



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:28 AM GMT

PDB ID : 3I55
Title : Co-crystal structure of Mycalamide A Bound to the Large Ribosomal Subunit
Authors : Gurel, G.; Blaha, G.; Steitz, T.A.; Moore, P.B.
Deposited on : 2009-07-03
Resolution : 3.11 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
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) : trunk26865

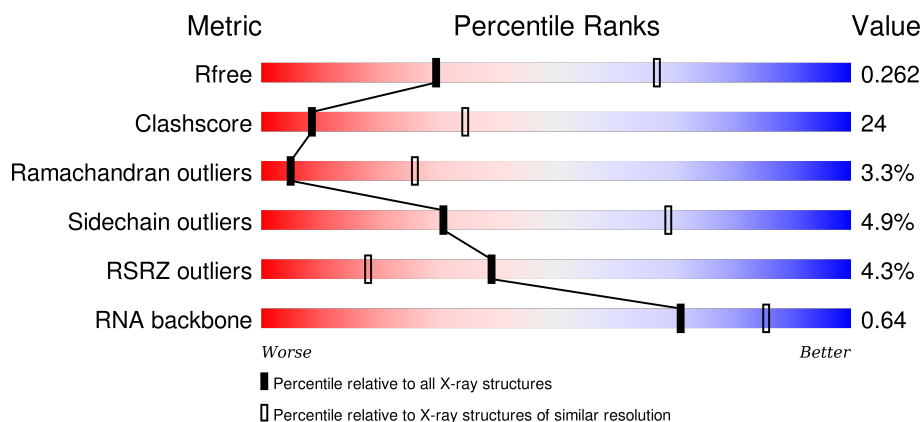
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.11 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.



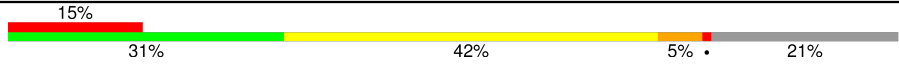

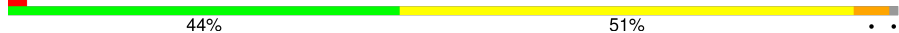




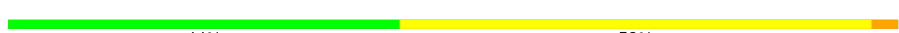







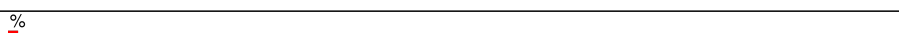
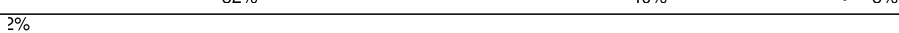





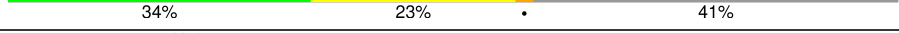


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1112 (3.16-3.08)
Clashscore	102246	1218 (3.16-3.08)
Ramachandran outliers	100387	1175 (3.16-3.08)
Sidechain outliers	100360	1175 (3.16-3.08)
RSRZ outliers	91569	1114 (3.16-3.08)
RNA backbone	2183	1010 (3.54-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 $\leq 5\%$. 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	
2	A	240	
3	B	338	
4	C	246	

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Mol	Chain	Length	Quality of chain
5	D	177	
6	E	178	
7	F	120	
8	G	348	
9	H	174	
10	I	162	
11	J	145	
12	K	132	
13	L	165	
14	M	194	
15	N	187	
16	O	116	
17	P	149	
18	Q	96	
19	R	155	
20	S	85	
21	T	120	
22	U	66	
23	V	71	
24	W	154	
25	X	92	
26	Y	241	
27	Z	116	
28	1	57	
29	2	50	

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Mol	Chain	Length	Quality of chain
30	3	92	
31	9	122	
32	4	8	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	5AA	4	76	-	-	X	-
33	MG	0	8043	-	-	-	X
33	MG	0	8047	-	-	-	X
33	MG	0	8076	-	-	-	X
33	MG	0	8080	-	-	-	X
33	MG	Y	8086	-	-	-	X
34	K	0	8401	-	-	-	X
34	K	0	8402	-	-	-	X
35	NA	0	8512	-	-	-	X
35	NA	0	8513	-	-	-	X
35	NA	0	8517	-	-	-	X
35	NA	0	8519	-	-	-	X
35	NA	0	8521	-	-	-	X
35	NA	0	8522	-	-	-	X
35	NA	0	8527	-	-	-	X
35	NA	0	8528	-	-	-	X
35	NA	0	8530	-	-	-	X
35	NA	0	8542	-	-	-	X
35	NA	0	8545	-	-	-	X
35	NA	0	8547	-	-	-	X
35	NA	0	8553	-	-	-	X
35	NA	0	8555	-	-	-	X
35	NA	0	8556	-	-	-	X
35	NA	0	8557	-	-	-	X
35	NA	0	8559	-	-	-	X
35	NA	0	8562	-	-	-	X
35	NA	0	8563	-	-	-	X
35	NA	0	8564	-	-	-	X
35	NA	0	8565	-	-	-	X
35	NA	0	8568	-	-	-	X
35	NA	0	8569	-	-	-	X
35	NA	M	8539	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
35	NA	Q	8540	-	-	-	X
36	CL	0	8805	-	-	-	X
37	SR	0	8904	-	-	-	X
37	SR	0	8949	-	-	-	X
37	SR	0	8962	-	-	-	X
37	SR	0	8992	-	-	-	X
37	SR	B	8987	-	-	-	X
37	SR	L	8969	-	-	-	X
38	MYL	0	2924	-	-	X	-
39	CD	3	8704	-	-	-	X

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 99287 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
1	0	2754	Total	C	N	O	P	0	0	0
			59021	26349	10873	19054	2745			

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

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

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

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

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

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

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

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

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

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

- 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
			1283	798	240	239	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
			519	323	81	114	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
			1136	683	229	224				

- 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
			1149	713	209	223	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
			641	389	111	138	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			
			950	568	180	202	0	0	0

- 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			
			410	244	75	86	5	0	0	0

- 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			
			499	304	94	100	1	0	0	0

- 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			
			1196	737	209	244	6	0	0	0

- 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			
			654	402	129	122	1	0	0	0

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

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

- 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			
			573	343	113	112	5	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	1	MET	-	EXPRESSION TAG	UNP P60619
Z	2	SER	-	EXPRESSION TAG	UNP P60619
Z	3	PRO	-	EXPRESSION TAG	UNP P60619
Z	4	ARG	-	EXPRESSION TAG	UNP P60619
Z	5	ALA	-	EXPRESSION TAG	UNP P60619
Z	6	ARG	-	EXPRESSION TAG	UNP P60619
Z	7	ARG	-	EXPRESSION TAG	UNP P60619
Z	8	GLU	-	EXPRESSION TAG	UNP P60619
Z	9	PRO	-	EXPRESSION TAG	UNP P60619
Z	10	ASN	-	EXPRESSION TAG	UNP P60619
Z	11	LEU	-	EXPRESSION TAG	UNP P60619
Z	12	GLU	-	EXPRESSION TAG	UNP P60619
Z	13	GLY	-	EXPRESSION TAG	UNP P60619
Z	14	LEU	-	EXPRESSION TAG	UNP P60619
Z	15	MET	-	EXPRESSION TAG	UNP P60619
Z	16	TRP	-	EXPRESSION TAG	UNP P60619
Z	17	PRO	-	EXPRESSION TAG	UNP P60619
Z	18	LEU	-	EXPRESSION TAG	UNP P60619
Z	19	GLY	-	EXPRESSION TAG	UNP P60619
Z	20	GLY	-	EXPRESSION TAG	UNP P60619
Z	21	GLN	-	EXPRESSION TAG	UNP P60619
Z	22	GLN	-	EXPRESSION TAG	UNP P60619
Z	23	THR	-	EXPRESSION TAG	UNP P60619
Z	24	THR	-	EXPRESSION TAG	UNP P60619

- 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 DNA/RNA hybrid called DNA/RNA (5'-R(*CP*CP*(5AA)P*(2OP)P*(PO2)P*AP*CP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	4	8	Total	C	N	O	P	0	0	0
			127	61	23	38	5			

- Molecule 33 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	83	Total	Mg	0	0
			83	83		
33	9	2	Total	Mg	0	0
			2	2		
33	K	1	Total	Mg	0	0
			1	1		
33	B	1	Total	Mg	0	0
			1	1		
33	A	2	Total	Mg	0	0
			2	2		
33	T	1	Total	Mg	0	0
			1	1		
33	2	1	Total	Mg	0	0
			1	1		
33	Y	1	Total	Mg	0	0
			1	1		
33	3	1	Total	Mg	0	0
			1	1		

- Molecule 34 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	0	2	Total	K	0	0
			2	2		

- Molecule 35 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	0	63	Total Na 63 63	0	0
35	J	1	Total Na 1 1	0	0
35	Q	1	Total Na 1 1	0	0
35	H	1	Total Na 1 1	0	0
35	B	1	Total Na 1 1	0	0
35	C	1	Total Na 1 1	0	0
35	R	3	Total Na 3 3	0	0
35	9	2	Total Na 2 2	0	0
35	S	1	Total Na 1 1	0	0
35	M	1	Total Na 1 1	0	0

- Molecule 36 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	0	10	Total Cl 10 10	0	0
36	J	3	Total Cl 3 3	0	0
36	B	1	Total Cl 1 1	0	0
36	A	1	Total Cl 1 1	0	0
36	N	1	Total Cl 1 1	0	0
36	O	1	Total Cl 1 1	0	0
36	R	1	Total Cl 1 1	0	0
36	Y	1	Total Cl 1 1	0	0
36	L	1	Total Cl 1 1	0	0
36	3	1	Total Cl 1 1	0	0

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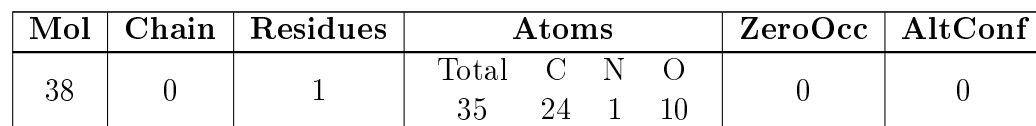
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	M	1	Total	Cl	0	0
			1	1		

- Molecule 37 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	0	93	Total	Sr	0	0
			93	93		
37	1	1	Total	Sr	0	0
			1	1		
37	H	1	Total	Sr	0	0
			1	1		
37	B	2	Total	Sr	0	0
			2	2		
37	3	2	Total	Sr	0	0
			2	2		
37	A	2	Total	Sr	0	0
			2	2		
37	R	1	Total	Sr	0	0
			1	1		
37	9	3	Total	Sr	0	0
			3	3		
37	L	1	Total	Sr	0	0
			1	1		
37	S	1	Total	Sr	0	0
			1	1		
37	F	1	Total	Sr	0	0
			1	1		

- Molecule 38 is MYCALAMIDE A (three-letter code: MYL) (formula: C₂₄H₄₁NO₁₀).



- | Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 39 | O | 1 | Total Cd
1 1 | 0 | 0 |
| 39 | Z | 1 | Total Cd
1 1 | 0 | 0 |
| 39 | 1 | 1 | Total Cd
1 1 | 0 | 0 |
| 39 | 3 | 1 | Total Cd
1 1 | 0 | 0 |
| 39 | U | 1 | Total Cd
1 1 | 0 | 0 |

- | Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|----------------------|---------|---------|
| 40 | 0 | 5841 | Total O
5841 5841 | 0 | 0 |
| 40 | A | 117 | Total O
117 117 | 0 | 0 |
| 40 | B | 151 | Total O
151 151 | 0 | 0 |



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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	C	175	Total 175	O 175	0	0
40	D	49	Total 49	O 49	0	0
40	E	40	Total 40	O 40	0	0
40	F	29	Total 29	O 29	0	0
40	G	18	Total 18	O 18	0	0
40	H	76	Total 76	O 76	0	0
40	I	10	Total 10	O 10	0	0
40	J	57	Total 57	O 57	0	0
40	K	62	Total 62	O 62	0	0
40	L	91	Total 91	O 91	0	0
40	M	148	Total 148	O 148	0	0
40	N	61	Total 61	O 61	0	0
40	O	41	Total 41	O 41	0	0
40	P	61	Total 61	O 61	0	0
40	Q	49	Total 49	O 49	0	0
40	R	83	Total 83	O 83	0	0
40	S	37	Total 37	O 37	0	0
40	T	36	Total 36	O 36	0	0
40	U	29	Total 29	O 29	0	0
40	V	13	Total 13	O 13	0	0
40	W	67	Total 67	O 67	0	0

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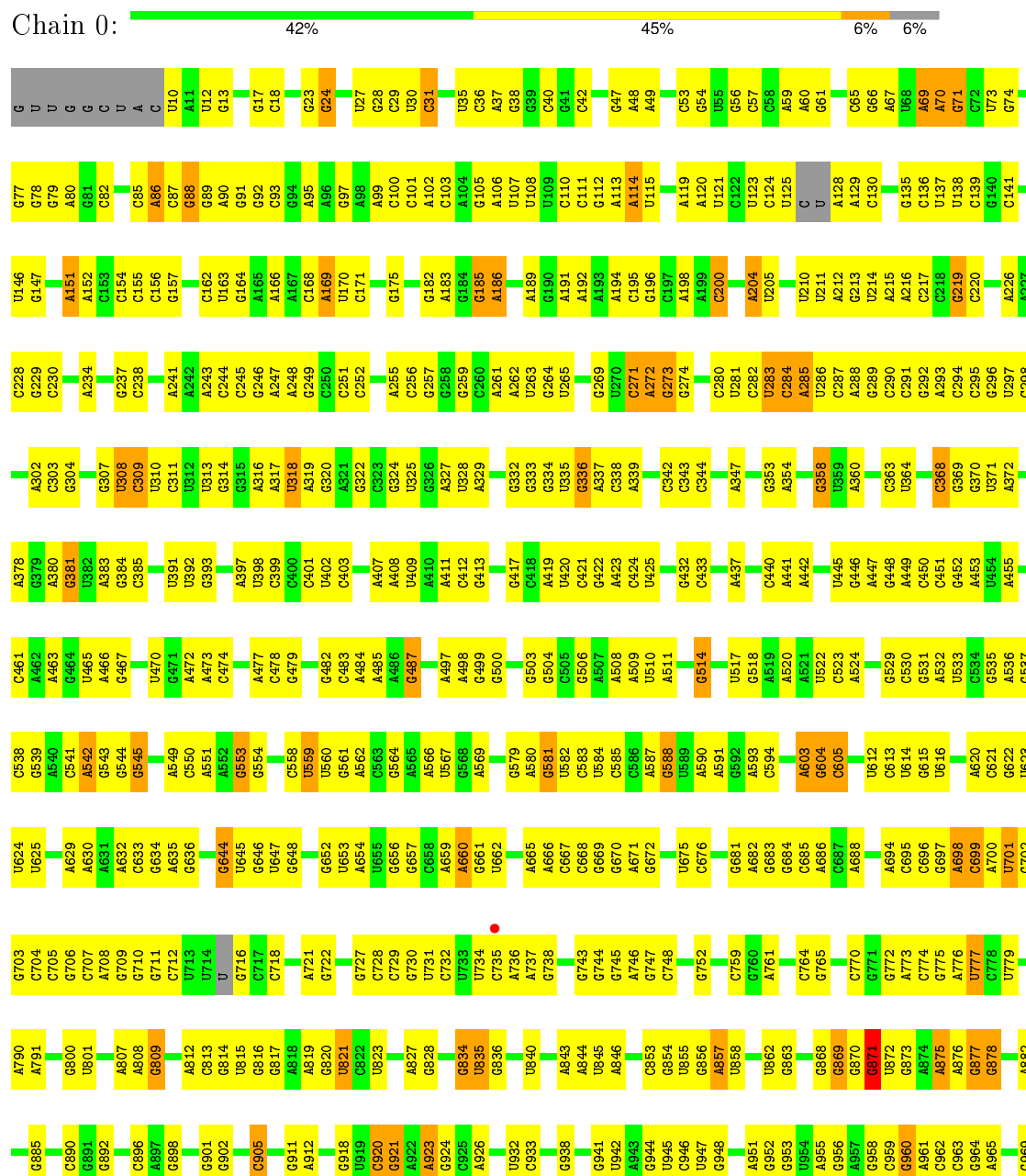
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	X	24	Total 24	O 24	0	0
40	Y	98	Total 98	O 98	0	0
40	Z	30	Total 30	O 30	0	0
40	1	58	Total 58	O 58	0	0
40	2	45	Total 45	O 45	0	0
40	3	70	Total 70	O 70	0	0
40	9	144	Total 144	O 144	0	0
40	4	13	Total 13	O 13	0	0

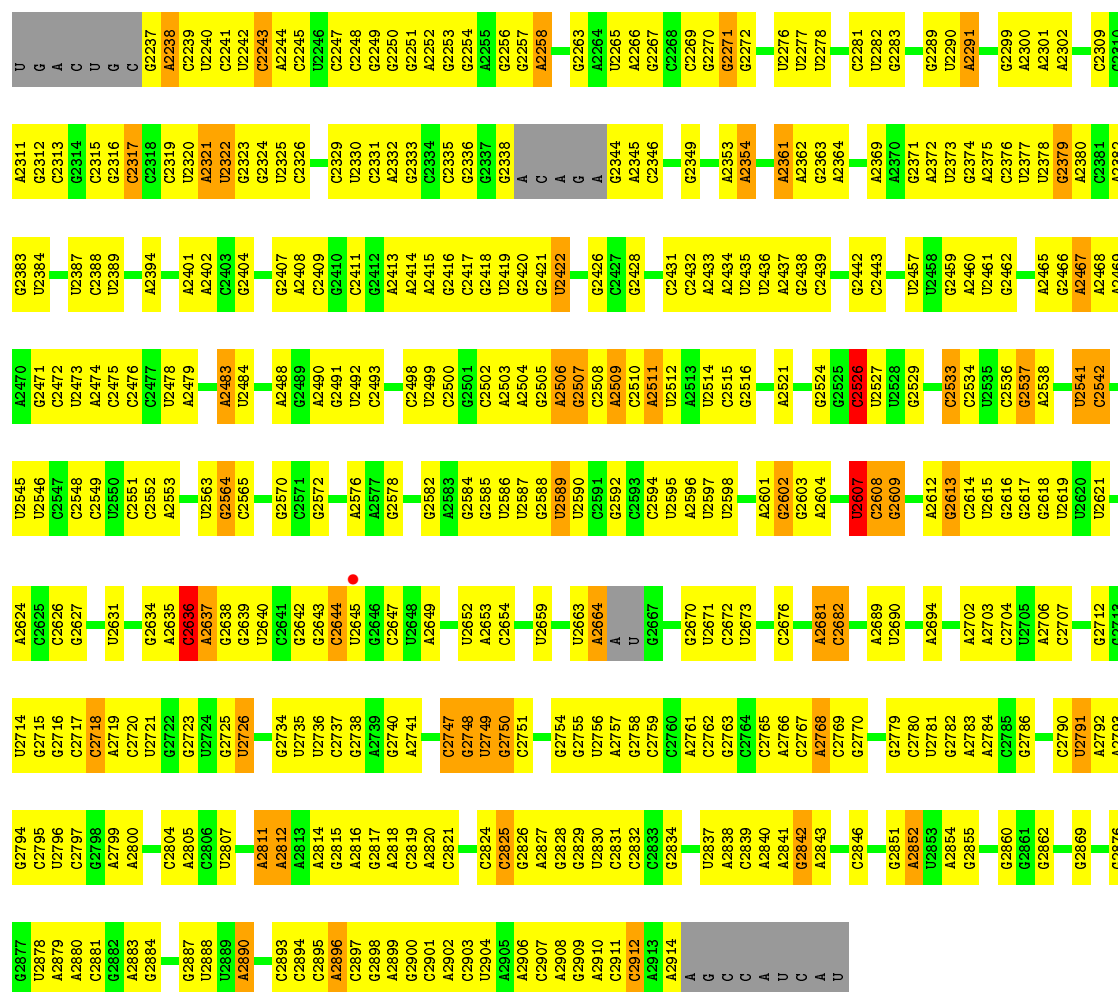
3 Residue-property plots

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 ($\text{RSRZ} > 2$). 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





