



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 8, 2023 – 05:34 PM EDT

PDB ID : 1Q86
Title : Crystal structure of CCA-Phe-cap-biotin bound simultaneously at half occupancy to both the A-site and P-site of the the 50S ribosomal Subunit.
Authors : Hansen, J.L.; Schmeing, T.M.; Moore, P.B.; Steitz, T.A.
Deposited on : 2003-08-20
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) 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
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

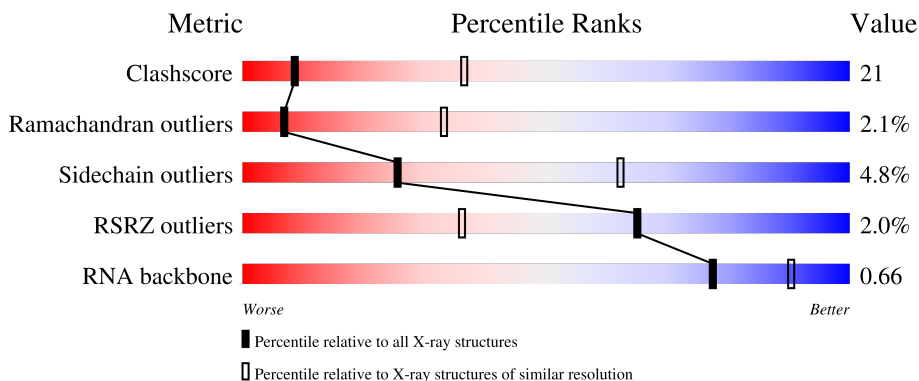
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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





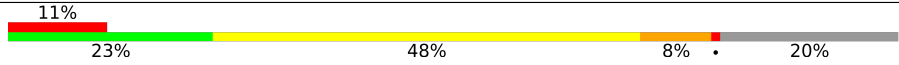
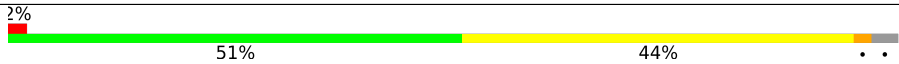
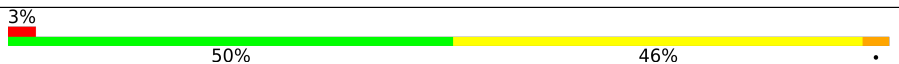
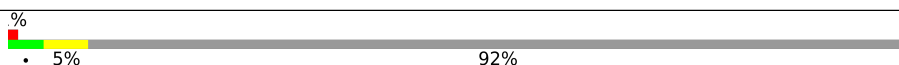
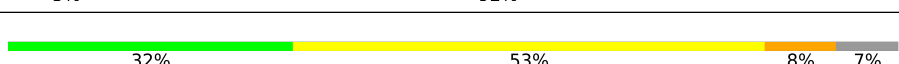

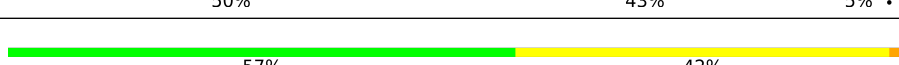

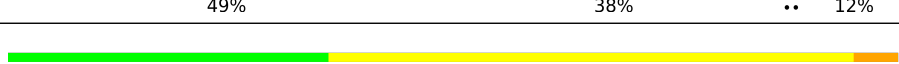
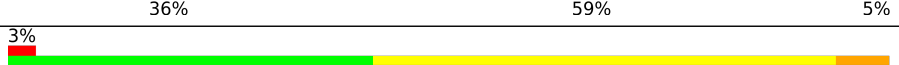
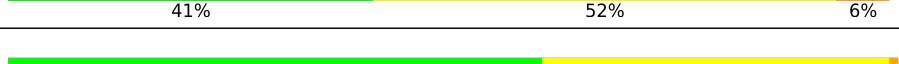
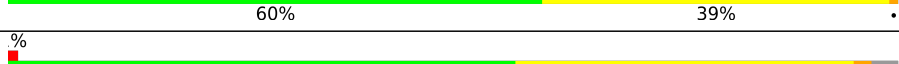


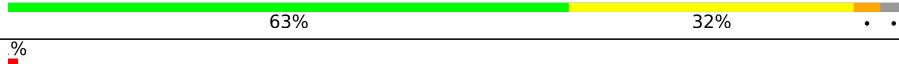


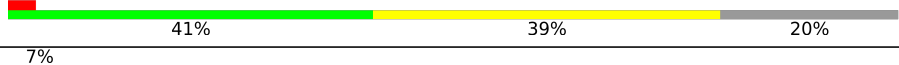
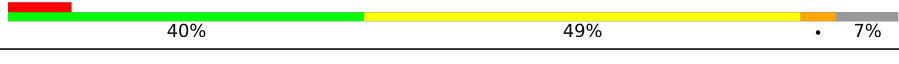


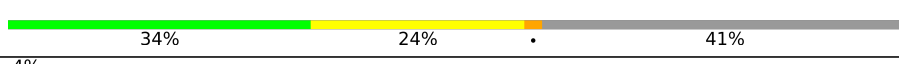
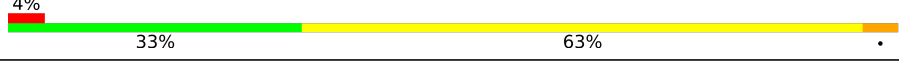
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)
RNA backbone	3102	1173 (3.30-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	A	2922	
2	B	122	
3	5	3	
3	6	3	
4	C	239	

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Mol	Chain	Length	Quality of chain
5	D	337	
6	E	246	
7	F	176	
8	G	177	
9	H	119	
10	I	348	
11	J	167	
12	K	145	
13	L	132	
14	M	164	
15	N	194	
16	O	186	
17	P	115	
18	Q	148	
19	R	95	
20	S	154	
21	T	84	
22	U	119	
23	V	66	
24	W	70	
25	X	154	
26	Y	91	
27	Z	240	
28	1	73	
29	2	56	

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Mol	Chain	Length	Quality of chain
30	3	48	
31	4	92	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	MG	1	8105	-	-	-	X
32	MG	6	8118	-	-	-	X
32	MG	A	8024	-	-	-	X
34	NA	A	8328	-	-	-	X
34	NA	A	8350	-	-	-	X
34	NA	A	8352	-	-	-	X
34	NA	A	8354	-	-	-	X
34	NA	A	8359	-	-	-	X
34	NA	A	8372	-	-	-	X
34	NA	A	8375	-	-	-	X
34	NA	A	8377	-	-	-	X
34	NA	A	8384	-	-	-	X
34	NA	S	8386	-	-	-	X
34	NA	T	8312	-	-	-	X
36	PHA	5	77	-	-	-	X
36	PHA	6	77	-	-	-	X

2 Entry composition [i](#)

There are 38 unique types of molecules in this entry. The entry contains 98659 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	A	2754	59017	26346	10878	19048	2745	0	0	0

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

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

- Molecule 3 is a RNA chain called CCA-phenylalanine-cariotic-acid-biotin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	5	3	59	28	11	18	2	0	0	0
3	6	3	59	28	11	18	2	0	0	0

- Molecule 4 is a protein called 50S ribosomal protein L2P.

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

- Molecule 5 is a protein called 50S ribosomal protein L3P.

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

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 6 is a protein called 50S ribosomal protein L4E.

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

- Molecule 7 is a protein called 50S ribosomal protein L5P.

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

- Molecule 8 is a protein called 50S ribosomal protein L6P.

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

- Molecule 9 is a protein called 50S ribosomal protein L7Ae.

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

- Molecule 10 is a protein called Acidic ribosomal protein P0 homolog.

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

- Molecule 11 is a protein called L10 Ribosomal Protein.

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

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

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

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

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

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

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

- Molecule 15 is a protein called L15 Ribosomal Protein.

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
28	1	73	563	359	111	86	7	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
29	2	56	430	258	86	82	4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
30	3	46	393	238	86	68	1	0	0	0

There is a discrepancy between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	4	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	A	108	Total	Mg	0	0
			108	108		
32	B	1	Total	Mg	0	0
			1	1		
32	6	1	Total	Mg	0	0
			1	1		
32	C	1	Total	Mg	0	0
			1	1		
32	D	2	Total	Mg	0	0
			2	2		
32	L	1	Total	Mg	0	0
			1	1		
32	U	1	Total	Mg	0	0
			1	1		
32	Z	1	Total	Mg	0	0
			1	1		
32	1	1	Total	Mg	0	0
			1	1		
32	4	1	Total	Mg	0	0
			1	1		

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	A	70	Total	Na	0	0
			70	70		
34	B	2	Total	Na	0	0
			2	2		
34	C	1	Total	Na	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	E	1	Total Na 1 1	0	0
34	J	2	Total Na 2 2	0	0
34	K	1	Total Na 1 1	0	0
34	M	1	Total Na 1 1	0	0
34	N	2	Total Na 2 2	0	0
34	R	1	Total Na 1 1	0	0
34	S	3	Total Na 3 3	0	0
34	T	1	Total Na 1 1	0	0
34	U	1	Total Na 1 1	0	0

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

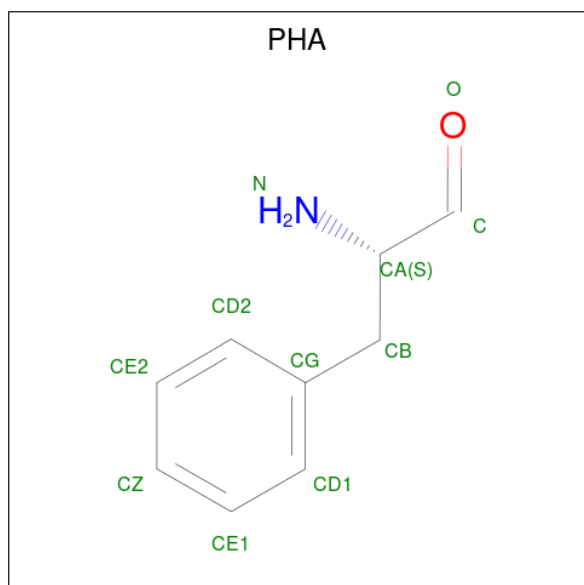
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	A	9	Total Cl 9 9	0	0
35	C	1	Total Cl 1 1	0	0
35	D	1	Total Cl 1 1	0	0
35	K	3	Total Cl 3 3	0	0
35	L	1	Total Cl 1 1	0	0
35	M	1	Total Cl 1 1	0	0
35	N	1	Total Cl 1 1	0	0
35	O	1	Total Cl 1 1	0	0
35	P	1	Total Cl 1 1	0	0
35	S	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	Z	1	Total Cl 1 1	0	0
35	4	1	Total Cl 1 1	0	0

