			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	0	85	Total	Mg	0	0
			85	85		
32	A	1	Total	Mg	0	0
			1	1		
32	B	1	Total	Mg	0	0
			1	1		
32	K	1	Total	Mg	0	0
			1	1		
32	T	1	Total	Mg	0	0
			1	1		
32	Y	1	Total	Mg	0	0
			1	1		
32	2	1	Total	Mg	0	0
			1	1		
32	9	2	Total	Mg	0	0
			2	2		

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

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	0	66	Total Na 66 66	0	0
34	C	1	Total Na 1 1	0	0
34	H	1	Total Na 1 1	0	0
34	J	1	Total Na 1 1	0	0
34	M	1	Total Na 1 1	0	0
34	Q	1	Total Na 1 1	0	0
34	R	1	Total Na 1 1	0	0
34	S	1	Total Na 1 1	0	0
34	9	2	Total Na 2 2	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	0	9	Total Cl 9 9	0	0
35	A	1	Total Cl 1 1	0	0
35	B	1	Total Cl 1 1	0	0
35	J	3	Total Cl 3 3	0	0
35	K	1	Total Cl 1 1	0	0
35	L	1	Total Cl 1 1	0	0
35	M	1	Total Cl 1 1	0	0
35	N	1	Total Cl 1 1	0	0

Continued on next page...

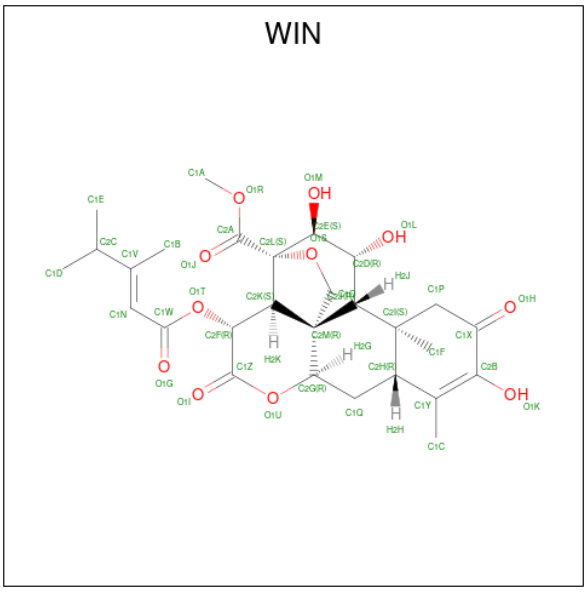
Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	O	1	Total Cl 1 1	0	0
35	R	1	Total Cl 1 1	0	0
35	Y	1	Total Cl 1 1	0	0
35	3	1	Total Cl 1 1	0	0

- Molecule 36 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	0	95	Total Sr 95 95	0	0
36	A	2	Total Sr 2 2	0	0
36	B	2	Total Sr 2 2	0	0
36	F	1	Total Sr 1 1	0	0
36	R	1	Total Sr 1 1	0	0
36	S	1	Total Sr 1 1	0	0
36	1	1	Total Sr 1 1	0	0
36	3	2	Total Sr 2 2	0	0
36	9	3	Total Sr 3 3	0	0

- Molecule 37 is methyl (5beta,7alpha,9beta,10alpha,11alpha,12alpha,13beta,15alpha)-15-{[(2E)-3,4-dimethylpent-2-enoyl]oxy}-3,11,12-trihydroxy-2,16-dioxo-13,20-epoxypicras-3-en-21-oate (three-letter code: WIN) (formula: $C_{28}H_{36}O_{11}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	0	1	Total C O 39 28 11	0	0

- Molecule 38 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	O	1	Total Cd 1 1	0	0
38	U	1	Total Cd 1 1	0	0
38	Z	1	Total Cd 1 1	0	0
38	1	1	Total Cd 1 1	0	0
38	3	1	Total Cd 1 1	0	0

- Molecule 39 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
39	0	5993	Total O 5993 5993	0	0
39	A	107	Total O 107 107	0	0
39	B	146	Total O 146 146	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
39	C	171	Total O 171 171	0	0
39	D	45	Total O 45 45	0	0
39	E	40	Total O 40 40	0	0
39	F	25	Total O 25 25	0	0
39	G	18	Total O 18 18	0	0
39	H	62	Total O 62 62	0	0
39	I	5	Total O 5 5	0	0
39	J	52	Total O 52 52	0	0
39	K	53	Total O 53 53	0	0
39	L	79	Total O 79 79	0	0
39	M	128	Total O 128 128	0	0
39	N	62	Total O 62 62	0	0
39	O	40	Total O 40 40	0	0
39	P	65	Total O 65 65	0	0
39	Q	43	Total O 43 43	0	0
39	R	77	Total O 77 77	0	0
39	S	28	Total O 28 28	0	0
39	T	32	Total O 32 32	0	0
39	U	27	Total O 27 27	0	0
39	V	12	Total O 12 12	0	0
39	W	65	Total O 65 65	0	0

Continued on next page...

Continued from previous page...

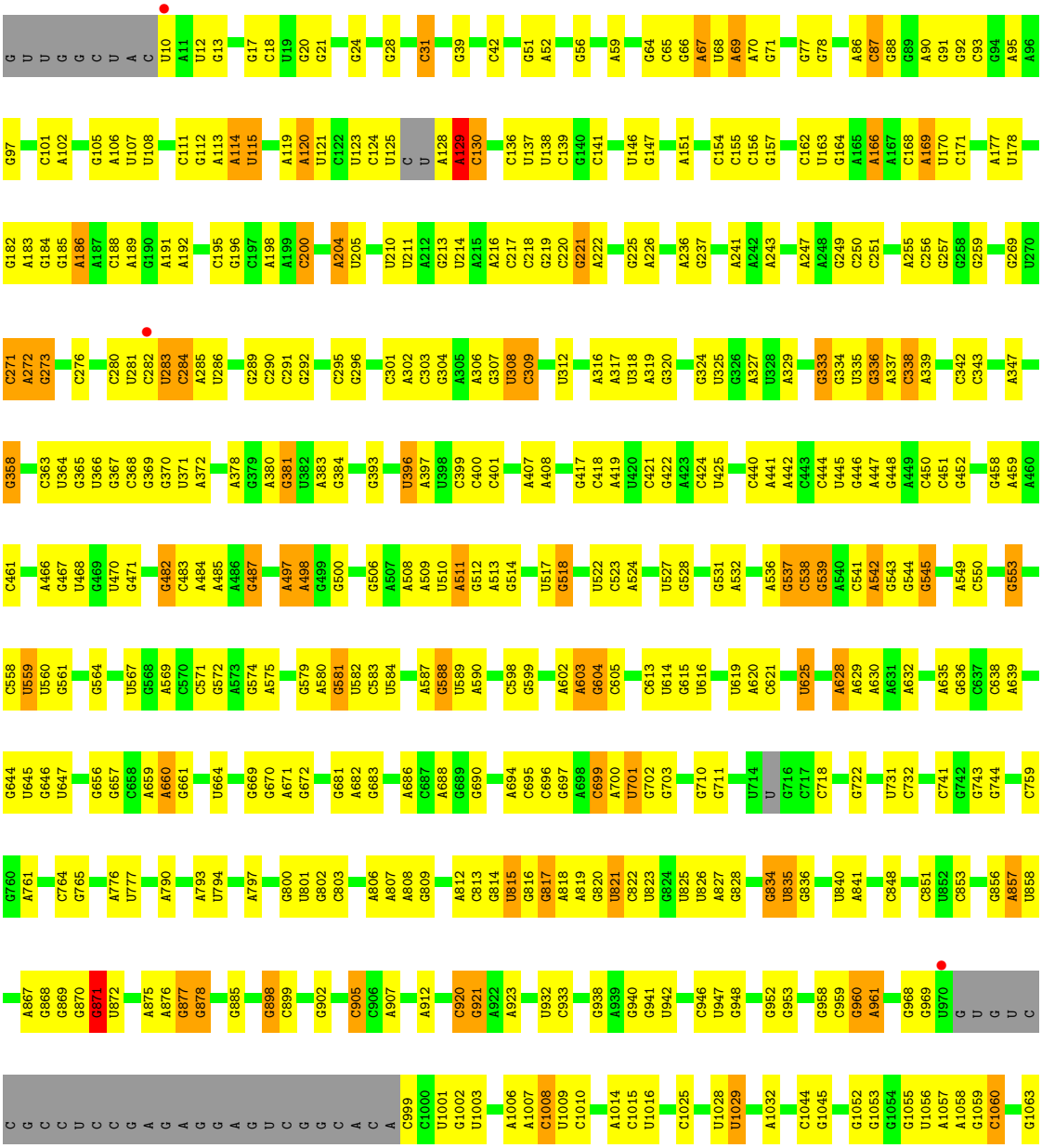
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
39	X	20	Total O 20 20	0	0
39	Y	94	Total O 94 94	0	0
39	Z	28	Total O 28 28	0	0
39	1	52	Total O 52 52	0	0
39	2	39	Total O 39 39	0	0
39	3	66	Total O 66 66	0	0
39	9	149	Total O 149 149	0	0