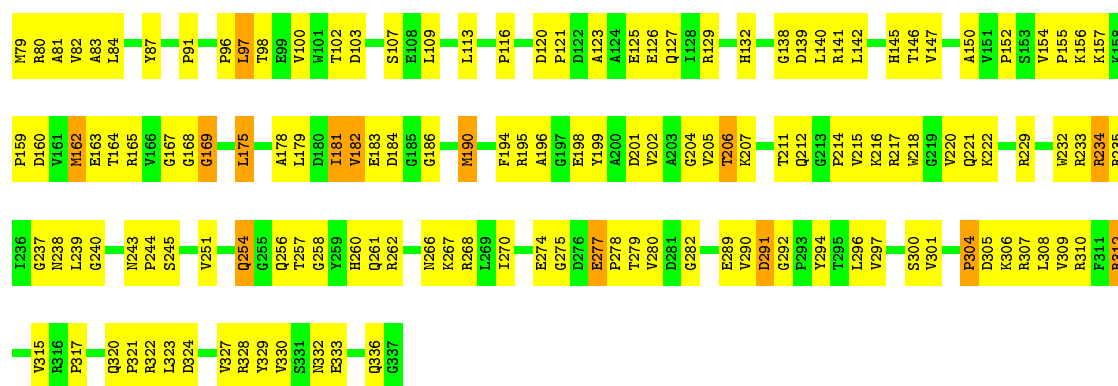


• Molecule 2: 50S ribosomal protein L2P



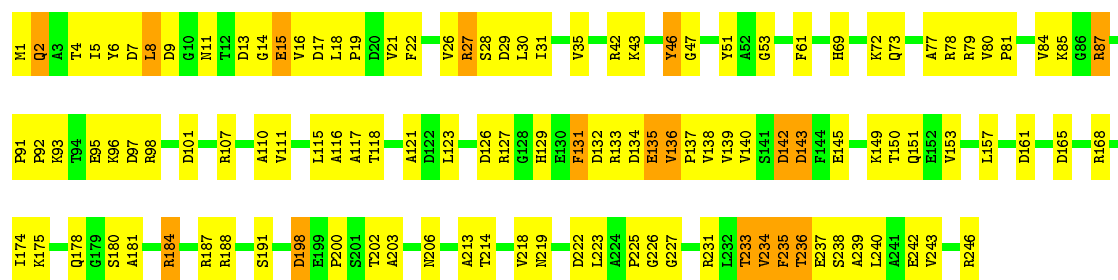
• Molecule 3: 50S ribosomal protein L3P





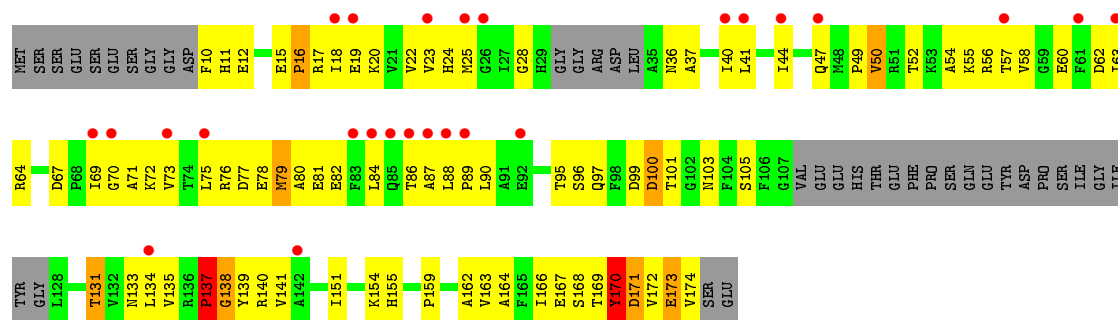
• Molecule 4: 50S ribosomal protein L4P

Chain C: 52% 41% 7%



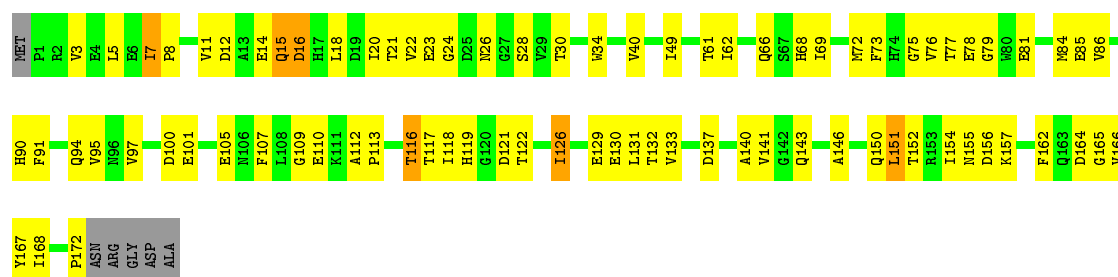
• Molecule 5: 50S ribosomal protein L5P

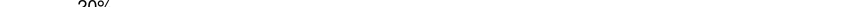
Chain D: 15% 31% 42% 5% 21%

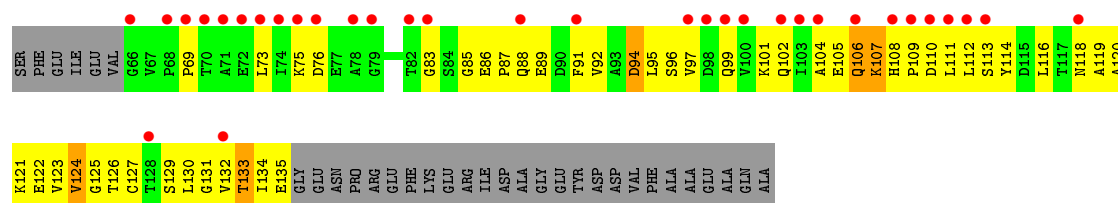


• Molecule 6: 50S ribosomal protein L6P

Chain E: 51% 42% 7%

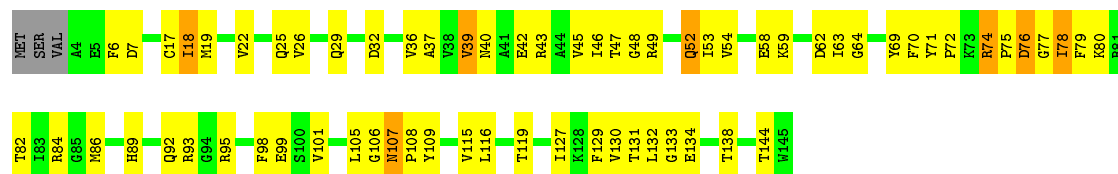


- Chain I: 
- | Amino Acid | Percentage |
|------------|------------|
| Met | 0% |
| Ala | 0% |
| Gly | 14% |
| Thr | 0% |
| Ile | 0% |
| Leu | 0% |
| Val | 0% |
| Pro | 0% |
| Gly | 14% |
| Glu | 0% |
| Asn | 0% |
| Pro | 0% |
| Gly | 14% |
| Pro | 0% |
| Leu | 0% |
| Gly | 14% |
| Pro | 0% |
| Glu | 0% |
| Leu | 0% |
| Gly | 14% |
| Pro | 0% |
| Thr | 0% |
| Val | 0% |
| Asp | 0% |
| Val | 0% |
| Gln | 0% |
| Ala | 0% |
| Val | 0% |
| Val | 0% |
| Gln | 0% |
| Glu | 0% |
| Ile | 0% |
| Asn | 0% |
| Asp | 0% |
| Gln | 0% |
| Thr | 0% |
| Ala | 0% |
| Phe | 0% |
| Asp | 0% |
| Gly | 14% |
| Thr | 0% |
| Glu | 0% |
| Val | 0% |
| Pro | 0% |
| Val | 0% |
| Thr | 0% |
| Val | 0% |
| Lys | 0% |
| Tyr | 0% |
| Asp | 0% |
| Asp | 0% |
| Gly | 14% |



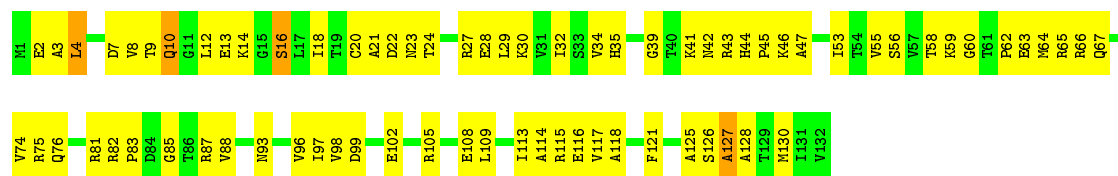
• Molecule 11: 50S ribosomal protein L13P

Chain J: 52% 41% 5%



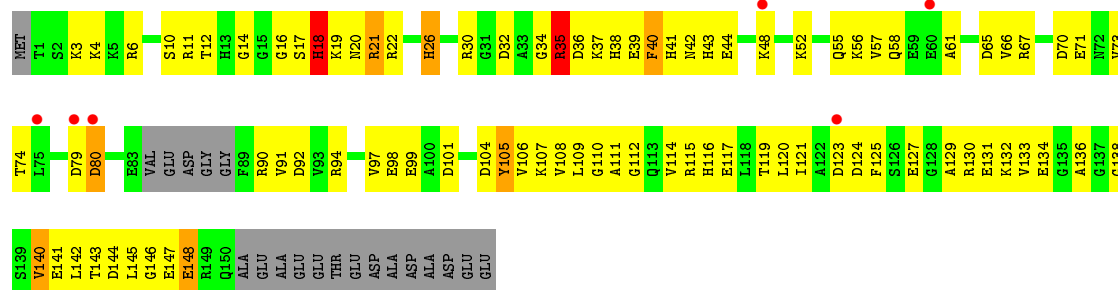
• Molecule 12: 50S ribosomal protein L14P

Chain K: 44% 53% 3%



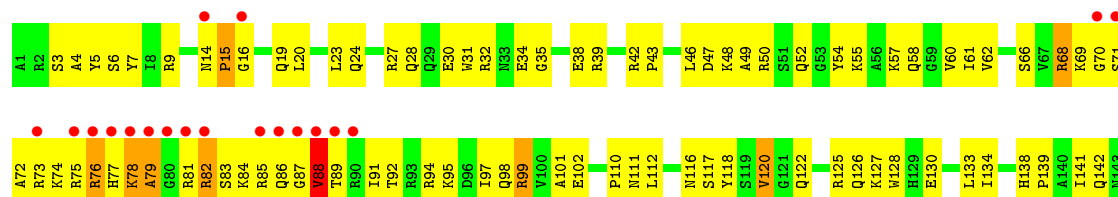
• Molecule 13: 50S ribosomal protein L15P

Chain L: 4% 34% 48% 12%



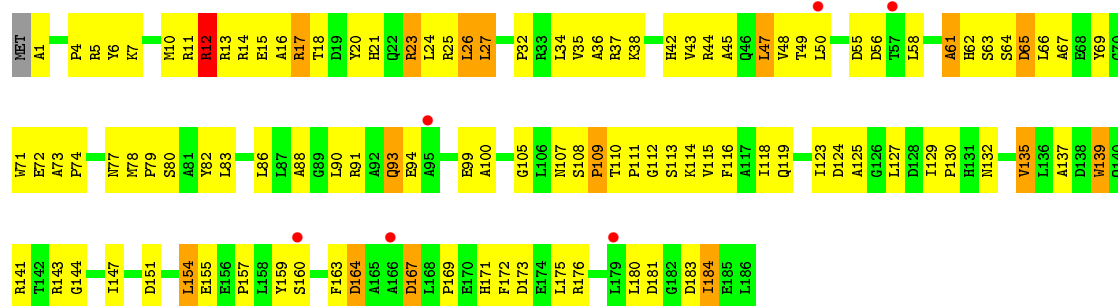
• Molecule 14: 50S ribosomal protein L15e

Chain M: 10% 42% 54% 2%

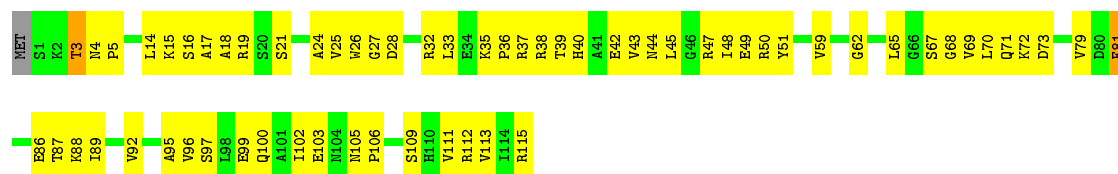




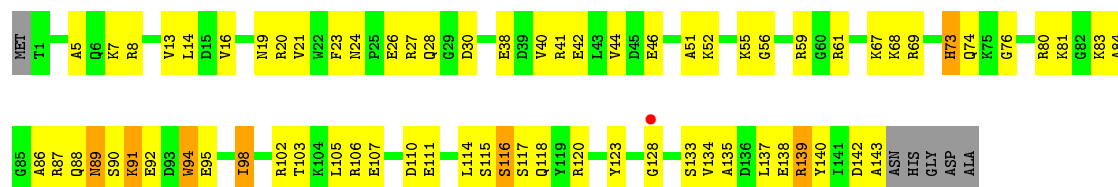
• Molecule 15: 50S ribosomal protein L18P