- Molecule 36 is PHENYLALANINAL (three-letter code: PHA) (formula: C₉H₁₁NO).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	5	1	Total C N O 11 9 1 1	0	0
36	6	1	Total C O 10 9 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	P	1	Total Cd 1 1	0	0
37	V	1	Total Cd 1 1	0	0
37	1	1	Total Cd 1 1	0	0
37	2	1	Total Cd 1 1	0	0
37	4	1	Total Cd 1 1	0	0

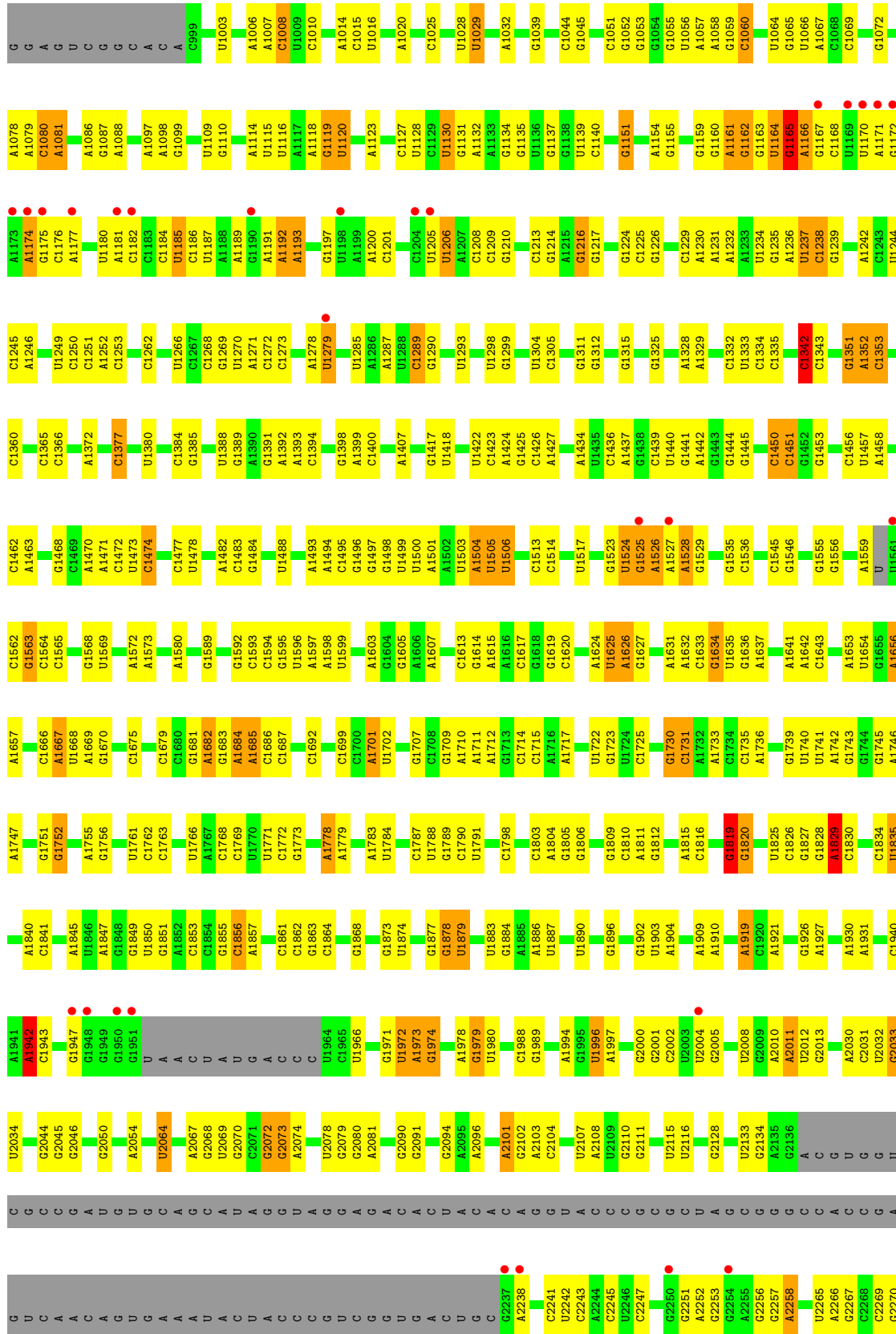
- Molecule 38 is water.

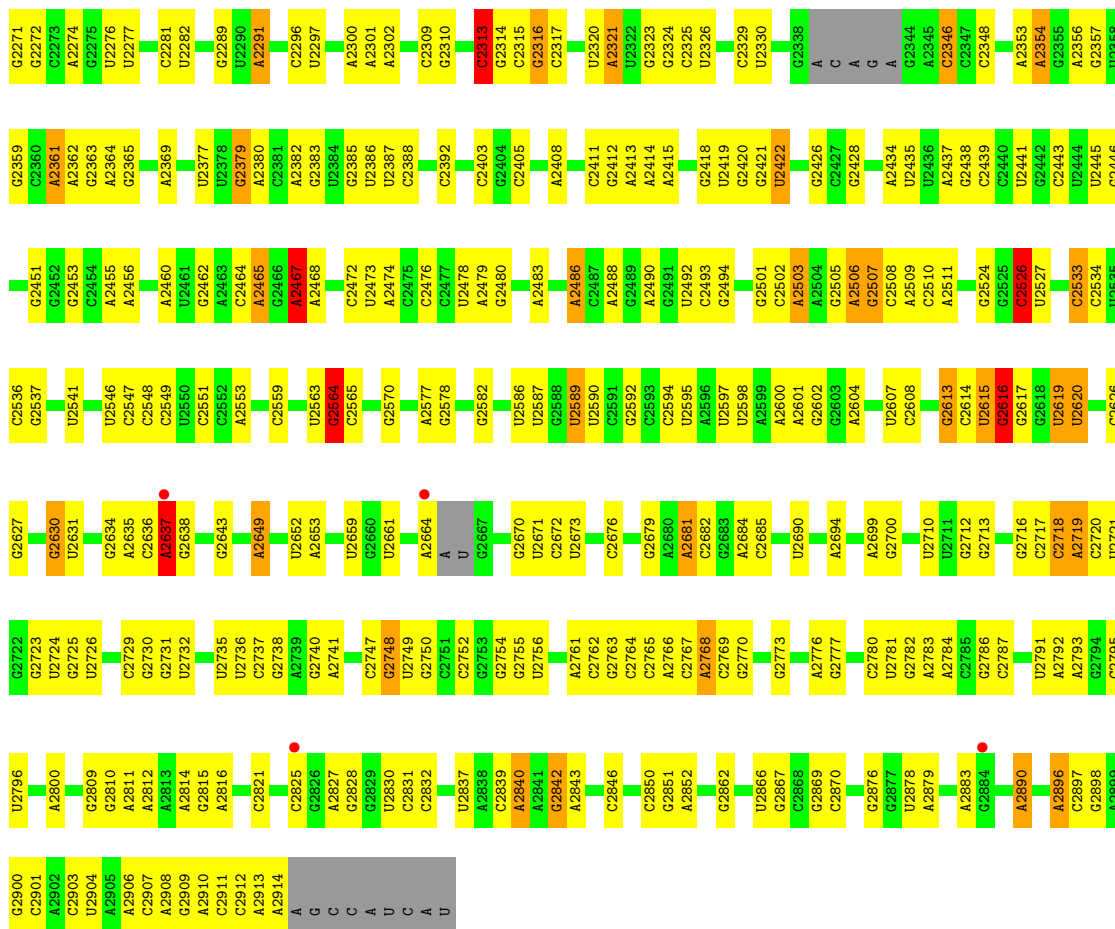
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	A	5892	Total 5892	O 5892	0	0
38	B	139	Total 139	O 139	0	0
38	C	116	Total 116	O 116	0	0
38	D	149	Total 149	O 149	0	0
38	E	173	Total 173	O 173	0	0
38	F	52	Total 52	O 52	0	0
38	G	43	Total 43	O 43	0	0
38	H	27	Total 27	O 27	0	0
38	I	21	Total 21	O 21	0	0
38	J	77	Total 77	O 77	0	0
38	K	54	Total 54	O 54	0	0
38	L	62	Total 62	O 62	0	0
38	M	82	Total 82	O 82	0	0
38	N	139	Total 139	O 139	0	0
38	O	70	Total 70	O 70	0	0
38	P	43	Total 43	O 43	0	0
38	Q	67	Total 67	O 67	0	0
38	R	54	Total 54	O 54	0	0
38	S	84	Total 84	O 84	0	0
38	T	37	Total 37	O 37	0	0
38	U	44	Total 44	O 44	0	0