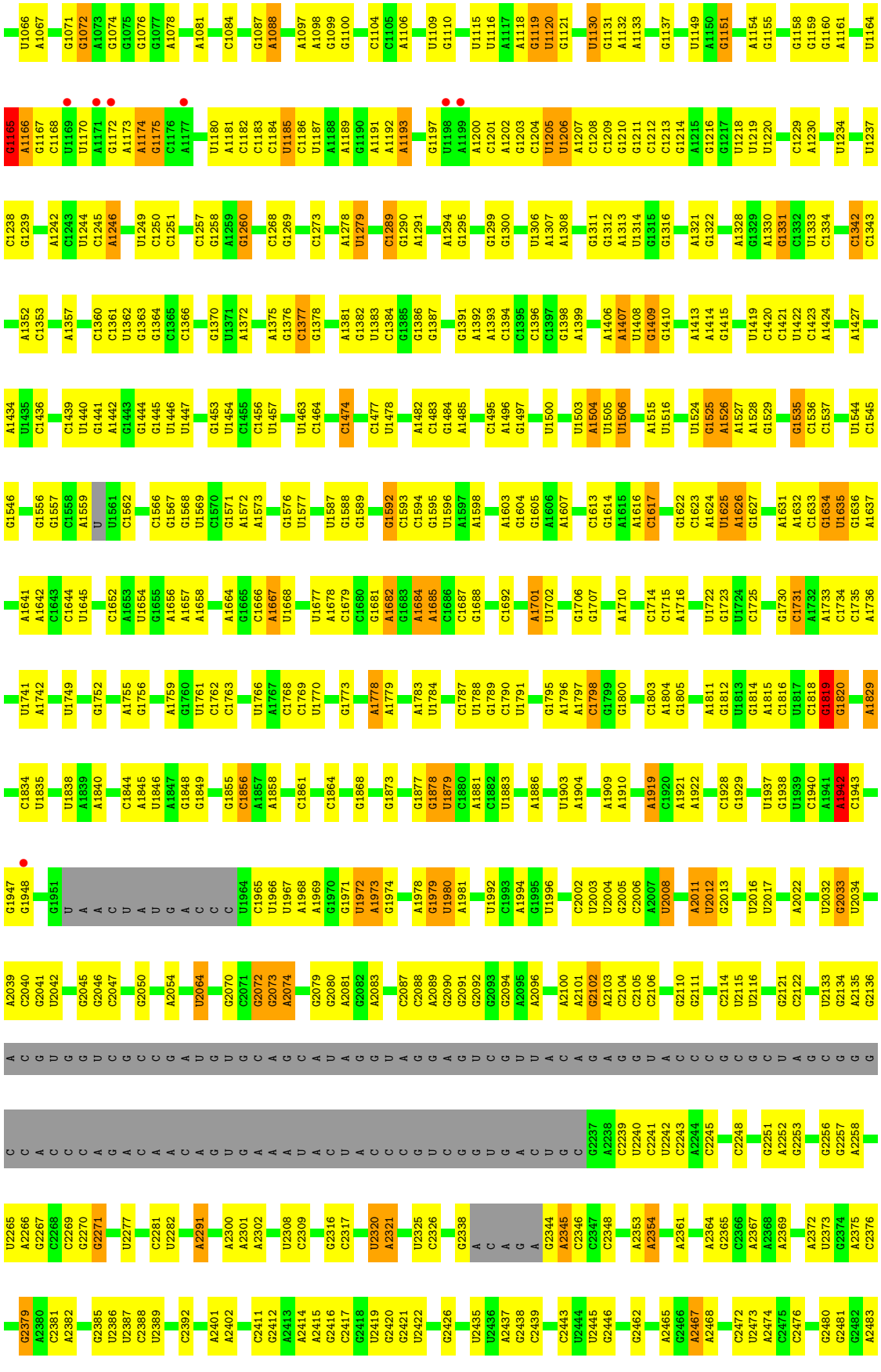
3 Residue-property plots (i)

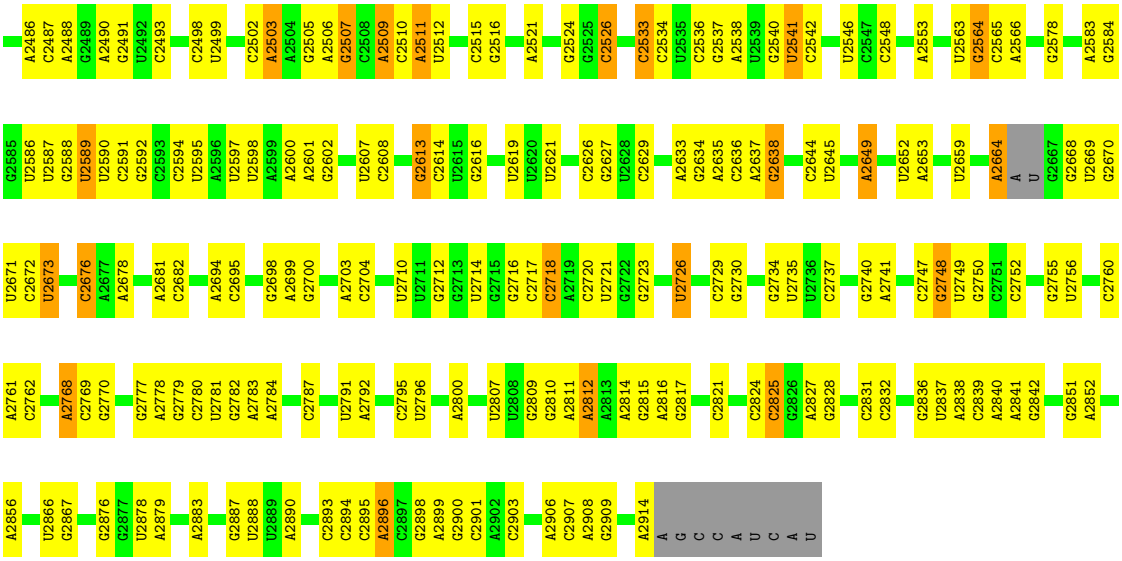
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: 23S ribosomal RNA

Chain 0:

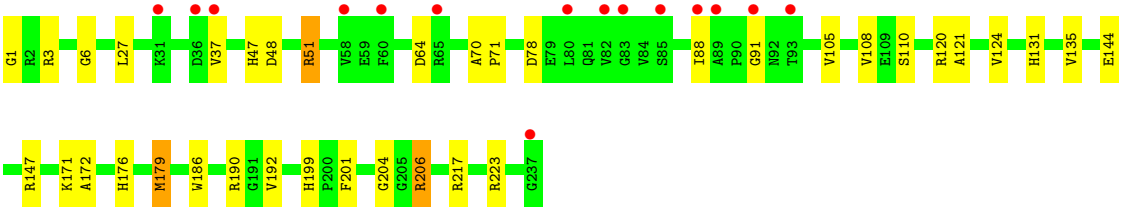






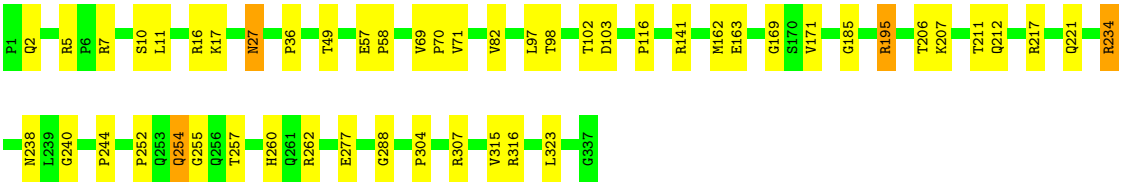
• Molecule 2: 50S ribosomal protein L2P

Chain A:



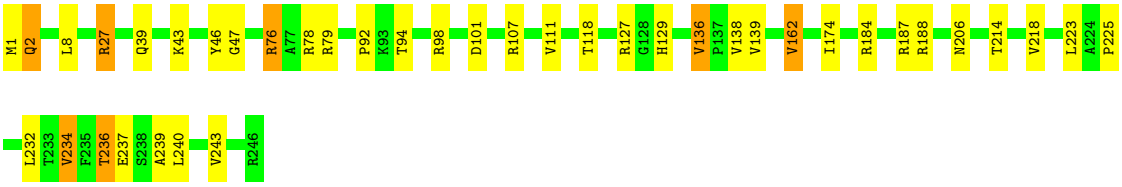
• Molecule 3: 50S ribosomal protein L3P

Chain B:



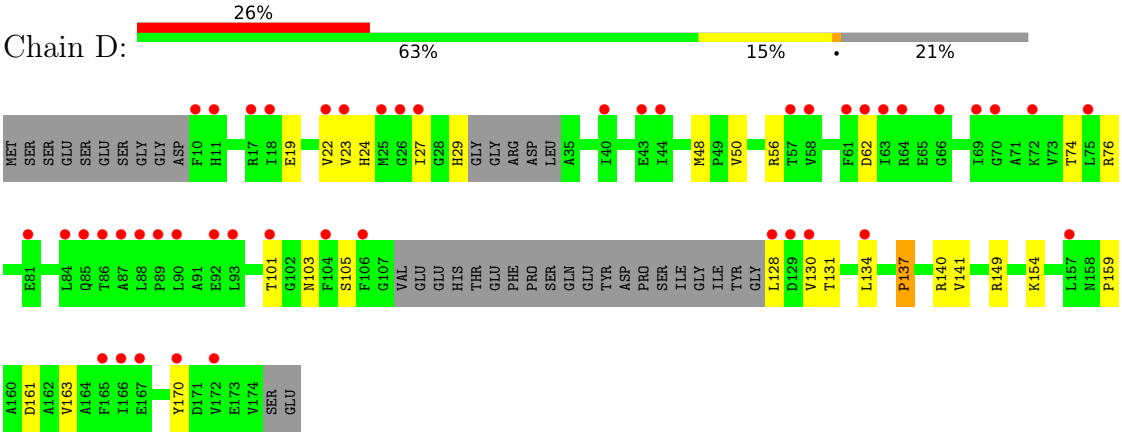
• Molecule 4: 50S ribosomal protein L4P

Chain C:



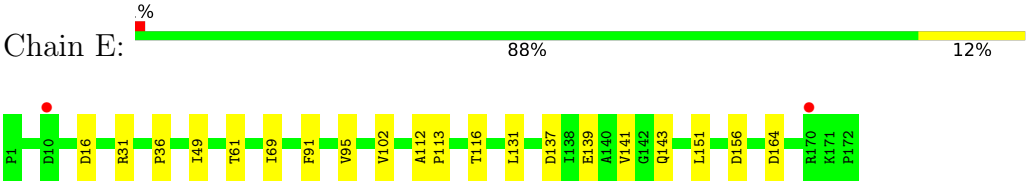
• Molecule 5: 50S ribosomal protein L5P

Chain D:



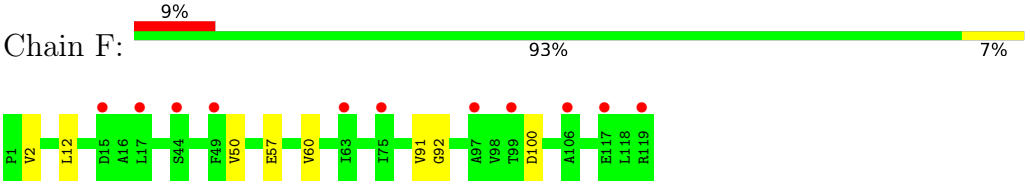
• Molecule 6: 50S ribosomal protein L6P

Chain E:



• Molecule 7: 50S ribosomal protein L7Ae

Chain F:

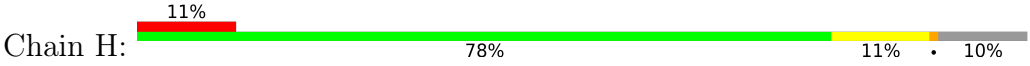


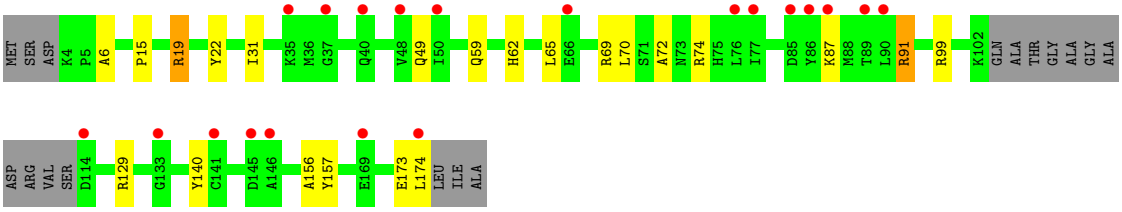
• Molecule 8: 50S ribosomal protein L10E