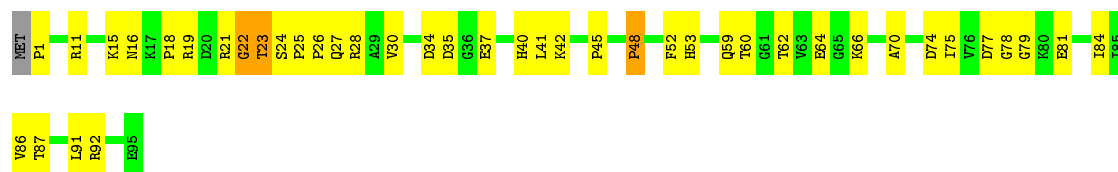
• Molecule 16: 50S ribosomal protein L18e



• Molecule 17: 50S ribosomal protein L19e

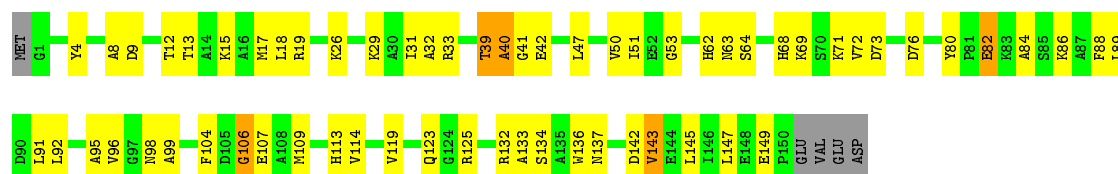


• Molecule 18: 50S ribosomal protein L21e

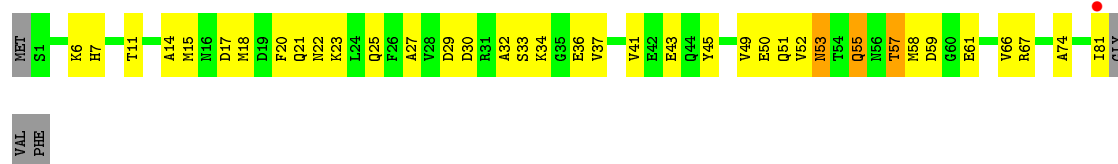


• Molecule 19: 50S ribosomal protein L22P

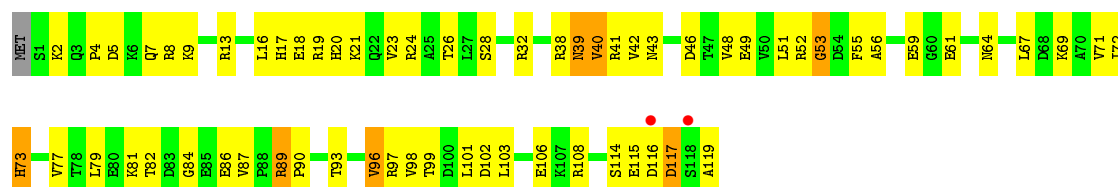




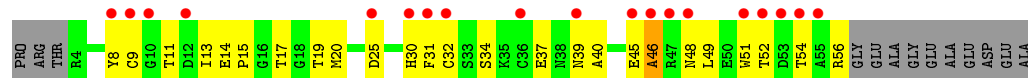
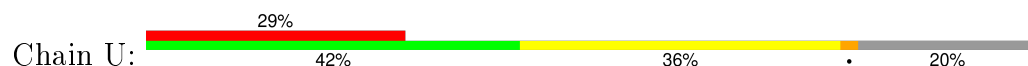
- Molecule 20: 50S ribosomal protein L23P



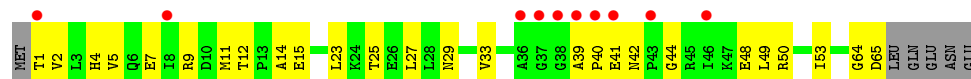
- Molecule 21: 50S ribosomal protein L24P



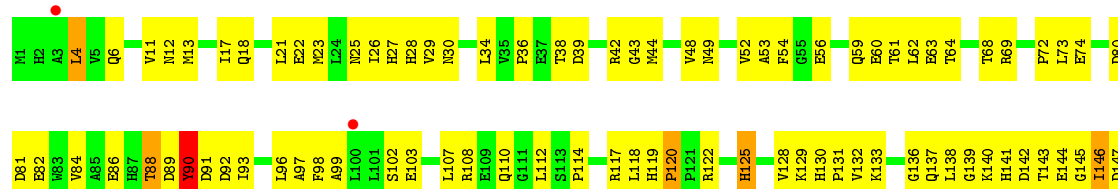
- Molecule 22: 50S ribosomal protein L24e



- Molecule 23: 50S ribosomal protein L29P

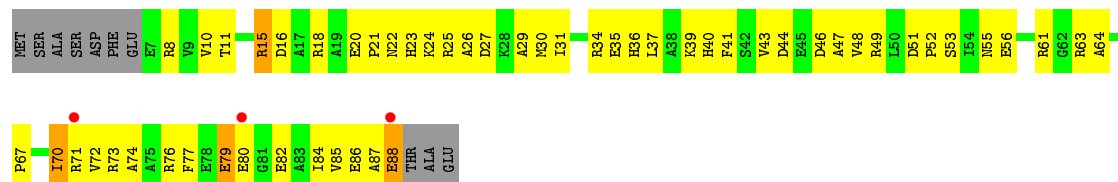


- Molecule 24: 50S ribosomal protein L30P

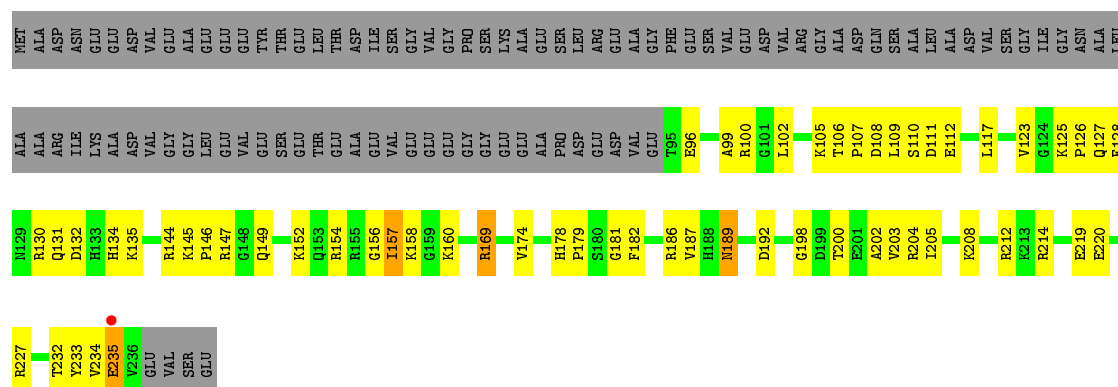




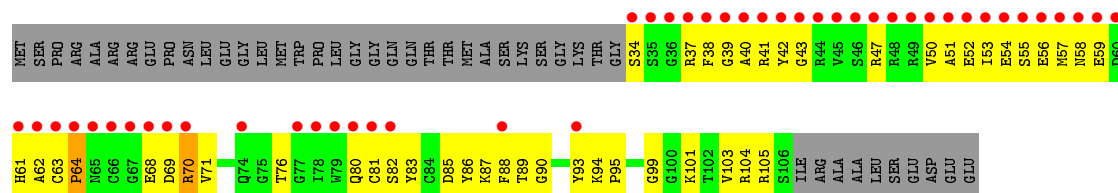
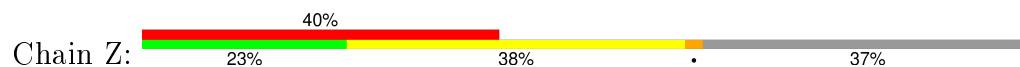
• Molecule 25: 50S ribosomal protein L31e



• Molecule 26: 50S ribosomal protein L32e



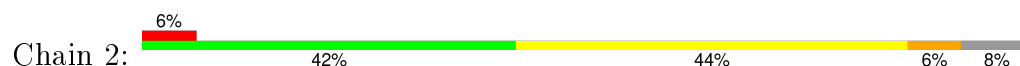
• Molecule 27: 50S ribosomal protein L37Ae

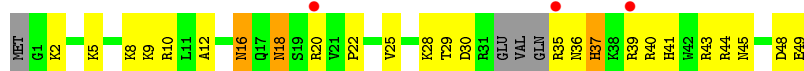


• Molecule 28: 50S ribosomal protein L37e

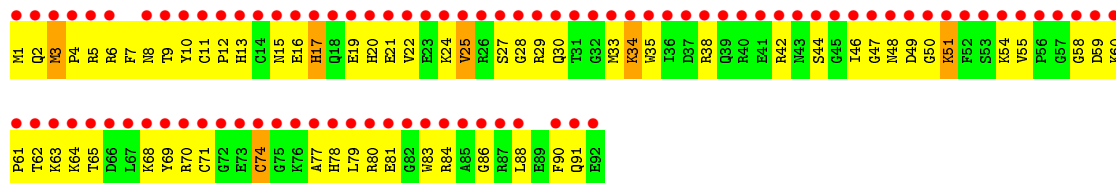


• Molecule 29: 50S ribosomal protein L39e

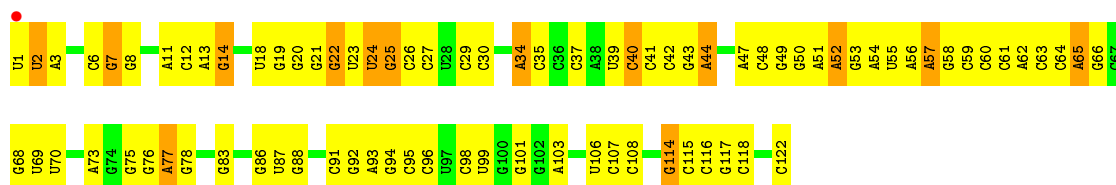




- Molecule 30: 50S ribosomal protein L44E



- Molecule 31: 5S ribosomal RNA



- Molecule 32: DNA/RNA (5'-R(*CP*CP*(5AA)P*(2OP)P*(PO2)P*AP*CP*C)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	211.32Å 299.65Å 574.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.98 – 3.11 85.39 – 2.40	Depositor EDS
% Data completeness (in resolution range)	93.4 (49.98-3.11) 93.9 (85.39-2.40)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 2.40Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.210 , 0.260 0.230 , 0.262	Depositor DCC
R_{free} test set	3147 reflections (1.05%)	DCC
Wilson B-factor (Å ²)	62.5	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 92.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 667086 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	99287	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: MG, OMG, CL, SR, NA, K, PO2, CD, 5AA, MYL, OMU, UR3, 2OP, 1MA, PSU

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	0.42	0/65958	0.68	6/102869 (0.0%)
2	A	0.33	0/1786	0.64	0/2408
3	B	0.36	0/2690	0.64	0/3652
4	C	0.38	0/1885	0.63	0/2552
5	D	0.31	0/1111	0.56	0/1498
6	E	0.35	0/1382	0.59	0/1880
7	F	0.32	0/901	0.59	0/1224
8	G	0.31	0/241	0.49	0/324
9	H	0.31	0/1303	0.63	0/1743
10	I	0.28	0/526	0.54	0/716
11	J	0.38	0/1136	0.62	0/1530
12	K	0.36	0/1004	0.65	0/1351
13	L	0.33	0/1130	0.62	0/1509
14	M	0.36	0/1583	0.59	0/2116
15	N	0.29	0/1474	0.62	0/1999
16	O	0.33	0/874	0.61	0/1181
17	P	0.36	0/1147	0.57	0/1528
18	Q	0.35	0/749	0.65	0/1005
19	R	0.40	0/1172	0.62	0/1578
20	S	0.35	0/648	0.58	0/875
21	T	0.33	0/958	0.63	0/1289
22	U	0.31	0/417	0.55	0/562
23	V	0.30	0/502	0.57	0/675
24	W	0.37	0/1219	0.66	0/1655
25	X	0.37	0/664	0.60	0/895
26	Y	0.38	0/1146	0.65	0/1536
27	Z	0.30	0/584	0.54	0/781
28	1	0.40	0/438	0.58	0/578
29	2	0.33	0/401	0.53	0/529
30	3	0.29	0/771	0.51	0/1024
31	9	0.35	0/2904	0.69	0/4526
32	4	0.46	0/102	0.73	0/149

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.39	0/98806	0.66	6/147737 (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	12
24	W	0	1
31	9	0	1
32	4	0	1
All	All	0	15

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1504	A	N9-C1'-C2'	6.22	122.09	114.00
1	0	1819	G	C5'-C4'-C3'	5.93	125.50	116.00
1	0	2726	U	N1-C1'-C2'	5.42	121.04	114.00
1	0	871	G	C5'-C4'-O4'	-5.40	102.62	109.10
1	0	1942	A	C5'-C4'-C3'	5.19	124.30	116.00

There are no chirality outliers.