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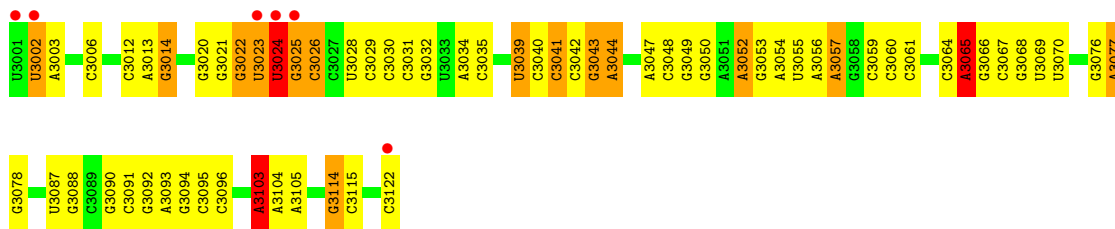
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	V	24	Total O 24 24	0	0
38	W	14	Total O 14 14	0	0
38	X	71	Total O 71 71	0	0
38	Y	31	Total O 31 31	0	0
38	Z	93	Total O 93 93	0	0
38	1	37	Total O 37 37	0	0
38	2	63	Total O 63 63	0	0
38	3	41	Total O 41 41	0	0
38	4	70	Total O 70 70	0	0