Chain G:

• Molecule 9: 50S ribosomal protein L10e

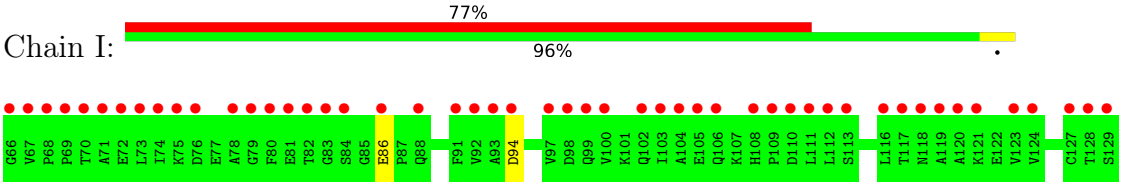
Chain H:





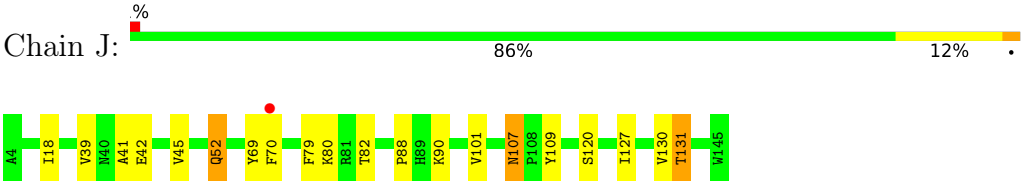
• Molecule 10: 50S ribosomal protein L11P

Chain I:



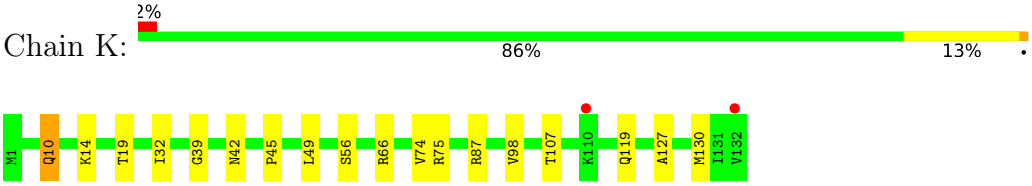
• Molecule 11: 50S ribosomal protein L13P

Chain J:



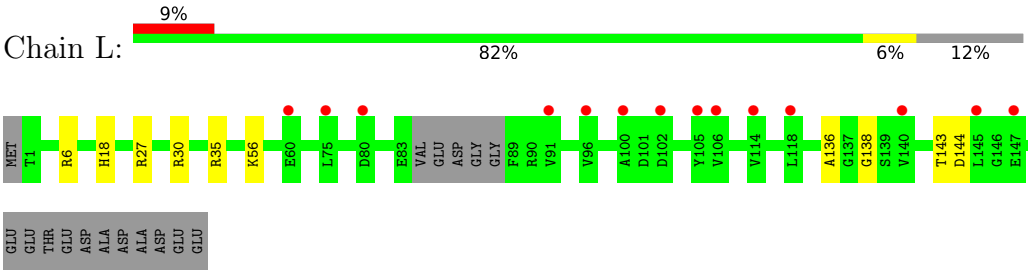
• Molecule 12: 50S ribosomal protein L14P

Chain K:



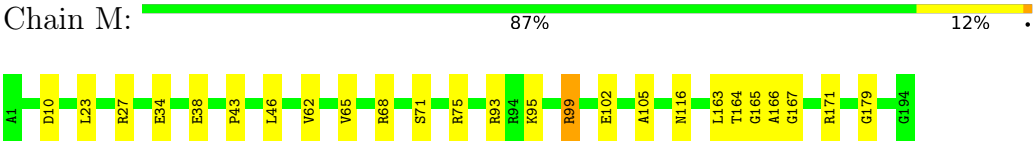
• Molecule 13: 50S ribosomal protein L15P

Chain L:



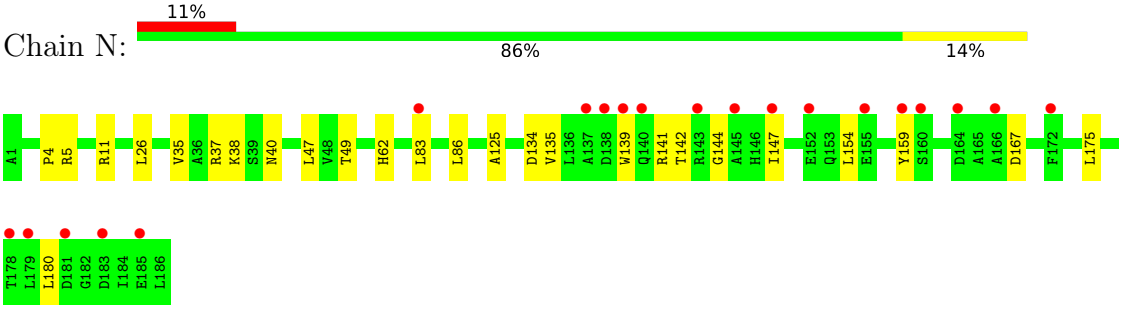
• Molecule 14: 50S ribosomal protein L15e

Chain M:



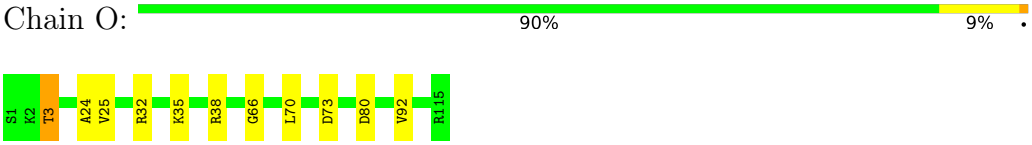
• Molecule 15: 50S ribosomal protein L18P

Chain N:



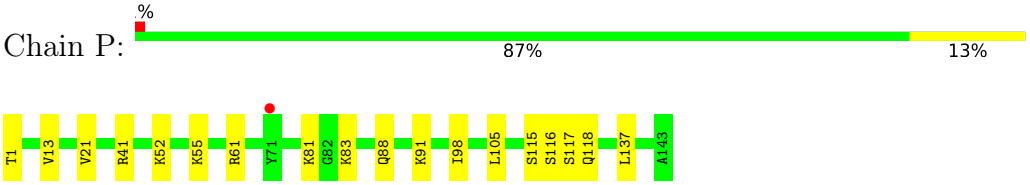
• Molecule 16: 50S ribosomal protein L18e

Chain O:



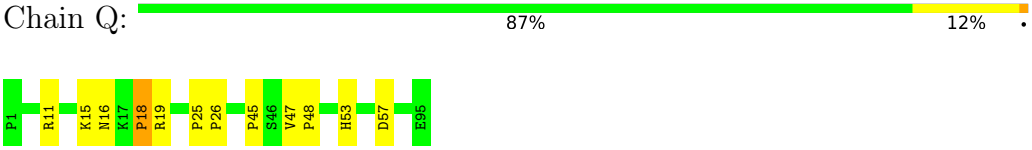
• Molecule 17: 50S ribosomal protein L19e

Chain P:



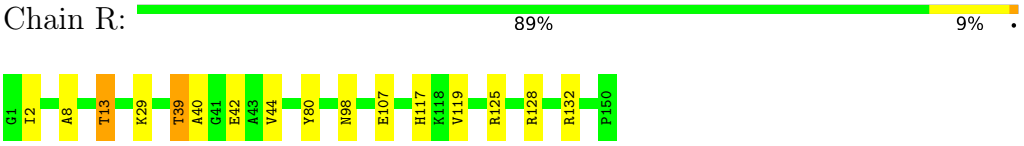
• Molecule 18: 50S ribosomal protein L21e

Chain Q:



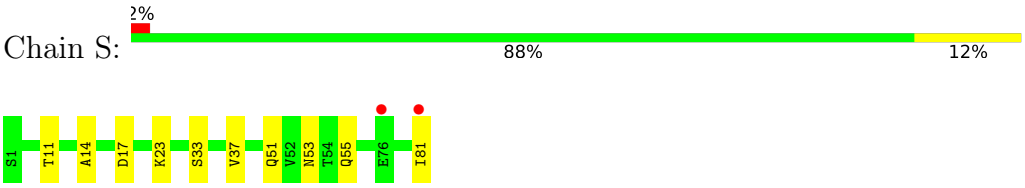
• Molecule 19: 50S ribosomal protein L22P

Chain R:



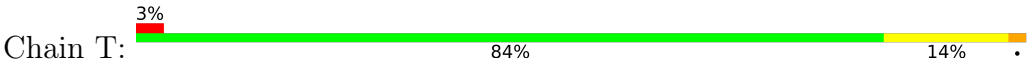
• Molecule 20: 50S ribosomal protein L23P

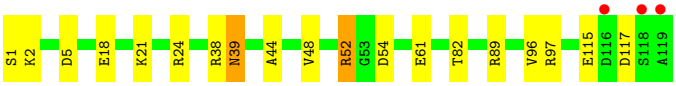
Chain S:



• Molecule 21: 50S ribosomal protein L24P

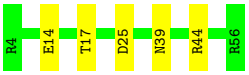
Chain T:





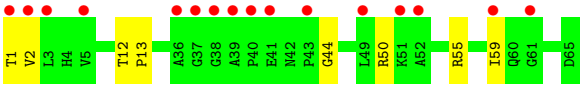
• Molecule 22: 50S ribosomal protein L24e

Chain U:



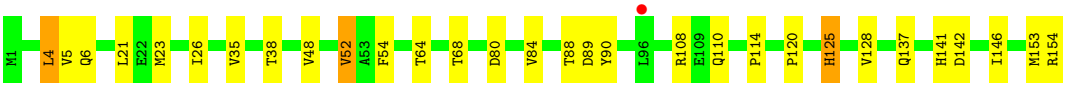
• Molecule 23: 50S ribosomal protein L29P

Chain V:



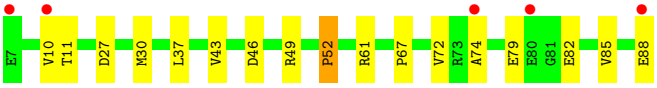
• Molecule 24: 50S ribosomal protein L30P

Chain W:



• Molecule 25: 50S ribosomal protein L31e

Chain X:

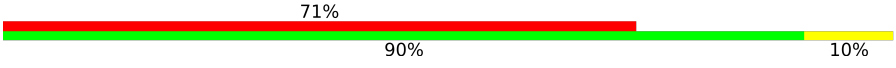


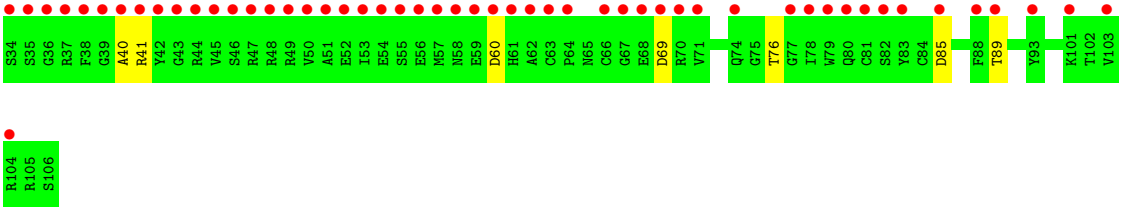
• Molecule 26: 50S ribosomal protein L32e

Chain Y:

• Molecule 27: 50S ribosomal protein L37Ae

Chain Z:



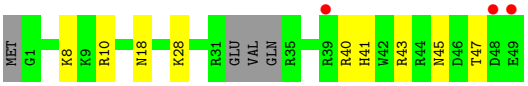


• Molecule 28: 50S ribosomal protein L37e

Chain 1:

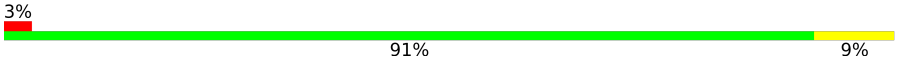
• Molecule 29: 50S ribosomal protein L39e

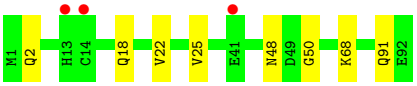
Chain 2:



• Molecule 30: 50S ribosomal protein L44E

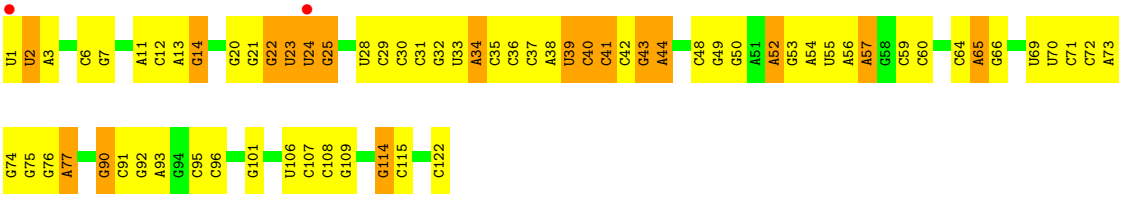
Chain 3:





• Molecule 31: 5S ribosomal RNA

Chain 9:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	212.21Å 299.54Å 574.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.76 – 2.85 85.61 – 2.40	Depositor EDS
% Data completeness (in resolution range)	91.2 (49.76-2.85) 91.0 (85.61-2.40)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.00 (at 2.40Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.186 , 0.233 0.181 , 0.226	Depositor DCC
R_{free} test set	6547 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å^2)	58.3	Xtriage
Anisotropy	0.215	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 80.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	99174	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.57% 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: 1MA, UR3, K, OMU, OMG, PSU, MG, WIN, CL, SR, CD, NA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	0	0.39	0/65958	0.68	10/102869 (0.0%)
2	A	0.51	1/1787 (0.1%)	0.76	0/2408
3	B	0.53	0/2690	0.77	0/3652
4	C	0.56	0/1885	0.79	0/2552
5	D	0.63	0/1111	0.71	2/1498 (0.1%)
6	E	0.60	0/1383	0.68	0/1880
7	F	0.54	0/901	0.70	0/1224
8	G	0.50	0/241	0.66	0/324
9	H	0.61	0/1302	0.76	0/1743
10	I	0.58	0/527	0.63	0/716
11	J	0.62	0/1136	0.73	0/1530
12	K	0.49	0/1004	0.80	0/1351
13	L	0.52	0/1130	0.74	0/1509
14	M	0.51	0/1583	0.74	0/2116
15	N	0.55	0/1474	0.75	0/1999
16	O	0.50	0/874	0.72	1/1181 (0.1%)
17	P	0.53	0/1148	0.66	0/1528
18	Q	0.51	0/749	0.75	0/1005
19	R	0.57	0/1173	0.76	0/1578
20	S	0.54	0/649	0.65	0/875
21	T	0.47	0/958	0.76	1/1289 (0.1%)
22	U	0.58	0/418	0.68	0/562
23	V	0.43	0/503	0.68	0/675
24	W	0.52	0/1219	0.77	1/1655 (0.1%)
25	X	0.52	0/665	0.75	0/895
26	Y	0.51	0/1147	0.72	0/1536
27	Z	0.68	0/585	0.71	0/781
28	1	0.55	0/438	0.73	0/578
29	2	0.45	0/401	0.70	0/529
30	3	0.56	0/771	0.67	0/1024
31	9	0.33	0/2904	0.69	1/4526 (0.0%)
All	All	0.44	1/98714 (0.0%)	0.70	16/147588 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	0	31
24	W	0	1
31	9	0	1
All	All	0	33

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	192	VAL	CB-CG1	-5.05	1.42	1.52

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	0	871	G	C5'-C4'-O4'	-7.01	100.69	109.10
1	0	2726	U	N1-C1'-C2'	5.93	121.71	114.00
1	0	1942	A	C5'-C4'-C3'	5.70	125.13	116.00
1	0	1504	A	C1'-O4'-C4'	-5.67	105.36	109.90
31	9	39	U	N1-C1'-C2'	5.64	121.34	114.00

There are no chirality outliers.

5 of 33 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	221	G	Sidechain
1	0	333	G	Sidechain
1	0	396	U	Sidechain
1	0	458	G	Sidechain
1	0	471	G	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	59021	0	29812	1012	0
2	A	1754	0	1766	26	0
3	B	2625	0	2533	33	0
4	C	1860	0	1813	23	0
5	D	1094	0	1085	14	0
6	E	1358	0	1266	10	0
7	F	890	0	843	2	0
8	G	240	0	231	1	0
9	H	1282	0	1292	14	0
10	I	520	0	500	2	0
11	J	1120	0	1098	16	0
12	K	994	0	1027	12	0
13	L	1118	0	1076	9	0
14	M	1559	0	1573	15	0
15	N	1445	0	1401	14	0
16	O	865	0	873	8	0
17	P	1137	0	1123	12	0
18	Q	735	0	729	7	0
19	R	1150	0	1122	11	0
20	S	642	0	605	6	0
21	T	950	0	924	9	0
22	U	411	0	364	3	0
23	V	500	0	511	6	0
24	W	1196	0	1137	20	0
25	X	655	0	653	7	0
26	Y	1131	0	1133	12	0
27	Z	574	0	534	6	0
28	1	431	0	426	10	0
29	2	396	0	413	8	0
30	3	755	0	729	5	0
31	9	2599	0	1325	77	0
32	0	85	0	0	0	0
32	2	1	0	0	0	0
32	9	2	0	0	0	0
32	A	1	0	0	0	0
32	B	1	0	0	0	0
32	K	1	0	0	0	0
32	T	1	0	0	0	0
32	Y	1	0	0	0	0
33	0	2	0	0	0	0
34	0	66	0	0	0	0
34	9	2	0	0	0	0
34	C	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	H	1	0	0	0	0
34	J	1	0	0	0	0
34	M	1	0	0	0	0
34	Q	1	0	0	0	0
34	R	1	0	0	0	0
34	S	1	0	0	0	0
35	0	9	0	0	0	0
35	3	1	0	0	0	0
35	A	1	0	0	0	0
35	B	1	0	0	0	0
35	J	3	0	0	1	0
35	K	1	0	0	1	0
35	L	1	0	0	0	0
35	M	1	0	0	0	0
35	N	1	0	0	0	0
35	O	1	0	0	0	0
35	R	1	0	0	0	0
35	Y	1	0	0	0	0
36	0	95	0	0	0	0
36	1	1	0	0	0	0
36	3	2	0	0	0	0
36	9	3	0	0	0	0
36	A	2	0	0	0	0
36	B	2	0	0	0	0
36	F	1	0	0	0	0
36	R	1	0	0	0	0
36	S	1	0	0	0	0
37	0	39	0	36	13	0
38	1	1	0	0	0	0
38	3	1	0	0	0	0
38	O	1	0	0	0	0
38	U	1	0	0	0	0
38	Z	1	0	0	0	0
39	0	5993	0	0	125	0
39	1	52	0	0	0	0
39	2	39	0	0	0	0
39	3	66	0	0	0	0
39	9	149	0	0	7	0
39	A	107	0	0	3	0
39	B	146	0	0	1	0
39	C	171	0	0	5	0
39	D	45	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	E	40	0	0	0	0
39	F	25	0	0	0	0
39	G	18	0	0	0	0
39	H	62	0	0	2	0
39	I	5	0	0	1	0
39	J	52	0	0	1	0
39	K	53	0	0	0	0
39	L	79	0	0	3	0
39	M	128	0	0	0	0
39	N	62	0	0	0	0
39	O	40	0	0	2	0
39	P	65	0	0	0	0
39	Q	43	0	0	0	0
39	R	77	0	0	1	0
39	S	28	0	0	0	0
39	T	32	0	0	0	0
39	U	27	0	0	0	0
39	V	12	0	0	0	0
39	W	65	0	0	1	0
39	X	20	0	0	0	0
39	Y	94	0	0	3	0
39	Z	28	0	0	1	0
All	All	99174	0	59953	1243	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 8.