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	1236	A	Sidechain
1	0	1430	G	Sidechain
1	0	1819	G	Sidechain
1	0	1829	A	Sidechain
1	0	24	G	Sidechain

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	0	59021	0	29812	1595	1
2	A	1753	0	1766	134	0
3	B	2625	0	2533	203	0
4	C	1860	0	1813	134	0
5	D	1094	0	1085	96	0
6	E	1357	0	1266	75	0
7	F	890	0	843	63	0
8	G	240	0	231	26	0
9	H	1283	0	1292	91	0
10	I	519	0	500	56	0
11	J	1120	0	1098	81	0
12	K	994	0	1027	84	0
13	L	1118	0	1076	94	0
14	M	1559	0	1573	155	0
15	N	1445	0	1401	122	0
16	O	865	0	873	59	0
17	P	1136	0	1123	84	0
18	Q	735	0	729	42	0
19	R	1149	0	1122	73	0
20	S	641	0	605	36	0
21	T	950	0	924	73	0
22	U	410	0	368	29	0
23	V	499	0	511	32	0
24	W	1196	0	1137	102	0
25	X	654	0	653	50	0
26	Y	1130	0	1133	62	0
27	Z	573	0	535	61	0
28	1	431	0	426	41	0
29	2	396	0	413	35	0
30	3	755	0	732	117	0
31	9	2599	0	1325	91	0
32	4	127	0	76	37	0
33	0	83	0	0	0	0
33	2	1	0	0	0	0
33	3	1	0	0	0	0
33	9	2	0	0	0	0
33	A	2	0	0	0	0
33	B	1	0	0	0	0
33	K	1	0	0	0	0
33	T	1	0	0	0	0
33	Y	1	0	0	0	0
34	0	2	0	0	0	0
35	0	63	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	9	2	0	0	0	0
35	B	1	0	0	0	0
35	C	1	0	0	0	0
35	H	1	0	0	0	0
35	J	1	0	0	0	0
35	M	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	3	0	0	0	0
35	S	1	0	0	0	0
36	0	10	0	0	2	0
36	3	1	0	0	0	0
36	A	1	0	0	0	0
36	B	1	0	0	0	0
36	J	3	0	0	2	0
36	L	1	0	0	0	0
36	M	1	0	0	1	0
36	N	1	0	0	0	0
36	O	1	0	0	0	0
36	R	1	0	0	0	0
36	Y	1	0	0	0	0
37	0	93	0	0	0	0
37	1	1	0	0	0	0
37	3	2	0	0	0	0
37	9	3	0	0	0	0
37	A	2	0	0	0	0
37	B	2	0	0	0	0
37	F	1	0	0	0	0
37	H	1	0	0	0	0
37	L	1	0	0	0	0
37	R	1	0	0	0	0
37	S	1	0	0	0	0
38	0	35	0	41	22	0
39	1	1	0	0	0	0
39	3	1	0	0	0	0
39	O	1	0	0	0	0
39	U	1	0	0	0	0
39	Z	1	0	0	0	0
40	0	5841	0	0	203	0
40	1	58	0	0	4	0
40	2	45	0	0	2	0
40	3	70	0	0	6	0
40	4	13	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	9	144	0	0	7	0
40	A	117	0	0	8	0
40	B	151	0	0	16	0
40	C	175	0	0	21	0
40	D	49	0	0	6	0
40	E	40	0	0	7	0
40	F	29	0	0	5	0
40	G	18	0	0	1	0
40	H	76	0	0	11	0
40	I	10	0	0	3	0
40	J	57	0	0	2	0
40	K	62	0	0	7	0
40	L	91	0	0	12	0
40	M	148	0	0	13	0
40	N	61	0	0	8	0
40	O	41	0	0	2	0
40	P	61	0	0	3	0
40	Q	49	0	0	3	0
40	R	83	0	0	3	0
40	S	37	0	0	1	0
40	T	36	0	0	4	0
40	U	29	0	0	2	0
40	V	13	0	0	3	0
40	W	67	0	0	6	0
40	X	24	0	0	1	0
40	Y	98	0	0	5	0
40	Z	30	0	0	6	0
All	All	99287	0	60042	3609	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 24.

The worst 5 of 3609 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)
40:0:4863:HOH:O	32:4:77:2OP:HB3	1.31	1.30
1:0:656:G:H5'	16:O:3:THR:HG22	1.20	1.15
1:0:871:G:C8	1:0:871:G:H5'	1.84	1.12
19:R:8:ALA:HB1	19:R:13:THR:HG21	1.28	1.11
1:0:1160:G:H5'	1:0:1161:A:H5'	1.28	1.10

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)
1:0:1171:A:N3	1:0:1964:U:O5'[3_655]	1.73	0.47

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	235/240 (98%)	193 (82%)	32 (14%)	10 (4%)	3	19
3	B	335/338 (99%)	285 (85%)	38 (11%)	12 (4%)	4	24
4	C	244/246 (99%)	204 (84%)	35 (14%)	5 (2%)	9	39
5	D	134/177 (76%)	91 (68%)	33 (25%)	10 (8%)	1	7
6	E	170/178 (96%)	149 (88%)	20 (12%)	1 (1%)	30	70
7	F	117/120 (98%)	95 (81%)	15 (13%)	7 (6%)	2	11
8	G	25/348 (7%)	18 (72%)	6 (24%)	1 (4%)	4	21
9	H	156/174 (90%)	134 (86%)	15 (10%)	7 (4%)	3	18
10	I	68/162 (42%)	43 (63%)	20 (29%)	5 (7%)	1	7
11	J	140/145 (97%)	120 (86%)	15 (11%)	5 (4%)	4	24
12	K	130/132 (98%)	113 (87%)	15 (12%)	2 (2%)	13	47
13	L	141/165 (86%)	105 (74%)	31 (22%)	5 (4%)	4	25
14	M	192/194 (99%)	153 (80%)	29 (15%)	10 (5%)	2	15
15	N	184/187 (98%)	147 (80%)	27 (15%)	10 (5%)	2	14
16	O	113/116 (97%)	89 (79%)	23 (20%)	1 (1%)	21	62
17	P	141/149 (95%)	118 (84%)	20 (14%)	3 (2%)	9	38
18	Q	93/96 (97%)	78 (84%)	10 (11%)	5 (5%)	2	14
19	R	148/155 (96%)	130 (88%)	16 (11%)	2 (1%)	14	49
20	S	79/85 (93%)	66 (84%)	12 (15%)	1 (1%)	15	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	T	117/120 (98%)	99 (85%)	15 (13%)	3 (3%)	7	32
22	U	51/66 (77%)	43 (84%)	6 (12%)	2 (4%)	4	22
23	V	63/71 (89%)	52 (82%)	11 (18%)	0	100	100
24	W	152/154 (99%)	121 (80%)	27 (18%)	4 (3%)	7	32
25	X	80/92 (87%)	65 (81%)	13 (16%)	2 (2%)	7	33
26	Y	140/241 (58%)	126 (90%)	13 (9%)	1 (1%)	26	67
27	Z	71/116 (61%)	58 (82%)	10 (14%)	3 (4%)	3	20
28	1	54/57 (95%)	46 (85%)	8 (15%)	0	100	100
29	2	42/50 (84%)	34 (81%)	7 (17%)	1 (2%)	7	34
30	3	90/92 (98%)	64 (71%)	23 (26%)	3 (3%)	5	26
All	All	3705/4466 (83%)	3039 (82%)	545 (15%)	121 (3%)	5	26

5 of 121 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	36	ASP
2	A	37	VAL
3	B	184	ASP
3	B	206	THR
4	C	8	LEU

5.3.2 Protein sidechains ⓘ

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	179/182 (98%)	170 (95%)	9 (5%)	30	68
3	B	282/283 (100%)	264 (94%)	18 (6%)	22	57
4	C	193/193 (100%)	174 (90%)	19 (10%)	10	35
5	D	117/148 (79%)	111 (95%)	6 (5%)	29	66
6	E	152/156 (97%)	145 (95%)	7 (5%)	33	70
7	F	93/94 (99%)	92 (99%)	1 (1%)	80	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	G	27/282 (10%)	26 (96%)	1 (4%)	41	77
9	H	134/143 (94%)	128 (96%)	6 (4%)	34	71
10	I	58/130 (45%)	56 (97%)	2 (3%)	44	79
11	J	118/121 (98%)	114 (97%)	4 (3%)	44	79
12	K	106/106 (100%)	101 (95%)	5 (5%)	32	70
13	L	113/127 (89%)	103 (91%)	10 (9%)	12	43
14	M	158/158 (100%)	153 (97%)	5 (3%)	46	80
15	N	149/150 (99%)	139 (93%)	10 (7%)	20	56
16	O	93/94 (99%)	90 (97%)	3 (3%)	46	80
17	P	113/117 (97%)	106 (94%)	7 (6%)	23	59
18	Q	79/80 (99%)	78 (99%)	1 (1%)	76	91
19	R	117/122 (96%)	112 (96%)	5 (4%)	35	73
20	S	71/74 (96%)	68 (96%)	3 (4%)	36	73
21	T	105/106 (99%)	98 (93%)	7 (7%)	20	56
22	U	44/52 (85%)	44 (100%)	0	100	100
23	V	51/57 (90%)	51 (100%)	0	100	100
24	W	130/130 (100%)	123 (95%)	7 (5%)	27	64
25	X	66/74 (89%)	60 (91%)	6 (9%)	12	40
26	Y	120/196 (61%)	116 (97%)	4 (3%)	45	79
27	Z	60/94 (64%)	59 (98%)	1 (2%)	68	89
28	1	46/47 (98%)	45 (98%)	1 (2%)	60	86
29	2	42/46 (91%)	40 (95%)	2 (5%)	31	69
30	3	79/79 (100%)	76 (96%)	3 (4%)	40	76
All	All	3095/3641 (85%)	2942 (95%)	153 (5%)	31	69