• Molecule 2: 5S ribosomal RNA



• Molecule 3: CCA-phenylalanine-cariotic-acid-biotin

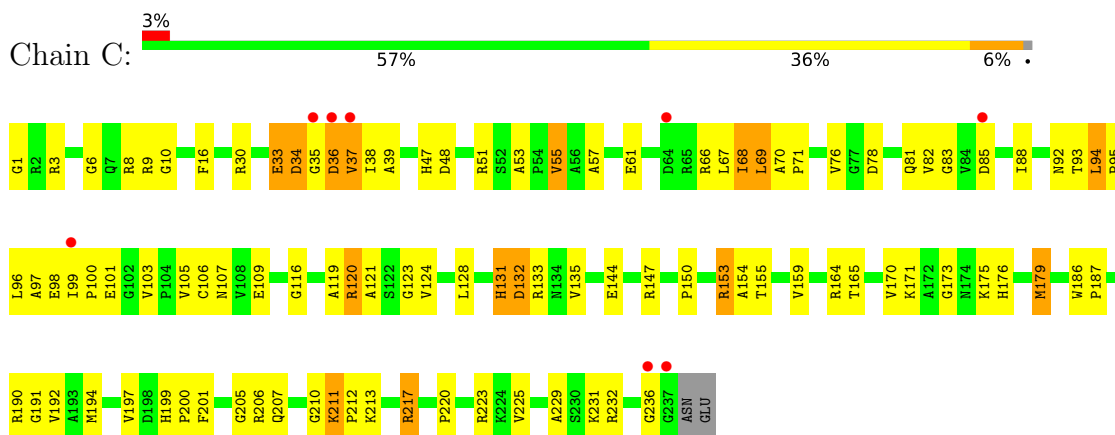


• Molecule 3: CCA-phenylalanine-cariotic-acid-biotin

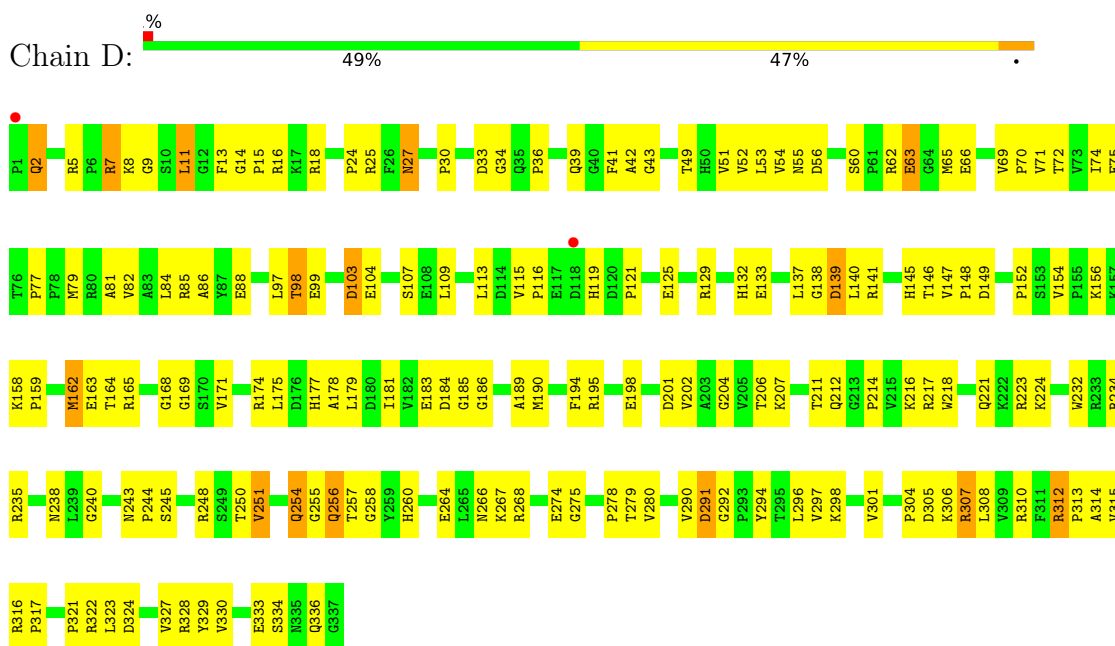


C74
C75
A76

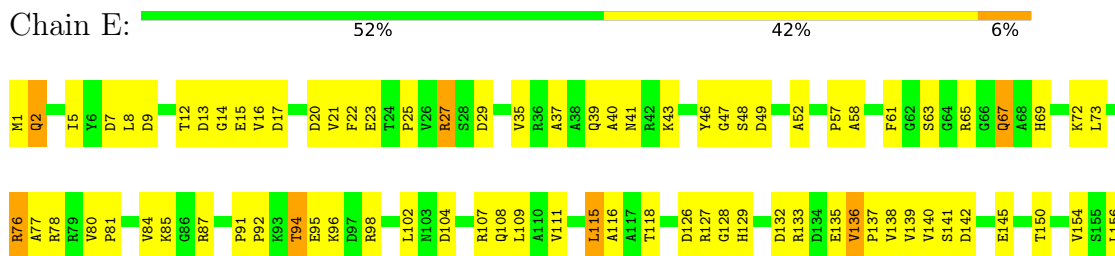
● Molecule 4: 50S ribosomal protein L2P

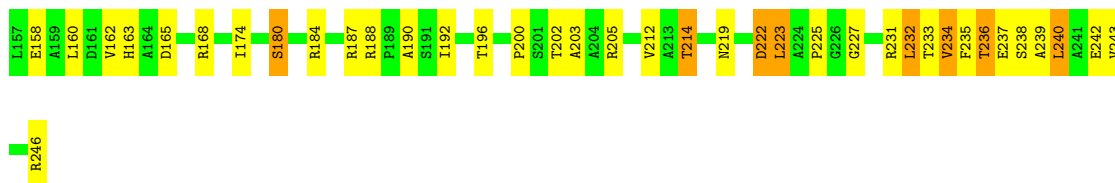


● Molecule 5: 50S ribosomal protein L3P

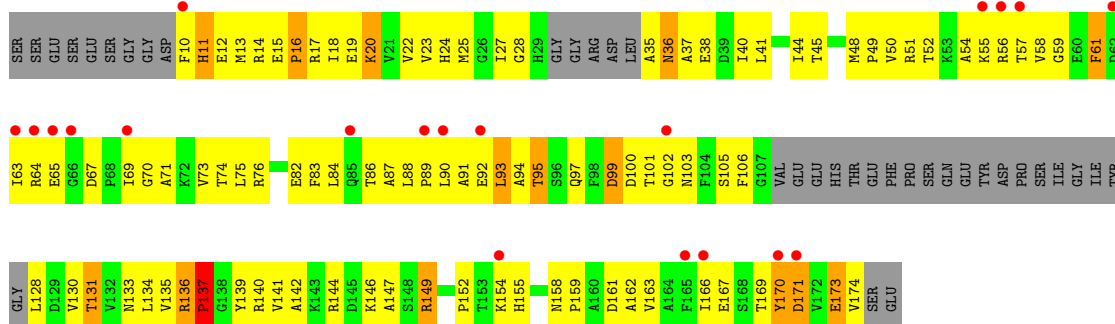


● Molecule 6: 50S ribosomal protein L4E

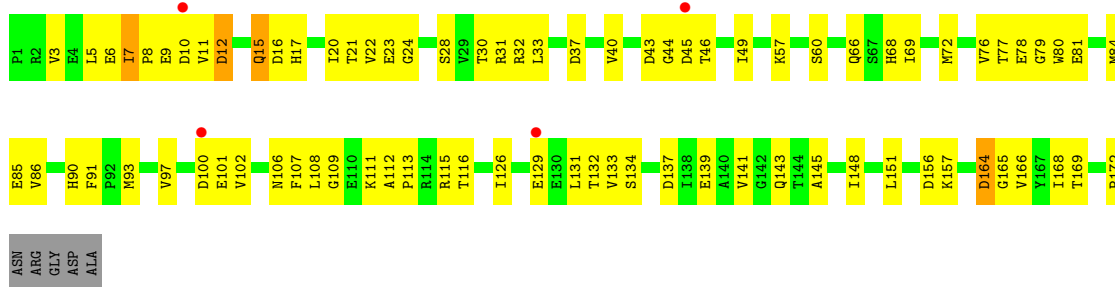




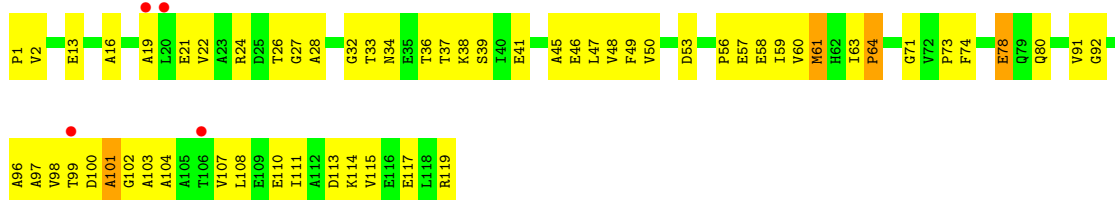
- Molecule 7: 50S ribosomal protein L5P



- Molecule 8: 50S ribosomal protein L6P

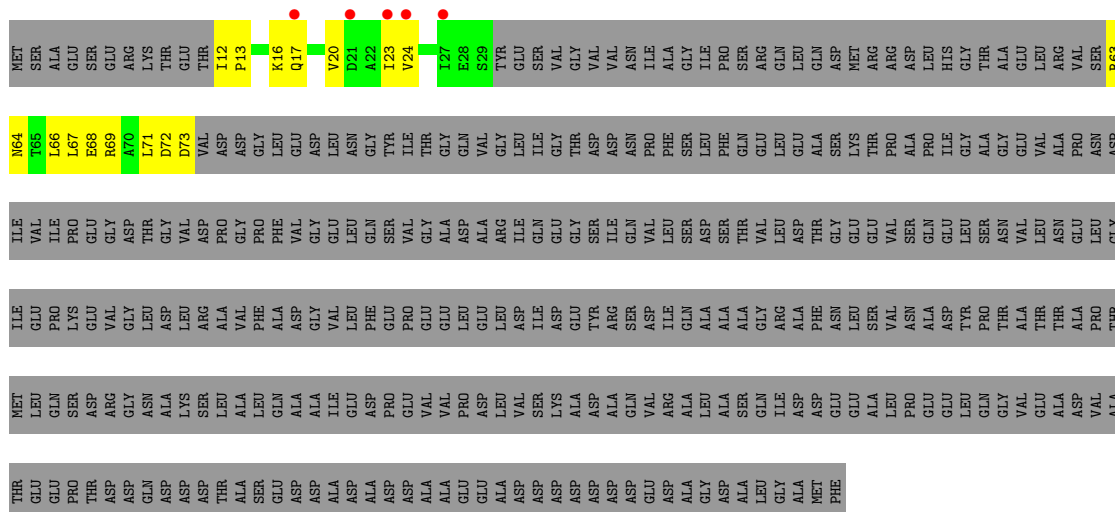


- Molecule 9: 50S ribosomal protein L7Ae



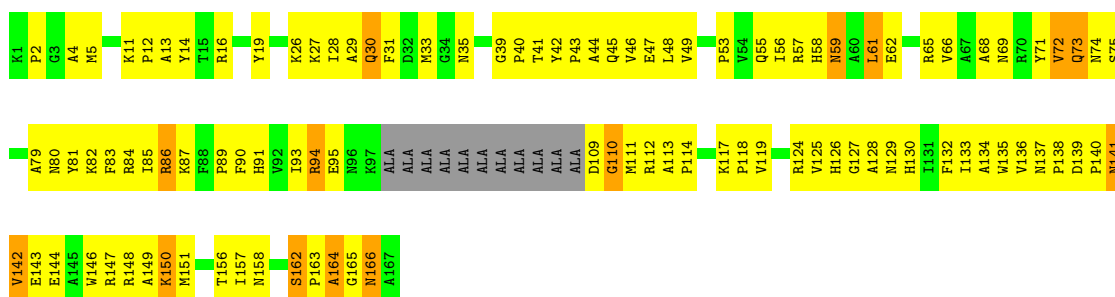
- Molecule 10: Acidic ribosomal protein P0 homolog





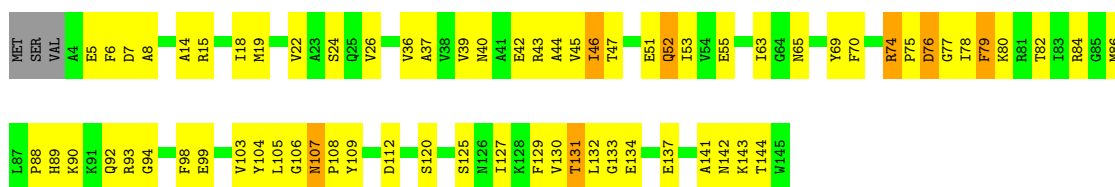