The worst 5 of 1243 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)
1:0:871:G:H5'	1:0:871:G:H8	1.10	1.15
1:0:1160:G:H5'	1:0:1161:A:H5'	1.26	1.12
1:0:871:G:H5'	1:0:871:G:C8	1.88	1.08
31:9:76:G:H3'	31:9:77:A:H5"	1.36	1.05
31:9:56:A:H2'	31:9:57:A:H5"	1.37	1.04

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	A	235/237 (99%)	218 (93%)	14 (6%)	3 (1%)	12 33
3	B	335/337 (99%)	307 (92%)	26 (8%)	2 (1%)	25 53
4	C	244/246 (99%)	224 (92%)	18 (7%)	2 (1%)	19 46
5	D	134/177 (76%)	121 (90%)	10 (8%)	3 (2%)	6 21
6	E	170/172 (99%)	161 (95%)	9 (5%)	0	100 100
7	F	117/119 (98%)	109 (93%)	7 (6%)	1 (1%)	17 43
8	G	25/348 (7%)	25 (100%)	0	0	100 100
9	H	156/177 (88%)	150 (96%)	5 (3%)	1 (1%)	25 53
10	I	68/70 (97%)	58 (85%)	10 (15%)	0	100 100
11	J	140/142 (99%)	134 (96%)	6 (4%)	0	100 100
12	K	130/132 (98%)	125 (96%)	4 (3%)	1 (1%)	19 46
13	L	141/165 (86%)	127 (90%)	14 (10%)	0	100 100
14	M	192/194 (99%)	187 (97%)	4 (2%)	1 (0%)	29 57
15	N	184/186 (99%)	173 (94%)	8 (4%)	3 (2%)	9 28
16	O	113/115 (98%)	111 (98%)	2 (2%)	0	100 100
17	P	141/143 (99%)	139 (99%)	2 (1%)	0	100 100
18	Q	93/95 (98%)	88 (95%)	4 (4%)	1 (1%)	14 38
19	R	148/150 (99%)	142 (96%)	6 (4%)	0	100 100
20	S	79/81 (98%)	75 (95%)	4 (5%)	0	100 100
21	T	117/119 (98%)	111 (95%)	5 (4%)	1 (1%)	17 43
22	U	51/53 (96%)	47 (92%)	4 (8%)	0	100 100
23	V	63/65 (97%)	61 (97%)	2 (3%)	0	100 100
24	W	152/154 (99%)	148 (97%)	4 (3%)	0	100 100
25	X	80/82 (98%)	77 (96%)	2 (2%)	1 (1%)	12 33
26	Y	140/142 (99%)	139 (99%)	1 (1%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	Z	71/73 (97%)	65 (92%)	6 (8%)	0	100	100
28	1	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
29	2	42/50 (84%)	41 (98%)	1 (2%)	0	100	100
30	3	90/92 (98%)	88 (98%)	2 (2%)	0	100	100
All	All	3705/4172 (89%)	3503 (94%)	182 (5%)	20 (0%)	29	57

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	37	VAL
5	D	137	PRO
15	N	154	LEU
15	N	139	TRP
3	B	2	GLN

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	
2	A	179/179 (100%)	168 (94%)	11 (6%)	18	43
3	B	282/282 (100%)	268 (95%)	14 (5%)	24	53
4	C	193/193 (100%)	176 (91%)	17 (9%)	10	26
5	D	117/148 (79%)	108 (92%)	9 (8%)	13	32
6	E	152/152 (100%)	146 (96%)	6 (4%)	32	63
7	F	93/93 (100%)	90 (97%)	3 (3%)	39	69
8	G	27/282 (10%)	27 (100%)	0	100	100
9	H	134/145 (92%)	128 (96%)	6 (4%)	27	57
10	I	58/58 (100%)	57 (98%)	1 (2%)	60	83
11	J	118/118 (100%)	110 (93%)	8 (7%)	16	38
12	K	106/106 (100%)	100 (94%)	6 (6%)	20	47
13	L	113/127 (89%)	112 (99%)	1 (1%)	78	92

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
14	M	158/158 (100%)	152 (96%)	6 (4%)	33 64
15	N	149/149 (100%)	140 (94%)	9 (6%)	19 45
16	O	93/93 (100%)	90 (97%)	3 (3%)	39 69
17	P	113/113 (100%)	108 (96%)	5 (4%)	28 58
18	Q	79/79 (100%)	75 (95%)	4 (5%)	24 52
19	R	117/117 (100%)	112 (96%)	5 (4%)	29 59
20	S	71/71 (100%)	70 (99%)	1 (1%)	67 86
21	T	105/105 (100%)	96 (91%)	9 (9%)	10 27
22	U	44/44 (100%)	44 (100%)	0	100 100
23	V	51/51 (100%)	49 (96%)	2 (4%)	32 63
24	W	130/130 (100%)	123 (95%)	7 (5%)	22 49
25	X	66/66 (100%)	57 (86%)	9 (14%)	3 9
26	Y	120/120 (100%)	116 (97%)	4 (3%)	38 68
27	Z	60/60 (100%)	59 (98%)	1 (2%)	60 83
28	1	46/46 (100%)	45 (98%)	1 (2%)	52 79
29	2	42/46 (91%)	41 (98%)	1 (2%)	49 77
30	3	79/79 (100%)	77 (98%)	2 (2%)	47 76
All	All	3095/3410 (91%)	2944 (95%)	151 (5%)	25 54

5 of 151 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
21	T	5	ASP
26	Y	174	VAL
21	T	82	THR
24	W	125	HIS
30	3	22	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 66 such sidechains are listed below:

Mol	Chain	Res	Type
28	1	16	HIS
29	2	16	ASN
30	3	48	ASN
13	L	41	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	L	18	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2923 (93%)	238 (8%)	26 (0%)
31	9	121/122 (99%)	17 (14%)	1 (0%)
All	All	2866/3045 (94%)	255 (8%)	27 (0%)

5 of 255 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	31	C
1	0	67	A
1	0	69	A
1	0	70	A
1	0	71	G

5 of 27 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1377	C
1	0	1684	A
1	0	2761	A
1	0	1667	A
1	0	1979	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	1MA	0	628	1,34	16,25,26	1.41	3 (18%)	18,37,40	1.20	3 (16%)
1	PSU	0	2621	1	18,21,22	1.52	2 (11%)	22,30,33	1.30	3 (13%)
1	OMU	0	2587	1,34	19,22,23	0.33	0	26,31,34	0.36	0
1	UR3	0	2619	1	19,22,23	0.49	0	26,32,35	0.61	1 (3%)
1	OMG	0	2588	1	18,26,27	1.05	2 (11%)	19,38,41	0.75	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	1MA	0	628	1,34	-	0/3/25/26	0/3/3/3
1	PSU	0	2621	1	-	0/7/25/26	0/2/2/2
1	OMU	0	2587	1,34	-	0/9/27/28	0/2/2/2
1	UR3	0	2619	1	-	0/7/25/26	0/2/2/2
1	OMG	0	2588	1	-	1/5/27/28	0/3/3/3

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C2-N1	4.95	1.43	1.36
1	0	628	1MA	C2-N3	3.69	1.33	1.29
1	0	2588	OMG	C5-C6	-2.79	1.41	1.47
1	0	2621	PSU	C6-C5	2.79	1.38	1.35
1	0	628	1MA	C6-N6	2.61	1.34	1.27

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	0	2621	PSU	C6-C5-C4	3.30	120.51	118.20
1	0	628	1MA	N1-C2-N3	2.88	129.37	126.02
1	0	2621	PSU	C6-N1-C2	-2.86	119.76	122.68
1	0	2621	PSU	O2-C2-N1	2.80	125.87	122.79
1	0	628	1MA	C5-C6-N1	2.52	117.66	113.90

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	0	2588	OMG	C3'-C2'-O2'-CM2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	0	628	1MA	1	0
1	0	2587	OMU	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 306 ligands modelled in this entry, 305 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	$\#\|Z\| > 2$
37	WIN	0	9101	-	41,43,43	1.87	9 (21%)	50,71,71	3.82	29 (58%)

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
37	WIN	0	9101	-	-	6/20/110/110	0/6/5/5

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	0	9101	WIN	C2M-C2G	5.40	1.61	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	0	9101	WIN	C1N-C1V	5.32	1.41	1.33
37	0	9101	WIN	C2B-C1X	-4.08	1.40	1.46
37	0	9101	WIN	C1C-C1Y	3.64	1.56	1.50
37	0	9101	WIN	C1N-C1W	-2.95	1.39	1.46

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	0	9101	WIN	O1R-C2A-C2L	9.27	125.14	111.41
37	0	9101	WIN	C2F-O1T-C1W	-9.15	104.94	116.94
37	0	9101	WIN	C1O-C2M-C2G	6.67	123.74	112.79
37	0	9101	WIN	O1J-C2A-C2L	-6.55	111.90	123.67
37	0	9101	WIN	O1U-C1Z-O1I	6.15	127.45	118.47

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
37	0	9101	WIN	C1B-C1V-C2C-C1E
37	0	9101	WIN	O1J-C2A-C2L-O1S
37	0	9101	WIN	O1R-C2A-C2L-O1S
37	0	9101	WIN	C1V-C1N-C1W-O1T
37	0	9101	WIN	O1R-C2A-C2L-C2K

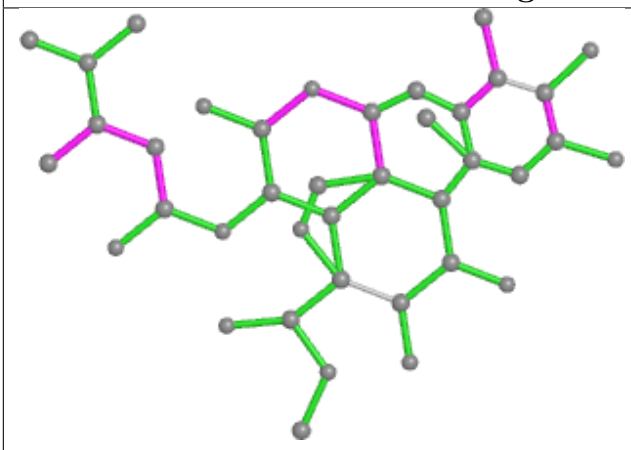
There are no ring outliers.

1 monomer is involved in 13 short contacts:

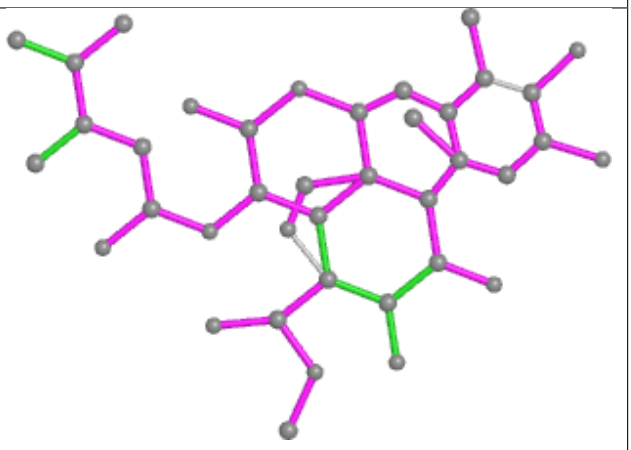
Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	0	9101	WIN	13	0