5 of 153 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	J	39	VAL
13	L	127	GLU
25	X	88	GLU
11	J	74	ARG
12	K	83	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 107 such sidechains are listed below:

Mol	Chain	Res	Type
13	L	58	GLN
17	P	28	GLN
29	2	41	HIS
14	M	24	GLN
14	M	98	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2923 (93%)	248 (9%)	18 (0%)
31	9	121/122 (99%)	18 (14%)	1 (0%)
32	4	1/8 (12%)	0	0
All	All	2867/3053 (93%)	266 (9%)	19 (0%)

5 of 266 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 19 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	871	G
1	0	2011	A
1	0	2718	C
1	0	857	A
1	0	2726	U

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

6 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	OMU	0	2587	1,35	12,22,23	1.05	1 (8%)	19,31,34	3.17	2 (10%)
1	OMG	0	2588	1,32	17,26,27	0.95	1 (5%)	21,38,41	2.52	3 (14%)
1	UR3	0	2619	1	12,22,23	0.77	0	16,32,35	0.75	0
1	PSU	0	2621	1	13,21,22	1.67	2 (15%)	18,30,33	6.10	3 (16%)
1	1MA	0	628	1	14,25,26	1.04	1 (7%)	15,37,40	1.16	1 (6%)
32	5AA	4	76	1,32	16,26,27	0.65	0	15,38,41	1.22	2 (13%)

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	OMU	0	2587	1,35	-	0/5/27/28	0/2/2/2
1	OMG	0	2588	1,32	-	0/5/27/28	0/3/3/3
1	UR3	0	2619	1	-	0/3/25/26	0/2/2/2
1	PSU	0	2621	1	-	0/7/25/26	0/2/2/2
1	1MA	0	628	1	-	0/3/25/26	0/3/3/3
32	5AA	4	76	1,32	-	0/7/29/30	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C5-C1'	-5.00	1.47	1.52
1	0	2587	OMU	C4-N3	2.59	1.37	1.33
1	0	2621	PSU	C4-N3	2.71	1.38	1.33
1	0	2588	OMG	C6-N1	2.83	1.38	1.33
1	0	628	1MA	C6-N6	2.85	1.34	1.29

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2621	PSU	N1-C2-N3	-21.39	114.69	128.33
1	0	2588	OMG	C5-C6-N1	-8.63	111.78	123.59
1	0	628	1MA	C2-N3-C4	-3.60	110.82	116.40
1	0	2587	OMU	C5-C4-N3	-3.34	114.54	123.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2588	OMG	N3-C2-N1	-2.26	124.00	127.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	0	2587	OMU	2	0
1	0	2588	OMG	5	0
1	0	2619	UR3	1	0
1	0	2621	PSU	1	0
32	4	76	5AA	10	0

5.5 Carbohydrates [i](#)

There are no carbohydrates 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	$\# Z > 2$
38	MYL	0	2924	-	35,37,37	1.19	2 (5%)	38,56,56	1.74	11 (28%)

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
38	MYL	0	2924	-	-	2/21/77/77	1/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	0	2924	MYL	CAA-CAV	2.66	1.39	1.32
38	0	2924	MYL	CBC-NAP	5.25	1.49	1.43

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	0	2924	MYL	CAN-CBH-CBB	-3.13	109.52	113.40
38	0	2924	MYL	OAR-CBC-CBG	-2.91	104.64	109.64
38	0	2924	MYL	CAO-CBA-CBE	-2.89	109.64	114.79
38	0	2924	MYL	CAB-OAQ-CBH	-2.22	110.45	116.36
38	0	2924	MYL	OAS-CBF-CBG	-2.13	106.40	110.23

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
38	0	2924	MYL	OAG-CAW-NAP-CBC
38	0	2924	MYL	CBB-CAW-NAP-CBC

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
38	0	2924	MYL	CAM-CBC-CBF-CBG-OAR-OAS

1 monomer is involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	0	2924	MYL	22	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, 95th 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%)	-0.34	5 (0%) 95 91	31, 61, 109, 181	0
2	A	237/240 (98%)	0.00	5 (2%) 67 45	37, 75, 110, 131	0
3	B	337/338 (99%)	-0.39	0 100 100	37, 65, 93, 103	0
4	C	246/246 (100%)	-0.29	0 100 100	34, 60, 84, 96	0
5	D	140/177 (79%)	1.01	26 (18%) 2 1	80, 118, 140, 148	0
6	E	172/178 (96%)	-0.23	0 100 100	54, 81, 102, 112	0
7	F	119/120 (99%)	0.17	2 (1%) 73 53	65, 93, 121, 135	0
8	G	29/348 (8%)	0.39	1 (3%) 49 25	86, 102, 109, 114	0
9	H	160/174 (91%)	0.13	5 (3%) 52 28	58, 79, 111, 121	0
10	I	70/162 (43%)	1.98	33 (47%) 0 0	137, 154, 180, 181	0
11	J	142/145 (97%)	-0.43	0 100 100	48, 63, 82, 98	0
12	K	132/132 (100%)	-0.28	0 100 100	46, 63, 88, 95	0
13	L	145/165 (87%)	0.21	6 (4%) 41 19	38, 86, 124, 133	0
14	M	194/194 (100%)	0.24	19 (9%) 10 3	38, 60, 136, 151	0
15	N	186/187 (99%)	0.24	6 (3%) 51 27	65, 89, 138, 146	0
16	O	115/116 (99%)	-0.33	0 100 100	51, 70, 84, 91	0
17	P	143/149 (95%)	-0.12	1 (0%) 89 79	52, 69, 87, 93	0
18	Q	95/96 (98%)	-0.15	0 100 100	51, 62, 77, 85	0
19	R	150/155 (96%)	-0.39	0 100 100	42, 56, 77, 89	0
20	S	81/85 (95%)	-0.09	1 (1%) 81 65	57, 76, 99, 111	0
21	T	119/120 (99%)	-0.00	2 (1%) 73 53	55, 73, 106, 125	0
22	U	53/66 (80%)	1.65	19 (35%) 0 0	95, 117, 133, 135	0
23	V	65/71 (91%)	0.84	10 (15%) 3 1	65, 90, 140, 144	0
24	W	154/154 (100%)	-0.23	2 (1%) 79 63	46, 62, 79, 95	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	X	82/92 (89%)	-0.01	3 (3%) 45 22	52, 70, 88, 105	0
26	Y	142/241 (58%)	-0.41	1 (0%) 89 79	39, 58, 80, 99	0
27	Z	73/116 (62%)	5.07	46 (63%) 0 0	107, 143, 170, 176	0
28	1	56/57 (98%)	-0.21	0 100 100	34, 47, 58, 62	0
29	2	46/50 (92%)	0.17	3 (6%) 22 8	47, 80, 113, 121	0
30	3	92/92 (100%)	7.73	90 (97%) 0 0	164, 175, 184, 189	0
31	9	122/122 (100%)	-0.56	1 (0%) 87 75	52, 86, 113, 166	0
32	4	5/8 (62%)	1.36	0 100 100	41, 43, 47, 47	0
All	All	6651/7519 (88%)	0.02	287 (4%) 39 18	31, 67, 132, 189	0

The worst 5 of 287 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
27	Z	34	SER	24.8
30	3	82	GLY	24.3
27	Z	35	SER	23.2
27	Z	58	ASN	21.8
27	Z	46	SER	20.9