● Molecule 11: L10 Ribosomal Protein

Chain J: 32% 53% 8% 7%



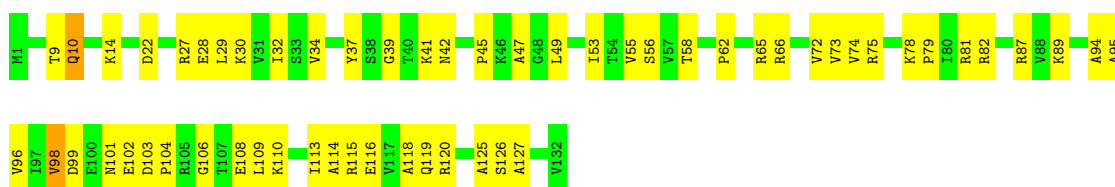
● Molecule 12: 50S ribosomal protein L13P

Chain K: 50% 43% 5%

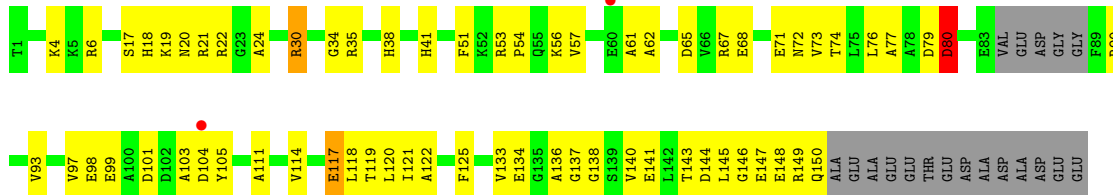


● Molecule 13: 50S ribosomal protein L14P

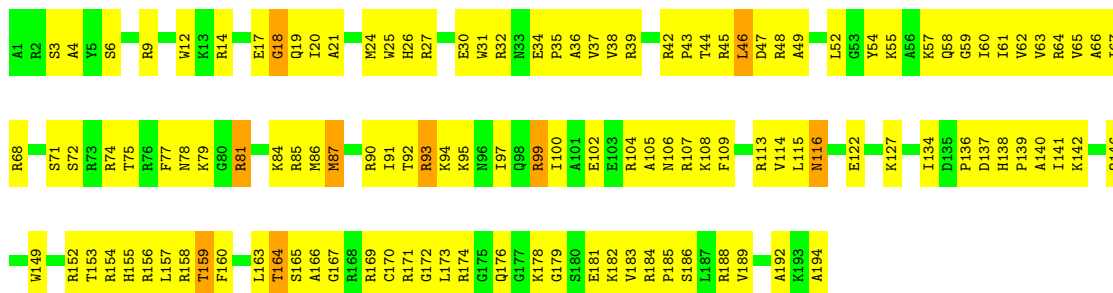
Chain L: 57% 42%



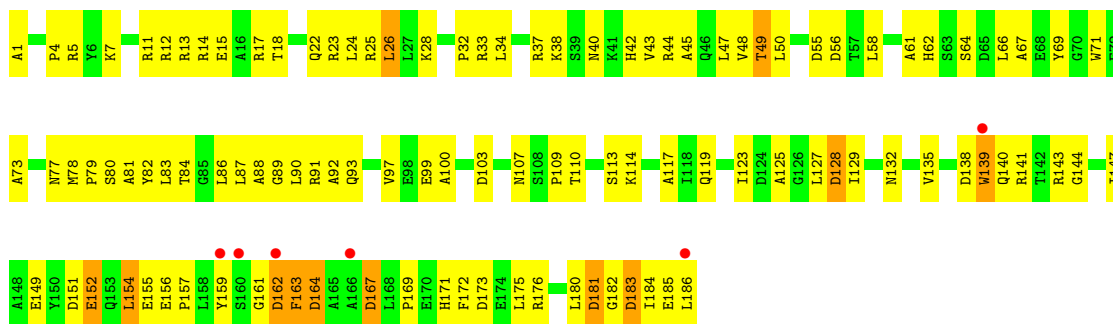
● Molecule 14: 50S ribosomal protein L15P



- Molecule 15: L15 Ribosomal Protein



- Molecule 16: 50S ribosomal protein L18P

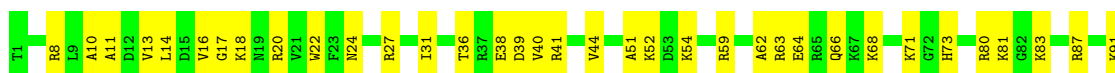


- Molecule 17: 50S ribosomal protein L18e



- Molecule 18: 50S ribosomal protein L19E

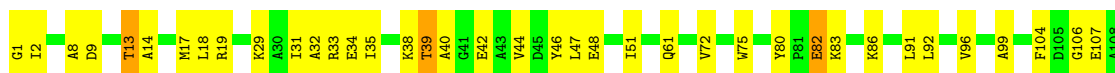




- Molecule 19: 50S ribosomal protein L21e



- Molecule 20: 50S ribosomal protein L22P



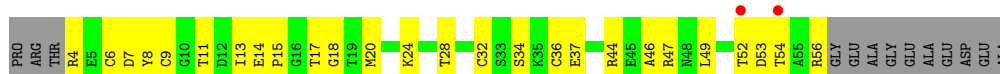
- Molecule 21: 50S ribosomal protein L23P



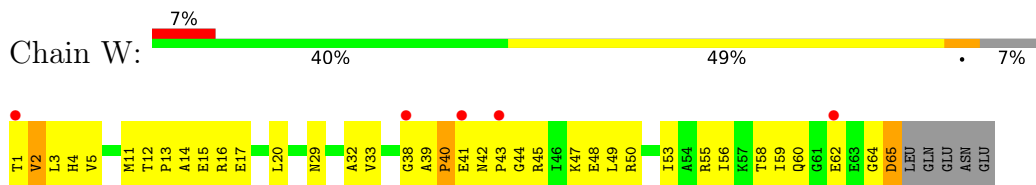
- Molecule 22: 50S ribosomal protein L24P