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

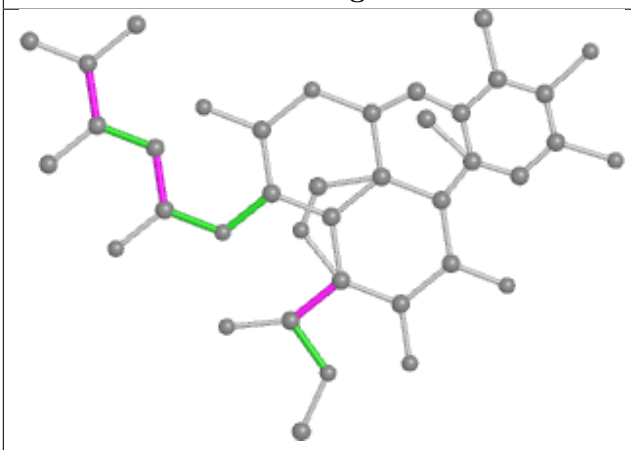
Ligand WIN 0 9101



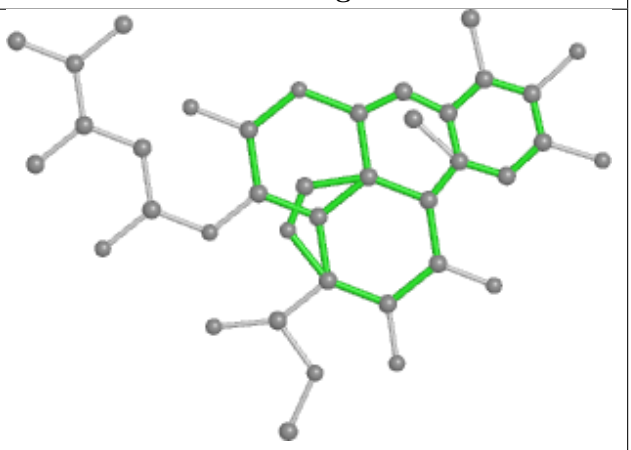
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	0	2749/2923 (94%)	-0.68	10 (0%) 92 92	24, 56, 105, 182	0
2	A	237/237 (100%)	0.07	15 (6%) 20 15	35, 71, 114, 133	0
3	B	337/337 (100%)	-0.43	0 100 100	34, 65, 95, 108	0
4	C	246/246 (100%)	-0.42	0 100 100	31, 56, 80, 91	0
5	D	140/177 (79%)	1.44	46 (32%) 0 0	80, 120, 142, 152	0
6	E	172/172 (100%)	-0.15	2 (1%) 79 78	55, 81, 105, 112	0
7	F	119/119 (100%)	0.64	11 (9%) 9 6	64, 90, 122, 137	0
8	G	29/348 (8%)	0.83	2 (6%) 16 12	89, 109, 116, 119	0
9	H	160/177 (90%)	0.64	20 (12%) 3 2	57, 84, 120, 128	0
10	I	70/70 (100%)	3.82	54 (77%) 0 0	142, 164, 183, 184	0
11	J	142/142 (100%)	-0.43	1 (0%) 87 87	47, 60, 82, 104	0
12	K	132/132 (100%)	-0.42	2 (1%) 73 72	44, 61, 86, 90	0
13	L	145/165 (87%)	0.43	15 (10%) 6 4	35, 87, 131, 142	0
14	M	194/194 (100%)	-0.43	0 100 100	38, 55, 75, 82	0
15	N	186/186 (100%)	0.38	20 (10%) 5 4	55, 83, 139, 146	0
16	O	115/115 (100%)	-0.41	0 100 100	43, 66, 84, 88	0
17	P	143/143 (100%)	-0.26	1 (0%) 87 87	50, 70, 86, 94	0
18	Q	95/95 (100%)	-0.50	0 100 100	49, 60, 76, 89	0
19	R	150/150 (100%)	-0.57	0 100 100	38, 56, 78, 84	0
20	S	81/81 (100%)	0.01	2 (2%) 57 54	56, 76, 100, 108	0
21	T	119/119 (100%)	-0.06	3 (2%) 57 54	48, 71, 100, 127	0
22	U	53/53 (100%)	-0.28	0 100 100	56, 72, 95, 102	0
23	V	65/65 (100%)	1.51	16 (24%) 0 0	66, 94, 137, 144	0
24	W	154/154 (100%)	-0.45	1 (0%) 89 89	44, 60, 79, 90	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
25	X	82/82 (100%)	-0.08	5 (6%) 21 17	55, 71, 97, 111	0
26	Y	142/142 (100%)	-0.58	1 (0%) 87 87	31, 53, 80, 102	0
27	Z	73/73 (100%)	4.55	52 (71%) 0 0	99, 132, 149, 150	0
28	1	56/56 (100%)	-0.48	0 100 100	33, 41, 52, 62	0
29	2	46/50 (92%)	0.04	3 (6%) 18 14	48, 79, 112, 122	0
30	3	92/92 (100%)	0.28	3 (3%) 46 41	58, 85, 99, 109	0
31	9	122/122 (100%)	-0.82	2 (1%) 72 70	46, 78, 108, 156	0
All	All	6646/7217 (92%)	-0.24	287 (4%) 35 30	24, 64, 122, 184	0

The worst 5 of 287 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
27	Z	46	SER	18.3
27	Z	58	ASN	18.3
27	Z	35	SER	17.0
27	Z	50	VAL	14.0
23	V	1	THR	13.9