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

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, 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	LLDF	B-factors(Å ²)	Q<0.9
1	UR3	0	2619	21/22	0.95	0.17	-	41,44,49,50	0
1	OMG	0	2588	24/25	0.96	0.16	-	37,42,44,45	0
1	PSU	0	2621	20/21	0.93	0.19	-	37,39,44,44	0
1	1MA	0	628	23/24	0.96	0.17	-	38,41,42,43	0
1	OMU	0	2587	21/22	0.95	0.14	-	43,46,50,50	0
32	5AA	4	76	24/25	0.77	0.29	-	38,44,48,48	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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, 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	LLDF	B-factors(Å ²)	Q<0.9
35	NA	0	8565	1/1	0.89	1.65	69.82	80,80,80,80	0
35	NA	0	8530	1/1	0.79	0.68	42.97	68,68,68,68	0
37	SR	L	8969	1/1	0.55	1.29	40.95	200,200,200,200	0
35	NA	0	8563	1/1	0.72	1.00	34.13	85,85,85,85	0
33	MG	0	8047	1/1	0.85	0.55	24.45	68,68,68,68	0
35	NA	0	8513	1/1	0.76	0.66	21.46	62,62,62,62	0
35	NA	0	8568	1/1	0.39	0.62	21.21	35,35,35,35	0
35	NA	0	8517	1/1	0.81	0.35	20.38	62,62,62,62	0
37	SR	B	8987	1/1	0.79	1.00	20.37	200,200,200,200	0
35	NA	0	8528	1/1	0.57	0.68	19.53	91,91,91,91	0
35	NA	0	8547	1/1	0.94	0.61	19.40	82,82,82,82	0
35	NA	0	8555	1/1	0.89	0.76	17.81	61,61,61,61	0
37	SR	0	8949	1/1	0.44	0.43	15.50	157,157,157,157	0
37	SR	0	8962	1/1	0.07	0.42	14.12	200,200,200,200	0
35	NA	0	8521	1/1	0.60	0.47	12.77	59,59,59,59	0
35	NA	0	8512	1/1	0.89	0.44	12.00	54,54,54,54	0
35	NA	0	8556	1/1	0.72	0.46	10.89	49,49,49,49	0
34	K	0	8401	1/1	0.83	0.36	10.00	132,132,132,132	0
35	NA	0	8519	1/1	0.92	0.36	9.30	69,69,69,69	0
35	NA	0	8527	1/1	0.97	0.34	8.05	75,75,75,75	0
35	NA	0	8553	1/1	0.90	0.36	7.05	98,98,98,98	0
35	NA	0	8559	1/1	0.69	0.32	6.84	99,99,99,99	0
35	NA	0	8542	1/1	0.94	0.34	6.58	51,51,51,51	0
35	NA	0	8569	1/1	0.81	0.37	6.03	63,63,63,63	0
37	SR	0	8992	1/1	0.73	0.29	5.80	164,164,164,164	0
35	NA	0	8562	1/1	0.92	0.21	5.76	49,49,49,49	0
33	MG	0	8080	1/1	0.91	2.92	4.99	126,126,126,126	0
33	MG	0	8043	1/1	0.92	0.21	4.87	48,48,48,48	0
36	CL	0	8805	1/1	0.88	0.24	4.78	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
35	NA	0	8522	1/1	0.57	0.27	4.44	71,71,71,71	0
37	SR	0	8904	1/1	0.99	0.23	3.74	65,65,65,65	0
35	NA	0	8564	1/1	0.84	0.21	3.42	94,94,94,94	0
35	NA	0	8557	1/1	0.57	0.16	3.32	72,72,72,72	0
35	NA	0	8545	1/1	0.91	0.26	2.83	25,25,25,25	0
35	NA	M	8539	1/1	0.84	0.26	2.65	51,51,51,51	0
33	MG	Y	8086	1/1	0.87	0.25	2.45	53,53,53,53	0
35	NA	Q	8540	1/1	0.74	0.30	2.29	84,84,84,84	0
33	MG	0	8076	1/1	0.81	0.25	2.25	52,52,52,52	0
35	NA	0	8534	1/1	0.81	0.40	1.97	53,53,53,53	0
34	K	0	8402	1/1	0.71	0.48	1.76	88,88,88,88	0
35	NA	0	8523	1/1	0.83	0.21	1.59	52,52,52,52	0
35	NA	R	8533	1/1	0.83	0.20	1.36	62,62,62,62	0
36	CL	B	8819	1/1	0.87	0.23	1.29	80,80,80,80	0
37	SR	0	8970	1/1	0.94	0.13	1.23	148,148,148,148	0
33	MG	0	8015	1/1	0.97	0.17	1.19	26,26,26,26	0
33	MG	0	8034	1/1	0.93	0.19	1.16	57,57,57,57	0
37	SR	0	8902	1/1	0.99	0.20	1.01	44,44,44,44	0
33	MG	0	8014	1/1	0.94	0.20	0.97	24,24,24,24	0
33	MG	0	8041	1/1	0.94	0.21	0.37	29,29,29,29	0
37	SR	0	8985	1/1	0.89	0.12	0.32	150,150,150,150	0
36	CL	M	8818	1/1	0.94	0.18	0.27	62,62,62,62	0
33	MG	0	8003	1/1	0.93	0.17	0.19	32,32,32,32	0
35	NA	R	8575	1/1	0.97	0.19	0.17	92,92,92,92	0
37	SR	0	8923	1/1	0.91	0.17	0.16	108,108,108,108	0
36	CL	J	8821	1/1	0.93	0.19	0.15	90,90,90,90	0
33	MG	0	8062	1/1	0.98	0.20	0.05	53,53,53,53	0
37	SR	0	8943	1/1	0.82	0.14	0.01	105,105,105,105	0
33	MG	A	8051	1/1	0.99	0.20	-0.05	81,81,81,81	0
33	MG	0	8006	1/1	0.98	0.16	-0.05	44,44,44,44	0
39	CD	U	8701	1/1	0.81	0.40	-0.28	200,200,200,200	0
39	CD	Z	8703	1/1	0.49	0.39	-0.34	200,200,200,200	0
33	MG	A	8050	1/1	0.91	0.18	-0.52	68,68,68,68	0
35	NA	0	8507	1/1	0.81	0.17	-0.53	27,27,27,27	0
33	MG	0	8044	1/1	0.59	0.16	-0.61	51,51,51,51	0
33	MG	0	8058	1/1	0.92	0.12	-0.65	22,22,22,22	0
33	MG	0	8088	1/1	0.53	0.18	-0.77	37,37,37,37	0
38	MYL	0	2924	35/35	0.84	0.26	-0.78	80,83,86,87	0
37	SR	A	8930	1/1	0.49	0.15	-0.82	168,168,168,168	0
37	SR	0	8903	1/1	0.96	0.15	-0.86	62,62,62,62	0
33	MG	0	8084	1/1	0.97	0.11	-0.91	31,31,31,31	0
35	NA	C	8503	1/1	0.88	0.17	-0.96	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	MG	0	8004	1/1	0.82	0.18	-1.01	25,25,25,25	0
33	MG	0	8016	1/1	0.96	0.19	-1.02	34,34,34,34	0
35	NA	J	8538	1/1	0.69	0.15	-1.10	56,56,56,56	0
35	NA	0	8515	1/1	0.92	0.18	-1.16	39,39,39,39	0
36	CL	L	8810	1/1	0.80	0.17	-1.16	76,76,76,76	0
33	MG	0	8001	1/1	0.98	0.17	-1.34	24,24,24,24	0
37	SR	0	8948	1/1	0.93	0.12	-1.35	113,113,113,113	0
36	CL	0	8812	1/1	0.95	0.11	-1.44	66,66,66,66	0
33	MG	0	8002	1/1	0.97	0.17	-1.48	40,40,40,40	0
35	NA	R	8532	1/1	0.93	0.08	-1.52	52,52,52,52	0
33	MG	0	8028	1/1	0.92	0.15	-1.54	13,13,13,13	0
33	MG	0	8065	1/1	0.73	0.12	-1.57	33,33,33,33	0
37	SR	0	8936	1/1	0.96	0.13	-1.61	125,125,125,125	0
35	NA	0	8537	1/1	0.84	0.09	-1.71	40,40,40,40	0
33	MG	0	8012	1/1	0.96	0.17	-1.75	23,23,23,23	0
37	SR	H	8972	1/1	0.96	0.11	-1.77	139,139,139,139	0
39	CD	1	8702	1/1	0.94	0.11	-1.89	78,78,78,78	0
37	SR	A	8929	1/1	0.82	0.07	-1.89	124,124,124,124	0
33	MG	0	8045	1/1	0.87	0.10	-1.93	64,64,64,64	0
37	SR	0	8910	1/1	0.89	0.13	-1.95	107,107,107,107	0
33	MG	0	8011	1/1	0.90	0.16	-2.05	14,14,14,14	0
33	MG	0	8025	1/1	0.91	0.14	-2.10	30,30,30,30	0
39	CD	3	8704	1/1	0.56	0.62	-2.29	200,200,200,200	0
37	SR	0	8935	1/1	0.93	0.09	-2.38	91,91,91,91	0
33	MG	T	8057	1/1	0.80	0.07	-2.65	68,68,68,68	0
33	MG	0	8009	1/1	0.98	0.13	-2.69	22,22,22,22	0
33	MG	0	8021	1/1	0.96	0.10	-2.89	53,53,53,53	0
33	MG	0	8052	1/1	0.91	0.13	-2.91	60,60,60,60	0
37	SR	0	8975	1/1	0.75	0.08	-3.21	158,158,158,158	0
33	MG	0	8010	1/1	0.57	0.14	-3.77	25,25,25,25	0
35	NA	9	8572	1/1	0.94	0.04	-3.91	78,78,78,78	0
35	NA	0	8504	1/1	0.99	0.13	-4.60	32,32,32,32	0
33	MG	0	8013	1/1	0.90	0.08	-13.05	24,24,24,24	0
35	NA	0	8574	1/1	0.56	0.62	-	72,72,72,72	0
37	SR	0	8991	1/1	0.68	0.14	-	197,197,197,197	0
33	MG	0	8083	1/1	0.83	0.18	-	50,50,50,50	0
33	MG	0	8039	1/1	0.83	0.18	-	55,55,55,55	0
35	NA	0	8520	1/1	0.87	0.18	-	63,63,63,63	0
33	MG	0	8078	1/1	0.95	0.85	-	91,91,91,91	0
37	SR	0	8907	1/1	0.96	0.14	-	59,59,59,59	0
37	SR	0	8951	1/1	0.85	0.06	-	144,144,144,144	0
35	NA	0	8573	1/1	0.92	0.15	-	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
37	SR	0	8941	1/1	0.38	0.30	-	152,152,152,152	0
33	MG	0	8048	1/1	0.91	0.29	-	41,41,41,41	0
37	SR	0	8920	1/1	0.95	0.14	-	130,130,130,130	0
33	MG	0	8017	1/1	0.82	0.17	-	26,26,26,26	0
36	CL	0	8811	1/1	0.92	0.21	-	87,87,87,87	0
36	CL	0	8815	1/1	0.94	0.21	-	83,83,83,83	0
36	CL	0	8822	1/1	0.89	0.90	-	123,123,123,123	0
35	NA	9	8543	1/1	0.74	0.18	-	68,68,68,68	0
33	MG	0	8082	1/1	0.88	0.23	-	61,61,61,61	0
33	MG	0	8007	1/1	0.96	0.12	-	27,27,27,27	0
37	SR	0	8934	1/1	0.89	0.31	-	168,168,168,168	0
33	MG	0	8069	1/1	0.64	0.43	-	63,63,63,63	0
37	SR	0	8945	1/1	0.77	0.13	-	131,131,131,131	0
37	SR	0	8908	1/1	0.57	0.21	-	116,116,116,116	0
35	NA	0	8561	1/1	0.71	0.26	-	66,66,66,66	0
37	SR	0	8989	1/1	0.68	0.16	-	129,129,129,129	0
35	NA	0	8529	1/1	0.83	0.09	-	45,45,45,45	0
37	SR	0	8973	1/1	0.85	0.12	-	162,162,162,162	0
35	NA	0	8546	1/1	0.84	0.63	-	65,65,65,65	0
37	SR	0	8971	1/1	-0.29	0.34	-	200,200,200,200	0
37	SR	0	8938	1/1	0.57	0.32	-	200,200,200,200	0
37	SR	0	8905	1/1	0.96	0.27	-	78,78,78,78	0
37	SR	0	8947	1/1	0.84	0.78	-	200,200,200,200	0
37	SR	0	8979	1/1	0.74	0.24	-	111,111,111,111	0
37	SR	0	8944	1/1	0.66	0.17	-	169,169,169,169	0
33	MG	0	8019	1/1	0.87	0.16	-	11,11,11,11	0
33	MG	0	8029	1/1	0.78	0.19	-	79,79,79,79	0
37	SR	0	8946	1/1	0.92	0.14	-	127,127,127,127	0
37	SR	0	8982	1/1	0.87	1.36	-	200,200,200,200	0
33	MG	3	8090	1/1	0.04	2.20	-	86,86,86,86	0
36	CL	0	8816	1/1	0.94	0.81	-	89,89,89,89	0