- Molecule 23: 50S ribosomal protein L24E



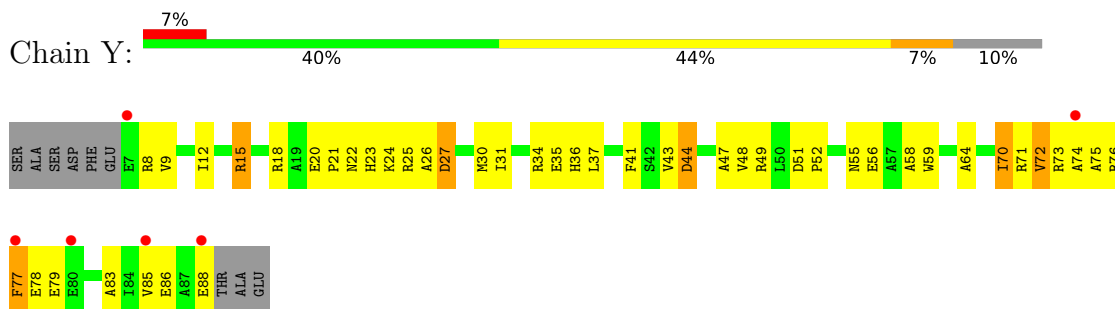
- Molecule 24: 50S ribosomal protein L29P



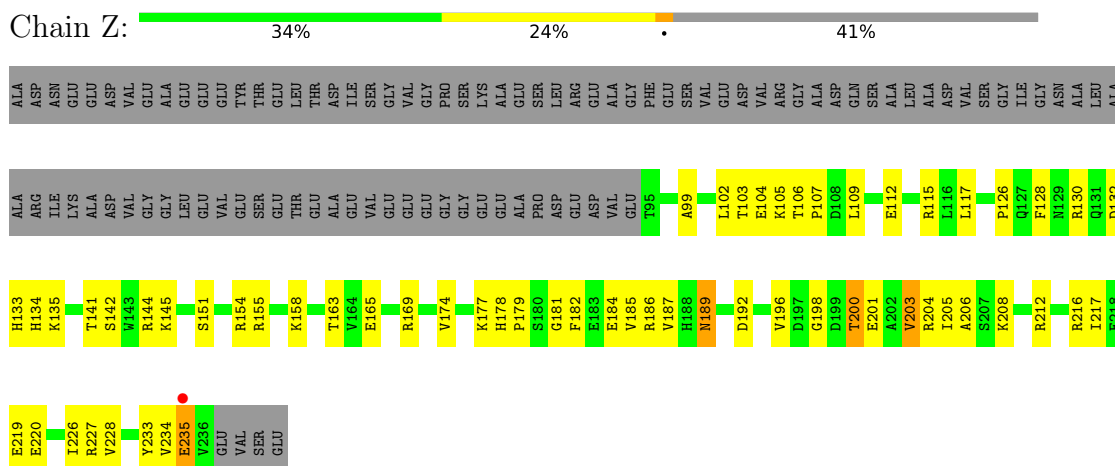
- Molecule 25: 50S ribosomal protein L30P



- Molecule 26: 50S ribosomal protein L31e

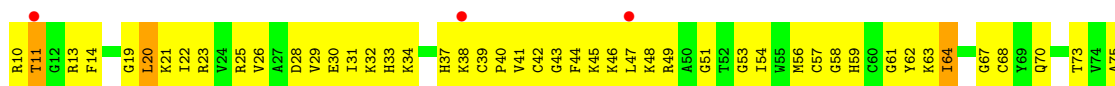


- Molecule 27: 50S ribosomal protein L32E



- Molecule 28: L37Ae 50S ribosomal protein

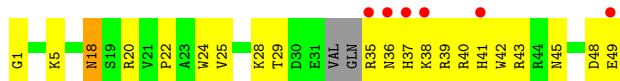




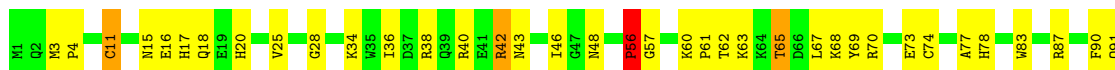
- Molecule 29: 50S ribosomal protein L37e



- Molecule 30: 50S ribosomal protein L39e



- Molecule 31: 50S ribosomal protein L44E



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	213.16Å 301.29Å 575.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 49.62 – 2.80	Depositor EDS
% Data completeness (in resolution range)	95.6 (20.00-3.00) 92.8 (49.62-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 2.81Å)	Xtrriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.234 , 0.264 0.234 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	47.1	Xtrriage
Anisotropy	0.292	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 70.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	98659	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.50% 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, 0.333 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: K, MG, PHA, CD, CL, 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	A	0.41	1/66076 (0.0%)	0.70	24/103052 (0.0%)
2	B	0.37	0/2905	0.75	4/4528 (0.1%)
3	5	0.67	0/65	0.86	0/99
3	6	1.66	2/65 (3.1%)	1.27	0/99
4	C	0.32	0/1787	0.65	0/2409
5	D	0.34	0/2689	0.64	0/3652
6	E	0.38	0/1883	0.65	0/2551
7	F	0.32	0/1111	0.59	0/1498
8	G	0.33	0/1382	0.59	0/1880
9	H	0.31	0/896	0.58	0/1219
10	I	0.29	0/241	0.50	0/324
11	J	0.40	0/1246	0.77	4/1686 (0.2%)
12	K	0.38	0/1135	0.63	0/1530
13	L	0.35	0/1003	0.68	0/1351
14	M	0.32	0/1126	0.65	0/1504
15	N	0.38	0/1633	0.68	0/2180
16	O	0.29	0/1473	0.64	0/1999
17	P	0.34	0/873	0.61	0/1181
18	Q	0.34	0/1143	0.54	0/1521
19	R	0.37	0/748	0.69	1/1005 (0.1%)
20	S	0.36	0/1172	0.67	0/1578
21	T	0.33	0/648	0.58	0/875
22	U	0.31	0/957	0.62	0/1289
23	V	0.33	0/417	0.59	0/562
24	W	0.29	0/502	0.56	0/675
25	X	0.35	0/1218	0.64	0/1655
26	Y	0.35	0/664	0.60	0/895
27	Z	0.36	0/1146	0.65	0/1536
28	1	0.37	0/575	0.69	0/763
29	2	0.37	0/437	0.63	0/578
30	3	0.30	0/398	0.52	0/527
31	4	0.41	0/771	0.62	0/1024

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.39	3/98385 (0.0%)	0.68	33/147225 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	2	50
2	B	1	3
3	6	0	1
25	X	0	1
All	All	3	55

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	6	75	C	O5'-C5'	5.83	1.53	1.44
1	A	2620	U	N1-C6	5.47	1.42	1.38
3	6	74	C	C2'-O2'	5.05	1.48	1.41

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1563	G	C2'-C3'-O3'	9.42	130.23	109.50
2	B	3024	U	C2'-C3'-O3'	9.17	129.68	109.50
1	A	2637	A	C4'-C3'-O3'	-7.22	94.24	109.40
2	B	3103	A	C5'-C4'-O4'	7.11	117.63	109.10
11	J	74	ASN	N-CA-C	-6.83	92.57	111.00

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1563	G	C3'
1	A	2616	G	C3'
2	B	3024	U	C3'

5 of 55 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	182	G	Sidechain

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Mol	Chain	Res	Type	Group
1	A	333	G	Sidechain
1	A	471	G	Sidechain
1	A	482	G	Sidechain
1	A	518	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	A	59017	0	29805	1077	0
2	B	2600	0	1326	84	0
3	5	59	0	34	4	0
3	6	59	0	34	0	0
4	C	1754	0	1763	112	0
5	D	2624	0	2533	183	0
6	E	1858	0	1816	135	0
7	F	1094	0	1085	146	0
8	G	1357	0	1266	77	0
9	H	885	0	854	71	0
10	I	240	0	231	23	0
11	J	1215	0	1215	170	0
12	K	1119	0	1098	77	0
13	L	993	0	1027	72	0
14	M	1114	0	1072	66	0
15	N	1605	0	1676	182	0
16	O	1444	0	1401	129	0
17	P	864	0	873	53	0
18	Q	1133	0	1127	62	0
19	R	734	0	729	26	0
20	S	1149	0	1122	67	0
21	T	641	0	605	31	0
22	U	949	0	923	62	0
23	V	410	0	364	35	0
24	W	499	0	511	33	0
25	X	1195	0	1137	118	0
26	Y	654	0	653	51	0
27	Z	1130	0	1133	71	0
28	1	563	0	597	66	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	2	430	0	426	28	0
30	3	393	0	406	32	0
31	4	755	0	728	40	0
32	1	1	0	0	0	0
32	4	1	0	0	0	0
32	6	1	0	0	0	0
32	A	108	0	0	0	0
32	B	1	0	0	0	0
32	C	1	0	0	0	0
32	D	2	0	0	0	0
32	L	1	0	0	0	0
32	U	1	0	0	0	0
32	Z	1	0	0	0	0
33	A	2	0	0	0	0
34	A	70	0	0	0	0
34	B	2	0	0	0	0
34	C	1	0	0	0	0
34	E	1	0	0	0	0
34	J	2	0	0	0	0
34	K	1	0	0	0	0
34	M	1	0	0	0	0
34	N	2	0	0	0	0
34	R	1	0	0	0	0
34	S	3	0	0	0	0
34	T	1	0	0	0	0
34	U	1	0	0	0	0
35	4	1	0	0	0	0
35	A	9	0	0	0	0
35	C	1	0	0	0	0
35	D	1	0	0	0	0
35	K	3	0	0	1	0
35	L	1	0	0	1	0
35	M	1	0	0	0	0
35	N	1	0	0	1	0
35	O	1	0	0	0	0
35	P	1	0	0	0	0
35	S	1	0	0	0	0
35	Z	1	0	0	0	0
36	5	11	0	10	5	0
36	6	10	0	7	4	0
37	1	1	0	0	0	0
37	2	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	4	1	0	0	0	0
37	P	1	0	0	0	0
37	V	1	0	0	0	0
38	1	37	0	0	14	0
38	2	63	0	0	4	0
38	3	41	0	0	3	0
38	4	70	0	0	10	0
38	A	5892	0	0	227	0
38	B	139	0	0	14	0
38	C	116	0	0	12	0
38	D	149	0	0	30	0
38	E	173	0	0	37	0
38	F	52	0	0	22	0
38	G	43	0	0	12	0
38	H	27	0	0	11	0
38	I	21	0	0	6	0
38	J	77	0	0	23	0
38	K	54	0	0	5	0
38	L	62	0	0	11	0
38	M	82	0	0	18	0
38	N	139	0	0	23	0
38	O	70	0	0	17	0
38	P	43	0	0	13	0
38	Q	67	0	0	5	0
38	R	54	0	0	5	0
38	S	84	0	0	7	0
38	T	37	0	0	6	0
38	U	44	0	0	7	0
38	V	24	0	0	5	0
38	W	14	0	0	3	0
38	X	71	0	0	14	0
38	Y	31	0	0	5	0
38	Z	93	0	0	14	0
All	All	98659	0	59587	3106	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 21.