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	1MA	0	628	23/24	0.98	0.15	34,36,38,39	0
1	UR3	0	2619	21/22	0.98	0.13	45,48,51,54	0
1	PSU	0	2621	20/21	0.98	0.12	30,35,50,51	0
1	OMU	0	2587	21/22	0.99	0.10	43,44,46,48	0
1	OMG	0	2588	24/25	0.99	0.12	42,44,46,48	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	MG	0	8090	1/1	-0.02	0.56	121,121,121,121	0
36	SR	0	8977	1/1	0.10	0.06	197,197,197,197	0
36	SR	0	8944	1/1	0.34	0.16	178,178,178,178	0
34	NA	0	8525	1/1	0.36	0.27	93,93,93,93	0
34	NA	0	8554	1/1	0.43	0.42	70,70,70,70	0
36	SR	9	9003	1/1	0.45	0.06	187,187,187,187	0
36	SR	0	8966	1/1	0.49	0.14	120,120,120,120	0
34	NA	9	8572	1/1	0.49	0.49	117,117,117,117	0
34	NA	0	8556	1/1	0.49	1.51	68,68,68,68	0
34	NA	0	8506	1/1	0.52	0.21	76,76,76,76	0
36	SR	0	8998	1/1	0.54	0.25	175,175,175,175	0
36	SR	0	8913	1/1	0.55	0.82	200,200,200,200	0
34	NA	C	8503	1/1	0.55	0.25	46,46,46,46	0
34	NA	0	8524	1/1	0.55	0.61	73,73,73,73	0
36	SR	0	9006	1/1	0.56	0.58	200,200,200,200	0
36	SR	0	8917	1/1	0.56	0.22	151,151,151,151	0
34	NA	0	8522	1/1	0.57	0.14	108,108,108,108	0
32	MG	0	8091	1/1	0.59	0.13	89,89,89,89	0
36	SR	0	8941	1/1	0.59	0.23	131,131,131,131	0
36	SR	0	8982	1/1	0.62	0.95	200,200,200,200	0
36	SR	0	8938	1/1	0.62	0.06	191,191,191,191	0
36	SR	0	8933	1/1	0.63	0.09	143,143,143,143	0
36	SR	0	8996	1/1	0.64	0.44	200,200,200,200	0
36	SR	0	8983	1/1	0.64	0.12	199,199,199,199	0
32	MG	0	8089	1/1	0.65	0.16	64,64,64,64	0
36	SR	0	8959	1/1	0.65	0.26	181,181,181,181	0
36	SR	0	8949	1/1	0.66	0.20	146,146,146,146	0
36	SR	0	8915	1/1	0.66	0.10	136,136,136,136	0
34	NA	0	8560	1/1	0.67	0.53	97,97,97,97	0
36	SR	0	8972	1/1	0.68	0.14	164,164,164,164	0
36	SR	0	8976	1/1	0.68	0.22	200,200,200,200	0
34	NA	0	8504	1/1	0.68	0.34	46,46,46,46	0
34	NA	0	8502	1/1	0.69	0.20	66,66,66,66	0
32	MG	0	8072	1/1	0.69	0.31	82,82,82,82	0
32	MG	9	8040	1/1	0.69	0.36	97,97,97,97	0
34	NA	0	8527	1/1	0.69	0.56	86,86,86,86	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
36	SR	0	8928	1/1	0.70	0.08	151,151,151,151	0
36	SR	0	8910	1/1	0.71	0.11	106,106,106,106	0
36	SR	0	9001	1/1	0.71	0.16	184,184,184,184	0
36	SR	0	8991	1/1	0.71	0.25	195,195,195,195	0
32	MG	0	8050	1/1	0.71	0.19	74,74,74,74	0
32	MG	0	8075	1/1	0.72	0.11	58,58,58,58	0
34	NA	0	8563	1/1	0.72	0.24	82,82,82,82	0
34	NA	0	8559	1/1	0.72	0.24	95,95,95,95	0
36	SR	0	8955	1/1	0.73	0.10	198,198,198,198	0
36	SR	0	8965	1/1	0.73	0.11	151,151,151,151	0
35	CL	3	8804	1/1	0.74	0.07	76,76,76,76	0
34	NA	0	8531	1/1	0.75	0.23	50,50,50,50	0
36	SR	0	8984	1/1	0.75	0.07	143,143,143,143	0
36	SR	0	8942	1/1	0.75	0.18	144,144,144,144	0
36	SR	B	8950	1/1	0.75	0.12	119,119,119,119	0
34	NA	0	8566	1/1	0.75	0.59	59,59,59,59	0
36	SR	0	9000	1/1	0.76	0.21	200,200,200,200	0
34	NA	0	8548	1/1	0.76	0.28	67,67,67,67	0
36	SR	0	8951	1/1	0.76	0.05	149,149,149,149	0
36	SR	0	9008	1/1	0.76	0.24	111,111,111,111	0
34	NA	H	8518	1/1	0.76	0.50	95,95,95,95	0
36	SR	0	8958	1/1	0.76	0.12	121,121,121,121	0
34	NA	0	8549	1/1	0.77	0.91	60,60,60,60	0
32	MG	0	8038	1/1	0.77	0.09	70,70,70,70	0
34	NA	0	8529	1/1	0.77	0.06	50,50,50,50	0
36	SR	B	8987	1/1	0.77	0.53	200,200,200,200	0
36	SR	0	8924	1/1	0.77	0.21	149,149,149,149	0
36	SR	0	8995	1/1	0.78	0.14	142,142,142,142	0
36	SR	0	8956	1/1	0.78	0.10	187,187,187,187	0
33	K	0	8401	1/1	0.78	0.88	123,123,123,123	0
34	NA	0	8523	1/1	0.78	0.16	65,65,65,65	0
36	SR	9	8978	1/1	0.78	0.12	169,169,169,169	0
36	SR	9	8980	1/1	0.78	0.05	175,175,175,175	0
32	MG	0	8030	1/1	0.78	0.33	79,79,79,79	0
36	SR	0	8994	1/1	0.80	0.40	199,199,199,199	0
36	SR	0	8964	1/1	0.80	0.10	139,139,139,139	0
34	NA	0	8555	1/1	0.80	0.58	53,53,53,53	0
36	SR	0	8997	1/1	0.80	1.19	200,200,200,200	0
34	NA	0	8542	1/1	0.80	0.70	62,62,62,62	0
34	NA	0	8557	1/1	0.80	0.04	74,74,74,74	0
32	MG	0	8006	1/1	0.80	0.17	33,33,33,33	0
36	SR	0	8908	1/1	0.81	0.29	175,175,175,175	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
36	SR	0	8922	1/1	0.81	0.27	156,156,156,156	0
34	NA	0	8565	1/1	0.81	1.90	100,100,100,100	0
32	MG	0	8062	1/1	0.82	0.28	61,61,61,61	0
32	MG	0	8092	1/1	0.82	0.10	80,80,80,80	0
36	SR	A	8930	1/1	0.82	0.26	169,169,169,169	0
34	NA	0	8536	1/1	0.82	0.07	65,65,65,65	0
32	MG	K	8054	1/1	0.82	0.21	47,47,47,47	0
32	MG	0	8069	1/1	0.82	0.19	49,49,49,49	0
34	NA	0	8515	1/1	0.82	0.15	50,50,50,50	0
34	NA	0	8550	1/1	0.82	0.49	59,59,59,59	0
36	SR	0	8968	1/1	0.83	0.06	165,165,165,165	0
36	SR	0	8920	1/1	0.83	0.59	185,185,185,185	0
36	SR	S	8961	1/1	0.83	0.12	145,145,145,145	0
37	WIN	0	9101	39/39	0.83	0.33	125,127,128,129	0
34	NA	0	8501	1/1	0.84	0.18	54,54,54,54	0
36	SR	0	9002	1/1	0.84	0.15	183,183,183,183	0
36	SR	0	8969	1/1	0.84	0.14	173,173,173,173	0
36	SR	0	8943	1/1	0.84	0.10	95,95,95,95	0
32	MG	0	8052	1/1	0.84	0.06	58,58,58,58	0
32	MG	0	8037	1/1	0.84	0.16	80,80,80,80	0
32	MG	0	8027	1/1	0.85	0.17	47,47,47,47	0
36	SR	0	8986	1/1	0.85	0.48	200,200,200,200	0
36	SR	0	8901	1/1	0.85	0.14	96,96,96,96	0
36	SR	0	8934	1/1	0.85	0.32	166,166,166,166	0
34	NA	0	8535	1/1	0.85	0.38	63,63,63,63	0
34	NA	J	8538	1/1	0.85	0.21	67,67,67,67	0
34	NA	0	8571	1/1	0.85	0.31	98,98,98,98	0
34	NA	0	8561	1/1	0.86	0.65	90,90,90,90	0
36	SR	0	8937	1/1	0.86	0.33	125,125,125,125	0
32	MG	0	8039	1/1	0.86	0.22	63,63,63,63	0
36	SR	0	8909	1/1	0.86	0.17	99,99,99,99	0
34	NA	Q	8540	1/1	0.87	0.13	58,58,58,58	0
34	NA	R	8532	1/1	0.87	0.11	59,59,59,59	0
32	MG	0	8066	1/1	0.87	0.34	88,88,88,88	0
34	NA	0	8558	1/1	0.87	0.50	63,63,63,63	0
36	SR	0	8989	1/1	0.87	0.17	185,185,185,185	0
34	NA	0	8568	1/1	0.87	0.22	57,57,57,57	0
34	NA	0	8553	1/1	0.87	0.42	69,69,69,69	0
32	MG	0	8063	1/1	0.87	0.22	80,80,80,80	0
36	SR	0	8954	1/1	0.87	0.11	109,109,109,109	0
34	NA	0	8511	1/1	0.87	0.22	67,67,67,67	0
32	MG	0	8080	1/1	0.87	0.29	87,87,87,87	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
36	SR	0	8981	1/1	0.87	0.21	158,158,158,158	0
36	SR	0	8962	1/1	0.88	0.17	180,180,180,180	0
34	NA	0	8567	1/1	0.88	0.51	87,87,87,87	0
35	CL	0	8815	1/1	0.88	0.14	83,83,83,83	0
36	SR	0	8988	1/1	0.88	0.12	158,158,158,158	0
32	MG	0	8085	1/1	0.88	0.11	69,69,69,69	0
32	MG	A	8051	1/1	0.88	0.29	98,98,98,98	0
32	MG	0	8053	1/1	0.88	0.06	69,69,69,69	0
34	NA	0	8505	1/1	0.88	1.08	44,44,44,44	0
34	NA	0	8537	1/1	0.88	0.21	50,50,50,50	0
32	MG	0	8018	1/1	0.88	0.28	54,54,54,54	0
32	MG	0	8084	1/1	0.88	0.14	36,36,36,36	0
36	SR	0	8916	1/1	0.88	0.10	129,129,129,129	0
36	SR	0	8902	1/1	0.89	0.17	70,70,70,70	0
32	MG	0	8002	1/1	0.89	0.18	26,26,26,26	0
34	NA	0	8562	1/1	0.89	0.62	82,82,82,82	0
36	SR	A	8929	1/1	0.89	0.10	142,142,142,142	0
36	SR	0	8971	1/1	0.89	0.06	185,185,185,185	0
32	MG	0	8047	1/1	0.89	0.39	71,71,71,71	0
34	NA	0	8544	1/1	0.89	0.19	73,73,73,73	0
34	NA	0	8509	1/1	0.89	0.28	77,77,77,77	0
34	NA	0	8533	1/1	0.89	0.15	72,72,72,72	0
33	K	0	8402	1/1	0.89	0.45	90,90,90,90	0
34	NA	0	8514	1/1	0.89	0.71	54,54,54,54	0
34	NA	0	8573	1/1	0.89	0.12	87,87,87,87	0
32	MG	0	8082	1/1	0.90	0.31	81,81,81,81	0
34	NA	0	8507	1/1	0.90	0.17	46,46,46,46	0
34	NA	0	8520	1/1	0.90	0.10	55,55,55,55	0
36	SR	0	8990	1/1	0.90	0.11	116,116,116,116	0
36	SR	0	8975	1/1	0.90	0.07	154,154,154,154	0
34	NA	0	8530	1/1	0.90	0.30	60,60,60,60	0
36	SR	0	8914	1/1	0.91	0.30	127,127,127,127	0
34	NA	0	8508	1/1	0.91	0.20	63,63,63,63	0
32	MG	0	8020	1/1	0.91	0.16	57,57,57,57	0
32	MG	0	8059	1/1	0.91	0.12	52,52,52,52	0
34	NA	0	8512	1/1	0.91	0.30	48,48,48,48	0
32	MG	T	8057	1/1	0.91	0.04	72,72,72,72	0
36	SR	0	8923	1/1	0.91	0.15	112,112,112,112	0
32	MG	0	8013	1/1	0.92	0.06	30,30,30,30	0
32	MG	0	8043	1/1	0.92	0.16	58,58,58,58	0
34	NA	0	8541	1/1	0.92	0.34	70,70,70,70	0
32	MG	0	8068	1/1	0.92	0.10	67,67,67,67	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
36	SR	1	8952	1/1	0.92	0.16	93,93,93,93	0
32	MG	2	8060	1/1	0.92	0.10	65,65,65,65	0
32	MG	0	8079	1/1	0.92	0.29	67,67,67,67	0
36	SR	0	8957	1/1	0.92	0.20	200,200,200,200	0
36	SR	0	8931	1/1	0.92	0.09	136,136,136,136	0
38	CD	Z	8703	1/1	0.92	0.06	172,172,172,172	0
32	MG	0	8078	1/1	0.93	0.29	54,54,54,54	0
36	SR	0	8939	1/1	0.93	0.07	145,145,145,145	0
35	CL	J	8801	1/1	0.93	0.09	82,82,82,82	0
36	SR	0	8919	1/1	0.93	0.08	179,179,179,179	0
34	NA	0	8516	1/1	0.93	0.15	37,37,37,37	0
32	MG	0	8034	1/1	0.93	0.14	47,47,47,47	0
36	SR	0	8948	1/1	0.93	0.16	122,122,122,122	0
36	SR	F	9005	1/1	0.93	0.04	149,149,149,149	0
34	NA	0	8574	1/1	0.93	0.41	69,69,69,69	0
32	MG	0	8049	1/1	0.93	0.53	116,116,116,116	0
32	MG	0	8036	1/1	0.93	0.13	60,60,60,60	0
32	MG	0	8071	1/1	0.93	0.12	71,71,71,71	0
32	MG	0	8031	1/1	0.93	0.36	73,73,73,73	0
32	MG	0	8064	1/1	0.93	0.18	51,51,51,51	0
34	NA	0	8528	1/1	0.93	0.17	60,60,60,60	0
32	MG	0	8019	1/1	0.94	0.23	30,30,30,30	0
34	NA	0	8521	1/1	0.94	0.26	71,71,71,71	0
35	CL	A	8809	1/1	0.94	0.31	96,96,96,96	0
32	MG	0	8001	1/1	0.94	0.15	26,26,26,26	0
35	CL	L	8810	1/1	0.94	0.09	69,69,69,69	0
36	SR	0	8970	1/1	0.94	0.06	135,135,135,135	0
32	MG	0	8081	1/1	0.94	0.17	81,81,81,81	0
36	SR	0	8992	1/1	0.94	0.11	137,137,137,137	0
32	MG	0	8024	1/1	0.94	0.20	54,54,54,54	0
34	NA	0	8546	1/1	0.94	0.73	85,85,85,85	0
36	SR	0	8921	1/1	0.94	0.11	99,99,99,99	0
32	MG	0	8044	1/1	0.94	0.05	55,55,55,55	0
36	SR	0	8979	1/1	0.94	0.10	195,195,195,195	0
36	SR	0	8960	1/1	0.94	0.11	151,151,151,151	0
34	NA	0	8526	1/1	0.94	0.12	45,45,45,45	0
32	MG	0	8032	1/1	0.95	0.06	42,42,42,42	0
36	SR	0	9004	1/1	0.95	0.47	200,200,200,200	0
36	SR	0	8985	1/1	0.95	0.05	148,148,148,148	0
32	MG	0	8045	1/1	0.95	0.08	30,30,30,30	0
32	MG	0	8041	1/1	0.95	0.23	32,32,32,32	0
35	CL	0	8803	1/1	0.95	0.07	62,62,62,62	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
34	NA	0	8545	1/1	0.95	0.14	48,48,48,48	0
32	MG	9	8074	1/1	0.95	0.14	101,101,101,101	0
36	SR	0	8974	1/1	0.95	0.23	179,179,179,179	0
34	NA	0	8547	1/1	0.95	0.87	71,71,71,71	0
34	NA	0	8534	1/1	0.95	0.26	47,47,47,47	0
34	NA	0	8575	1/1	0.95	0.27	87,87,87,87	0
32	MG	0	8073	1/1	0.95	0.08	80,80,80,80	0
32	MG	0	8056	1/1	0.95	0.15	62,62,62,62	0
32	MG	0	8033	1/1	0.95	0.20	63,63,63,63	0
36	SR	0	8945	1/1	0.95	0.07	131,131,131,131	0
36	SR	0	8993	1/1	0.96	0.05	178,178,178,178	0
36	SR	0	8940	1/1	0.96	0.10	94,94,94,94	0
36	SR	0	8967	1/1	0.96	0.04	147,147,147,147	0
32	MG	0	8005	1/1	0.96	0.23	35,35,35,35	0
32	MG	0	8029	1/1	0.96	0.18	69,69,69,69	0
34	NA	0	8519	1/1	0.96	0.33	50,50,50,50	0
34	NA	9	8543	1/1	0.96	0.17	57,57,57,57	0
32	MG	0	8046	1/1	0.96	0.18	53,53,53,53	0
36	SR	0	8946	1/1	0.96	0.17	129,129,129,129	0
36	SR	0	8947	1/1	0.96	0.25	200,200,200,200	0
32	MG	0	8023	1/1	0.96	0.20	30,30,30,30	0
36	SR	0	9007	1/1	0.96	0.67	199,199,199,199	0
35	CL	0	8811	1/1	0.96	0.11	72,72,72,72	0
34	NA	0	8551	1/1	0.96	0.20	60,60,60,60	0
34	NA	0	8552	1/1	0.96	0.27	80,80,80,80	0
32	MG	0	8061	1/1	0.96	0.22	36,36,36,36	0
35	CL	J	8821	1/1	0.96	0.09	78,78,78,78	0
34	NA	0	8570	1/1	0.96	0.08	59,59,59,59	0
32	MG	0	8048	1/1	0.96	0.23	28,28,28,28	0
32	MG	0	8087	1/1	0.96	0.13	36,36,36,36	0
36	SR	3	8932	1/1	0.96	0.10	94,94,94,94	0
32	MG	0	8035	1/1	0.96	0.19	70,70,70,70	0
32	MG	0	8076	1/1	0.96	0.10	38,38,38,38	0
36	SR	0	8963	1/1	0.96	0.09	133,133,133,133	0
34	NA	0	8513	1/1	0.96	0.34	56,56,56,56	0
32	MG	0	8016	1/1	0.96	0.16	30,30,30,30	0
32	MG	Y	8086	1/1	0.97	0.10	55,55,55,55	0
35	CL	0	8814	1/1	0.97	0.09	66,66,66,66	0
32	MG	0	8007	1/1	0.97	0.19	40,40,40,40	0
35	CL	0	8822	1/1	0.97	0.35	86,86,86,86	0
32	MG	0	8065	1/1	0.97	0.07	41,41,41,41	0
34	NA	M	8539	1/1	0.97	0.29	53,53,53,53	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	MG	0	8093	1/1	0.97	0.07	45,45,45,45	0
32	MG	0	8014	1/1	0.97	0.20	33,33,33,33	0
35	CL	N	8807	1/1	0.97	0.18	72,72,72,72	0
35	CL	O	8808	1/1	0.97	0.20	79,79,79,79	0
34	NA	S	8510	1/1	0.97	0.15	50,50,50,50	0
32	MG	0	8025	1/1	0.97	0.10	37,37,37,37	0
36	SR	0	8926	1/1	0.97	0.12	142,142,142,142	0
36	SR	0	8927	1/1	0.97	0.11	167,167,167,167	0
36	SR	0	8973	1/1	0.97	0.11	141,141,141,141	0
34	NA	0	8517	1/1	0.97	0.11	36,36,36,36	0
36	SR	0	8904	1/1	0.97	0.21	64,64,64,64	0
32	MG	0	8058	1/1	0.97	0.07	23,23,23,23	0
35	CL	0	8805	1/1	0.97	0.10	76,76,76,76	0
32	MG	0	8017	1/1	0.98	0.08	34,34,34,34	0
35	CL	Y	8820	1/1	0.98	0.05	46,46,46,46	0
32	MG	B	8042	1/1	0.98	0.13	62,62,62,62	0
36	SR	0	8935	1/1	0.98	0.09	93,93,93,93	0
36	SR	0	8936	1/1	0.98	0.07	108,108,108,108	0
32	MG	0	8011	1/1	0.98	0.24	30,30,30,30	0
32	MG	0	8070	1/1	0.98	0.28	64,64,64,64	0
34	NA	0	8569	1/1	0.98	0.16	61,61,61,61	0
32	MG	0	8012	1/1	0.98	0.20	26,26,26,26	0
32	MG	0	8003	1/1	0.98	0.15	35,35,35,35	0
35	CL	0	8813	1/1	0.98	0.02	54,54,54,54	0
32	MG	0	8021	1/1	0.98	0.10	43,43,43,43	0
32	MG	0	8088	1/1	0.98	0.18	46,46,46,46	0
35	CL	0	8816	1/1	0.98	0.22	75,75,75,75	0
35	CL	0	8817	1/1	0.98	0.05	68,68,68,68	0
32	MG	0	8008	1/1	0.98	0.16	32,32,32,32	0
32	MG	0	8015	1/1	0.98	0.14	33,33,33,33	0
35	CL	B	8819	1/1	0.98	0.10	57,57,57,57	0
32	MG	0	8077	1/1	0.98	0.06	43,43,43,43	0
36	SR	0	8953	1/1	0.98	0.19	164,164,164,164	0
35	CL	J	8802	1/1	0.98	0.07	79,79,79,79	0
32	MG	0	8010	1/1	0.98	0.11	34,34,34,34	0
36	SR	3	8999	1/1	0.98	0.10	140,140,140,140	0
35	CL	K	8812	1/1	0.98	0.11	57,57,57,57	0
36	SR	0	8925	1/1	0.98	0.11	95,95,95,95	0
32	MG	0	8067	1/1	0.98	0.26	34,34,34,34	0
35	CL	M	8818	1/1	0.98	0.04	49,49,49,49	0
38	CD	O	8705	1/1	0.98	0.06	105,105,105,105	0
34	NA	0	8564	1/1	0.98	0.65	95,95,95,95	0