37	SR	0	8966	1/1	0.76	0.13	-	117,117,117,117	0
33	MG	0	8072	1/1	0.95	0.40	-	60,60,60,60	0
33	MG	2	8060	1/1	0.73	0.11	-	62,62,62,62	0
33	MG	0	8038	1/1	0.68	0.20	-	92,92,92,92	0
37	SR	0	8960	1/1	0.76	0.09	-	175,175,175,175	0
37	SR	0	8958	1/1	0.96	0.16	-	120,120,120,120	0
33	MG	9	8074	1/1	0.83	0.11	-	87,87,87,87	0
33	MG	0	8049	1/1	0.94	0.35	-	82,82,82,82	0
36	CL	J	8802	1/1	0.89	0.24	-	84,84,84,84	0
33	MG	0	8059	1/1	0.90	0.15	-	56,56,56,56	0
36	CL	0	8813	1/1	0.82	0.10	-	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
37	SR	0	8917	1/1	0.83	0.23	-	157,157,157,157	0
33	MG	0	8070	1/1	0.88	0.09	-	58,58,58,58	0
36	CL	0	8803	1/1	0.63	0.12	-	68,68,68,68	0
36	CL	Y	8820	1/1	0.87	0.21	-	58,58,58,58	0
36	CL	O	8808	1/1	0.67	0.14	-	109,109,109,109	0
39	CD	O	8705	1/1	0.95	0.07	-	117,117,117,117	0
35	NA	0	8511	1/1	0.91	0.26	-	54,54,54,54	0
37	SR	0	8965	1/1	0.16	0.19	-	158,158,158,158	0
37	SR	0	8977	1/1	0.20	0.12	-	200,200,200,200	0
37	SR	0	8983	1/1	0.16	0.28	-	199,199,199,199	0
35	NA	0	8524	1/1	0.96	0.12	-	67,67,67,67	0
33	MG	9	8040	1/1	0.93	0.23	-	89,89,89,89	0
33	MG	0	8033	1/1	0.96	0.20	-	79,79,79,79	0
37	SR	9	8980	1/1	0.39	0.37	-	192,192,192,192	0
35	NA	0	8554	1/1	0.71	0.44	-	106,106,106,106	0
33	MG	0	8018	1/1	0.88	0.14	-	32,32,32,32	0
35	NA	0	8544	1/1	0.05	0.45	-	75,75,75,75	0
37	SR	0	8974	1/1	0.27	0.20	-	163,163,163,163	0
37	SR	0	8911	1/1	0.75	0.10	-	99,99,99,99	0
33	MG	0	8077	1/1	0.89	0.64	-	60,60,60,60	0
35	NA	0	8516	1/1	0.89	0.20	-	39,39,39,39	0
37	SR	0	8955	1/1	0.89	0.13	-	200,200,200,200	0
33	MG	0	8053	1/1	0.76	0.10	-	61,61,61,61	0
33	MG	0	8089	1/1	0.88	0.21	-	42,42,42,42	0
35	NA	0	8536	1/1	0.55	0.19	-	72,72,72,72	0
37	SR	0	8993	1/1	0.36	0.23	-	186,186,186,186	0
36	CL	J	8801	1/1	0.90	0.34	-	88,88,88,88	0
36	CL	A	8809	1/1	0.81	0.79	-	128,128,128,128	0
35	NA	0	8548	1/1	0.39	0.33	-	67,67,67,67	0
33	MG	0	8061	1/1	0.93	0.41	-	48,48,48,48	0
33	MG	0	8030	1/1	0.95	0.39	-	88,88,88,88	0
37	SR	0	8924	1/1	0.82	0.20	-	140,140,140,140	0
35	NA	0	8549	1/1	0.76	0.34	-	124,124,124,124	0
33	MG	0	8008	1/1	0.93	0.15	-	23,23,23,23	0
37	SR	B	8950	1/1	0.90	0.15	-	125,125,125,125	0
37	SR	0	8953	1/1	0.76	1.12	-	200,200,200,200	0
35	NA	0	8535	1/1	0.92	0.76	-	72,72,72,72	0
37	SR	0	9004	1/1	0.93	0.25	-	172,172,172,172	0
35	NA	0	8566	1/1	0.91	0.38	-	64,64,64,64	0
37	SR	0	8916	1/1	0.74	0.17	-	126,126,126,126	0
37	SR	0	8988	1/1	0.78	0.17	-	183,183,183,183	0
37	SR	0	8939	1/1	0.90	0.15	-	166,166,166,166	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	MG	0	8063	1/1	0.89	0.16	-	62,62,62,62	0
37	SR	9	8978	1/1	0.94	0.10	-	154,154,154,154	0
35	NA	0	8508	1/1	0.71	0.44	-	68,68,68,68	0
35	NA	0	8506	1/1	0.45	0.80	-	65,65,65,65	0
33	MG	0	8087	1/1	0.95	0.10	-	29,29,29,29	0
35	NA	0	8550	1/1	0.86	0.28	-	76,76,76,76	0
37	SR	0	8918	1/1	0.85	0.14	-	92,92,92,92	0
37	SR	0	9001	1/1	0.79	0.18	-	200,200,200,200	0
37	SR	0	8957	1/1	0.77	0.29	-	200,200,200,200	0
35	NA	0	8505	1/1	0.88	0.48	-	58,58,58,58	0
33	MG	0	8068	1/1	0.99	0.12	-	64,64,64,64	0
35	NA	B	8552	1/1	0.92	0.22	-	111,111,111,111	0
37	SR	3	8999	1/1	0.66	0.71	-	200,200,200,200	0
37	SR	R	8912	1/1	0.96	0.16	-	93,93,93,93	0
33	MG	0	8023	1/1	0.94	0.18	-	41,41,41,41	0
35	NA	0	8502	1/1	0.70	0.39	-	53,53,53,53	0
37	SR	0	8963	1/1	0.92	0.12	-	146,146,146,146	0
37	SR	0	8968	1/1	0.60	0.15	-	180,180,180,180	0
37	SR	0	9002	1/1	0.42	0.12	-	169,169,169,169	0
37	SR	0	8926	1/1	0.79	0.16	-	127,127,127,127	0
35	NA	0	8525	1/1	0.85	0.26	-	67,67,67,67	0
35	NA	0	8501	1/1	0.89	0.24	-	41,41,41,41	0
33	MG	0	8071	1/1	0.74	0.30	-	67,67,67,67	0
37	SR	0	8959	1/1	0.39	0.37	-	194,194,194,194	0
37	SR	0	8984	1/1	0.84	0.07	-	118,118,118,118	0
37	SR	0	8964	1/1	0.81	0.08	-	160,160,160,160	0
37	SR	0	8928	1/1	0.92	0.12	-	148,148,148,148	0
37	SR	0	8954	1/1	0.93	0.15	-	108,108,108,108	0
33	MG	0	8026	1/1	0.87	0.20	-	39,39,39,39	0
37	SR	0	8906	1/1	0.95	0.21	-	64,64,64,64	0
35	NA	0	8526	1/1	0.94	0.13	-	40,40,40,40	0
33	MG	0	8037	1/1	0.99	0.10	-	67,67,67,67	0
35	NA	0	8541	1/1	0.82	0.38	-	65,65,65,65	0
33	MG	0	8031	1/1	0.82	0.62	-	77,77,77,77	0
37	SR	0	8915	1/1	0.74	0.14	-	131,131,131,131	0
37	SR	0	9007	1/1	0.79	0.38	-	200,200,200,200	0
37	SR	0	8986	1/1	0.53	0.84	-	200,200,200,200	0
35	NA	0	8509	1/1	0.62	0.58	-	90,90,90,90	0
37	SR	0	8927	1/1	0.77	0.16	-	176,176,176,176	0
33	MG	0	8022	1/1	0.94	0.07	-	56,56,56,56	0
33	MG	0	8032	1/1	0.92	0.16	-	66,66,66,66	0
33	MG	0	8073	1/1	0.73	0.09	-	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	MG	0	8067	1/1	0.97	0.17	-	33,33,33,33	0
37	SR	S	8961	1/1	0.90	0.12	-	150,150,150,150	0
37	SR	0	8931	1/1	0.89	0.09	-	147,147,147,147	0
37	SR	0	8967	1/1	0.92	0.07	-	164,164,164,164	0
37	SR	0	8942	1/1	0.86	0.21	-	139,139,139,139	0
37	SR	0	9000	1/1	0.52	1.08	-	200,200,200,200	0
37	SR	0	8940	1/1	0.96	0.16	-	110,110,110,110	0
35	NA	S	8510	1/1	0.83	0.12	-	56,56,56,56	0
37	SR	0	8996	1/1	0.96	0.22	-	200,200,200,200	0
37	SR	0	9006	1/1	0.80	0.13	-	190,190,190,190	0
37	SR	0	8990	1/1	0.98	0.19	-	108,108,108,108	0
37	SR	9	9003	1/1	0.64	0.06	-	195,195,195,195	0
36	CL	N	8807	1/1	0.89	0.29	-	98,98,98,98	0
35	NA	0	8570	1/1	0.69	0.26	-	61,61,61,61	0
33	MG	0	8081	1/1	0.63	0.59	-	80,80,80,80	0
33	MG	0	8035	1/1	0.94	0.25	-	52,52,52,52	0
33	MG	0	8075	1/1	0.30	0.14	-	64,64,64,64	0
33	MG	0	8020	1/1	0.83	0.15	-	56,56,56,56	0
33	MG	0	8036	1/1	0.79	0.16	-	59,59,59,59	0
33	MG	0	8066	1/1	0.56	0.24	-	75,75,75,75	0
33	MG	0	8055	1/1	0.63	0.54	-	87,87,87,87	0
37	SR	0	8914	1/1	0.88	0.15	-	109,109,109,109	0
37	SR	0	8909	1/1	0.96	0.18	-	105,105,105,105	0
35	NA	H	8518	1/1	0.65	0.77	-	92,92,92,92	0
35	NA	0	8531	1/1	0.74	0.18	-	45,45,45,45	0
37	SR	0	8919	1/1	0.88	0.09	-	81,81,81,81	0
33	MG	0	8027	1/1	0.98	0.08	-	47,47,47,47	0
37	SR	0	8901	1/1	0.91	0.15	-	78,78,78,78	0
37	SR	0	8922	1/1	0.74	0.64	-	182,182,182,182	0
37	SR	1	8952	1/1	0.94	0.16	-	81,81,81,81	0
33	MG	0	8092	1/1	0.69	0.48	-	133,133,133,133	0
33	MG	0	8064	1/1	0.80	0.29	-	53,53,53,53	0
35	NA	0	8551	1/1	0.48	0.79	-	86,86,86,86	0
36	CL	0	8814	1/1	0.97	0.17	-	55,55,55,55	0
37	SR	F	9005	1/1	0.61	0.07	-	153,153,153,153	0
35	NA	0	8514	1/1	0.95	0.56	-	38,38,38,38	0
35	NA	0	8571	1/1	0.70	0.35	-	101,101,101,101	0
37	SR	3	8932	1/1	-0.02	0.28	-	184,184,184,184	0
37	SR	0	8976	1/1	0.78	0.38	-	200,200,200,200	0
33	MG	0	8085	1/1	0.93	0.13	-	73,73,73,73	0
37	SR	0	9008	1/1	0.93	0.16	-	107,107,107,107	0
35	NA	0	8560	1/1	0.78	0.80	-	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	MG	K	8054	1/1	0.72	0.19	-	29,29,29,29	0
33	MG	0	8046	1/1	0.85	0.13	-	46,46,46,46	0
37	SR	0	8933	1/1	0.83	0.06	-	122,122,122,122	0
36	CL	3	8804	1/1	0.08	0.58	-	121,121,121,121	0
37	SR	0	8937	1/1	0.93	0.10	-	116,116,116,116	0
33	MG	0	8005	1/1	0.90	0.31	-	46,46,46,46	0
37	SR	0	8997	1/1	0.79	0.74	-	200,200,200,200	0
33	MG	0	8056	1/1	0.81	0.13	-	44,44,44,44	0
33	MG	0	8093	1/1	0.59	0.11	-	29,29,29,29	0
33	MG	B	8042	1/1	0.92	0.47	-	121,121,121,121	0
37	SR	0	8956	1/1	0.88	0.09	-	154,154,154,154	0
37	SR	0	8998	1/1	0.95	0.21	-	196,196,196,196	0
37	SR	0	8995	1/1	0.86	0.45	-	191,191,191,191	0
35	NA	0	8567	1/1	0.78	0.81	-	57,57,57,57	0
35	NA	0	8558	1/1	0.70	0.58	-	60,60,60,60	0
36	CL	0	8817	1/1	0.95	0.34	-	80,80,80,80	0
37	SR	0	8913	1/1	0.89	0.77	-	181,181,181,181	0
33	MG	0	8024	1/1	0.79	0.24	-	55,55,55,55	0
37	SR	0	8981	1/1	0.94	0.28	-	198,198,198,198	0
37	SR	0	8994	1/1	0.97	0.59	-	200,200,200,200	0
37	SR	0	8921	1/1	0.92	0.16	-	98,98,98,98	0
33	MG	0	8091	1/1	0.78	0.10	-	111,111,111,111	0
37	SR	0	8925	1/1	0.97	0.10	-	99,99,99,99	0
33	MG	0	8079	1/1	0.87	0.41	-	76,76,76,76	0
36	CL	R	8806	1/1	0.95	0.08	-	56,56,56,56	0

6.5 Other polymers

There are no such residues in this entry.