The worst 5 of 3106 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)
6:E:236:THR:HG22	6:E:239:ALA:H	1.05	1.18
11:J:45:GLN:HB3	11:J:163:PRO:HD2	1.31	1.12
11:J:86:ARG:NH1	11:J:133:ILE:HG13	1.64	1.11
1:A:1119:G:H2'	12:K:52:GLN:HE22	1.10	1.10
1:A:156:C:H5''	15:N:171:ARG:HD3	1.29	1.09

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	
4	C	235/239 (98%)	202 (86%)	27 (12%)	6 (3%)	5	27
5	D	335/337 (99%)	291 (87%)	36 (11%)	8 (2%)	6	29
6	E	244/246 (99%)	210 (86%)	31 (13%)	3 (1%)	13	48
7	F	134/176 (76%)	95 (71%)	28 (21%)	11 (8%)	1	4
8	G	170/177 (96%)	159 (94%)	10 (6%)	1 (1%)	25	64
9	H	117/119 (98%)	100 (86%)	13 (11%)	4 (3%)	3	20
10	I	25/348 (7%)	23 (92%)	1 (4%)	1 (4%)	3	17
11	J	152/167 (91%)	129 (85%)	18 (12%)	5 (3%)	4	21
12	K	140/145 (97%)	126 (90%)	8 (6%)	6 (4%)	2	15
13	L	130/132 (98%)	115 (88%)	13 (10%)	2 (2%)	10	42
14	M	141/164 (86%)	117 (83%)	22 (16%)	2 (1%)	11	43
15	N	192/194 (99%)	164 (85%)	25 (13%)	3 (2%)	9	40
16	O	184/186 (99%)	160 (87%)	17 (9%)	7 (4%)	3	18
17	P	113/115 (98%)	105 (93%)	8 (7%)	0	100	100
18	Q	141/148 (95%)	132 (94%)	8 (6%)	1 (1%)	22	60
19	R	93/95 (98%)	88 (95%)	4 (4%)	1 (1%)	14	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	S	148/154 (96%)	134 (90%)	14 (10%)	0	100	100
21	T	79/84 (94%)	71 (90%)	8 (10%)	0	100	100
22	U	117/119 (98%)	103 (88%)	12 (10%)	2 (2%)	9	39
23	V	51/66 (77%)	44 (86%)	6 (12%)	1 (2%)	7	34
24	W	63/70 (90%)	55 (87%)	5 (8%)	3 (5%)	2	13
25	X	152/154 (99%)	142 (93%)	8 (5%)	2 (1%)	12	45
26	Y	80/91 (88%)	70 (88%)	8 (10%)	2 (2%)	5	28
27	Z	140/240 (58%)	135 (96%)	5 (4%)	0	100	100
28	1	71/73 (97%)	59 (83%)	10 (14%)	2 (3%)	5	25
29	2	54/56 (96%)	51 (94%)	3 (6%)	0	100	100
30	3	42/48 (88%)	42 (100%)	0	0	100	100
31	4	90/92 (98%)	84 (93%)	4 (4%)	2 (2%)	6	31
All	All	3633/4235 (86%)	3206 (88%)	352 (10%)	75 (2%)	7	33

5 of 75 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	D	139	ASP
5	D	184	ASP
6	E	8	LEU
7	F	93	LEU
7	F	95	THR

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	
4	C	179/181 (99%)	166 (93%)	13 (7%)	14	44
5	D	282/282 (100%)	267 (95%)	15 (5%)	22	58
6	E	193/193 (100%)	177 (92%)	16 (8%)	11	39
7	F	117/147 (80%)	108 (92%)	9 (8%)	13	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	G	152/155 (98%)	147 (97%)	5 (3%)	38	73
9	H	92/92 (100%)	91 (99%)	1 (1%)	73	90
10	I	27/283 (10%)	27 (100%)	0	100	100
11	J	122/122 (100%)	111 (91%)	11 (9%)	9	35
12	K	118/121 (98%)	107 (91%)	11 (9%)	9	33
13	L	106/106 (100%)	104 (98%)	2 (2%)	57	84
14	M	112/126 (89%)	107 (96%)	5 (4%)	27	64
15	N	166/166 (100%)	157 (95%)	9 (5%)	22	57
16	O	149/149 (100%)	144 (97%)	5 (3%)	37	72
17	P	93/93 (100%)	92 (99%)	1 (1%)	73	90
18	Q	113/116 (97%)	109 (96%)	4 (4%)	36	71
19	R	79/79 (100%)	75 (95%)	4 (5%)	24	60
20	S	117/121 (97%)	113 (97%)	4 (3%)	37	72
21	T	71/73 (97%)	70 (99%)	1 (1%)	67	88
22	U	105/105 (100%)	99 (94%)	6 (6%)	20	56
23	V	44/52 (85%)	44 (100%)	0	100	100
24	W	51/56 (91%)	50 (98%)	1 (2%)	55	83
25	X	130/130 (100%)	124 (95%)	6 (5%)	27	64
26	Y	66/73 (90%)	61 (92%)	5 (8%)	13	43
27	Z	120/195 (62%)	115 (96%)	5 (4%)	30	66
28	1	56/56 (100%)	54 (96%)	2 (4%)	35	70
29	2	46/46 (100%)	46 (100%)	0	100	100
30	3	42/44 (96%)	41 (98%)	1 (2%)	49	79
31	4	79/79 (100%)	75 (95%)	4 (5%)	24	60
All	All	3027/3441 (88%)	2881 (95%)	146 (5%)	25	62

5 of 146 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
21	T	10	VAL
31	4	42	ARG
22	U	39	ASN
26	Y	27	ASP
7	F	131	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 97 such sidechains are listed below:

Mol	Chain	Res	Type
19	R	16	ASN
25	X	12	ASN
20	S	61	GLN
21	T	53	ASN
25	X	87	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2747/2922 (94%)	244 (8%)	32 (1%)
2	B	121/122 (99%)	16 (13%)	3 (2%)
3	5	2/3 (66%)	1 (50%)	0
3	6	2/3 (66%)	0	0
All	All	2872/3050 (94%)	261 (9%)	35 (1%)

5 of 261 RNA backbone outliers are listed below:

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

5 of 35 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	2616	G
1	A	2649	A
2	B	3024	U
1	A	1080	C
1	A	898	G

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 235 ligands modelled in this entry, 233 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	PHA	5	77	3	10,11,11	0.86	0	10,13,13	0.79	0
36	PHA	6	77	3	10,10,11	0.63	0	11,11,13	0.48	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	PHA	5	77	3	-	3/5/6/6	0/1/1/1
36	PHA	6	77	3	-	1/3/4/6	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
36	5	77	PHA	CA-CB-CG-CD1
36	5	77	PHA	CA-CB-CG-CD2
36	5	77	PHA	C-CA-CB-CG
36	6	77	PHA	C-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	5	77	PHA	5	0
36	6	77	PHA	4	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	A	2754/2922 (94%)	0.14	41 (1%) 73 46	19, 47, 95, 154	0
2	B	122/122 (100%)	0.11	6 (4%) 29 11	30, 62, 92, 154	0
3	5	3/3 (100%)	1.61	1 (33%) 0 0	29, 29, 31, 35	3 (100%)
3	6	3/3 (100%)	2.43	3 (100%) 0 0	15, 15, 17, 31	3 (100%)
4	C	237/239 (99%)	0.19	8 (3%) 45 19	27, 52, 91, 115	0
5	D	337/337 (100%)	0.02	2 (0%) 89 72	26, 55, 84, 96	0
6	E	246/246 (100%)	-0.25	0 100 100	19, 47, 71, 80	0
7	F	140/176 (79%)	0.87	20 (14%) 2 1	53, 101, 124, 131	0
8	G	172/177 (97%)	0.24	4 (2%) 60 31	41, 68, 91, 99	0
9	H	119/119 (100%)	0.44	4 (3%) 45 19	53, 77, 104, 111	0
10	I	29/348 (8%)	1.19	5 (17%) 1 0	66, 86, 97, 103	0
11	J	156/167 (93%)	-0.12	0 100 100	30, 52, 77, 81	0
12	K	142/145 (97%)	-0.21	0 100 100	34, 47, 71, 90	0
13	L	132/132 (100%)	-0.04	0 100 100	31, 53, 78, 86	0
14	M	145/164 (88%)	0.04	2 (1%) 75 49	21, 67, 108, 116	0
15	N	194/194 (100%)	-0.05	0 100 100	30, 47, 68, 80	0
16	O	186/186 (100%)	0.13	6 (3%) 47 20	35, 65, 112, 125	0
17	P	115/115 (100%)	-0.15	0 100 100	36, 54, 74, 83	0
18	Q	143/148 (96%)	0.33	1 (0%) 87 69	36, 57, 71, 80	0
19	R	95/95 (100%)	-0.28	0 100 100	32, 42, 57, 73	0
20	S	150/154 (97%)	-0.05	0 100 100	29, 43, 64, 75	0
21	T	81/84 (96%)	0.21	1 (1%) 79 54	41, 62, 81, 85	0
22	U	119/119 (100%)	0.28	4 (3%) 45 19	38, 60, 86, 105	0
23	V	53/66 (80%)	0.35	2 (3%) 40 16	42, 53, 71, 80	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
24	W	65/70 (92%)	0.72	5 (7%) 13 4	56, 79, 120, 125	0
25	X	154/154 (100%)	-0.42	0 100 100	29, 45, 62, 74	0
26	Y	82/91 (90%)	0.46	6 (7%) 15 4	42, 56, 79, 100	0
27	Z	142/240 (59%)	-0.17	1 (0%) 87 69	25, 45, 67, 86	0
28	1	73/73 (100%)	0.26	3 (4%) 37 14	43, 61, 76, 81	0
29	2	56/56 (100%)	-0.29	0 100 100	24, 33, 39, 41	0
30	3	46/48 (95%)	0.84	6 (13%) 3 1	34, 65, 118, 126	0
31	4	92/92 (100%)	0.00	0 100 100	39, 55, 69, 78	0
All	All	6583/7285 (90%)	0.11	131 (1%) 65 36	15, 52, 97, 154	6 (0%)