Continued on next page...

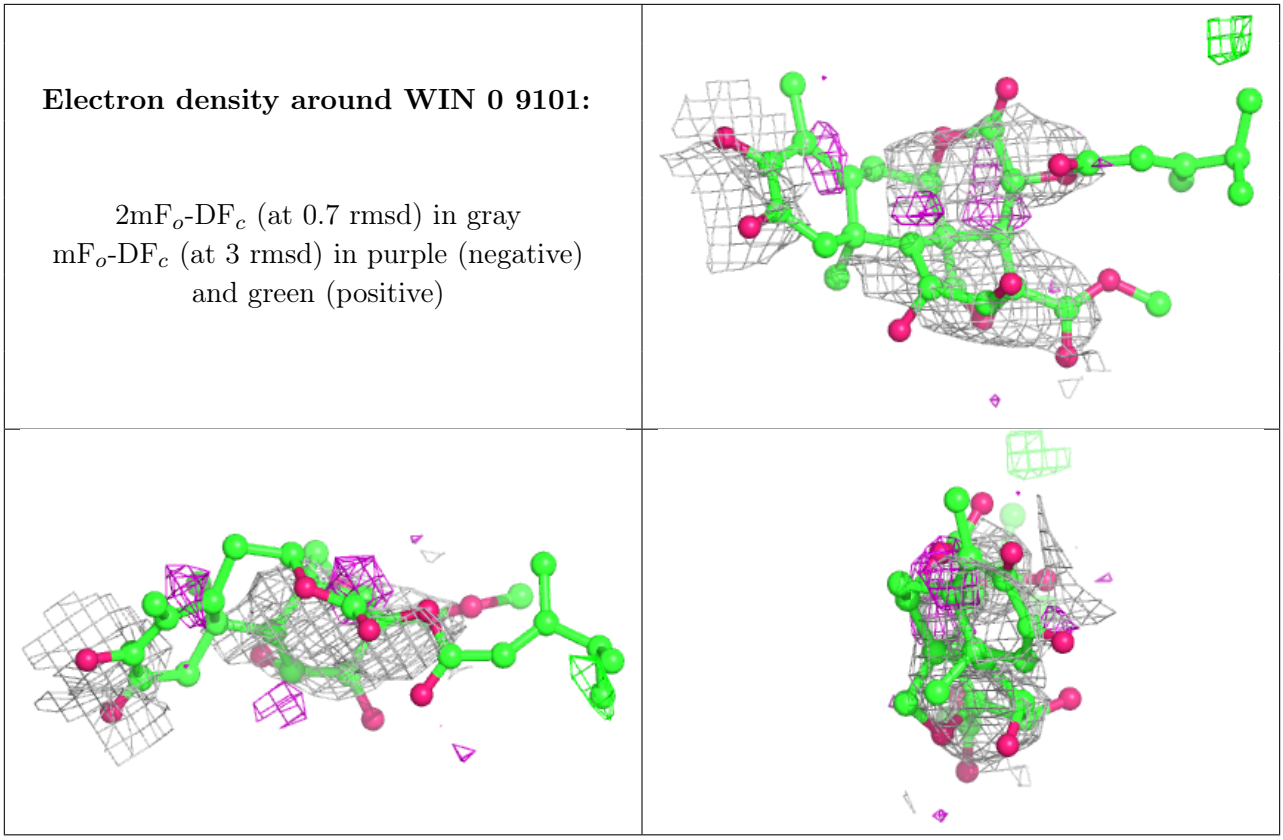
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	MG	0	8028	1/1	0.99	0.25	30,30,30,30	0
36	SR	R	8912	1/1	0.99	0.19	93,93,93,93	0
32	MG	0	8009	1/1	0.99	0.35	42,42,42,42	0
32	MG	0	8022	1/1	0.99	0.17	37,37,37,37	0
32	MG	0	8055	1/1	0.99	0.20	49,49,49,49	0
36	SR	0	8905	1/1	0.99	0.26	73,73,73,73	0
36	SR	0	8918	1/1	0.99	0.14	94,94,94,94	0
36	SR	0	8906	1/1	0.99	0.23	67,67,67,67	0
32	MG	0	8083	1/1	0.99	0.27	74,74,74,74	0
32	MG	0	8026	1/1	0.99	0.13	55,55,55,55	0
32	MG	0	8004	1/1	0.99	0.17	29,29,29,29	0
36	SR	0	8911	1/1	0.99	0.08	95,95,95,95	0
38	CD	1	8702	1/1	0.99	0.14	72,72,72,72	0
38	CD	3	8704	1/1	0.99	0.06	94,94,94,94	0
38	CD	U	8701	1/1	1.00	0.12	71,71,71,71	0
35	CL	R	8806	1/1	1.00	0.10	55,55,55,55	0
36	SR	0	8907	1/1	1.00	0.14	62,62,62,62	0
36	SR	0	8903	1/1	1.00	0.21	66,66,66,66	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 WIN 0 9101:

$2mF_o$-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.