The worst 5 of 131 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
24	W	1	THR	11.8
2	B	3001	U	7.4
1	A	1172	G	5.1
1	A	2237	G	5.1
7	F	66	GLY	4.9

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
34	NA	A	8384	1/1	0.23	0.68	101,101,101,101	0
34	NA	S	8386	1/1	0.37	0.78	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	MG	A	8046	1/1	0.40	0.19	45,45,45,45	0
32	MG	A	8114	1/1	0.44	0.28	51,51,51,51	0
34	NA	A	8366	1/1	0.46	0.26	51,51,51,51	0
32	MG	A	8076	1/1	0.54	0.16	37,37,37,37	0
32	MG	A	8041	1/1	0.56	0.20	79,79,79,79	0
32	MG	C	8065	1/1	0.58	0.16	40,40,40,40	0
34	NA	A	8369	1/1	0.60	0.39	59,59,59,59	0
34	NA	A	8324	1/1	0.60	0.31	58,58,58,58	0
32	MG	A	8106	1/1	0.60	0.17	45,45,45,45	0
34	NA	A	8359	1/1	0.61	0.73	48,48,48,48	0
34	NA	A	8385	1/1	0.63	0.28	43,43,43,43	0
34	NA	A	8372	1/1	0.64	0.56	55,55,55,55	0
32	MG	A	8029	1/1	0.64	0.14	53,53,53,53	0
32	MG	A	8040	1/1	0.65	0.17	71,71,71,71	0
32	MG	A	8024	1/1	0.65	0.81	95,95,95,95	0
32	MG	6	8118	1/1	0.65	0.69	61,61,61,61	0
34	NA	A	8317	1/1	0.66	0.20	63,63,63,63	0
32	MG	1	8105	1/1	0.67	0.46	30,30,30,30	0
32	MG	U	8073	1/1	0.68	0.23	52,52,52,52	0
34	NA	B	8351	1/1	0.69	0.30	85,85,85,85	0
36	PHA	6	77	10/11	0.69	0.43	35,38,41,41	10
36	PHA	5	77	11/11	0.70	0.52	24,25,29,29	11
32	MG	A	8113	1/1	0.70	0.18	43,43,43,43	0
34	NA	A	8382	1/1	0.71	0.25	54,54,54,54	0
34	NA	T	8312	1/1	0.71	0.47	108,108,108,108	0
32	MG	4	8078	1/1	0.72	0.13	63,63,63,63	0
32	MG	A	8011	1/1	0.73	0.10	37,37,37,37	0
35	CL	P	8508	1/1	0.73	0.22	72,72,72,72	0
32	MG	A	8080	1/1	0.73	0.15	33,33,33,33	0
32	MG	A	8059	1/1	0.73	0.20	65,65,65,65	0
37	CD	P	8405	1/1	0.73	0.12	184,184,184,184	0
32	MG	A	8115	1/1	0.74	0.20	36,36,36,36	0
32	MG	A	8096	1/1	0.74	0.18	46,46,46,46	0
34	NA	A	8327	1/1	0.74	0.21	34,34,34,34	0
34	NA	A	8329	1/1	0.74	0.38	65,65,65,65	0
34	NA	A	8377	1/1	0.74	0.41	76,76,76,76	0
32	MG	A	8044	1/1	0.75	0.20	50,50,50,50	0
32	MG	A	8110	1/1	0.75	0.14	29,29,29,29	0
34	NA	A	8352	1/1	0.75	0.43	51,51,51,51	0
32	MG	A	8071	1/1	0.76	0.19	80,80,80,80	0
34	NA	A	8328	1/1	0.76	0.55	54,54,54,54	0
32	MG	A	8016	1/1	0.76	0.21	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
35	CL	A	8514	1/1	0.76	0.29	55,55,55,55	0
34	NA	A	8340	1/1	0.77	0.31	38,38,38,38	0
34	NA	A	8350	1/1	0.77	0.43	36,36,36,36	0
32	MG	A	8104	1/1	0.77	0.29	51,51,51,51	0
32	MG	A	8081	1/1	0.77	0.09	51,51,51,51	0
32	MG	A	8035	1/1	0.77	0.11	54,54,54,54	0
34	NA	A	8319	1/1	0.77	0.15	33,33,33,33	0
34	NA	J	8322	1/1	0.77	0.31	68,68,68,68	0
35	CL	K	8501	1/1	0.78	0.13	69,69,69,69	0
32	MG	A	8090	1/1	0.78	0.34	62,62,62,62	0
34	NA	A	8374	1/1	0.78	0.27	60,60,60,60	0
34	NA	A	8375	1/1	0.78	0.73	63,63,63,63	0
32	MG	A	8092	1/1	0.78	0.33	92,92,92,92	0
34	NA	A	8370	1/1	0.79	0.29	50,50,50,50	0
34	NA	A	8307	1/1	0.79	0.22	53,53,53,53	0
34	NA	A	8354	1/1	0.79	0.55	31,31,31,31	0
34	NA	A	8336	1/1	0.79	0.18	41,41,41,41	0
32	MG	A	8091	1/1	0.79	0.09	53,53,53,53	0
32	MG	A	8111	1/1	0.79	0.15	67,67,67,67	0
34	NA	A	8368	1/1	0.80	0.22	69,69,69,69	0
34	NA	A	8320	1/1	0.80	0.25	24,24,24,24	0
34	NA	A	8310	1/1	0.80	0.38	33,33,33,33	0
32	MG	A	8116	1/1	0.80	0.12	67,67,67,67	0
32	MG	A	8117	1/1	0.80	0.14	26,26,26,26	0
32	MG	A	8019	1/1	0.81	0.09	15,15,15,15	0
34	NA	A	8357	1/1	0.81	0.09	53,53,53,53	0
34	NA	A	8330	1/1	0.81	0.39	42,42,42,42	0
34	NA	A	8313	1/1	0.81	0.26	44,44,44,44	0
32	MG	A	8084	1/1	0.82	0.14	56,56,56,56	0
35	CL	A	8515	1/1	0.82	0.58	85,85,85,85	0
32	MG	A	8054	1/1	0.82	0.12	37,37,37,37	0
35	CL	L	8512	1/1	0.82	0.16	47,47,47,47	0
34	NA	A	8381	1/1	0.83	0.16	54,54,54,54	0
32	MG	Z	8109	1/1	0.83	0.12	28,28,28,28	0
32	MG	A	8015	1/1	0.83	0.09	38,38,38,38	0
34	NA	A	8358	1/1	0.83	0.47	113,113,113,113	0
32	MG	A	8009	1/1	0.84	0.08	15,15,15,15	0
32	MG	A	8068	1/1	0.84	0.15	58,58,58,58	0
32	MG	A	8058	1/1	0.84	0.15	33,33,33,33	0
34	NA	C	8345	1/1	0.84	0.17	48,48,48,48	0
32	MG	A	8075	1/1	0.84	0.15	64,64,64,64	0
34	NA	A	8316	1/1	0.85	0.23	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	MG	A	8063	1/1	0.85	0.10	54,54,54,54	0
34	NA	A	8373	1/1	0.85	0.39	45,45,45,45	0
34	NA	K	8346	1/1	0.85	0.30	33,33,33,33	0
34	NA	S	8338	1/1	0.85	0.22	48,48,48,48	0
32	MG	A	8006	1/1	0.85	0.09	34,34,34,34	0
32	MG	A	8021	1/1	0.85	0.11	22,22,22,22	0
35	CL	A	8511	1/1	0.85	0.19	65,65,65,65	0
34	NA	A	8342	1/1	0.86	0.21	34,34,34,34	0
32	MG	A	8094	1/1	0.86	0.15	67,67,67,67	0
34	NA	A	8305	1/1	0.86	0.22	27,27,27,27	0
34	NA	N	8365	1/1	0.86	0.49	46,46,46,46	0
32	MG	A	8045	1/1	0.86	0.19	52,52,52,52	0
32	MG	A	8086	1/1	0.86	0.17	49,49,49,49	0
32	MG	A	8088	1/1	0.86	0.21	23,23,23,23	0
34	NA	A	8326	1/1	0.86	1.05	54,54,54,54	0
37	CD	1	8403	1/1	0.86	0.09	60,60,60,60	0
34	NA	A	8333	1/1	0.87	0.11	24,24,24,24	0
32	MG	A	8062	1/1	0.87	0.09	61,61,61,61	0
35	CL	A	8516	1/1	0.87	0.19	51,51,51,51	0
32	MG	A	8039	1/1	0.87	0.10	52,52,52,52	0
32	MG	A	8032	1/1	0.87	0.10	24,24,24,24	0
32	MG	A	8037	1/1	0.87	0.12	46,46,46,46	0
32	MG	A	8061	1/1	0.87	0.11	25,25,25,25	0
34	NA	A	8318	1/1	0.87	0.60	37,37,37,37	0
35	CL	A	8505	1/1	0.87	0.16	60,60,60,60	0
32	MG	A	8112	1/1	0.87	0.26	43,43,43,43	0
34	NA	B	8383	1/1	0.88	0.29	72,72,72,72	0
32	MG	A	8066	1/1	0.88	0.10	72,72,72,72	0
34	NA	A	8306	1/1	0.88	0.89	42,42,42,42	0
32	MG	A	8087	1/1	0.88	0.10	56,56,56,56	0
32	MG	A	8030	1/1	0.88	0.10	23,23,23,23	0
32	MG	A	8028	1/1	0.89	0.06	30,30,30,30	0
34	NA	N	8347	1/1	0.89	0.16	36,36,36,36	0
34	NA	A	8353	1/1	0.89	0.13	26,26,26,26	0
35	CL	K	8502	1/1	0.89	0.14	62,62,62,62	0
32	MG	A	8099	1/1	0.89	0.14	32,32,32,32	0
35	CL	M	8510	1/1	0.89	0.19	57,57,57,57	0
34	NA	A	8355	1/1	0.89	0.65	72,72,72,72	0
35	CL	Z	8520	1/1	0.89	0.12	39,39,39,39	0
33	K	A	8201	1/1	0.89	0.31	76,76,76,76	0
32	MG	D	8055	1/1	0.89	0.10	34,34,34,34	0
32	MG	A	8013	1/1	0.89	0.15	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
37	CD	V	8401	1/1	0.89	0.07	69,69,69,69	0
32	MG	A	8020	1/1	0.89	0.14	27,27,27,27	0
35	CL	A	8503	1/1	0.90	0.24	47,47,47,47	0
34	NA	A	8356	1/1	0.90	0.69	44,44,44,44	0
35	CL	O	8507	1/1	0.90	0.34	63,63,63,63	0
34	NA	A	8360	1/1	0.90	0.49	45,45,45,45	0
34	NA	A	8371	1/1	0.90	0.53	62,62,62,62	0
35	CL	4	8504	1/1	0.90	0.26	56,56,56,56	0
34	NA	S	8337	1/1	0.90	0.16	45,45,45,45	0
34	NA	A	8379	1/1	0.90	0.13	34,34,34,34	0
32	MG	A	8082	1/1	0.90	0.28	51,51,51,51	0
32	MG	A	8010	1/1	0.90	0.09	26,26,26,26	0
35	CL	K	8521	1/1	0.90	0.19	51,51,51,51	0
32	MG	A	8102	1/1	0.91	0.09	53,53,53,53	0
32	MG	A	8033	1/1	0.91	0.06	22,22,22,22	0
32	MG	A	8001	1/1	0.91	0.09	23,23,23,23	0
32	MG	A	8085	1/1	0.91	0.17	61,61,61,61	0
32	MG	A	8007	1/1	0.91	0.09	19,19,19,19	0
34	NA	A	8301	1/1	0.91	0.14	26,26,26,26	0
34	NA	A	8334	1/1	0.91	0.11	46,46,46,46	0
34	NA	A	8302	1/1	0.91	0.32	39,39,39,39	0
32	MG	A	8067	1/1	0.91	0.29	55,55,55,55	0
32	MG	A	8048	1/1	0.91	0.09	57,57,57,57	0
32	MG	A	8089	1/1	0.91	0.22	60,60,60,60	0
32	MG	A	8070	1/1	0.91	0.27	36,36,36,36	0
32	MG	A	8049	1/1	0.91	0.24	67,67,67,67	0
34	NA	A	8314	1/1	0.91	0.17	21,21,21,21	0
32	MG	A	8008	1/1	0.91	0.07	20,20,20,20	0
32	MG	B	8095	1/1	0.91	0.10	69,69,69,69	0
32	MG	A	8004	1/1	0.91	0.09	28,28,28,28	0
32	MG	A	8022	1/1	0.91	0.06	17,17,17,17	0
32	MG	A	8043	1/1	0.91	0.16	38,38,38,38	0
34	NA	A	8321	1/1	0.91	0.37	49,49,49,49	0
34	NA	A	8323	1/1	0.91	0.30	34,34,34,34	0
32	MG	L	8069	1/1	0.91	0.08	56,56,56,56	0
34	NA	A	8335	1/1	0.92	0.21	58,58,58,58	0
34	NA	A	8376	1/1	0.92	0.21	42,42,42,42	0
34	NA	E	8304	1/1	0.92	0.18	39,39,39,39	0
32	MG	A	8097	1/1	0.92	0.12	27,27,27,27	0
35	CL	S	8506	1/1	0.92	0.22	41,41,41,41	0
32	MG	A	8064	1/1	0.92	0.20	29,29,29,29	0
34	NA	A	8315	1/1	0.92	0.29	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
32	MG	A	8100	1/1	0.92	0.23	53,53,53,53	0
35	CL	A	8522	1/1	0.92	0.33	78,78,78,78	0
32	MG	D	8056	1/1	0.92	0.14	44,44,44,44	0
34	NA	A	8311	1/1	0.92	0.17	52,52,52,52	0
34	NA	A	8361	1/1	0.92	0.25	48,48,48,48	0
34	NA	U	8343	1/1	0.93	0.18	23,23,23,23	0
34	NA	A	8332	1/1	0.93	0.31	35,35,35,35	0
32	MG	A	8018	1/1	0.93	0.09	44,44,44,44	0
34	NA	A	8378	1/1	0.93	0.56	46,46,46,46	0
32	MG	A	8014	1/1	0.93	0.12	21,21,21,21	0
34	NA	A	8325	1/1	0.93	0.25	49,49,49,49	0
34	NA	A	8308	1/1	0.93	0.12	49,49,49,49	0
32	MG	A	8077	1/1	0.93	0.11	33,33,33,33	0
35	CL	D	8519	1/1	0.93	0.27	47,47,47,47	0
32	MG	A	8042	1/1	0.93	0.12	35,35,35,35	0
34	NA	A	8303	1/1	0.93	0.21	55,55,55,55	0
32	MG	A	8053	1/1	0.93	0.11	39,39,39,39	0
34	NA	A	8331	1/1	0.94	0.12	34,34,34,34	0
32	MG	A	8036	1/1	0.94	0.10	27,27,27,27	0
34	NA	M	8380	1/1	0.94	0.27	61,61,61,61	0
32	MG	A	8098	1/1	0.94	0.20	28,28,28,28	0
32	MG	A	8072	1/1	0.94	0.13	44,44,44,44	0
32	MG	A	8083	1/1	0.94	0.05	43,43,43,43	0
32	MG	A	8101	1/1	0.94	0.22	54,54,54,54	0
32	MG	A	8060	1/1	0.94	0.10	49,49,49,49	0
34	NA	A	8363	1/1	0.94	0.20	46,46,46,46	0
34	NA	A	8364	1/1	0.94	0.20	39,39,39,39	0
32	MG	A	8103	1/1	0.94	0.13	73,73,73,73	0
34	NA	A	8344	1/1	0.94	0.10	17,17,17,17	0
32	MG	A	8023	1/1	0.94	0.09	34,34,34,34	0
35	CL	A	8513	1/1	0.94	0.13	50,50,50,50	0
32	MG	A	8057	1/1	0.94	0.10	34,34,34,34	0
32	MG	A	8108	1/1	0.94	0.12	72,72,72,72	0
32	MG	A	8050	1/1	0.94	0.09	65,65,65,65	0
37	CD	2	8402	1/1	0.94	0.07	64,64,64,64	0
32	MG	A	8025	1/1	0.95	0.09	63,63,63,63	0
34	NA	A	8362	1/1	0.95	0.29	70,70,70,70	0
32	MG	A	8005	1/1	0.95	0.10	32,32,32,32	0
32	MG	A	8047	1/1	0.95	0.17	58,58,58,58	0
32	MG	A	8002	1/1	0.95	0.07	33,33,33,33	0
34	NA	A	8349	1/1	0.95	0.20	40,40,40,40	0
32	MG	A	8031	1/1	0.96	0.11	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	NA	A	8341	1/1	0.96	0.10	28,28,28,28	0
35	CL	N	8518	1/1	0.96	0.12	41,41,41,41	0
32	MG	A	8107	1/1	0.96	0.05	39,39,39,39	0
32	MG	A	8074	1/1	0.96	0.05	15,15,15,15	0
32	MG	A	8026	1/1	0.96	0.10	20,20,20,20	0
32	MG	A	8003	1/1	0.96	0.10	29,29,29,29	0
35	CL	A	8517	1/1	0.96	0.09	61,61,61,61	0
32	MG	A	8051	1/1	0.96	0.21	87,87,87,87	0
35	CL	C	8509	1/1	0.96	0.16	55,55,55,55	0
32	MG	A	8093	1/1	0.96	0.13	48,48,48,48	0
32	MG	A	8079	1/1	0.96	0.07	27,27,27,27	0
32	MG	A	8052	1/1	0.96	0.11	39,39,39,39	0
34	NA	J	8309	1/1	0.96	0.12	31,31,31,31	0
34	NA	A	8367	1/1	0.97	0.32	48,48,48,48	0
32	MG	A	8038	1/1	0.97	0.09	29,29,29,29	0
32	MG	A	8034	1/1	0.97	0.06	24,24,24,24	0
32	MG	A	8017	1/1	0.97	0.04	24,24,24,24	0
34	NA	A	8339	1/1	0.97	0.21	14,14,14,14	0
37	CD	4	8404	1/1	0.97	0.08	63,63,63,63	0
32	MG	A	8012	1/1	0.98	0.11	33,33,33,33	0
32	MG	A	8027	1/1	0.98	0.07	35,35,35,35	0
33	K	A	8202	1/1	0.98	0.08	53,53,53,53	0
34	NA	R	8348	1/1	0.99	0.10	29,29,29,29	0

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.